



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:26 am BST

PDB ID : 2VKZ  
Title : Structure of the cerulenin-inhibited fungal fatty acid synthase type I multienzyme complex  
Authors : Johansson, P.; Wiltschi, B.; Kumari, P.; Kessler, B.; Vonrhein, C.; Vonck, J.; Oesterhelt, D.; Grininger, M.  
Deposited on : 2008-01-07  
Resolution : 4.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

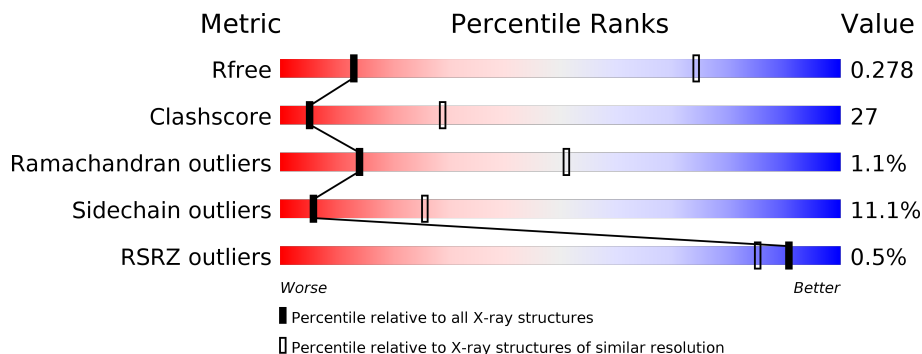
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1887	 50% 31% 14%
1	B	1887	 50% 30% 5% 14%
1	C	1887	 49% 32% 5% 14%
2	G	2051	 51% 40% 8%
2	H	2051	 51% 40% 8%
2	I	2051	 51% 40% 8%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 85959 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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.

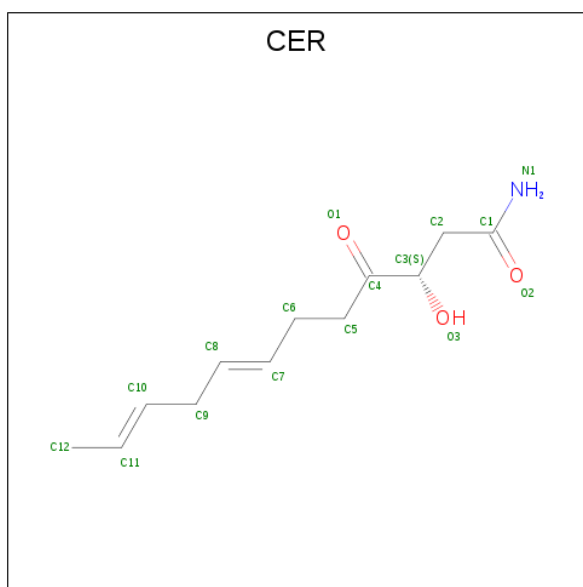
- Molecule 1 is a protein called FATTY ACID SYNTHASE SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1614	12615	7997	2127	2443	48	0	0	0
1	B	1614	12615	7997	2127	2443	48	0	0	0
1	C	1614	12615	7997	2127	2443	48	0	0	0

- Molecule 2 is a protein called FATTY ACID SYNTHASE SUBUNIT BETA.

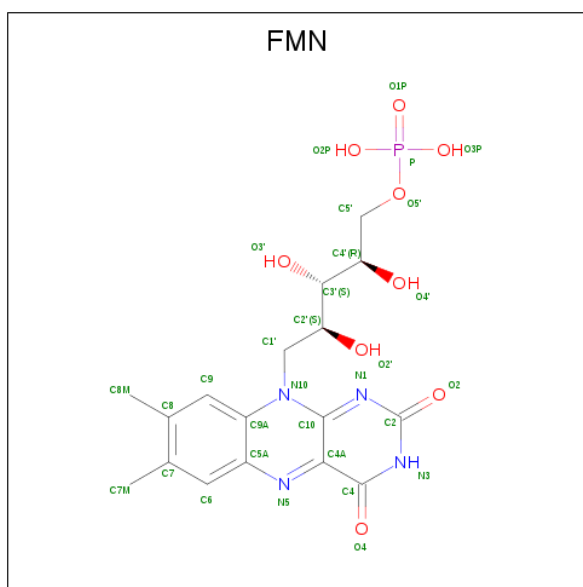
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	2033	15995	10253	2660	3026	56	0	0	0
2	H	2033	15995	10253	2660	3026	56	0	0	0
2	I	2033	15995	10253	2660	3026	56	0	0	0

- Molecule 3 is (2S, 3R)-3-HYDROXY-4-OXO-7,10-TRANS,TRANS-DODECADIENAMIDE (three-letter code: CER) (formula: C<sub>12</sub>H<sub>19</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	8	1	3		
3	B	1	Total	C	N	O	0	0
			12	8	1	3		
3	C	1	Total	C	N	O	0	0
			12	8	1	3		

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

*Continued on next page...*

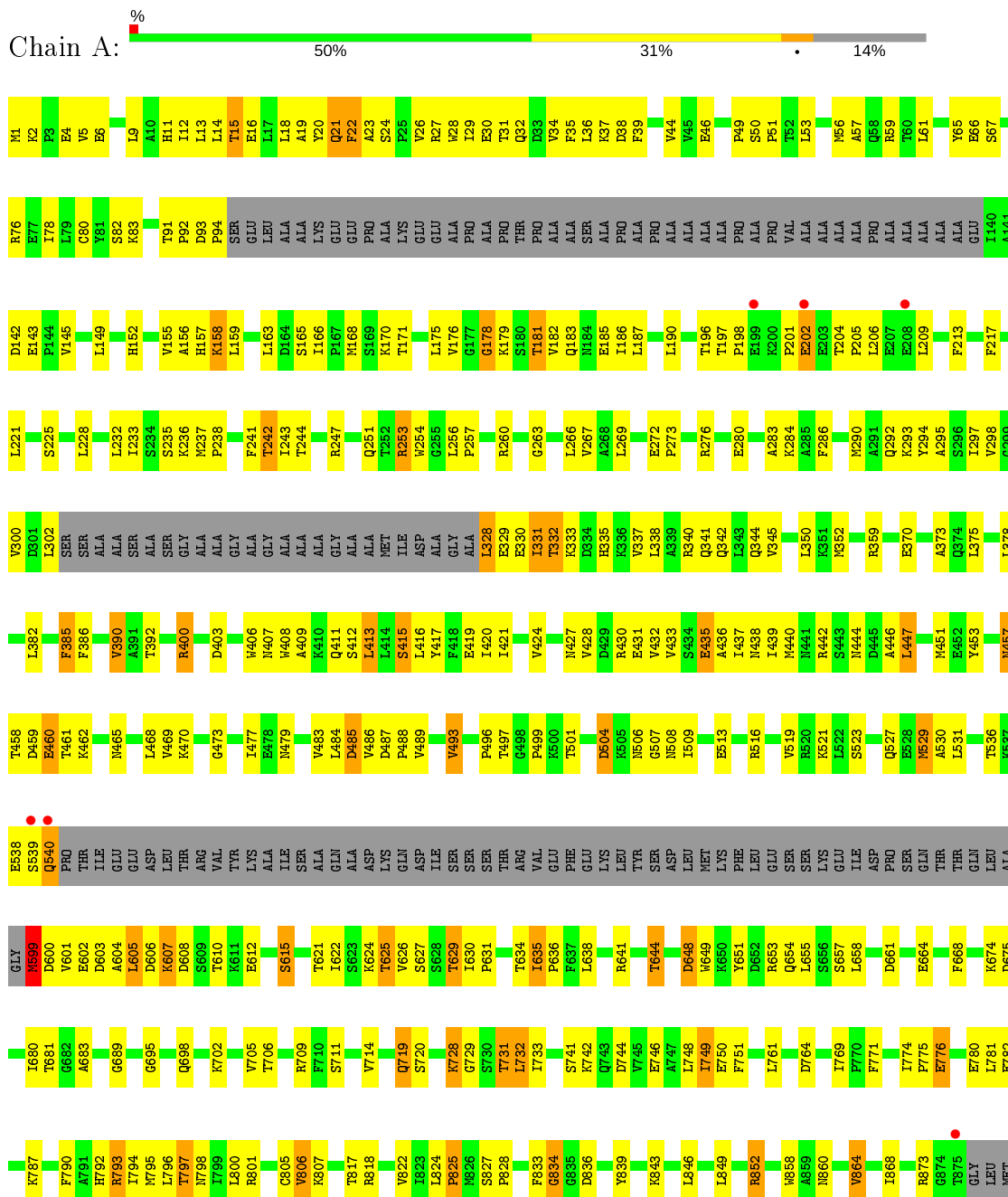
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>					<b>ZeroOcc</b>	<b>AltConf</b>
4	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	I	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

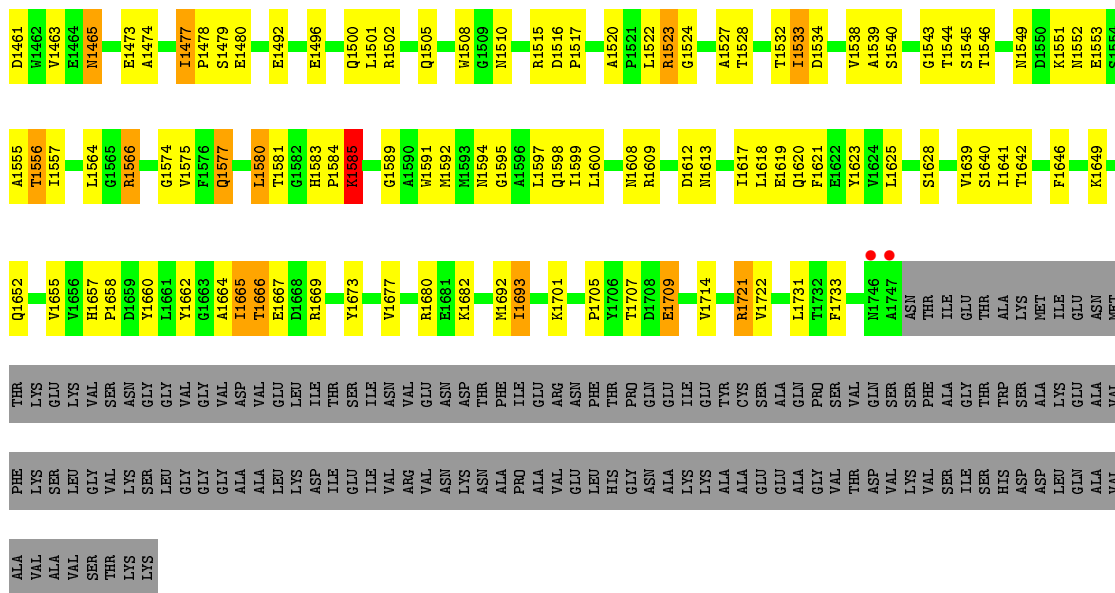
- Molecule 1: FATTY ACID SYNTHASE SUBUNIT ALPHA



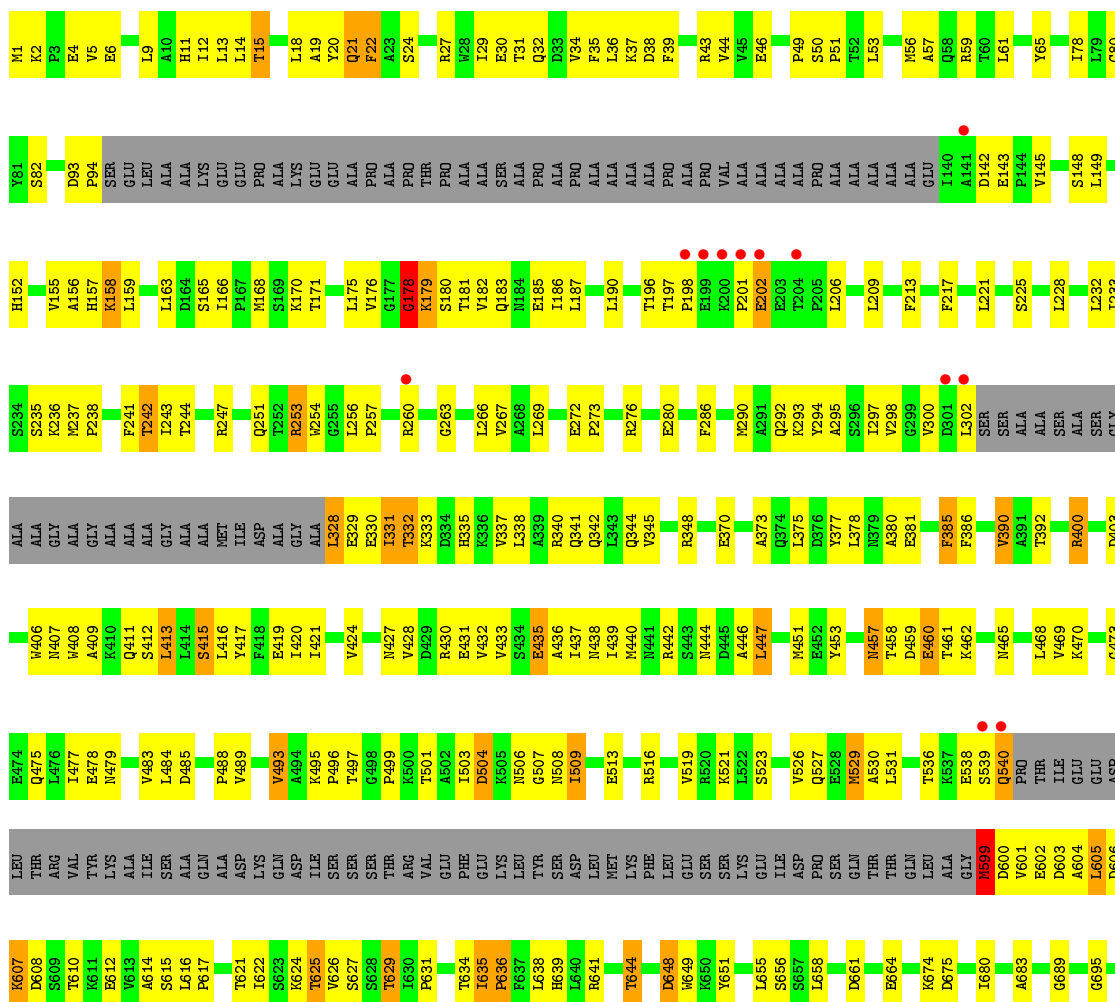








● Molecule 1: FATTY ACID SYNTHASE SUBUNIT ALPHA



Q698	F790	R882	P984	K1081	Q1188	V1270	R1360	K1450	S1540	V1624	R1721	GLU
K702	A791	I883	R985	K1087	I1189	I1274	T1381	Q1451	G1543	L1628	V1722	ILE
V705	R792	E886	A986	D1088	P1189	L1275	P1362	Q1455	T1544	P1627	L1731	TVR
T706	R793	G887	N987	V1089	P1190	Q1276	A1363	R1455	S1545	S1628	F1732	ALA
R709	I794	I888	Q988	T1095	W1193	F1279	E1364	Q1458	T1546	V1639	F1733	SER
F710	R796	E889	Q989	S1096	N1194	I1280	M1366	I1459	M1549	S1640	I1738	ALA
S711	L797	R891	F992	I1097	A1195	M1281	R1367	K1460	D1550	I1641	Q1739	ALA
V714	T798	G892	Y998	S1101	T1197	M1283	T1370	W1461	K1551	T1642	Y1744	VAL
Q719	R801	V893	I1004	S1104	I1200	M1284	T1371	V1463	E1553	F1646	A1747	ASP
S720	C805	R894	L1009	R1104	S1201	A1285	R1373	E1464	A1555	K1649	A1747	ASP
G726	V806	L906	L1009	L1105	D1202	M1289	M1374	M1465	I1555	G1650	ASN	SER
K728	R807	G907	E1010	L1106	V1208	L1290	G1375	E1473	I1557	G1651	THR	PHE
G729	R818	L908	G1011	E1107	D1209	A1474	F1376	E1475	L1564	Q1652	ILE	ALA
T731	V822	V913	L1012	P1108	T1212	I1292	Q1380	E1476	G1565	V1655	THR	THR
L732	I823	L916	D1014	Y1114	V1215	G1296	G1381	I1477	R1566	V1656	ALA	THR
I733	M824	P921	E1014	M1115	V1215	P1297	I1382	S1478	I1573	H1657	LYS	LYS
F737	P825	V922	I1019	K1119	S1218	T1300	G1383	S1479	G1574	P1658	ILE	LYS
Q738	M826	R921	V1020	K1119	V1219	P1301	I1384	L1487	W1575	D1659	GLU	GLU
R739	L824	N927	V1021	Q1123	V1220	G1303	Q1385	R1488	F1576	Y1660	ASN	ALA
M739	P828	G928	T1022	E1124	I1224	A1304	I1386	R1489	Q1577	Y1662	THR	VAL
Q739	F833	G929	T1022	E1125	T1229	I1307	M1396	T1490	L1580	G1663	THR	VAL
M739	R834	G929	P1029	T1126	I1229	T1307	M1396	T1490	L1580	A1664	GLU	VAL
G740	L930	G929	W1030	Y1126	I1229	E1492	E1496	Q1500	H1583	I1665	LYS	LYS
S741	G835	Q931	W1030	V1127	S1226	C1305	L1392	L1501	G1589	P1666	GLY	GLY
K742	F932	Q931	W1030	V1127	S1226	R1491	L1392	R1502	A1590	E1667	GLY	VAL
Q743	D836	V933	R1036	L1131	T1229	V1308	M1396	Q1505	W1591	D1668	GLY	VAL
D744	Y839	P934	W1037	E1132	T1229	V1309	M1396	M1500	M1592	E1668	ASP	ALA
E745	R843	R937	M1039	P1133	Y1232	E1310	I4400	Q1500	L1597	R1669	ASP	VAL
L748	E938	E937	E1040	P1133	E1233	E1310	Y4401	L1501	Q1598	Y1670	GLY	LEU
I749	L846	F939	E1040	K1138	M1234	V1312	A4408	R1502	W1592	Y1673	GLY	LEU
E750	L849	R944	F1045	D1153	V1238	V1316	T1411	Q1505	M1594	V1677	VAL	VAL
F751	R852	L947	S1046	I1154	H1239	E1317	D1412	M1540	L1597	V1677	VAL	VAL
L761	L947	V948	L1047	I1154	V1240	E1317	K1413	R1545	L1597	R1680	GLY	LEU
D764	E948	E949	E1048	P1158	S1241	I1318	I1414	D1516	Q1598	E1681	ILE	LEU
I769	E856	E949	C1050	E1159	E1242	I1324	I1414	P1517	L1599	K1682	THR	LEU
F771	S857	T950	C1050	E1163	G1244	I1326	V1418	P1517	L1600	M1682	SER	LEU
I774	S858	S951	E1052	Y1163	S1247	G1327	P1419	A1520	P1606	M1692	ILE	ILE
E776	S859	S952	E1056	K1166	G1248	I1328	A1420	P1521	G1607	I1693	VAL	VAL
E782	M860	F953	I1056	T1172	S1249	V1329	L1426	R1524	M1608	F1698	ARG	VAL
H783	V864	R954	M1057	L1173	V1249	Y1332	L1426	G1524	R1609	K1701	ASN	ASN
I784	I868	I959	S1061	Y1174	G1252	Y1337	R1430	A1527	D1612	K1701	THR	ASN
G874	R873	V968	Y1062	L1175	E1253	E1337	E1431	T1528	M1613	P1705	PHE	ALA
H83	G874	H969	H1063	P1176	V1254	E1338	H1432	T1528	M1613	Y1706	PRO	ALA
I787	T875	H969	L1087	K1177	S1255	F1341	H1433	T1532	I1617	T1707	GLU	ALA
L788	T875	G970	R1070	A1178	A1256	F1341	S1434	I1533	I1617	D1708	ARG	VAL
K787	LEU	G970	R1070	R1180	R1258	G1344	M1442	I1533	E1619	E1709	ASN	ASN
S788	MET	V980	V1076	D1182	G1259	K1347	L1443	L1536	Q1620	ASP	PHE	LEU
E789	SER	E981	D1077	R1183	D1263	K1347	H1444	G1537	F1621	V1714	THR	HIS
	ALA	I982	S1078	L1184	R1264	K1347	M1445	V1538	E1622	A1720	PRO	GLY
	M881	Q983	V1185	V1185	K1446	T1352	K1446	A1539	Y1623		GLN	ASN

● Molecule 2: FATTY ACID SYNTHASE SUBUNIT BETA



MET ASP TYR T6 R7 P8 L9 L11 S15 L16 V22 P23 T24 A25 S26 F27 F28 L33 L40 L41 L42 E43 P44 T45 E46 G47 F48 A49 A50 D61 D62 E53 P64 K63 F64 L65 V72 E73 K76 Q155 L156 Q157 F80 I159

L84 M85 L86 T89 M83 C94 Y95 N99 D100 I101 H102 A105 L109 M112 D113 T114 T115 L116 V117 K118 L119 K120 P121 E121 A122 L122 L123 K124 L127 T128 T129 I131 M132 K133 A134 P135 P136 F137 D138 K139 L142 M144 L145 L146 V149 E153 M153 A154 Q155 L156 V157 A158 I159

I236 S237 C238 P239 L240 L241 L244 Q245 Q246 A247 H248 Y249 V250 V251 L255 L258 T259 P260 G261 L1683 E262 L263 R264 A270 T271 G272 H273 G276 L277 V278 T279 V281 A282 L283 T286 W289 S295 V296 R297 K298 A299 I300 T301 V302 F304 F305 I306 R309 P315

L319 L324 L328 E332 G333 V334 F335 L339 S340 S342 S344 N343 L344 T345 Q346 E347 Q348 V349 Q350 V353 R354 K355 T356 N357 S358 R359 Q365 S369 L370 V371 A374 R375 N376 L377 S380 L386 R389 N390 L391 T392 R394 K397 L402 D403 Q404

F416 S417 R419 F420 P422 V423 A424 S425 P426 F427 H428 H430 L431 L432 L439 N440 N441 D442 L443 V444 T445 N446 U447 V448 T455 Q456 L457 V459 Y460 D461 F463 D464 Q465 S466 D467 R468 V470 S472 R469 N553 K556 R557 N558 P559 N560 Y563 K562 L563 R564 L565 Y566

P487 V488 K489 N490 E491 T492 T493 P494 Q495 F496 T499 S500 L501 L502 D503 D504 G505 F504 S506 P506 G507 H508 L512 L513 T516 H517 K520 M521 N522 R526 G531 T532 L533 D539 F543 K544 Q545 V550 T551 S552 V553 K556 R557 N558 P559 N560 Y563 K562 L563 R564 L565 Y566

L569 L570 K571 N572 S573 C575 K576 L577 F578 F579 T580 T581 K582 F583 S584 L585 L586 S587 G588 L592 L593 V594 P595 G596 M597 T598 P599 G600 T601 S603 F606 L607 T610 N612 K613 Q614 Y615 T616 G617 E618 Y619 L620 G621 G622 K624 Y624 Y625 Y626 Y627 Y628 Y629 Y630 Y631 Y632 Y633 Y634 Y635 Y636 Y637 Y638 Y639 Y640 Y641 Y642 Y643 Y644 Y645 Y646 Y647 Y648 Y649 Y650 Y651 Y652 Y653 Y654 Y655 Y656 Y657 Y658 Y659 Y660 Y661 Y662 Y663 Y664 Y665 Y666 Y667 Y668 Y669 Y670 Y671 Y672 Y673 Y674 Y675 Y676 Y677 Y678 Y679 Y680 Y681 Y682 Y683 Y684 Y685 Y686 Y687 Y688 Y689 Y690 Y691 Y692 Y693 Y694 Y695 Y696 Y697 Y698 Y699 Y700 Y701 Y702 Y703 Y704 Y705 Y706 Y707 Y708 Y709 Y710 Y711 Y712 Y713 Y714 Y715 Y716

I717 M718 L719 K720 A721 A722 H723 F726 P727 T728 T729 L730 Q731 W732 G735 R736 G739 H740 H741 S742 D745 A746 H747 T748 P749 M750 L751 Q752 M753 Y754 I757 R758 R759 H760 W761 M762 N763 M764 L765 I766 F767 G768 S769 G772 S773 A774 D775 T776 T777 Y780 E784 W785

S786 I787 F788 F789 D790 E791 T792 F793 W794 P795 L796 D797 G798 F799 L800 R804 V805 W806 L807 E810 V811 W812 K812 T813 D816 A817 K818 F820 F821 L821 T825 G826 V827 P828 W832 T835 T840 G841 G842 L843 W844 T845 W846 E852 P853 L854 B855 K856 L857 L858 T859 R860 W865

K866 E867 D868 E870 E871 T872 L873 F873 K879 P880 V881 W882 T883 L884 K887 Q888 L889 S893 R894 D898 F899 Q900 K901 P902 W903 F904 A905 T906 V907 Q910 A911 R912 D913 T916 E921 L926 L929 I932 I933 W938 F939 T942 W943 R944 T945 W946 E952 P953 L954 B955 K956 L957 L958 T959 R960 W965

F950 L951 R952 R953 V954 E955 E956 R957 K960 S961 K962 T963 L964 S965 L966 R967 Q968 S969 Y970 S971 L972 L973 Y987 E992 Q993 F994 L995 Q998 D999 I1000 H1002 A1003 L1004 S1005 M1006 P1010 M1011 Q1012 K1013 P1014 V1015 P1016 F1017 V1018 P1019 V1020 L1021 R1024 A1025 E1026 I1027 K1031

D1032 L1040 E1041 A1042 V1043 S1044 D1045 Q1046 V1047 D1048 A1049 R1050 T1051 C1052 I1053 L1054 H1055 V1058 A1059 A1060 Q1061 T1062 T1063 I1066 D1067 E1068 P1069 I1070 K1071 M1074 D1075 G1076 I1077 H1078 D1079 G1080 H1081 I1082 K1083 K1084 L1085 L1086 Y1090 G1091 D1092 D1093 K1096 I1097 P1098 A1099 V1100 E1101 Y1102 F1103

P1108 P1109 ASP VAL GLN SER GLN VAL ASP SER SER SER VAL V1128 A1129 T1130 T1133 D1134 E1135 W1138 T1145 S1145 H1148 W1149 H1150 H1151 I1159 T1160 Q1161 T1162 K1163 V1166 S1167 M1168 P1169 I1170 K1171 K1172 V1173 F1174 K1175 P1176 S1177 M1180 V1181 T1189

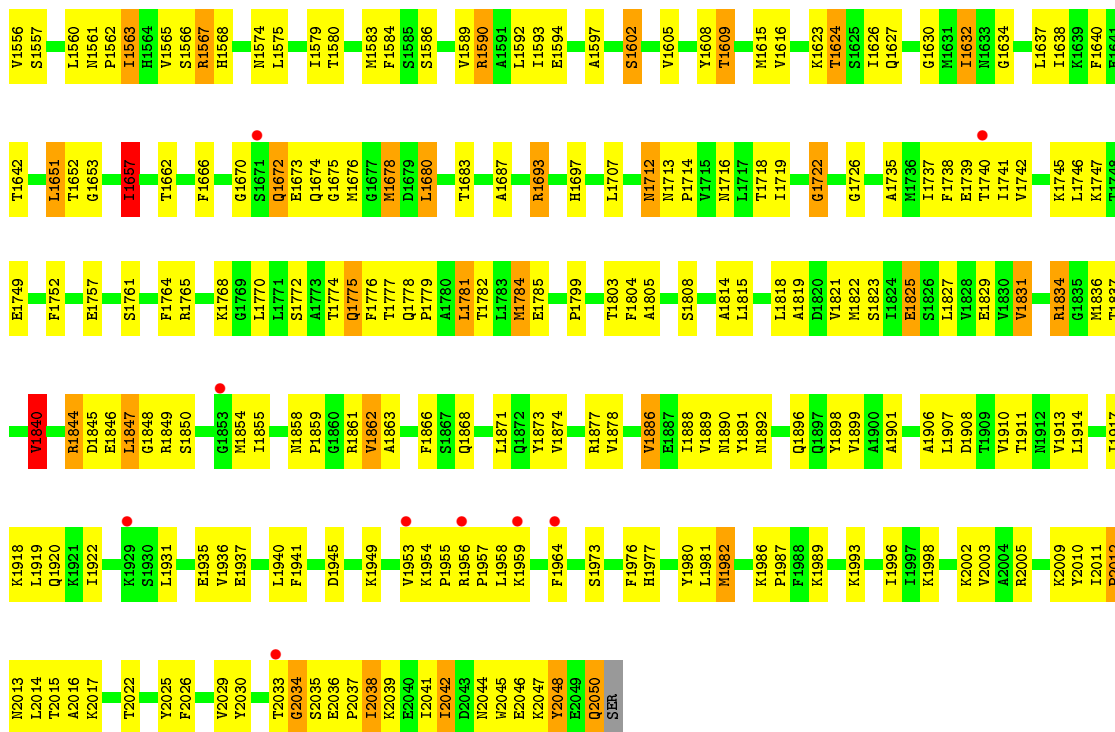
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S1198	V1284	I1378	T1468	V1565	K1765	R1765	L1847	L1919	L2014
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		V1381	E1470	E1567	F1666	K1768	R1849	F1921	A2016
		V1382	T1470	H1568	G1670	G1769	S1850	L1922	K2017
		M1383	V1472	M1569	S1671	L1770	M1854	L1931	T2022
		T1293	T1473	L1574	Q1672	L1771	L1931	T1932	T2022
		A1294	F1474	M1575	E1673	S1772	L1855	S1932	T2025
		K1295	K1475	L1579	Q1674	A1773	A1856	E1935	Y2026
		E1296	K1475	T1579	G1675	T1774	L1857	V1936	F2026
		F1300	S1481	T1580	M1676	Q1775	M1858	E1937	V2029
		A1303	S1482	M1583	G1677	F1776	P1859	E1937	F2030
		Q1308	V1483	F1584	M1678	T1777	G1860	L1940	Y2030
		E1309	F1486	F1585	D1679	P1779	V1862	F1941	T2033
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		V1312	I1489	V1589	T1683	L1782	F1866	K1949	S2035
		S1313	R1490	M1590	A1687	L1783	M1949	K1949	E2036
		R1314	E1492	A1591	M1687	M1783	Q1868	V1953	P2037
		T1318	L1493	L1592	R1693	E1785	L1871	K1954	I2038
		M1319	P1494	I1593	H1697	P1789	L1871	P1955	K2039
		P1232	T1495	E1594	H1697	L1789	I1872	F1956	E2040
		V1234	K1496	A1597	I1706	T1803	V1873	R1956	I2041
		S1235	R1496	S1602	L1707	F1804	V1874	P1957	I2042
		L1236	E1501	V1605	L1707	L1815	E1876	L1958	N2044
		L1238	I1502	R1606	I1711	A1805	L1877	V1964	V2045
		L1239	G1503	G1607	M1712	H1807	V1878	F1964	E2046
		Y1240	F1504	F1607	M1716	S1808	V1884	S1973	K2047
		M1241	A1510	T1608	I1718	A1814	L1885	F1976	E2049
		F1242	S1511	T1609	I1719	L1815	V1886	H1977	Q2050
		M1243	H1512	M1615	G1722	L1818	I1888	S1978	SER
		P1244	T1526	V1616	G1726	A1819	V1889	T1979	
		G1247	E1528	K1623	F1738	D1820	M1890	Y1980	
		S1252	Q1529	T1624	E1739	M1821	V1891	L1981	
		E1256	L1533	S1625	L1740	S1823	M1892	M1982	
		D1257	D1543	Q1627	I1742	I1824	E1894	K1986	
		R1258	D1543	Q1627	V1742	E1825	V1895	F1988	
		H1259	D1543	Q1627	I1742	S1826	Q1897	K1989	
		Q1260	D1543	Q1627	K1745	V1828	V1898	F1991	
		R1261	D1543	Q1627	L1746	E1829	V1899	L1992	
		L1262	D1543	Q1627	K1747	V1830	A1900	K1993	
		K1263	D1543	Q1627	T1748	V1831	A1901	I1996	
		M1265	D1543	Q1627	E1749	R1834	A1906	I1997	
		Y1266	D1543	Q1627	F1752	G1835	L1907	K1998	
		L1269	D1543	Q1627	F1752	M1836	T1908	V2003	
		D1272	D1543	Q1627	I1755	T1837	V1910	A2004	
			D1560	L1651	M1756	V1840	L1911	R2005	
			L1560	L1652	E1757	V1842	V1913	K2009	

● Molecule 2: FATTY ACID SYNTHASE SUBUNIT BETA



MET	L84	I159	T234
ASP	M85	F160	P235
ALA	L86	G161	L236
TYR	S85	G162	S237
	T89	Q163	C238
	R7	T166	P239
	P8	D167	L240
	L9	G168	L241
	T10	Y169	L244
	L11	F170	Q245
	S15	L173	L246
	L16	R174	A247
	V22	D175	E248
	P23	L176	V250
	T24	V177	V251
	A25	Q178	L255
	S26	T179	F258
	F27	Y180	H181
	F28	V182	D113
	L33	L183	T259
	M38	V184	P260
	R39	G185	G261
	T40	D186	E262
	L41	L187	L263
	L42	L188	R264
	L43	L189	T271
	L44	F190	G272
	L45	L191	H273
	L46	S192	R274
	L47	A193	S274
	L48	T194	Q275
	L49	L195	G276
	L50	L196	L277
	L51	E197	V278
	L52	L198	T279
	L53	I199	A280
	L54	L203	V281
	L55	F209	A282
	L56	T210	L283
	L57	L213	T286
	L58	M214	M289
	L59	L215	E290
	L60	L216	S295
	L61	E217	V296
	L62	L218	R297
	L63	M219	K298
	L64	V149	A299
	L65	M153	I300
	L66	V72	L303
	L67	E73	P304
	L68	L154	F305
	L69	Q155	L306
	L70	L156	R309
	L71	V157	L232
	L72	A158	L232
	L73	L157	L232
	L74	L158	S233

D1468	T1374	F1279	L1197	VAL	L1040	T945	A858	E784	V716	I694	Y565	C482	L402	P345
K1462	V1377	D1280	S1198	GLN	E1041	F946	T859	W785	I717	W638	Y569	F483	D403	F485
T1463	I1378	P1281	SER	GLN	A1042	T947	R860	T787	W718	L669	L569	R485	Q404	S318
T1468	V1381	V1284	VAL	VAL	V1043	G948	W865	K788	A720	I641	N572	L486	R406	L319
E1469	V1382	L1282	ASP	ASP	D1045	D949	K866	F789	K721	E642	K573	P487	I407	P320
T1470	M1383	I1210	SER	SER	Q1046	R952	F868	W791	A722	K643	S574	V488	P408	P321
V1472	G1387	L1211	SER	VAL	V1048	F792	D869	F792	F727	S644	S575	K489	F409	L324
L1473	G1395	K1212	VAL	VAL	Q1049	V954	E870	M793	F727	G648	K575	W490	F416	S417
L1474	K1368	L1213	SER	GLU	R1050	E955	T871	M794	T492	I649	L577	T492	S417	L328
K1475	I1389	L1214	GLU	D1123	C1052	E956	L872	T051	L872	W796	V579	T494	R419	E332
S1481	V1390	I1219	D1123	L1053	L1053	K960	D797	L790	L790	I682	E580	Q495	F420	E332
S1482	L1396	Q1220	K1128	L1054	L1054	R879	R879	Q731	Q731	W653	T581	F496	L421	P335
V1483	S1397	M1221	A1129	L1067	L1067	L880	L880	W732	W732	W654	K582	P422	P422	P422
F1486	V1403	M1223	T1130	V1058	V1058	P882	P882	T733	T733	W658	F583	T499	V423	M338
V1491	M1404	R1227	T1133	A1060	A1060	R804	R804	R796	R796	I659	S584	H500	A424	L339
E1492	T1407	T1228	D1134	Q1061	Q1061	W805	W805	R796	R796	I661	K585	I501	S425	S340
L1493	S1408	G1231	E1135	T1063	T1063	I807	I807	H741	H741	I663	G588	G505	H428	N343
P1494	F1409	G1232	W1138	I1066	I1066	R893	R893	S742	S742	I665	L586	F504	L431	L344
K1496	F1410	K1232	S1145	E1068	E1068	R894	R894	D745	D745	I666	V594	T516	L432	T345
E1497	F1411	V1234	E1146	E1068	E1068	L896	L896	K812	K812	I667	W594	H517	V349	E347
T1498	G1414	S1235	I1147	P1069	P1069	Q993	Q993	T813	T813	E688	P595	H517	Q348	Q348
V1499	N1415	A1321	M1148	F1070	F1070	R995	R995	D816	D816	E689	G596	R526	V349	V349
E1500	Y1416	P1322	W1149	K1071	K1071	L995	L995	A817	A817	R670	G596	R526	N443	Q350
I1501	T1417	L1238	H1151	M1074	M1074	Q998	Q998	K818	K818	I674	T598	D521	K441	N353
G1502	D1418	M1241	A1152	D1075	D1075	P999	P999	L751	L751	P675	P599	G522	D442	N354
L1503	F1419	F1242	I1159	G1076	G1076	I1000	I1000	Q752	Q752	P676	G600	R526	L443	K386
V1504	E1420	M1243	M1168	I1077	I1077	D1001	D1001	W753	W753	I677	T601	R526	V444	T356
V1505	M1421	P1244	P1169	H1078	H1078	H1002	H1002	F904	F904	Q677	V602	V602	K445	N357
A1510	K1425	G1247	I1170	D1079	D1079	F1003	F1003	G824	G824	F678	S603	N446	N446	S358
H1511	T1426	Y1252	H1163	G1080	G1080	T906	T906	T825	T825	W757	F606	L533	N447	R360
H1512	E1428	S1252	K1083	H1081	H1081	P907	P907	G826	G826	R758	V607	N536	V448	P361
P1515	Y1431	E1256	V1166	K1084	K1084	Q910	Q910	R827	R827	R759	P537	N537	I455	S369
T1526	H1434	D1257	N1167	L1085	L1085	P1010	P1010	F828	F828	H760	T610	D538	L370	L370
L1527	I1435	F1344	N1168	L1086	L1086	M1011	M1011	W832	W832	N762	T611	D639	V371	V371
Q1529	T1437	P1340	P1169	L1086	L1086	Q1012	Q1012	E833	E833	N763	N612	D540	V459	V459
K1530	K1437	V1343	I1170	Y1090	Y1090	V1015	V1015	Q834	Q834	W764	Y615	F543	Y460	Y460
L1533	S1438	D1344	R1171	G1091	G1091	P1016	P1016	T835	T835	L765	T616	R544	D461	D461
E1528	I1439	D1344	K1172	D1092	D1092	F1017	F1017	W836	W836	I766	K594	R544	T462	T462
Q1529	T1437	L1347	V1173	D1093	D1093	L1262	L1262	L698	L698	F767	Q545	R544	F462	F462
K1530	S1438	L1347	F1174	D1093	D1093	P1018	P1018	G768	G768	E618	E618	D464	D464	D464
L1533	I1441	L1349	K1175	K1096	K1096	P1019	P1019	L926	L926	L619	V550	G465	G465	G465
D1543	A1442	L1350	P1176	L1097	L1097	V1020	V1020	L929	L929	Y702	T551	S552	S466	S466
P1547	V1443	V1351	S1177	I1097	I1097	L1021	L1021	W844	W844	L703	S552	S552	R469	R469
S1548	L1444	H1352	M1180	V1100	V1100	R1024	R1024	T845	T845	G704	N553	N553	V470	V470
T1549	R1445	H1352	V1181	F1025	F1025	E1026	E1026	W846	W846	L705	G623	G623	L471	L471
M1550	S1446	M1355	T1189	E1026	E1026	I1027	I1027	K706	K706	F707	Y624	K556	L471	L471
M1551	L1462	M1359	V1189	I1027	I1027	K1031	K1031	E852	E852	A712	G629	N558	S476	S476
P1552	F1457	L1360	V1194	P1109	P1109	ASP	ASP	P863	P863	I713	M630	P559	E477	E477
		V1368	V1195	V1109	V1109			R856	R856	W780	A632	M560	R478	R478
			T1196	ASP	ASP			I857	I857	Q715	A633	L562	D481	D481



• Molecule 2: FATTY ACID SYNTHASE SUBUNIT BETA

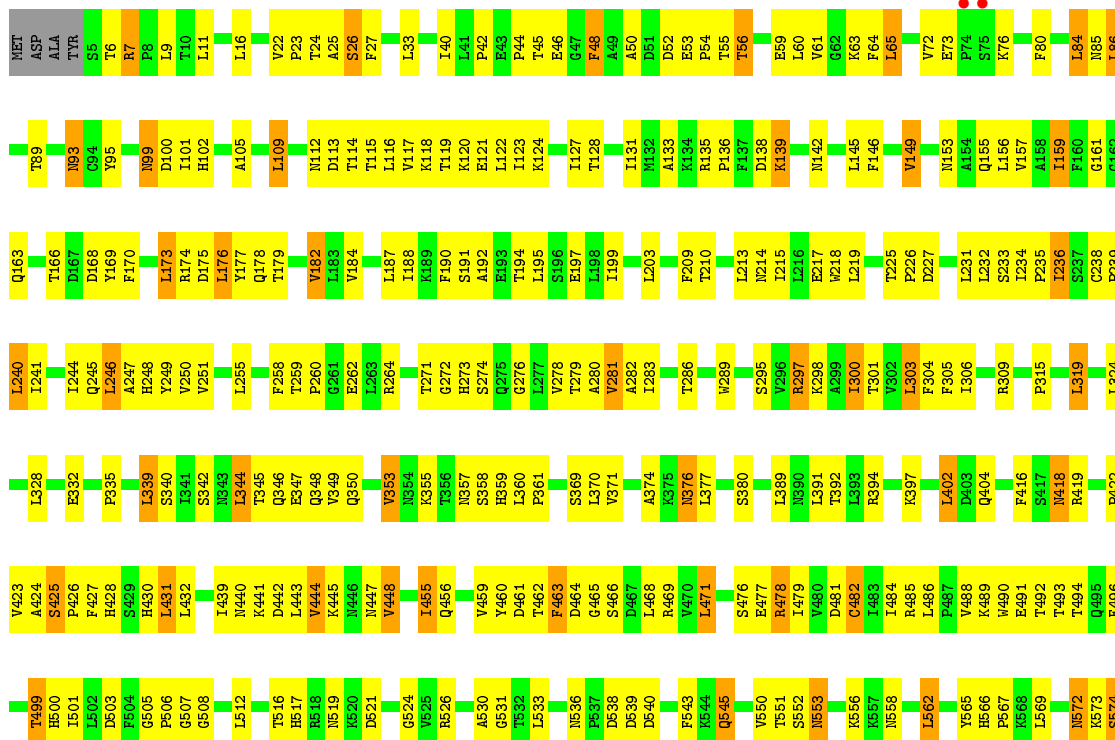
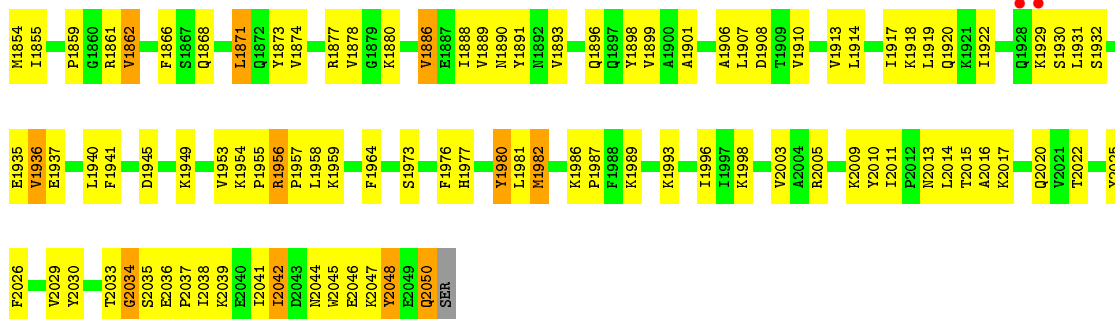


Table with 3 columns of residue labels (e.g., S1761, F1764, R1765) and their corresponding B-factors. The labels are color-coded by range and include red and green markers. The table contains approximately 40 columns of labels, each with a corresponding numerical value representing the B-factor. The values range from approximately 0.7 to 105.9.





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	231.90Å 231.90Å 756.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.99 – 4.00 24.99 – 4.00	Depositor EDS
% Data completeness (in resolution range)	97.3 (24.99-4.00) 97.3 (24.99-4.00)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 3.97Å)	Xtrriage
Refinement program		Depositor
R, $R_{free}$	0.268 , 0.268 0.276 , 0.278	Depositor DCC
$R_{free}$ test set	8547 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	130.2	Xtrriage
Anisotropy	0.319	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 76.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.19$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	85959	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	164.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, CER

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.50	9/12855 (0.1%)	0.61	8/17369 (0.0%)
1	B	0.44	3/12855 (0.0%)	0.62	9/17369 (0.1%)
1	C	0.48	8/12855 (0.1%)	0.61	7/17369 (0.0%)
2	G	0.42	11/16360 (0.1%)	0.58	7/22198 (0.0%)
2	H	0.55	13/16360 (0.1%)	0.61	9/22198 (0.0%)
2	I	0.42	8/16360 (0.0%)	0.59	12/22198 (0.1%)
All	All	0.47	52/87645 (0.1%)	0.60	52/118701 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	G	0	1
2	H	0	3
2	I	0	1
All	All	0	5

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1657	ILE	C-N	-32.81	0.58	1.34
2	H	559	PRO	C-N	23.37	1.87	1.34
1	A	485	ASP	C-N	18.89	1.77	1.34
1	C	1430	ARG	C-N	-13.61	1.02	1.34
2	H	1422	THR	C-N	-13.47	1.03	1.34
1	A	992	PHE	C-N	13.35	1.59	1.34
2	H	315	PRO	C-N	13.20	1.64	1.34
1	C	992	PHE	C-N	13.18	1.59	1.34
1	C	181	THR	C-N	-12.39	1.05	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	933	VAL	C-N	12.23	1.57	1.34
2	H	1530	LYS	C-N	11.67	1.60	1.34
2	I	842	GLY	C-N	11.12	1.59	1.34
2	G	315	PRO	C-N	10.45	1.58	1.34
1	A	932	PHE	C-N	-9.64	1.11	1.34
1	C	485	ASP	C-N	9.61	1.56	1.34
2	H	1529	GLN	C-N	-9.44	1.12	1.34
2	H	1256	GLU	C-N	9.35	1.55	1.34
2	H	138	ASP	C-N	9.07	1.54	1.34
2	H	1840	VAL	C-N	8.47	1.53	1.34
1	A	1118	LYS	C-N	-8.42	1.14	1.34
2	G	1657	ILE	C-N	8.15	1.52	1.34
2	I	1530	LYS	C-N	7.92	1.52	1.34
2	I	315	PRO	C-N	7.84	1.52	1.34
1	A	668	PHE	C-N	7.73	1.51	1.34
2	I	1980	TYR	C-N	7.70	1.51	1.34
2	G	1841	ALA	C-N	-7.11	1.17	1.34
1	A	181	THR	C-N	7.05	1.50	1.34
2	G	422	PRO	C-N	6.97	1.50	1.34
2	I	1422	THR	C-N	-6.96	1.18	1.34
2	G	559	PRO	C-N	-6.78	1.18	1.34
2	G	1422	THR	C-N	-6.67	1.18	1.34
1	C	381	GLU	C-N	-6.65	1.18	1.34
2	I	1018	VAL	C-N	-6.57	1.21	1.34
2	G	1256	GLU	C-N	6.43	1.48	1.34
1	C	1520	ALA	C-N	-6.36	1.22	1.34
1	C	932	PHE	C-N	-6.35	1.19	1.34
2	I	903	TRP	C-N	6.33	1.48	1.34
2	H	1053	ILE	C-N	6.30	1.48	1.34
2	H	422	PRO	C-N	6.29	1.48	1.34
2	I	1529	GLN	C-N	-6.27	1.19	1.34
2	G	842	GLY	C-N	6.06	1.48	1.34
2	H	137	PHE	C-N	5.95	1.47	1.34
1	A	1520	ALA	C-N	5.79	1.45	1.34
2	H	1982	MET	C-N	5.67	1.47	1.34
1	B	181	THR	C-N	-5.65	1.21	1.34
2	G	1529	GLN	C-N	-5.50	1.21	1.34
2	G	1840	VAL	C-N	5.48	1.46	1.34
2	G	1980	TYR	C-N	5.38	1.46	1.34
1	C	636	PRO	C-N	-5.29	1.21	1.34
1	B	668	PHE	C-N	5.29	1.46	1.34
1	B	1430	ARG	C-N	-5.19	1.22	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1181	PHE	C-N	5.13	1.45	1.34

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1657	ILE	O-C-N	-17.23	95.13	122.70
2	H	1657	ILE	CA-C-N	12.14	143.92	117.20
1	B	1116	PRO	O-C-N	-11.67	104.02	122.70
2	H	1657	ILE	C-N-CA	11.19	149.68	121.70
1	C	178	GLY	O-C-N	10.12	138.89	122.70
2	I	1982	MET	O-C-N	-9.44	107.59	122.70
2	G	842	GLY	O-C-N	-8.86	108.52	122.70
2	G	1053	ILE	O-C-N	-8.58	108.97	122.70
1	B	992	PHE	O-C-N	8.47	137.19	121.10
2	I	422	PRO	O-C-N	-8.30	109.42	122.70
2	H	1530	LYS	O-C-N	8.28	135.95	122.70
1	B	992	PHE	C-N-CD	8.15	145.52	128.40
2	I	1982	MET	C-N-CA	8.08	141.89	121.70
1	B	1116	PRO	CA-C-N	8.00	134.79	117.20
1	C	178	GLY	CA-C-N	-7.55	100.59	117.20
2	I	1657	ILE	O-C-N	-7.47	110.75	122.70
1	C	1520	ALA	O-C-N	7.43	135.22	121.10
1	A	1430	ARG	O-C-N	-7.40	110.85	122.70
1	B	1116	PRO	C-N-CA	7.29	139.94	121.70
1	B	599	MET	N-CA-C	-6.93	92.27	111.00
1	C	599	MET	N-CA-C	-6.92	92.32	111.00
1	A	599	MET	N-CA-C	-6.90	92.37	111.00
1	A	992	PHE	C-N-CD	6.65	142.37	128.40
2	I	422	PRO	CA-C-N	6.52	131.55	117.20
2	H	1840	VAL	O-C-N	-6.51	112.29	122.70
2	I	1982	MET	CA-C-N	6.50	131.50	117.20
2	H	1530	LYS	C-N-CA	-6.37	105.79	121.70
1	C	1116	PRO	O-C-N	-6.36	112.52	122.70
2	H	1530	LYS	CA-C-N	-6.32	103.30	117.20
2	I	1530	LYS	O-C-N	6.31	132.79	122.70
1	B	992	PHE	CA-C-N	-6.11	100.00	117.10
2	G	1053	ILE	CA-C-N	6.05	130.50	117.20
1	A	992	PHE	O-C-N	5.97	132.45	121.10
2	G	1842	VAL	O-C-N	5.80	132.12	121.10
2	I	315	PRO	O-C-N	-5.75	113.50	122.70
1	B	540	GLN	N-CA-C	-5.65	95.74	111.00
1	A	540	GLN	N-CA-C	-5.64	95.77	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	540	GLN	N-CA-C	-5.63	95.80	111.00
1	B	178	GLY	O-C-N	5.57	131.61	122.70
2	I	422	PRO	C-N-CA	5.52	135.50	121.70
2	G	138	ASP	O-C-N	-5.44	113.99	122.70
1	A	933	VAL	O-C-N	5.44	131.44	121.10
1	A	1520	ALA	O-C-N	5.44	131.44	121.10
2	H	1256	GLU	CA-C-N	-5.39	105.35	117.20
2	I	1657	ILE	CA-C-N	5.34	128.95	117.20
2	G	842	GLY	CA-C-N	5.30	128.86	117.20
1	C	178	GLY	C-N-CA	-5.24	108.61	121.70
1	A	1116	PRO	O-C-N	-5.17	114.43	122.70
2	H	138	ASP	O-C-N	-5.08	114.56	122.70
2	G	138	ASP	C-N-CA	5.05	134.32	121.70
2	I	1657	ILE	C-N-CA	5.03	134.27	121.70
2	I	1530	LYS	CA-C-N	-5.02	106.15	117.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	1108	PRO	Peptide
2	H	1108	PRO	Peptide
2	H	1256	GLU	Mainchain
2	H	1657	ILE	Mainchain
2	I	1108	PRO	Peptide

## 5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12615	0	12589	601	1
1	B	12615	0	12591	582	6
1	C	12615	0	12587	588	0
2	G	15995	0	15975	998	10
2	H	15995	0	15974	997	7
2	I	15995	0	15976	977	12
3	A	12	0	10	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	10	4	0
3	C	12	0	10	4	0
4	G	31	0	19	7	0
4	H	31	0	19	6	0
4	I	31	0	19	8	0
All	All	85959	0	85779	4568	18

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 27.

All (4568) 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)
1:A:485:ASP:C	1:A:486:VAL:N	1.77	1.36
2:H:559:PRO:C	2:H:560:ASN:N	1.87	1.26
2:H:1956:ARG:HB2	2:H:1957:PRO:HD3	1.24	1.18
2:G:28:PHE:CE2	2:H:7:ARG:HD2	1.80	1.16
2:G:1859:PRO:HG3	2:G:1871:LEU:HD12	1.29	1.15
2:H:1834:ARG:HH11	2:H:1834:ARG:HG2	1.06	1.15
2:H:490:TRP:HE1	2:H:516:THR:HG22	1.12	1.14
2:H:499:THR:HB	2:H:500:HIS:HD2	1.10	1.12
2:I:490:TRP:HE1	2:I:516:THR:HG22	1.10	1.12
2:G:1956:ARG:HB2	2:G:1957:PRO:HD3	1.23	1.12
2:G:131:ILE:HD12	2:G:182:VAL:HB	1.18	1.12
2:H:131:ILE:HD12	2:H:182:VAL:CB	1.79	1.11
2:I:601:THR:HG21	2:I:618:GLU:O	1.50	1.11
2:I:1956:ARG:HB2	2:I:1957:PRO:HD3	1.23	1.11
1:A:253:ARG:HG3	1:A:254:TRP:HD1	1.15	1.10
1:A:1721:ARG:HG2	1:A:1721:ARG:HH11	1.16	1.10
2:H:601:THR:HG21	2:H:618:GLU:O	1.50	1.10
2:G:601:THR:HG21	2:G:618:GLU:O	1.52	1.10
2:G:499:THR:HB	2:G:500:HIS:HD2	1.08	1.09
2:H:131:ILE:CB	2:H:182:VAL:HG11	1.82	1.09
2:I:297:ARG:HD3	2:I:447:ASN:HD21	1.15	1.09
2:G:131:ILE:HB	2:G:182:VAL:HG11	1.31	1.09
2:I:499:THR:HB	2:I:500:HIS:HD2	1.07	1.08
2:G:490:TRP:HE1	2:G:516:THR:HG22	1.12	1.08
1:C:852:ARG:HG2	1:C:852:ARG:HH11	1.14	1.08
2:H:131:ILE:HG21	2:H:182:VAL:HG12	1.35	1.07
2:H:128:THR:HA	2:H:182:VAL:HG21	1.31	1.07
2:I:1227:ARG:HH11	2:I:1227:ARG:HG3	1.18	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:297:ARG:HD3	2:G:447:ASN:HD21	1.17	1.06
2:G:28:PHE:CZ	2:H:7:ARG:HD2	1.91	1.06
2:I:1834:ARG:HG2	2:I:1834:ARG:HH11	1.16	1.06
1:C:1367:ARG:NH1	1:C:1372:THR:HB	1.71	1.06
2:G:903:TRP:O	2:G:906:THR:HG22	1.57	1.05
1:C:1721:ARG:HG2	1:C:1721:ARG:HH11	1.19	1.05
2:G:1834:ARG:HG2	2:G:1834:ARG:HH11	1.16	1.05
2:I:7:ARG:HH21	2:I:27:PHE:HB3	1.20	1.05
1:B:253:ARG:HG3	1:B:254:TRP:HD1	1.17	1.04
1:A:1367:ARG:NH1	1:A:1372:THR:HB	1.72	1.04
1:C:253:ARG:HG3	1:C:254:TRP:HD1	1.15	1.04
2:G:932:ILE:HD11	2:G:1042:ALA:HB2	1.36	1.04
2:I:1739:GLU:HB2	2:I:1987:PRO:HB3	1.40	1.04
1:B:1367:ARG:NH1	1:B:1372:THR:HB	1.73	1.04
2:H:1227:ARG:HG3	2:H:1227:ARG:HH11	1.19	1.03
2:G:1227:ARG:HH11	2:G:1227:ARG:HG3	1.18	1.03
2:H:297:ARG:HD3	2:H:447:ASN:HD21	1.16	1.03
1:B:1721:ARG:HH11	1:B:1721:ARG:HG2	1.21	1.03
1:B:1722:VAL:HG11	1:B:1731:LEU:HB3	1.37	1.03
1:C:1722:VAL:HG11	1:C:1731:LEU:HB3	1.37	1.02
2:G:7:ARG:HH21	2:G:27:PHE:HB3	1.22	1.02
1:B:599:MET:HB2	1:B:624:LYS:HD2	1.42	1.02
2:H:7:ARG:HH21	2:H:27:PHE:HB3	1.22	1.02
1:B:852:ARG:HH11	1:B:852:ARG:HG2	1.20	1.02
1:A:852:ARG:HH11	1:A:852:ARG:HG2	1.23	1.02
2:H:1739:GLU:HB2	2:H:1987:PRO:HB3	1.42	1.02
2:H:1859:PRO:HG3	2:H:1871:LEU:HD12	1.37	1.01
2:I:1859:PRO:HG3	2:I:1871:LEU:HD12	1.41	1.01
2:H:131:ILE:HB	2:H:182:VAL:CG1	1.89	1.01
1:C:1219:VAL:HA	1:C:1384:ILE:HD11	1.40	1.01
2:H:131:ILE:CD1	2:H:182:VAL:HB	1.91	1.00
1:C:1014:ASP:H	1:C:1510:ASN:HD21	1.03	1.00
2:H:903:TRP:O	2:H:906:THR:HG22	1.59	1.00
1:A:1722:VAL:HG11	1:A:1731:LEU:HB3	1.40	1.00
2:I:741:HIS:NE2	2:I:855:HIS:CE1	2.30	1.00
1:A:599:MET:HB2	1:A:624:LYS:HD2	1.43	0.99
2:H:1567:ARG:HG3	2:H:1567:ARG:HH11	1.27	0.99
1:C:599:MET:HB2	1:C:624:LYS:HD2	1.43	0.99
1:C:253:ARG:HG3	1:C:254:TRP:CD1	1.98	0.99
2:G:499:THR:HB	2:G:500:HIS:CD2	1.97	0.98
2:I:892:ILE:HD11	2:I:903:TRP:CE2	1.98	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ARG:HG3	1:A:254:TRP:CD1	1.98	0.98
1:B:1219:VAL:HA	1:B:1384:ILE:HD11	1.45	0.98
2:H:1803:THR:HG22	2:H:2009:LYS:HA	1.45	0.98
2:H:762:ASN:H	2:H:762:ASN:HD22	1.03	0.98
2:H:131:ILE:HB	2:H:182:VAL:HG11	1.00	0.98
2:I:499:THR:HB	2:I:500:HIS:CD2	1.97	0.98
2:I:903:TRP:O	2:I:906:THR:HG22	1.63	0.98
1:A:400:ARG:HG2	1:A:400:ARG:HH11	1.28	0.97
2:G:892:ILE:HD11	2:G:903:TRP:CE2	1.98	0.97
1:A:400:ARG:CG	1:A:400:ARG:HH11	1.76	0.97
2:H:499:THR:HB	2:H:500:HIS:CD2	1.99	0.97
2:H:1172:LYS:HE3	2:H:1574:ASN:OD1	1.64	0.97
1:B:198:PRO:HG3	1:B:209:LEU:HD21	1.47	0.97
1:B:253:ARG:HG3	1:B:254:TRP:CD1	1.99	0.96
2:H:594:VAL:HB	2:H:617:ILE:HG13	1.44	0.96
2:I:490:TRP:NE1	2:I:516:THR:HG22	1.79	0.96
2:I:762:ASN:HD22	2:I:762:ASN:H	1.08	0.96
1:A:1014:ASP:H	1:A:1510:ASN:HD21	1.10	0.96
2:H:490:TRP:NE1	2:H:516:THR:HG22	1.81	0.96
2:H:131:ILE:HD12	2:H:182:VAL:HB	0.96	0.96
1:A:12:ILE:HD11	2:G:2041:ILE:HD12	1.47	0.95
1:C:198:PRO:HG3	1:C:209:LEU:HD21	1.48	0.95
2:G:490:TRP:NE1	2:G:516:THR:HG22	1.81	0.95
2:H:1567:ARG:HH11	2:H:1567:ARG:CG	1.79	0.95
2:H:892:ILE:HD11	2:H:903:TRP:CE2	2.01	0.95
2:G:1803:THR:HG22	2:G:2009:LYS:HA	1.48	0.95
2:I:1567:ARG:HH11	2:I:1567:ARG:HG3	1.29	0.95
2:I:594:VAL:HB	2:I:617:ILE:HG13	1.46	0.95
2:I:1567:ARG:HH11	2:I:1567:ARG:CG	1.79	0.95
2:H:1199:GLU:OE2	2:H:1567:ARG:NH1	2.00	0.95
2:G:1878:VAL:HG11	2:G:1910:VAL:HG22	1.48	0.95
2:G:1741:ILE:HD12	2:G:1986:LYS:HD2	1.47	0.95
1:A:198:PRO:HG3	1:A:209:LEU:HD21	1.47	0.95
2:I:741:HIS:CE1	2:I:855:HIS:CE1	2.55	0.95
2:G:1567:ARG:CG	2:G:1567:ARG:HH11	1.80	0.95
1:A:444:ASN:HB2	1:A:447:LEU:H	1.31	0.95
2:H:741:HIS:HE1	2:H:845:THR:CG2	1.80	0.95
2:H:835:THR:HG21	2:H:855:HIS:CD2	1.99	0.94
2:G:1739:GLU:HB2	2:G:1987:PRO:HB3	1.43	0.94
2:G:1589:VAL:HA	2:G:1592:LEU:HD12	1.49	0.94
2:H:55:THR:HG22	2:H:56:THR:HG22	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:ASN:HB2	1:B:447:LEU:H	1.31	0.94
2:I:1741:ILE:HD12	2:I:1986:LYS:HD2	1.49	0.94
1:C:400:ARG:HG2	1:C:400:ARG:HH11	1.33	0.94
1:C:2:LYS:HD2	2:I:2050:GLN:HB3	1.50	0.94
2:I:1878:VAL:HG11	2:I:1910:VAL:HG22	1.50	0.94
2:H:1314:ARG:HH11	2:H:1314:ARG:HG3	1.31	0.94
2:G:762:ASN:H	2:G:762:ASN:HD22	1.03	0.93
2:G:942:THR:HB	2:G:1012:GLN:HG2	1.50	0.93
1:A:1219:VAL:HA	1:A:1384:ILE:HD11	1.45	0.93
1:B:529:MET:HE3	1:B:529:MET:HA	1.47	0.93
2:I:741:HIS:HE1	2:I:845:THR:CG2	1.81	0.93
2:H:1845:ASP:HB2	2:H:1849:ARG:H	1.34	0.93
2:H:652:ILE:H	2:H:658:MET:HE3	1.30	0.93
1:B:400:ARG:HH11	1:B:400:ARG:CG	1.81	0.93
2:H:1589:VAL:HA	2:H:1592:LEU:HD12	1.49	0.93
2:I:1314:ARG:HG3	2:I:1314:ARG:HH11	1.32	0.93
1:A:12:ILE:HD11	2:G:2041:ILE:CD1	1.99	0.93
2:I:56:THR:HG23	2:I:59:GLU:HG3	1.49	0.93
2:G:1567:ARG:HG3	2:G:1567:ARG:HH11	1.30	0.93
2:G:128:THR:HA	2:G:182:VAL:HG21	1.51	0.92
1:A:1523:ARG:HG3	1:A:1523:ARG:HH11	1.33	0.92
1:C:1523:ARG:HH11	1:C:1523:ARG:HG3	1.32	0.92
2:I:741:HIS:CE1	2:I:845:THR:CG2	2.52	0.92
2:G:55:THR:HG21	2:G:113:ASP:HB2	1.52	0.92
1:A:152:HIS:CD2	1:A:163:LEU:HB2	2.05	0.92
2:G:741:HIS:NE2	2:G:855:HIS:CE1	2.38	0.92
2:I:55:THR:HG22	2:I:56:THR:HG22	1.51	0.91
2:I:667:LYS:HD2	2:I:697:THR:HG22	1.51	0.91
2:G:1845:ASP:HB2	2:G:1849:ARG:H	1.34	0.91
2:I:741:HIS:CE1	2:I:845:THR:HG22	2.04	0.91
1:A:1721:ARG:CG	1:A:1721:ARG:HH11	1.84	0.91
1:C:400:ARG:HH11	1:C:400:ARG:CG	1.81	0.91
2:G:1314:ARG:HH11	2:G:1314:ARG:HG3	1.32	0.91
1:C:152:HIS:CD2	1:C:163:LEU:HB2	2.05	0.91
2:G:56:THR:HG23	2:G:59:GLU:HG3	1.50	0.91
2:G:741:HIS:CE1	2:G:855:HIS:CE1	2.57	0.91
2:I:1803:THR:HG22	2:I:2009:LYS:HA	1.51	0.91
2:I:707:PRO:HG3	2:I:716:VAL:HG21	1.52	0.91
1:A:1693:ILE:HD11	2:G:998:GLN:HB2	1.51	0.91
1:B:1523:ARG:HH11	1:B:1523:ARG:HG3	1.36	0.91
1:C:793:ARG:HA	1:C:797:THR:HG23	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1741:ILE:HD12	2:H:1986:LYS:HD2	1.54	0.90
2:I:942:THR:HB	2:I:1012:GLN:HG2	1.52	0.90
2:H:707:PRO:HG3	2:H:716:VAL:HG21	1.54	0.90
2:I:1441:ILE:HD11	2:I:1445:ARG:CZ	2.02	0.90
2:I:652:ILE:H	2:I:658:MET:HE3	1.36	0.90
2:G:55:THR:HG22	2:G:56:THR:HG22	1.52	0.90
2:G:131:ILE:HD12	2:G:182:VAL:CB	2.01	0.89
2:G:1847:LEU:H	2:G:1847:LEU:HD12	1.37	0.89
1:C:444:ASN:HB2	1:C:447:LEU:H	1.33	0.89
2:G:594:VAL:HB	2:G:617:ILE:HG13	1.52	0.89
1:B:1721:ARG:HH11	1:B:1721:ARG:CG	1.85	0.89
1:B:793:ARG:HA	1:B:797:THR:HG23	1.54	0.89
2:I:1589:VAL:HA	2:I:1592:LEU:HD12	1.51	0.89
1:A:253:ARG:HE	1:A:254:TRP:HE1	1.21	0.89
2:G:1441:ILE:HD11	2:G:1445:ARG:CZ	2.02	0.89
2:H:1847:LEU:H	2:H:1847:LEU:HD12	1.37	0.89
2:H:55:THR:HG21	2:H:113:ASP:HB2	1.53	0.89
1:A:529:MET:HA	1:A:529:MET:HE3	1.53	0.89
2:H:56:THR:HG23	2:H:59:GLU:HG3	1.54	0.89
1:A:1474:ALA:HA	1:A:1478:PRO:HG2	1.54	0.88
2:G:667:LYS:HD2	2:G:697:THR:HG22	1.55	0.88
2:H:667:LYS:HD2	2:H:697:THR:HG22	1.55	0.88
1:A:1367:ARG:HH12	1:A:1372:THR:HB	1.35	0.88
1:A:403:ASP:HB2	1:A:1613:ASN:HD21	1.38	0.88
1:B:31:THR:HG23	2:H:2011:ILE:HG21	1.56	0.88
2:H:942:THR:HB	2:H:1012:GLN:HG2	1.54	0.88
2:I:55:THR:HG21	2:I:113:ASP:HB2	1.53	0.88
1:B:1367:ARG:HH12	1:B:1372:THR:HB	1.38	0.88
1:B:152:HIS:CD2	1:B:163:LEU:HB2	2.09	0.88
2:I:1227:ARG:HH11	2:I:1227:ARG:CG	1.87	0.88
1:C:1721:ARG:CG	1:C:1721:ARG:HH11	1.87	0.87
2:G:707:PRO:HG3	2:G:716:VAL:HG21	1.56	0.87
2:H:1441:ILE:HD11	2:H:1445:ARG:CZ	2.04	0.87
2:I:131:ILE:HD12	2:I:182:VAL:HB	1.55	0.87
1:A:793:ARG:HA	1:A:797:THR:HG23	1.53	0.87
1:C:59:ARG:HH11	2:I:1896:GLN:NE2	1.71	0.87
2:I:369:SER:OG	2:I:380:SER:HB3	1.74	0.87
2:I:298:LYS:HG2	2:I:448:VAL:HG22	1.56	0.87
1:C:529:MET:HA	1:C:529:MET:HE3	1.57	0.87
2:H:131:ILE:CG2	2:H:182:VAL:HG12	2.04	0.87
2:I:1845:ASP:HB2	2:I:1849:ARG:H	1.38	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ARG:HH12	1:B:300:VAL:HG21	1.38	0.87
2:I:932:ILE:HD11	2:I:1042:ALA:HB2	1.57	0.87
1:C:253:ARG:HE	1:C:254:TRP:HE1	1.21	0.87
1:A:340:ARG:NH1	1:A:344:GLN:HG2	1.88	0.87
1:B:893:VAL:HG11	1:B:930:LEU:HD23	1.55	0.87
2:H:741:HIS:HE1	2:H:845:THR:HG22	1.38	0.86
1:C:1474:ALA:HA	1:C:1478:PRO:HG2	1.57	0.86
2:H:1878:VAL:HG11	2:H:1910:VAL:HG22	1.55	0.86
2:I:1739:GLU:HB3	2:I:1746:LEU:HD11	1.58	0.86
1:B:1474:ALA:HA	1:B:1478:PRO:HG2	1.58	0.86
2:G:741:HIS:HE1	2:G:845:THR:CG2	1.88	0.86
2:H:1533:LEU:HD13	2:H:1630:GLY:HA2	1.55	0.86
1:B:400:ARG:HH11	1:B:400:ARG:HG2	1.41	0.85
2:H:1739:GLU:HB3	2:H:1746:LEU:HD11	1.56	0.85
2:G:741:HIS:CE1	2:G:845:THR:CG2	2.59	0.85
2:I:1533:LEU:HD13	2:I:1630:GLY:HA2	1.59	0.85
2:H:1425:LYS:HG2	2:H:1471:GLU:HG3	1.58	0.85
2:H:774:ALA:HB1	2:H:1081:HIS:HD2	1.41	0.85
2:G:1425:LYS:HG2	2:G:1471:GLU:HG3	1.57	0.85
2:I:1847:LEU:HD12	2:I:1847:LEU:H	1.40	0.85
1:B:340:ARG:NH1	1:B:344:GLN:HG2	1.91	0.85
2:G:28:PHE:HE2	2:H:7:ARG:HD2	1.36	0.85
2:H:1844:ARG:HH11	2:H:1844:ARG:CG	1.89	0.85
2:H:1844:ARG:HH11	2:H:1844:ARG:HG2	1.41	0.85
2:G:28:PHE:CZ	2:H:7:ARG:CD	2.59	0.85
2:H:932:ILE:HD11	2:H:1042:ALA:HB2	1.58	0.84
2:H:297:ARG:HD3	2:H:447:ASN:ND2	1.91	0.84
2:G:369:SER:OG	2:G:380:SER:HB3	1.75	0.84
2:H:777:THR:CG2	2:H:1081:HIS:NE2	2.41	0.84
1:A:893:VAL:HG11	1:A:930:LEU:HD23	1.59	0.84
2:G:131:ILE:HG21	2:G:182:VAL:HG12	1.57	0.84
1:C:340:ARG:NH1	1:C:344:GLN:HG2	1.91	0.84
2:I:297:ARG:HD3	2:I:447:ASN:ND2	1.92	0.84
2:G:1054:LEU:HB2	4:G:3051:FMN:HM72	1.60	0.84
2:G:652:ILE:H	2:G:658:MET:HE3	1.42	0.84
2:H:2038:ILE:HG22	2:H:2042:ILE:HD11	1.60	0.84
2:H:369:SER:OG	2:H:380:SER:HB3	1.78	0.84
1:C:852:ARG:HG2	1:C:852:ARG:NH1	1.93	0.84
2:I:774:ALA:HB2	2:I:1077:ILE:HA	1.58	0.84
1:B:11:HIS:ND1	2:H:1998:LYS:HA	1.93	0.84
1:C:1303:GLY:HA2	1:C:1649:LYS:HE2	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:995:LEU:HD23	2:I:1000:ILE:HD13	1.60	0.84
2:H:741:HIS:CE1	2:H:845:THR:HG22	2.12	0.84
1:C:31:THR:HG23	2:I:2011:ILE:HG21	1.59	0.84
2:G:1533:LEU:HD13	2:G:1630:GLY:HA2	1.60	0.83
2:G:774:ALA:HB2	2:G:1077:ILE:HA	1.61	0.83
1:A:980:VAL:HG23	2:G:968:GLN:OE1	1.78	0.83
1:B:253:ARG:HE	1:B:254:TRP:HE1	1.21	0.83
2:G:1227:ARG:HH11	2:G:1227:ARG:CG	1.89	0.83
2:I:774:ALA:HB1	2:I:1081:HIS:HD2	1.43	0.83
2:H:1227:ARG:HH11	2:H:1227:ARG:CG	1.90	0.83
2:H:1672:GLN:HG2	2:H:1777:THR:HG23	1.59	0.83
2:H:741:HIS:CE1	2:H:845:THR:CG2	2.60	0.83
2:I:1844:ARG:HH11	2:I:1844:ARG:HG2	1.43	0.83
1:C:893:VAL:HG11	1:C:930:LEU:HD23	1.59	0.83
2:G:1293:THR:HG23	2:G:1296:GLU:H	1.44	0.83
2:I:1425:LYS:HG2	2:I:1471:GLU:HG3	1.61	0.83
2:I:598:THR:HG22	2:I:622:GLY:HA3	1.61	0.83
1:B:403:ASP:HB2	1:B:1613:ASN:HD21	1.44	0.82
2:G:777:THR:CG2	2:G:1081:HIS:NE2	2.41	0.82
1:A:20:TYR:CG	2:G:2033:THR:OG1	2.32	0.82
2:G:297:ARG:HD3	2:G:447:ASN:ND2	1.94	0.82
2:H:85:ASN:HD22	2:H:135:ARG:HH11	1.26	0.82
1:C:1367:ARG:HH12	1:C:1372:THR:HB	1.37	0.82
2:G:1739:GLU:HB3	2:G:1746:LEU:HD11	1.60	0.82
2:G:131:ILE:CB	2:G:182:VAL:HG11	2.07	0.82
2:G:298:LYS:HG2	2:G:448:VAL:HG22	1.61	0.82
2:I:1672:GLN:HG2	2:I:1777:THR:HG23	1.61	0.82
1:A:1249:SER:HB3	1:A:1280:ILE:HG23	1.62	0.82
1:A:36:LEU:HD22	1:A:61:LEU:HD21	1.60	0.82
1:B:1014:ASP:H	1:B:1510:ASN:HD21	1.28	0.82
2:H:995:LEU:HD23	2:H:1000:ILE:HD13	1.58	0.82
2:I:1931:LEU:HB3	2:I:1935:GLU:HG2	1.62	0.82
2:I:2038:ILE:HG22	2:I:2042:ILE:HD11	1.61	0.82
1:A:335:HIS:HE1	1:B:335:HIS:CE1	1.98	0.82
1:B:12:ILE:HD11	2:H:2041:ILE:CD1	2.10	0.82
1:C:333:LYS:O	1:C:337:VAL:HG23	1.80	0.81
2:G:995:LEU:HD23	2:G:1000:ILE:HD13	1.60	0.81
2:G:1844:ARG:CG	2:G:1844:ARG:HH11	1.93	0.81
2:G:1847:LEU:HD13	2:G:1849:ARG:HD2	1.62	0.81
2:I:128:THR:HA	2:I:182:VAL:HG21	1.62	0.81
2:H:1159:ILE:HG12	2:H:1168:ASN:HA	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:543:PHE:HB2	2:H:545:GLN:HE22	1.45	0.81
2:I:1844:ARG:CG	2:I:1844:ARG:HH11	1.93	0.81
2:I:1054:LEU:HB2	4:I:3051:FMN:C7M	2.11	0.81
1:B:1249:SER:HB3	1:B:1280:ILE:HG23	1.62	0.81
2:G:543:PHE:HB2	2:G:545:GLN:HE22	1.46	0.81
2:I:777:THR:CG2	2:I:1081:HIS:NE2	2.43	0.81
2:I:345:THR:HG22	2:I:347:GLU:H	1.46	0.81
2:G:1931:LEU:HB3	2:G:1935:GLU:HG2	1.61	0.81
2:H:1149:TRP:HA	2:H:1242:PHE:CE1	2.15	0.81
1:C:59:ARG:HH11	2:I:1896:GLN:HE22	1.25	0.81
1:B:881:ASN:HA	1:B:944:ARG:NH2	1.96	0.81
1:B:93:ASP:HB3	1:B:94:PRO:HD2	1.62	0.81
1:A:1203:ASP:HB3	1:B:179:LYS:NZ	1.95	0.81
2:G:2038:ILE:HG22	2:G:2042:ILE:HD11	1.60	0.81
1:A:335:HIS:CE1	1:C:335:HIS:HE1	1.98	0.81
2:I:345:THR:HB	2:I:348:GLN:H	1.46	0.81
1:A:93:ASP:HB3	1:A:94:PRO:HD2	1.63	0.81
2:G:1844:ARG:HG2	2:G:1844:ARG:HH11	1.46	0.81
2:I:1159:ILE:HG12	2:I:1168:ASN:HA	1.63	0.81
1:A:400:ARG:HG2	1:A:400:ARG:NH1	1.91	0.80
2:I:1693:ARG:HD2	2:I:1825:GLU:OE2	1.80	0.80
1:A:1552:ASN:O	1:A:1556:THR:HG22	1.80	0.80
1:A:333:LYS:O	1:A:337:VAL:HG23	1.82	0.80
2:G:1693:ARG:HD2	2:G:1825:GLU:OE2	1.81	0.80
2:I:584:SER:HB3	2:I:591:PRO:HG3	1.63	0.80
1:B:1030:TRP:CD1	1:B:1580:LEU:HD22	2.17	0.80
2:H:1931:LEU:HB3	2:H:1935:GLU:HG2	1.62	0.80
2:H:298:LYS:HG2	2:H:448:VAL:HG22	1.63	0.80
1:A:340:ARG:HH12	1:A:344:GLN:HG2	1.45	0.80
1:A:20:TYR:CE1	2:G:2035:SER:HB2	2.17	0.80
2:I:259:THR:HG22	2:I:262:GLU:HG3	1.63	0.80
2:G:1672:GLN:HG2	2:G:1777:THR:HG23	1.61	0.80
1:B:36:LEU:HD22	1:B:61:LEU:HD21	1.64	0.80
2:H:1159:ILE:HG12	2:H:1169:PRO:HD3	1.63	0.80
1:B:24:SER:CB	2:H:2014:LEU:HD12	2.11	0.80
2:G:741:HIS:CE1	2:G:845:THR:HG22	2.17	0.80
2:H:1847:LEU:HD13	2:H:1849:ARG:HD2	1.63	0.80
2:I:192:ALA:HA	2:I:215:ILE:HD12	1.64	0.80
1:C:1249:SER:HB3	1:C:1280:ILE:HG23	1.63	0.80
2:I:1242:PHE:HE2	2:I:1244:PRO:HG3	1.46	0.80
2:H:598:THR:HG22	2:H:622:GLY:HA3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:907:VAL:HG21	2:H:921:GLU:HG2	1.64	0.79
2:I:455:ILE:HD11	2:I:469:ARG:HD3	1.63	0.79
2:I:1293:THR:HG23	2:I:1296:GLU:H	1.47	0.79
2:H:1199:GLU:OE2	2:H:1567:ARG:CZ	2.31	0.79
2:I:55:THR:CG2	2:I:113:ASP:HB2	2.12	0.79
1:A:31:THR:HG23	2:G:2011:ILE:HG21	1.64	0.79
2:I:1310:ASP:OD2	2:I:1602:SER:HB3	1.82	0.79
2:H:774:ALA:HB2	2:H:1077:ILE:HA	1.64	0.79
2:H:455:ILE:HD11	2:H:469:ARG:HD3	1.63	0.79
2:I:238:CYS:HB2	2:I:239:PRO:HD3	1.64	0.79
2:I:543:PHE:HB2	2:I:545:GLN:HE22	1.46	0.79
2:G:634:ILE:HD11	2:G:649:ILE:HD11	1.63	0.79
2:I:907:VAL:HG21	2:I:921:GLU:HG2	1.65	0.79
2:G:1314:ARG:CG	2:G:1314:ARG:HH11	1.95	0.79
1:B:260:ARG:NH1	1:B:300:VAL:HG21	1.97	0.79
1:C:403:ASP:HB2	1:C:1613:ASN:HD21	1.46	0.79
2:G:774:ALA:HB1	2:G:1081:HIS:HD2	1.47	0.79
1:B:1303:GLY:HA2	1:B:1649:LYS:HE2	1.63	0.79
2:G:55:THR:CG2	2:G:113:ASP:HB2	2.13	0.79
2:H:105:ALA:HB1	2:H:119:THR:HG23	1.65	0.79
2:H:757:ILE:HG21	2:H:765:LEU:HD13	1.64	0.79
2:I:1847:LEU:HD13	2:I:1849:ARG:HD2	1.64	0.79
1:B:1722:VAL:CG1	1:B:1731:LEU:HB3	2.13	0.78
1:C:1523:ARG:CG	1:C:1523:ARG:HH11	1.96	0.78
2:G:85:ASN:HD22	2:G:135:ARG:HH11	1.28	0.78
2:I:1149:TRP:HA	2:I:1242:PHE:CE1	2.19	0.78
1:C:328:LEU:O	1:C:331:ILE:HG22	1.84	0.78
2:H:1567:ARG:NH1	2:H:1567:ARG:HG3	1.98	0.78
2:H:345:THR:HB	2:H:348:GLN:H	1.48	0.78
2:H:960:LYS:HA	2:H:960:LYS:HE2	1.65	0.78
2:I:85:ASN:HD22	2:I:135:ARG:HH11	1.28	0.78
1:B:12:ILE:HD11	2:H:2041:ILE:HD12	1.63	0.78
2:G:7:ARG:NH2	2:G:27:PHE:HB3	1.99	0.78
2:H:131:ILE:CB	2:H:182:VAL:CG1	2.53	0.78
1:A:328:LEU:O	1:A:331:ILE:HG22	1.84	0.78
1:B:333:LYS:O	1:B:337:VAL:HG23	1.81	0.78
2:I:741:HIS:HE1	2:I:845:THR:HG22	1.41	0.78
1:C:1014:ASP:N	1:C:1510:ASN:HD21	1.82	0.78
2:I:138:ASP:O	2:I:139:LYS:HG3	1.83	0.78
2:I:1770:LEU:HD23	2:I:1776:PHE:CE2	2.19	0.78
1:A:2:LYS:HD2	2:G:2050:GLN:HB3	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:PRO:HG3	1:B:209:LEU:CD2	2.13	0.78
1:B:24:SER:O	2:H:1977:HIS:HD2	1.67	0.78
2:H:55:THR:CG2	2:H:113:ASP:HB2	2.13	0.78
2:I:7:ARG:NH2	2:I:27:PHE:HB3	1.97	0.78
2:I:634:ILE:HD11	2:I:649:ILE:HD11	1.66	0.78
2:G:1227:ARG:HD2	2:G:1565:VAL:HG11	1.66	0.77
2:G:1770:LEU:HD23	2:G:1776:PHE:CE2	2.20	0.77
2:H:1693:ARG:HD2	2:H:1825:GLU:OE2	1.83	0.77
1:A:335:HIS:CE1	1:C:335:HIS:CE1	2.72	0.77
2:H:1293:THR:HG23	2:H:1296:GLU:H	1.49	0.77
1:C:1665:ILE:HG13	1:C:1669:ARG:HD3	1.66	0.77
2:G:455:ILE:HD11	2:G:469:ARG:HD3	1.66	0.77
2:G:355:LYS:O	2:G:358:SER:HB3	1.84	0.77
2:H:131:ILE:CG2	2:H:182:VAL:CG1	2.63	0.77
2:G:28:PHE:HZ	2:H:7:ARG:CD	1.97	0.77
2:I:741:HIS:CE1	2:I:855:HIS:NE2	2.52	0.77
1:A:1523:ARG:CG	1:A:1523:ARG:HH11	1.97	0.77
2:H:1310:ASP:OD2	2:H:1602:SER:HB3	1.82	0.77
1:A:24:SER:HB3	2:G:2014:LEU:HD12	1.64	0.77
1:B:1239:HIS:HD2	1:B:1241:SER:OG	1.67	0.77
2:I:1314:ARG:CG	2:I:1314:ARG:HH11	1.98	0.77
1:C:1030:TRP:CD1	1:C:1580:LEU:HD22	2.20	0.77
2:G:1284:VAL:HG13	2:G:1377:VAL:HG22	1.65	0.77
2:G:345:THR:HG22	2:G:347:GLU:H	1.47	0.77
2:G:598:THR:HG22	2:G:622:GLY:HA3	1.67	0.77
1:C:1693:ILE:HD11	2:I:998:GLN:HB2	1.67	0.77
1:C:93:ASP:HB3	1:C:94:PRO:HD2	1.65	0.77
1:B:29:ILE:HG13	2:H:1891:TYR:O	1.85	0.77
1:C:1030:TRP:NE1	1:C:1580:LEU:HD22	2.00	0.77
1:C:12:ILE:HD11	2:I:2041:ILE:HD12	1.67	0.77
1:C:340:ARG:HH12	1:C:344:GLN:HG2	1.49	0.77
2:G:907:VAL:HG21	2:G:921:GLU:HG2	1.65	0.77
1:A:1665:ILE:HG13	1:A:1669:ARG:HD3	1.66	0.76
2:H:1834:ARG:NH1	2:H:1834:ARG:HG2	1.86	0.76
2:I:1567:ARG:HG3	2:I:1567:ARG:NH1	2.00	0.76
2:I:1834:ARG:HG2	2:I:1834:ARG:NH1	1.93	0.76
2:I:1956:ARG:CB	2:I:1957:PRO:HD3	2.09	0.76
1:A:1030:TRP:NE1	1:A:1580:LEU:HD22	1.99	0.76
1:B:1030:TRP:NE1	1:B:1580:LEU:HD22	2.00	0.76
1:A:198:PRO:HG3	1:A:209:LEU:CD2	2.14	0.76
1:C:198:PRO:HG3	1:C:209:LEU:CD2	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1678:MET:HE3	2:G:1707:LEU:HD22	1.66	0.76
1:C:400:ARG:HG2	1:C:400:ARG:NH1	1.94	0.76
2:H:762:ASN:N	2:H:762:ASN:HD22	1.82	0.76
2:G:146:PHE:HA	2:G:149:VAL:CG1	2.15	0.76
2:G:345:THR:HB	2:G:348:GLN:H	1.50	0.76
2:I:355:LYS:O	2:I:358:SER:HB3	1.85	0.76
1:A:1030:TRP:CD1	1:A:1580:LEU:HD22	2.21	0.76
2:G:1149:TRP:HA	2:G:1242:PHE:CE1	2.20	0.76
2:G:964:LEU:H	2:G:964:LEU:HD23	1.50	0.76
2:H:598:THR:OG1	2:H:599:PRO:HD3	1.86	0.76
2:I:2015:THR:HG22	2:I:2017:LYS:H	1.51	0.76
1:C:1722:VAL:CG1	1:C:1731:LEU:HB3	2.14	0.76
1:C:24:SER:O	2:I:1977:HIS:HD2	1.68	0.76
2:H:1956:ARG:HB2	2:H:1957:PRO:CD	2.12	0.76
1:C:1239:HIS:HD2	1:C:1241:SER:OG	1.68	0.76
2:H:584:SER:HB3	2:H:591:PRO:HG3	1.67	0.76
1:A:988:ILE:HD13	1:A:1048:GLU:CB	2.15	0.75
2:G:2015:THR:HG22	2:G:2017:LYS:H	1.51	0.75
2:H:1314:ARG:HH11	2:H:1314:ARG:CG	1.97	0.75
2:I:707:PRO:CG	2:I:716:VAL:HG21	2.15	0.75
1:B:1523:ARG:HH11	1:B:1523:ARG:CG	1.98	0.75
1:B:340:ARG:HH12	1:B:344:GLN:HG2	1.48	0.75
2:H:192:ALA:HA	2:H:215:ILE:HD12	1.68	0.75
2:I:1054:LEU:HB2	4:I:3051:FMN:HM72	1.66	0.75
1:B:1665:ILE:HG13	1:B:1669:ARG:HD3	1.66	0.75
2:G:1159:ILE:HG12	2:G:1168:ASN:HA	1.67	0.75
2:G:1956:ARG:HB2	2:G:1957:PRO:CD	2.11	0.75
2:H:7:ARG:NH2	2:H:27:PHE:HB3	1.99	0.75
2:I:856:LYS:HG2	2:I:1054:LEU:HD12	1.68	0.75
2:G:960:LYS:HE2	2:G:960:LYS:HA	1.67	0.75
2:H:355:LYS:O	2:H:358:SER:HB3	1.85	0.75
2:H:84:LEU:HD13	2:H:133:ALA:HB2	1.69	0.75
1:B:328:LEU:O	1:B:331:ILE:HG22	1.86	0.75
2:H:1770:LEU:HD23	2:H:1776:PHE:CE2	2.22	0.75
2:H:259:THR:HG22	2:H:262:GLU:HG3	1.68	0.75
1:B:1208:VAL:HG13	1:B:1212:THR:HB	1.68	0.75
2:H:2015:THR:HG22	2:H:2017:LYS:H	1.51	0.75
2:H:579:VAL:HG23	2:H:1078:HIS:CD2	2.21	0.75
1:A:1303:GLY:HA2	1:A:1649:LYS:HE2	1.68	0.75
1:A:1310:GLU:OE1	1:A:1649:LYS:HE3	1.86	0.75
2:G:192:ALA:HA	2:G:215:ILE:HD12	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:572:ASN:HB3	2:G:576:LYS:H	1.52	0.75
2:H:455:ILE:HD11	2:H:469:ARG:CD	2.17	0.75
2:H:741:HIS:CB	2:H:853:PRO:HB2	2.16	0.75
2:I:960:LYS:HA	2:I:960:LYS:HE2	1.67	0.75
2:I:1129:ALA:HB2	2:I:1138:TRP:CZ3	2.22	0.75
2:I:1956:ARG:HB2	2:I:1957:PRO:CD	2.11	0.75
2:I:572:ASN:HB3	2:I:576:LYS:H	1.52	0.75
2:I:757:ILE:HG21	2:I:765:LEU:HD13	1.69	0.75
2:H:943:TRP:CH2	2:H:1016:PRO:HG3	2.22	0.74
2:H:1834:ARG:CG	2:H:1834:ARG:HH11	1.92	0.74
2:I:1159:ILE:HG12	2:I:1169:PRO:HD3	1.67	0.74
2:I:1284:VAL:HG13	2:I:1377:VAL:HG22	1.69	0.74
1:A:427:ASN:HD21	1:A:610:THR:H	1.33	0.74
1:B:1552:ASN:O	1:B:1556:THR:HG22	1.88	0.74
2:H:1678:MET:HE3	2:H:1707:LEU:HD22	1.67	0.74
1:A:20:TYR:CD2	2:G:2033:THR:OG1	2.40	0.74
2:H:1242:PHE:HE2	2:H:1244:PRO:HG3	1.51	0.74
2:H:1672:GLN:HA	2:H:1676:MET:HE1	1.68	0.74
2:I:943:TRP:CH2	2:I:1016:PRO:HG3	2.21	0.74
2:H:1784:MET:HG3	2:H:1785:GLU:N	2.03	0.74
1:A:1239:HIS:HD2	1:A:1241:SER:OG	1.69	0.74
1:A:335:HIS:CE1	1:B:335:HIS:CE1	2.74	0.74
1:B:335:HIS:HE1	1:C:335:HIS:CE1	2.06	0.74
1:C:749:ILE:HD13	1:C:806:VAL:HG12	1.70	0.74
2:H:1129:ALA:HB2	2:H:1138:TRP:CZ3	2.21	0.74
2:H:1672:GLN:HA	2:H:1676:MET:CE	2.18	0.74
2:H:1956:ARG:CB	2:H:1957:PRO:HD3	2.11	0.74
2:I:105:ALA:HB1	2:I:119:THR:HG23	1.67	0.74
2:I:131:ILE:HB	2:I:182:VAL:HG11	1.69	0.74
1:C:1552:ASN:O	1:C:1556:THR:HG22	1.88	0.74
2:G:1310:ASP:OD2	2:G:1602:SER:HB3	1.88	0.74
2:I:2035:SER:HB3	2:I:2038:ILE:HG13	1.69	0.74
2:I:835:THR:HG21	2:I:855:HIS:CD2	2.23	0.74
1:B:1551:LYS:HD2	1:B:1617:ILE:HG21	1.70	0.74
2:G:705:LEU:HD12	2:G:716:VAL:HG13	1.70	0.74
2:I:741:HIS:CE1	2:I:845:THR:HG21	2.22	0.74
2:G:757:ILE:HG21	2:G:765:LEU:HD13	1.67	0.74
1:B:18:LEU:HD21	2:H:1815:LEU:HD12	1.70	0.74
2:I:1889:VAL:HG13	2:I:1977:HIS:HB2	1.69	0.74
1:A:44:VAL:CG1	1:A:78:ILE:HG12	2.18	0.73
1:B:833:PHE:HA	1:B:937:LYS:HD2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1194:VAL:HG22	2:H:1212:LYS:HB3	1.70	0.73
2:H:7:ARG:NH1	2:H:24:THR:HG23	2.03	0.73
2:H:1004:LEU:HD21	2:H:1020:VAL:HG23	1.70	0.73
1:C:36:LEU:HD22	1:C:61:LEU:HD21	1.68	0.73
2:G:1159:ILE:HG12	2:G:1169:PRO:HD3	1.71	0.73
1:A:982:ILE:HD11	2:G:965:SER:HB2	1.69	0.73
2:H:705:LEU:HD12	2:H:716:VAL:HG13	1.70	0.73
2:H:1680:LEU:HD13	2:H:1687:ALA:HB2	1.71	0.73
2:I:1784:MET:HG3	2:I:1785:GLU:N	2.02	0.73
2:G:105:ALA:HB1	2:G:119:THR:HG23	1.70	0.73
2:G:7:ARG:NH1	2:G:24:THR:HG23	2.03	0.73
2:I:455:ILE:HD11	2:I:469:ARG:CD	2.19	0.73
1:B:749:ILE:HD13	1:B:806:VAL:HG12	1.70	0.73
2:G:259:THR:HG22	2:G:262:GLU:HG3	1.68	0.73
2:G:777:THR:HG22	2:G:1081:HIS:NE2	2.03	0.73
2:I:7:ARG:NH1	2:I:24:THR:HG23	2.03	0.73
1:A:1551:LYS:HD2	1:A:1617:ILE:HG21	1.70	0.73
2:G:194:THR:HG23	2:G:300:ILE:HD11	1.70	0.73
2:H:1300:PHE:CA	2:H:1556:VAL:HG11	2.19	0.73
2:H:345:THR:HG22	2:H:347:GLU:H	1.51	0.73
1:C:260:ARG:HH12	1:C:300:VAL:HG21	1.52	0.73
2:G:652:ILE:H	2:G:658:MET:CE	2.01	0.73
2:H:1331:TRP:CZ2	2:H:1335:ILE:HG13	2.23	0.73
2:H:1355:ASN:HA	2:H:1407:THR:O	1.88	0.73
2:H:194:THR:HG23	2:H:300:ILE:HD11	1.71	0.73
2:H:146:PHE:HA	2:H:149:VAL:CG1	2.18	0.73
2:H:1300:PHE:HA	2:H:1556:VAL:HG11	1.70	0.73
2:H:7:ARG:HH21	2:H:27:PHE:CB	2.01	0.73
1:B:44:VAL:CG1	1:B:78:ILE:HG12	2.18	0.72
2:H:1284:VAL:HG13	2:H:1377:VAL:HG22	1.71	0.72
2:H:579:VAL:HG23	2:H:1078:HIS:NE2	2.03	0.72
2:I:707:PRO:HG3	2:I:716:VAL:CG2	2.18	0.72
2:G:762:ASN:N	2:G:762:ASN:HD22	1.82	0.72
2:I:579:VAL:HG23	2:I:1078:HIS:CD2	2.24	0.72
1:A:1045:PHE:HB3	1:A:1049:GLY:HA3	1.71	0.72
1:A:655:LEU:HD22	1:A:916:LEU:HD11	1.71	0.72
1:C:1208:VAL:HG13	1:C:1212:THR:HB	1.71	0.72
1:C:1551:LYS:HD2	1:C:1617:ILE:HG21	1.70	0.72
2:G:1889:VAL:HG13	2:G:1977:HIS:HB2	1.72	0.72
2:H:128:THR:HA	2:H:182:VAL:CG2	2.16	0.72
2:H:634:ILE:HD11	2:H:649:ILE:HD11	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1672:GLN:HA	2:I:1676:MET:HE1	1.70	0.72
1:A:1722:VAL:CG1	1:A:1731:LEU:HB3	2.19	0.72
1:C:473:GLY:O	1:C:477:ILE:HG13	1.88	0.72
2:I:191:SER:HA	2:I:194:THR:HG22	1.71	0.72
2:I:194:THR:HG23	2:I:300:ILE:HD11	1.70	0.72
1:C:427:ASN:HD21	1:C:610:THR:H	1.38	0.72
1:A:24:SER:CB	2:G:2014:LEU:HD12	2.19	0.72
2:H:109:LEU:HD11	2:H:116:LEU:HD23	1.72	0.72
1:A:1208:VAL:HG13	1:A:1212:THR:HB	1.70	0.72
1:B:254:TRP:CZ3	1:B:302:LEU:HD13	2.24	0.72
2:I:1672:GLN:HA	2:I:1676:MET:CE	2.20	0.72
2:I:777:THR:HG22	2:I:1081:HIS:NE2	2.04	0.72
2:I:7:ARG:HH21	2:I:27:PHE:CB	1.99	0.72
1:B:24:SER:HB3	2:H:2014:LEU:HD12	1.69	0.72
2:G:584:SER:HB3	2:G:591:PRO:HG3	1.70	0.72
2:H:455:ILE:CD1	2:H:469:ARG:HD3	2.20	0.72
2:H:455:ILE:CG1	2:H:469:ARG:HD3	2.20	0.72
2:I:259:THR:HG22	2:I:262:GLU:CG	2.20	0.72
1:B:473:GLY:O	1:B:477:ILE:HG13	1.89	0.72
2:G:1680:LEU:HD13	2:G:1687:ALA:HB2	1.71	0.72
2:G:598:THR:OG1	2:G:599:PRO:HD3	1.89	0.72
2:H:572:ASN:HB3	2:H:576:LYS:H	1.54	0.72
2:G:131:ILE:CD1	2:G:182:VAL:HB	2.09	0.72
2:H:777:THR:HG22	2:H:1081:HIS:NE2	2.04	0.72
2:G:751:LEU:HD23	2:G:791:TYR:CE2	2.25	0.72
2:G:741:HIS:CE1	2:G:845:THR:HG21	2.24	0.72
2:G:741:HIS:CE1	2:G:855:HIS:NE2	2.58	0.72
2:I:1086:LEU:HG	2:I:1092:ASP:HA	1.72	0.72
2:I:84:LEU:HD13	2:I:133:ALA:HB2	1.71	0.72
1:B:1232:TYR:CZ	1:B:1701:LYS:HD2	2.26	0.71
2:G:1567:ARG:HG3	2:G:1567:ARG:NH1	2.02	0.71
2:G:161:GLY:H	2:G:505:GLY:HA3	1.54	0.71
2:I:2036:GLU:HB2	2:I:2037:PRO:HD3	1.72	0.71
1:B:888:ILE:HD12	1:B:939:PHE:HE2	1.55	0.71
1:C:59:ARG:NH1	2:I:1896:GLN:NE2	2.38	0.71
2:H:652:ILE:H	2:H:658:MET:CE	2.03	0.71
2:H:741:HIS:NE2	2:H:855:HIS:CE1	2.58	0.71
2:I:1419:PHE:O	2:I:1422:THR:HG22	1.90	0.71
2:I:1673:GLU:H	2:I:1676:MET:HE3	1.55	0.71
1:B:1030:TRP:NE1	1:B:1580:LEU:CD2	2.54	0.71
2:G:1638:ILE:HD12	2:G:1657:ILE:HD12	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:762:ASN:H	2:G:762:ASN:ND2	1.85	0.71
2:H:1227:ARG:HD2	2:H:1565:VAL:HG11	1.71	0.71
2:I:1670:GLY:H	2:I:1672:GLN:HE21	1.38	0.71
1:A:733:ILE:HD13	1:A:761:LEU:HD11	1.71	0.71
1:A:982:ILE:HD11	2:G:965:SER:CB	2.21	0.71
2:G:2036:GLU:HB2	2:G:2037:PRO:HD3	1.73	0.71
2:G:50:ALA:HB3	2:G:53:GLU:HG3	1.72	0.71
1:A:983:GLN:NE2	2:G:962:LYS:HD2	2.05	0.71
2:H:1819:ALA:HA	2:H:2005:ARG:HH11	1.55	0.71
1:B:2:LYS:HD2	2:H:2050:GLN:HB3	1.72	0.71
2:I:1331:TRP:CZ2	2:I:1335:ILE:HG13	2.25	0.71
2:I:455:ILE:CG1	2:I:469:ARG:HD3	2.21	0.71
1:C:733:ILE:HD13	1:C:761:LEU:HD11	1.72	0.71
2:H:1054:LEU:HB2	4:H:3051:FMN:C7M	2.21	0.71
2:I:732:TRP:CG	2:I:750:MET:CE	2.73	0.71
1:A:1208:VAL:CG1	1:A:1212:THR:HB	2.21	0.71
1:C:1219:VAL:HG22	1:C:1384:ILE:HD12	1.73	0.71
2:G:1199:GLU:OE2	2:G:1567:ARG:NH1	2.23	0.71
2:G:1672:GLN:HA	2:G:1676:MET:HE1	1.72	0.71
2:G:1917:ILE:HG23	2:G:1922:ILE:HB	1.72	0.71
2:G:238:CYS:HB2	2:G:239:PRO:HD3	1.71	0.71
2:G:949:ASP:HB3	2:G:1006:MET:HE2	1.71	0.71
2:H:238:CYS:HB2	2:H:239:PRO:HD3	1.71	0.71
2:I:1058:VAL:O	2:I:1061:GLN:HG2	1.90	0.71
2:G:109:LEU:HD11	2:G:116:LEU:HD23	1.71	0.71
1:B:18:LEU:HD21	2:H:1815:LEU:CD1	2.20	0.71
1:B:655:LEU:HD22	1:B:916:LEU:HD11	1.72	0.71
2:G:707:PRO:CG	2:G:716:VAL:HG21	2.20	0.71
2:H:964:LEU:HD23	2:H:964:LEU:H	1.56	0.71
1:C:459:ASP:HB3	1:C:462:LYS:HG3	1.73	0.70
2:I:1242:PHE:CE2	2:I:1244:PRO:HG3	2.26	0.70
1:C:59:ARG:NH1	2:I:1896:GLN:HE22	1.88	0.70
2:I:751:LEU:HD23	2:I:791:TYR:CE2	2.25	0.70
1:B:1721:ARG:NH1	1:B:1721:ARG:HG2	2.00	0.70
2:H:707:PRO:CG	2:H:716:VAL:HG21	2.21	0.70
1:A:1:MET:CE	1:A:6:GLU:HA	2.21	0.70
1:C:631:PRO:HB2	1:C:634:THR:OG1	1.91	0.70
2:G:1672:GLN:HA	2:G:1676:MET:CE	2.21	0.70
1:C:12:ILE:HD11	2:I:2041:ILE:CD1	2.21	0.70
2:I:964:LEU:H	2:I:964:LEU:HD23	1.56	0.70
1:C:881:ASN:HA	1:C:944:ARG:NH2	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:650:ASN:HD21	4:G:3051:FMN:HN3	1.40	0.70
2:I:1680:LEU:HD13	2:I:1687:ALA:HB2	1.72	0.70
2:I:732:TRP:CG	2:I:750:MET:HE1	2.26	0.70
1:B:1208:VAL:CG1	1:B:1212:THR:HB	2.20	0.70
2:G:579:VAL:HG23	2:G:1078:HIS:CD2	2.27	0.70
2:G:123:ILE:HD11	2:G:533:LEU:CD2	2.21	0.70
2:I:455:ILE:CD1	2:I:469:ARG:HD3	2.20	0.70
2:I:748:THR:HB	2:I:749:PRO:HD3	1.74	0.70
1:B:459:ASP:HB3	1:B:462:LYS:HG3	1.73	0.70
2:G:1956:ARG:CB	2:G:1957:PRO:HD3	2.10	0.70
2:G:707:PRO:HG3	2:G:716:VAL:CG2	2.22	0.70
2:G:732:TRP:CG	2:G:750:MET:HE1	2.27	0.70
2:I:146:PHE:HA	2:I:149:VAL:CG1	2.20	0.70
1:A:1312:VAL:HG22	1:A:1329:VAL:HG11	1.73	0.70
1:B:1:MET:CE	1:B:6:GLU:HA	2.21	0.70
2:G:1242:PHE:HE2	2:G:1244:PRO:HG3	1.55	0.70
1:B:968:VAL:HG23	2:H:1515:PRO:HG3	1.74	0.70
1:C:260:ARG:NH1	1:C:300:VAL:HG21	2.06	0.70
2:G:1355:ASN:HA	2:G:1407:THR:O	1.92	0.70
2:H:234:ILE:HG13	2:H:235:PRO:HD3	1.73	0.70
2:I:1264:GLU:HA	2:I:1275:PHE:CE1	2.27	0.70
1:C:655:LEU:HD22	1:C:916:LEU:HD11	1.74	0.70
2:G:455:ILE:HD11	2:G:469:ARG:CD	2.22	0.70
2:H:741:HIS:CE1	2:H:845:THR:HG21	2.26	0.70
1:A:12:ILE:HA	1:A:15:THR:CG2	2.21	0.70
2:G:1331:TRP:CZ2	2:G:1335:ILE:HG13	2.26	0.70
2:G:1673:GLU:H	2:G:1676:MET:HE3	1.57	0.70
2:H:2036:GLU:HB2	2:H:2037:PRO:HD3	1.72	0.70
1:A:1232:TYR:CZ	1:A:1701:LYS:HD2	2.27	0.69
2:G:7:ARG:HH21	2:G:27:PHE:CB	2.01	0.69
2:H:1673:GLU:H	2:H:1676:MET:HE3	1.57	0.69
2:H:499:THR:CB	2:H:500:HIS:HD2	1.99	0.69
2:H:835:THR:HB	2:H:845:THR:HG23	1.73	0.69
2:I:926:LEU:HD13	2:I:947:THR:HG22	1.73	0.69
1:B:427:ASN:HD21	1:B:610:THR:H	1.40	0.69
2:G:1194:VAL:HG22	2:G:1212:LYS:HB3	1.74	0.69
2:H:1670:GLY:H	2:H:1672:GLN:HE21	1.40	0.69
2:I:1862:VAL:HG11	2:I:1866:PHE:CD1	2.26	0.69
1:A:749:ILE:HD13	1:A:806:VAL:HG12	1.72	0.69
1:C:12:ILE:HA	1:C:15:THR:CG2	2.22	0.69
1:C:852:ARG:CG	1:C:852:ARG:HH11	2.00	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1054:LEU:HB2	4:G:3051:FMN:C7M	2.22	0.69
2:H:1195:VAL:CG1	2:H:1211:LEU:HB3	2.23	0.69
2:H:1381:VAL:HG13	2:H:1390:VAL:HG22	1.74	0.69
2:I:652:ILE:H	2:I:658:MET:CE	2.04	0.69
1:A:254:TRP:CZ3	1:A:292:GLN:HG3	2.26	0.69
1:B:254:TRP:CZ3	1:B:292:GLN:HG3	2.27	0.69
2:I:1770:LEU:HD23	2:I:1776:PHE:HE2	1.55	0.69
2:G:84:LEU:HD13	2:G:133:ALA:HB2	1.75	0.69
2:G:964:LEU:CD2	2:G:964:LEU:H	2.05	0.69
2:I:1678:MET:HE3	2:I:1707:LEU:HD22	1.75	0.69
1:C:1208:VAL:CG1	1:C:1212:THR:HB	2.23	0.69
2:G:856:LYS:HG2	2:G:1054:LEU:HD12	1.73	0.69
2:H:1917:ILE:HG23	2:H:1922:ILE:HB	1.74	0.69
2:H:1889:VAL:HG13	2:H:1977:HIS:CB	2.22	0.69
1:A:1721:ARG:NH1	1:A:1721:ARG:HG2	1.97	0.69
1:A:749:ILE:HD11	1:A:805:CYS:HB3	1.75	0.69
1:B:1376:PHE:HB3	1:B:1544:THR:HG22	1.74	0.69
2:G:191:SER:HA	2:G:194:THR:HG22	1.74	0.69
2:I:109:LEU:HD11	2:I:116:LEU:HD23	1.73	0.69
2:I:1194:VAL:HG22	2:I:1212:LYS:HB3	1.75	0.69
2:G:1172:LYS:HE3	2:G:1574:ASN:OD1	1.92	0.69
2:G:1670:GLY:H	2:G:1672:GLN:HE21	1.39	0.69
2:H:1889:VAL:HG13	2:H:1977:HIS:HB2	1.72	0.69
2:H:2022:THR:HG23	2:H:2025:TYR:H	1.58	0.69
1:A:1693:ILE:CD1	2:G:998:GLN:HB2	2.23	0.69
2:H:663:ILE:HB	2:H:664:PRO:HD3	1.75	0.69
2:H:751:LEU:HD23	2:H:791:TYR:CE2	2.27	0.69
2:I:652:ILE:N	2:I:658:MET:HE3	2.08	0.69
1:A:631:PRO:HB2	1:A:634:THR:OG1	1.92	0.69
2:G:1264:GLU:HA	2:G:1275:PHE:CE1	2.28	0.69
2:G:1496:LYS:HE2	2:G:1693:ARG:HH21	1.57	0.69
2:H:1172:LYS:CE	2:H:1574:ASN:OD1	2.40	0.69
2:H:1739:GLU:CB	2:H:1987:PRO:HB3	2.21	0.69
2:H:305:PHE:CE1	2:H:442:ASP:HB3	2.28	0.69
2:I:1739:GLU:CB	2:I:1987:PRO:HB3	2.20	0.69
2:I:663:ILE:HB	2:I:664:PRO:HD3	1.75	0.69
2:I:768:GLY:HA3	2:I:800:LEU:HD21	1.74	0.69
1:A:1376:PHE:HB3	1:A:1544:THR:HG22	1.74	0.69
1:A:257:PRO:HD2	1:A:260:ARG:HB2	1.75	0.69
1:C:1219:VAL:HA	1:C:1384:ILE:CD1	2.20	0.69
1:C:1021:VAL:HG11	1:C:1597:LEU:HD11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:663:ILE:HB	2:G:664:PRO:HD3	1.74	0.69
2:H:54:PRO:HG3	2:H:63:LYS:HG3	1.72	0.69
2:H:652:ILE:N	2:H:658:MET:HE3	2.05	0.69
2:I:1917:ILE:HG23	2:I:1922:ILE:HB	1.74	0.69
2:I:499:THR:CB	2:I:500:HIS:HD2	1.95	0.69
2:H:1419:PHE:O	2:H:1422:THR:HG22	1.93	0.68
2:H:259:THR:HG22	2:H:262:GLU:CG	2.22	0.68
2:I:234:ILE:HG13	2:I:235:PRO:HD3	1.73	0.68
1:A:1203:ASP:HB3	1:B:179:LYS:HZ3	1.58	0.68
2:G:1058:VAL:O	2:G:1061:GLN:HG2	1.93	0.68
1:A:1431:GLU:HG3	1:A:1433:HIS:CE1	2.28	0.68
1:C:1045:PHE:HB3	1:C:1049:GLY:HA3	1.74	0.68
2:G:2035:SER:HB3	2:G:2038:ILE:HG13	1.74	0.68
2:H:1101:GLU:HB3	2:H:1147:ILE:HG22	1.76	0.68
2:H:161:GLY:H	2:H:505:GLY:HA3	1.59	0.68
1:C:1376:PHE:HB3	1:C:1544:THR:HG22	1.74	0.68
2:G:1834:ARG:HG2	2:G:1834:ARG:NH1	1.93	0.68
2:I:1227:ARG:NH1	2:I:1227:ARG:HG3	2.00	0.68
2:I:598:THR:CG2	2:I:622:GLY:HA3	2.23	0.68
1:B:1312:VAL:HG22	1:B:1329:VAL:HG11	1.73	0.68
1:B:400:ARG:HG2	1:B:400:ARG:NH1	2.00	0.68
2:I:187:LEU:HA	2:I:190:PHE:HB3	1.76	0.68
2:I:161:GLY:H	2:I:505:GLY:HA3	1.56	0.68
1:C:985:ARG:NH1	2:I:953:ARG:CZ	2.57	0.68
1:C:1014:ASP:H	1:C:1510:ASN:ND2	1.84	0.68
2:G:1784:MET:HG3	2:G:1785:GLU:N	2.07	0.68
2:G:259:THR:HG22	2:G:262:GLU:CG	2.22	0.68
2:G:54:PRO:HG3	2:G:63:LYS:HG3	1.76	0.68
2:G:732:TRP:CG	2:G:750:MET:CE	2.76	0.68
2:I:1638:ILE:HD12	2:I:1657:ILE:HD12	1.75	0.68
2:I:594:VAL:HG21	2:I:610:THR:HG21	1.75	0.68
1:A:1474:ALA:HA	1:A:1478:PRO:CG	2.24	0.68
1:C:987:ASN:HD22	2:I:957:ARG:HD2	1.58	0.68
2:H:648:GLY:HA3	2:H:678:PHE:CE2	2.29	0.68
1:A:504:ASP:HB3	1:A:508:ASN:H	1.56	0.68
1:A:332:THR:HG22	1:B:331:ILE:HD11	1.76	0.68
2:G:455:ILE:CG1	2:G:469:ARG:HD3	2.23	0.68
2:H:187:LEU:HA	2:H:190:PHE:HB3	1.75	0.68
2:I:305:PHE:CE1	2:I:442:ASP:HB3	2.28	0.68
1:B:1219:VAL:HG22	1:B:1384:ILE:HD12	1.75	0.68
1:C:1310:GLU:OE1	1:C:1649:LYS:HE3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:455:ILE:CD1	2:G:469:ARG:HD3	2.24	0.68
2:H:641:ILE:HG12	2:H:645:SER:HB2	1.76	0.68
1:A:1056:ILE:HD13	1:A:1193:TRP:HD1	1.59	0.68
2:G:1176:PRO:O	2:G:1177:SER:HB3	1.93	0.68
2:H:1058:VAL:O	2:H:1061:GLN:HG2	1.94	0.68
1:A:1303:GLY:H	1:A:1307:THR:HG22	1.59	0.67
1:A:1594:ASN:O	1:A:1598:GLN:HG3	1.94	0.67
1:B:183:GLN:HE21	1:B:202:GLU:HG2	1.59	0.67
1:C:1303:GLY:H	1:C:1307:THR:HG22	1.60	0.67
1:C:254:TRP:CZ3	1:C:292:GLN:HG3	2.29	0.67
1:C:44:VAL:CG1	1:C:78:ILE:HG12	2.24	0.67
2:G:1475:LYS:CG	2:G:1481:SER:HB2	2.24	0.67
2:G:187:LEU:HA	2:G:190:PHE:HB3	1.74	0.67
2:H:1054:LEU:HB2	4:H:3051:FMN:HM72	1.76	0.67
2:H:707:PRO:HG3	2:H:716:VAL:CG2	2.24	0.67
2:H:191:SER:HA	2:H:194:THR:HG22	1.77	0.67
1:C:1232:TYR:CZ	1:C:1701:LYS:HD2	2.29	0.67
1:C:1455:ARG:HH11	1:C:1458:GLN:HE21	1.42	0.67
2:G:1889:VAL:HG13	2:G:1977:HIS:CB	2.24	0.67
2:G:163:GLN:HG2	2:G:423:VAL:HG12	1.77	0.67
2:H:50:ALA:HB3	2:H:53:GLU:HG3	1.76	0.67
2:I:579:VAL:HG23	2:I:1078:HIS:NE2	2.10	0.67
1:C:504:ASP:HB3	1:C:508:ASN:H	1.60	0.67
2:G:1129:ALA:HB2	2:G:1138:TRP:CZ3	2.30	0.67
2:I:598:THR:OG1	2:I:599:PRO:HD3	1.94	0.67
1:A:459:ASP:HB3	1:A:462:LYS:HG3	1.76	0.67
1:B:1303:GLY:H	1:B:1307:THR:HG22	1.59	0.67
1:C:1056:ILE:HD13	1:C:1193:TRP:HD1	1.60	0.67
1:C:1523:ARG:CG	1:C:1523:ARG:NH1	2.57	0.67
1:C:409:ALA:HB2	1:C:442:ARG:HD2	1.76	0.67
2:G:768:GLY:HA3	2:G:800:LEU:HD21	1.76	0.67
2:G:910:GLN:HE21	2:G:912:ARG:HH21	1.42	0.67
2:H:1638:ILE:HD12	2:H:1657:ILE:HD12	1.76	0.67
2:H:902:PRO:HG2	2:H:929:LEU:HD21	1.74	0.67
2:I:904:PHE:HB2	2:I:1017:PHE:CD1	2.28	0.67
2:I:910:GLN:HE21	2:I:912:ARG:HH21	1.40	0.67
1:A:1360:ARG:HH11	1:A:1364:GLU:HG2	1.60	0.67
1:B:1039:MET:O	1:B:1609:ARG:NH2	2.27	0.67
2:G:1741:ILE:HG12	2:G:1746:LEU:HD13	1.77	0.67
1:B:1310:GLU:OE1	1:B:1649:LYS:HE3	1.94	0.67
2:I:1675:GLY:O	2:I:1678:MET:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:LEU:O	1:A:328:LEU:HD22	1.94	0.67
1:C:746:GLU:O	1:C:750:GLU:HG3	1.95	0.67
2:H:545:GLN:HE21	2:H:545:GLN:H	1.41	0.67
2:H:594:VAL:HG21	2:H:610:THR:HG21	1.77	0.67
2:H:768:GLY:HA3	2:H:800:LEU:HD21	1.77	0.67
2:I:54:PRO:HG3	2:I:63:LYS:HG3	1.75	0.67
2:G:1004:LEU:HD21	2:G:1020:VAL:HG23	1.77	0.67
2:G:1676:MET:HE1	2:G:1781:LEU:HD21	1.76	0.67
2:G:1770:LEU:HD23	2:G:1776:PHE:HE2	1.58	0.67
2:H:1086:LEU:HG	2:H:1092:ASP:HA	1.77	0.67
2:H:1242:PHE:CE2	2:H:1244:PRO:HG3	2.30	0.67
2:H:1264:GLU:HA	2:H:1275:PHE:CE1	2.29	0.67
2:I:703:LEU:HD21	2:I:705:LEU:HD21	1.76	0.67
2:G:353:VAL:HG23	2:G:357:ASN:ND2	2.10	0.67
2:H:1256:GLU:O	2:H:1257:ASP:HB2	1.93	0.67
2:I:1889:VAL:HG13	2:I:1977:HIS:CB	2.24	0.67
2:I:949:ASP:HB3	2:I:1006:MET:HE2	1.77	0.67
1:A:1030:TRP:NE1	1:A:1580:LEU:CD2	2.57	0.66
1:C:183:GLN:HE21	1:C:202:GLU:HG2	1.61	0.66
1:C:257:PRO:HD2	1:C:260:ARG:HB2	1.76	0.66
1:C:888:ILE:HD12	1:C:939:PHE:HE2	1.60	0.66
2:G:670:ARG:HD3	2:G:699:GLY:O	1.95	0.66
2:H:1159:ILE:CG1	2:H:1169:PRO:HD3	2.24	0.66
2:H:1862:VAL:HG11	2:H:1866:PHE:CD1	2.30	0.66
2:I:1227:ARG:HD2	2:I:1565:VAL:HG11	1.77	0.66
2:I:163:GLN:HG2	2:I:423:VAL:HG12	1.76	0.66
2:I:50:ALA:HB3	2:I:53:GLU:HG3	1.76	0.66
1:A:1662:TYR:O	1:A:1665:ILE:HG22	1.95	0.66
1:A:473:GLY:O	1:A:477:ILE:HG13	1.95	0.66
1:B:328:LEU:O	1:B:328:LEU:HD22	1.95	0.66
1:B:335:HIS:CE1	1:C:335:HIS:CE1	2.82	0.66
1:C:294:TYR:CE1	1:C:298:VAL:HG21	2.29	0.66
1:C:328:LEU:HD22	1:C:328:LEU:O	1.95	0.66
2:H:670:ARG:HD3	2:H:699:GLY:O	1.95	0.66
2:I:1920:GLN:HG2	2:I:1922:ILE:HD11	1.75	0.66
2:I:1739:GLU:O	2:I:1987:PRO:HG3	1.95	0.66
1:A:183:GLN:HE21	1:A:202:GLU:HG2	1.59	0.66
1:B:1045:PHE:HB3	1:B:1049:GLY:HA3	1.76	0.66
1:B:27:ARG:HB2	2:H:2016:ALA:HB2	1.76	0.66
1:C:1030:TRP:NE1	1:C:1580:LEU:CD2	2.58	0.66
1:C:460:GLU:HG2	1:C:470:LYS:HD3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:507:GLY:N	1:C:954:ARG:HG2	2.11	0.66
2:H:910:GLN:HE21	2:H:912:ARG:HH21	1.43	0.66
2:I:762:ASN:ND2	2:I:762:ASN:H	1.88	0.66
2:I:750:MET:HG3	2:I:796:PHE:HZ	1.60	0.66
1:A:864:VAL:HG22	1:A:921:PRO:HB3	1.78	0.66
1:B:12:ILE:HA	1:B:15:THR:CG2	2.25	0.66
2:I:705:LEU:HD12	2:I:716:VAL:HG13	1.75	0.66
1:B:504:ASP:HB3	1:B:508:ASN:H	1.60	0.66
2:G:1300:PHE:HA	2:G:1556:VAL:HG11	1.77	0.66
2:G:1862:VAL:HG11	2:G:1866:PHE:CD1	2.30	0.66
2:G:61:VAL:O	2:G:65:LEU:HB2	1.96	0.66
2:H:826:GLY:HA3	2:H:1061:GLN:HB3	1.75	0.66
2:H:835:THR:HG21	2:H:855:HIS:HD2	1.59	0.66
2:H:741:HIS:CE1	2:H:855:HIS:CE1	2.84	0.66
1:A:988:ILE:HD13	1:A:1048:GLU:HB3	1.76	0.66
2:G:579:VAL:HG23	2:G:1078:HIS:NE2	2.10	0.66
2:H:1173:VAL:HG21	2:H:1221:MET:HE1	1.77	0.66
2:H:1986:LYS:N	2:H:1987:PRO:HD2	2.11	0.66
1:A:836:ASP:HB3	1:A:839:TYR:HB3	1.76	0.66
1:B:1540:SER:HA	1:B:1575:VAL:HG22	1.78	0.66
1:B:497:THR:OG1	1:B:513:GLU:HG2	1.95	0.66
2:G:1920:GLN:HG2	2:G:1922:ILE:HD11	1.78	0.66
2:H:904:PHE:HB2	2:H:1017:PHE:CD1	2.30	0.66
2:H:1741:ILE:HG12	2:H:1746:LEU:HD13	1.76	0.66
2:H:61:VAL:O	2:H:65:LEU:HB2	1.96	0.66
1:B:733:ILE:HD13	1:B:761:LEU:HD11	1.78	0.66
2:G:1419:PHE:O	2:G:1422:THR:HG22	1.95	0.66
2:G:1457:PHE:CZ	2:G:1501:ILE:HD11	2.30	0.66
2:G:1808:SER:H	2:G:2013:ASN:ND2	1.93	0.66
2:H:131:ILE:HG21	2:H:182:VAL:CG1	2.18	0.66
2:I:1173:VAL:HG21	2:I:1221:MET:HE1	1.77	0.66
2:I:1195:VAL:CG1	2:I:1211:LEU:HB3	2.25	0.66
1:A:254:TRP:CH2	1:A:292:GLN:HG3	2.31	0.66
1:B:1219:VAL:HA	1:B:1384:ILE:CD1	2.24	0.66
1:C:295:ALA:HB2	1:C:302:LEU:HD11	1.77	0.66
2:H:1770:LEU:HD23	2:H:1776:PHE:HE2	1.59	0.66
2:I:1381:VAL:HG13	2:I:1390:VAL:HG22	1.78	0.66
2:I:1808:SER:H	2:I:2013:ASN:ND2	1.94	0.66
1:B:501:THR:N	1:B:886:GLU:OE1	2.21	0.66
1:C:1360:ARG:HH11	1:C:1364:GLU:HG2	1.60	0.66
2:G:843:ILE:HD11	2:G:1055:HIS:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1352:HIS:CD2	2:G:1410:PHE:CE2	2.84	0.66
2:G:33:LEU:HD11	2:G:80:PHE:HD2	1.61	0.66
2:G:904:PHE:HB2	2:G:1017:PHE:CD1	2.30	0.66
2:I:1819:ALA:HA	2:I:2005:ARG:HH11	1.61	0.66
1:A:497:THR:OG1	1:A:513:GLU:HG2	1.96	0.65
1:B:529:MET:CG	1:B:638:LEU:HG	2.26	0.65
1:C:1317:GLU:HA	1:C:1317:GLU:OE1	1.96	0.65
1:C:1:MET:CE	1:C:6:GLU:HA	2.25	0.65
2:G:1976:PHE:HA	2:G:1981:LEU:HD22	1.78	0.65
2:G:652:ILE:N	2:G:658:MET:HE3	2.11	0.65
2:H:2035:SER:HB3	2:H:2038:ILE:HG13	1.78	0.65
1:B:836:ASP:HB3	1:B:839:TYR:HB3	1.79	0.65
1:C:1312:VAL:HG22	1:C:1329:VAL:HG11	1.78	0.65
1:C:330:GLU:HA	1:C:333:LYS:HD2	1.79	0.65
1:C:836:ASP:HB3	1:C:839:TYR:HB3	1.77	0.65
2:G:1352:HIS:HE1	2:G:1583:MET:HE1	1.60	0.65
2:G:1986:LYS:N	2:G:1987:PRO:HD2	2.12	0.65
2:H:1325:PHE:CZ	2:H:1328:VAL:HG11	2.32	0.65
2:H:732:TRP:CG	2:H:750:MET:CE	2.79	0.65
2:I:1782:THR:HG22	2:I:1827:LEU:HD21	1.78	0.65
1:A:27:ARG:HB2	2:G:2016:ALA:HB2	1.77	0.65
2:G:597:MET:HA	4:G:3051:FMN:N5	2.10	0.65
1:A:27:ARG:HD2	1:A:30:GLU:OE2	1.97	0.65
1:A:331:ILE:HD11	1:C:332:THR:HG22	1.79	0.65
1:B:1317:GLU:OE1	1:B:1317:GLU:HA	1.96	0.65
1:B:460:GLU:HG2	1:B:470:LYS:HD3	1.78	0.65
1:C:32:GLN:HA	1:C:35:PHE:CE2	2.31	0.65
2:G:1086:LEU:HG	2:G:1092:ASP:HA	1.77	0.65
2:G:234:ILE:HG13	2:G:235:PRO:HD3	1.77	0.65
2:G:259:THR:HG23	2:G:262:GLU:H	1.62	0.65
2:G:902:PRO:HG2	2:G:929:LEU:HD21	1.79	0.65
2:H:1719:ILE:O	2:H:1761:SER:HB2	1.97	0.65
2:I:251:VAL:O	2:I:255:LEU:HB2	1.96	0.65
1:B:257:PRO:HD2	1:B:260:ARG:HB2	1.78	0.65
1:B:749:ILE:HD11	1:B:805:CYS:HB3	1.77	0.65
2:G:736:ARG:NH1	2:G:769:SER:O	2.29	0.65
1:A:1219:VAL:HG22	1:A:1384:ILE:HD12	1.77	0.65
1:A:331:ILE:CD1	1:C:332:THR:HG22	2.26	0.65
2:G:131:ILE:HG21	2:G:182:VAL:CG1	2.26	0.65
2:I:545:GLN:HE21	2:I:545:GLN:H	1.42	0.65
1:C:435:GLU:O	1:C:439:ILE:HG13	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1381:VAL:HG13	2:G:1390:VAL:HG22	1.77	0.65
1:A:968:VAL:O	2:G:1512:HIS:HB2	1.97	0.65
2:G:1740:THR:HG22	2:G:1742:VAL:HG23	1.78	0.65
1:B:294:TYR:CE1	1:B:298:VAL:HG21	2.32	0.65
1:C:497:THR:OG1	1:C:513:GLU:HG2	1.97	0.65
2:G:826:GLY:HA3	2:G:1061:GLN:HB3	1.77	0.65
2:H:667:LYS:HB2	2:H:698:LEU:HD23	1.79	0.65
2:H:748:THR:HB	2:H:749:PRO:HD3	1.78	0.65
2:H:949:ASP:HB3	2:H:1006:MET:HE2	1.79	0.65
1:A:1219:VAL:HA	1:A:1384:ILE:CD1	2.23	0.65
1:A:340:ARG:HH12	1:A:344:GLN:CG	2.09	0.65
1:A:529:MET:CG	1:A:638:LEU:HG	2.27	0.65
2:G:1242:PHE:CE2	2:G:1244:PRO:HG3	2.31	0.65
2:G:259:THR:CG2	2:G:262:GLU:H	2.10	0.65
1:A:294:TYR:CE1	1:A:298:VAL:HG21	2.32	0.65
1:C:1292:ILE:CD1	1:C:1328:ILE:HD11	2.27	0.65
2:I:1176:PRO:O	2:I:1177:SER:HB3	1.95	0.65
1:C:11:HIS:ND1	2:I:1998:LYS:HA	2.12	0.65
1:B:254:TRP:CH2	1:B:292:GLN:HG3	2.32	0.64
2:H:1195:VAL:HG13	2:H:1211:LEU:HB3	1.80	0.64
2:H:741:HIS:HB3	2:H:853:PRO:HB2	1.77	0.64
2:I:1475:LYS:CG	2:I:1481:SER:HB2	2.27	0.64
2:I:490:TRP:HE1	2:I:516:THR:CG2	2.00	0.64
1:B:599:MET:HB2	1:B:624:LYS:CD	2.24	0.64
1:C:1721:ARG:CG	1:C:1721:ARG:NH1	2.56	0.64
2:G:1906:ALA:O	2:G:1910:VAL:HG23	1.97	0.64
2:G:353:VAL:HG23	2:G:357:ASN:HD22	1.61	0.64
2:H:1859:PRO:O	2:H:1862:VAL:HG13	1.98	0.64
2:I:1355:ASN:HA	2:I:1407:THR:O	1.97	0.64
2:I:719:ILE:O	2:I:722:ALA:HB3	1.97	0.64
1:A:421:ILE:CG1	1:A:469:VAL:HG21	2.28	0.64
1:B:864:VAL:HG22	1:B:921:PRO:HB3	1.77	0.64
1:C:749:ILE:HD11	1:C:805:CYS:HB3	1.78	0.64
2:H:115:THR:HB	2:H:118:LYS:HB2	1.80	0.64
1:C:604:ALA:HB3	1:C:612:GLU:HG2	1.80	0.64
2:G:138:ASP:O	2:G:139:LYS:HG3	1.97	0.64
2:H:1352:HIS:CD2	2:H:1410:PHE:CE2	2.85	0.64
2:H:1906:ALA:O	2:H:1910:VAL:HG23	1.98	0.64
2:H:259:THR:HG23	2:H:262:GLU:H	1.63	0.64
2:I:1265:MET:HE1	2:I:1562:PRO:HG2	1.78	0.64
1:A:1039:MET:O	1:A:1609:ARG:NH2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:746:GLU:O	1:B:750:GLU:HG3	1.97	0.64
2:G:1359:MET:HE3	2:G:1404:MET:HB3	1.79	0.64
2:G:490:TRP:HE1	2:G:516:THR:CG2	1.99	0.64
2:H:1823:SER:OG	2:H:1825:GLU:HG2	1.96	0.64
2:H:259:THR:CG2	2:H:262:GLU:H	2.10	0.64
2:H:658:MET:HA	2:H:661:TRP:NE1	2.13	0.64
2:I:1422:THR:CG2	2:I:1474:PHE:HB2	2.27	0.64
1:B:504:ASP:HB2	1:B:508:ASN:HB2	1.79	0.64
1:C:1540:SER:HA	1:C:1575:VAL:HG22	1.79	0.64
1:C:1594:ASN:O	1:C:1598:GLN:HG3	1.97	0.64
2:G:1195:VAL:CG1	2:G:1211:LEU:HB3	2.27	0.64
2:G:1103:PHE:O	2:G:1247:GLY:HA3	1.97	0.64
2:I:61:VAL:O	2:I:65:LEU:HB2	1.96	0.64
2:I:826:GLY:HA3	2:I:1061:GLN:HB3	1.78	0.64
1:A:1022:THR:HG22	1:A:1226:SER:HB2	1.80	0.64
1:A:504:ASP:HB2	1:A:508:ASN:HB2	1.78	0.64
1:A:746:GLU:O	1:A:750:GLU:HG3	1.97	0.64
1:C:833:PHE:HA	1:C:937:LYS:HD2	1.78	0.64
2:G:499:THR:CB	2:G:500:HIS:HD2	1.97	0.64
2:H:1808:SER:H	2:H:2013:ASN:HD21	1.46	0.64
2:I:1457:PHE:CZ	2:I:1501:ILE:HD11	2.33	0.64
2:I:7:ARG:HE	2:I:27:PHE:HB2	1.62	0.64
1:B:330:GLU:HA	1:B:333:LYS:HD2	1.80	0.64
1:B:852:ARG:NH1	1:B:852:ARG:HG2	1.98	0.64
1:C:1194:ASN:HB3	1:C:1197:THR:CG2	2.27	0.64
2:G:1739:GLU:CB	2:G:1987:PRO:HB3	2.23	0.64
2:H:1457:PHE:CZ	2:H:1501:ILE:HD11	2.32	0.64
2:H:232:LEU:O	2:H:232:LEU:HD23	1.98	0.64
2:I:1676:MET:HE1	2:I:1781:LEU:HD21	1.79	0.64
2:I:2022:THR:HG23	2:I:2025:TYR:H	1.63	0.64
2:I:648:GLY:HA3	2:I:678:PHE:CE2	2.32	0.64
1:A:1317:GLU:OE1	1:A:1317:GLU:HA	1.96	0.64
1:B:421:ILE:CG1	1:B:469:VAL:HG21	2.27	0.64
2:G:545:GLN:H	2:G:545:GLN:HE21	1.46	0.64
2:H:1205:LEU:O	2:H:1206:LYS:HG3	1.97	0.64
2:H:1676:MET:HE1	2:H:1781:LEU:HD21	1.80	0.64
2:I:892:ILE:HD11	2:I:903:TRP:NE1	2.12	0.64
2:I:964:LEU:CD2	2:I:964:LEU:H	2.11	0.64
1:B:1474:ALA:HA	1:B:1478:PRO:CG	2.27	0.64
2:G:305:PHE:CE1	2:G:442:ASP:HB3	2.32	0.64
2:H:163:GLN:HG2	2:H:423:VAL:HG12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:703:LEU:HD21	2:H:705:LEU:HD21	1.79	0.64
2:I:670:ARG:HD3	2:I:699:GLY:O	1.98	0.64
1:A:1021:VAL:HG11	1:A:1597:LEU:HD11	1.79	0.63
1:A:152:HIS:HD2	1:A:163:LEU:HB2	1.61	0.63
1:C:1474:ALA:HA	1:C:1478:PRO:CG	2.27	0.63
2:G:648:GLY:HA3	2:G:678:PHE:CE2	2.33	0.63
2:H:1176:PRO:O	2:H:1177:SER:HB3	1.97	0.63
2:H:1266:TYR:CB	2:H:1347:LEU:HD23	2.28	0.63
2:H:964:LEU:CD2	2:H:964:LEU:H	2.09	0.63
1:C:24:SER:CB	2:I:2014:LEU:HD12	2.27	0.63
2:I:641:ILE:HG12	2:I:645:SER:HB2	1.79	0.63
1:A:504:ASP:CB	1:A:508:ASN:H	2.10	0.63
1:B:438:ASN:HD21	1:B:698:GLN:HE21	1.46	0.63
1:C:436:ALA:O	1:C:440:MET:HG3	1.98	0.63
1:C:504:ASP:HB2	1:C:508:ASN:HB2	1.80	0.63
1:C:989:GLN:NE2	2:I:993:GLN:OE1	2.32	0.63
2:G:1205:LEU:O	2:G:1206:LYS:HG3	1.98	0.63
2:G:2022:THR:HG23	2:G:2025:TYR:H	1.63	0.63
2:H:1227:ARG:CG	2:H:1227:ARG:NH1	2.57	0.63
2:H:1808:SER:H	2:H:2013:ASN:ND2	1.95	0.63
2:I:1279:PHE:HB2	2:I:1340:PRO:HG3	1.79	0.63
2:I:1266:TYR:CB	2:I:1347:LEU:HD23	2.28	0.63
2:I:1378:ILE:HD11	2:I:1381:VAL:CG2	2.28	0.63
2:I:902:PRO:HG2	2:I:929:LEU:HD21	1.79	0.63
1:A:1292:ILE:CD1	1:A:1328:ILE:HD11	2.28	0.63
1:A:1461:ASP:O	1:A:1465:ASN:HB2	1.99	0.63
1:A:956:ALA:O	1:A:959:ILE:HG22	1.98	0.63
1:B:992:PHE:CE2	1:B:1399:PRO:HG3	2.34	0.63
1:C:1721:ARG:HG2	1:C:1721:ARG:NH1	2.00	0.63
2:G:259:THR:OG1	2:G:260:PRO:HD2	1.97	0.63
2:G:7:ARG:HE	2:G:27:PHE:HB2	1.63	0.63
2:G:745:ASP:HA	2:G:832:TRP:HH2	1.64	0.63
2:H:353:VAL:HG23	2:H:357:ASN:ND2	2.13	0.63
2:I:1890:ASN:HB2	2:I:1899:VAL:HB	1.81	0.63
2:I:1976:PHE:HA	2:I:1981:LEU:HD22	1.81	0.63
1:A:824:LEU:HD12	1:A:846:LEU:HB3	1.80	0.63
1:A:852:ARG:NH1	1:A:852:ARG:HG2	2.00	0.63
1:B:881:ASN:HA	1:B:944:ARG:HH21	1.63	0.63
1:C:599:MET:HB2	1:C:624:LYS:CD	2.25	0.63
1:C:680:ILE:HG13	1:C:769:ILE:HB	1.80	0.63
2:G:1266:TYR:CB	2:G:1347:LEU:HD23	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:835:THR:HG21	2:G:855:HIS:CD2	2.33	0.63
2:H:1422:THR:CG2	2:H:1474:PHE:HB2	2.29	0.63
2:H:1740:THR:HG22	2:H:1742:VAL:HG23	1.79	0.63
2:I:1159:ILE:CG1	2:I:1169:PRO:HD3	2.28	0.63
1:B:421:ILE:HG13	1:B:469:VAL:HG21	1.81	0.63
2:G:1859:PRO:O	2:G:1862:VAL:HG13	1.99	0.63
2:H:598:THR:CG2	2:H:622:GLY:HA3	2.28	0.63
2:I:1195:VAL:HG13	2:I:1211:LEU:HB3	1.79	0.63
2:I:159:ILE:HD11	2:I:512:LEU:HG	1.80	0.63
1:A:330:GLU:HA	1:A:333:LYS:HD2	1.80	0.63
1:B:1721:ARG:CG	1:B:1721:ARG:NH1	2.55	0.63
1:B:444:ASN:HB3	1:B:446:ALA:H	1.63	0.63
1:B:1:MET:HE3	1:B:5:VAL:HG12	1.81	0.63
1:C:158:LYS:HD3	1:C:185:GLU:HB3	1.79	0.63
2:G:115:THR:HB	2:G:118:LYS:HB2	1.80	0.63
2:G:251:VAL:O	2:G:255:LEU:HB2	1.99	0.63
2:H:1475:LYS:CG	2:H:1481:SER:HB2	2.29	0.63
2:H:601:THR:CG2	2:H:618:GLU:O	2.38	0.63
2:H:835:THR:HG22	2:H:845:THR:N	2.14	0.63
2:I:1741:ILE:HG12	2:I:1746:LEU:HD13	1.80	0.63
2:I:1859:PRO:O	2:I:1862:VAL:HG13	1.98	0.63
1:A:1194:ASN:HB3	1:A:1197:THR:CG2	2.28	0.63
1:A:233:ILE:HD13	1:A:237:MET:HE2	1.81	0.63
1:A:436:ALA:O	1:A:440:MET:HG3	1.99	0.63
2:I:241:ILE:HG23	2:I:506:PRO:HG3	1.81	0.63
1:B:27:ARG:HH21	2:H:2015:THR:HA	1.64	0.63
1:C:864:VAL:HG22	1:C:921:PRO:HB3	1.79	0.63
2:G:1360:ILE:HG23	2:G:1403:VAL:O	1.99	0.63
2:G:748:THR:HB	2:G:749:PRO:HD3	1.78	0.63
2:H:892:ILE:HD11	2:H:903:TRP:NE1	2.14	0.63
2:I:1194:VAL:HG12	2:I:1194:VAL:O	1.99	0.63
1:A:460:GLU:HG2	1:A:470:LYS:HD3	1.79	0.63
1:C:742:LYS:HD3	1:C:746:GLU:OE2	1.98	0.63
2:G:490:TRP:O	2:G:494:THR:HG22	1.99	0.63
2:I:115:THR:HB	2:I:118:LYS:HB2	1.80	0.63
2:I:259:THR:HG23	2:I:262:GLU:H	1.64	0.63
2:I:259:THR:OG1	2:I:260:PRO:HD2	1.98	0.63
1:A:411:GLN:HE22	1:A:1628:SER:H	1.47	0.62
1:B:1056:ILE:HD13	1:B:1193:TRP:HD1	1.64	0.62
1:C:956:ALA:O	1:C:959:ILE:HG22	1.98	0.62
2:G:1227:ARG:HG3	2:G:1227:ARG:NH1	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1874:VAL:O	2:H:1878:VAL:HG12	1.98	0.62
2:H:33:LEU:HD11	2:H:80:PHE:HD2	1.63	0.62
1:A:13:LEU:HB2	2:G:2026:PHE:CE1	2.34	0.62
1:A:158:LYS:HD3	1:A:185:GLU:HB3	1.81	0.62
1:B:529:MET:HG3	1:B:638:LEU:HG	1.80	0.62
2:G:943:TRP:CH2	2:G:1016:PRO:HG3	2.34	0.62
2:G:1173:VAL:HG21	2:G:1221:MET:HE1	1.80	0.62
2:G:1378:ILE:HD11	2:G:1381:VAL:CG2	2.29	0.62
2:G:85:ASN:ND2	2:G:135:ARG:HH11	1.97	0.62
2:H:1374:THR:HG23	2:H:1396:LEU:HD12	1.81	0.62
2:H:1931:LEU:HD22	2:H:1935:GLU:HG2	1.81	0.62
2:H:251:VAL:O	2:H:255:LEU:HB2	1.99	0.62
1:A:1259:GLY:HA2	1:A:1263:ASP:HB2	1.81	0.62
1:A:440:MET:HE3	1:A:483:VAL:HG21	1.81	0.62
1:C:254:TRP:CH2	1:C:292:GLN:HG3	2.34	0.62
1:C:529:MET:CG	1:C:638:LEU:HG	2.30	0.62
2:G:726:PHE:O	2:G:762:ASN:HB2	1.98	0.62
2:H:750:MET:HG3	2:H:796:PHE:HZ	1.64	0.62
2:H:856:LYS:HG2	2:H:1054:LEU:HD12	1.81	0.62
2:I:1472:VAL:HG22	2:I:1483:VAL:HG22	1.81	0.62
2:I:1624:THR:HB	2:I:1642:THR:HG23	1.81	0.62
2:I:324:LEU:HD12	2:I:328:LEU:HG	1.82	0.62
1:C:1431:GLU:HG3	1:C:1433:HIS:CE1	2.33	0.62
2:H:1472:VAL:HG22	2:H:1483:VAL:HG22	1.79	0.62
2:H:871:THR:HB	2:H:872:ILE:HD12	1.80	0.62
2:I:1868:GLN:HG3	2:I:1898:TYR:OH	1.99	0.62
2:I:1906:ALA:O	2:I:1910:VAL:HG23	2.00	0.62
1:A:1292:ILE:HD11	1:A:1328:ILE:HD11	1.81	0.62
1:A:1455:ARG:HH11	1:A:1458:GLN:HE21	1.46	0.62
1:B:1584:PRO:HG3	1:B:1591:TRP:CZ3	2.35	0.62
1:B:507:GLY:N	1:B:954:ARG:HG2	2.15	0.62
1:C:1039:MET:O	1:C:1609:ARG:NH2	2.31	0.62
2:G:1102:TYR:HB3	2:G:1244:PRO:HA	1.80	0.62
2:G:1782:THR:HG22	2:G:1827:LEU:HD21	1.81	0.62
2:G:1819:ALA:HA	2:G:2005:ARG:HH11	1.65	0.62
2:H:601:THR:O	2:H:601:THR:HG22	2.00	0.62
1:B:1455:ARG:HH11	1:B:1458:GLN:HE21	1.47	0.62
1:C:822:VAL:HG12	1:C:824:LEU:HD22	1.82	0.62
2:H:1168:ASN:ND2	2:H:1171:ARG:HB2	2.14	0.62
2:I:1740:THR:HG22	2:I:1742:VAL:HG23	1.79	0.62
2:I:464:ASP:HB3	2:I:466:SER:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:846:VAL:HG13	2:I:865:TRP:NE1	2.15	0.62
1:A:1540:SER:HA	1:A:1575:VAL:HG22	1.81	0.62
1:A:749:ILE:CD1	1:A:805:CYS:HB3	2.29	0.62
1:C:233:ILE:HD13	1:C:237:MET:CE	2.30	0.62
2:G:1908:ASP:HB2	2:G:1958:LEU:HD21	1.81	0.62
2:G:241:ILE:HG23	2:G:506:PRO:HG3	1.80	0.62
2:G:871:THR:HB	2:G:872:ILE:HD12	1.82	0.62
2:H:131:ILE:HD12	2:H:182:VAL:CG1	2.29	0.62
2:I:184:VAL:HG13	2:I:187:LEU:HD21	1.80	0.62
2:I:259:THR:CG2	2:I:262:GLU:H	2.11	0.62
1:C:444:ASN:HB3	1:C:446:ALA:H	1.65	0.62
2:G:1300:PHE:CA	2:G:1556:VAL:HG11	2.29	0.62
2:G:159:ILE:HD11	2:G:512:LEU:HG	1.80	0.62
2:G:641:ILE:HG12	2:G:645:SER:HB2	1.80	0.62
2:H:85:ASN:ND2	2:H:135:ARG:HH11	1.96	0.62
2:I:1805:ALA:HB2	2:I:2011:ILE:HB	1.82	0.62
1:A:1523:ARG:CG	1:A:1523:ARG:NH1	2.57	0.62
1:A:20:TYR:HE1	2:G:2035:SER:HB2	1.60	0.62
1:B:27:ARG:HD2	1:B:30:GLU:OE2	2.00	0.62
1:C:501:THR:N	1:C:886:GLU:OE1	2.21	0.62
2:G:750:MET:HG3	2:G:796:PHE:HZ	1.65	0.62
2:H:490:TRP:O	2:H:494:THR:HG22	2.00	0.62
1:A:1326:ILE:HG12	1:A:1388:MET:HG3	1.82	0.62
2:G:1719:ILE:O	2:G:1761:SER:HB2	2.00	0.62
2:G:1931:LEU:HD22	2:G:1935:GLU:HG2	1.82	0.62
2:H:1149:TRP:CD1	2:H:1213:LEU:HD12	2.34	0.62
2:I:1086:LEU:HD12	2:I:1090:TYR:HB2	1.82	0.62
2:I:1823:SER:OG	2:I:1825:GLU:HG2	2.00	0.62
2:I:745:ASP:HA	2:I:832:TRP:HH2	1.65	0.62
1:C:1057:MET:SD	1:C:1097:ILE:HG23	2.40	0.61
1:C:233:ILE:HD13	1:C:237:MET:HE2	1.80	0.61
1:C:509:ILE:HG12	1:C:951:SER:HB2	1.82	0.61
2:G:1199:GLU:OE2	2:G:1567:ARG:CZ	2.46	0.61
2:G:719:ILE:O	2:G:722:ALA:HB3	2.00	0.61
2:H:100:ASP:OD2	2:H:102:HIS:HD2	1.82	0.61
2:H:159:ILE:HD11	2:H:512:LEU:HG	1.82	0.61
2:H:1675:GLY:O	2:H:1678:MET:HB2	1.99	0.61
1:B:1292:ILE:CD1	1:B:1328:ILE:HD11	2.30	0.61
1:B:631:PRO:HB2	1:B:634:THR:OG1	2.00	0.61
2:H:7:ARG:HE	2:H:27:PHE:HB2	1.64	0.61
2:H:353:VAL:HG23	2:H:357:ASN:HD22	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:LYS:HD3	1:B:185:GLU:HB3	1.82	0.61
1:B:340:ARG:HH12	1:B:344:GLN:CG	2.13	0.61
1:B:824:LEU:HD12	1:B:846:LEU:HB3	1.82	0.61
2:H:856:LYS:NZ	2:H:1052:CYS:SG	2.70	0.61
2:H:589:ARG:HB3	2:H:590:PRO:HD2	1.82	0.61
2:I:1054:LEU:HB2	4:I:3051:FMN:HM71	1.82	0.61
2:I:860:ARG:HB3	2:I:898:ASP:HB3	1.81	0.61
1:A:1721:ARG:NH1	1:A:1721:ARG:CG	2.52	0.61
1:B:1555:ALA:HA	1:B:1621:PHE:CE1	2.36	0.61
2:G:1739:GLU:O	2:G:1987:PRO:HG3	2.00	0.61
2:H:1378:ILE:HD11	2:H:1381:VAL:CG2	2.31	0.61
2:H:565:TYR:CZ	2:H:758:ARG:HD2	2.35	0.61
2:H:835:THR:HG21	2:H:855:HIS:NE2	2.14	0.61
2:I:100:ASP:OD2	2:I:102:HIS:HD2	1.83	0.61
2:I:1808:SER:H	2:I:2013:ASN:HD21	1.47	0.61
1:C:20:TYR:CE1	2:I:2035:SER:HB2	2.35	0.61
1:A:24:SER:O	2:G:1977:HIS:HD2	1.84	0.61
1:B:20:TYR:CE1	2:H:2035:SER:HB2	2.35	0.61
1:B:644:THR:HG23	1:B:648:ASP:H	1.65	0.61
1:C:1292:ILE:HD11	1:C:1328:ILE:HD11	1.81	0.61
2:G:324:LEU:HD12	2:G:328:LEU:HG	1.81	0.61
2:H:1086:LEU:HD12	2:H:1090:TYR:HB2	1.83	0.61
2:H:1279:PHE:HB2	2:H:1340:PRO:HG3	1.81	0.61
2:H:174:ARG:NH2	2:H:225:THR:OG1	2.33	0.61
2:H:33:LEU:HD11	2:H:80:PHE:CD2	2.35	0.61
1:C:20:TYR:CG	2:I:2033:THR:OG1	2.53	0.61
2:I:56:THR:HG23	2:I:59:GLU:CG	2.28	0.61
1:A:705:VAL:HG23	1:A:732:LEU:HD21	1.82	0.61
1:B:1431:GLU:HG3	1:B:1433:HIS:CE1	2.36	0.61
1:B:1693:ILE:HD11	2:H:998:GLN:HB2	1.83	0.61
1:B:24:SER:O	2:H:1977:HIS:CD2	2.53	0.61
2:H:603:SER:O	2:H:607:VAL:HG12	2.00	0.61
1:A:644:THR:HG23	1:A:648:ASP:H	1.65	0.61
1:A:822:VAL:HG12	1:A:824:LEU:HD22	1.82	0.61
1:B:1194:ASN:HB3	1:B:1197:THR:CG2	2.30	0.61
1:C:824:LEU:HD12	1:C:846:LEU:HB3	1.82	0.61
2:I:1325:PHE:CZ	2:I:1328:VAL:HG11	2.36	0.61
2:I:1352:HIS:HE1	2:I:1583:MET:HE1	1.65	0.61
1:C:24:SER:HB3	2:I:2014:LEU:HD12	1.82	0.61
2:I:663:ILE:HG13	2:I:694:TYR:HE1	1.66	0.61
1:B:1052:GLU:O	1:B:1056:ILE:HG23	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1594:ASN:O	1:B:1598:GLN:HG3	2.00	0.61
1:A:599:MET:HB2	1:A:624:LYS:CD	2.25	0.61
1:A:488:PRO:HG3	1:A:728:LYS:HG3	1.81	0.61
1:B:1292:ILE:HD11	1:B:1328:ILE:HD11	1.82	0.61
1:B:1360:ARG:HH11	1:B:1364:GLU:HG2	1.66	0.61
2:G:1123:ASP:N	2:G:1123:ASP:OD1	2.34	0.61
2:G:1976:PHE:HB3	2:G:1981:LEU:HD21	1.82	0.61
1:A:11:HIS:ND1	2:G:1998:LYS:HA	2.15	0.61
2:G:601:THR:O	2:G:601:THR:HG22	2.01	0.61
2:H:260:PRO:HD3	2:H:289:TRP:CE2	2.36	0.61
1:A:1:MET:HE3	1:A:5:VAL:HG12	1.82	0.61
2:G:856:LYS:NZ	2:G:1052:CYS:SG	2.69	0.61
2:G:1472:VAL:HG22	2:G:1483:VAL:HG22	1.83	0.61
2:H:1805:ALA:HB2	2:H:2011:ILE:HB	1.83	0.61
2:H:184:VAL:HG13	2:H:187:LEU:HD21	1.83	0.61
2:I:1219:ILE:HD11	2:I:1242:PHE:HB2	1.83	0.61
1:C:504:ASP:CB	1:C:508:ASN:H	2.14	0.60
2:H:846:VAL:HG13	2:H:865:TRP:NE1	2.16	0.60
2:I:565:TYR:CZ	2:I:758:ARG:HD2	2.35	0.60
1:A:32:GLN:HA	1:A:35:PHE:CE2	2.35	0.60
1:B:233:ILE:HD13	1:B:237:MET:HE2	1.82	0.60
2:G:174:ARG:NH2	2:G:225:THR:OG1	2.34	0.60
2:G:33:LEU:HD11	2:G:80:PHE:CD2	2.35	0.60
2:I:856:LYS:NZ	2:I:1052:CYS:SG	2.70	0.60
2:I:1300:PHE:HA	2:I:1556:VAL:HG11	1.84	0.60
1:C:2:LYS:CD	2:I:2050:GLN:HB3	2.30	0.60
2:I:33:LEU:HD11	2:I:80:PHE:CD2	2.36	0.60
1:A:232:LEU:HD22	1:A:269:LEU:HA	1.83	0.60
2:G:1808:SER:H	2:G:2013:ASN:HD21	1.47	0.60
2:G:607:VAL:HA	2:G:617:ILE:HD13	1.82	0.60
2:G:747:HIS:HE1	2:G:780:TYR:OH	1.84	0.60
2:I:1198:SER:HB3	2:I:1205:LEU:HD21	1.82	0.60
2:I:1908:ASP:HB2	2:I:1958:LEU:HD21	1.83	0.60
1:B:400:ARG:HH11	1:B:400:ARG:HG3	1.64	0.60
1:A:20:TYR:OH	2:G:2035:SER:HB2	2.01	0.60
2:G:846:VAL:HG13	2:G:865:TRP:NE1	2.16	0.60
2:H:1198:SER:HB3	2:H:1205:LEU:HD21	1.83	0.60
2:H:1219:ILE:HD11	2:H:1242:PHE:HB2	1.83	0.60
2:H:324:LEU:HD12	2:H:328:LEU:HG	1.84	0.60
2:I:1352:HIS:CD2	2:I:1410:PHE:CE2	2.90	0.60
2:I:1360:ILE:HG23	2:I:1403:VAL:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:674:TYR:HB3	2:I:676:ILE:HG22	1.84	0.60
1:B:1523:ARG:NH1	1:B:1523:ARG:CG	2.59	0.60
1:B:509:ILE:HG12	1:B:951:SER:HB2	1.82	0.60
1:C:221:LEU:O	1:C:225:SER:HB3	2.02	0.60
2:G:1325:PHE:CZ	2:G:1328:VAL:HG11	2.37	0.60
2:G:499:THR:CB	2:G:500:HIS:CD2	2.80	0.60
2:G:61:VAL:HG21	2:G:95:TYR:HE1	1.67	0.60
2:G:926:LEU:HD13	2:G:947:THR:HG22	1.84	0.60
2:H:745:ASP:HA	2:H:832:TRP:HH2	1.66	0.60
2:I:1123:ASP:OD1	2:I:1123:ASP:N	2.35	0.60
2:I:1205:LEU:O	2:I:1206:LYS:HG3	2.00	0.60
2:I:667:LYS:HB2	2:I:698:LEU:HD23	1.82	0.60
2:I:817:ALA:O	2:I:821:ILE:HG13	2.01	0.60
1:C:644:THR:HG23	1:C:648:ASP:H	1.65	0.60
2:G:1822:MET:HE2	2:G:1996:ILE:HG12	1.84	0.60
2:G:816:ASP:HB3	2:G:1048:VAL:HG21	1.83	0.60
2:H:1624:THR:HB	2:H:1642:THR:HG23	1.82	0.60
2:I:1976:PHE:HB3	2:I:1981:LEU:HD21	1.83	0.60
2:I:589:ARG:HB3	2:I:590:PRO:HD2	1.83	0.60
1:A:1194:ASN:O	1:A:1197:THR:HG23	2.02	0.60
1:A:529:MET:HG3	1:A:638:LEU:HG	1.84	0.60
1:B:513:GLU:OE2	1:B:873:ARG:NH1	2.33	0.60
2:G:184:VAL:HG13	2:G:187:LEU:HD21	1.84	0.60
2:G:271:THR:OG1	2:G:460:TYR:HB2	2.01	0.60
2:I:33:LEU:HD11	2:I:80:PHE:HD2	1.65	0.60
1:A:233:ILE:HD13	1:A:237:MET:CE	2.32	0.60
1:C:1062:TYR:CD2	1:C:1693:ILE:HG23	2.36	0.60
2:H:1149:TRP:CD1	2:H:1213:LEU:CD1	2.85	0.60
2:H:1739:GLU:O	2:H:1987:PRO:HG3	2.02	0.60
2:I:1986:LYS:N	2:I:1987:PRO:HD2	2.16	0.60
1:B:1657:HIS:ND1	1:B:1658:PRO:HD2	2.17	0.60
1:B:604:ALA:HB3	1:B:612:GLU:HG2	1.82	0.60
1:C:529:MET:HG3	1:C:638:LEU:HG	1.82	0.60
2:G:732:TRP:CD2	2:G:750:MET:CE	2.85	0.60
2:G:892:ILE:HD11	2:G:903:TRP:NE1	2.17	0.60
2:H:719:ILE:O	2:H:722:ALA:HB3	2.02	0.60
1:B:1021:VAL:HG11	1:B:1597:LEU:HD11	1.83	0.60
1:B:1057:MET:SD	1:B:1097:ILE:HG23	2.42	0.60
1:C:1662:TYR:O	1:C:1665:ILE:HG22	2.01	0.60
2:H:1093:ASP:HB3	2:H:1096:LYS:HG3	1.84	0.60
2:I:1874:VAL:O	2:I:1878:VAL:HG12	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1989:LYS:O	2:I:1993:LYS:HG3	2.02	0.60
2:I:601:THR:HG22	2:I:601:THR:O	2.02	0.60
2:I:741:HIS:CB	2:I:853:PRO:HB2	2.32	0.60
1:B:1189:ILE:HD12	1:B:1380:GLN:HG3	1.82	0.59
1:C:1461:ASP:O	1:C:1465:ASN:HB2	2.02	0.59
1:C:1585:LYS:HB3	3:C:2748:CER:H52	1.84	0.59
2:G:100:ASP:OD2	2:G:102:HIS:HD2	1.85	0.59
2:G:598:THR:CG2	2:G:622:GLY:HA3	2.30	0.59
2:H:1494:PRO:HB2	2:H:1823:SER:HB2	1.84	0.59
2:I:732:TRP:CD2	2:I:750:MET:CE	2.84	0.59
1:A:37:LYS:HB2	1:A:65:TYR:HE1	1.67	0.59
1:A:67:SER:OG	2:I:359:HIS:HE1	1.85	0.59
1:B:1062:TYR:CD2	1:B:1693:ILE:HG23	2.36	0.59
1:B:1184:LEU:HB2	1:B:1352:THR:HG21	1.83	0.59
1:B:80:CYS:SG	1:B:82:SER:HB3	2.42	0.59
2:H:813:THR:HB	2:H:818:LYS:HE3	1.84	0.59
2:I:1378:ILE:HD11	2:I:1381:VAL:HG21	1.84	0.59
2:I:163:GLN:CG	2:I:423:VAL:HG12	2.32	0.59
1:A:435:GLU:O	1:A:439:ILE:HG13	2.03	0.59
1:B:32:GLN:HA	1:B:35:PHE:CE2	2.38	0.59
1:B:680:ILE:HG13	1:B:769:ILE:HB	1.83	0.59
1:C:705:VAL:HG23	1:C:732:LEU:HD21	1.83	0.59
2:G:594:VAL:HG21	2:G:610:THR:HG21	1.84	0.59
2:H:1314:ARG:NH1	2:H:1314:ARG:CG	2.62	0.59
2:I:1575:LEU:HD13	2:I:1579:ILE:HD12	1.84	0.59
1:A:1584:PRO:HG3	1:A:1591:TRP:CZ3	2.37	0.59
1:B:1259:GLY:HA2	1:B:1263:ASP:HB2	1.84	0.59
1:B:221:LEU:O	1:B:225:SER:HB3	2.02	0.59
1:C:421:ILE:CG1	1:C:469:VAL:HG21	2.32	0.59
1:C:56:MET:HG3	2:I:1893:VAL:CG2	2.32	0.59
2:G:2038:ILE:O	2:G:2042:ILE:HG12	2.02	0.59
2:G:565:TYR:CZ	2:G:758:ARG:HD2	2.37	0.59
2:G:754:TYR:CD2	2:G:794:MET:HG3	2.38	0.59
2:H:1223:MET:HE3	2:H:1238:LEU:HD12	1.84	0.59
2:H:409:PHE:HB3	2:H:833:GLU:OE1	2.02	0.59
2:H:241:ILE:HG23	2:H:506:PRO:HG3	1.83	0.59
2:H:860:ARG:HB3	2:H:898:ASP:HB3	1.83	0.59
2:I:658:MET:HA	2:I:661:TRP:NE1	2.17	0.59
1:A:1432:HIS:CE1	1:A:1434:SER:OG	2.55	0.59
1:B:233:ILE:HD13	1:B:237:MET:CE	2.32	0.59
1:B:956:ALA:O	1:B:959:ILE:HG22	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1194:ASN:O	1:C:1197:THR:HG23	2.02	0.59
1:C:1492:GLU:O	1:C:1496:GLU:HG3	2.01	0.59
2:G:1805:ALA:HB2	2:G:2011:ILE:HB	1.84	0.59
2:G:443:LEU:HD22	2:G:448:VAL:HG11	1.84	0.59
2:I:1149:TRP:CD1	2:I:1213:LEU:HD12	2.37	0.59
2:I:85:ASN:ND2	2:I:135:ARG:HH11	1.99	0.59
2:I:402:LEU:HD13	2:I:402:LEU:O	2.02	0.59
1:B:504:ASP:CB	1:B:508:ASN:H	2.15	0.59
1:C:1584:PRO:HG3	1:C:1591:TRP:CZ3	2.38	0.59
2:G:1195:VAL:HG13	2:G:1211:LEU:HB3	1.84	0.59
2:G:603:SER:O	2:G:607:VAL:HG12	2.03	0.59
2:G:932:ILE:HD11	2:G:1042:ALA:CB	2.24	0.59
2:H:817:ALA:O	2:H:821:ILE:HG13	2.02	0.59
1:A:417:TYR:OH	1:A:458:THR:HG22	2.02	0.59
1:A:516:ARG:NH2	1:A:889:GLU:OE1	2.35	0.59
1:B:1585:LYS:HB3	3:B:2748:CER:H52	1.85	0.59
1:C:733:ILE:HD12	1:C:761:LEU:HD21	1.85	0.59
2:H:663:ILE:HG13	2:H:694:TYR:HE1	1.66	0.59
2:H:726:PHE:O	2:H:762:ASN:HB2	2.03	0.59
2:I:1086:LEU:HD12	2:I:1090:TYR:CB	2.33	0.59
2:I:1496:LYS:HE2	2:I:1693:ARG:HH21	1.67	0.59
2:I:99:ASN:HA	2:I:550:VAL:CG2	2.32	0.59
1:A:409:ALA:HB2	1:A:442:ARG:HD2	1.84	0.59
2:G:131:ILE:CG2	2:G:182:VAL:CG1	2.80	0.59
2:H:197:GLU:HA	2:H:197:GLU:OE1	2.02	0.59
2:H:455:ILE:HG13	2:H:469:ARG:HD3	1.83	0.59
1:A:50:SER:HB2	1:A:51:PRO:HD3	1.85	0.59
1:C:1555:ALA:HA	1:C:1621:PHE:CE1	2.38	0.59
2:G:1086:LEU:HD12	2:G:1090:TYR:HB2	1.84	0.59
2:G:402:LEU:HD13	2:G:402:LEU:O	2.03	0.59
2:H:2038:ILE:O	2:H:2042:ILE:HG12	2.03	0.59
1:B:1474:ALA:O	1:B:1478:PRO:HD2	2.03	0.59
1:B:417:TYR:OH	1:B:458:THR:HG22	2.03	0.59
2:G:1210:ILE:HB	2:G:1222:GLU:HB3	1.85	0.59
2:G:1293:THR:CG2	2:G:1296:GLU:H	2.14	0.59
2:G:1374:THR:HG23	2:G:1396:LEU:HD12	1.85	0.59
2:H:1130:THR:H	2:H:1133:THR:HG23	1.68	0.59
2:H:259:THR:OG1	2:H:260:PRO:HD2	2.03	0.59
2:I:174:ARG:NH2	2:I:225:THR:OG1	2.36	0.59
2:I:353:VAL:HG23	2:I:357:ASN:ND2	2.18	0.59
2:I:490:TRP:O	2:I:494:THR:HG22	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1524:GLY:O	1:A:1528:THR:HG23	2.03	0.58
1:A:1585:LYS:HB3	3:A:2748:CER:H52	1.85	0.58
1:B:1234:MET:HG2	1:B:1326:ILE:HD12	1.85	0.58
1:C:488:PRO:HG3	1:C:728:LYS:HG3	1.83	0.58
2:G:1198:SER:HB3	2:G:1205:LEU:HD21	1.85	0.58
2:G:1279:PHE:HB2	2:G:1340:PRO:HG3	1.85	0.58
2:G:1378:ILE:HD11	2:G:1381:VAL:HG21	1.85	0.58
2:H:273:HIS:HB3	2:H:512:LEU:HD22	1.85	0.58
2:I:455:ILE:HG13	2:I:469:ARG:HD3	1.85	0.58
1:A:421:ILE:HG12	1:A:469:VAL:HG21	1.85	0.58
1:A:531:LEU:HD21	1:A:629:THR:HG22	1.85	0.58
1:B:1392:LEU:HD22	1:B:1396:MET:HG3	1.84	0.58
1:C:1657:HIS:ND1	1:C:1658:PRO:HD2	2.17	0.58
1:C:749:ILE:CD1	1:C:805:CYS:HB3	2.32	0.58
1:C:80:CYS:SG	1:C:82:SER:HB3	2.42	0.58
2:G:1149:TRP:CD1	2:G:1213:LEU:HD12	2.38	0.58
2:H:1010:PRO:O	2:H:1011:MET:HB2	2.03	0.58
2:H:665:LEU:O	2:H:669:LEU:HB2	2.04	0.58
2:I:1822:MET:CE	2:I:1996:ILE:HG12	2.34	0.58
2:I:499:THR:CB	2:I:500:HIS:CD2	2.79	0.58
2:I:907:VAL:O	2:I:910:GLN:HB3	2.03	0.58
1:B:37:LYS:HB2	1:B:65:TYR:HE1	1.69	0.58
2:G:166:THR:HG22	2:G:168:ASP:N	2.19	0.58
2:G:28:PHE:CZ	2:H:7:ARG:NE	2.70	0.58
2:I:1227:ARG:NH1	2:I:1227:ARG:CG	2.55	0.58
2:I:1374:THR:HG23	2:I:1396:LEU:HD12	1.83	0.58
2:I:601:THR:CG2	2:I:618:GLU:O	2.39	0.58
1:A:260:ARG:HH12	1:A:300:VAL:HG21	1.68	0.58
1:A:444:ASN:HB3	1:A:446:ALA:H	1.66	0.58
1:B:409:ALA:HB2	1:B:442:ARG:HD2	1.86	0.58
1:C:1233:GLU:OE2	1:C:1680:ARG:NH2	2.36	0.58
1:C:24:SER:O	2:I:1977:HIS:CD2	2.54	0.58
2:H:1103:PHE:O	2:H:1247:GLY:HA3	2.03	0.58
2:H:1360:ILE:HG23	2:H:1403:VAL:O	2.04	0.58
2:I:127:ILE:O	2:I:131:ILE:HG13	2.03	0.58
2:I:736:ARG:NH1	2:I:769:SER:O	2.36	0.58
1:B:436:ALA:O	1:B:440:MET:HG3	2.04	0.58
1:C:1009:LEU:HA	1:C:1445:MET:HE2	1.85	0.58
1:C:232:LEU:HD22	1:C:269:LEU:HA	1.83	0.58
2:G:1597:ALA:HB1	2:G:1638:ILE:CD1	2.33	0.58
2:G:1823:SER:OG	2:G:1825:GLU:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:807:ILE:CG2	2:G:1066:ILE:HA	2.34	0.58
2:H:271:THR:OG1	2:H:460:TYR:HB2	2.03	0.58
2:H:499:THR:CB	2:H:500:HIS:CD2	2.81	0.58
2:H:762:ASN:H	2:H:762:ASN:ND2	1.85	0.58
2:I:1269:LEU:O	2:I:1560:LEU:HD23	2.03	0.58
1:A:986:ALA:HB2	1:A:1047:LEU:HD13	1.85	0.58
1:B:1461:ASP:O	1:B:1465:ASN:HB2	2.03	0.58
1:C:1665:ILE:HD11	1:C:1669:ARG:HG2	1.85	0.58
1:C:232:LEU:HD13	1:C:272:GLU:HB2	1.85	0.58
1:C:340:ARG:HH12	1:C:344:GLN:CG	2.13	0.58
1:C:421:ILE:HG13	1:C:469:VAL:HG21	1.84	0.58
2:G:1223:MET:HE3	2:G:1238:LEU:HD12	1.85	0.58
2:G:131:ILE:CG2	2:G:182:VAL:HG12	2.33	0.58
2:G:907:VAL:O	2:G:910:GLN:HB3	2.02	0.58
2:I:707:PRO:HG2	2:I:730:LEU:HD13	1.85	0.58
1:A:1600:LEU:HD13	1:A:1657:HIS:HA	1.85	0.58
1:C:419:GLU:HG2	1:C:424:VAL:HB	1.86	0.58
2:G:1159:ILE:CG1	2:G:1169:PRO:HD3	2.33	0.58
2:G:260:PRO:HD3	2:G:289:TRP:CE2	2.38	0.58
2:G:674:TYR:HB3	2:G:676:ILE:HG22	1.85	0.58
1:B:29:ILE:HG13	2:H:1891:TYR:C	2.23	0.58
2:H:490:TRP:CH2	2:H:512:LEU:HD21	2.39	0.58
2:H:543:PHE:CB	2:H:545:GLN:HE22	2.17	0.58
2:I:942:THR:HG21	2:I:1012:GLN:HA	1.85	0.58
1:C:968:VAL:O	2:I:1512:HIS:HB2	2.04	0.58
2:I:1719:ILE:O	2:I:1761:SER:HB2	2.01	0.58
1:B:198:PRO:CG	1:B:209:LEU:HD21	2.26	0.58
1:B:286:PHE:O	1:B:290:MET:HG2	2.03	0.58
1:C:1020:VAL:HG13	1:C:1400:ILE:HG23	1.84	0.58
2:G:638:VAL:HA	2:G:641:ILE:HG22	1.86	0.58
2:H:163:GLN:CG	2:H:423:VAL:HG12	2.32	0.58
2:I:1822:MET:HE2	2:I:1996:ILE:HG12	1.86	0.58
1:A:198:PRO:CG	1:A:209:LEU:HD21	2.28	0.58
1:A:987:ASN:HD22	2:G:957:ARG:HD2	1.68	0.58
1:B:1473:GLU:O	1:B:1478:PRO:HD3	2.04	0.58
1:B:1662:TYR:O	1:B:1665:ILE:HG22	2.04	0.58
1:B:232:LEU:HD22	1:B:269:LEU:HA	1.85	0.58
1:B:749:ILE:CD1	1:B:805:CYS:HB3	2.33	0.58
1:C:1247:SER:HB2	1:C:1332:TYR:HE2	1.68	0.58
2:G:1359:MET:HA	2:G:1359:MET:HE3	1.86	0.58
1:A:20:TYR:CZ	2:G:2035:SER:HB2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:232:LEU:HD23	2:G:232:LEU:O	2.03	0.58
2:G:273:HIS:HB3	2:G:512:LEU:HD22	1.86	0.58
2:G:611:THR:CG2	2:G:641:ILE:HG13	2.34	0.58
2:G:817:ALA:O	2:G:821:ILE:HG13	2.04	0.58
2:G:860:ARG:HB3	2:G:898:ASP:HB3	1.85	0.58
2:H:1210:ILE:HB	2:H:1222:GLU:HB3	1.85	0.58
1:C:27:ARG:HH21	2:I:2015:THR:HA	1.68	0.58
1:A:1062:TYR:CD2	1:A:1693:ILE:HG23	2.39	0.57
1:A:1189:ILE:HD12	1:A:1380:GLN:HG3	1.86	0.57
1:A:1419:PRO:HB3	1:A:1646:PHE:CZ	2.39	0.57
1:A:329:GLU:O	1:A:333:LYS:HG3	2.04	0.57
1:B:1247:SER:HB2	1:B:1332:TYR:HE2	1.69	0.57
1:B:419:GLU:HG2	1:B:424:VAL:HB	1.86	0.57
1:C:1219:VAL:CA	1:C:1384:ILE:HD11	2.27	0.57
1:C:433:VAL:O	1:C:437:ILE:HG13	2.04	0.57
2:G:146:PHE:HA	2:G:149:VAL:HG12	1.86	0.57
2:G:376:ASN:HD22	2:G:377:LEU:N	2.02	0.57
2:G:526:ARG:HH11	2:G:558:ASN:HD21	1.49	0.57
2:G:56:THR:HG23	2:G:59:GLU:CG	2.29	0.57
2:G:7:ARG:NH1	2:G:24:THR:HA	2.19	0.57
2:I:239:PRO:HG3	2:I:304:PHE:HA	1.86	0.57
2:I:376:ASN:HD22	2:I:377:LEU:N	2.02	0.57
1:A:1056:ILE:CD1	1:A:1193:TRP:HD1	2.17	0.57
1:A:1203:ASP:HB3	1:B:179:LYS:HZ1	1.68	0.57
1:A:1247:SER:HB2	1:A:1332:TYR:HE2	1.66	0.57
1:A:11:HIS:O	1:A:15:THR:HG22	2.04	0.57
1:B:1496:GLU:O	1:B:1500:GLN:HG3	2.03	0.57
1:B:232:LEU:HD13	1:B:272:GLU:HB2	1.87	0.57
1:C:1052:GLU:O	1:C:1056:ILE:HG23	2.04	0.57
2:G:1149:TRP:CD1	2:G:1213:LEU:CD1	2.87	0.57
2:G:658:MET:HA	2:G:661:TRP:NE1	2.19	0.57
2:H:1331:TRP:CE2	2:H:1335:ILE:HG13	2.38	0.57
2:H:722:ALA:HB1	2:H:723:HIS:CE1	2.38	0.57
2:I:726:PHE:O	2:I:762:ASN:HB2	2.04	0.57
1:A:1538:VAL:HB	1:A:1639:VAL:HG22	1.86	0.57
1:B:1022:THR:HG22	1:B:1226:SER:HB2	1.87	0.57
1:B:1125:VAL:HG21	1:B:1175:ILE:HD12	1.86	0.57
1:B:50:SER:HB2	1:B:51:PRO:HD3	1.86	0.57
1:C:1056:ILE:CD1	1:C:1193:TRP:HD1	2.16	0.57
2:G:942:THR:HG21	2:G:1012:GLN:HA	1.86	0.57
2:G:826:GLY:O	2:G:827:VAL:HG23	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:124:LYS:HG2	2:H:179:THR:HA	1.86	0.57
1:B:413:LEU:HD13	1:B:451:MET:HG2	1.85	0.57
1:B:705:VAL:HG23	1:B:732:LEU:HD21	1.85	0.57
2:G:163:GLN:CG	2:G:423:VAL:HG12	2.33	0.57
2:H:1086:LEU:HD12	2:H:1090:TYR:CB	2.34	0.57
2:H:1231:GLY:O	2:H:1233:PRO:HD3	2.04	0.57
2:H:1567:ARG:HH12	2:H:1568:HIS:HB3	1.70	0.57
2:H:1908:ASP:HB2	2:H:1958:LEU:HD21	1.86	0.57
2:H:601:THR:HG22	2:H:620:ALA:H	1.69	0.57
2:H:732:TRP:CG	2:H:750:MET:HE3	2.39	0.57
2:H:907:VAL:O	2:H:910:GLN:HB3	2.03	0.57
2:I:145:LEU:O	2:I:149:VAL:HG12	2.03	0.57
2:I:654:VAL:HG23	2:I:683:ALA:HB1	1.87	0.57
1:A:232:LEU:HD13	1:A:272:GLU:HB2	1.85	0.57
1:C:1189:ILE:HD12	1:C:1380:GLN:HG3	1.86	0.57
1:C:1600:LEU:HD13	1:C:1657:HIS:HA	1.87	0.57
1:C:198:PRO:CG	1:C:209:LEU:HD21	2.28	0.57
1:C:771:PHE:CD1	1:C:825:PRO:HG3	2.40	0.57
2:G:1010:PRO:O	2:G:1011:MET:HB2	2.05	0.57
2:G:932:ILE:CD1	2:G:1042:ALA:HB2	2.24	0.57
2:H:736:ARG:NH1	2:H:769:SER:O	2.36	0.57
2:H:89:THR:O	2:H:93:ASN:HB2	2.04	0.57
2:I:1130:THR:H	2:I:1133:THR:HG23	1.69	0.57
1:A:604:ALA:HB3	1:A:612:GLU:HG2	1.86	0.57
1:A:828:PRO:HG3	1:A:868:ILE:HG22	1.86	0.57
1:B:980:VAL:HG21	2:H:952:ARG:HH21	1.70	0.57
1:C:1184:LEU:HB2	1:C:1352:THR:HG21	1.85	0.57
1:C:1473:GLU:O	1:C:1478:PRO:HD3	2.05	0.57
1:C:251:GLN:HA	1:C:256:LEU:H	1.69	0.57
2:G:1314:ARG:CG	2:G:1314:ARG:NH1	2.61	0.57
2:G:1954:LYS:HD3	2:G:1958:LEU:HD13	1.86	0.57
2:G:517:HIS:C	2:G:517:HIS:CD2	2.78	0.57
2:H:1782:THR:HG22	2:H:1827:LEU:HD21	1.86	0.57
2:H:522:GLY:HA3	2:H:561:TRP:CZ3	2.40	0.57
2:H:732:TRP:CG	2:H:750:MET:HE1	2.40	0.57
2:I:2038:ILE:O	2:I:2042:ILE:HG12	2.04	0.57
2:I:813:THR:HB	2:I:818:LYS:HE3	1.85	0.57
1:A:988:ILE:HA	1:A:1048:GLU:HG2	1.84	0.57
1:A:655:LEU:CD2	1:A:916:LEU:HD11	2.35	0.57
2:G:1775:GLN:HG2	2:G:1836:MET:SD	2.44	0.57
2:G:1778:GLN:HB3	2:G:1831:VAL:HG13	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1890:ASN:HB2	2:G:1899:VAL:HB	1.86	0.57
2:G:741:HIS:HE1	2:G:845:THR:HG22	1.58	0.57
2:H:166:THR:HG22	2:H:168:ASP:N	2.19	0.57
2:H:61:VAL:HG21	2:H:95:TYR:HE1	1.69	0.57
2:I:665:LEU:O	2:I:669:LEU:HB2	2.05	0.57
1:A:1285:ALA:O	1:A:1289:MET:HG3	2.04	0.57
1:A:1474:ALA:O	1:A:1478:PRO:HD2	2.04	0.57
1:A:680:ILE:HG13	1:A:769:ILE:HB	1.87	0.57
1:B:140:ILE:HD13	1:B:255:GLY:O	2.05	0.57
1:B:440:MET:HE3	1:B:483:VAL:HG21	1.87	0.57
2:G:1266:TYR:CG	2:G:1347:LEU:HD23	2.40	0.57
2:G:703:LEU:HD21	2:G:705:LEU:HD21	1.86	0.57
2:H:1123:ASP:OD1	2:H:1123:ASP:N	2.36	0.57
2:H:1100:VAL:HG21	2:H:1147:ILE:CD1	2.34	0.57
2:H:1575:LEU:HD13	2:H:1579:ILE:HD12	1.85	0.57
2:H:2029:VAL:O	2:H:2033:THR:HG22	2.05	0.57
2:H:732:TRP:CD2	2:H:750:MET:CE	2.87	0.57
2:I:1292:ILE:O	2:I:1368:VAL:O	2.23	0.57
2:I:273:HIS:HB3	2:I:512:LEU:HD22	1.87	0.57
2:I:353:VAL:HG23	2:I:357:ASN:HD22	1.69	0.57
1:A:415:SER:O	1:A:419:GLU:HB2	2.05	0.57
1:A:80:CYS:SG	1:A:82:SER:HB3	2.45	0.57
1:C:1474:ALA:O	1:C:1478:PRO:HD2	2.04	0.57
2:G:1168:ASN:ND2	2:G:1171:ARG:HB2	2.20	0.57
2:G:1547:PRO:HD3	2:G:1584:PHE:CE2	2.40	0.57
2:G:463:PHE:HD1	2:G:486:LEU:HD13	1.70	0.57
2:G:455:ILE:HG13	2:G:469:ARG:HD3	1.86	0.57
2:G:584:SER:HA	2:G:587:ILE:HG23	1.87	0.57
2:G:667:LYS:HB2	2:G:698:LEU:HD23	1.85	0.57
2:G:89:THR:O	2:G:93:ASN:HB2	2.05	0.57
2:H:777:THR:CG2	2:H:1081:HIS:CE1	2.88	0.57
2:H:127:ILE:O	2:H:131:ILE:HG13	2.04	0.57
2:H:1589:VAL:HG11	2:H:1640:PHE:CE1	2.39	0.57
2:I:777:THR:CG2	2:I:1081:HIS:CE1	2.88	0.57
2:I:1199:GLU:OE2	2:I:1567:ARG:NH1	2.37	0.57
2:I:463:PHE:HD1	2:I:486:LEU:HD13	1.70	0.57
2:I:807:ILE:CG2	2:I:1066:ILE:HA	2.35	0.57
1:B:1431:GLU:HB3	1:B:1520:ALA:HB2	1.86	0.57
1:B:529:MET:HE3	1:B:529:MET:CA	2.31	0.57
1:B:742:LYS:HD3	1:B:746:GLU:OE2	2.05	0.57
1:C:341:GLN:O	1:C:345:VAL:HG12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1675:GLY:O	2:G:1678:MET:HB2	2.05	0.57
2:H:1266:TYR:CG	2:H:1347:LEU:HD23	2.40	0.57
2:H:1871:LEU:HD22	2:H:1888:ILE:HD11	1.85	0.57
2:H:1976:PHE:HA	2:H:1981:LEU:HD22	1.86	0.57
2:I:1210:ILE:HB	2:I:1222:GLU:HB3	1.85	0.57
2:I:1231:GLY:O	2:I:1233:PRO:HD3	2.05	0.57
2:I:2029:VAL:O	2:I:2033:THR:HG22	2.05	0.57
2:I:607:VAL:HA	2:I:617:ILE:HD13	1.86	0.57
1:A:263:GLY:O	1:A:267:VAL:HG23	2.05	0.56
1:A:742:LYS:HD3	1:A:746:GLU:OE2	2.05	0.56
1:B:1524:GLY:O	1:B:1528:THR:HG23	2.05	0.56
1:B:152:HIS:HD2	1:B:163:LEU:HB2	1.66	0.56
1:B:251:GLN:HA	1:B:256:LEU:H	1.70	0.56
2:G:1868:GLN:HG3	2:G:1898:TYR:OH	2.04	0.56
2:G:653:TYR:CD1	2:G:659:LEU:HD21	2.39	0.56
1:B:964:GLU:HG2	2:H:1515:PRO:HB3	1.86	0.56
2:H:517:HIS:CD2	2:H:517:HIS:C	2.78	0.56
2:H:526:ARG:HH11	2:H:558:ASN:HD21	1.53	0.56
2:H:56:THR:HG23	2:H:59:GLU:CG	2.32	0.56
2:H:653:TYR:CD1	2:H:659:LEU:HD21	2.40	0.56
2:H:740:HIS:CE1	2:H:852:GLU:OE1	2.58	0.56
2:I:120:LYS:O	2:I:124:LYS:HG3	2.05	0.56
2:I:2030:TYR:CE1	2:I:2034:GLY:HA2	2.39	0.56
1:A:419:GLU:HG2	1:A:424:VAL:HB	1.86	0.56
1:C:1326:ILE:HG12	1:C:1388:MET:HG3	1.86	0.56
1:C:1524:GLY:O	1:C:1528:THR:HG23	2.05	0.56
1:C:1538:VAL:HB	1:C:1639:VAL:HG22	1.86	0.56
1:C:626:VAL:HG23	1:C:664:GLU:OE2	2.05	0.56
2:G:1567:ARG:HG3	2:G:1568:HIS:N	2.20	0.56
2:G:1804:PHE:CZ	2:G:2010:TYR:HB2	2.40	0.56
2:G:654:VAL:HG23	2:G:683:ALA:HB1	1.87	0.56
2:H:1352:HIS:HE1	2:H:1583:MET:HE1	1.69	0.56
2:H:638:VAL:HA	2:H:641:ILE:HG22	1.86	0.56
2:G:28:PHE:HZ	2:H:7:ARG:NE	2.02	0.56
2:H:839:PRO:HA	2:H:844:VAL:HG13	1.86	0.56
2:H:926:LEU:HD13	2:H:947:THR:HG22	1.86	0.56
2:I:1223:MET:HE3	2:I:1238:LEU:HD12	1.87	0.56
2:I:197:GLU:OE1	2:I:197:GLU:HA	2.05	0.56
1:C:20:TYR:HE1	2:I:2035:SER:HB2	1.69	0.56
2:I:281:VAL:HG23	2:I:459:VAL:HG11	1.87	0.56
2:I:741:HIS:HB3	2:I:853:PRO:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:89:THR:O	2:I:93:ASN:HB2	2.05	0.56
1:A:1014:ASP:N	1:A:1510:ASN:HD21	1.92	0.56
1:B:152:HIS:CE1	1:B:168:MET:HG3	2.40	0.56
2:G:1194:VAL:HG12	2:G:1194:VAL:O	2.05	0.56
2:G:1989:LYS:O	2:G:1993:LYS:HG3	2.05	0.56
2:G:1086:LEU:HD12	2:G:1090:TYR:CB	2.35	0.56
2:G:663:ILE:HG13	2:G:694:TYR:HE1	1.70	0.56
2:H:702:TYR:CB	2:H:727:PRO:HB2	2.36	0.56
2:I:1149:TRP:CD1	2:I:1213:LEU:CD1	2.88	0.56
2:I:443:LEU:HD22	2:I:448:VAL:HG11	1.87	0.56
2:I:481:ASP:OD2	2:I:485:ARG:NH1	2.38	0.56
2:I:490:TRP:CH2	2:I:512:LEU:HD21	2.40	0.56
2:I:543:PHE:CB	2:I:545:GLN:HE22	2.17	0.56
1:B:488:PRO:HG3	1:B:728:LYS:HG3	1.87	0.56
1:C:635:ILE:HG22	1:C:651:TYR:CD1	2.41	0.56
2:G:813:THR:HB	2:G:818:LYS:HE3	1.87	0.56
2:H:1223:MET:CE	2:H:1238:LEU:HD12	2.35	0.56
2:H:1834:ARG:NH1	2:H:1834:ARG:CG	2.60	0.56
2:H:376:ASN:HD22	2:H:377:LEU:N	2.03	0.56
2:H:835:THR:HG22	2:H:844:VAL:C	2.26	0.56
2:I:1722:GLY:N	2:I:1726:GLY:HA3	2.21	0.56
2:I:1804:PHE:CZ	2:I:2010:TYR:HB2	2.40	0.56
1:A:1009:LEU:HA	1:A:1445:MET:HE2	1.87	0.56
1:A:21:GLN:O	2:G:1977:HIS:CD2	2.59	0.56
1:B:411:GLN:HE22	1:B:1628:SER:H	1.52	0.56
1:C:152:HIS:HD2	1:C:163:LEU:HB2	1.63	0.56
2:G:1834:ARG:HH11	2:G:1834:ARG:CG	2.03	0.56
2:G:543:PHE:CB	2:G:545:GLN:HE22	2.17	0.56
2:G:758:ARG:NH2	2:G:797:ASP:OD1	2.33	0.56
2:H:120:LYS:O	2:H:124:LYS:HG3	2.06	0.56
2:H:606:PHE:HZ	2:H:805:VAL:HG11	1.68	0.56
1:A:1057:MET:SD	1:A:1097:ILE:HG23	2.45	0.56
1:A:221:LEU:O	1:A:225:SER:HB3	2.05	0.56
1:B:1419:PRO:HB3	1:B:1646:PHE:CZ	2.40	0.56
1:C:1022:THR:HG22	1:C:1226:SER:HB2	1.87	0.56
1:C:741:SER:HB3	1:C:744:ASP:HB2	1.86	0.56
2:H:1920:GLN:HG2	2:H:1922:ILE:HD11	1.87	0.56
1:B:1009:LEU:HG	1:B:1664:ALA:HB2	1.87	0.56
1:C:695:GLY:HA3	1:C:906:LEU:HD11	1.88	0.56
2:G:1722:GLY:N	2:G:1726:GLY:HA3	2.21	0.56
2:G:634:ILE:HD11	2:G:649:ILE:CD1	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1890:ASN:HB2	2:H:1899:VAL:HB	1.88	0.56
2:H:443:LEU:HD22	2:H:448:VAL:HG11	1.86	0.56
2:H:463:PHE:HD1	2:H:486:LEU:HD13	1.71	0.56
2:I:1567:ARG:HH12	2:I:1568:HIS:HB3	1.71	0.56
2:I:835:THR:HG23	2:I:843:ILE:O	2.05	0.56
1:A:1036:ARG:NH1	1:A:1040:GLU:OE1	2.39	0.56
1:A:152:HIS:CE1	1:A:168:MET:HG3	2.41	0.56
1:A:251:GLN:HA	1:A:256:LEU:H	1.68	0.56
1:B:1138:LYS:HG3	1:B:1163:TYR:CE1	2.41	0.56
1:B:1492:GLU:O	1:B:1496:GLU:HG3	2.06	0.56
1:B:644:THR:HG22	1:B:648:ASP:O	2.06	0.56
2:G:577:ILE:HD13	2:G:1097:ILE:CD1	2.35	0.56
2:G:589:ARG:HB3	2:G:590:PRO:HD2	1.87	0.56
2:G:599:PRO:HD2	4:G:3051:FMN:H6	1.88	0.56
2:H:1868:GLN:HG3	2:H:1898:TYR:OH	2.05	0.56
2:H:607:VAL:HA	2:H:617:ILE:HD13	1.88	0.56
2:I:601:THR:HG22	2:I:620:ALA:H	1.71	0.56
2:I:702:TYR:CB	2:I:727:PRO:HB2	2.36	0.56
2:I:732:TRP:CG	2:I:750:MET:HE3	2.39	0.56
2:I:774:ALA:HB1	2:I:1081:HIS:CD2	2.33	0.56
2:I:871:THR:HB	2:I:872:ILE:HD12	1.88	0.56
1:B:529:MET:HG2	1:B:638:LEU:CD1	2.35	0.56
1:C:1259:GLY:HA2	1:C:1263:ASP:HB2	1.87	0.56
1:C:329:GLU:O	1:C:333:LYS:HG3	2.06	0.56
1:C:531:LEU:HD21	1:C:629:THR:HG22	1.88	0.56
1:C:881:ASN:HA	1:C:944:ARG:HH21	1.70	0.56
2:G:1130:THR:H	2:G:1133:THR:HG23	1.70	0.56
2:G:1422:THR:CG2	2:G:1474:PHE:HB2	2.36	0.56
2:G:1567:ARG:HH12	2:G:1568:HIS:HB3	1.71	0.56
2:G:702:TYR:CB	2:G:727:PRO:HB2	2.35	0.56
2:H:1100:VAL:HG21	2:H:1147:ILE:HD13	1.88	0.56
2:H:1194:VAL:O	2:H:1194:VAL:HG12	2.05	0.56
2:H:1778:GLN:HB3	2:H:1831:VAL:HG13	1.88	0.56
2:H:1989:LYS:O	2:H:1993:LYS:HG3	2.06	0.56
2:I:1931:LEU:HD22	2:I:1935:GLU:HG2	1.86	0.56
1:A:1052:GLU:O	1:A:1056:ILE:HG23	2.06	0.56
1:A:1665:ILE:CG1	1:A:1669:ARG:HD3	2.36	0.56
1:C:1419:PRO:HB3	1:C:1646:PHE:CZ	2.41	0.56
2:G:120:LYS:O	2:G:124:LYS:HG3	2.05	0.56
2:G:1308:CYS:HB3	2:G:1311:PHE:CD2	2.41	0.56
2:G:1874:VAL:O	2:G:1878:VAL:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1308:CYS:HB3	2:H:1311:PHE:CD2	2.41	0.56
2:H:1328:VAL:HG23	2:H:1557:SER:HA	1.88	0.56
2:I:826:GLY:HA2	2:I:1060:ALA:HB3	1.88	0.56
2:I:577:ILE:HD13	2:I:1097:ILE:CD1	2.36	0.56
2:I:1589:VAL:HG11	2:I:1640:PHE:CE1	2.41	0.56
2:I:732:TRP:CD1	2:I:750:MET:HE3	2.40	0.56
1:A:1524:GLY:HA2	1:A:1527:ALA:HB3	1.89	0.55
1:A:295:ALA:HB2	1:A:302:LEU:HD11	1.87	0.55
1:B:11:HIS:O	1:B:15:THR:HG22	2.06	0.55
1:B:1233:GLU:OE2	1:B:1680:ARG:NH2	2.40	0.55
1:C:1496:GLU:O	1:C:1500:GLN:HG3	2.06	0.55
2:G:1475:LYS:HG3	2:G:1481:SER:HB2	1.88	0.55
2:G:1561:ASN:OD1	2:G:1563:ILE:HB	2.05	0.55
2:G:732:TRP:CD2	2:G:750:MET:HE1	2.41	0.55
2:H:1493:LEU:HD11	2:H:1499:VAL:CG2	2.36	0.55
2:H:16:LEU:HG	2:H:48:PHE:CZ	2.40	0.55
2:H:239:PRO:HG3	2:H:304:PHE:HA	1.88	0.55
2:I:1308:CYS:HB3	2:I:1311:PHE:CD2	2.40	0.55
1:C:29:ILE:HG13	2:I:1891:TYR:O	2.06	0.55
2:I:7:ARG:NH1	2:I:24:THR:HA	2.20	0.55
2:I:653:TYR:CD1	2:I:659:LEU:HD21	2.40	0.55
1:A:1114:TYR:CD1	1:A:1337:GLU:HG3	2.41	0.55
1:A:1555:ALA:HA	1:A:1621:PHE:CE1	2.41	0.55
1:A:864:VAL:CG2	1:A:921:PRO:HB3	2.36	0.55
1:B:1538:VAL:HB	1:B:1639:VAL:HG22	1.87	0.55
1:B:733:ILE:HD12	1:B:761:LEU:HD21	1.88	0.55
1:B:988:ILE:HD13	1:B:1048:GLU:HB3	1.89	0.55
1:C:335:HIS:HD2	1:C:335:HIS:O	1.89	0.55
2:G:652:ILE:HB	2:G:658:MET:CE	2.36	0.55
2:H:7:ARG:NH1	2:H:24:THR:HA	2.21	0.55
2:I:1382:VAL:HA	2:I:1422:THR:OG1	2.07	0.55
2:I:1931:LEU:HB3	2:I:1935:GLU:CG	2.35	0.55
2:I:232:LEU:HD23	2:I:232:LEU:O	2.06	0.55
1:A:1665:ILE:HD11	1:A:1669:ARG:HG2	1.88	0.55
1:B:1665:ILE:HD11	1:B:1669:ARG:HG2	1.88	0.55
1:B:433:VAL:O	1:B:437:ILE:HG13	2.07	0.55
1:C:12:ILE:HA	1:C:15:THR:HG23	1.88	0.55
1:C:417:TYR:OH	1:C:458:THR:HG22	2.06	0.55
2:G:1931:LEU:HB3	2:G:1935:GLU:CG	2.33	0.55
2:G:2036:GLU:O	2:G:2039:LYS:HG2	2.06	0.55
2:G:722:ALA:HB1	2:G:723:HIS:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1822:MET:HE2	2:H:1996:ILE:HG12	1.89	0.55
2:H:490:TRP:HA	2:H:493:THR:CG2	2.36	0.55
2:I:124:LYS:HG2	2:I:179:THR:HA	1.87	0.55
2:I:634:ILE:HD11	2:I:649:ILE:CD1	2.35	0.55
1:A:825:PRO:HB2	1:A:843:LYS:NZ	2.21	0.55
1:B:1036:ARG:NH1	1:B:1040:GLU:OE1	2.40	0.55
1:C:1347:LYS:HD3	1:C:1347:LYS:O	2.05	0.55
1:C:1:MET:HE3	1:C:9:LEU:HD12	1.89	0.55
2:G:1678:MET:CE	2:G:1707:LEU:HD22	2.35	0.55
2:G:665:LEU:O	2:G:669:LEU:HB2	2.06	0.55
2:H:1431:TYR:CE1	2:H:1526:THR:HG23	2.41	0.55
1:C:254:TRP:CZ3	1:C:302:LEU:HD13	2.41	0.55
1:C:27:ARG:HD2	1:C:30:GLU:OE2	2.06	0.55
1:C:807:LYS:HG3	1:C:858:TRP:HB3	1.87	0.55
2:G:1475:LYS:HB2	2:G:1481:SER:HB2	1.89	0.55
2:H:1166:VAL:HG12	2:H:1167:SER:N	2.21	0.55
2:H:2038:ILE:HG22	2:H:2042:ILE:CD1	2.36	0.55
2:I:166:THR:HG22	2:I:168:ASP:N	2.21	0.55
2:I:638:VAL:HA	2:I:641:ILE:HG22	1.88	0.55
2:I:926:LEU:HB3	2:I:947:THR:HG22	1.88	0.55
2:I:61:VAL:HG21	2:I:95:TYR:HE1	1.72	0.55
1:A:1238:VAL:HG12	1:A:1239:HIS:N	2.21	0.55
1:C:1125:VAL:HG21	1:C:1175:ILE:HD12	1.88	0.55
1:C:152:HIS:CE1	1:C:168:MET:HG3	2.41	0.55
1:C:11:HIS:O	1:C:15:THR:HG22	2.06	0.55
2:G:1496:LYS:HE2	2:G:1693:ARG:NH2	2.20	0.55
2:G:197:GLU:OE1	2:G:197:GLU:HA	2.06	0.55
2:H:807:ILE:CG2	2:H:1066:ILE:HA	2.36	0.55
2:H:1359:MET:HE3	2:H:1359:MET:HA	1.88	0.55
2:I:2015:THR:HG22	2:I:2017:LYS:N	2.21	0.55
1:A:1056:ILE:HD13	1:A:1193:TRP:CD1	2.42	0.55
1:A:1233:GLU:OE2	1:A:1680:ARG:NH2	2.40	0.55
1:A:12:ILE:HD11	2:G:2041:ILE:HD11	1.83	0.55
1:A:1473:GLU:O	1:A:1478:PRO:HD3	2.06	0.55
1:A:529:MET:HG2	1:A:638:LEU:CD1	2.36	0.55
1:A:771:PHE:CD1	1:A:825:PRO:HG3	2.42	0.55
1:B:1285:ALA:O	1:B:1289:MET:HG3	2.07	0.55
1:B:1432:HIS:CE1	1:B:1434:SER:OG	2.60	0.55
1:B:328:LEU:C	1:B:328:LEU:HD22	2.28	0.55
1:A:332:THR:HG22	1:B:331:ILE:CD1	2.36	0.55
1:C:883:ILE:HD12	1:C:947:LEU:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:239:PRO:HG3	2:G:304:PHE:HA	1.88	0.55
2:H:584:SER:HA	2:H:587:ILE:HG23	1.89	0.55
2:H:707:PRO:HG2	2:H:730:LEU:HD13	1.89	0.55
2:I:1873:TYR:HE1	2:I:1877:ARG:HH21	1.54	0.55
2:I:603:SER:O	2:I:607:VAL:HG12	2.06	0.55
1:C:635:ILE:HG22	1:C:651:TYR:CG	2.42	0.55
2:G:777:THR:CG2	2:G:1081:HIS:CE1	2.89	0.55
2:G:1822:MET:CE	2:G:1996:ILE:HG12	2.37	0.55
2:H:1173:VAL:CG2	2:H:1221:MET:HE1	2.35	0.55
2:H:1822:MET:CE	2:H:1996:ILE:HG12	2.37	0.55
2:H:264:ARG:NH1	2:H:456:GLN:HG3	2.22	0.55
2:H:740:HIS:HA	2:H:854:ILE:HD13	1.89	0.55
2:I:1427:VAL:HG12	2:I:1427:VAL:O	2.07	0.55
2:I:741:HIS:CE1	2:I:855:HIS:CD2	2.95	0.55
1:A:56:MET:HG3	2:G:1893:VAL:CG2	2.37	0.55
1:A:982:ILE:HG13	2:G:965:SER:N	2.22	0.55
1:C:50:SER:HB2	1:C:51:PRO:HD3	1.88	0.55
2:G:127:ILE:O	2:G:131:ILE:HG13	2.07	0.55
2:G:1624:THR:HB	2:G:1642:THR:HG23	1.86	0.55
2:G:747:HIS:O	2:G:751:LEU:HB2	2.07	0.55
2:G:835:THR:HG23	2:G:843:ILE:O	2.06	0.55
2:H:1350:LEU:HD11	2:H:1410:PHE:HB3	1.89	0.55
2:H:1567:ARG:NH1	2:H:1567:ARG:CG	2.50	0.55
2:H:1697:HIS:CE1	2:H:1829:GLU:HG2	2.42	0.55
2:H:1844:ARG:CG	2:H:1844:ARG:NH1	2.58	0.55
2:H:402:LEU:O	2:H:402:LEU:HD13	2.07	0.55
2:I:1010:PRO:O	2:I:1011:MET:HB2	2.05	0.55
2:I:1168:ASN:ND2	2:I:1171:ARG:HB2	2.22	0.55
1:A:1392:LEU:HD22	1:A:1396:MET:HG3	1.89	0.55
1:B:1123:GLN:HG3	1:B:1124:GLU:N	2.22	0.55
1:B:1566:ARG:HB3	1:B:1623:TYR:CE1	2.42	0.55
1:B:49:PRO:O	1:B:82:SER:HB2	2.07	0.55
1:C:1009:LEU:HD13	1:C:1445:MET:HE1	1.89	0.55
1:C:1455:ARG:NH2	1:C:1459:ILE:HG12	2.22	0.55
2:G:1844:ARG:NH1	2:G:1844:ARG:CG	2.62	0.55
2:G:264:ARG:NH1	2:G:456:GLN:HG3	2.22	0.55
2:H:1475:LYS:HB2	2:H:1481:SER:HB2	1.88	0.55
2:H:2036:GLU:O	2:H:2039:LYS:HG2	2.07	0.55
2:I:1293:THR:HG22	2:I:1296:GLU:CD	2.28	0.55
2:I:1624:THR:HB	2:I:1642:THR:OG1	2.06	0.55
2:I:260:PRO:HD3	2:I:289:TRP:CE2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1194:ASN:HB3	1:A:1197:THR:HG22	1.88	0.54
1:B:1373:ARG:HB2	1:B:1545:SER:O	2.07	0.54
1:C:1501:LEU:O	1:C:1505:GLN:HG3	2.07	0.54
1:C:1:MET:HE3	1:C:5:VAL:HG12	1.88	0.54
2:G:1227:ARG:CG	2:G:1227:ARG:NH1	2.56	0.54
2:G:1313:SER:O	2:G:1314:ARG:HD3	2.07	0.54
2:G:598:THR:HG23	4:G:3051:FMN:O4	2.06	0.54
2:H:1159:ILE:HG12	2:H:1169:PRO:CD	2.36	0.54
2:I:1382:VAL:HA	2:I:1422:THR:HG1	1.72	0.54
2:I:1493:LEU:HD11	2:I:1499:VAL:CG2	2.37	0.54
1:A:1455:ARG:NH2	1:A:1459:ILE:HG12	2.22	0.54
1:A:236:LYS:HE2	1:A:273:PRO:O	2.07	0.54
1:A:733:ILE:CD1	1:A:761:LEU:HD11	2.37	0.54
1:A:741:SER:HB3	1:A:744:ASP:HB2	1.89	0.54
1:B:263:GLY:O	1:B:267:VAL:HG23	2.07	0.54
1:B:771:PHE:CD1	1:B:825:PRO:HG3	2.42	0.54
1:C:1373:ARG:HB2	1:C:1545:SER:O	2.07	0.54
1:C:286:PHE:O	1:C:290:MET:HG2	2.07	0.54
2:G:1859:PRO:CG	2:G:1871:LEU:HD12	2.20	0.54
2:G:464:ASP:HB3	2:G:466:SER:HB3	1.88	0.54
2:H:1293:THR:HG22	2:H:1296:GLU:CD	2.28	0.54
2:H:1976:PHE:HB3	2:H:1981:LEU:HD21	1.89	0.54
2:I:131:ILE:HD12	2:I:182:VAL:CB	2.33	0.54
2:I:1331:TRP:CE2	2:I:1335:ILE:HG13	2.42	0.54
2:I:145:LEU:HD21	2:I:156:LEU:HD21	1.89	0.54
2:I:606:PHE:HZ	2:I:805:VAL:HG11	1.71	0.54
1:A:430:ARG:NH2	1:A:605:LEU:HD13	2.23	0.54
2:G:1292:ILE:O	2:G:1368:VAL:O	2.25	0.54
2:G:332:GLU:OE2	2:G:394:ARG:HD3	2.07	0.54
2:G:462:THR:HB	2:G:482:CYS:SG	2.48	0.54
2:H:1497:GLU:OE1	2:H:2002:LYS:HE3	2.07	0.54
2:H:2015:THR:HG22	2:H:2017:LYS:N	2.21	0.54
2:H:732:TRP:CD2	2:H:750:MET:HE3	2.43	0.54
2:I:1567:ARG:CG	2:I:1567:ARG:NH1	2.50	0.54
2:I:517:HIS:CD2	2:I:517:HIS:C	2.80	0.54
1:A:733:ILE:HD12	1:A:761:LEU:HD21	1.89	0.54
1:A:20:TYR:CD1	2:G:2033:THR:HG21	2.42	0.54
2:H:1102:TYR:HB3	2:H:1244:PRO:HA	1.90	0.54
2:H:490:TRP:HE1	2:H:516:THR:CG2	2.01	0.54
2:H:611:THR:CG2	2:H:641:ILE:HG13	2.38	0.54
2:I:1093:ASP:HB3	2:I:1096:LYS:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1166:VAL:HG12	2:I:1167:SER:N	2.23	0.54
2:I:490:TRP:HA	2:I:493:THR:CG2	2.38	0.54
1:A:1657:HIS:ND1	1:A:1658:PRO:HD2	2.21	0.54
1:A:183:GLN:O	1:A:187:LEU:HG	2.08	0.54
1:B:1501:LEU:O	1:B:1505:GLN:HG3	2.08	0.54
1:B:1401:TYR:C	1:B:1658:PRO:HG3	2.27	0.54
1:C:479:ASN:O	1:C:483:VAL:HG23	2.07	0.54
2:G:1575:LEU:HD13	2:G:1579:ILE:HD12	1.89	0.54
2:G:344:LEU:HB3	2:G:349:VAL:HG23	1.90	0.54
2:H:85:ASN:HD22	2:H:135:ARG:NH1	2.02	0.54
2:I:1475:LYS:HB2	2:I:1481:SER:HB2	1.89	0.54
2:I:1547:PRO:HD3	2:I:1584:PHE:CE2	2.43	0.54
2:I:2046:GLU:C	2:I:2048:TYR:H	2.11	0.54
2:I:584:SER:HA	2:I:587:ILE:HG23	1.89	0.54
1:A:1234:MET:CE	1:A:1326:ILE:HG21	2.38	0.54
1:A:328:LEU:C	1:A:328:LEU:HD22	2.28	0.54
1:B:385:PHE:HD2	1:B:787:LYS:HA	1.73	0.54
1:B:824:LEU:HD11	1:B:849:LEU:HD12	1.89	0.54
1:C:1123:GLN:HG3	1:C:1124:GLU:N	2.23	0.54
2:G:1697:HIS:CE1	2:G:1829:GLU:HG2	2.43	0.54
2:G:2030:TYR:CE1	2:G:2034:GLY:HA2	2.43	0.54
2:G:807:ILE:HG21	2:G:1066:ILE:HA	1.88	0.54
2:H:1547:PRO:HD3	2:H:1584:PHE:CE2	2.42	0.54
2:H:464:ASP:HB3	2:H:466:SER:HB3	1.90	0.54
2:I:1778:GLN:HB3	2:I:1831:VAL:HG13	1.88	0.54
2:I:123:ILE:HD11	2:I:533:LEU:CD2	2.37	0.54
2:I:611:THR:CG2	2:I:641:ILE:HG13	2.37	0.54
2:I:652:ILE:HB	2:I:658:MET:CE	2.37	0.54
1:A:1184:LEU:HB2	1:A:1352:THR:HG21	1.89	0.54
1:B:23:ALA:O	2:H:1977:HIS:HA	2.07	0.54
2:G:1428:GLU:HB2	2:G:1468:THR:HG22	1.88	0.54
1:B:236:LYS:HE2	1:B:273:PRO:O	2.07	0.54
1:B:280:GLU:O	1:B:280:GLU:HG2	2.08	0.54
1:B:655:LEU:CD2	1:B:916:LEU:HD11	2.38	0.54
2:G:601:THR:CG2	2:G:618:GLU:O	2.41	0.54
2:H:1378:ILE:HD11	2:H:1381:VAL:HG21	1.90	0.54
2:H:964:LEU:N	2:H:964:LEU:CD2	2.70	0.54
2:I:1452:LEU:HA	2:I:1502:GLY:HA3	1.88	0.54
2:I:545:GLN:NE2	2:I:545:GLN:H	2.06	0.54
2:I:722:ALA:HB1	2:I:723:HIS:CE1	2.42	0.54
2:I:99:ASN:HA	2:I:550:VAL:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1496:GLU:O	1:A:1500:GLN:HG3	2.07	0.54
1:B:695:GLY:HA3	1:B:906:LEU:HD11	1.90	0.54
1:C:1477:ILE:H	1:C:1478:PRO:CD	2.20	0.54
1:C:37:LYS:HB2	1:C:65:TYR:HE1	1.72	0.54
2:I:826:GLY:O	2:I:827:VAL:HG23	2.07	0.54
1:A:1138:LYS:HG3	1:A:1163:TYR:CE1	2.43	0.54
1:A:340:ARG:HH12	1:A:344:GLN:NE2	2.06	0.54
1:A:644:THR:HG22	1:A:648:ASP:O	2.08	0.54
1:A:625:THR:HG23	1:A:661:ASP:OD1	2.08	0.54
1:B:1600:LEU:HD13	1:B:1657:HIS:HA	1.90	0.54
1:B:635:ILE:HG22	1:B:651:TYR:CG	2.43	0.54
1:C:1682:LYS:HB3	2:I:994:PHE:CE2	2.43	0.54
1:C:516:ARG:NH2	1:C:889:GLU:OE1	2.41	0.54
2:G:1231:GLY:O	2:G:1233:PRO:HD3	2.08	0.54
2:I:1054:LEU:CB	4:I:3051:FMN:C7M	2.85	0.54
2:I:1172:LYS:HE3	2:I:1574:ASN:OD1	2.08	0.54
2:I:332:GLU:OE2	2:I:394:ARG:HD3	2.08	0.54
2:I:868:PHE:HB3	2:I:873:PHE:CE2	2.43	0.54
1:A:1125:VAL:HG21	1:A:1175:ILE:HD12	1.88	0.53
1:B:1010:GLU:HA	1:B:1664:ALA:HA	1.89	0.53
1:C:1194:ASN:HB3	1:C:1197:THR:HG22	1.89	0.53
1:C:529:MET:HG2	1:C:638:LEU:CD1	2.39	0.53
2:H:1313:SER:O	2:H:1314:ARG:HD3	2.09	0.53
2:H:1325:PHE:CE1	2:H:1328:VAL:HG11	2.43	0.53
2:H:146:PHE:HA	2:H:149:VAL:HG12	1.89	0.53
2:I:754:TYR:CD2	2:I:794:MET:HG3	2.42	0.53
1:A:1566:ARG:HB3	1:A:1623:TYR:CE1	2.42	0.53
1:B:807:LYS:HG3	1:B:858:TRP:HB3	1.90	0.53
1:C:825:PRO:HB2	1:C:843:LYS:NZ	2.24	0.53
2:G:1331:TRP:CE2	2:G:1335:ILE:HG13	2.43	0.53
2:H:1177:SER:O	2:H:1180:MET:HG2	2.08	0.53
2:H:606:PHE:CE1	2:H:811:VAL:HG13	2.43	0.53
2:I:615:TYR:CZ	2:I:1074:MET:HB3	2.42	0.53
2:I:1844:ARG:CG	2:I:1844:ARG:NH1	2.61	0.53
2:I:1954:LYS:HD3	2:I:1958:LEU:HD13	1.89	0.53
1:A:1153:ASP:OD2	1:B:359:ARG:NH2	2.41	0.53
1:A:1123:GLN:HB2	1:A:1177:LYS:HE2	1.90	0.53
1:A:1392:LEU:CD2	1:A:1396:MET:HG3	2.38	0.53
1:B:1194:ASN:O	1:B:1197:THR:HG23	2.08	0.53
1:C:236:LYS:HE2	1:C:273:PRO:O	2.08	0.53
2:G:1269:LEU:O	2:G:1560:LEU:HD23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:281:VAL:HG23	2:H:459:VAL:HG11	1.90	0.53
2:H:674:TYR:HB3	2:H:676:ILE:HG22	1.88	0.53
2:H:826:GLY:O	2:H:827:VAL:HG23	2.07	0.53
2:I:873:PHE:CD1	2:I:1026:GLU:HB2	2.43	0.53
2:I:234:ILE:CG1	2:I:235:PRO:HD3	2.38	0.53
2:I:491:GLU:HA	2:I:494:THR:HG22	1.89	0.53
2:I:582:LYS:HE2	2:I:1108:PRO:HB3	1.91	0.53
1:A:1373:ARG:HB2	1:A:1545:SER:O	2.08	0.53
1:A:807:LYS:HG3	1:A:858:TRP:HB3	1.91	0.53
1:B:1392:LEU:CD2	1:B:1396:MET:HG3	2.38	0.53
1:B:1020:VAL:HG13	1:B:1400:ILE:HG23	1.91	0.53
1:C:263:GLY:O	1:C:267:VAL:HG23	2.08	0.53
1:C:824:LEU:HD11	1:C:849:LEU:HD12	1.90	0.53
2:G:741:HIS:CB	2:G:853:PRO:HB2	2.38	0.53
2:G:892:ILE:HG12	2:G:903:TRP:CG	2.43	0.53
2:G:964:LEU:CD2	2:G:964:LEU:N	2.68	0.53
2:H:55:THR:CG2	2:H:56:THR:HG22	2.30	0.53
2:I:1745:LYS:HE2	2:I:1747:LYS:HG2	1.91	0.53
2:I:271:THR:OG1	2:I:460:TYR:HB2	2.08	0.53
1:A:421:ILE:HG13	1:A:469:VAL:HG21	1.89	0.53
1:B:1665:ILE:CG1	1:B:1669:ARG:HD3	2.36	0.53
1:B:607:LYS:HG2	1:B:608:ASP:N	2.23	0.53
1:B:751:PHE:CZ	1:B:761:LEU:HD13	2.42	0.53
1:C:1401:TYR:C	1:C:1658:PRO:HG3	2.29	0.53
1:C:176:VAL:HG11	1:C:179:LYS:O	2.08	0.53
1:C:385:PHE:HD2	1:C:787:LYS:HA	1.73	0.53
2:G:707:PRO:HG2	2:G:730:LEU:HD13	1.90	0.53
2:H:1804:PHE:CZ	2:H:2010:TYR:HB2	2.44	0.53
2:H:173:LEU:HD13	2:H:219:LEU:HD21	1.90	0.53
2:H:816:ASP:HB3	2:H:1048:VAL:HG21	1.91	0.53
2:I:1102:TYR:HB3	2:I:1244:PRO:HA	1.91	0.53
2:I:1177:SER:O	2:I:1180:MET:HG2	2.09	0.53
2:I:1314:ARG:CG	2:I:1314:ARG:NH1	2.63	0.53
2:I:1567:ARG:HG3	2:I:1568:HIS:N	2.22	0.53
2:I:526:ARG:HH11	2:I:558:ASN:HD21	1.55	0.53
1:C:985:ARG:HH12	2:I:953:ARG:CZ	2.21	0.53
1:A:1020:VAL:HG13	1:A:1400:ILE:HG23	1.90	0.53
1:A:1665:ILE:HG12	1:A:1666:THR:N	2.23	0.53
1:A:50:SER:HB2	1:A:51:PRO:CD	2.39	0.53
1:A:635:ILE:HG22	1:A:651:TYR:CG	2.43	0.53
1:A:529:MET:CE	1:A:894:ARG:HD2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:825:PRO:HB2	1:C:843:LYS:HZ2	1.73	0.53
2:G:1382:VAL:HA	2:G:1422:THR:OG1	2.08	0.53
2:G:2015:THR:HG22	2:G:2017:LYS:N	2.22	0.53
2:G:913:ASP:H	2:G:916:THR:CG2	2.22	0.53
2:H:1567:ARG:HG3	2:H:1568:HIS:N	2.23	0.53
2:H:652:ILE:HB	2:H:658:MET:CE	2.39	0.53
2:I:1173:VAL:CG2	2:I:1221:MET:HE1	2.39	0.53
2:I:1293:THR:HG22	2:I:1296:GLU:CG	2.39	0.53
2:I:2036:GLU:HG2	2:I:2039:LYS:NZ	2.23	0.53
1:A:1492:GLU:O	1:A:1496:GLU:HG3	2.09	0.53
1:B:1123:GLN:HB2	1:B:1177:LYS:HE2	1.91	0.53
1:B:1577:GLN:HE22	1:B:1591:TRP:C	2.12	0.53
1:C:1012:LEU:HD23	1:C:1445:MET:CE	2.39	0.53
1:C:1037:TRP:HB2	1:C:1598:GLN:OE1	2.09	0.53
2:G:1166:VAL:HG12	2:G:1167:SER:N	2.23	0.53
2:G:346:GLN:HA	2:G:377:LEU:HD21	1.89	0.53
2:G:606:PHE:HZ	2:G:805:VAL:HG11	1.74	0.53
2:H:1382:VAL:HA	2:H:1422:THR:OG1	2.09	0.53
2:H:1913:VAL:O	2:H:1917:ILE:HG13	2.08	0.53
2:H:402:LEU:HD12	2:H:404:GLN:HG2	1.90	0.53
2:H:774:ALA:HB1	2:H:1081:HIS:CD2	2.32	0.53
2:I:1327:ILE:HG12	2:I:1583:MET:HE3	1.91	0.53
1:A:1014:ASP:H	1:A:1510:ASN:ND2	1.93	0.53
1:A:385:PHE:HD2	1:A:787:LYS:HA	1.74	0.53
1:B:12:ILE:HA	1:B:15:THR:HG23	1.90	0.53
1:C:1524:GLY:HA2	1:C:1527:ALA:HB3	1.91	0.53
2:G:490:TRP:CH2	2:G:512:LEU:HD21	2.43	0.53
2:G:750:MET:CG	2:G:796:PHE:HZ	2.21	0.53
2:G:85:ASN:HD22	2:G:135:ARG:NH1	2.03	0.53
2:H:1040:LEU:HD21	2:H:1048:VAL:HA	1.89	0.53
2:H:1452:LEU:HA	2:H:1502:GLY:HA3	1.90	0.53
2:H:1954:LYS:HD3	2:H:1958:LEU:HD13	1.90	0.53
2:H:346:GLN:HA	2:H:377:LEU:HD21	1.91	0.53
2:I:1040:LEU:HD21	2:I:1048:VAL:HA	1.90	0.53
2:I:1441:ILE:HD11	2:I:1445:ARG:NH2	2.23	0.53
2:I:1861:ARG:HD2	2:I:1964:PHE:O	2.08	0.53
2:I:2038:ILE:HG22	2:I:2042:ILE:CD1	2.37	0.53
2:I:892:ILE:HG12	2:I:903:TRP:CG	2.44	0.53
1:A:1455:ARG:O	1:A:1459:ILE:HG13	2.08	0.53
1:A:12:ILE:HA	1:A:15:THR:HG23	1.88	0.53
1:C:1036:ARG:NH1	1:C:1040:GLU:OE1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1040:LEU:HD21	2:G:1048:VAL:HA	1.90	0.53
2:G:2038:ILE:HG22	2:G:2042:ILE:CD1	2.37	0.53
2:G:281:VAL:HG23	2:G:459:VAL:HG11	1.91	0.53
2:H:1745:LYS:HE2	2:H:1747:LYS:HG2	1.91	0.53
2:I:1266:TYR:CG	2:I:1347:LEU:HD23	2.43	0.53
2:I:2035:SER:HB3	2:I:2038:ILE:CG1	2.37	0.53
2:I:240:LEU:O	2:I:244:ILE:HG13	2.08	0.53
2:I:871:THR:HG21	2:I:887:LYS:NZ	2.24	0.53
1:B:1326:ILE:HG12	1:B:1388:MET:HG3	1.91	0.53
1:C:1285:ALA:O	1:C:1289:MET:HG3	2.09	0.53
1:C:625:THR:HG23	1:C:661:ASP:OD1	2.09	0.53
2:G:1173:VAL:CG2	2:G:1221:MET:HE1	2.38	0.53
2:G:102:HIS:HE1	2:G:180:TYR:OH	1.92	0.53
2:G:1861:ARG:HD2	2:G:1964:PHE:O	2.09	0.53
2:H:1101:GLU:HB2	2:H:1147:ILE:O	2.09	0.53
2:H:1697:HIS:HE1	2:H:1829:GLU:HG2	1.74	0.53
2:H:234:ILE:CG1	2:H:235:PRO:HD3	2.39	0.53
2:H:455:ILE:HG12	2:H:469:ARG:HG2	1.91	0.53
2:I:264:ARG:NH1	2:I:456:GLN:HG3	2.24	0.53
1:A:529:MET:HG2	1:A:638:LEU:HG	1.89	0.52
1:B:340:ARG:HH12	1:B:344:GLN:NE2	2.08	0.52
1:C:864:VAL:CG2	1:C:921:PRO:HB3	2.39	0.52
2:G:55:THR:CG2	2:G:56:THR:HG22	2.33	0.52
2:I:1040:LEU:O	2:I:1046:GLN:HG3	2.09	0.52
2:I:606:PHE:CE1	2:I:811:VAL:HG13	2.44	0.52
1:A:156:ALA:HA	1:A:166:ILE:CD1	2.39	0.52
1:A:341:GLN:O	1:A:345:VAL:HG12	2.09	0.52
1:A:986:ALA:CA	1:A:1047:LEU:HD13	2.39	0.52
1:B:12:ILE:HD11	2:H:2041:ILE:HD11	1.89	0.52
1:B:1234:MET:CE	1:B:1326:ILE:HG21	2.40	0.52
2:H:1159:ILE:CG1	2:H:1169:PRO:CD	2.87	0.52
2:H:1427:VAL:O	2:H:1427:VAL:HG12	2.08	0.52
2:H:145:LEU:O	2:H:149:VAL:HG12	2.10	0.52
2:H:1697:HIS:HE1	2:H:1829:GLU:CG	2.22	0.52
2:H:2026:PHE:CD2	2:H:2045:TRP:HZ3	2.27	0.52
2:I:2036:GLU:O	2:I:2039:LYS:HG2	2.09	0.52
2:I:465:GLY:HA2	2:I:493:THR:HA	1.91	0.52
2:I:598:THR:O	2:I:602:VAL:HB	2.09	0.52
1:B:784:ILE:HG23	1:B:788:SER:HB2	1.92	0.52
1:C:1056:ILE:HD13	1:C:1193:TRP:CD1	2.41	0.52
1:C:1305:CYS:SG	1:C:1583:HIS:NE2	2.82	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:615:TYR:CZ	2:G:1074:MET:HB3	2.44	0.52
2:H:194:THR:CG2	2:H:300:ILE:HD11	2.39	0.52
2:H:768:GLY:HA3	2:H:800:LEU:CD2	2.39	0.52
1:B:980:VAL:HG21	2:H:952:ARG:NH2	2.24	0.52
2:I:418:ASN:HD22	2:I:418:ASN:N	2.07	0.52
1:A:335:HIS:HD2	1:A:335:HIS:O	1.92	0.52
1:A:824:LEU:HD11	1:A:849:LEU:HD12	1.89	0.52
1:B:329:GLU:O	1:B:333:LYS:HG3	2.08	0.52
1:C:1411:THR:HG22	1:C:1412:ASP:N	2.24	0.52
1:C:260:ARG:HH12	1:C:300:VAL:CG2	2.22	0.52
1:C:530:ALA:HA	1:C:636:PRO:HB3	1.91	0.52
2:G:1159:ILE:HG12	2:G:1169:PRO:CD	2.39	0.52
2:G:1359:MET:CE	2:G:1404:MET:HB3	2.39	0.52
2:G:1438:SER:O	2:G:1441:ILE:HG23	2.09	0.52
2:G:490:TRP:HA	2:G:493:THR:CG2	2.40	0.52
2:H:955:GLU:HG2	2:H:987:TYR:CE2	2.45	0.52
2:I:1486:PHE:HA	2:I:1504:VAL:O	2.10	0.52
1:A:988:ILE:HD13	1:A:1048:GLU:CA	2.39	0.52
1:C:406:TRP:CE3	1:C:1619:GLU:HG3	2.44	0.52
1:C:465:ASN:O	1:C:469:VAL:HG23	2.10	0.52
2:G:1389:ILE:HG13	2:G:1411:PHE:HD1	1.75	0.52
2:G:145:LEU:HD21	2:G:156:LEU:HD21	1.91	0.52
2:G:871:THR:HG21	2:G:887:LYS:NZ	2.25	0.52
2:H:1722:GLY:N	2:H:1726:GLY:HA3	2.24	0.52
2:H:754:TYR:CD2	2:H:794:MET:HG3	2.44	0.52
2:I:1350:LEU:HD11	2:I:1410:PHE:HB3	1.91	0.52
2:I:1438:SER:O	2:I:1441:ILE:HG23	2.08	0.52
2:I:1475:LYS:HG3	2:I:1481:SER:HB2	1.92	0.52
2:I:1300:PHE:CA	2:I:1556:VAL:HG11	2.40	0.52
2:I:1774:THR:HA	2:I:1777:THR:HB	1.92	0.52
2:I:741:HIS:HE1	2:I:855:HIS:NE2	2.06	0.52
1:A:1477:ILE:H	1:A:1478:PRO:CD	2.21	0.52
1:A:998:TYR:CE2	1:A:1667:GLU:HB2	2.44	0.52
1:A:501:THR:N	1:A:886:GLU:OE1	2.30	0.52
1:B:341:GLN:O	1:B:345:VAL:HG12	2.10	0.52
2:G:1475:LYS:CB	2:G:1481:SER:HB2	2.39	0.52
2:G:1567:ARG:HG2	2:G:1567:ARG:HH11	1.72	0.52
2:G:1593:ILE:HD13	2:G:1626:ILE:HD13	1.92	0.52
2:G:1932:SER:O	2:G:1936:VAL:HG22	2.10	0.52
2:H:1359:MET:HE3	2:H:1404:MET:HB3	1.92	0.52
2:I:702:TYR:HB2	2:I:727:PRO:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:964:LEU:CD2	2:I:964:LEU:N	2.72	0.52
1:A:1305:CYS:SG	1:A:1583:HIS:NE2	2.83	0.52
1:A:430:ARG:NH1	1:A:493:VAL:O	2.40	0.52
1:A:59:ARG:HH11	2:G:1896:GLN:NE2	2.07	0.52
2:G:2026:PHE:CD2	2:G:2045:TRP:HZ3	2.27	0.52
1:A:2:LYS:CD	2:G:2050:GLN:HB3	2.38	0.52
2:G:955:GLU:HG2	2:G:987:TYR:CE2	2.45	0.52
2:H:615:TYR:CZ	2:H:1074:MET:HB3	2.43	0.52
2:H:1292:ILE:O	2:H:1368:VAL:O	2.27	0.52
2:H:1776:PHE:O	2:H:1779:PRO:HD2	2.09	0.52
2:H:747:HIS:O	2:H:751:LEU:HB2	2.10	0.52
2:I:1004:LEU:HD21	2:I:1020:VAL:HG23	1.91	0.52
2:I:1159:ILE:HG12	2:I:1169:PRO:CD	2.39	0.52
2:I:913:ASP:H	2:I:916:THR:CG2	2.23	0.52
1:B:529:MET:HG2	1:B:638:LEU:HG	1.92	0.52
1:B:893:VAL:HG11	1:B:930:LEU:CD2	2.36	0.52
1:C:27:ARG:HB2	2:I:2016:ALA:HB2	1.91	0.52
1:C:607:LYS:HG2	1:C:608:ASP:N	2.24	0.52
2:G:1177:SER:O	2:G:1180:MET:HG2	2.09	0.52
2:G:926:LEU:HB3	2:G:947:THR:HG22	1.92	0.52
2:H:599:PRO:HD2	4:H:3051:FMN:H6	1.92	0.52
2:H:418:ASN:HD22	2:H:418:ASN:N	2.08	0.52
2:I:1597:ALA:HB1	2:I:1638:ILE:CD1	2.39	0.52
2:I:1918:LYS:HG2	2:I:1919:LEU:HD23	1.92	0.52
2:I:751:LEU:HD23	2:I:791:TYR:CZ	2.44	0.52
1:A:521:LYS:HE2	1:A:605:LEU:HD11	1.92	0.52
1:A:705:VAL:CG2	1:A:732:LEU:HD21	2.39	0.52
1:C:1577:GLN:HE22	1:C:1591:TRP:C	2.13	0.52
1:C:340:ARG:HH12	1:C:344:GLN:NE2	2.08	0.52
1:C:705:VAL:CG2	1:C:732:LEU:HD21	2.40	0.52
2:G:1093:ASP:HB3	2:G:1096:LYS:HG3	1.90	0.52
2:G:121:GLU:HA	2:G:124:LYS:HD2	1.91	0.52
2:G:1745:LYS:HD3	2:G:1747:LYS:HE2	1.91	0.52
2:G:176:LEU:HD22	2:G:247:ALA:HB1	1.90	0.52
2:G:1873:TYR:CE1	2:G:1877:ARG:NE	2.75	0.52
2:G:768:GLY:HA3	2:G:800:LEU:CD2	2.38	0.52
2:H:278:VAL:HG11	2:H:303:LEU:HD13	1.92	0.52
2:I:1223:MET:CE	2:I:1238:LEU:HD12	2.40	0.52
2:I:273:HIS:CB	2:I:512:LEU:HD22	2.40	0.52
2:I:747:HIS:O	2:I:751:LEU:HB2	2.10	0.52
1:A:1183:ARG:NH1	1:A:1344:GLY:HA2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1577:GLN:HE22	1:A:1591:TRP:C	2.13	0.52
1:A:280:GLU:O	1:A:280:GLU:HG2	2.10	0.52
1:A:607:LYS:HG2	1:A:608:ASP:N	2.25	0.52
1:A:674:LYS:O	1:A:675:ASP:HB2	2.09	0.52
1:C:156:ALA:HA	1:C:166:ILE:CD1	2.40	0.52
2:G:278:VAL:HG11	2:G:303:LEU:HD13	1.92	0.52
2:H:281:VAL:HG12	2:H:282:ALA:N	2.24	0.52
2:H:522:GLY:HA3	2:H:561:TRP:CH2	2.45	0.52
2:H:577:ILE:HD13	2:H:1097:ILE:CD1	2.40	0.52
2:H:892:ILE:HG12	2:H:903:TRP:CG	2.45	0.52
2:I:1871:LEU:HD22	2:I:1888:ILE:HD11	1.92	0.52
2:I:2026:PHE:CD2	2:I:2045:TRP:HZ3	2.27	0.52
1:A:881:ASN:HA	1:A:944:ARG:NH2	2.25	0.51
1:B:1056:ILE:CD1	1:B:1193:TRP:HD1	2.22	0.51
1:B:1238:VAL:HG12	1:B:1239:HIS:N	2.25	0.51
1:C:1431:GLU:HB3	1:C:1520:ALA:HB2	1.92	0.51
1:C:1665:ILE:CG1	1:C:1669:ARG:HD3	2.36	0.51
2:G:1774:THR:HA	2:G:1777:THR:HB	1.90	0.51
2:G:234:ILE:CG1	2:G:235:PRO:HD3	2.40	0.51
2:H:1673:GLU:N	2:H:1676:MET:HE3	2.25	0.51
2:H:654:VAL:HG23	2:H:683:ALA:HB1	1.92	0.51
1:B:985:ARG:HH12	2:H:953:ARG:NH2	2.07	0.51
2:I:1745:LYS:HD3	2:I:1747:LYS:HE2	1.93	0.51
1:A:1123:GLN:HG3	1:A:1124:GLU:N	2.24	0.51
1:A:1411:THR:HG22	1:A:1412:ASP:N	2.25	0.51
1:B:1104:ARG:O	1:B:1185:VAL:HG13	2.11	0.51
1:B:1665:ILE:HG12	1:B:1666:THR:N	2.25	0.51
1:C:1238:VAL:HG12	1:C:1239:HIS:N	2.25	0.51
1:C:1303:GLY:N	1:C:1307:THR:HG22	2.26	0.51
1:C:156:ALA:HA	1:C:166:ILE:HD12	1.92	0.51
2:G:376:ASN:C	2:G:376:ASN:HD22	2.13	0.51
2:H:131:ILE:CD1	2:H:182:VAL:CG1	2.88	0.51
2:I:1697:HIS:CE1	2:I:1829:GLU:HG2	2.45	0.51
2:I:1868:GLN:HG3	2:I:1898:TYR:CZ	2.45	0.51
2:I:715:GLN:O	2:I:719:ILE:HG12	2.10	0.51
1:A:1303:GLY:N	1:A:1307:THR:HG22	2.25	0.51
1:A:1411:THR:HG22	1:A:1412:ASP:H	1.76	0.51
1:A:1474:ALA:HA	1:A:1478:PRO:CD	2.41	0.51
1:C:46:GLU:OE1	1:C:53:LEU:HB2	2.11	0.51
1:C:674:LYS:O	1:C:675:ASP:HB2	2.11	0.51
2:G:1293:THR:HG22	2:G:1296:GLU:CG	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1328:VAL:HG23	2:G:1557:SER:HA	1.92	0.51
2:G:1493:LEU:HD11	2:G:1499:VAL:CG2	2.40	0.51
2:G:124:LYS:HG2	2:G:179:THR:HA	1.90	0.51
2:G:213:LEU:HG	2:G:213:LEU:O	2.10	0.51
2:G:489:LYS:O	2:G:493:THR:HG22	2.10	0.51
2:G:702:TYR:HB2	2:G:727:PRO:HB2	1.93	0.51
2:H:1293:THR:HG22	2:H:1296:GLU:CG	2.41	0.51
2:H:1475:LYS:CB	2:H:1481:SER:HB2	2.40	0.51
2:H:545:GLN:NE2	2:H:545:GLN:H	2.07	0.51
2:H:758:ARG:NH2	2:H:797:ASP:OD1	2.35	0.51
1:B:985:ARG:NH1	2:H:953:ARG:CZ	2.73	0.51
2:H:318:SER:HB3	2:I:1595:ASN:HD21	1.76	0.51
1:B:1411:THR:HG22	1:B:1412:ASP:N	2.26	0.51
1:B:335:HIS:HD2	1:B:335:HIS:O	1.93	0.51
1:C:983:GLN:NE2	2:I:962:LYS:HD2	2.25	0.51
2:G:1081:HIS:O	2:G:1085:LEU:HB2	2.10	0.51
1:A:12:ILE:CD1	2:G:2041:ILE:CD1	2.83	0.51
2:G:654:VAL:HG12	2:G:654:VAL:O	2.09	0.51
2:H:1081:HIS:O	2:H:1085:LEU:HB2	2.10	0.51
2:H:582:LYS:HE2	2:H:1108:PRO:HB3	1.92	0.51
2:H:1475:LYS:HG3	2:H:1481:SER:HB2	1.93	0.51
2:H:1491:VAL:HB	2:H:1501:ILE:HD12	1.92	0.51
2:I:1475:LYS:CB	2:I:1481:SER:HB2	2.41	0.51
2:I:652:ILE:HD12	2:I:652:ILE:N	2.25	0.51
2:I:732:TRP:CD2	2:I:750:MET:HE3	2.45	0.51
2:I:732:TRP:CD2	2:I:750:MET:HE1	2.43	0.51
2:G:816:ASP:HB3	2:G:1048:VAL:CG2	2.41	0.51
2:H:1561:ASN:OD1	2:H:1563:ILE:HB	2.10	0.51
2:I:460:TYR:HA	2:I:466:SER:O	2.11	0.51
1:A:157:HIS:HE1	1:A:228:LEU:HD22	1.76	0.51
1:B:1194:ASN:HB3	1:B:1197:THR:HG22	1.91	0.51
1:B:1477:ILE:H	1:B:1478:PRO:CD	2.24	0.51
1:B:338:LEU:O	1:B:342:GLN:HG3	2.10	0.51
1:B:415:SER:O	1:B:419:GLU:HB2	2.10	0.51
1:C:328:LEU:HD22	1:C:328:LEU:C	2.30	0.51
1:C:644:THR:HG22	1:C:648:ASP:O	2.10	0.51
2:G:1427:VAL:HG12	2:G:1427:VAL:O	2.09	0.51
2:G:145:LEU:O	2:G:149:VAL:HG12	2.10	0.51
2:H:1493:LEU:HD11	2:H:1499:VAL:HG21	1.93	0.51
2:H:432:LEU:HB3	2:H:484:ILE:HG23	1.92	0.51
2:H:55:THR:HB	2:H:59:GLU:OE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1015:VAL:HG11	2:I:1017:PHE:CE1	2.45	0.51
1:A:1310:GLU:OE1	1:A:1649:LYS:CE	2.56	0.51
2:G:1431:TYR:CE1	2:G:1526:THR:HG23	2.45	0.51
2:G:1589:VAL:HG11	2:G:1640:PHE:CE1	2.45	0.51
2:G:1579:ILE:HD11	2:G:1615:MET:SD	2.51	0.51
2:G:1764:PHE:HB2	2:G:1770:LEU:HD21	1.93	0.51
2:H:1716:ASN:OD1	2:H:1765:ARG:HA	2.11	0.51
2:H:260:PRO:HD3	2:H:289:TRP:CZ2	2.46	0.51
2:H:1054:LEU:HB3	4:H:3051:FMN:HM82	1.93	0.51
2:H:732:TRP:CD1	2:H:750:MET:HE3	2.46	0.51
2:I:1428:GLU:HB2	2:I:1468:THR:HG22	1.93	0.51
2:I:1566:SER:HB3	2:I:1568:HIS:CE1	2.45	0.51
2:I:306:ILE:HA	2:I:439:ILE:CD1	2.40	0.51
1:A:254:TRP:HZ3	1:A:292:GLN:HG3	1.75	0.51
1:A:465:ASN:O	1:A:469:VAL:HG23	2.11	0.51
1:B:864:VAL:CG2	1:B:921:PRO:HB3	2.40	0.51
1:C:1123:GLN:HB2	1:C:1177:LYS:HE2	1.93	0.51
1:C:1411:THR:HG22	1:C:1412:ASP:H	1.75	0.51
1:C:1009:LEU:HG	1:C:1664:ALA:HB2	1.93	0.51
1:C:513:GLU:OE2	1:C:873:ARG:NH1	2.44	0.51
2:G:1986:LYS:HA	2:G:1989:LYS:HB3	1.92	0.51
2:H:1236:LEU:HD11	2:H:1262:ILE:HG12	1.92	0.51
2:H:533:LEU:HD13	2:H:545:GLN:HG3	1.92	0.51
2:H:667:LYS:HD2	2:H:697:THR:CG2	2.35	0.51
2:I:157:VAL:HG11	2:I:496:PHE:CZ	2.46	0.51
2:I:346:GLN:HA	2:I:377:LEU:HD21	1.92	0.51
2:I:950:PHE:O	2:I:954:VAL:HG23	2.11	0.51
1:B:1705:PRO:HB2	1:B:1733:PHE:CE1	2.46	0.51
1:C:733:ILE:CD1	1:C:761:LEU:HD11	2.40	0.51
2:G:1382:VAL:HA	2:G:1422:THR:HG1	1.76	0.51
2:G:16:LEU:HG	2:G:48:PHE:CZ	2.45	0.51
2:G:443:LEU:HD22	2:G:448:VAL:CG1	2.41	0.51
2:G:786:SER:CB	2:G:794:MET:HE2	2.41	0.51
2:H:807:ILE:HG21	2:H:1066:ILE:HA	1.92	0.51
2:H:2046:GLU:C	2:H:2048:TYR:H	2.14	0.51
2:H:332:GLU:OE2	2:H:394:ARG:HD3	2.10	0.51
2:H:461:ASP:HB3	2:H:464:ASP:HB2	1.93	0.51
2:I:1313:SER:O	2:I:1314:ARG:HD3	2.11	0.51
2:I:1359:MET:HA	2:I:1359:MET:HE3	1.92	0.51
2:I:807:ILE:HG21	2:I:1066:ILE:HA	1.93	0.51
1:A:400:ARG:HH11	1:A:400:ARG:HG3	1.67	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:889:GLU:HG3	1:A:893:VAL:O	2.11	0.51
1:B:1455:ARG:NH2	1:B:1459:ILE:HG12	2.26	0.51
1:B:822:VAL:HG12	1:B:824:LEU:HD22	1.93	0.51
1:C:157:HIS:HE1	1:C:228:LEU:HD22	1.75	0.51
1:C:411:GLN:HE22	1:C:1628:SER:H	1.58	0.51
2:G:1135:GLU:OE2	2:G:1175:LYS:HE3	2.11	0.51
2:G:1452:LEU:HA	2:G:1502:GLY:HA3	1.92	0.51
2:G:418:ASN:N	2:G:418:ASN:HD22	2.09	0.51
2:G:751:LEU:HD23	2:G:791:TYR:CZ	2.46	0.51
2:G:868:PHE:HB3	2:G:873:PHE:CE2	2.46	0.51
2:H:1678:MET:CE	2:H:1707:LEU:HD22	2.40	0.51
2:H:2026:PHE:HD2	2:H:2045:TRP:HZ3	1.59	0.51
2:H:233:SER:HA	2:H:424:ALA:CB	2.41	0.51
2:H:460:TYR:HA	2:H:466:SER:O	2.11	0.51
2:H:741:HIS:HB2	2:H:853:PRO:O	2.11	0.51
2:I:1431:TYR:CE1	2:I:1526:THR:HG23	2.46	0.51
1:A:1105:LEU:HD23	1:A:1185:VAL:HG22	1.93	0.50
1:A:635:ILE:HG22	1:A:651:TYR:CD1	2.46	0.50
1:A:985:ARG:NH1	2:G:953:ARG:CZ	2.74	0.50
1:B:1524:GLY:HA2	1:B:1527:ALA:HB3	1.93	0.50
1:B:386:PHE:O	1:B:390:VAL:HB	2.11	0.50
1:B:50:SER:HB2	1:B:51:PRO:CD	2.40	0.50
2:G:1223:MET:CE	2:G:1238:LEU:HD12	2.40	0.50
2:G:1697:HIS:HE1	2:G:1829:GLU:HG2	1.74	0.50
2:G:194:THR:CG2	2:G:300:ILE:HD11	2.41	0.50
2:G:601:THR:HG22	2:G:620:ALA:H	1.75	0.50
2:H:1265:MET:HE1	2:H:1562:PRO:HG2	1.92	0.50
2:H:1422:THR:HG21	2:H:1474:PHE:HB2	1.94	0.50
2:H:408:PRO:HG3	2:H:836:TYR:CD2	2.46	0.50
2:I:1493:LEU:HD11	2:I:1499:VAL:HG21	1.93	0.50
2:I:1776:PHE:O	2:I:1779:PRO:HD2	2.10	0.50
1:A:1533:ILE:HD11	1:A:1564:LEU:HD13	1.93	0.50
1:A:433:VAL:O	1:A:437:ILE:HG13	2.12	0.50
1:B:1158:PRO:HD2	1:B:1159:GLU:OE2	2.10	0.50
1:B:1196:LYS:HE3	1:B:1202:ASP:CG	2.31	0.50
1:B:1411:THR:HG22	1:B:1412:ASP:H	1.75	0.50
1:B:635:ILE:HG22	1:B:651:TYR:CD1	2.46	0.50
1:C:34:VAL:O	1:C:38:ASP:HB2	2.11	0.50
1:C:828:PRO:HG3	1:C:868:ILE:HG22	1.94	0.50
1:C:655:LEU:CD2	1:C:916:LEU:HD11	2.41	0.50
2:G:281:VAL:HG12	2:G:282:ALA:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:7:ARG:CZ	2:G:24:THR:HA	2.41	0.50
2:H:1597:ALA:HB1	2:H:1638:ILE:CD1	2.41	0.50
2:H:1861:ARG:HD2	2:H:1964:PHE:O	2.12	0.50
2:I:281:VAL:HG12	2:I:282:ALA:N	2.25	0.50
2:I:611:THR:HA	2:I:615:TYR:O	2.11	0.50
2:I:750:MET:CG	2:I:796:PHE:HZ	2.24	0.50
2:I:85:ASN:HD22	2:I:135:ARG:NH1	2.04	0.50
1:A:20:TYR:CE1	2:G:2033:THR:HG21	2.47	0.50
1:A:24:SER:O	2:G:1977:HIS:CD2	2.65	0.50
1:A:34:VAL:O	1:A:38:ASP:HB2	2.10	0.50
1:A:59:ARG:HH11	2:G:1896:GLN:HE22	1.58	0.50
1:C:176:VAL:CG1	1:C:179:LYS:O	2.59	0.50
2:G:1272:ASP:O	2:G:1273:GLU:HG3	2.11	0.50
2:G:1918:LYS:HG2	2:G:1919:LEU:HD23	1.93	0.50
2:G:652:ILE:CD1	2:G:658:MET:HE3	2.42	0.50
2:H:1774:THR:HA	2:H:1777:THR:HB	1.93	0.50
2:H:1775:GLN:HG2	2:H:1836:MET:SD	2.51	0.50
2:H:344:LEU:HB3	2:H:349:VAL:HG23	1.94	0.50
2:H:491:GLU:HA	2:H:494:THR:HG22	1.93	0.50
2:I:1027:ILE:O	2:I:1031:LYS:HB2	2.11	0.50
2:I:1945:ASP:O	2:I:1949:LYS:HG3	2.10	0.50
2:I:173:LEU:HD13	2:I:219:LEU:HD21	1.94	0.50
2:I:376:ASN:C	2:I:376:ASN:HD22	2.14	0.50
1:A:286:PHE:O	1:A:290:MET:HG2	2.10	0.50
1:B:1303:GLY:N	1:B:1307:THR:HG22	2.25	0.50
1:B:421:ILE:HG12	1:B:469:VAL:HG21	1.93	0.50
1:C:1116:PRO:HB2	1:C:1184:LEU:HD12	1.93	0.50
1:C:280:GLU:O	1:C:280:GLU:HG2	2.11	0.50
1:C:415:SER:O	1:C:419:GLU:HB2	2.12	0.50
1:C:702:LYS:HE2	1:C:729:GLY:O	2.11	0.50
2:G:545:GLN:NE2	2:G:545:GLN:H	2.09	0.50
2:H:1148:ASN:ND2	2:H:1151:HIS:H	2.08	0.50
2:H:1102:TYR:CE2	2:H:1152:ALA:HB2	2.47	0.50
2:H:1389:ILE:HG13	2:H:1411:PHE:HD1	1.76	0.50
2:H:1435:ILE:HG22	2:H:1435:ILE:O	2.10	0.50
2:H:463:PHE:CE1	2:H:486:LEU:HD22	2.47	0.50
2:I:1491:VAL:HB	2:I:1501:ILE:HD12	1.93	0.50
1:A:1004:ILE:HG22	1:A:1660:TYR:CE2	2.46	0.50
1:B:156:ALA:HA	1:B:166:ILE:CD1	2.41	0.50
1:B:156:ALA:HA	1:B:166:ILE:HD12	1.93	0.50
2:G:1871:LEU:HD22	2:G:1888:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:611:THR:HA	2:G:615:TYR:O	2.11	0.50
2:G:663:ILE:HB	2:G:664:PRO:CD	2.40	0.50
2:G:676:ILE:HG12	2:G:676:ILE:O	2.11	0.50
2:G:732:TRP:CG	2:G:750:MET:HE3	2.46	0.50
2:G:784:GLU:O	2:G:787:THR:HB	2.11	0.50
2:H:1382:VAL:HA	2:H:1422:THR:HG1	1.76	0.50
2:H:1428:GLU:HB2	2:H:1468:THR:HG22	1.94	0.50
2:I:1135:GLU:OE2	2:I:1175:LYS:HE3	2.12	0.50
2:I:1716:ASN:OD1	2:I:1765:ARG:HA	2.11	0.50
2:I:2035:SER:HB3	2:I:2038:ILE:CD1	2.40	0.50
2:I:955:GLU:HG2	2:I:987:TYR:CE2	2.46	0.50
1:A:1523:ARG:NH2	1:A:1564:LEU:O	2.45	0.50
1:B:1009:LEU:HA	1:B:1445:MET:HE2	1.93	0.50
1:C:1019:ILE:HG21	1:C:1316:VAL:HG22	1.94	0.50
1:C:1474:ALA:HA	1:C:1478:PRO:CD	2.42	0.50
1:C:985:ARG:HH12	2:I:953:ARG:NH2	2.09	0.50
2:G:1350:LEU:HD11	2:G:1410:PHE:HB3	1.94	0.50
2:G:774:ALA:HB1	2:G:1081:HIS:CD2	2.37	0.50
2:H:826:GLY:HA2	2:H:1060:ALA:HB3	1.94	0.50
2:H:2036:GLU:HG2	2:H:2039:LYS:NZ	2.27	0.50
2:I:1953:VAL:HG12	2:I:1953:VAL:O	2.11	0.50
2:I:712:ALA:O	2:I:715:GLN:HB3	2.12	0.50
2:I:866:LYS:O	2:I:870:GLU:HG3	2.12	0.50
1:A:1104:ARG:O	1:A:1185:VAL:HG13	2.12	0.50
1:A:12:ILE:CD1	2:G:2041:ILE:HD11	2.41	0.50
1:A:359:ARG:NH2	1:C:1153:ASP:OD2	2.43	0.50
1:B:1347:LYS:O	1:B:1347:LYS:HD3	2.11	0.50
1:B:825:PRO:HB2	1:B:843:LYS:NZ	2.27	0.50
2:G:440:ASN:ND2	2:G:477:GLU:HG2	2.26	0.50
2:G:894:ARG:NH1	2:G:898:ASP:OD2	2.43	0.50
2:G:949:ASP:CB	2:G:1006:MET:HE2	2.38	0.50
2:H:121:GLU:HA	2:H:124:LYS:HD2	1.93	0.50
1:B:20:TYR:OH	2:H:2035:SER:HB2	2.12	0.50
2:H:161:GLY:HA3	2:H:506:PRO:HD2	1.93	0.50
2:H:638:VAL:HG22	2:H:675:PRO:HG2	1.93	0.50
2:I:1986:LYS:HA	2:I:1989:LYS:HB3	1.93	0.50
1:C:13:LEU:HB2	2:I:2026:PHE:CE1	2.45	0.50
1:B:408:TRP:CZ3	1:B:1628:SER:HB3	2.47	0.50
1:C:157:HIS:CE1	1:C:228:LEU:HD22	2.47	0.50
1:C:328:LEU:HD13	1:C:329:GLU:N	2.27	0.50
1:C:702:LYS:HD3	1:C:731:THR:CG2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1776:PHE:O	2:G:1779:PRO:HD2	2.12	0.50
2:G:2035:SER:HB3	2:G:2038:ILE:CD1	2.42	0.50
2:G:24:THR:O	2:G:26:SER:N	2.44	0.50
2:G:306:ILE:HA	2:G:439:ILE:CD1	2.42	0.50
2:G:606:PHE:CE1	2:G:811:VAL:HG13	2.46	0.50
2:G:60:LEU:O	2:G:63:LYS:HB2	2.12	0.50
2:G:682:GLY:O	2:G:683:ALA:HB3	2.12	0.50
2:H:2035:SER:HB3	2:H:2038:ILE:CD1	2.42	0.50
2:H:747:HIS:HE1	2:H:780:TYR:OH	1.95	0.50
2:I:344:LEU:HB3	2:I:349:VAL:HG23	1.93	0.50
1:A:1125:VAL:HG21	1:A:1175:ILE:CD1	2.42	0.50
1:A:1116:PRO:HB2	1:A:1184:LEU:HD12	1.94	0.50
1:A:1347:LYS:HD3	1:A:1347:LYS:O	2.11	0.50
1:A:1459:ILE:O	1:A:1463:VAL:HG23	2.12	0.50
1:A:156:ALA:HA	1:A:166:ILE:HD12	1.93	0.50
1:B:46:GLU:OE1	1:B:53:LEU:HB2	2.12	0.50
1:C:1566:ARG:HB3	1:C:1623:TYR:CE1	2.46	0.50
1:C:1705:PRO:HB2	1:C:1733:PHE:CE1	2.46	0.50
2:G:1552:PRO:O	2:G:1556:VAL:HG23	2.12	0.50
2:G:1716:ASN:OD1	2:G:1765:ARG:HA	2.12	0.50
2:G:1697:HIS:HE1	2:G:1829:GLU:CG	2.25	0.50
2:G:1845:ASP:HB2	2:G:1849:ARG:N	2.15	0.50
2:G:428:HIS:CD2	2:G:488:VAL:HG23	2.47	0.50
2:H:1004:LEU:HD21	2:H:1020:VAL:CG2	2.41	0.50
2:H:2030:TYR:CE1	2:H:2034:GLY:HA2	2.46	0.50
2:H:441:LYS:O	2:H:444:VAL:HG12	2.12	0.50
2:H:7:ARG:CZ	2:H:24:THR:HA	2.42	0.50
2:I:777:THR:HG23	2:I:1081:HIS:CE1	2.47	0.50
2:I:1673:GLU:N	2:I:1676:MET:HE3	2.25	0.50
2:I:455:ILE:HG12	2:I:469:ARG:HG2	1.93	0.50
1:A:142:ASP:CG	1:A:257:PRO:HB2	2.32	0.49
1:B:1451:GLN:OE1	1:B:1451:GLN:HA	2.12	0.49
1:B:1533:ILE:HG13	1:B:1564:LEU:HB3	1.94	0.49
1:B:413:LEU:HB2	1:B:439:ILE:HD13	1.94	0.49
1:C:1665:ILE:HG12	1:C:1666:THR:N	2.27	0.49
1:C:267:VAL:O	1:C:290:MET:HE1	2.12	0.49
2:G:131:ILE:CB	2:G:182:VAL:CG1	2.85	0.49
2:G:1441:ILE:HD11	2:G:1445:ARG:NH2	2.25	0.49
2:G:1868:GLN:HG3	2:G:1898:TYR:CZ	2.48	0.49
2:G:2029:VAL:O	2:G:2033:THR:HG22	2.12	0.49
2:H:1227:ARG:HG3	2:H:1227:ARG:NH1	2.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:777:THR:HG23	2:H:1081:HIS:CE1	2.47	0.49
2:I:1632:ILE:HG23	2:I:1632:ILE:O	2.12	0.49
2:I:72:VAL:HG12	2:I:73:GLU:N	2.27	0.49
2:I:7:ARG:HE	2:I:27:PHE:CB	2.24	0.49
1:A:335:HIS:O	1:A:338:LEU:HB3	2.12	0.49
1:B:1125:VAL:HG21	1:B:1175:ILE:CD1	2.42	0.49
1:B:1474:ALA:HA	1:B:1478:PRO:CD	2.41	0.49
1:B:674:LYS:O	1:B:675:ASP:HB2	2.11	0.49
2:G:871:THR:HG21	2:G:887:LYS:HZ2	1.77	0.49
2:H:1148:ASN:HD22	2:H:1151:HIS:H	1.60	0.49
2:H:1162:ASP:O	2:H:1163:LYS:HB2	2.11	0.49
2:H:1745:LYS:HD3	2:H:1747:LYS:HE2	1.94	0.49
2:H:7:ARG:HE	2:H:27:PHE:CB	2.26	0.49
2:H:871:THR:HG21	2:H:887:LYS:NZ	2.26	0.49
2:I:24:THR:O	2:I:26:SER:N	2.45	0.49
2:I:259:THR:HG22	2:I:262:GLU:CB	2.41	0.49
2:H:28:PHE:CE1	2:I:27:PHE:CE2	3.00	0.49
2:I:274:SER:OG	2:I:428:HIS:HE1	1.95	0.49
2:I:60:LEU:O	2:I:63:LYS:HB2	2.11	0.49
1:A:1276:GLN:O	1:A:1282:THR:HG21	2.13	0.49
1:C:1264:ARG:NH1	1:C:1270:VAL:HB	2.27	0.49
1:C:1455:ARG:O	1:C:1459:ILE:HG13	2.12	0.49
1:C:889:GLU:HG3	1:C:893:VAL:O	2.13	0.49
2:G:1425:LYS:HG2	2:G:1471:GLU:CG	2.37	0.49
2:G:1493:LEU:HD11	2:G:1499:VAL:HG21	1.93	0.49
2:G:1486:PHE:HA	2:G:1504:VAL:O	2.12	0.49
2:G:463:PHE:CE1	2:G:486:LEU:HD22	2.47	0.49
2:G:463:PHE:O	2:G:463:PHE:HD2	1.95	0.49
2:H:894:ARG:NH1	2:H:898:ASP:OD2	2.41	0.49
2:I:1352:HIS:HE1	2:I:1583:MET:CE	2.25	0.49
2:I:324:LEU:HD12	2:I:324:LEU:O	2.12	0.49
2:I:751:LEU:HA	2:I:794:MET:HE3	1.94	0.49
1:A:1189:ILE:HG23	1:A:1190:PRO:HD2	1.95	0.49
1:A:1009:LEU:HD13	1:A:1445:MET:HE1	1.94	0.49
1:C:1392:LEU:HD22	1:C:1396:MET:HG3	1.93	0.49
1:C:790:PHE:CE2	1:C:794:ILE:HD11	2.48	0.49
2:G:1427:VAL:HG22	2:G:1469:GLU:HG2	1.94	0.49
2:G:677:GLN:O	2:G:678:PHE:HB3	2.13	0.49
2:G:706:LYS:HE2	2:G:731:GLN:OE1	2.13	0.49
2:G:950:PHE:O	2:G:954:VAL:HG23	2.13	0.49
2:H:942:THR:HG21	2:H:1012:GLN:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1889:VAL:HG13	2:H:1977:HIS:HB3	1.93	0.49
2:H:273:HIS:CB	2:H:512:LEU:HD22	2.41	0.49
2:H:682:GLY:O	2:H:683:ALA:HB3	2.13	0.49
2:I:1293:THR:CG2	2:I:1296:GLU:H	2.20	0.49
2:I:1678:MET:CE	2:I:1707:LEU:HD22	2.41	0.49
2:I:238:CYS:CB	2:I:239:PRO:HD3	2.40	0.49
1:A:1234:MET:HG2	1:A:1326:ILE:HD12	1.94	0.49
1:A:20:TYR:CD1	2:G:2033:THR:OG1	2.59	0.49
1:A:46:GLU:OE1	1:A:53:LEU:HB2	2.12	0.49
1:B:1305:CYS:SG	1:B:1583:HIS:NE2	2.85	0.49
1:B:435:GLU:O	1:B:439:ILE:HG13	2.12	0.49
1:C:1050:CYS:HB3	1:C:1089:VAL:HG12	1.94	0.49
1:C:50:SER:HB2	1:C:51:PRO:CD	2.43	0.49
2:H:1303:ALA:HB2	2:H:1556:VAL:HG21	1.93	0.49
2:H:598:THR:O	2:H:602:VAL:HB	2.11	0.49
1:A:1451:GLN:OE1	1:A:1451:GLN:HA	2.12	0.49
1:A:157:HIS:CE1	1:A:228:LEU:HD22	2.48	0.49
1:B:1362:PRO:HA	1:B:1365:MET:HG3	1.94	0.49
1:B:1600:LEU:HD11	1:B:1655:VAL:HG12	1.94	0.49
1:B:170:LYS:HD3	1:B:175:LEU:HD23	1.93	0.49
1:B:764:ASP:OD2	1:B:818:ARG:HD3	2.11	0.49
2:G:465:GLY:HA2	2:G:493:THR:HA	1.95	0.49
2:H:138:ASP:O	2:H:139:LYS:HG3	2.12	0.49
2:H:1566:SER:HB3	2:H:1568:HIS:CE1	2.47	0.49
2:H:7:ARG:HH11	2:H:24:THR:HG23	1.75	0.49
2:H:22:VAL:HG11	2:H:27:PHE:HA	1.94	0.49
2:H:369:SER:O	2:H:370:LEU:HD23	2.13	0.49
2:H:715:GLN:O	2:H:719:ILE:HG12	2.13	0.49
2:H:949:ASP:CB	2:H:1006:MET:HE2	2.42	0.49
2:I:1015:VAL:HG13	2:I:1017:PHE:CE2	2.47	0.49
2:I:1265:MET:CE	2:I:1562:PRO:HG2	2.41	0.49
2:I:1435:ILE:O	2:I:1435:ILE:HG22	2.12	0.49
2:I:7:ARG:CZ	2:I:24:THR:HA	2.42	0.49
2:I:16:LEU:HG	2:I:48:PHE:CZ	2.48	0.49
2:I:161:GLY:HA3	2:I:506:PRO:HD2	1.93	0.49
2:I:55:THR:CG2	2:I:56:THR:HG22	2.33	0.49
1:A:1264:ARG:NH1	1:A:1270:VAL:HB	2.28	0.49
1:A:1705:PRO:HB2	1:A:1733:PHE:CE1	2.47	0.49
1:A:256:LEU:HD22	1:A:260:ARG:HB3	1.94	0.49
1:A:328:LEU:HD13	1:A:329:GLU:N	2.27	0.49
1:B:1105:LEU:HD23	1:B:1185:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:636:PRO:HB2	1:C:638:LEU:O	2.13	0.49
1:C:980:VAL:HG23	2:I:968:GLN:OE1	2.13	0.49
2:G:1266:TYR:HB2	2:G:1347:LEU:HD23	1.95	0.49
1:A:18:LEU:HD21	2:G:1815:LEU:HD12	1.95	0.49
2:G:618:GLU:HG2	2:G:678:PHE:CZ	2.48	0.49
2:H:161:GLY:N	2:H:505:GLY:HA3	2.25	0.49
2:H:1873:TYR:HE1	2:H:1877:ARG:HH21	1.59	0.49
2:H:463:PHE:O	2:H:463:PHE:HD2	1.96	0.49
2:H:455:ILE:HD11	2:H:469:ARG:NE	2.27	0.49
2:I:1169:PRO:O	2:I:1173:VAL:HG23	2.13	0.49
2:I:1873:TYR:CE2	2:I:1940:LEU:HD21	2.47	0.49
2:I:740:HIS:CE1	2:I:852:GLU:OE1	2.65	0.49
1:A:21:GLN:HG3	2:G:2013:ASN:HB2	1.93	0.49
1:B:1642:THR:HG22	1:B:1652:GLN:HG3	1.93	0.49
1:C:1114:TYR:CD1	1:C:1337:GLU:HG3	2.48	0.49
1:C:176:VAL:HG12	1:C:178:GLY:H	1.77	0.49
2:G:157:VAL:HG11	2:G:496:PHE:CZ	2.47	0.49
2:G:491:GLU:HA	2:G:494:THR:HG22	1.95	0.49
2:G:732:TRP:CD1	2:G:750:MET:HE3	2.47	0.49
2:H:569:LEU:HD12	2:H:1090:TYR:CD1	2.48	0.49
2:H:1425:LYS:HG2	2:H:1471:GLU:CG	2.38	0.49
2:H:1593:ILE:O	2:H:1597:ALA:HB3	2.12	0.49
2:H:1634:GLY:HA3	2:H:1799:PRO:HA	1.94	0.49
2:H:1666:PHE:CD1	2:H:1814:ALA:HA	2.48	0.49
2:H:173:LEU:O	2:H:173:LEU:HD22	2.13	0.49
2:H:702:TYR:HB2	2:H:727:PRO:HB2	1.94	0.49
2:H:932:ILE:HD12	2:H:939:PHE:HD1	1.78	0.49
2:I:949:ASP:CB	2:I:1006:MET:HE2	2.43	0.49
2:I:573:LYS:HE3	2:I:1101:GLU:OE1	2.12	0.49
2:I:597:MET:H	2:I:601:THR:HB	1.78	0.49
2:I:11:LEU:HD11	2:I:64:PHE:CD2	2.48	0.49
1:C:982:ILE:HD11	2:I:965:SER:HB2	1.95	0.49
1:A:1362:PRO:HA	1:A:1365:MET:HG3	1.95	0.49
1:A:1219:VAL:CA	1:A:1384:ILE:HD11	2.31	0.49
1:B:186:ILE:O	1:B:190:LEU:HG	2.13	0.49
1:C:1020:VAL:CG1	1:C:1400:ILE:HG23	2.42	0.49
1:C:267:VAL:HG12	1:C:290:MET:CE	2.42	0.49
2:G:1130:THR:H	2:G:1133:THR:CG2	2.26	0.49
2:G:161:GLY:N	2:G:505:GLY:HA3	2.24	0.49
2:G:273:HIS:CB	2:G:512:LEU:HD22	2.42	0.49
2:H:1749:GLU:OE2	2:H:1840:VAL:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:428:HIS:HD2	2:H:486:LEU:O	1.96	0.49
2:I:1567:ARG:HH11	2:I:1567:ARG:HG2	1.70	0.49
2:I:173:LEU:O	2:I:173:LEU:HD22	2.13	0.49
1:C:18:LEU:HD21	2:I:1815:LEU:HD12	1.94	0.49
1:C:20:TYR:CD2	2:I:2033:THR:OG1	2.66	0.49
2:I:306:ILE:HA	2:I:439:ILE:HD13	1.94	0.49
1:A:1009:LEU:HG	1:A:1664:ALA:HB2	1.95	0.49
1:A:1022:THR:HG22	1:A:1226:SER:CB	2.43	0.49
1:B:1312:VAL:CG2	1:B:1329:VAL:HG11	2.39	0.49
1:C:335:HIS:O	1:C:335:HIS:CD2	2.65	0.49
1:C:32:GLN:NE2	1:C:57:ALA:HA	2.28	0.49
2:G:1666:PHE:CD1	2:G:1814:ALA:HA	2.48	0.49
2:G:173:LEU:HD22	2:G:173:LEU:O	2.13	0.49
2:G:1913:VAL:O	2:G:1917:ILE:HG13	2.12	0.49
2:G:2036:GLU:HG2	2:G:2039:LYS:NZ	2.28	0.49
2:G:259:THR:HG22	2:G:262:GLU:CB	2.43	0.49
2:G:653:TYR:HD1	2:G:659:LEU:HD21	1.78	0.49
2:G:715:GLN:O	2:G:719:ILE:HG12	2.13	0.49
2:G:807:ILE:HD12	2:G:1063:THR:HG23	1.95	0.49
2:H:1002:HIS:NE2	2:H:1006:MET:HE3	2.27	0.49
2:H:860:ARG:HB2	2:H:1049:GLN:HG3	1.94	0.49
2:I:1567:ARG:NH1	2:I:1568:HIS:HB3	2.28	0.49
2:I:428:HIS:HD2	2:I:486:LEU:O	1.95	0.49
2:I:881:VAL:N	2:I:882:PRO:CD	2.76	0.49
1:A:1021:VAL:HG22	1:A:1387:ILE:HG22	1.95	0.48
1:A:1312:VAL:CG2	1:A:1329:VAL:HG11	2.41	0.48
1:B:182:VAL:O	1:B:186:ILE:HG13	2.12	0.48
1:B:916:LEU:HD22	1:B:922:VAL:HG22	1.94	0.48
1:C:1105:LEU:HD23	1:C:1185:VAL:HG22	1.94	0.48
2:G:402:LEU:HD12	2:G:404:GLN:HG2	1.95	0.48
2:G:598:THR:O	2:G:602:VAL:HB	2.13	0.48
2:H:739:GLY:HA2	2:H:1054:LEU:HG	1.95	0.48
2:H:1931:LEU:HB3	2:H:1935:GLU:CG	2.36	0.48
2:H:465:GLY:HA2	2:H:493:THR:HA	1.95	0.48
2:I:1697:HIS:HE1	2:I:1829:GLU:CG	2.26	0.48
2:I:161:GLY:N	2:I:505:GLY:HA3	2.24	0.48
2:I:663:ILE:HB	2:I:664:PRO:CD	2.42	0.48
2:I:835:THR:HG22	2:I:844:VAL:HA	1.95	0.48
1:C:1693:ILE:CD1	2:I:998:GLN:HB2	2.40	0.48
1:B:187:LEU:HD22	1:B:201:PRO:HB2	1.94	0.48
1:B:465:ASN:O	1:B:469:VAL:HG23	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1745:LYS:HE2	2:G:1747:LYS:HG2	1.95	0.48
2:G:2046:GLU:C	2:G:2048:TYR:H	2.15	0.48
2:G:376:ASN:C	2:G:376:ASN:ND2	2.67	0.48
2:G:597:MET:H	2:G:601:THR:HB	1.77	0.48
2:G:11:LEU:HD11	2:G:64:PHE:CD2	2.48	0.48
2:H:901:LYS:NZ	2:H:1031:LYS:O	2.46	0.48
2:H:1272:ASP:O	2:H:1273:GLU:HG3	2.13	0.48
2:H:1417:THR:O	2:H:1419:PHE:N	2.45	0.48
2:H:1868:GLN:HG3	2:H:1898:TYR:CZ	2.48	0.48
2:H:259:THR:HG22	2:H:262:GLU:CB	2.42	0.48
2:H:306:ILE:HA	2:H:439:ILE:CD1	2.42	0.48
2:H:786:SER:CB	2:H:794:MET:HE2	2.43	0.48
2:I:1674:GLN:OE1	2:I:1712:ASN:HA	2.13	0.48
2:I:629:GLY:O	2:I:632:ALA:HB3	2.13	0.48
2:I:682:GLY:O	2:I:683:ALA:HB3	2.13	0.48
2:I:970:TYR:O	2:I:973:LEU:HB2	2.14	0.48
1:A:1477:ILE:H	1:A:1478:PRO:HD3	1.78	0.48
1:B:157:HIS:HE1	1:B:228:LEU:HD22	1.77	0.48
1:B:413:LEU:C	1:B:415:SER:H	2.17	0.48
1:B:2:LYS:HE2	1:B:4:GLU:CD	2.34	0.48
1:C:1305:CYS:SG	3:C:2748:CER:C5	3.01	0.48
1:C:1523:ARG:NH2	1:C:1564:LEU:O	2.46	0.48
1:C:256:LEU:HD22	1:C:260:ARG:HB3	1.95	0.48
2:G:1330:GLY:HA2	2:G:1374:THR:HG21	1.94	0.48
2:G:1428:GLU:HG2	2:G:1470:THR:HG22	1.94	0.48
2:G:533:LEU:HD13	2:G:545:GLN:HG3	1.94	0.48
2:G:754:TYR:CE2	2:G:794:MET:HG3	2.48	0.48
2:G:7:ARG:HE	2:G:27:PHE:CB	2.25	0.48
2:H:33:LEU:HD21	2:H:80:PHE:CE2	2.49	0.48
2:H:40:ILE:O	2:H:42:PRO:HD3	2.13	0.48
2:H:463:PHE:CD1	2:H:486:LEU:HD22	2.48	0.48
2:H:955:GLU:HG2	2:H:987:TYR:HE2	1.78	0.48
2:I:1130:THR:H	2:I:1133:THR:CG2	2.25	0.48
2:I:1873:TYR:CE1	2:I:1877:ARG:NE	2.77	0.48
2:I:278:VAL:HG11	2:I:303:LEU:HD13	1.95	0.48
2:I:786:SER:CB	2:I:794:MET:HE2	2.42	0.48
1:A:340:ARG:HH12	1:A:344:GLN:HE21	1.60	0.48
1:B:328:LEU:HD13	1:B:329:GLU:N	2.29	0.48
1:B:335:HIS:O	1:B:338:LEU:HB3	2.14	0.48
1:B:702:LYS:HD3	1:B:731:THR:CG2	2.44	0.48
1:B:332:THR:HG22	1:C:331:ILE:CD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:ILE:HG23	1:C:332:THR:N	2.28	0.48
2:G:1980:TYR:HD1	2:G:1981:LEU:HD12	1.79	0.48
2:G:455:ILE:HG12	2:G:469:ARG:HG2	1.94	0.48
2:G:720:ALA:HA	2:G:728:ILE:CD1	2.43	0.48
2:H:1624:THR:HB	2:H:1642:THR:OG1	2.14	0.48
2:H:428:HIS:CD2	2:H:488:VAL:HG23	2.49	0.48
2:H:995:LEU:HB3	2:H:1000:ILE:HD11	1.94	0.48
2:I:146:PHE:HA	2:I:149:VAL:HG12	1.92	0.48
2:I:1850:SER:HB2	2:I:1973:SER:HB2	1.95	0.48
2:I:249:TYR:CD2	2:I:283:ILE:HD11	2.48	0.48
2:I:402:LEU:HD12	2:I:404:GLN:HG2	1.94	0.48
2:I:455:ILE:O	2:I:455:ILE:HG13	2.13	0.48
2:I:551:THR:HG22	2:I:552:SER:N	2.29	0.48
2:I:593:LEU:HD21	2:I:800:LEU:HB3	1.95	0.48
2:I:995:LEU:HB3	2:I:1000:ILE:HD11	1.95	0.48
1:A:1714:VAL:HG22	1:A:1738:ILE:HD11	1.96	0.48
1:B:408:TRP:CH2	1:B:1628:SER:HB3	2.47	0.48
1:B:21:GLN:HG3	2:H:2013:ASN:HB2	1.95	0.48
1:B:998:TYR:CE2	1:B:1667:GLU:HB2	2.49	0.48
1:C:988:ILE:HD13	1:C:1048:GLU:CB	2.43	0.48
1:C:1477:ILE:H	1:C:1478:PRO:HD3	1.78	0.48
1:C:1642:THR:HG22	1:C:1652:GLN:HG3	1.96	0.48
2:G:1344:ASP:O	2:G:1416:TYR:HE2	1.97	0.48
2:G:1567:ARG:CG	2:G:1567:ARG:NH1	2.51	0.48
2:G:995:LEU:HB3	2:G:1000:ILE:HD11	1.96	0.48
2:H:1100:VAL:CG2	2:H:1147:ILE:HG21	2.43	0.48
2:H:145:LEU:HD21	2:H:156:LEU:HD21	1.95	0.48
2:H:1918:LYS:HG2	2:H:1919:LEU:HD23	1.96	0.48
2:H:1953:VAL:O	2:H:1953:VAL:HG12	2.14	0.48
2:H:1986:LYS:HA	2:H:1989:LYS:HB3	1.95	0.48
2:I:1081:HIS:O	2:I:1085:LEU:HB2	2.14	0.48
2:I:569:LEU:HD12	2:I:1090:TYR:CD1	2.48	0.48
2:I:1266:TYR:HB2	2:I:1347:LEU:HD23	1.95	0.48
1:A:1401:TYR:C	1:A:1658:PRO:HG3	2.33	0.48
1:A:19:ALA:O	1:A:22:PHE:HB2	2.14	0.48
1:A:444:ASN:HB2	1:A:447:LEU:N	2.14	0.48
1:B:503:ILE:HD12	1:B:950:THR:HG21	1.96	0.48
1:C:430:ARG:NH1	1:C:493:VAL:O	2.44	0.48
1:C:764:ASP:OD2	1:C:818:ARG:HD3	2.12	0.48
2:G:569:LEU:HD12	2:G:1090:TYR:CD1	2.48	0.48
2:G:1148:ASN:C	2:G:1148:ASN:HD22	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1213:LEU:O	2:G:1214:LEU:HD23	2.12	0.48
1:A:20:TYR:CE1	2:G:2033:THR:CG2	2.97	0.48
2:G:593:LEU:HD21	2:G:800:LEU:HB3	1.96	0.48
2:G:72:VAL:HG12	2:G:73:GLU:N	2.28	0.48
2:H:1632:ILE:O	2:H:1632:ILE:HG23	2.13	0.48
2:H:397:LYS:HB3	2:H:416:PHE:CE2	2.48	0.48
2:H:99:ASN:HA	2:H:550:VAL:HG21	1.95	0.48
2:H:784:GLU:O	2:H:787:THR:HB	2.13	0.48
2:I:1159:ILE:CG1	2:I:1169:PRO:CD	2.90	0.48
2:I:121:GLU:HA	2:I:124:LYS:HD2	1.96	0.48
2:I:1738:PHE:CE1	2:I:1837:THR:HG23	2.48	0.48
2:I:7:ARG:HH11	2:I:24:THR:HG23	1.77	0.48
2:I:533:LEU:HG	2:I:533:LEU:O	2.13	0.48
2:I:586:LEU:HD12	2:I:764:MET:SD	2.54	0.48
1:A:988:ILE:HA	1:A:1048:GLU:CG	2.44	0.48
1:A:182:VAL:O	1:A:186:ILE:HG13	2.14	0.48
1:A:420:ILE:HG22	1:A:469:VAL:HG22	1.96	0.48
1:A:485:ASP:C	1:A:486:VAL:CA	2.76	0.48
1:C:1276:GLN:O	1:C:1282:THR:HG21	2.13	0.48
1:C:1300:THR:HA	1:C:1301:PRO:HD3	1.67	0.48
1:C:1312:VAL:CG2	1:C:1329:VAL:HG11	2.44	0.48
1:C:1396:MET:O	1:C:1680:ARG:NH1	2.46	0.48
1:C:1451:GLN:OE1	1:C:1451:GLN:HA	2.13	0.48
1:C:1617:ILE:O	1:C:1620:GLN:HG2	2.13	0.48
1:C:852:ARG:CG	1:C:852:ARG:NH1	2.66	0.48
2:G:1590:ARG:HG3	2:G:1608:TYR:CD2	2.48	0.48
2:G:2026:PHE:HD2	2:G:2045:TRP:HZ3	1.59	0.48
2:G:240:LEU:O	2:G:244:ILE:HG13	2.13	0.48
2:H:1674:GLN:OE1	2:H:1712:ASN:HA	2.12	0.48
2:H:751:LEU:HD23	2:H:791:TYR:CZ	2.49	0.48
2:I:1697:HIS:HE1	2:I:1829:GLU:HG2	1.77	0.48
2:I:667:LYS:HD2	2:I:697:THR:CG2	2.35	0.48
2:I:762:ASN:HD22	2:I:762:ASN:N	1.88	0.48
1:A:1037:TRP:HB2	1:A:1598:GLN:OE1	2.13	0.48
1:A:539:SER:O	1:A:540:GLN:C	2.52	0.48
1:B:1056:ILE:HD13	1:B:1193:TRP:CD1	2.45	0.48
1:B:1183:ARG:NH1	1:B:1344:GLY:HA2	2.29	0.48
1:B:625:THR:HG23	1:B:661:ASP:OD1	2.13	0.48
1:B:790:PHE:CE2	1:B:794:ILE:HD11	2.47	0.48
1:C:1738:ILE:O	1:C:1739:GLN:HB2	2.14	0.48
1:C:888:ILE:HD12	1:C:939:PHE:CE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1180:MET:HB2	2:G:1197:LEU:HD21	1.95	0.48
2:G:522:GLY:O	2:G:560:ASN:HA	2.13	0.48
2:H:1040:LEU:O	2:H:1046:GLN:HG3	2.13	0.48
2:H:169:TYR:CG	2:H:170:PHE:N	2.81	0.48
2:H:214:ASN:ND2	2:H:217:GLU:HB2	2.27	0.48
2:H:490:TRP:HA	2:H:493:THR:HG22	1.96	0.48
2:H:597:MET:H	2:H:601:THR:HB	1.78	0.48
2:I:1325:PHE:CE1	2:I:1328:VAL:HG11	2.49	0.48
2:I:1586:SER:O	2:I:1590:ARG:HB2	2.14	0.48
2:I:845:THR:HG22	2:I:855:HIS:CD2	2.49	0.48
1:A:427:ASN:HB2	1:A:468:LEU:HD21	1.95	0.48
1:A:695:GLY:HA3	1:A:906:LEU:HD11	1.94	0.48
1:B:243:ILE:O	1:B:247:ARG:HG3	2.13	0.48
2:G:306:ILE:HA	2:G:439:ILE:HD13	1.96	0.48
2:G:432:LEU:HB3	2:G:484:ILE:HG23	1.96	0.48
2:G:481:ASP:OD2	2:G:485:ARG:NH1	2.47	0.48
2:H:489:LYS:O	2:H:493:THR:HG22	2.13	0.48
2:H:868:PHE:HB3	2:H:873:PHE:CE2	2.48	0.48
2:I:1159:ILE:HG22	2:I:1160:THR:N	2.28	0.48
2:I:772:GLY:O	2:I:804:ARG:HD3	2.14	0.48
1:A:1639:VAL:HG12	1:A:1640:SER:N	2.28	0.48
1:A:328:LEU:N	1:A:330:GLU:H	2.12	0.48
1:A:927:ASN:O	1:A:929:GLY:N	2.41	0.48
1:B:1319:ILE:HA	1:B:1324:ALA:O	2.13	0.48
1:B:328:LEU:N	1:B:330:GLU:H	2.11	0.48
1:B:683:ALA:HA	1:B:689:GLY:HA3	1.95	0.48
1:B:930:LEU:HD23	1:B:930:LEU:HA	1.67	0.48
1:C:386:PHE:O	1:C:390:VAL:HB	2.14	0.48
1:C:751:PHE:CZ	1:C:761:LEU:HD13	2.49	0.48
2:G:1148:ASN:ND2	2:G:1151:HIS:H	2.12	0.48
2:G:1325:PHE:CE1	2:G:1328:VAL:HG11	2.48	0.48
2:G:173:LEU:HD13	2:G:219:LEU:HD21	1.94	0.48
2:G:461:ASP:HB3	2:G:464:ASP:HB2	1.95	0.48
2:H:157:VAL:HG11	2:H:496:PHE:CZ	2.49	0.48
2:H:232:LEU:HD21	2:H:423:VAL:HA	1.95	0.48
2:H:706:LYS:HE2	2:H:731:GLN:OE1	2.14	0.48
2:I:2026:PHE:HD2	2:I:2045:TRP:HZ3	1.60	0.48
2:I:214:ASN:ND2	2:I:217:GLU:HB2	2.28	0.48
2:I:489:LYS:O	2:I:493:THR:HG22	2.13	0.48
2:I:753:MET:O	2:I:757:ILE:HG13	2.14	0.48
1:A:187:LEU:HD22	1:A:201:PRO:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1646:PHE:CE1	3:B:2748:CER:H31	2.49	0.47
1:B:1:MET:HE3	1:B:9:LEU:HD12	1.96	0.47
1:C:1392:LEU:CD2	1:C:1396:MET:HG3	2.44	0.47
1:C:182:VAL:O	1:C:186:ILE:HG13	2.14	0.47
1:C:187:LEU:HD22	1:C:201:PRO:HB2	1.96	0.47
1:C:440:MET:HE3	1:C:483:VAL:HG21	1.95	0.47
1:C:529:MET:HG2	1:C:638:LEU:HG	1.95	0.47
2:G:1027:ILE:O	2:G:1031:LYS:HB2	2.14	0.47
2:G:1566:SER:HB3	2:G:1568:HIS:CE1	2.49	0.47
2:G:22:VAL:HG11	2:G:27:PHE:HA	1.96	0.47
2:H:873:PHE:CD1	2:H:1026:GLU:HB2	2.49	0.47
2:H:1590:ARG:NH2	2:H:1594:GLU:OE2	2.47	0.47
2:H:943:TRP:CZ2	2:H:1016:PRO:HG3	2.49	0.47
2:I:1002:HIS:NE2	2:I:1006:MET:HE3	2.29	0.47
2:I:1015:VAL:HA	2:I:1016:PRO:HD3	1.74	0.47
2:I:176:LEU:HD22	2:I:247:ALA:HB1	1.96	0.47
2:I:1834:ARG:NH1	2:I:1834:ARG:CG	2.66	0.47
2:I:594:VAL:CG2	2:I:610:THR:HG21	2.44	0.47
2:I:900:GLN:NE2	2:I:1051:THR:HA	2.28	0.47
1:A:1501:LEU:O	1:A:1505:GLN:HG3	2.14	0.47
1:A:176:VAL:HG12	1:A:178:GLY:H	1.79	0.47
1:B:1367:ARG:HH12	1:B:1372:THR:CB	2.20	0.47
1:B:256:LEU:HD22	1:B:260:ARG:HB3	1.95	0.47
1:C:1021:VAL:HG11	1:C:1597:LEU:CD1	2.44	0.47
1:C:1125:VAL:HG21	1:C:1175:ILE:CD1	2.43	0.47
1:C:427:ASN:HB2	1:C:468:LEU:HD21	1.95	0.47
2:G:777:THR:HG23	2:G:1081:HIS:CE1	2.49	0.47
2:G:40:ILE:O	2:G:42:PRO:HD3	2.14	0.47
2:H:159:ILE:CG2	2:H:501:ILE:HG22	2.44	0.47
2:H:1749:GLU:OE2	2:H:1840:VAL:CG1	2.62	0.47
2:H:213:LEU:HG	2:H:213:LEU:O	2.14	0.47
2:H:732:TRP:CD2	2:H:750:MET:HE1	2.49	0.47
2:H:950:PHE:O	2:H:954:VAL:HG23	2.13	0.47
1:A:1238:VAL:CG1	1:A:1242:GLU:HB2	2.44	0.47
1:A:1303:GLY:C	1:A:1307:THR:HG22	2.35	0.47
1:A:683:ALA:HA	1:A:689:GLY:HA3	1.95	0.47
1:A:852:ARG:HB3	1:A:858:TRP:HZ2	1.80	0.47
1:A:893:VAL:HG11	1:A:930:LEU:CD2	2.38	0.47
1:B:1116:PRO:HB2	1:B:1184:LEU:HD12	1.95	0.47
1:B:1209:ASP:OD2	1:B:1253:GLY:HA2	2.14	0.47
1:B:530:ALA:HA	1:B:636:PRO:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1516:ASP:HA	1:C:1517:PRO:HD3	1.66	0.47
1:C:1010:GLU:HA	1:C:1664:ALA:HA	1.95	0.47
2:G:1417:THR:O	2:G:1419:PHE:N	2.46	0.47
2:G:1624:THR:HB	2:G:1642:THR:OG1	2.15	0.47
2:G:1666:PHE:CD1	2:G:1814:ALA:HB2	2.49	0.47
2:G:428:HIS:HD2	2:G:486:LEU:O	1.97	0.47
2:G:804:ARG:NH2	2:G:1068:GLU:OE1	2.48	0.47
2:H:1417:THR:C	2:H:1419:PHE:H	2.18	0.47
2:H:1438:SER:O	2:H:1441:ILE:HG23	2.13	0.47
2:H:589:ARG:HB3	2:H:590:PRO:CD	2.43	0.47
2:I:1579:ILE:HD11	2:I:1615:MET:SD	2.53	0.47
2:I:1752:PHE:HZ	2:I:1836:MET:HE3	1.80	0.47
2:I:926:LEU:HB3	2:I:947:THR:CG2	2.43	0.47
1:C:1133:PRO:HG3	1:C:1166:LYS:HG3	1.96	0.47
1:C:1138:LYS:HG3	1:C:1163:TYR:CE1	2.48	0.47
1:C:998:TYR:CE2	1:C:1667:GLU:HB2	2.49	0.47
1:C:370:GLU:O	1:C:373:ALA:HB3	2.14	0.47
1:C:526:VAL:HG12	1:C:626:VAL:HG11	1.96	0.47
1:C:987:ASN:HD22	2:I:957:ARG:CD	2.26	0.47
2:G:169:TYR:CG	2:G:170:PHE:N	2.83	0.47
2:G:33:LEU:HD21	2:G:80:PHE:CE2	2.50	0.47
2:G:512:LEU:O	2:G:516:THR:HG23	2.15	0.47
2:H:1472:VAL:CG2	2:H:1483:VAL:HG22	2.44	0.47
2:H:1486:PHE:HA	2:H:1504:VAL:O	2.14	0.47
2:H:597:MET:HA	4:H:3051:FMN:N5	2.30	0.47
2:H:634:ILE:HD11	2:H:649:ILE:CD1	2.40	0.47
2:H:677:GLN:O	2:H:678:PHE:HB3	2.15	0.47
2:I:1804:PHE:CD2	2:I:1818:LEU:HD22	2.49	0.47
2:I:233:SER:HA	2:I:424:ALA:CB	2.44	0.47
2:I:562:LEU:HG	2:I:793:PRO:CB	2.44	0.47
1:A:1208:VAL:HG11	1:A:1212:THR:HB	1.96	0.47
1:A:1319:ILE:HA	1:A:1324:ALA:O	2.14	0.47
1:A:1012:LEU:HD23	1:A:1445:MET:CE	2.43	0.47
1:B:1477:ILE:H	1:B:1478:PRO:HD3	1.79	0.47
1:B:20:TYR:CG	2:H:2033:THR:OG1	2.67	0.47
1:B:331:ILE:HG23	1:B:332:THR:N	2.29	0.47
1:B:531:LEU:HD21	1:B:629:THR:HG22	1.97	0.47
1:C:1303:GLY:CA	1:C:1649:LYS:HE2	2.36	0.47
1:C:142:ASP:CG	1:C:257:PRO:HB2	2.34	0.47
1:C:328:LEU:N	1:C:330:GLU:H	2.12	0.47
2:G:1651:LEU:O	2:G:1652:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1949:LYS:O	2:G:1953:VAL:HG23	2.15	0.47
2:G:463:PHE:CD1	2:G:486:LEU:HD22	2.48	0.47
2:G:123:ILE:CD1	2:G:533:LEU:CD2	2.93	0.47
2:G:732:TRP:CD2	2:G:750:MET:HE3	2.48	0.47
2:H:2037:PRO:O	2:H:2041:ILE:HG13	2.15	0.47
2:H:376:ASN:C	2:H:376:ASN:HD22	2.18	0.47
2:H:455:ILE:HG13	2:H:455:ILE:O	2.13	0.47
2:H:750:MET:CG	2:H:796:PHE:HZ	2.25	0.47
2:H:860:ARG:H	2:H:1049:GLN:HG3	1.79	0.47
2:I:873:PHE:CE1	2:I:1026:GLU:HB2	2.49	0.47
2:I:1378:ILE:O	2:I:1378:ILE:HG12	2.14	0.47
2:I:2037:PRO:O	2:I:2041:ILE:HG13	2.14	0.47
2:I:350:GLN:HA	2:I:353:VAL:HG13	1.96	0.47
2:I:55:THR:HB	2:I:59:GLU:OE2	2.13	0.47
1:A:983:GLN:HE22	2:G:962:LYS:HD2	1.77	0.47
1:B:157:HIS:CE1	1:B:228:LEU:HD22	2.49	0.47
1:B:1305:CYS:SG	3:B:2748:CER:C5	3.03	0.47
1:C:335:HIS:O	1:C:338:LEU:HB3	2.14	0.47
2:H:579:VAL:CG2	2:H:1078:HIS:CD2	2.95	0.47
2:H:1854:MET:CG	2:H:1901:ALA:HB2	2.45	0.47
2:H:355:LYS:HB3	2:H:355:LYS:HE2	1.65	0.47
2:H:652:ILE:N	2:H:652:ILE:HD12	2.30	0.47
2:H:751:LEU:HD23	2:H:791:TYR:CD2	2.49	0.47
2:I:1103:PHE:O	2:I:1247:GLY:HA3	2.14	0.47
2:I:1389:ILE:HG13	2:I:1411:PHE:HD1	1.80	0.47
2:I:1590:ARG:NH2	2:I:1594:GLU:OE2	2.48	0.47
2:I:455:ILE:HD11	2:I:469:ARG:NE	2.29	0.47
2:I:553:ASN:O	2:I:556:LYS:HE3	2.15	0.47
2:I:706:LYS:HE2	2:I:731:GLN:OE1	2.15	0.47
2:I:748:THR:CB	2:I:749:PRO:HD3	2.44	0.47
1:A:1061:SER:HB2	1:A:1078:SER:HB3	1.96	0.47
1:A:1010:GLU:HA	1:A:1664:ALA:HA	1.97	0.47
1:A:243:ILE:O	1:A:247:ARG:HG3	2.14	0.47
1:A:413:LEU:HD13	1:A:451:MET:HG2	1.97	0.47
1:B:34:VAL:O	1:B:38:ASP:HB2	2.14	0.47
1:B:776:GLU:OE1	1:B:795:MET:HE1	2.13	0.47
1:B:827:SER:HA	1:B:828:PRO:HD3	1.73	0.47
1:B:889:GLU:HG3	1:B:893:VAL:O	2.15	0.47
1:C:1183:ARG:NH1	1:C:1344:GLY:HA2	2.30	0.47
1:C:1305:CYS:SG	1:C:1585:LYS:HA	2.55	0.47
1:C:254:TRP:HZ3	1:C:292:GLN:HG3	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1102:TYR:HB3	2:G:1244:PRO:CA	2.44	0.47
2:G:232:LEU:HD21	2:G:423:VAL:HA	1.97	0.47
2:G:732:TRP:CE2	2:G:750:MET:HE3	2.50	0.47
2:H:1130:THR:H	2:H:1133:THR:CG2	2.27	0.47
2:H:1378:ILE:HG12	2:H:1378:ILE:O	2.13	0.47
2:H:176:LEU:HD22	2:H:247:ALA:HB1	1.95	0.47
2:H:606:PHE:HZ	2:H:805:VAL:CG1	2.28	0.47
2:H:11:LEU:HD11	2:H:64:PHE:CD2	2.50	0.47
2:H:741:HIS:HE1	2:H:845:THR:HG21	1.61	0.47
2:I:1148:ASN:ND2	2:I:1151:HIS:H	2.13	0.47
2:I:22:VAL:HG11	2:I:27:PHE:HA	1.97	0.47
2:I:461:ASP:HB3	2:I:464:ASP:HB2	1.95	0.47
2:I:732:TRP:CE2	2:I:750:MET:HE3	2.50	0.47
1:A:1158:PRO:HD2	1:A:1159:GLU:OE2	2.14	0.47
1:A:406:TRP:CE3	1:A:1619:GLU:HG3	2.49	0.47
1:B:1276:GLN:O	1:B:1282:THR:HG21	2.14	0.47
1:B:705:VAL:CG2	1:B:732:LEU:HD21	2.43	0.47
1:B:968:VAL:O	2:H:1512:HIS:HB2	2.14	0.47
1:C:186:ILE:O	1:C:190:LEU:HG	2.14	0.47
1:C:338:LEU:O	1:C:342:GLN:HG3	2.15	0.47
2:G:1567:ARG:NH1	2:G:1568:HIS:HB3	2.28	0.47
2:G:369:SER:O	2:G:370:LEU:HD23	2.14	0.47
2:G:629:GLY:O	2:G:632:ALA:HB3	2.15	0.47
2:H:1980:TYR:HD1	2:H:1981:LEU:HD12	1.79	0.47
2:H:1819:ALA:CA	2:H:2005:ARG:HH11	2.26	0.47
2:H:967:ILE:HD12	2:H:972:LEU:HD22	1.96	0.47
2:I:1004:LEU:CD2	2:I:1019:PRO:HB2	2.44	0.47
2:I:443:LEU:HD22	2:I:448:VAL:CG1	2.45	0.47
2:I:747:HIS:HE1	2:I:780:TYR:OH	1.97	0.47
2:I:768:GLY:HA3	2:I:800:LEU:CD2	2.41	0.47
2:I:955:GLU:HG2	2:I:987:TYR:HE2	1.79	0.47
1:A:479:ASN:O	1:A:483:VAL:HG23	2.15	0.47
1:A:529:MET:HE3	1:A:529:MET:CA	2.36	0.47
1:A:988:ILE:HD13	1:A:1048:GLU:HA	1.97	0.47
1:B:1523:ARG:NH2	1:B:1564:LEU:O	2.48	0.47
1:B:253:ARG:O	1:B:254:TRP:CD1	2.68	0.47
1:B:142:ASP:CG	1:B:257:PRO:HB2	2.35	0.47
1:C:1544:THR:O	1:C:1545:SER:HB3	2.15	0.47
2:G:1159:ILE:CG1	2:G:1169:PRO:CD	2.93	0.47
2:G:1666:PHE:CE1	2:G:1814:ALA:HA	2.50	0.47
2:G:1873:TYR:CE2	2:G:1940:LEU:HD21	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:55:THR:HB	2:G:59:GLU:OE2	2.14	0.47
2:H:1004:LEU:CD2	2:H:1019:PRO:HB2	2.44	0.47
2:H:586:LEU:HD12	2:H:764:MET:SD	2.55	0.47
2:H:826:GLY:HA3	2:H:1061:GLN:CB	2.44	0.47
2:I:194:THR:CG2	2:I:300:ILE:HD11	2.40	0.47
2:I:376:ASN:C	2:I:376:ASN:ND2	2.68	0.47
2:I:42:PRO:HG2	2:I:52:ASP:CG	2.35	0.47
1:B:1305:CYS:SG	3:B:2748:CER:H51	2.54	0.47
1:C:1012:LEU:HD23	1:C:1445:MET:HE3	1.97	0.47
1:C:237:MET:HG3	1:C:241:PHE:HB3	1.95	0.47
2:G:826:GLY:HA2	2:G:1060:ALA:HB3	1.97	0.47
2:G:1850:SER:HB2	2:G:1973:SER:HB2	1.96	0.47
2:G:730:LEU:C	2:G:730:LEU:HD12	2.35	0.47
2:G:772:GLY:O	2:G:804:ARG:HD3	2.15	0.47
2:H:127:ILE:HD12	2:H:180:TYR:HD2	1.80	0.47
2:H:131:ILE:CD1	2:H:182:VAL:CB	2.71	0.47
2:I:1553:TYR:OH	2:I:1583:MET:HB3	2.15	0.47
1:C:18:LEU:HD21	2:I:1815:LEU:CD1	2.45	0.47
2:I:606:PHE:HZ	2:I:805:VAL:CG1	2.28	0.47
1:A:1430:ARG:O	1:A:1430:ARG:HG2	2.15	0.47
1:A:36:LEU:CD2	1:A:61:LEU:HD21	2.37	0.47
1:B:1009:LEU:HD13	1:B:1445:MET:HE1	1.97	0.47
1:B:254:TRP:HZ3	1:B:292:GLN:HG3	1.76	0.47
1:B:32:GLN:NE2	1:B:57:ALA:HA	2.29	0.47
1:B:883:ILE:HD12	1:B:947:LEU:HD12	1.97	0.47
1:C:1189:ILE:HG23	1:C:1190:PRO:HD2	1.97	0.47
2:G:1273:GLU:HB3	2:G:1274:PRO:CD	2.45	0.47
2:G:1493:LEU:HB3	2:G:1494:PRO:HD2	1.96	0.47
1:A:29:ILE:HG13	2:G:1891:TYR:O	2.15	0.47
2:G:739:GLY:HA2	2:G:1054:LEU:HG	1.97	0.47
2:G:745:ASP:HA	2:G:832:TRP:CH2	2.48	0.47
2:G:881:VAL:N	2:G:882:PRO:CD	2.78	0.47
2:H:1015:VAL:HG11	2:H:1017:PHE:CE1	2.50	0.47
2:H:1054:LEU:HB2	4:H:3051:FMN:HM71	1.96	0.47
2:H:1273:GLU:HB3	2:H:1274:PRO:CD	2.45	0.47
2:H:1428:GLU:HG2	2:H:1470:THR:HG22	1.97	0.47
2:H:1473:THR:O	2:H:1481:SER:HB3	2.15	0.47
2:H:1764:PHE:HB2	2:H:1770:LEU:HD21	1.97	0.47
2:H:238:CYS:CB	2:H:239:PRO:HD3	2.43	0.47
2:H:720:ALA:HA	2:H:728:ILE:CD1	2.45	0.47
2:I:1148:ASN:HD22	2:I:1148:ASN:C	2.19	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:490:TRP:HA	2:I:493:THR:HG22	1.96	0.47
1:A:186:ILE:O	1:A:190:LEU:HG	2.14	0.46
1:A:702:LYS:HD3	1:A:731:THR:CG2	2.44	0.46
1:B:1544:THR:O	1:B:1545:SER:HB3	2.15	0.46
1:C:709:ARG:O	1:C:714:VAL:HG21	2.16	0.46
2:G:1015:VAL:HG11	2:G:1017:PHE:CE1	2.50	0.46
2:G:1417:THR:C	2:G:1419:PHE:H	2.18	0.46
2:G:1738:PHE:CE1	2:G:1837:THR:HG23	2.50	0.46
2:G:2035:SER:HB3	2:G:2038:ILE:CG1	2.41	0.46
2:G:249:TYR:CD2	2:G:283:ILE:HD11	2.50	0.46
2:H:7:ARG:NH2	2:H:24:THR:O	2.48	0.46
2:H:440:ASN:ND2	2:H:477:GLU:HG2	2.30	0.46
2:I:1344:ASP:O	2:I:1416:TYR:HE2	1.98	0.46
2:I:1913:VAL:O	2:I:1917:ILE:HG13	2.15	0.46
2:I:533:LEU:HD13	2:I:545:GLN:HG3	1.97	0.46
2:I:573:LYS:C	2:I:575:GLY:H	2.19	0.46
2:I:99:ASN:HA	2:I:550:VAL:HG23	1.97	0.46
1:A:1056:ILE:HG13	1:A:1057:MET:N	2.30	0.46
1:A:1238:VAL:CG1	1:A:1239:HIS:N	2.78	0.46
1:A:183:GLN:NE2	1:A:202:GLU:HG2	2.29	0.46
1:A:908:LEU:HA	1:A:913:VAL:HG21	1.96	0.46
1:A:930:LEU:HD23	1:A:930:LEU:HA	1.70	0.46
1:B:1133:PRO:HG3	1:B:1166:LYS:HG3	1.97	0.46
1:C:1303:GLY:C	1:C:1307:THR:HG22	2.35	0.46
1:C:1646:PHE:CE1	3:C:2748:CER:H31	2.50	0.46
1:C:293:LYS:O	1:C:297:ILE:HG13	2.15	0.46
1:C:499:PRO:HD3	1:C:516:ARG:HH21	1.80	0.46
1:C:893:VAL:HG11	1:C:930:LEU:CD2	2.40	0.46
2:G:1293:THR:HG22	2:G:1296:GLU:CD	2.35	0.46
2:G:279:THR:O	2:G:283:ILE:HB	2.15	0.46
2:G:598:THR:CB	2:G:599:PRO:HD3	2.46	0.46
2:G:652:ILE:HD12	2:G:652:ILE:N	2.29	0.46
2:G:751:LEU:HA	2:G:794:MET:HE3	1.96	0.46
2:H:101:ILE:H	2:H:101:ILE:HG13	1.30	0.46
2:H:1258:ARG:O	2:H:1262:ILE:HG13	2.15	0.46
2:H:1269:LEU:O	2:H:1560:LEU:HD23	2.15	0.46
2:H:1804:PHE:CD2	2:H:1818:LEU:HD22	2.50	0.46
2:H:218:TRP:HB3	2:H:225:THR:OG1	2.15	0.46
2:H:736:ARG:H	2:H:736:ARG:HG3	1.55	0.46
2:H:926:LEU:HB3	2:H:947:THR:HG22	1.97	0.46
2:I:1080:GLY:O	2:I:1084:LYS:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1148:ASN:HD22	2:I:1151:HIS:H	1.63	0.46
2:I:213:LEU:HG	2:I:213:LEU:O	2.16	0.46
2:I:345:THR:HG22	2:I:347:GLU:N	2.23	0.46
2:I:758:ARG:NH2	2:I:797:ASP:OD1	2.38	0.46
1:A:232:LEU:HD13	1:A:272:GLU:CB	2.44	0.46
1:A:702:LYS:HE2	1:A:729:GLY:O	2.15	0.46
1:B:1239:HIS:CD2	1:B:1241:SER:H	2.33	0.46
1:B:1303:GLY:C	1:B:1307:THR:HG22	2.35	0.46
1:B:1114:TYR:CD1	1:B:1337:GLU:HG3	2.50	0.46
1:B:1639:VAL:CG1	1:B:1640:SER:N	2.79	0.46
1:B:237:MET:HG3	1:B:241:PHE:HB3	1.97	0.46
1:C:1004:ILE:HG22	1:C:1660:TYR:CE2	2.49	0.46
1:C:420:ILE:HG22	1:C:469:VAL:HG22	1.96	0.46
1:C:908:LEU:HA	1:C:913:VAL:HG21	1.96	0.46
2:G:1579:ILE:HG22	2:G:1580:THR:O	2.15	0.46
2:G:9:LEU:HB2	2:G:27:PHE:HE1	1.81	0.46
2:G:7:ARG:NH2	2:G:24:THR:O	2.48	0.46
2:G:826:GLY:HA3	2:G:1061:GLN:CB	2.44	0.46
2:H:1079:ASP:O	2:H:1082:ILE:HG22	2.16	0.46
2:H:1359:MET:CE	2:H:1404:MET:HB3	2.44	0.46
2:H:1552:PRO:O	2:H:1556:VAL:HG23	2.15	0.46
1:B:14:LEU:HD11	2:H:1821:VAL:HG11	1.97	0.46
2:H:1945:ASP:O	2:H:1949:LYS:HG3	2.15	0.46
2:H:350:GLN:HA	2:H:353:VAL:HG13	1.97	0.46
2:H:598:THR:CB	2:H:599:PRO:HD3	2.44	0.46
2:H:72:VAL:HG12	2:H:73:GLU:N	2.30	0.46
2:H:879:LYS:HA	2:H:879:LYS:HD3	1.71	0.46
2:I:1417:THR:C	2:I:1419:PHE:H	2.18	0.46
2:I:1593:ILE:HD13	2:I:1626:ILE:HD13	1.97	0.46
2:I:826:GLY:HA3	2:I:1061:GLN:CB	2.46	0.46
1:A:986:ALA:CB	1:A:1047:LEU:HD13	2.45	0.46
1:A:1544:THR:O	1:A:1545:SER:HB3	2.15	0.46
1:A:1639:VAL:CG1	1:A:1640:SER:N	2.78	0.46
1:A:1646:PHE:CE1	3:A:2748:CER:H31	2.50	0.46
1:A:338:LEU:O	1:A:342:GLN:HG3	2.16	0.46
1:B:1305:CYS:SG	1:B:1585:LYS:HA	2.56	0.46
1:B:741:SER:HB3	1:B:744:ASP:HB2	1.97	0.46
1:C:1238:VAL:CG1	1:C:1242:GLU:HB2	2.45	0.46
1:C:451:MET:HE2	1:C:451:MET:HB3	1.71	0.46
1:C:784:ILE:HG23	1:C:788:SER:HB2	1.98	0.46
1:C:933:VAL:HA	1:C:934:PRO:HD3	1.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:355:LYS:HE2	2:G:355:LYS:HB3	1.64	0.46
2:H:807:ILE:HD12	2:H:1063:THR:HG23	1.96	0.46
2:H:1266:TYR:HB2	2:H:1347:LEU:HD23	1.97	0.46
2:H:1666:PHE:CD1	2:H:1814:ALA:HB2	2.49	0.46
2:H:1908:ASP:HA	2:H:1911:THR:HG22	1.98	0.46
2:H:42:PRO:HG2	2:H:52:ASP:CG	2.36	0.46
2:H:573:LYS:HE3	2:H:1101:GLU:OE1	2.15	0.46
2:H:881:VAL:N	2:H:882:PRO:CD	2.79	0.46
2:I:1272:ASP:O	2:I:1273:GLU:HG3	2.15	0.46
2:I:131:ILE:HG21	2:I:182:VAL:HG12	1.97	0.46
2:I:1624:THR:HB	2:I:1642:THR:CG2	2.43	0.46
2:I:1764:PHE:HB2	2:I:1770:LEU:HD21	1.97	0.46
1:A:1050:CYS:HB3	1:A:1089:VAL:HG12	1.98	0.46
1:B:1618:LEU:HD23	1:B:1621:PHE:CE2	2.51	0.46
1:B:183:GLN:NE2	1:B:202:GLU:HG2	2.29	0.46
1:B:451:MET:HE2	1:B:451:MET:HB3	1.73	0.46
1:C:256:LEU:HA	1:C:257:PRO:HD3	1.72	0.46
1:C:2:LYS:HE2	1:C:4:GLU:CD	2.35	0.46
2:G:873:PHE:CD1	2:G:1026:GLU:HB2	2.50	0.46
2:G:109:LEU:HD11	2:G:116:LEU:CD2	2.41	0.46
2:G:1834:ARG:CG	2:G:1834:ARG:NH1	2.68	0.46
1:A:26:VAL:CG2	2:G:1890:ASN:ND2	2.78	0.46
2:G:455:ILE:O	2:G:455:ILE:HG13	2.14	0.46
2:G:702:TYR:HB3	2:G:727:PRO:HB2	1.97	0.46
2:H:1169:PRO:O	2:H:1173:VAL:HG23	2.15	0.46
2:H:1195:VAL:HG13	2:H:1211:LEU:CB	2.44	0.46
2:H:1441:ILE:HD11	2:H:1445:ARG:NH2	2.27	0.46
2:H:1567:ARG:NH1	2:H:1568:HIS:HB3	2.29	0.46
2:I:1666:PHE:CD1	2:I:1814:ALA:HA	2.50	0.46
2:I:584:SER:CB	2:I:591:PRO:HG3	2.41	0.46
1:A:170:LYS:HD3	1:A:175:LEU:HD23	1.97	0.46
1:A:2:LYS:HE2	1:A:4:GLU:CD	2.36	0.46
1:B:1303:GLY:CA	1:B:1649:LYS:HE2	2.40	0.46
1:B:702:LYS:HE2	1:B:729:GLY:O	2.15	0.46
1:C:1319:ILE:HA	1:C:1324:ALA:O	2.14	0.46
1:C:1362:PRO:HA	1:C:1365:MET:HG3	1.97	0.46
1:C:1367:ARG:HH12	1:C:1372:THR:CB	2.20	0.46
1:C:1533:ILE:HD11	1:C:1564:LEU:HD13	1.98	0.46
1:C:243:ILE:O	1:C:247:ARG:HG3	2.16	0.46
2:G:1886:VAL:HG22	2:G:1906:ALA:HB1	1.97	0.46
2:G:209:PHE:CE2	2:G:213:LEU:HD22	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:214:ASN:ND2	2:G:217:GLU:HB2	2.30	0.46
2:G:309:ARG:HA	2:G:309:ARG:HD3	1.64	0.46
2:G:441:LYS:O	2:G:444:VAL:HG12	2.15	0.46
2:G:669:LEU:HD12	2:G:669:LEU:HA	1.62	0.46
2:G:719:ILE:H	2:G:719:ILE:HG12	1.57	0.46
2:G:844:VAL:HG22	2:G:858:ALA:HB2	1.98	0.46
2:H:582:LYS:HE2	2:H:761:PRO:O	2.16	0.46
2:I:1071:LYS:HE3	2:I:1075:ASP:OD2	2.14	0.46
2:H:321:PRO:HD2	2:I:1599:ASP:OD1	2.16	0.46
2:I:1932:SER:O	2:I:1936:VAL:HG22	2.16	0.46
2:I:2026:PHE:HB3	2:I:2042:ILE:HD13	1.98	0.46
2:I:843:ILE:HD11	2:I:1055:HIS:HB3	1.98	0.46
1:A:1270:VAL:HG11	1:A:1274:ILE:HD13	1.97	0.46
1:A:1487:LEU:C	1:A:1487:LEU:HD23	2.35	0.46
1:A:1617:ILE:O	1:A:1620:GLN:HG2	2.16	0.46
1:A:709:ARG:O	1:A:714:VAL:HG21	2.16	0.46
1:B:11:HIS:C	1:B:11:HIS:CD2	2.89	0.46
1:B:792:HIS:CE1	1:B:796:LEU:HD23	2.51	0.46
1:C:1263:ASP:HB2	1:C:1270:VAL:HG21	1.98	0.46
1:C:1577:GLN:NE2	1:C:1591:TRP:HB3	2.30	0.46
1:C:1233:GLU:CD	1:C:1680:ARG:HH21	2.19	0.46
1:C:183:GLN:O	1:C:187:LEU:HG	2.15	0.46
1:C:774:ILE:HA	1:C:775:PRO:HD3	1.74	0.46
2:G:1378:ILE:O	2:G:1378:ILE:HG12	2.13	0.46
2:G:1854:MET:CG	2:G:1901:ALA:HB2	2.46	0.46
2:G:553:ASN:O	2:G:556:LYS:HE3	2.16	0.46
2:H:1180:MET:HB2	2:H:1197:LEU:HD21	1.98	0.46
2:H:1624:THR:HB	2:H:1642:THR:CG2	2.45	0.46
2:H:1738:PHE:CE1	2:H:1837:THR:HG23	2.50	0.46
2:H:1850:SER:HB2	2:H:1973:SER:HB2	1.97	0.46
2:H:1858:ASN:HA	2:H:1896:GLN:O	2.16	0.46
2:H:306:ILE:HA	2:H:439:ILE:HD13	1.96	0.46
2:H:481:ASP:OD2	2:H:485:ARG:NH1	2.48	0.46
2:H:553:ASN:O	2:H:556:LYS:HE3	2.16	0.46
2:H:653:TYR:HD1	2:H:659:LEU:HD21	1.80	0.46
2:H:845:THR:HG22	2:H:855:HIS:CD2	2.51	0.46
2:I:860:ARG:HB2	2:I:1049:GLN:HG3	1.97	0.46
2:I:109:LEU:HD11	2:I:116:LEU:CD2	2.43	0.46
2:I:109:LEU:HD22	2:I:114:THR:HG23	1.96	0.46
2:I:589:ARG:HB3	2:I:590:PRO:CD	2.43	0.46
2:I:653:TYR:HD1	2:I:659:LEU:HD21	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LYS:HB2	1:A:65:TYR:CE1	2.48	0.46
1:A:427:ASN:ND2	1:A:610:THR:H	2.08	0.46
1:A:49:PRO:O	1:A:82:SER:HB2	2.16	0.46
1:B:1021:VAL:HG22	1:B:1387:ILE:HG22	1.98	0.46
1:B:1595:GLY:O	1:B:1599:ILE:HG13	2.15	0.46
2:G:1168:ASN:HA	2:G:1169:PRO:HD3	1.81	0.46
2:G:1303:ALA:HB2	2:G:1556:VAL:HG21	1.98	0.46
2:G:131:ILE:CG2	2:G:182:VAL:HG11	2.43	0.46
2:G:2037:PRO:O	2:G:2041:ILE:HG13	2.16	0.46
2:G:785:TRP:CG	2:G:786:SER:N	2.83	0.46
2:G:845:THR:HG22	2:G:855:HIS:CD2	2.50	0.46
2:G:955:GLU:HG2	2:G:987:TYR:HE2	1.80	0.46
2:H:1344:ASP:O	2:H:1416:TYR:HE2	1.99	0.46
2:H:1427:VAL:HG22	2:H:1469:GLU:HG2	1.96	0.46
2:H:1491:VAL:HB	2:H:1501:ILE:CD1	2.45	0.46
2:H:1651:LEU:O	2:H:1652:THR:HG23	2.16	0.46
2:H:1846:GLU:C	2:H:1848:GLY:H	2.19	0.46
2:H:1873:TYR:CE1	2:H:1877:ARG:NE	2.77	0.46
2:H:551:THR:HG22	2:H:552:SER:N	2.30	0.46
2:H:60:LEU:O	2:H:63:LYS:HB2	2.16	0.46
2:I:1180:MET:HB3	2:I:1199:GLU:HG2	1.98	0.46
2:I:1543:ASP:OD1	2:I:1623:LYS:HG2	2.15	0.46
2:I:490:TRP:CZ2	2:I:512:LEU:HD21	2.51	0.46
1:A:331:ILE:HG23	1:A:332:THR:N	2.31	0.46
1:A:35:PHE:HA	1:A:39:PHE:HD2	1.81	0.46
1:A:507:GLY:N	1:A:954:ARG:HG2	2.31	0.46
1:C:1196:LYS:HE3	1:C:1202:ASP:CG	2.37	0.46
1:C:11:His:C	1:C:11:His:CD2	2.89	0.46
1:C:1209:ASP:OD2	1:C:1253:GLY:HA2	2.16	0.46
2:G:123:ILE:HD11	2:G:533:LEU:HD22	1.98	0.46
2:G:1842:VAL:HA	2:G:1843:PRO:HD2	1.89	0.46
2:G:970:TYR:O	2:G:973:LEU:HB2	2.16	0.46
2:H:1236:LEU:HA	2:H:1237:PRO:HD3	1.78	0.46
2:H:1374:THR:HG23	2:H:1396:LEU:CD1	2.46	0.46
2:H:1227:ARG:NE	2:H:1565:VAL:HG12	2.30	0.46
2:H:490:TRP:CZ2	2:H:512:LEU:HD21	2.51	0.46
2:H:702:TYR:HB3	2:H:727:PRO:HB2	1.97	0.46
2:I:1031:LYS:O	2:I:1032:ASP:C	2.54	0.46
2:I:1054:LEU:HB3	4:I:3051:FMN:HM82	1.98	0.46
2:I:1228:THR:HG21	2:I:1234:VAL:HG23	1.98	0.46
2:I:740:His:HE1	2:I:852:GLU:OE1	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:860:ARG:H	2:I:1049:GLN:HG3	1.80	0.46
1:A:1709:GLU:HG3	1:A:1709:GLU:H	1.46	0.46
1:A:386:PHE:O	1:A:390:VAL:HB	2.16	0.46
1:B:143:GLU:H	1:B:260:ARG:HG2	1.81	0.46
1:B:601:VAL:O	1:B:602:GLU:C	2.54	0.46
1:C:1459:ILE:O	1:C:1463:VAL:HG23	2.16	0.46
1:C:539:SER:O	1:C:540:GLN:C	2.52	0.46
2:G:1002:HIS:NE2	2:G:1006:MET:CE	2.79	0.46
2:G:1311:PHE:HD1	2:G:1320:LEU:O	1.99	0.46
2:G:1435:ILE:O	2:G:1435:ILE:HG22	2.15	0.46
2:G:233:SER:HA	2:G:424:ALA:CB	2.46	0.46
2:H:1021:LEU:HA	2:H:1021:LEU:HD22	1.58	0.46
2:H:913:ASP:H	2:H:916:THR:CG2	2.29	0.46
2:I:1222:GLU:HG3	2:I:1235:SER:OG	2.16	0.46
2:I:1561:ASN:OD1	2:I:1563:ILE:HB	2.15	0.46
2:I:232:LEU:HD21	2:I:423:VAL:HA	1.98	0.46
2:I:391:LEU:CD2	2:I:394:ARG:NH2	2.78	0.46
2:I:670:ARG:HD2	2:I:676:ILE:O	2.16	0.46
2:I:785:TRP:CG	2:I:786:SER:N	2.84	0.46
2:I:751:LEU:HD11	2:I:789:PHE:CD1	2.51	0.46
2:I:844:VAL:HG22	2:I:858:ALA:HB2	1.97	0.46
1:A:1533:ILE:HG13	1:A:1564:LEU:HB3	1.98	0.45
1:A:411:GLN:NE2	1:A:1628:SER:H	2.13	0.45
1:A:1557:ILE:HD11	1:A:1642:THR:HG21	1.97	0.45
1:A:792:HIS:CE1	1:A:796:LEU:HD23	2.51	0.45
1:B:1234:MET:HG2	1:B:1326:ILE:CD1	2.46	0.45
1:B:516:ARG:NH2	1:B:889:GLU:OE1	2.49	0.45
1:B:881:ASN:HA	1:B:944:ARG:HH22	1.78	0.45
1:C:1040:GLU:HB2	1:C:1580:LEU:HD12	1.98	0.45
1:C:1432:HIS:CE1	1:C:1434:SER:OG	2.69	0.45
1:C:1376:PHE:CB	1:C:1544:THR:HG22	2.45	0.45
1:C:1573:ILE:HG23	1:C:1627:PRO:HG3	1.98	0.45
1:C:400:ARG:HH11	1:C:400:ARG:HG3	1.72	0.45
2:G:1586:SER:O	2:G:1590:ARG:HB2	2.16	0.45
2:G:159:ILE:CG2	2:G:501:ILE:HG22	2.46	0.45
2:H:1031:LYS:O	2:H:1032:ASP:C	2.54	0.45
2:H:1135:GLU:OE2	2:H:1175:LYS:HE3	2.15	0.45
2:H:1388:LYS:HE3	2:H:1418:ASP:OD2	2.16	0.45
2:H:1593:ILE:HD13	2:H:1626:ILE:HD13	1.97	0.45
2:H:1666:PHE:CE1	2:H:1814:ALA:HA	2.50	0.45
2:H:1873:TYR:CE1	2:H:1877:ARG:NH2	2.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2026:PHE:HB3	2:H:2042:ILE:HD13	1.98	0.45
2:H:391:LEU:CD2	2:H:394:ARG:NH2	2.80	0.45
2:H:730:LEU:HD12	2:H:730:LEU:C	2.36	0.45
2:I:738:GLY:HA3	4:I:3051:FMN:HM81	1.98	0.45
2:I:807:ILE:HD12	2:I:1063:THR:HG23	1.98	0.45
1:A:1114:TYR:CE1	1:A:1337:GLU:HG3	2.50	0.45
1:A:408:TRP:CZ3	1:A:1628:SER:HB3	2.51	0.45
1:A:764:ASP:OD2	1:A:818:ARG:HD3	2.17	0.45
1:B:1431:GLU:OE2	1:B:1433:HIS:HE1	2.00	0.45
1:B:19:ALA:O	1:B:22:PHE:HB2	2.15	0.45
1:B:26:VAL:HG13	2:H:2013:ASN:ND2	2.31	0.45
1:B:2:LYS:HE2	1:B:4:GLU:OE1	2.15	0.45
1:B:719:GLN:HG3	1:B:720:SER:N	2.31	0.45
1:C:170:LYS:HD3	1:C:175:LEU:HD23	1.97	0.45
1:C:430:ARG:NH2	1:C:605:LEU:HD13	2.31	0.45
1:C:529:MET:CE	1:C:894:ARG:HD2	2.46	0.45
1:C:931:GLN:HG3	1:C:931:GLN:H	1.31	0.45
2:G:1219:ILE:HD11	2:G:1242:PHE:HB2	1.98	0.45
2:G:1222:GLU:HG3	2:G:1235:SER:OG	2.16	0.45
2:G:1472:VAL:CG2	2:G:1483:VAL:HG22	2.46	0.45
2:G:1673:GLU:N	2:G:1676:MET:HE3	2.25	0.45
2:G:191:SER:HA	2:G:194:THR:CG2	2.46	0.45
2:G:1976:PHE:HA	2:G:1981:LEU:CD2	2.46	0.45
2:G:161:GLY:HA3	2:G:506:PRO:HD2	1.98	0.45
2:H:1579:ILE:HG22	2:H:1580:THR:O	2.16	0.45
2:H:1768:LYS:HE2	2:H:1772:SER:HB3	1.98	0.45
2:H:246:LEU:HD12	2:H:246:LEU:HA	1.85	0.45
2:H:324:LEU:HD12	2:H:324:LEU:O	2.16	0.45
2:H:612:ASN:HD21	2:H:641:ILE:HA	1.81	0.45
2:I:1359:MET:HE3	2:I:1404:MET:HB3	1.98	0.45
2:I:369:SER:O	2:I:370:LEU:HD23	2.16	0.45
2:I:601:THR:HB	2:I:620:ALA:HB2	1.98	0.45
2:I:669:LEU:HD12	2:I:669:LEU:HA	1.65	0.45
1:A:1367:ARG:HH12	1:A:1372:THR:CB	2.18	0.45
1:A:1431:GLU:OE2	1:A:1523:ARG:NH1	2.48	0.45
1:A:751:PHE:CZ	1:A:761:LEU:HD13	2.51	0.45
1:B:1639:VAL:HG12	1:B:1640:SER:N	2.31	0.45
1:B:235:SER:HA	1:B:276:ARG:NH2	2.32	0.45
1:B:37:LYS:HB2	1:B:65:TYR:CE1	2.51	0.45
1:B:444:ASN:HB2	1:B:447:LEU:N	2.15	0.45
1:C:827:SER:HA	1:C:828:PRO:HD3	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:982:ILE:HD11	2:I:965:SER:CB	2.46	0.45
1:A:18:LEU:HD21	2:G:1815:LEU:CD1	2.46	0.45
2:G:1953:VAL:O	2:G:1953:VAL:HG12	2.16	0.45
2:G:247:ALA:O	2:G:251:VAL:HG13	2.15	0.45
2:G:460:TYR:HA	2:G:466:SER:O	2.17	0.45
2:G:860:ARG:HB2	2:G:1049:GLN:HG3	1.97	0.45
2:H:1590:ARG:HG3	2:H:1608:TYR:CD2	2.51	0.45
2:H:1776:PHE:C	2:H:1779:PRO:HD2	2.37	0.45
2:H:249:TYR:CD2	2:H:283:ILE:HD11	2.52	0.45
2:H:439:ILE:HD12	2:H:484:ILE:CD1	2.46	0.45
2:I:1180:MET:HB2	2:I:1197:LEU:HD21	1.97	0.45
2:I:1775:GLN:HG2	2:I:1836:MET:SD	2.57	0.45
2:I:1854:MET:CG	2:I:1901:ALA:HB2	2.47	0.45
2:I:618:GLU:HG2	2:I:678:PHE:CZ	2.51	0.45
2:I:739:GLY:HA2	2:I:1054:LEU:HG	1.97	0.45
1:A:168:MET:HA	1:A:206:LEU:HB2	1.98	0.45
1:A:413:LEU:C	1:A:415:SER:H	2.18	0.45
1:A:625:THR:HG23	1:A:627:SER:H	1.82	0.45
1:A:630:ILE:O	1:A:653:ARG:NH2	2.48	0.45
1:A:798:ASN:HA	1:A:801:ARG:HB2	1.98	0.45
1:B:1310:GLU:OE1	1:B:1649:LYS:CE	2.62	0.45
1:B:32:GLN:NE2	1:B:57:ALA:CA	2.80	0.45
1:B:988:ILE:HD13	1:B:1048:GLU:CB	2.47	0.45
1:C:1533:ILE:HG13	1:C:1564:LEU:HB3	1.98	0.45
2:G:1015:VAL:HG13	2:G:1017:PHE:CE2	2.52	0.45
2:G:1148:ASN:HD22	2:G:1151:HIS:H	1.63	0.45
2:G:1314:ARG:HA	2:G:1314:ARG:HD3	1.62	0.45
2:G:582:LYS:HE2	2:G:1108:PRO:HB3	1.97	0.45
2:G:807:ILE:HA	2:G:818:LYS:HG2	1.97	0.45
2:H:1735:ALA:O	2:H:1737:ILE:HG13	2.16	0.45
2:H:463:PHE:CD2	2:H:463:PHE:C	2.90	0.45
2:H:601:THR:O	2:H:601:THR:CG2	2.65	0.45
2:H:835:THR:CB	2:H:845:THR:HG23	2.43	0.45
2:I:1199:GLU:OE2	2:I:1567:ARG:CZ	2.65	0.45
2:I:1327:ILE:HA	2:I:1327:ILE:HD12	1.80	0.45
2:I:1609:THR:O	2:I:1653:GLY:HA3	2.16	0.45
2:I:463:PHE:CE1	2:I:486:LEU:HD22	2.51	0.45
1:A:1196:LYS:HE3	1:A:1202:ASP:CG	2.36	0.45
1:A:143:GLU:H	1:A:260:ARG:HG2	1.81	0.45
1:A:293:LYS:O	1:A:297:ILE:HG13	2.16	0.45
1:B:1020:VAL:CG1	1:B:1400:ILE:HG23	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1061:SER:HB2	1:B:1078:SER:HB3	1.99	0.45
1:B:1019:ILE:HG21	1:B:1316:VAL:HG22	1.98	0.45
1:B:1376:PHE:CB	1:B:1544:THR:HG22	2.45	0.45
1:C:1104:ARG:O	1:C:1185:VAL:HG13	2.17	0.45
1:C:776:GLU:OE1	1:C:795:MET:HE1	2.17	0.45
2:G:357:ASN:OD1	2:G:365:GLN:HB3	2.16	0.45
2:H:1027:ILE:O	2:H:1031:LYS:HB2	2.16	0.45
2:H:1383:ASN:HD21	2:H:1418:ASP:CB	2.30	0.45
2:H:24:THR:O	2:H:26:SER:N	2.49	0.45
2:H:319:LEU:HA	2:H:319:LEU:HD22	1.68	0.45
2:H:611:THR:HA	2:H:615:TYR:O	2.16	0.45
2:H:659:LEU:HA	2:H:659:LEU:HD12	1.82	0.45
2:H:754:TYR:CE2	2:H:794:MET:HG3	2.52	0.45
2:I:1776:PHE:C	2:I:1779:PRO:HD2	2.37	0.45
2:I:1976:PHE:CB	2:I:1981:LEU:CD2	2.94	0.45
2:I:2036:GLU:HG2	2:I:2039:LYS:HZ3	1.82	0.45
2:I:894:ARG:NH1	2:I:898:ASP:OD2	2.42	0.45
2:I:938:TRP:CD1	2:I:944:ARG:HG3	2.52	0.45
1:C:1682:LYS:HB3	2:I:994:PHE:CD2	2.51	0.45
1:A:776:GLU:OE1	1:A:795:MET:HE1	2.16	0.45
1:A:658:LEU:HD13	1:A:916:LEU:HD12	1.99	0.45
1:B:1533:ILE:HD11	1:B:1564:LEU:HD13	1.98	0.45
1:C:1491:ARG:NH1	1:C:1744:TYR:O	2.50	0.45
1:C:197:THR:HG22	1:C:198:PRO:O	2.15	0.45
1:C:225:SER:OG	1:C:266:LEU:HD21	2.16	0.45
1:C:143:GLU:H	1:C:260:ARG:HG2	1.81	0.45
1:B:332:THR:HG22	1:C:331:ILE:HD11	1.98	0.45
2:G:1080:GLY:O	2:G:1084:LYS:HG3	2.16	0.45
2:G:1241:ASN:N	2:G:1252:SER:O	2.49	0.45
2:G:142:ASN:HB2	2:G:550:VAL:HG13	1.99	0.45
2:G:1466:PHE:HE2	2:G:1489:ILE:HD13	1.81	0.45
2:G:1976:PHE:CB	2:G:1981:LEU:CD2	2.95	0.45
2:G:315:PRO:O	2:H:1314:ARG:NH2	2.50	0.45
2:G:712:ALA:O	2:G:715:GLN:HB3	2.16	0.45
2:H:1085:LEU:HD12	2:H:1085:LEU:HA	1.85	0.45
2:H:1159:ILE:HG22	2:H:1160:THR:N	2.32	0.45
2:H:1325:PHE:O	2:H:1328:VAL:HG12	2.16	0.45
2:H:618:GLU:HG2	2:H:678:PHE:CZ	2.52	0.45
2:H:785:TRP:CG	2:H:786:SER:N	2.84	0.45
2:I:1195:VAL:HG13	2:I:1211:LEU:CB	2.46	0.45
2:I:1637:LEU:HD23	2:I:1637:LEU:HA	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:440:ASN:ND2	2:I:477:GLU:HG2	2.31	0.45
2:I:23:PRO:HG2	2:I:86:LEU:HD11	1.98	0.45
1:A:1300:THR:HA	1:A:1301:PRO:HD3	1.70	0.45
1:B:66:GLU:HA	1:B:66:GLU:OE1	2.15	0.45
1:C:1670:TYR:O	1:C:1674:VAL:HG23	2.17	0.45
1:C:1305:CYS:SG	3:C:2748:CER:H51	2.57	0.45
1:C:521:LYS:HB3	1:C:523:SER:HB3	1.98	0.45
2:G:1858:ASN:ND2	2:G:1861:ARG:HG3	2.32	0.45
2:G:1873:TYR:HE1	2:G:1877:ARG:HH21	1.59	0.45
2:G:665:LEU:O	2:G:665:LEU:HD22	2.17	0.45
2:G:754:TYR:CG	2:G:794:MET:HG2	2.51	0.45
2:H:1678:MET:HE3	2:H:1707:LEU:CD2	2.41	0.45
2:H:2035:SER:HB3	2:H:2038:ILE:CG1	2.44	0.45
2:H:594:VAL:CG2	2:H:610:THR:HG21	2.45	0.45
2:I:1162:ASP:O	2:I:1163:LYS:HB2	2.16	0.45
2:I:1949:LYS:O	2:I:1953:VAL:HG23	2.17	0.45
1:C:21:GLN:HG3	2:I:2013:ASN:HB2	1.98	0.45
2:I:478:ARG:O	2:I:482:CYS:HB2	2.17	0.45
2:I:784:GLU:O	2:I:787:THR:HB	2.17	0.45
1:A:1239:HIS:CD2	1:A:1241:SER:H	2.35	0.45
1:A:1443:LEU:HA	1:A:1443:LEU:HD23	1.75	0.45
1:B:1004:ILE:HG22	1:B:1660:TYR:CE2	2.52	0.45
1:B:1459:ILE:O	1:B:1463:VAL:HG23	2.17	0.45
1:B:1584:PRO:CG	1:B:1591:TRP:CZ3	3.00	0.45
1:B:1239:HIS:HE1	1:B:1714:VAL:O	2.00	0.45
2:G:101:ILE:HG13	2:G:101:ILE:H	1.31	0.45
2:G:1265:MET:HE1	2:G:1562:PRO:HG2	1.98	0.45
2:G:218:TRP:HB3	2:G:225:THR:OG1	2.16	0.45
2:G:350:GLN:HA	2:G:353:VAL:HG13	1.97	0.45
2:G:455:ILE:HD11	2:G:469:ARG:NE	2.32	0.45
2:G:879:LYS:HA	2:G:879:LYS:HD3	1.68	0.45
2:H:1100:VAL:HG23	2:H:1147:ILE:HB	1.99	0.45
2:H:1845:ASP:HB2	2:H:1849:ARG:N	2.15	0.45
2:H:751:LEU:HA	2:H:794:MET:HE3	1.98	0.45
2:I:1002:HIS:NE2	2:I:1006:MET:CE	2.80	0.45
2:I:943:TRP:CZ2	2:I:1016:PRO:HG3	2.52	0.45
2:I:1258:ARG:O	2:I:1262:ILE:HG13	2.17	0.45
2:I:1308:CYS:HB3	2:I:1311:PHE:CE2	2.51	0.45
2:I:1417:THR:O	2:I:1419:PHE:N	2.45	0.45
2:I:161:GLY:H	2:I:505:GLY:CA	2.28	0.45
2:I:355:LYS:HE2	2:I:355:LYS:HB3	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:654:VAL:O	2:I:654:VAL:HG12	2.17	0.45
2:I:677:GLN:O	2:I:678:PHE:HB3	2.17	0.45
1:A:485:ASP:CA	1:A:486:VAL:N	2.72	0.45
1:B:1617:ILE:O	1:B:1620:GLN:HG2	2.17	0.45
1:B:340:ARG:HH12	1:B:344:GLN:HE21	1.64	0.45
1:B:420:ILE:HG22	1:B:469:VAL:HG22	1.99	0.45
1:C:927:ASN:O	1:C:929:GLY:N	2.41	0.45
2:G:1491:VAL:HB	2:G:1501:ILE:HD12	1.99	0.45
2:G:1543:ASP:OD1	2:G:1623:LYS:HG2	2.16	0.45
2:G:1227:ARG:CZ	2:G:1565:VAL:HG12	2.47	0.45
2:G:624:TYR:HB2	2:G:630:MET:HE3	1.99	0.45
2:H:1327:ILE:HG12	2:H:1583:MET:HE3	1.99	0.45
2:H:512:LEU:O	2:H:516:THR:HG23	2.17	0.45
2:I:1491:VAL:HB	2:I:1501:ILE:CD1	2.47	0.45
2:I:653:TYR:OH	2:I:690:VAL:HG11	2.17	0.45
1:A:1516:ASP:HA	1:A:1517:PRO:HD3	1.61	0.45
1:A:204:THR:HA	1:A:205:PRO:HD3	1.85	0.45
1:A:335:HIS:CD2	1:A:335:HIS:O	2.69	0.45
1:B:1119:LYS:HE2	1:B:1341:PHE:CG	2.52	0.45
1:B:1300:THR:HA	1:B:1301:PRO:HD3	1.69	0.45
1:B:1592:MET:HE2	1:B:1641:ILE:HG23	1.98	0.45
1:B:196:THR:O	1:B:213:PHE:HE2	2.00	0.45
1:B:43:ARG:O	2:H:1662:THR:HA	2.16	0.45
1:B:32:GLN:HE21	1:B:57:ALA:HB2	1.82	0.45
1:B:67:SER:OG	2:G:359:HIS:HE1	1.99	0.45
1:B:44:VAL:HG13	1:B:78:ILE:HG12	1.98	0.45
1:C:1061:SER:HB2	1:C:1078:SER:HB3	1.99	0.45
1:C:478:GLU:OE1	1:C:478:GLU:HA	2.17	0.45
1:C:916:LEU:HD22	1:C:922:VAL:HG22	1.99	0.45
2:G:1002:HIS:NE2	2:G:1006:MET:HE3	2.32	0.45
2:G:109:LEU:HA	2:G:109:LEU:HD23	1.79	0.45
2:G:1325:PHE:O	2:G:1328:VAL:HG12	2.17	0.45
2:G:1389:ILE:HG13	2:G:1411:PHE:CD1	2.52	0.45
2:G:42:PRO:HG2	2:G:52:ASP:CG	2.38	0.45
2:H:315:PRO:O	2:I:1314:ARG:NH2	2.50	0.45
2:H:641:ILE:HG12	2:H:645:SER:CB	2.46	0.45
2:I:1256:GLU:O	2:I:1257:ASP:HB2	2.17	0.45
2:I:231:LEU:HA	2:I:236:ILE:HD12	1.99	0.45
2:I:298:LYS:HG2	2:I:448:VAL:CG2	2.38	0.45
1:A:1283:MET:O	1:A:1287:VAL:HG23	2.18	0.44
1:A:242:THR:HG22	1:A:243:ILE:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:PRO:HB2	1:A:638:LEU:O	2.16	0.44
1:A:931:GLN:H	1:A:931:GLN:HG3	1.30	0.44
1:B:1029:PRO:HA	1:B:1188:GLN:O	2.17	0.44
1:B:1455:ARG:HD2	1:B:1455:ARG:HA	1.86	0.44
1:B:411:GLN:NE2	1:B:1628:SER:H	2.15	0.44
1:B:427:ASN:HB2	1:B:468:LEU:HD21	1.99	0.44
1:B:612:GLU:O	1:B:615:SER:HB3	2.17	0.44
1:B:626:VAL:HG23	1:B:664:GLU:OE2	2.17	0.44
1:B:733:ILE:CD1	1:B:761:LEU:HD11	2.46	0.44
1:C:1257:LEU:HA	1:C:1257:LEU:HD23	1.83	0.44
1:C:253:ARG:O	1:C:254:TRP:CD1	2.70	0.44
1:C:641:ARG:HD3	1:C:649:TRP:O	2.17	0.44
2:G:1071:LYS:HE3	2:G:1075:ASP:OD2	2.16	0.44
2:G:1294:ALA:HA	2:G:1368:VAL:CG2	2.47	0.44
2:G:1855:ILE:HB	2:G:1907:LEU:HD12	2.00	0.44
2:G:607:VAL:O	2:G:611:THR:HB	2.17	0.44
2:G:717:ILE:O	2:G:720:ALA:HB3	2.18	0.44
2:G:741:HIS:HB3	2:G:853:PRO:HB2	1.98	0.44
2:G:741:HIS:HE1	2:G:855:HIS:NE2	2.13	0.44
2:G:926:LEU:HB3	2:G:947:THR:CG2	2.46	0.44
2:H:109:LEU:HD22	2:H:114:THR:HG23	1.99	0.44
2:H:1308:CYS:HB3	2:H:1311:PHE:CE2	2.52	0.44
2:H:1321:ALA:HA	2:H:1322:PRO:HD3	1.84	0.44
1:B:13:LEU:HB2	2:H:2026:PHE:CE1	2.52	0.44
2:H:443:LEU:HD22	2:H:448:VAL:CG1	2.46	0.44
2:I:1159:ILE:CG2	2:I:1160:THR:N	2.81	0.44
2:I:1589:VAL:HG21	2:I:1651:LEU:HD12	1.99	0.44
2:I:272:GLY:HA3	2:I:276:GLY:C	2.37	0.44
1:A:1012:LEU:HD23	1:A:1445:MET:HE2	1.99	0.44
1:A:1373:ARG:NE	1:A:1550:ASP:HB2	2.32	0.44
1:A:1666:THR:HG23	1:A:1669:ARG:CB	2.47	0.44
1:A:225:SER:OG	1:A:266:LEU:HD21	2.16	0.44
1:B:168:MET:HA	1:B:206:LEU:HB2	2.00	0.44
1:B:256:LEU:HA	1:B:257:PRO:HD3	1.73	0.44
1:B:330:GLU:O	1:B:330:GLU:HG2	2.16	0.44
1:C:1234:MET:HG2	1:C:1326:ILE:HD12	1.98	0.44
1:C:1238:VAL:CG1	1:C:1239:HIS:N	2.80	0.44
2:G:1609:THR:O	2:G:1653:GLY:HA3	2.16	0.44
2:G:7:ARG:HH11	2:G:24:THR:HG23	1.76	0.44
2:G:463:PHE:C	2:G:463:PHE:CD2	2.90	0.44
2:G:595:PRO:HD3	2:G:800:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:120:LYS:HB3	2:H:124:LYS:HE3	1.99	0.44
2:H:1330:GLY:HA2	2:H:1374:THR:HG21	1.98	0.44
2:H:1543:ASP:OD1	2:H:1623:LYS:HG2	2.17	0.44
2:H:786:SER:HB2	2:H:794:MET:HE2	1.99	0.44
2:H:854:ILE:HG22	2:H:856:LYS:HG3	1.99	0.44
2:I:1303:ALA:HB2	2:I:1556:VAL:HG21	1.98	0.44
2:I:1314:ARG:HD3	2:I:1314:ARG:HA	1.64	0.44
2:I:191:SER:HA	2:I:194:THR:CG2	2.43	0.44
2:I:441:LYS:O	2:I:444:VAL:HG12	2.17	0.44
2:I:659:LEU:HA	2:I:659:LEU:HD12	1.84	0.44
1:A:1431:GLU:HB3	1:A:1520:ALA:HB2	1.99	0.44
1:A:27:ARG:HH21	2:G:2015:THR:HA	1.82	0.44
1:A:267:VAL:HG12	1:A:290:MET:CE	2.48	0.44
1:B:183:GLN:O	1:B:187:LEU:HG	2.17	0.44
1:B:225:SER:OG	1:B:266:LEU:HD21	2.18	0.44
1:B:479:ASN:O	1:B:483:VAL:HG23	2.17	0.44
1:B:539:SER:O	1:B:540:GLN:C	2.54	0.44
1:B:655:LEU:HD23	1:B:655:LEU:HA	1.82	0.44
1:B:833:PHE:O	1:B:834:GLY:O	2.35	0.44
1:C:1487:LEU:C	1:C:1487:LEU:HD23	2.38	0.44
2:G:1015:VAL:HA	2:G:1016:PRO:HD3	1.79	0.44
2:G:120:LYS:HB3	2:G:124:LYS:HE3	1.99	0.44
2:G:231:LEU:HA	2:G:236:ILE:HD12	2.00	0.44
2:H:161:GLY:H	2:H:505:GLY:CA	2.29	0.44
2:H:427:PHE:HB3	2:H:428:HIS:ND1	2.32	0.44
2:H:607:VAL:O	2:H:611:THR:HB	2.17	0.44
2:I:1735:ALA:O	2:I:1737:ILE:HG13	2.17	0.44
2:I:1757:GLU:H	2:I:1757:GLU:HG3	1.50	0.44
2:I:703:LEU:HD21	2:I:705:LEU:CD2	2.45	0.44
2:I:780:TYR:HB2	2:I:799:PHE:CE2	2.53	0.44
2:I:901:LYS:NZ	2:I:1031:LYS:O	2.51	0.44
1:A:1020:VAL:CG1	1:A:1400:ILE:HG23	2.47	0.44
1:A:1056:ILE:CD1	1:A:1193:TRP:CD1	3.00	0.44
1:A:66:GLU:HA	1:A:66:GLU:OE1	2.17	0.44
1:B:1040:GLU:OE2	1:B:1577:GLN:HB2	2.18	0.44
1:B:232:LEU:HD13	1:B:272:GLU:CB	2.47	0.44
1:B:32:GLN:HE22	1:B:57:ALA:N	2.16	0.44
1:C:1022:THR:HG22	1:C:1226:SER:CB	2.47	0.44
1:C:1657:HIS:CG	1:C:1658:PRO:HD2	2.53	0.44
1:C:625:THR:HG23	1:C:627:SER:H	1.83	0.44
2:G:1590:ARG:NH2	2:G:1594:GLU:OE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1752:PHE:HZ	2:G:1836:MET:HE3	1.82	0.44
2:G:1873:TYR:CE1	2:G:1877:ARG:NH2	2.84	0.44
2:G:1908:ASP:HA	2:G:1911:THR:HG22	2.00	0.44
2:G:1945:ASP:O	2:G:1949:LYS:HG3	2.17	0.44
2:G:932:ILE:HD12	2:G:939:PHE:HD1	1.83	0.44
2:H:1311:PHE:HD1	2:H:1320:LEU:O	2.00	0.44
2:H:1697:HIS:CE1	2:H:1829:GLU:CG	3.00	0.44
2:H:209:PHE:CE2	2:H:213:LEU:HD22	2.52	0.44
2:H:663:ILE:HB	2:H:664:PRO:CD	2.44	0.44
2:H:778:TYR:N	2:H:779:PRO:CD	2.80	0.44
2:I:1330:GLY:HA2	2:I:1374:THR:HG21	1.99	0.44
2:I:1420:GLU:HG3	2:I:1420:GLU:H	1.41	0.44
2:I:1651:LEU:HA	2:I:1651:LEU:HD23	1.73	0.44
2:I:1054:LEU:CB	4:I:3051:FMN:HM71	2.46	0.44
2:I:665:LEU:HD22	2:I:665:LEU:O	2.18	0.44
1:B:496:PRO:HB2	1:B:519:VAL:HG12	1.99	0.44
1:C:503:ILE:HD12	1:C:950:THR:HG21	1.98	0.44
1:C:44:VAL:HG13	1:C:78:ILE:HG12	1.99	0.44
2:G:109:LEU:HD22	2:G:114:THR:HG23	2.00	0.44
2:G:1632:ILE:O	2:G:1632:ILE:HG23	2.16	0.44
2:G:297:ARG:O	2:G:301:THR:HG22	2.17	0.44
2:G:490:TRP:HA	2:G:493:THR:HG22	1.98	0.44
2:G:562:LEU:HG	2:G:793:PRO:CB	2.48	0.44
2:G:589:ARG:HB3	2:G:590:PRO:CD	2.48	0.44
2:H:109:LEU:HD11	2:H:116:LEU:CD2	2.43	0.44
2:H:641:ILE:CG1	2:H:645:SER:HB2	2.45	0.44
2:I:1590:ARG:HG3	2:I:1608:TYR:CD2	2.53	0.44
2:I:1846:GLU:C	2:I:1848:GLY:H	2.20	0.44
2:I:468:LEU:O	2:I:471:LEU:HB2	2.18	0.44
2:I:245:GLN:HG2	2:I:505:GLY:HA2	2.00	0.44
2:I:835:THR:HG22	2:I:844:VAL:CA	2.48	0.44
2:I:9:LEU:HB2	2:I:27:PHE:HE1	1.82	0.44
1:A:1022:THR:CG2	1:A:1226:SER:OG	2.66	0.44
1:A:1135:GLU:CD	1:B:242:THR:HG21	2.38	0.44
1:A:1305:CYS:SG	1:A:1585:LYS:HA	2.57	0.44
1:B:1238:VAL:CG1	1:B:1239:HIS:N	2.81	0.44
1:B:1516:ASP:HA	1:B:1517:PRO:HD3	1.65	0.44
1:B:267:VAL:HG12	1:B:290:MET:CE	2.48	0.44
1:C:1557:ILE:HD11	1:C:1642:THR:HG21	2.00	0.44
1:C:503:ILE:HD11	1:C:947:LEU:HD22	1.98	0.44
2:G:1784:MET:HE2	2:G:1784:MET:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:551:THR:C	2:G:553:ASN:H	2.20	0.44
2:G:551:THR:HG22	2:G:552:SER:N	2.31	0.44
2:G:751:LEU:HD11	2:G:789:PHE:CD1	2.53	0.44
2:G:751:LEU:HD23	2:G:791:TYR:CD2	2.53	0.44
2:H:1389:ILE:HG13	2:H:1411:PHE:CD1	2.52	0.44
2:H:305:PHE:CD1	2:H:442:ASP:HB3	2.53	0.44
2:H:807:ILE:HA	2:H:818:LYS:HG2	1.99	0.44
2:I:1257:ASP:O	2:I:1261:ARG:HG3	2.17	0.44
2:I:159:ILE:CG2	2:I:501:ILE:HG22	2.47	0.44
2:I:1896:GLN:HE21	2:I:1896:GLN:HB3	1.58	0.44
2:I:305:PHE:CD1	2:I:442:ASP:HB3	2.52	0.44
2:I:40:ILE:O	2:I:42:PRO:HD3	2.17	0.44
2:I:720:ALA:HA	2:I:728:ILE:CD1	2.47	0.44
1:A:1194:ASN:OD1	1:A:1196:LYS:HB2	2.18	0.44
1:A:1220:VAL:O	1:A:1224:ILE:HG12	2.18	0.44
1:A:458:THR:OG1	1:A:470:LYS:HD2	2.18	0.44
1:B:1012:LEU:HD23	1:B:1445:MET:CE	2.48	0.44
1:B:1195:ALA:HB1	1:B:1200:ILE:HD12	1.99	0.44
1:C:1673:TYR:CZ	1:C:1677:VAL:HG21	2.51	0.44
2:H:1148:ASN:HD22	2:H:1148:ASN:C	2.21	0.44
2:H:1579:ILE:HD11	2:H:1615:MET:SD	2.58	0.44
1:B:29:ILE:HG12	2:H:1892:ASN:C	2.37	0.44
2:H:272:GLY:HA3	2:H:276:GLY:C	2.38	0.44
2:H:376:ASN:C	2:H:376:ASN:ND2	2.70	0.44
2:H:455:ILE:C	2:H:455:ILE:HD12	2.38	0.44
2:H:562:LEU:HG	2:H:793:PRO:CB	2.47	0.44
2:I:1739:GLU:HB2	2:I:1987:PRO:CB	2.29	0.44
2:I:184:VAL:HG12	2:I:188:ILE:HG12	1.99	0.44
2:I:1976:PHE:HB3	2:I:1981:LEU:CD2	2.48	0.44
2:I:297:ARG:O	2:I:301:THR:HG22	2.18	0.44
2:I:517:HIS:CE1	2:I:540:ASP:O	2.71	0.44
1:A:1133:PRO:HG3	1:A:1166:LYS:HG3	1.99	0.44
1:A:11:HIS:CD2	1:A:11:HIS:C	2.92	0.44
1:A:499:PRO:HD3	1:A:516:ARG:HH21	1.83	0.44
1:A:530:ALA:HA	1:A:636:PRO:HB3	1.99	0.44
1:B:1037:TRP:HB2	1:B:1598:GLN:OE1	2.18	0.44
1:B:1455:ARG:O	1:B:1459:ILE:HG13	2.18	0.44
1:B:42:GLU:O	1:B:77:GLU:N	2.47	0.44
1:C:1270:VAL:HG11	1:C:1274:ILE:HD13	1.99	0.44
1:C:1234:MET:CE	1:C:1326:ILE:HG21	2.48	0.44
1:C:601:VAL:O	1:C:602:GLU:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:706:THR:HB	1:C:737:PHE:HB3	2.00	0.44
1:C:852:ARG:HB3	1:C:858:TRP:HZ2	1.83	0.44
2:G:615:TYR:CE2	2:G:1074:MET:HB3	2.52	0.44
2:G:1257:ASP:O	2:G:1261:ARG:HG3	2.18	0.44
2:G:1551:GLU:HB2	2:G:1552:PRO:HD3	2.00	0.44
2:G:1589:VAL:HG21	2:G:1651:LEU:HD12	1.99	0.44
2:G:1776:PHE:C	2:G:1779:PRO:HD2	2.38	0.44
2:G:1662:THR:HB	2:G:1799:PRO:HG2	1.99	0.44
2:H:1228:THR:HG21	2:H:1234:VAL:HG23	2.00	0.44
2:H:184:VAL:HG12	2:H:188:ILE:HG12	2.00	0.44
1:B:20:TYR:CD2	2:H:2033:THR:OG1	2.71	0.44
2:H:732:TRP:CE2	2:H:750:MET:HE3	2.52	0.44
2:H:780:TYR:HB2	2:H:799:PHE:CE2	2.53	0.44
2:H:938:TRP:CE2	2:H:944:ARG:HG3	2.52	0.44
2:I:142:ASN:HB2	2:I:550:VAL:HG13	1.99	0.44
2:I:1579:ILE:HG22	2:I:1580:THR:O	2.18	0.44
2:I:1666:PHE:CE1	2:I:1814:ALA:HA	2.53	0.44
2:I:1886:VAL:HG22	2:I:1906:ALA:HB1	1.98	0.44
1:B:1430:ARG:HG2	1:B:1430:ARG:O	2.18	0.44
1:B:267:VAL:O	1:B:290:MET:HE1	2.17	0.44
1:C:1181:PHE:CZ	1:C:1341:PHE:HA	2.53	0.44
1:C:1291:LEU:HD21	1:C:1698:PHE:CE1	2.53	0.44
1:C:295:ALA:HB1	1:C:300:VAL:O	2.18	0.44
1:C:833:PHE:O	1:C:834:GLY:O	2.36	0.44
2:G:1004:LEU:CD2	2:G:1019:PRO:HB2	2.48	0.44
2:G:1352:HIS:HE1	2:G:1583:MET:CE	2.27	0.44
2:G:159:ILE:HD11	2:G:512:LEU:CG	2.48	0.44
2:G:459:VAL:HG12	2:G:468:LEU:HD12	2.00	0.44
2:G:901:LYS:NZ	2:G:1031:LYS:O	2.50	0.44
2:H:102:HIS:HE1	2:H:180:TYR:OH	2.00	0.44
2:H:1496:LYS:HE2	2:H:1693:ARG:HH21	1.82	0.44
2:H:1739:GLU:HB2	2:H:1987:PRO:CB	2.30	0.44
2:I:914:LEU:HD21	2:I:1003:PHE:CD2	2.53	0.44
2:I:1493:LEU:HB3	2:I:1494:PRO:CD	2.48	0.44
2:I:1684:SER:O	2:I:1688:GLN:HG3	2.18	0.44
2:I:218:TRP:HB3	2:I:225:THR:OG1	2.18	0.44
2:I:246:LEU:O	2:I:250:VAL:HG23	2.18	0.44
1:A:181:THR:O	1:A:185:GLU:HG3	2.18	0.43
1:A:406:TRP:CE3	1:A:407:ASN:HB2	2.53	0.43
1:B:35:PHE:HA	1:B:39:PHE:HD2	1.83	0.43
1:B:888:ILE:HD12	1:B:939:PHE:CE2	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1332:TYR:HB3	1:C:1382:ALA:CB	2.48	0.43
1:C:1373:ARG:NE	1:C:1550:ASP:HB2	2.33	0.43
1:C:178:GLY:O	1:C:180:SER:N	2.50	0.43
1:B:1129:GLU:OE1	1:C:348:ARG:HD3	2.18	0.43
1:C:413:LEU:C	1:C:415:SER:H	2.21	0.43
2:G:1236:LEU:HD11	2:G:1262:ILE:HG12	1.99	0.43
2:G:245:GLN:HG2	2:G:505:GLY:HA2	1.99	0.43
2:G:543:PHE:CB	2:G:545:GLN:NE2	2.81	0.43
2:G:726:PHE:HA	2:G:727:PRO:HD3	1.89	0.43
2:G:753:MET:O	2:G:757:ILE:HG13	2.18	0.43
2:G:866:LYS:O	2:G:870:GLU:HG3	2.18	0.43
2:H:1222:GLU:HG3	2:H:1235:SER:OG	2.17	0.43
2:H:1586:SER:O	2:H:1590:ARG:HB2	2.17	0.43
2:H:9:LEU:HB2	2:H:27:PHE:HE1	1.83	0.43
2:H:123:ILE:HD11	2:H:533:LEU:CD2	2.48	0.43
2:H:670:ARG:HD2	2:H:676:ILE:O	2.18	0.43
2:I:1427:VAL:HG22	2:I:1469:GLU:HG2	1.99	0.43
2:I:1551:GLU:HB2	2:I:1552:PRO:HD3	2.00	0.43
2:I:1782:THR:CG2	2:I:1827:LEU:HD21	2.45	0.43
2:I:427:PHE:HB3	2:I:428:HIS:ND1	2.33	0.43
2:I:432:LEU:HB3	2:I:484:ILE:HG23	2.00	0.43
2:I:932:ILE:HD12	2:I:939:PHE:HD1	1.83	0.43
1:A:1584:PRO:CG	1:A:1591:TRP:CZ3	3.02	0.43
1:A:626:VAL:HG23	1:A:664:GLU:OE2	2.18	0.43
1:B:1279:PHE:HB2	1:B:1282:THR:HG23	2.00	0.43
1:C:1279:PHE:HB2	1:C:1282:THR:HG23	2.00	0.43
1:C:1720:ALA:O	1:C:1721:ARG:HG2	2.17	0.43
1:C:196:THR:O	1:C:213:PHE:HE2	2.01	0.43
1:C:168:MET:HA	1:C:206:LEU:HB2	2.00	0.43
2:G:1195:VAL:HG13	2:G:1211:LEU:CB	2.48	0.43
2:G:1227:ARG:CD	2:G:1565:VAL:HG11	2.44	0.43
2:G:195:LEU:O	2:G:199:ILE:HG13	2.18	0.43
2:G:581:THR:O	2:G:585:LYS:HB2	2.18	0.43
2:G:754:TYR:CD2	2:G:794:MET:CG	3.01	0.43
2:G:900:GLN:NE2	2:G:1051:THR:HA	2.32	0.43
2:H:666:ILE:HG22	2:H:698:LEU:HD22	2.00	0.43
2:I:1778:GLN:HB2	2:I:1779:PRO:HD3	2.00	0.43
2:I:1976:PHE:HA	2:I:1981:LEU:CD2	2.48	0.43
2:I:428:HIS:CD2	2:I:488:VAL:HG23	2.53	0.43
2:I:751:LEU:HD23	2:I:791:TYR:CD2	2.53	0.43
2:I:938:TRP:CE2	2:I:944:ARG:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1209:ASP:OD2	1:A:1253:GLY:HA2	2.19	0.43
1:A:237:MET:HG3	1:A:241:PHE:HB3	2.00	0.43
1:A:235:SER:HA	1:A:276:ARG:NH2	2.32	0.43
1:A:28:TRP:HB3	2:G:1892:ASN:HA	2.00	0.43
1:A:411:GLN:O	1:A:415:SER:HB2	2.18	0.43
1:B:1248:GLY:HA3	1:B:1301:PRO:HD2	1.99	0.43
1:B:1014:ASP:N	1:B:1510:ASN:HD21	2.06	0.43
1:B:807:LYS:HD3	1:B:807:LYS:C	2.39	0.43
1:C:988:ILE:HD13	1:C:1048:GLU:HB3	2.01	0.43
1:C:1056:ILE:CD1	1:C:1193:TRP:CD1	2.99	0.43
1:C:340:ARG:HH12	1:C:344:GLN:HE21	1.65	0.43
1:C:421:ILE:HG12	1:C:469:VAL:HG21	1.98	0.43
1:C:627:SER:HB3	1:C:661:ASP:OD1	2.18	0.43
1:C:639:HIS:HB2	1:C:656:SER:OG	2.18	0.43
2:G:1327:ILE:HD12	2:G:1327:ILE:HA	1.79	0.43
2:G:1473:THR:O	2:G:1481:SER:HB3	2.18	0.43
2:G:1768:LYS:HE2	2:G:1772:SER:HB3	2.00	0.43
2:H:856:LYS:CE	2:H:1052:CYS:SG	3.06	0.43
2:H:369:SER:C	2:H:370:LEU:HD23	2.38	0.43
2:H:439:ILE:HD12	2:H:484:ILE:HD11	1.99	0.43
2:H:732:TRP:CH2	2:H:749:PRO:HG2	2.53	0.43
2:H:772:GLY:O	2:H:804:ARG:HD3	2.18	0.43
2:H:970:TYR:O	2:H:973:LEU:HB2	2.18	0.43
2:I:1241:ASN:N	2:I:1252:SER:O	2.50	0.43
2:I:159:ILE:HG12	2:I:512:LEU:HD23	2.01	0.43
2:I:1624:THR:CB	2:I:1642:THR:HG23	2.47	0.43
2:I:551:THR:C	2:I:553:ASN:H	2.22	0.43
2:I:572:ASN:CB	2:I:576:LYS:H	2.27	0.43
2:I:754:TYR:CG	2:I:794:MET:HG2	2.53	0.43
2:I:843:ILE:HD13	2:I:1055:HIS:O	2.18	0.43
1:B:1244:GLY:C	1:B:1327:CYS:HB2	2.38	0.43
1:B:176:VAL:HG12	1:B:178:GLY:H	1.83	0.43
1:C:980:VAL:HG21	2:I:952:ARG:HH21	1.83	0.43
2:G:1016:PRO:HD2	2:G:1017:PHE:CE2	2.53	0.43
2:G:1040:LEU:O	2:G:1046:GLN:HG3	2.19	0.43
2:G:1162:ASP:O	2:G:1163:LYS:HB2	2.19	0.43
2:G:1223:MET:HE3	2:G:1238:LEU:CD1	2.49	0.43
2:G:1308:CYS:HB3	2:G:1311:PHE:CE2	2.53	0.43
2:G:1674:GLN:OE1	2:G:1712:ASN:HA	2.18	0.43
2:G:1678:MET:HE3	2:G:1707:LEU:CD2	2.43	0.43
2:G:1804:PHE:CD2	2:G:1818:LEU:HD22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1846:GLU:C	2:G:1848:GLY:H	2.20	0.43
2:G:455:ILE:C	2:G:455:ILE:HD12	2.39	0.43
2:G:967:ILE:HD12	2:G:972:LEU:HD22	2.00	0.43
2:H:309:ARG:HD3	2:H:309:ARG:HA	1.63	0.43
2:I:1210:ILE:O	2:I:1210:ILE:HG22	2.18	0.43
2:I:1325:PHE:O	2:I:1328:VAL:HG12	2.18	0.43
2:I:1428:GLU:HG2	2:I:1470:THR:HG22	1.99	0.43
2:I:430:HIS:CE1	2:I:431:LEU:HD13	2.53	0.43
2:I:439:ILE:HD12	2:I:484:ILE:CD1	2.48	0.43
2:I:835:THR:HG21	2:I:855:HIS:NE2	2.33	0.43
1:A:1291:LEU:HD21	1:A:1698:PHE:CE1	2.53	0.43
1:A:1375:GLY:HA2	1:A:1546:THR:HG22	2.01	0.43
1:A:1553:GLU:HA	1:A:1556:THR:HG23	2.01	0.43
1:A:1556:THR:O	1:A:1560:MET:HG2	2.18	0.43
1:A:1673:TYR:CZ	1:A:1677:VAL:HG21	2.53	0.43
1:A:254:TRP:CZ3	1:A:302:LEU:HD13	2.53	0.43
1:A:413:LEU:HG	1:A:413:LEU:O	2.17	0.43
1:A:496:PRO:HB2	1:A:519:VAL:HG12	2.01	0.43
1:B:242:THR:HB	1:B:244:THR:HB	2.01	0.43
1:C:1021:VAL:HG22	1:C:1387:ILE:HG22	2.01	0.43
1:C:1625:LEU:O	1:C:1627:PRO:HD3	2.18	0.43
1:C:221:LEU:HA	1:C:221:LEU:HD23	1.89	0.43
1:C:235:SER:HA	1:C:276:ARG:NH2	2.33	0.43
2:G:1458:ASP:O	2:G:1462:LYS:HE3	2.19	0.43
2:G:1493:LEU:HB3	2:G:1494:PRO:CD	2.48	0.43
2:G:272:GLY:HA3	2:G:276:GLY:C	2.38	0.43
2:G:397:LYS:HB3	2:G:416:PHE:CE2	2.53	0.43
2:G:156:LEU:HD23	2:G:500:HIS:HB2	1.99	0.43
2:G:653:TYR:OH	2:G:690:VAL:HG11	2.18	0.43
2:H:1015:VAL:HG13	2:H:1017:PHE:CE2	2.53	0.43
2:H:726:PHE:HA	2:H:727:PRO:HD3	1.88	0.43
2:H:745:ASP:HA	2:H:832:TRP:CH2	2.51	0.43
2:I:1651:LEU:O	2:I:1652:THR:HG23	2.17	0.43
2:I:1496:LYS:CE	2:I:1693:ARG:HH21	2.31	0.43
2:I:397:LYS:HB3	2:I:416:PHE:CE2	2.53	0.43
2:I:439:ILE:HD12	2:I:484:ILE:HD11	1.99	0.43
2:I:562:LEU:HD23	2:I:562:LEU:HA	1.79	0.43
2:I:852:GLU:HG3	2:I:852:GLU:H	1.39	0.43
2:I:972:LEU:HD23	2:I:979:ALA:HB2	2.00	0.43
1:A:242:THR:HB	1:A:244:THR:HB	2.00	0.43
1:A:641:ARG:HD3	1:A:649:TRP:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:SER:HB2	1:A:657:SER:CB	2.48	0.43
1:A:790:PHE:CE2	1:A:794:ILE:HD11	2.53	0.43
1:B:1208:VAL:HG11	1:B:1212:THR:HB	1.97	0.43
1:B:1270:VAL:HG11	1:B:1274:ILE:HD13	2.00	0.43
1:C:1234:MET:HE3	1:C:1326:ILE:HG21	2.01	0.43
1:C:1446:LYS:O	1:C:1450:ARG:HG3	2.18	0.43
1:C:232:LEU:HD13	1:C:272:GLU:CB	2.48	0.43
1:C:378:LEU:HA	1:C:378:LEU:HD12	1.85	0.43
1:C:930:LEU:HD23	1:C:930:LEU:HA	1.68	0.43
2:G:1889:VAL:HG13	2:G:1977:HIS:HB3	1.97	0.43
2:G:419:ARG:HG3	2:G:420:PHE:N	2.33	0.43
2:G:99:ASN:HA	2:G:550:VAL:CG2	2.49	0.43
2:H:1241:ASN:N	2:H:1252:SER:O	2.51	0.43
2:H:360:LEU:HA	2:H:361:PRO:HD3	1.90	0.43
2:H:160:PHE:CE2	2:H:504:PHE:HB2	2.54	0.43
2:H:73:GLU:OE2	2:H:76:LYS:HD2	2.18	0.43
2:I:1079:ASP:O	2:I:1082:ILE:HG22	2.19	0.43
2:I:1236:LEU:HD22	2:I:1238:LEU:HG	1.99	0.43
2:I:1959:LYS:HG2	2:I:1959:LYS:O	2.19	0.43
2:I:279:THR:O	2:I:283:ILE:HB	2.19	0.43
2:I:871:THR:HG21	2:I:887:LYS:HZ1	1.83	0.43
1:A:1431:GLU:OE2	1:A:1433:HIS:HE1	2.02	0.43
1:A:267:VAL:O	1:A:290:MET:HE1	2.19	0.43
1:A:988:ILE:CD1	1:A:1048:GLU:HA	2.48	0.43
1:B:1219:VAL:CA	1:B:1384:ILE:HD11	2.32	0.43
1:B:1233:GLU:CD	1:B:1680:ARG:HH21	2.22	0.43
1:B:370:GLU:O	1:B:373:ALA:HB3	2.19	0.43
1:C:1248:GLY:HA3	1:C:1301:PRO:HD2	2.01	0.43
1:C:1431:GLU:OE2	1:C:1433:HIS:HE1	2.00	0.43
1:C:1375:GLY:HA2	1:C:1546:THR:HG22	1.99	0.43
1:C:1553:GLU:HA	1:C:1556:THR:HG23	2.01	0.43
1:C:1539:ALA:O	1:C:1574:GLY:HA2	2.18	0.43
1:C:1599:ILE:HD11	1:C:1606:PRO:HD2	2.01	0.43
1:C:49:PRO:O	1:C:82:SER:HB2	2.19	0.43
2:G:184:VAL:HG12	2:G:188:ILE:HG12	2.00	0.43
2:G:184:VAL:O	2:G:184:VAL:HG12	2.19	0.43
2:G:324:LEU:O	2:G:324:LEU:HD12	2.18	0.43
2:G:573:LYS:C	2:G:575:GLY:H	2.21	0.43
2:G:652:ILE:HD13	2:G:658:MET:HE3	1.99	0.43
2:G:854:ILE:HG22	2:G:856:LYS:HG3	2.01	0.43
2:H:1223:MET:HE3	2:H:1238:LEU:CD1	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1422:THR:HG23	2:H:1474:PHE:CD1	2.54	0.43
2:H:573:LYS:C	2:H:575:GLY:H	2.21	0.43
2:H:629:GLY:O	2:H:632:ALA:HB3	2.18	0.43
2:H:643:LYS:HA	2:H:1163:LYS:HG2	1.99	0.43
2:H:653:TYR:OH	2:H:690:VAL:HG11	2.18	0.43
2:I:607:VAL:O	2:I:611:THR:HB	2.18	0.43
2:I:7:ARG:NH2	2:I:24:THR:O	2.52	0.43
1:A:1009:LEU:CD1	1:A:1445:MET:HE1	2.48	0.43
1:A:644:THR:HG23	1:A:648:ASP:N	2.34	0.43
1:A:827:SER:HA	1:A:828:PRO:HD3	1.70	0.43
1:B:1375:GLY:HA2	1:B:1546:THR:HG22	2.01	0.43
1:B:1446:LYS:O	1:B:1450:ARG:HG3	2.19	0.43
1:B:681:THR:HA	1:B:706:THR:OG1	2.19	0.43
1:C:1158:PRO:HD2	1:C:1159:GLU:OE2	2.18	0.43
1:A:335:HIS:ND1	1:C:335:HIS:HE1	2.17	0.43
2:G:1004:LEU:HD21	2:G:1020:VAL:CG2	2.48	0.43
2:G:1175:LYS:HG3	2:G:1176:PRO:HD2	2.00	0.43
2:G:324:LEU:O	2:G:328:LEU:HG	2.18	0.43
2:G:601:THR:O	2:G:601:THR:CG2	2.67	0.43
2:G:786:SER:HB3	2:G:794:MET:HE2	2.01	0.43
2:G:860:ARG:H	2:G:1049:GLN:HG3	1.83	0.43
2:H:1567:ARG:HH11	2:H:1567:ARG:HG2	1.72	0.43
2:H:1940:LEU:HD12	2:H:1941:PHE:N	2.34	0.43
2:H:654:VAL:HG12	2:H:654:VAL:O	2.18	0.43
2:I:1168:ASN:HA	2:I:1169:PRO:HD3	1.84	0.43
2:I:1552:PRO:O	2:I:1556:VAL:HG23	2.19	0.43
2:I:169:TYR:CG	2:I:170:PHE:N	2.87	0.43
2:I:2030:TYR:CD1	2:I:2034:GLY:HA2	2.54	0.43
2:I:425:SER:HA	2:I:426:PRO:HD3	1.78	0.43
2:I:846:VAL:CG1	2:I:865:TRP:NE1	2.82	0.43
1:A:1431:GLU:CG	1:A:1433:HIS:CE1	3.00	0.43
1:A:1670:TYR:O	1:A:1674:VAL:HG23	2.18	0.43
1:A:933:VAL:HA	1:A:934:PRO:HD3	1.84	0.43
1:A:833:PHE:HA	1:A:937:LYS:HD2	2.00	0.43
1:B:1431:GLU:CG	1:B:1433:HIS:CE1	3.02	0.43
1:B:1657:HIS:HA	1:B:1658:PRO:HD3	1.89	0.43
1:B:460:GLU:CG	1:B:470:LYS:HD3	2.48	0.43
1:C:1600:LEU:HD11	1:C:1655:VAL:HG12	2.00	0.43
2:G:884:LEU:HD22	2:G:1021:LEU:CD1	2.49	0.43
2:G:1219:ILE:HB	2:G:1240:TYR:HB2	2.01	0.43
2:G:1875:VAL:HG22	2:G:1910:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2042:ILE:HG12	2:G:2042:ILE:H	1.39	0.43
2:G:28:PHE:CE2	2:H:7:ARG:CD	2.73	0.43
2:G:486:LEU:HA	2:G:487:PRO:HD3	1.90	0.43
2:G:15:SER:H	2:G:48:PHE:HE2	1.67	0.43
2:G:835:THR:HG22	2:G:844:VAL:HA	2.00	0.43
2:H:1862:VAL:HG22	2:H:1863:ALA:N	2.33	0.43
2:H:543:PHE:CB	2:H:545:GLN:NE2	2.81	0.43
2:H:717:ILE:HG23	2:H:760:HIS:CE1	2.54	0.43
2:I:615:TYR:CE2	2:I:1074:MET:HB3	2.53	0.43
2:I:1561:ASN:HA	2:I:1562:PRO:HD3	1.80	0.43
2:I:1662:THR:HB	2:I:1799:PRO:HG2	2.00	0.43
2:I:1873:TYR:CE1	2:I:1877:ARG:NH2	2.81	0.43
2:I:209:PHE:CE2	2:I:213:LEU:HD22	2.53	0.43
2:I:573:LYS:C	2:I:575:GLY:N	2.72	0.43
2:I:702:TYR:HB3	2:I:727:PRO:HB2	2.00	0.43
2:I:967:ILE:HD12	2:I:972:LEU:HD22	2.00	0.43
1:A:1107:GLU:HA	1:A:1108:PRO:HD3	1.90	0.43
1:A:196:THR:O	1:A:213:PHE:HE2	2.01	0.43
1:A:460:GLU:CG	1:A:470:LYS:HD3	2.49	0.43
1:A:32:GLN:HE22	1:A:57:ALA:N	2.16	0.43
1:A:44:VAL:HG11	1:A:78:ILE:HG12	1.96	0.43
1:B:1283:MET:O	1:B:1287:VAL:HG23	2.18	0.43
1:B:1553:GLU:HA	1:B:1556:THR:HG23	2.00	0.43
1:B:260:ARG:HH12	1:B:300:VAL:CG2	2.20	0.43
1:B:335:HIS:C	1:B:335:HIS:CD2	2.92	0.43
1:B:411:GLN:O	1:B:415:SER:HB2	2.18	0.43
1:C:1047:LEU:O	1:C:1051:VAL:HG23	2.19	0.43
1:C:1107:GLU:HA	1:C:1108:PRO:HD3	1.89	0.43
1:C:1208:VAL:HG11	1:C:1212:THR:HB	1.98	0.43
1:C:1430:ARG:O	1:C:1430:ARG:HG2	2.19	0.43
1:C:852:ARG:NH1	1:C:856:GLU:OE1	2.52	0.43
2:G:1339:PHE:N	2:G:1340:PRO:CD	2.82	0.43
2:G:1348:LEU:HD12	2:G:1348:LEU:HA	1.81	0.43
2:G:1327:ILE:HG12	2:G:1583:MET:HE3	2.01	0.43
2:G:1858:ASN:HA	2:G:1896:GLN:O	2.18	0.43
2:G:339:LEU:HD23	2:G:419:ARG:O	2.19	0.43
2:G:441:LYS:O	2:G:445:LYS:HG3	2.18	0.43
2:G:634:ILE:CD1	2:G:649:ILE:HD11	2.43	0.43
2:H:1293:THR:CG2	2:H:1296:GLU:H	2.24	0.43
2:H:595:PRO:HD3	2:H:800:LEU:HB2	2.01	0.43
2:I:652:ILE:CD1	2:I:658:MET:HE3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:950:PHE:O	2:I:953:ARG:HB3	2.19	0.43
1:A:1396:MET:O	1:A:1680:ARG:NH1	2.52	0.42
1:A:1539:ALA:O	1:A:1574:GLY:HA2	2.18	0.42
1:A:155:VAL:O	1:A:159:LEU:HG	2.19	0.42
1:A:2:LYS:HE2	1:A:4:GLU:OE1	2.19	0.42
1:A:705:VAL:HG23	1:A:732:LEU:CD2	2.48	0.42
1:B:1050:CYS:HB3	1:B:1089:VAL:HG12	2.00	0.42
1:B:1263:ASP:HB2	1:B:1270:VAL:HG21	2.00	0.42
1:B:1406:MET:HE1	1:B:1428:THR:HB	2.01	0.42
1:B:335:HIS:CD2	1:B:335:HIS:O	2.70	0.42
1:B:350:LEU:HB2	1:B:352:MET:HG2	2.01	0.42
1:B:430:ARG:NH2	1:B:605:LEU:HD13	2.33	0.42
1:C:1175:ILE:HA	1:C:1176:PRO:HD3	1.89	0.42
1:C:1243:VAL:O	1:C:1296:GLY:HA3	2.18	0.42
1:C:1431:GLU:CG	1:C:1433:HIS:CE1	3.01	0.42
2:G:23:PRO:HG2	2:G:86:LEU:HD11	2.00	0.42
2:H:1257:ASP:O	2:H:1261:ARG:HG3	2.19	0.42
2:H:1458:ASP:O	2:H:1462:LYS:HE3	2.19	0.42
2:H:1847:LEU:H	2:H:1847:LEU:CD1	2.12	0.42
2:H:551:THR:C	2:H:553:ASN:H	2.21	0.42
2:I:1311:PHE:HD1	2:I:1320:LEU:O	2.02	0.42
2:I:1868:GLN:HG3	2:I:1898:TYR:HH	1.83	0.42
2:I:1878:VAL:CG1	2:I:1910:VAL:HG22	2.36	0.42
2:I:7:ARG:CG	2:I:22:VAL:O	2.67	0.42
2:I:516:THR:O	2:I:519:ASN:HB2	2.19	0.42
2:I:736:ARG:HG3	2:I:736:ARG:H	1.57	0.42
2:I:835:THR:HB	2:I:845:THR:HG23	2.01	0.42
1:A:1195:ALA:HB1	1:A:1200:ILE:HD12	2.02	0.42
1:A:1495:ASN:HD22	1:A:1495:ASN:HA	1.67	0.42
1:A:32:GLN:NE2	1:A:57:ALA:HA	2.34	0.42
1:B:1119:LYS:HE2	1:B:1341:PHE:CD1	2.54	0.42
1:B:417:TYR:HH	1:B:458:THR:HG22	1.84	0.42
1:C:1308:SER:HB3	1:C:1589:GLY:HA3	2.01	0.42
1:C:1618:LEU:HD23	1:C:1621:PHE:CE2	2.55	0.42
1:C:1657:HIS:CE1	1:C:1658:PRO:HD2	2.54	0.42
1:C:1239:HIS:HE1	1:C:1714:VAL:O	2.02	0.42
1:C:949:GLU:O	1:C:953:VAL:CG1	2.67	0.42
2:G:1320:LEU:HD12	2:G:1320:LEU:HA	1.88	0.42
2:G:238:CYS:CB	2:G:239:PRO:HD3	2.45	0.42
2:G:612:ASN:HD21	2:G:641:ILE:HA	1.85	0.42
2:H:1070:ILE:CD1	2:H:1074:MET:HG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1149:TRP:HA	2:H:1242:PHE:CD1	2.54	0.42
2:H:1335:ILE:O	2:H:1338:ILE:HG12	2.19	0.42
2:H:127:ILE:HD12	2:H:180:TYR:CD2	2.54	0.42
1:B:12:ILE:CD1	2:H:2041:ILE:HD11	2.49	0.42
2:H:245:GLN:HG2	2:H:505:GLY:HA2	2.00	0.42
2:H:274:SER:OG	2:H:428:HIS:HE1	2.02	0.42
2:H:279:THR:O	2:H:283:ILE:HB	2.20	0.42
2:H:665:LEU:HD22	2:H:665:LEU:O	2.19	0.42
2:H:866:LYS:O	2:H:870:GLU:HG3	2.19	0.42
2:H:938:TRP:CD1	2:H:944:ARG:HG3	2.53	0.42
2:I:896:ASN:O	2:I:1050:ARG:NH2	2.52	0.42
2:I:1321:ALA:HA	2:I:1322:PRO:HD3	1.83	0.42
2:I:1666:PHE:CD1	2:I:1814:ALA:HB2	2.54	0.42
2:I:503:ASP:O	2:I:530:ALA:HB3	2.19	0.42
2:I:538:ASP:HB2	2:I:540:ASP:HB2	2.01	0.42
2:I:810:GLU:OE2	2:I:1070:ILE:N	2.43	0.42
2:I:856:LYS:CE	2:I:1052:CYS:SG	3.07	0.42
1:A:1131:LEU:HD12	1:A:1131:LEU:HA	1.76	0.42
1:A:1132:GLU:HA	1:A:1133:PRO:HD3	1.94	0.42
1:A:290:MET:HB3	1:A:290:MET:HE2	1.93	0.42
1:B:1145:LYS:HD3	1:B:1154:ILE:HG12	2.01	0.42
1:B:1420:ALA:HA	1:B:1421:PRO:HD3	1.74	0.42
1:B:155:VAL:HG22	1:B:186:ILE:CG2	2.50	0.42
1:B:280:GLU:O	1:B:284:LYS:HG3	2.20	0.42
1:B:828:PRO:HG3	1:B:868:ILE:HG22	2.00	0.42
1:B:908:LEU:HA	1:B:913:VAL:HG21	2.00	0.42
1:C:1114:TYR:CE1	1:C:1337:GLU:HG3	2.55	0.42
1:C:408:TRP:CH2	1:C:1628:SER:HB3	2.55	0.42
1:C:330:GLU:O	1:C:330:GLU:HG2	2.18	0.42
2:G:1031:LYS:O	2:G:1032:ASP:C	2.57	0.42
2:G:1986:LYS:N	2:G:1987:PRO:CD	2.82	0.42
2:G:2026:PHE:HB3	2:G:2042:ILE:HD13	2.00	0.42
2:G:421:LEU:HA	2:G:422:PRO:HD3	1.81	0.42
2:G:543:PHE:HB2	2:G:545:GLN:NE2	2.25	0.42
2:G:586:LEU:HD12	2:G:764:MET:SD	2.59	0.42
2:H:1080:GLY:O	2:H:1084:LYS:HG3	2.19	0.42
2:H:1159:ILE:CG2	2:H:1160:THR:N	2.82	0.42
2:H:1383:ASN:HD21	2:H:1418:ASP:HB3	1.84	0.42
2:H:1497:GLU:OE1	2:H:2002:LYS:CE	2.66	0.42
2:H:1551:GLU:HB2	2:H:1552:PRO:HD3	2.00	0.42
2:H:240:LEU:HA	2:H:240:LEU:HD12	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:258:PHE:N	2:H:258:PHE:CD1	2.87	0.42
2:H:38:ASN:HA	2:H:41:LEU:HD12	2.01	0.42
2:H:967:ILE:CD1	2:H:972:LEU:HD22	2.50	0.42
2:I:1085:LEU:HD12	2:I:1085:LEU:HA	1.82	0.42
2:I:190:PHE:O	2:I:194:THR:HG22	2.19	0.42
2:I:234:ILE:HG13	2:I:235:PRO:CD	2.46	0.42
2:I:309:ARG:HD3	2:I:309:ARG:HA	1.61	0.42
2:I:726:PHE:HA	2:I:727:PRO:HD3	1.86	0.42
2:I:778:TYR:N	2:I:779:PRO:CD	2.82	0.42
1:A:460:GLU:H	1:A:460:GLU:HG3	1.34	0.42
1:B:874:GLY:O	1:B:875:THR:C	2.58	0.42
1:C:1219:VAL:CA	1:C:1384:ILE:CD1	2.94	0.42
1:C:183:GLN:NE2	1:C:202:GLU:HG2	2.31	0.42
1:C:21:GLN:HB3	1:C:21:GLN:HE21	1.69	0.42
1:C:406:TRP:CE3	1:C:407:ASN:HB2	2.53	0.42
1:C:798:ASN:HA	1:C:801:ARG:HB2	2.02	0.42
2:G:1749:GLU:OE2	2:G:1840:VAL:HG13	2.19	0.42
2:G:1878:VAL:CG1	2:G:1910:VAL:HG22	2.34	0.42
2:G:503:ASP:OD2	2:G:513:GLY:N	2.50	0.42
2:H:1159:ILE:HG13	2:H:1169:PRO:CD	2.50	0.42
2:H:1427:VAL:HG22	2:H:1469:GLU:CG	2.50	0.42
2:H:176:LEU:CD2	2:H:184:VAL:HG21	2.50	0.42
2:H:1986:LYS:N	2:H:1987:PRO:CD	2.81	0.42
2:H:520:LYS:O	2:H:521:ASP:C	2.58	0.42
2:H:536:ASN:HD21	2:H:540:ASP:HB3	1.84	0.42
2:H:741:HIS:CE1	2:H:855:HIS:NE2	2.88	0.42
2:I:1102:TYR:HB3	2:I:1244:PRO:CA	2.49	0.42
2:I:1175:LYS:HG3	2:I:1176:PRO:HD2	2.00	0.42
2:I:120:LYS:HB3	2:I:124:LYS:HE3	2.01	0.42
2:I:1590:ARG:HG3	2:I:1608:TYR:CG	2.54	0.42
2:I:2042:ILE:HG12	2:I:2042:ILE:H	1.36	0.42
2:I:441:LYS:O	2:I:445:LYS:HG3	2.19	0.42
2:I:674:TYR:HA	2:I:675:PRO:HD3	1.69	0.42
1:A:1195:ALA:CB	1:A:1213:LEU:HD13	2.49	0.42
1:A:382:LEU:HA	1:A:382:LEU:HD23	1.79	0.42
1:B:1022:THR:HG22	1:B:1226:SER:CB	2.49	0.42
1:B:1234:MET:HE3	1:B:1326:ILE:HG21	2.01	0.42
1:B:1385:GLN:HE21	1:B:1385:GLN:HB3	1.66	0.42
1:B:1534:ASP:OD1	1:B:1566:ARG:HD3	2.19	0.42
1:B:157:HIS:CE1	1:B:269:LEU:HD11	2.55	0.42
1:B:272:GLU:HA	1:B:273:PRO:HD3	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1455:ARG:HD2	1:C:1455:ARG:HA	1.82	0.42
1:C:1592:MET:HE2	1:C:1641:ILE:HG23	2.00	0.42
1:C:408:TRP:CZ3	1:C:1628:SER:HB3	2.54	0.42
1:C:413:LEU:O	1:C:413:LEU:HG	2.19	0.42
1:C:32:GLN:NE2	1:C:57:ALA:CA	2.82	0.42
2:G:1135:GLU:HG2	2:G:1176:PRO:HG2	2.02	0.42
2:G:517:HIS:CE1	2:G:540:ASP:O	2.73	0.42
2:G:638:VAL:HG22	2:G:675:PRO:HG2	2.01	0.42
2:H:1149:TRP:NE1	2:H:1213:LEU:HD12	2.34	0.42
2:H:1294:ALA:HA	2:H:1368:VAL:CG2	2.49	0.42
1:B:20:TYR:HE1	2:H:2035:SER:HB2	1.82	0.42
2:H:676:ILE:O	2:H:676:ILE:HG12	2.17	0.42
2:H:751:LEU:HD11	2:H:789:PHE:CD1	2.55	0.42
2:I:463:PHE:CD1	2:I:486:LEU:HD22	2.54	0.42
2:I:730:LEU:C	2:I:730:LEU:HD12	2.40	0.42
2:I:786:SER:HB3	2:I:794:MET:HE2	2.01	0.42
2:I:754:TYR:CE2	2:I:794:MET:HG3	2.53	0.42
2:I:835:THR:HG22	2:I:844:VAL:C	2.40	0.42
1:A:1420:ALA:HA	1:A:1421:PRO:HD3	1.75	0.42
1:A:529:MET:HG2	1:A:638:LEU:CG	2.50	0.42
1:B:1239:HIS:CD2	1:B:1241:SER:OG	2.59	0.42
1:B:706:THR:HB	1:B:737:PHE:HB3	2.01	0.42
1:B:982:ILE:HG23	2:H:956:GLU:HG2	2.01	0.42
1:C:1220:VAL:O	1:C:1224:ILE:HG12	2.19	0.42
1:C:406:TRP:CD2	1:C:1619:GLU:HG3	2.55	0.42
1:C:1639:VAL:CG1	1:C:1640:SER:N	2.82	0.42
1:C:475:GLN:CD	1:C:614:ALA:HB2	2.40	0.42
2:G:1180:MET:HB3	2:G:1199:GLU:HG2	2.00	0.42
2:G:786:SER:HB2	2:G:794:MET:HE2	2.00	0.42
2:H:345:THR:HG22	2:H:347:GLU:N	2.25	0.42
2:H:60:LEU:HD23	2:H:60:LEU:O	2.20	0.42
2:H:900:GLN:NE2	2:H:1051:THR:HA	2.34	0.42
2:I:1217:ASN:HD22	2:I:1217:ASN:HA	1.60	0.42
2:I:1359:MET:CE	2:I:1404:MET:HB3	2.50	0.42
2:I:298:LYS:HA	2:I:448:VAL:CG2	2.49	0.42
2:I:33:LEU:HD21	2:I:80:PHE:CE2	2.54	0.42
1:A:1019:ILE:HG13	1:A:1316:VAL:HG13	2.01	0.42
1:A:1263:ASP:HB2	1:A:1270:VAL:HG21	2.01	0.42
1:A:181:THR:HG22	1:A:185:GLU:OE2	2.19	0.42
1:A:1:MET:HE3	1:A:9:LEU:HD12	2.01	0.42
1:B:1238:VAL:CG1	1:B:1242:GLU:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1264:ARG:NH1	1:B:1270:VAL:HB	2.35	0.42
1:B:1244:GLY:O	1:B:1327:CYS:HB2	2.20	0.42
1:B:1682:LYS:HB3	2:H:994:PHE:CE2	2.54	0.42
1:B:242:THR:HG22	1:B:243:ILE:H	1.83	0.42
1:B:625:THR:HG23	1:B:627:SER:H	1.84	0.42
1:C:1067:LEU:HA	1:C:1067:LEU:HD23	1.76	0.42
1:C:377:TYR:O	1:C:380:ALA:HB3	2.19	0.42
1:C:438:ASN:HD21	1:C:698:GLN:HE21	1.66	0.42
2:G:1044:VAL:HG21	2:G:1050:ARG:NE	2.34	0.42
2:G:856:LYS:CE	2:G:1052:CYS:SG	3.08	0.42
2:G:1149:TRP:NE1	2:G:1213:LEU:HD12	2.35	0.42
2:G:507:GLY:O	2:G:508:GLY:C	2.58	0.42
2:G:810:GLU:OE2	2:G:1070:ILE:N	2.44	0.42
2:G:938:TRP:CE2	2:G:944:ARG:HG3	2.54	0.42
2:H:1002:HIS:NE2	2:H:1006:MET:CE	2.82	0.42
2:H:804:ARG:NH1	2:H:1062:PHE:O	2.52	0.42
2:H:1175:LYS:HG3	2:H:1176:PRO:HD2	2.02	0.42
2:H:1339:PHE:N	2:H:1340:PRO:CD	2.83	0.42
2:H:581:THR:O	2:H:585:LYS:HB2	2.20	0.42
2:H:712:ALA:O	2:H:716:VAL:HG23	2.20	0.42
2:H:754:TYR:CG	2:H:794:MET:HG2	2.55	0.42
2:H:949:ASP:HB3	2:H:1006:MET:CE	2.47	0.42
2:I:1129:ALA:HB2	2:I:1138:TRP:CH2	2.55	0.42
2:I:1273:GLU:HB3	2:I:1274:PRO:CD	2.50	0.42
2:I:1343:VAL:HG22	2:I:1343:VAL:O	2.20	0.42
2:I:1989:LYS:NZ	2:I:2037:PRO:HG2	2.35	0.42
2:I:2046:GLU:C	2:I:2048:TYR:N	2.73	0.42
2:I:44:PRO:HA	2:I:53:GLU:OE2	2.19	0.42
2:I:703:LEU:CD2	2:I:705:LEU:HG	2.50	0.42
2:I:73:GLU:OE2	2:I:76:LYS:HD2	2.18	0.42
2:I:740:HIS:HA	2:I:854:ILE:HD13	2.01	0.42
2:I:745:ASP:HA	2:I:832:TRP:CH2	2.49	0.42
1:A:1260:MET:HB2	1:A:1274:ILE:HD12	2.02	0.42
1:A:408:TRP:CH2	1:A:1628:SER:HB3	2.55	0.42
1:A:655:LEU:HA	1:A:655:LEU:HD23	1.81	0.42
1:A:800:LEU:HA	1:A:800:LEU:HD23	1.84	0.42
1:B:1012:LEU:HD23	1:B:1445:MET:HE3	2.00	0.42
1:B:458:THR:OG1	1:B:470:LYS:HD2	2.20	0.42
1:B:798:ASN:HA	1:B:801:ARG:HB2	2.02	0.42
1:C:1310:GLU:OE1	1:C:1649:LYS:CE	2.65	0.42
1:C:155:VAL:O	1:C:159:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:LYS:HE2	1:C:4:GLU:OE1	2.19	0.42
1:C:37:LYS:HB2	1:C:65:TYR:CE1	2.52	0.42
2:G:1014:PRO:HG2	2:G:1032:ASP:HB2	2.01	0.42
2:G:1079:ASP:O	2:G:1082:ILE:HG22	2.19	0.42
2:G:1217:ASN:HA	2:G:1217:ASN:HD22	1.62	0.42
2:G:1383:ASN:OD1	2:G:1388:LYS:HG3	2.20	0.42
2:G:237:SER:O	2:G:241:ILE:HG13	2.20	0.42
2:G:258:PHE:HD1	2:G:258:PHE:N	2.18	0.42
2:G:732:TRP:CH2	2:G:749:PRO:HG2	2.55	0.42
2:G:7:ARG:NH1	2:G:24:THR:CG2	2.79	0.42
2:G:827:VAL:HG21	2:G:840:THR:CG2	2.49	0.42
1:A:987:ASN:HD22	2:G:957:ARG:CD	2.30	0.42
2:H:1642:THR:HB	2:H:1651:LEU:HB2	2.01	0.42
2:H:33:LEU:HD13	2:H:68:VAL:HG22	2.02	0.42
2:H:624:TYR:HB2	2:H:630:MET:HE3	2.02	0.42
2:H:844:VAL:HG22	2:H:858:ALA:HB2	2.01	0.42
2:I:732:TRP:CH2	2:I:749:PRO:HG2	2.55	0.42
1:A:1332:TYR:HB3	1:A:1382:ALA:CB	2.50	0.42
1:A:1618:LEU:HD23	1:A:1621:PHE:CE2	2.54	0.42
1:A:155:VAL:HG22	1:A:186:ILE:CG2	2.50	0.42
1:A:335:HIS:CD2	1:A:335:HIS:C	2.92	0.42
1:A:444:ASN:CB	1:A:446:ALA:H	2.32	0.42
1:A:453:TYR:O	1:A:457:ASN:HB2	2.20	0.42
1:B:1189:ILE:HG23	1:B:1190:PRO:HD2	2.01	0.42
1:B:1539:ALA:O	1:B:1574:GLY:HA2	2.20	0.42
1:B:1705:PRO:HB2	1:B:1733:PHE:CD1	2.55	0.42
1:B:1:MET:HE3	1:B:6:GLU:HA	2.01	0.42
1:B:780:GLU:O	1:B:781:LEU:C	2.58	0.42
1:B:44:VAL:HG11	1:B:78:ILE:HG12	2.00	0.42
1:C:1012:LEU:HD23	1:C:1445:MET:HE2	2.02	0.42
1:C:1154:ILE:O	1:C:1154:ILE:HG13	2.20	0.42
1:C:1244:GLY:HA3	1:C:1297:PRO:HD2	2.02	0.42
2:G:1666:PHE:CD1	2:G:1814:ALA:CB	3.02	0.42
2:G:2036:GLU:HB2	2:G:2037:PRO:CD	2.48	0.42
2:G:892:ILE:HD11	2:G:903:TRP:CD2	2.51	0.42
2:H:1889:VAL:HG22	2:H:1977:HIS:O	2.19	0.42
1:B:31:THR:CG2	2:H:2011:ILE:HG21	2.40	0.42
1:B:20:TYR:CZ	2:H:2035:SER:HB2	2.53	0.42
2:H:433:VAL:N	2:H:434:PRO:CD	2.83	0.42
2:H:641:ILE:CD1	2:H:645:SER:HB2	2.50	0.42
2:H:995:LEU:HB3	2:H:1000:ILE:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1135:GLU:HG2	2:I:1176:PRO:HG2	2.02	0.42
2:I:1223:MET:HE3	2:I:1238:LEU:CD1	2.49	0.42
2:I:1593:ILE:O	2:I:1597:ALA:HB3	2.20	0.42
2:I:360:LEU:HA	2:I:361:PRO:HD3	1.89	0.42
2:I:879:LYS:HA	2:I:879:LYS:HD3	1.73	0.42
1:A:1234:MET:HE3	1:A:1326:ILE:HG21	2.02	0.42
1:A:998:TYR:CD2	1:A:1667:GLU:HG3	2.55	0.42
1:A:350:LEU:HD23	1:A:350:LEU:HA	1.89	0.42
1:A:483:VAL:O	1:A:486:VAL:HB	2.20	0.42
1:A:521:LYS:HB3	1:A:523:SER:HB3	2.01	0.42
1:A:32:GLN:HE21	1:A:57:ALA:HB2	1.85	0.42
1:A:780:GLU:O	1:A:781:LEU:C	2.59	0.42
1:B:1175:ILE:HA	1:B:1176:PRO:HD3	1.89	0.42
1:B:140:ILE:CG2	1:B:141:ALA:N	2.83	0.42
1:B:438:ASN:ND2	1:B:698:GLN:HE21	2.14	0.42
1:C:1029:PRO:HA	1:C:1188:GLN:O	2.20	0.42
1:C:1370:THR:HG22	1:C:1371:THR:N	2.35	0.42
1:C:19:ALA:O	1:C:22:PHE:HB2	2.19	0.42
2:G:1236:LEU:HA	2:G:1237:PRO:HD3	1.76	0.42
2:G:1360:ILE:HA	2:G:1361:PRO:HD3	1.91	0.42
2:G:1383:ASN:HD21	2:G:1418:ASP:HB3	1.85	0.42
2:G:1782:THR:CG2	2:G:1827:LEU:HD21	2.48	0.42
2:G:298:LYS:HA	2:G:448:VAL:CG2	2.50	0.42
2:G:427:PHE:HB3	2:G:428:HIS:ND1	2.34	0.42
2:G:468:LEU:O	2:G:471:LEU:HB2	2.20	0.42
2:G:670:ARG:HD2	2:G:676:ILE:O	2.20	0.42
2:G:736:ARG:H	2:G:736:ARG:HG3	1.59	0.42
2:H:1180:MET:HB3	2:H:1199:GLU:HG2	2.02	0.42
2:H:1343:VAL:HG22	2:H:1343:VAL:O	2.20	0.42
2:H:1666:PHE:CD1	2:H:1814:ALA:CB	3.03	0.42
2:H:1855:ILE:HB	2:H:1907:LEU:HD12	2.01	0.42
2:H:2036:GLU:HB2	2:H:2037:PRO:CD	2.47	0.42
2:H:234:ILE:HG13	2:H:235:PRO:CD	2.47	0.42
2:H:23:PRO:HG2	2:H:86:LEU:HD11	2.01	0.42
2:H:421:LEU:HA	2:H:422:PRO:HD3	1.78	0.42
2:I:804:ARG:NH2	2:I:1068:GLU:OE1	2.53	0.42
2:I:1214:LEU:HD11	2:I:1220:GLN:NE2	2.35	0.42
2:I:1335:ILE:O	2:I:1338:ILE:HG12	2.20	0.42
2:I:1738:PHE:HE1	2:I:1837:THR:HG23	1.85	0.42
2:I:258:PHE:N	2:I:258:PHE:CD1	2.87	0.42
1:A:1279:PHE:HB2	1:A:1282:THR:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1308:SER:HB3	1:A:1589:GLY:HA3	2.01	0.41
1:A:1019:ILE:HG21	1:A:1316:VAL:HG22	2.01	0.41
1:A:1657:HIS:CG	1:A:1658:PRO:HD2	2.55	0.41
1:A:32:GLN:NE2	1:A:57:ALA:CA	2.83	0.41
1:B:1019:ILE:HG13	1:B:1316:VAL:HG13	2.02	0.41
1:B:1673:TYR:CZ	1:B:1677:VAL:HG21	2.55	0.41
1:C:1215:VAL:O	1:C:1219:VAL:HG23	2.20	0.41
1:C:12:ILE:HD11	2:I:2041:ILE:HD11	2.01	0.41
1:C:616:LEU:HB2	1:C:617:PRO:HD3	2.01	0.41
1:C:635:ILE:CG2	1:C:651:TYR:CG	3.03	0.41
2:G:1128:LYS:HG2	2:G:1181:VAL:HG22	2.02	0.41
2:G:1579:ILE:CD1	2:G:1615:MET:SD	3.08	0.41
2:G:1496:LYS:CE	2:G:1693:ARG:HH21	2.28	0.41
2:G:439:ILE:HD12	2:G:484:ILE:HD11	2.01	0.41
2:G:638:VAL:HA	2:G:641:ILE:CG2	2.50	0.41
2:H:896:ASN:O	2:H:1050:ARG:NH2	2.53	0.41
2:H:2010:TYR:O	2:H:2012:PRO:HD3	2.20	0.41
2:H:240:LEU:O	2:H:244:ILE:HG13	2.19	0.41
2:H:258:PHE:N	2:H:258:PHE:HD1	2.18	0.41
2:I:1815:LEU:O	2:I:1821:VAL:HG23	2.20	0.41
2:I:1697:HIS:CE1	2:I:1829:GLU:CG	3.03	0.41
2:I:1980:TYR:HD1	2:I:1981:LEU:HD12	1.85	0.41
2:I:441:LYS:HG2	2:I:445:LYS:HE3	2.02	0.41
2:I:512:LEU:O	2:I:516:THR:HG23	2.20	0.41
2:I:659:LEU:O	2:I:663:ILE:HG12	2.20	0.41
1:A:1233:GLU:CD	1:A:1680:ARG:HH21	2.24	0.41
1:A:280:GLU:O	1:A:284:LYS:HG3	2.21	0.41
1:A:28:TRP:CE2	1:A:53:LEU:HD22	2.55	0.41
1:A:340:ARG:NH1	1:A:344:GLN:CG	2.70	0.41
1:A:50:SER:CB	1:A:51:PRO:CD	2.98	0.41
1:B:290:MET:HE2	1:B:290:MET:HB3	1.96	0.41
1:C:1584:PRO:CG	1:C:1591:TRP:CZ3	3.03	0.41
1:C:12:ILE:O	1:C:15:THR:HG23	2.20	0.41
1:C:889:GLU:C	1:C:891:MET:H	2.24	0.41
2:G:1553:TYR:OH	2:G:1583:MET:HB3	2.20	0.41
2:G:1755:ILE:HD11	2:G:1762:TYR:HB2	2.03	0.41
1:A:29:ILE:HD13	2:G:1894:GLU:HA	2.01	0.41
2:G:2035:SER:OG	2:G:2037:PRO:HD2	2.21	0.41
2:G:717:ILE:HG23	2:G:760:HIS:CE1	2.55	0.41
1:A:983:GLN:HE21	2:G:962:LYS:HD2	1.80	0.41
2:G:992:GLU:HA	2:G:992:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:142:ASN:HB2	2:H:550:VAL:HG13	2.01	0.41
2:H:1713:ASN:HA	2:H:1714:PRO:HD3	1.89	0.41
2:H:15:SER:H	2:H:48:PHE:HE2	1.66	0.41
2:H:584:SER:CB	2:H:591:PRO:HG3	2.46	0.41
2:I:1149:TRP:HA	2:I:1242:PHE:CD1	2.54	0.41
2:I:1495:THR:O	2:I:1496:LYS:HB2	2.20	0.41
2:I:524:GLY:HA2	2:I:558:ASN:O	2.20	0.41
2:I:592:LEU:O	2:I:616:THR:HG23	2.19	0.41
2:I:84:LEU:HA	2:I:84:LEU:HD23	1.89	0.41
1:A:1666:THR:HG23	1:A:1669:ARG:HB2	2.01	0.41
1:B:1047:LEU:O	1:B:1051:VAL:HG23	2.20	0.41
1:B:455:ILE:HD13	1:B:455:ILE:HA	1.84	0.41
1:B:852:ARG:HB3	1:B:858:TRP:HZ2	1.83	0.41
1:C:1047:LEU:HD23	1:C:1047:LEU:HA	1.89	0.41
1:C:1208:VAL:HG13	1:C:1209:ASP:O	2.20	0.41
1:C:335:HIS:C	1:C:335:HIS:CD2	2.91	0.41
1:C:792:HIS:CE1	1:C:796:LEU:HD23	2.55	0.41
2:G:1258:ARG:O	2:G:1262:ILE:HG13	2.20	0.41
2:G:1359:MET:HB3	2:G:1606:ARG:NH2	2.35	0.41
2:G:1624:THR:HB	2:G:1642:THR:CG2	2.50	0.41
2:G:520:LYS:O	2:G:521:ASP:C	2.58	0.41
2:G:667:LYS:HD2	2:G:697:THR:CG2	2.38	0.41
2:G:888:ARG:O	2:G:892:ILE:HB	2.21	0.41
2:H:1314:ARG:HD3	2:H:1314:ARG:HA	1.63	0.41
2:I:1493:LEU:HB3	2:I:1494:PRO:HD2	2.02	0.41
2:I:195:LEU:O	2:I:199:ILE:HG13	2.20	0.41
2:I:339:LEU:HD23	2:I:419:ARG:O	2.20	0.41
2:I:507:GLY:O	2:I:508:GLY:C	2.59	0.41
2:I:581:THR:O	2:I:585:LYS:HB2	2.20	0.41
2:I:807:ILE:HA	2:I:818:LYS:HG2	2.02	0.41
1:A:1154:ILE:O	1:A:1154:ILE:HG13	2.19	0.41
1:A:1305:CYS:SG	3:A:2748:CER:C5	3.08	0.41
1:A:12:ILE:O	1:A:15:THR:HG23	2.20	0.41
1:A:1720:ALA:O	1:A:1721:ARG:HG2	2.21	0.41
1:A:330:GLU:O	1:A:330:GLU:HG2	2.20	0.41
1:A:28:TRP:CZ2	1:A:53:LEU:HD22	2.56	0.41
1:A:807:LYS:C	1:A:807:LYS:HD3	2.40	0.41
1:B:1216:LEU:HA	1:B:1216:LEU:HD23	1.93	0.41
1:B:1448:ARG:HD2	1:B:1508:TRP:O	2.21	0.41
1:B:378:LEU:HA	1:B:378:LEU:HD12	1.75	0.41
1:B:992:PHE:CD2	1:B:1399:PRO:HG3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:495:LYS:HA	1:C:496:PRO:HD3	1.86	0.41
1:C:496:PRO:HB2	1:C:519:VAL:HG12	2.02	0.41
1:C:521:LYS:HE2	1:C:605:LEU:HD11	2.02	0.41
1:C:719:GLN:HG3	1:C:720:SER:N	2.35	0.41
2:G:439:ILE:HD12	2:G:484:ILE:CD1	2.50	0.41
2:G:760:HIS:HA	2:G:761:PRO:HD3	1.85	0.41
2:G:846:VAL:HG13	2:G:865:TRP:CD1	2.55	0.41
2:G:950:PHE:O	2:G:953:ARG:HB3	2.20	0.41
2:H:1071:LYS:HE3	2:H:1075:ASP:OD2	2.20	0.41
2:H:1752:PHE:HZ	2:H:1836:MET:HE3	1.84	0.41
2:H:1886:VAL:HG22	2:H:1906:ALA:HB1	2.02	0.41
2:H:455:ILE:HG12	2:H:469:ARG:CG	2.49	0.41
2:H:601:THR:HB	2:H:620:ALA:HB2	2.01	0.41
2:I:1021:LEU:HD22	2:I:1021:LEU:HA	1.61	0.41
2:I:1383:ASN:HD21	2:I:1418:ASP:CB	2.34	0.41
2:I:1388:LYS:HE3	2:I:1418:ASP:OD2	2.21	0.41
2:I:1457:PHE:CD2	2:I:1459:LEU:HD23	2.55	0.41
2:I:1458:ASP:O	2:I:1462:LYS:HE3	2.21	0.41
2:I:156:LEU:HD23	2:I:500:HIS:HB2	2.02	0.41
2:I:258:PHE:HD1	2:I:258:PHE:N	2.18	0.41
2:I:654:VAL:CG2	2:I:683:ALA:HB1	2.50	0.41
2:I:949:ASP:HB3	2:I:1006:MET:CE	2.48	0.41
1:A:12:ILE:O	1:A:16:GLU:HG2	2.20	0.41
1:A:1477:ILE:N	1:A:1478:PRO:CD	2.83	0.41
1:A:601:VAL:O	1:A:602:GLU:C	2.59	0.41
1:A:82:SER:OG	1:A:83:LYS:HG3	2.20	0.41
1:B:1244:GLY:HA3	1:B:1297:PRO:HD2	2.03	0.41
1:B:1257:LEU:HD23	1:B:1257:LEU:HA	1.76	0.41
1:B:1303:GLY:H	1:B:1307:THR:CG2	2.31	0.41
1:B:1308:SER:HB3	1:B:1589:GLY:HA3	2.03	0.41
1:B:1232:TYR:CE2	1:B:1701:LYS:HD2	2.55	0.41
1:B:453:TYR:O	1:B:457:ASN:HB2	2.21	0.41
1:B:504:ASP:CB	1:B:508:ASN:HB2	2.49	0.41
1:B:949:GLU:O	1:B:953:VAL:HG12	2.21	0.41
1:C:1408:ALA:O	1:C:1651:GLY:HA2	2.21	0.41
1:C:1443:LEU:HA	1:C:1443:LEU:HD23	1.77	0.41
1:C:242:THR:HB	1:C:244:THR:HB	2.02	0.41
2:G:1676:MET:HE1	2:G:1781:LEU:CD2	2.47	0.41
2:G:1706:ILE:HD12	2:G:1706:ILE:HA	1.89	0.41
2:G:1862:VAL:HG22	2:G:1863:ALA:N	2.36	0.41
1:A:9:LEU:HD21	2:G:2047:LYS:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:LYS:CD	2:H:2050:GLN:HB3	2.44	0.41
2:H:231:LEU:HA	2:H:236:ILE:HD12	2.03	0.41
2:H:339:LEU:HD23	2:H:419:ARG:O	2.20	0.41
2:H:478:ARG:O	2:H:482:CYS:HB2	2.20	0.41
2:I:177:TYR:CD1	2:I:188:ILE:HG21	2.55	0.41
2:I:1940:LEU:HD12	2:I:1941:PHE:N	2.35	0.41
2:I:566:HIS:ND1	2:I:567:PRO:HD2	2.35	0.41
2:I:572:ASN:HA	2:I:572:ASN:HD22	1.70	0.41
2:I:712:ALA:O	2:I:716:VAL:HG23	2.21	0.41
2:I:780:TYR:HB2	2:I:799:PHE:HE2	1.85	0.41
2:I:786:SER:HB2	2:I:794:MET:HE2	2.02	0.41
2:I:800:LEU:H	2:I:800:LEU:HD23	1.85	0.41
1:A:370:GLU:O	1:A:373:ALA:HB3	2.20	0.41
1:A:825:PRO:HB2	1:A:843:LYS:HZ2	1.86	0.41
1:A:529:MET:HE1	1:A:894:ARG:HD2	2.00	0.41
1:B:1066:ASN:HD22	1:B:1071:PRO:HA	1.86	0.41
1:B:238:PRO:CG	1:B:283:ALA:HB2	2.50	0.41
1:B:406:TRP:CD2	1:B:1619:GLU:HG3	2.55	0.41
1:B:495:LYS:HA	1:B:496:PRO:HD3	1.89	0.41
1:C:1709:GLU:H	1:C:1709:GLU:HG3	1.42	0.41
1:C:155:VAL:HG22	1:C:186:ILE:CG2	2.50	0.41
2:G:1169:PRO:O	2:G:1173:VAL:HG23	2.20	0.41
2:G:1352:HIS:HD2	2:G:1410:PHE:CD2	2.38	0.41
2:G:1495:THR:O	2:G:1496:LYS:HB2	2.20	0.41
2:G:1642:THR:HB	2:G:1651:LEU:HB2	2.01	0.41
2:G:1815:LEU:O	2:G:1821:VAL:HG23	2.20	0.41
2:G:1979:THR:O	2:G:1982:MET:HB2	2.21	0.41
2:G:597:MET:HA	4:G:3051:FMN:C5A	2.51	0.41
2:G:490:TRP:CZ2	2:G:512:LEU:HD21	2.55	0.41
2:G:754:TYR:CG	2:G:794:MET:CG	3.04	0.41
2:H:1236:LEU:HD22	2:H:1238:LEU:HG	2.03	0.41
2:H:1680:LEU:HD13	2:H:1687:ALA:CB	2.45	0.41
2:H:624:TYR:CD1	2:H:630:MET:HE2	2.56	0.41
2:H:712:ALA:O	2:H:715:GLN:HB3	2.20	0.41
2:H:717:ILE:CG2	2:H:760:HIS:CE1	3.04	0.41
2:H:722:ALA:CB	2:H:723:HIS:CE1	3.04	0.41
2:H:950:PHE:O	2:H:953:ARG:HB3	2.20	0.41
2:I:1054:LEU:HD22	4:I:3051:FMN:HM72	2.03	0.41
2:I:663:ILE:HG13	2:I:694:TYR:CE1	2.51	0.41
2:I:638:VAL:HG22	2:I:675:PRO:HG2	2.03	0.41
1:A:32:GLN:O	1:A:36:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:774:ILE:HA	1:A:775:PRO:HD3	1.76	0.41
1:A:988:ILE:HD13	1:A:1048:GLU:CG	2.50	0.41
1:B:1105:LEU:HA	1:B:1105:LEU:HD23	1.89	0.41
1:B:1126:ILE:CD1	1:B:1172:THR:HG22	2.51	0.41
1:B:1666:THR:HG23	1:B:1669:ARG:CB	2.50	0.41
1:C:1119:LYS:HE2	1:C:1341:PHE:CG	2.55	0.41
1:C:1131:LEU:HA	1:C:1131:LEU:HD12	1.69	0.41
1:C:1418:VAL:N	1:C:1419:PRO:CD	2.83	0.41
1:C:35:PHE:HA	1:C:39:PHE:HD2	1.86	0.41
2:G:843:ILE:CD1	2:G:1055:HIS:HB3	2.50	0.41
2:G:571:LYS:HB2	2:G:1099:ALA:HB2	2.02	0.41
2:G:1388:LYS:HE3	2:G:1418:ASP:OD2	2.20	0.41
2:G:1427:VAL:HG22	2:G:1469:GLU:CG	2.51	0.41
2:G:1749:GLU:OE2	2:G:1840:VAL:CG1	2.68	0.41
2:G:246:LEU:HD12	2:G:246:LEU:HA	1.82	0.41
2:G:425:SER:HA	2:G:426:PRO:HD3	1.79	0.41
2:G:587:ILE:HD11	2:G:589:ARG:HB2	2.03	0.41
2:G:835:THR:HG21	2:G:855:HIS:NE2	2.35	0.41
2:H:1128:LYS:HG2	2:H:1181:VAL:HG22	2.01	0.41
2:H:11:LEU:HD23	2:H:11:LEU:HA	1.93	0.41
2:H:1503:ILE:HG22	2:H:1504:VAL:C	2.41	0.41
2:H:236:ILE:C	2:H:236:ILE:HD13	2.40	0.41
2:H:821:ILE:HA	2:H:857:ILE:HD11	2.02	0.41
2:H:827:VAL:HG12	2:H:828:PRO:O	2.19	0.41
2:I:1357:TYR:HD1	2:I:1406:VAL:HG22	1.85	0.41
2:I:159:ILE:HD11	2:I:512:LEU:CG	2.49	0.41
2:I:1642:THR:HB	2:I:1651:LEU:HB2	2.03	0.41
2:I:1981:LEU:HD12	2:I:1981:LEU:N	2.36	0.41
2:I:463:PHE:O	2:I:463:PHE:HD2	2.04	0.41
2:I:634:ILE:CD1	2:I:649:ILE:HD11	2.44	0.41
2:I:595:PRO:HD3	2:I:800:LEU:HB2	2.01	0.41
1:A:16:GLU:HA	1:A:16:GLU:OE2	2.21	0.41
1:A:1239:HIS:HE1	1:A:1714:VAL:O	2.03	0.41
1:A:91:THR:HA	1:A:92:PRO:HD3	1.81	0.41
1:B:521:LYS:HB3	1:B:523:SER:HB3	2.03	0.41
1:B:949:GLU:O	1:B:953:VAL:CG1	2.68	0.41
1:C:1420:ALA:HA	1:C:1421:PRO:HD3	1.78	0.41
1:C:658:LEU:HD13	1:C:916:LEU:HD12	2.02	0.41
2:G:1070:ILE:O	2:G:1070:ILE:HD13	2.21	0.41
2:G:131:ILE:HD12	2:G:182:VAL:CG1	2.49	0.41
2:G:1428:GLU:CG	2:G:1468:THR:HG22	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:236:ILE:HG12	2:G:240:LEU:HD22	2.02	0.41
2:G:270:ALA:O	2:G:459:VAL:HA	2.20	0.41
2:G:123:ILE:CD1	2:G:533:LEU:HD23	2.50	0.41
2:H:159:ILE:HG12	2:H:512:LEU:HD23	2.02	0.41
2:H:1662:THR:HB	2:H:1799:PRO:HG2	2.02	0.41
2:H:1959:LYS:HG2	2:H:1959:LYS:O	2.20	0.41
2:H:320:PRO:HA	2:H:321:PRO:HD3	1.92	0.41
2:H:674:TYR:HA	2:H:675:PRO:HD3	1.73	0.41
2:H:719:ILE:HG12	2:H:719:ILE:H	1.63	0.41
2:H:805:VAL:HG12	2:H:805:VAL:O	2.21	0.41
2:I:1374:THR:HG23	2:I:1396:LEU:CD1	2.49	0.41
2:I:2035:SER:OG	2:I:2037:PRO:HD2	2.21	0.41
2:I:705:LEU:HD23	2:I:705:LEU:HA	1.80	0.41
1:A:152:HIS:HD2	1:A:163:LEU:CB	2.32	0.41
1:A:612:GLU:O	1:A:615:SER:HB3	2.21	0.41
1:A:719:GLN:HG3	1:A:720:SER:N	2.36	0.41
1:B:1418:VAL:N	1:B:1419:PRO:CD	2.83	0.41
1:B:1618:LEU:HD23	1:B:1621:PHE:HE2	1.85	0.41
1:B:1709:GLU:HG3	1:B:1709:GLU:H	1.45	0.41
1:C:1239:HIS:CD2	1:C:1241:SER:H	2.38	0.41
1:C:1244:GLY:C	1:C:1327:CYS:HB2	2.41	0.41
1:C:453:TYR:O	1:C:457:ASN:HB2	2.19	0.41
1:C:32:GLN:HE22	1:C:57:ALA:N	2.19	0.41
1:C:683:ALA:HA	1:C:689:GLY:HA3	2.02	0.41
2:G:1210:ILE:O	2:G:1210:ILE:HG22	2.19	0.41
2:G:1383:ASN:HD21	2:G:1418:ASP:CB	2.33	0.41
2:G:1884:TRP:HB3	2:G:1885:LEU:H	1.74	0.41
2:H:1300:PHE:CB	2:H:1556:VAL:HG11	2.50	0.41
2:H:1815:LEU:O	2:H:1821:VAL:HG23	2.21	0.41
2:H:1868:GLN:HG3	2:H:1898:TYR:HH	1.83	0.41
2:H:195:LEU:O	2:H:199:ILE:HG13	2.20	0.41
2:H:827:VAL:HG21	2:H:840:THR:CG2	2.51	0.41
2:I:1219:ILE:HB	2:I:1240:TYR:HB2	2.03	0.41
2:I:1503:ILE:HG22	2:I:1504:VAL:C	2.41	0.41
2:I:1514:ASN:HA	2:I:1515:PRO:HD3	1.86	0.41
2:I:1579:ILE:CD1	2:I:1615:MET:SD	3.09	0.41
2:I:827:VAL:HG12	2:I:828:PRO:O	2.20	0.41
1:A:253:ARG:O	1:A:254:TRP:CD1	2.74	0.41
1:A:438:ASN:HD21	1:A:698:GLN:HE21	1.68	0.41
1:B:1657:HIS:CG	1:B:1658:PRO:HD2	2.55	0.41
1:B:444:ASN:CB	1:B:446:ALA:H	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1076:VAL:CG1	1:C:1081:LYS:HA	2.50	0.41
1:C:1705:PRO:HB2	1:C:1733:PHE:CD1	2.56	0.41
1:C:739:GLN:HB3	1:C:794:ILE:HG23	2.03	0.41
1:C:949:GLU:O	1:C:953:VAL:HG12	2.21	0.41
2:G:1352:HIS:CD2	2:G:1410:PHE:CD2	3.09	0.41
2:G:1778:GLN:HB2	2:G:1779:PRO:HD3	2.02	0.41
2:G:1889:VAL:HG22	2:G:1977:HIS:O	2.20	0.41
2:G:1981:LEU:HD12	2:G:1981:LEU:N	2.36	0.41
2:G:1989:LYS:NZ	2:G:2037:PRO:HG2	2.35	0.41
2:G:258:PHE:N	2:G:258:PHE:CD1	2.87	0.41
2:G:260:PRO:HD3	2:G:289:TRP:CZ2	2.54	0.41
2:G:735:GLY:O	2:G:741:HIS:CD2	2.73	0.41
2:G:748:THR:CB	2:G:749:PRO:HD3	2.47	0.41
2:G:780:TYR:HB2	2:G:799:PHE:CE2	2.56	0.41
2:G:995:LEU:HB3	2:G:1000:ILE:CD1	2.50	0.41
2:H:615:TYR:CE2	2:H:1074:MET:HB3	2.56	0.41
2:H:1213:LEU:O	2:H:1214:LEU:HD23	2.19	0.41
2:H:1270:TRP:HZ3	2:H:1347:LEU:HD21	1.85	0.41
2:H:1589:VAL:HG21	2:H:1651:LEU:HD12	2.02	0.41
2:H:425:SER:HA	2:H:426:PRO:HD3	1.78	0.41
2:H:753:MET:O	2:H:757:ILE:HG13	2.21	0.41
2:H:804:ARG:NH2	2:H:1068:GLU:OE1	2.54	0.41
2:H:892:ILE:HD11	2:H:903:TRP:CD2	2.53	0.41
2:I:248:HIS:CE1	2:I:531:GLY:HA2	2.55	0.41
2:I:455:ILE:C	2:I:455:ILE:HD12	2.42	0.41
2:I:582:LYS:HE2	2:I:761:PRO:O	2.21	0.41
1:A:1705:PRO:HB2	1:A:1733:PHE:CD1	2.56	0.41
1:A:36:LEU:O	1:A:76:ARG:NH1	2.53	0.41
1:A:487:ASP:HA	1:A:488:PRO:HD3	1.88	0.41
1:A:908:LEU:O	1:A:913:VAL:HG22	2.21	0.41
1:B:1029:PRO:HG2	1:B:1581:THR:O	2.21	0.41
1:B:197:THR:HG22	1:B:198:PRO:O	2.21	0.41
1:B:187:LEU:CD2	1:B:201:PRO:HB2	2.51	0.41
1:B:32:GLN:HE22	1:B:57:ALA:CA	2.34	0.41
1:B:489:VAL:HG22	1:B:670:GLY:HA3	2.02	0.41
1:B:427:ASN:ND2	1:B:610:THR:H	2.14	0.41
1:B:82:SER:OG	1:B:83:LYS:HG3	2.20	0.41
1:B:504:ASP:O	1:B:954:ARG:HD3	2.21	0.41
1:C:1019:ILE:HG13	1:C:1316:VAL:HG13	2.03	0.41
1:C:1666:THR:HG23	1:C:1669:ARG:CB	2.51	0.41
1:C:237:MET:HA	1:C:238:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:TYR:CZ	1:C:298:VAL:HG21	2.55	0.41
1:C:427:ASN:HB2	1:C:468:LEU:CD2	2.51	0.41
1:C:644:THR:HG23	1:C:648:ASP:N	2.34	0.41
2:G:2049:GLU:O	2:G:2050:GLN:C	2.59	0.41
2:G:339:LEU:HB2	2:G:386:LEU:HD22	2.03	0.41
2:G:44:PRO:HA	2:G:53:GLU:OE2	2.21	0.41
2:G:455:ILE:HD13	2:G:457:ILE:O	2.21	0.41
2:H:1063:THR:HG22	2:H:1063:THR:O	2.21	0.41
2:H:1387:GLY:HA2	2:H:1414:GLY:O	2.21	0.41
2:H:1949:LYS:O	2:H:1953:VAL:HG23	2.21	0.41
2:I:118:LYS:O	2:I:121:GLU:HB2	2.20	0.41
2:I:1327:ILE:O	2:I:1331:TRP:HB2	2.21	0.41
2:I:2020:GLN:NE2	2:I:2020:GLN:HA	2.36	0.41
2:I:319:LEU:HA	2:I:319:LEU:HD22	1.67	0.41
2:I:717:ILE:O	2:I:720:ALA:HB3	2.21	0.41
2:I:754:TYR:CG	2:I:794:MET:CG	3.04	0.41
2:I:827:VAL:HG21	2:I:840:THR:CG2	2.51	0.41
1:A:1418:VAL:N	1:A:1419:PRO:CD	2.84	0.40
1:A:197:THR:HG22	1:A:198:PRO:O	2.21	0.40
1:A:232:LEU:O	1:A:236:LYS:HB2	2.21	0.40
1:A:681:THR:HA	1:A:706:THR:OG1	2.21	0.40
1:B:1056:ILE:HG13	1:B:1057:MET:N	2.36	0.40
1:B:1557:ILE:HD11	1:B:1642:THR:HG21	2.03	0.40
1:B:483:VAL:O	1:B:483:VAL:HG12	2.21	0.40
1:B:91:THR:HA	1:B:92:PRO:HD3	1.81	0.40
1:B:933:VAL:HA	1:B:934:PRO:HD3	1.63	0.40
1:B:989:GLN:NE2	2:H:993:GLN:OE1	2.53	0.40
1:B:998:TYR:CD2	1:B:1667:GLU:HG3	2.56	0.40
1:C:1308:SER:OG	1:C:1590:ALA:N	2.54	0.40
2:G:1343:VAL:HG22	2:G:1343:VAL:O	2.20	0.40
1:A:29:ILE:HG21	2:G:1894:GLU:HB2	2.04	0.40
2:G:430:HIS:CE1	2:G:431:LEU:HD13	2.56	0.40
2:G:159:ILE:HG12	2:G:512:LEU:HD23	2.03	0.40
2:G:73:GLU:OE2	2:G:76:LYS:HD2	2.21	0.40
2:G:938:TRP:CD1	2:G:944:ARG:HG3	2.56	0.40
2:H:1227:ARG:CZ	2:H:1565:VAL:HG12	2.51	0.40
2:H:338:MET:HG3	2:H:423:VAL:HG21	2.02	0.40
2:H:888:ARG:O	2:H:892:ILE:HB	2.21	0.40
2:I:1676:MET:HE1	2:I:1781:LEU:CD2	2.50	0.40
2:I:1880:LYS:HB2	2:I:1880:LYS:HE3	1.90	0.40
2:I:1889:VAL:HG21	2:I:1901:ALA:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2036:GLU:HB2	2:I:2037:PRO:CD	2.47	0.40
2:I:2039:LYS:HA	2:I:2042:ILE:HG13	2.03	0.40
2:I:247:ALA:O	2:I:251:VAL:HG13	2.21	0.40
2:I:280:ALA:O	2:I:283:ILE:HG22	2.21	0.40
2:I:846:VAL:CG2	2:I:866:LYS:HB2	2.51	0.40
1:A:1021:VAL:HG11	1:A:1597:LEU:CD1	2.50	0.40
1:A:1146:HIS:O	1:A:1146:HIS:HD2	2.04	0.40
1:A:1665:ILE:HD11	1:A:1669:ARG:CG	2.51	0.40
1:A:44:VAL:HG13	1:A:78:ILE:HG12	1.99	0.40
1:A:833:PHE:O	1:A:834:GLY:O	2.39	0.40
1:B:1583:HIS:HA	1:B:1584:PRO:HD3	1.84	0.40
1:C:1105:LEU:HA	1:C:1105:LEU:HD23	1.84	0.40
1:C:148:SER:O	1:C:152:HIS:HB2	2.21	0.40
1:C:411:GLN:O	1:C:415:SER:HB2	2.21	0.40
2:G:1227:ARG:NE	2:G:1565:VAL:HG12	2.36	0.40
2:G:1678:MET:HG2	2:G:1711:ILE:HG12	2.03	0.40
2:G:1940:LEU:HD12	2:G:1941:PHE:N	2.37	0.40
1:A:23:ALA:O	2:G:1977:HIS:HA	2.20	0.40
2:G:601:THR:HB	2:G:620:ALA:HB2	2.01	0.40
2:G:638:VAL:O	2:G:641:ILE:HG22	2.20	0.40
2:G:805:VAL:O	2:G:805:VAL:HG12	2.21	0.40
2:G:827:VAL:HG12	2:G:828:PRO:O	2.21	0.40
2:H:1214:LEU:HD11	2:H:1220:GLN:NE2	2.36	0.40
2:H:1506:TYR:CZ	2:H:1515:PRO:HG2	2.56	0.40
2:H:1609:THR:O	2:H:1653:GLY:HA3	2.21	0.40
2:H:203:LEU:HD12	2:H:203:LEU:HA	1.91	0.40
2:H:462:THR:HB	2:H:482:CYS:SG	2.61	0.40
2:H:573:LYS:C	2:H:575:GLY:N	2.75	0.40
2:H:590:PRO:HA	2:H:591:PRO:HD3	1.81	0.40
2:H:638:VAL:HA	2:H:641:ILE:CG2	2.52	0.40
2:H:723:HIS:ND1	2:H:723:HIS:N	2.70	0.40
2:H:960:LYS:CE	2:H:960:LYS:HA	2.44	0.40
2:I:1091:GLY:O	2:I:1093:ASP:N	2.55	0.40
2:I:1339:PHE:N	2:I:1340:PRO:CD	2.85	0.40
2:I:1359:MET:HB3	2:I:1606:ARG:NH2	2.36	0.40
2:I:1889:VAL:HG13	2:I:1977:HIS:HB3	2.00	0.40
2:I:246:LEU:HA	2:I:246:LEU:HD12	1.79	0.40
2:I:536:ASN:HD21	2:I:540:ASP:HB3	1.85	0.40
2:I:543:PHE:CB	2:I:545:GLN:NE2	2.82	0.40
2:I:703:LEU:HD23	2:I:705:LEU:HG	2.04	0.40
2:I:816:ASP:HB3	2:I:1048:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:PRO:CG	1:A:283:ALA:HB2	2.51	0.40
1:A:852:ARG:NH1	1:A:852:ARG:CG	2.73	0.40
1:B:1303:GLY:CA	1:B:1307:THR:HG22	2.52	0.40
1:B:221:LEU:HD23	1:B:221:LEU:HA	1.94	0.40
1:B:293:LYS:O	1:B:297:ILE:HG13	2.20	0.40
1:B:774:ILE:HA	1:B:775:PRO:HD3	1.74	0.40
1:C:1303:GLY:CA	1:C:1307:THR:HG22	2.52	0.40
1:C:43:ARG:O	2:I:1662:THR:HA	2.22	0.40
2:G:1637:LEU:HA	2:G:1637:LEU:HD23	1.77	0.40
2:G:1875:VAL:HA	2:G:1878:VAL:CG1	2.52	0.40
2:G:248:HIS:CE1	2:G:531:GLY:HA2	2.56	0.40
2:G:319:LEU:HA	2:G:319:LEU:HD22	1.62	0.40
2:G:391:LEU:CD2	2:G:394:ARG:NH2	2.85	0.40
2:G:441:LYS:HG2	2:G:445:LYS:HE3	2.02	0.40
2:G:573:LYS:C	2:G:575:GLY:N	2.75	0.40
2:G:582:LYS:HE2	2:G:761:PRO:O	2.22	0.40
2:G:852:GLU:H	2:G:852:GLU:HG3	1.40	0.40
2:H:1166:VAL:CG1	2:H:1167:SER:N	2.85	0.40
2:H:517:HIS:HB2	2:H:527:VAL:HG21	2.04	0.40
2:H:517:HIS:CE1	2:H:540:ASP:O	2.75	0.40
2:H:810:GLU:OE2	2:H:1070:ILE:N	2.45	0.40
2:H:912:ARG:HB2	2:H:916:THR:HG23	2.03	0.40
2:I:1213:LEU:O	2:I:1214:LEU:HD23	2.20	0.40
2:I:1271:ILE:HG22	2:I:1273:GLU:HB2	2.04	0.40
2:I:1855:ILE:HB	2:I:1907:LEU:HD12	2.02	0.40
2:I:612:ASN:HD21	2:I:641:ILE:HA	1.84	0.40
2:I:864:LEU:HD13	2:I:894:ARG:HB3	2.04	0.40
1:A:1209:ASP:OD1	1:A:1210:PRO:HD2	2.21	0.40
1:A:1406:MET:CE	1:A:1428:THR:HB	2.52	0.40
1:A:157:HIS:CE1	1:A:269:LEU:HD11	2.57	0.40
1:A:916:LEU:HD22	1:A:922:VAL:HG22	2.02	0.40
1:B:1370:THR:HG22	1:B:1371:THR:N	2.36	0.40
1:B:12:ILE:O	1:B:16:GLU:HG2	2.20	0.40
1:B:509:ILE:HG13	1:B:509:ILE:H	1.50	0.40
1:B:74:LEU:O	1:B:74:LEU:HD12	2.22	0.40
1:C:1063:HIS:CE1	1:C:1067:LEU:CD2	3.04	0.40
1:C:1195:ALA:HB1	1:C:1200:ILE:HD12	2.03	0.40
1:C:1639:VAL:HG12	1:C:1640:SER:N	2.35	0.40
1:C:406:TRP:CZ3	1:C:407:ASN:HB2	2.57	0.40
1:C:655:LEU:HD23	1:C:655:LEU:HA	1.79	0.40
2:G:260:PRO:HD3	2:G:289:TRP:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:612:ASN:C	2:G:614:GLY:H	2.24	0.40
2:H:1281:PRO:O	2:H:1378:ILE:HG23	2.22	0.40
2:H:1593:ILE:HD13	2:H:1626:ILE:CD1	2.51	0.40
2:H:1716:ASN:HA	2:H:1770:LEU:HD11	2.04	0.40
2:H:538:ASP:HB2	2:H:540:ASP:HB2	2.03	0.40
2:H:607:VAL:HG23	2:H:617:ILE:CG2	2.51	0.40
2:I:240:LEU:HA	2:I:240:LEU:HD12	1.81	0.40
2:I:717:ILE:CG2	2:I:760:HIS:CE1	3.05	0.40
2:I:812:LYS:HA	2:I:812:LYS:HD3	1.82	0.40
1:A:350:LEU:HB2	1:A:352:MET:HG2	2.03	0.40
1:A:427:ASN:HB2	1:A:468:LEU:CD2	2.51	0.40
1:B:1577:GLN:NE2	1:B:1591:TRP:HB3	2.36	0.40
1:B:709:ARG:O	1:B:714:VAL:HG21	2.21	0.40
1:C:413:LEU:HD13	1:C:451:MET:HG2	2.03	0.40
2:G:119:THR:HG22	2:G:120:LYS:N	2.36	0.40
2:G:1830:VAL:HA	2:G:1991:PHE:HE2	1.86	0.40
2:G:2039:LYS:HA	2:G:2042:ILE:HG13	2.03	0.40
2:G:533:LEU:HG	2:G:533:LEU:O	2.21	0.40
2:G:606:PHE:HZ	2:G:805:VAL:CG1	2.33	0.40
2:H:1172:LYS:HZ1	2:H:1574:ASN:HA	1.85	0.40
2:H:1327:ILE:HA	2:H:1327:ILE:HD12	1.77	0.40
2:H:283:ILE:HD12	2:H:283:ILE:HA	1.89	0.40
2:H:233:SER:HA	2:H:424:ALA:HB3	2.03	0.40
2:H:441:LYS:O	2:H:445:LYS:HG3	2.22	0.40
2:H:298:LYS:HA	2:H:448:VAL:CG2	2.52	0.40
2:H:156:LEU:HD23	2:H:500:HIS:HB2	2.04	0.40
2:H:816:ASP:HB3	2:H:1048:VAL:CG2	2.52	0.40
2:I:225:THR:HA	2:I:226:PRO:HD3	1.98	0.40
2:I:601:THR:O	2:I:601:THR:CG2	2.68	0.40
2:I:612:ASN:C	2:I:614:GLY:H	2.25	0.40

All (18) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1480:GLU:OE2	2:H:290:GLU:CB[6_555]	0.75	1.45
1:B:1480:GLU:CD	2:H:290:GLU:CB[6_555]	1.29	0.91
2:G:77:VAL:CB	2:I:1929:LYS:CD[6_455]	1.32	0.88
1:B:1480:GLU:OE2	2:H:290:GLU:CG[6_555]	1.43	0.77
2:G:77:VAL:CG2	2:I:1929:LYS:NZ[6_455]	1.47	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:77:VAL:CG2	2:I:1929:LYS:CE[6_455]	1.51	0.69
2:G:79:GLN:OE1	2:I:1930:SER:O[6_455]	1.65	0.55
2:G:77:VAL:CB	2:I:1929:LYS:CE[6_455]	1.72	0.48
1:B:1480:GLU:OE1	2:H:290:GLU:CB[6_555]	1.82	0.38
2:G:77:VAL:O	2:I:1929:LYS:CB[6_455]	1.93	0.27
2:G:77:VAL:O	2:I:1929:LYS:CA[6_455]	1.93	0.27
2:G:77:VAL:CG1	2:I:1929:LYS:CD[6_455]	1.95	0.25
2:G:77:VAL:O	2:I:1929:LYS:CG[6_455]	1.98	0.22
2:H:6:THR:CG2	2:I:1935:GLU:OE2[6_455]	2.06	0.14
2:H:6:THR:CG2	2:I:1935:GLU:CD[6_455]	2.06	0.14
2:G:77:VAL:CB	2:I:1929:LYS:CG[6_455]	2.14	0.06
1:A:852:ARG:NH2	1:B:837:GLY:O[7_645]	2.19	0.01
1:B:1480:GLU:OE1	2:H:290:GLU:CA[6_555]	2.19	0.01

## 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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1604/1887 (85%)	1498 (93%)	92 (6%)	14 (1%)	17	55
1	B	1604/1887 (85%)	1497 (93%)	94 (6%)	13 (1%)	19	58
1	C	1604/1887 (85%)	1499 (94%)	90 (6%)	15 (1%)	17	55
2	G	2029/2051 (99%)	1836 (90%)	167 (8%)	26 (1%)	12	48
2	H	2029/2051 (99%)	1836 (90%)	170 (8%)	23 (1%)	14	51
2	I	2029/2051 (99%)	1833 (90%)	171 (8%)	25 (1%)	13	49
All	All	10899/11814 (92%)	9999 (92%)	784 (7%)	116 (1%)	14	51

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	504	ASP
1	A	538	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	605	LEU
1	A	834	GLY
1	B	504	ASP
1	B	538	GLU
1	B	605	LEU
1	B	834	GLY
1	C	504	ASP
1	C	538	GLU
1	C	605	LEU
1	C	834	GLY
2	G	521	ASP
2	G	1177	SER
2	G	1418	ASP
2	G	1955	PRO
2	H	521	ASP
2	H	1418	ASP
2	H	1955	PRO
2	I	521	ASP
2	I	1418	ASP
2	I	1955	PRO
1	A	1252	GLY
1	A	1585	LYS
1	A	1608	ASN
1	B	179	LYS
1	B	1252	GLY
1	B	1585	LYS
1	B	1608	ASN
1	C	1252	GLY
1	C	1585	LYS
1	C	1608	ASN
2	G	203	LEU
2	G	1044	VAL
2	G	1722	GLY
2	H	203	LEU
2	H	1044	VAL
2	H	1177	SER
2	H	1722	GLY
2	I	203	LEU
2	I	1044	VAL
2	I	1177	SER
2	I	1722	GLY
1	A	179	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	179	LYS
2	G	112	ASN
2	G	139	LYS
2	G	1101	GLU
2	G	2034	GLY
2	H	112	ASN
2	H	1101	GLU
2	I	374	ALA
2	I	1092	ASP
2	I	1101	GLU
2	I	2034	GLY
2	G	25	ALA
2	G	26	SER
2	G	374	ALA
2	G	742	SER
2	G	769	SER
2	G	1092	ASP
2	G	1510	ALA
2	H	26	SER
2	H	374	ALA
2	H	742	SER
2	H	823	ALA
2	H	1510	ALA
2	H	2034	GLY
2	I	26	SER
2	I	112	ASN
2	I	742	SER
1	A	1130	ASP
1	A	1477	ILE
1	A	1536	LEU
1	B	970	GLY
1	B	1477	ILE
1	C	1477	ILE
2	H	769	SER
2	H	1092	ASP
2	H	1257	ASP
2	I	25	ALA
2	I	136	PRO
2	I	769	SER
2	I	823	ALA
2	I	1510	ALA
1	A	178	GLY

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Mol	Chain	Res	Type
1	A	970	GLY
1	C	970	GLY
1	C	1536	LEU
2	G	574	SER
2	I	139	LYS
2	I	574	SER
1	A	1543	GLY
1	B	1543	GLY
1	C	178	GLY
1	C	1543	GLY
2	G	136	PRO
2	G	335	PRO
2	H	136	PRO
2	H	335	PRO
1	B	178	GLY
2	G	1340	PRO
2	G	1956	ARG
2	H	772	GLY
1	C	1240	VAL
2	G	772	GLY
2	G	1176	PRO
2	I	772	GLY
1	B	726	GLY
1	C	726	GLY
2	G	470	VAL
2	H	470	VAL
2	H	2012	PRO
2	I	335	PRO
2	I	1956	ARG
2	I	1340	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1367/1566 (87%)	1224 (90%)	143 (10%)	<b>7</b> <b>27</b>

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1367/1566 (87%)	1225 (90%)	142 (10%)	7	28
1	C	1367/1566 (87%)	1227 (90%)	140 (10%)	7	28
2	G	1772/1789 (99%)	1567 (88%)	205 (12%)	5	24
2	H	1772/1789 (99%)	1566 (88%)	206 (12%)	5	24
2	I	1772/1789 (99%)	1562 (88%)	210 (12%)	5	24
All	All	9417/10065 (94%)	8371 (89%)	1046 (11%)	6	26

All (1046) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	15	THR
1	A	21	GLN
1	A	22	PHE
1	A	145	VAL
1	A	149	LEU
1	A	158	LYS
1	A	165	SER
1	A	171	THR
1	A	202	GLU
1	A	217	PHE
1	A	242	THR
1	A	253	ARG
1	A	328	LEU
1	A	331	ILE
1	A	332	THR
1	A	375	LEU
1	A	378	LEU
1	A	385	PHE
1	A	390	VAL
1	A	392	THR
1	A	400	ARG
1	A	412	SER
1	A	413	LEU
1	A	415	SER
1	A	416	LEU
1	A	428	VAL
1	A	431	GLU
1	A	432	VAL
1	A	435	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	447	LEU
1	A	457	ASN
1	A	460	GLU
1	A	461	THR
1	A	484	LEU
1	A	489	VAL
1	A	493	VAL
1	A	506	ASN
1	A	509	ILE
1	A	527	GLN
1	A	529	MET
1	A	536	THR
1	A	599	MET
1	A	600	ASP
1	A	603	ASP
1	A	606	ASP
1	A	607	LYS
1	A	615	SER
1	A	621	THR
1	A	622	ILE
1	A	625	THR
1	A	629	THR
1	A	635	ILE
1	A	644	THR
1	A	648	ASP
1	A	654	GLN
1	A	711	SER
1	A	719	GLN
1	A	728	LYS
1	A	731	THR
1	A	732	LEU
1	A	748	LEU
1	A	749	ILE
1	A	776	GLU
1	A	782	GLU
1	A	793	ARG
1	A	797	THR
1	A	806	VAL
1	A	817	THR
1	A	825	PRO
1	A	852	ARG
1	A	860	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	864	VAL
1	A	873	ARG
1	A	881	ASN
1	A	891	MET
1	A	913	VAL
1	A	930	LEU
1	A	933	VAL
1	A	947	LEU
1	A	949	GLU
1	A	953	VAL
1	A	964	GLU
1	A	980	VAL
1	A	1016	GLU
1	A	1020	VAL
1	A	1022	THR
1	A	1047	LEU
1	A	1056	ILE
1	A	1070	ARG
1	A	1087	LYS
1	A	1095	THR
1	A	1101	SER
1	A	1125	VAL
1	A	1127	VAL
1	A	1131	LEU
1	A	1172	THR
1	A	1173	LEU
1	A	1179	LEU
1	A	1184	LEU
1	A	1196	LYS
1	A	1197	THR
1	A	1208	VAL
1	A	1218	SER
1	A	1226	SER
1	A	1229	THR
1	A	1255	SER
1	A	1274	ILE
1	A	1283	MET
1	A	1307	THR
1	A	1327	CYS
1	A	1338	GLU
1	A	1367	ARG
1	A	1372	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1384	ILE
1	A	1385	GLN
1	A	1392	LEU
1	A	1414	ILE
1	A	1426	LEU
1	A	1442	ASN
1	A	1465	ASN
1	A	1479	SER
1	A	1489	ARG
1	A	1502	ARG
1	A	1515	ARG
1	A	1522	LEU
1	A	1523	ARG
1	A	1532	THR
1	A	1533	ILE
1	A	1549	ASN
1	A	1556	THR
1	A	1566	ARG
1	A	1580	LEU
1	A	1585	LYS
1	A	1612	ASP
1	A	1625	LEU
1	A	1665	ILE
1	A	1666	THR
1	A	1692	MET
1	A	1693	ILE
1	A	1707	THR
1	A	1709	GLU
1	A	1721	ARG
1	B	14	LEU
1	B	15	THR
1	B	21	GLN
1	B	22	PHE
1	B	145	VAL
1	B	149	LEU
1	B	158	LYS
1	B	165	SER
1	B	171	THR
1	B	202	GLU
1	B	217	PHE
1	B	242	THR
1	B	253	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	300	VAL
1	B	328	LEU
1	B	331	ILE
1	B	332	THR
1	B	375	LEU
1	B	385	PHE
1	B	390	VAL
1	B	392	THR
1	B	400	ARG
1	B	401	THR
1	B	412	SER
1	B	413	LEU
1	B	415	SER
1	B	416	LEU
1	B	428	VAL
1	B	432	VAL
1	B	435	GLU
1	B	447	LEU
1	B	457	ASN
1	B	460	GLU
1	B	461	THR
1	B	484	LEU
1	B	489	VAL
1	B	493	VAL
1	B	499	PRO
1	B	506	ASN
1	B	509	ILE
1	B	510	THR
1	B	527	GLN
1	B	529	MET
1	B	536	THR
1	B	599	MET
1	B	600	ASP
1	B	603	ASP
1	B	606	ASP
1	B	607	LYS
1	B	615	SER
1	B	621	THR
1	B	622	ILE
1	B	625	THR
1	B	629	THR
1	B	635	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	644	THR
1	B	648	ASP
1	B	711	SER
1	B	719	GLN
1	B	728	LYS
1	B	731	THR
1	B	732	LEU
1	B	748	LEU
1	B	749	ILE
1	B	776	GLU
1	B	782	GLU
1	B	793	ARG
1	B	797	THR
1	B	806	VAL
1	B	852	ARG
1	B	860	ASN
1	B	864	VAL
1	B	873	ARG
1	B	881	ASN
1	B	891	MET
1	B	913	VAL
1	B	930	LEU
1	B	933	VAL
1	B	947	LEU
1	B	949	GLU
1	B	953	VAL
1	B	964	GLU
1	B	980	VAL
1	B	1016	GLU
1	B	1020	VAL
1	B	1047	LEU
1	B	1056	ILE
1	B	1070	ARG
1	B	1078	SER
1	B	1080	THR
1	B	1087	LYS
1	B	1095	THR
1	B	1101	SER
1	B	1125	VAL
1	B	1127	VAL
1	B	1131	LEU
1	B	1172	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	1173	LEU
1	B	1179	LEU
1	B	1184	LEU
1	B	1196	LYS
1	B	1197	THR
1	B	1208	VAL
1	B	1218	SER
1	B	1229	THR
1	B	1255	SER
1	B	1274	ILE
1	B	1283	MET
1	B	1307	THR
1	B	1327	CYS
1	B	1338	GLU
1	B	1367	ARG
1	B	1372	THR
1	B	1384	ILE
1	B	1385	GLN
1	B	1392	LEU
1	B	1414	ILE
1	B	1426	LEU
1	B	1442	ASN
1	B	1465	ASN
1	B	1479	SER
1	B	1502	ARG
1	B	1515	ARG
1	B	1522	LEU
1	B	1523	ARG
1	B	1532	THR
1	B	1533	ILE
1	B	1549	ASN
1	B	1556	THR
1	B	1566	ARG
1	B	1577	GLN
1	B	1580	LEU
1	B	1585	LYS
1	B	1612	ASP
1	B	1625	LEU
1	B	1665	ILE
1	B	1666	THR
1	B	1692	MET
1	B	1693	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	1707	THR
1	B	1709	GLU
1	B	1721	ARG
1	C	14	LEU
1	C	15	THR
1	C	21	GLN
1	C	22	PHE
1	C	145	VAL
1	C	149	LEU
1	C	158	LYS
1	C	165	SER
1	C	171	THR
1	C	202	GLU
1	C	217	PHE
1	C	242	THR
1	C	253	ARG
1	C	328	LEU
1	C	331	ILE
1	C	332	THR
1	C	375	LEU
1	C	385	PHE
1	C	390	VAL
1	C	392	THR
1	C	400	ARG
1	C	412	SER
1	C	413	LEU
1	C	415	SER
1	C	416	LEU
1	C	428	VAL
1	C	431	GLU
1	C	432	VAL
1	C	435	GLU
1	C	447	LEU
1	C	457	ASN
1	C	460	GLU
1	C	461	THR
1	C	484	LEU
1	C	489	VAL
1	C	493	VAL
1	C	506	ASN
1	C	509	ILE
1	C	527	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	529	MET
1	C	536	THR
1	C	599	MET
1	C	600	ASP
1	C	603	ASP
1	C	606	ASP
1	C	607	LYS
1	C	615	SER
1	C	621	THR
1	C	622	ILE
1	C	625	THR
1	C	629	THR
1	C	635	ILE
1	C	644	THR
1	C	648	ASP
1	C	711	SER
1	C	719	GLN
1	C	728	LYS
1	C	731	THR
1	C	732	LEU
1	C	748	LEU
1	C	749	ILE
1	C	776	GLU
1	C	782	GLU
1	C	797	THR
1	C	806	VAL
1	C	824	LEU
1	C	852	ARG
1	C	860	ASN
1	C	864	VAL
1	C	873	ARG
1	C	881	ASN
1	C	891	MET
1	C	913	VAL
1	C	930	LEU
1	C	933	VAL
1	C	947	LEU
1	C	949	GLU
1	C	951	SER
1	C	953	VAL
1	C	980	VAL
1	C	1016	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	1020	VAL
1	C	1047	LEU
1	C	1056	ILE
1	C	1070	ARG
1	C	1078	SER
1	C	1087	LYS
1	C	1095	THR
1	C	1101	SER
1	C	1125	VAL
1	C	1127	VAL
1	C	1131	LEU
1	C	1172	THR
1	C	1173	LEU
1	C	1179	LEU
1	C	1184	LEU
1	C	1196	LYS
1	C	1197	THR
1	C	1208	VAL
1	C	1218	SER
1	C	1229	THR
1	C	1255	SER
1	C	1274	ILE
1	C	1283	MET
1	C	1307	THR
1	C	1327	CYS
1	C	1338	GLU
1	C	1367	ARG
1	C	1372	THR
1	C	1384	ILE
1	C	1385	GLN
1	C	1392	LEU
1	C	1414	ILE
1	C	1426	LEU
1	C	1442	ASN
1	C	1455	ARG
1	C	1465	ASN
1	C	1479	SER
1	C	1489	ARG
1	C	1502	ARG
1	C	1515	ARG
1	C	1522	LEU
1	C	1523	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	1532	THR
1	C	1533	ILE
1	C	1549	ASN
1	C	1556	THR
1	C	1566	ARG
1	C	1577	GLN
1	C	1580	LEU
1	C	1585	LYS
1	C	1612	ASP
1	C	1625	LEU
1	C	1665	ILE
1	C	1666	THR
1	C	1692	MET
1	C	1693	ILE
1	C	1707	THR
1	C	1709	GLU
1	C	1721	ARG
2	G	6	THR
2	G	7	ARG
2	G	45	THR
2	G	46	GLU
2	G	48	PHE
2	G	56	THR
2	G	65	LEU
2	G	84	LEU
2	G	86	LEU
2	G	93	ASN
2	G	99	ASN
2	G	101	ILE
2	G	109	LEU
2	G	117	VAL
2	G	122	LEU
2	G	149	VAL
2	G	153	ASN
2	G	155	GLN
2	G	159	ILE
2	G	173	LEU
2	G	175	ASP
2	G	176	LEU
2	G	178	GLN
2	G	182	VAL
2	G	210	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	G	227	ASP
2	G	236	ILE
2	G	240	LEU
2	G	246	LEU
2	G	281	VAL
2	G	286	THR
2	G	295	SER
2	G	297	ARG
2	G	300	ILE
2	G	303	LEU
2	G	319	LEU
2	G	339	LEU
2	G	340	SER
2	G	342	SER
2	G	344	LEU
2	G	353	VAL
2	G	371	VAL
2	G	376	ASN
2	G	389	LEU
2	G	392	THR
2	G	402	LEU
2	G	418	ASN
2	G	425	SER
2	G	431	LEU
2	G	448	VAL
2	G	455	ILE
2	G	462	THR
2	G	463	PHE
2	G	471	LEU
2	G	476	SER
2	G	478	ARG
2	G	482	CYS
2	G	492	THR
2	G	499	THR
2	G	539	ASP
2	G	545	GLN
2	G	553	ASN
2	G	562	LEU
2	G	574	SER
2	G	586	LEU
2	G	587	ILE
2	G	598	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	G	607	VAL
2	G	611	THR
2	G	616	THR
2	G	653	TYR
2	G	665	LEU
2	G	669	LEU
2	G	670	ARG
2	G	676	ILE
2	G	693	GLU
2	G	714	SER
2	G	719	ILE
2	G	723	HIS
2	G	730	LEU
2	G	736	ARG
2	G	741	HIS
2	G	750	MET
2	G	751	LEU
2	G	762	ASN
2	G	767	PHE
2	G	775	ASP
2	G	777	THR
2	G	787	THR
2	G	794	MET
2	G	800	LEU
2	G	810	GLU
2	G	825	THR
2	G	832	TRP
2	G	835	THR
2	G	844	VAL
2	G	852	GLU
2	G	855	HIS
2	G	857	ILE
2	G	869	ASP
2	G	880	LEU
2	G	881	VAL
2	G	892	ILE
2	G	907	VAL
2	G	929	LEU
2	G	945	THR
2	G	952	ARG
2	G	953	ARG
2	G	964	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	G	971	SER
2	G	993	GLN
2	G	1015	VAL
2	G	1021	LEU
2	G	1024	ARG
2	G	1048	VAL
2	G	1066	ILE
2	G	1070	ILE
2	G	1082	ILE
2	G	1109	VAL
2	G	1123	ASP
2	G	1124	SER
2	G	1145	SER
2	G	1148	ASN
2	G	1160	THR
2	G	1171	ARG
2	G	1189	THR
2	G	1197	LEU
2	G	1211	LEU
2	G	1219	ILE
2	G	1227	ARG
2	G	1260	GLN
2	G	1265	MET
2	G	1284	VAL
2	G	1314	ARG
2	G	1318	THR
2	G	1328	VAL
2	G	1335	ILE
2	G	1348	LEU
2	G	1359	MET
2	G	1360	ILE
2	G	1378	ILE
2	G	1397	SER
2	G	1407	THR
2	G	1408	SER
2	G	1420	GLU
2	G	1434	HIS
2	G	1437	THR
2	G	1441	ILE
2	G	1443	VAL
2	G	1446	SER
2	G	1452	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	G	1463	THR
2	G	1468	THR
2	G	1470	THR
2	G	1472	VAL
2	G	1473	THR
2	G	1501	ILE
2	G	1511	SER
2	G	1526	THR
2	G	1527	LEU
2	G	1528	GLU
2	G	1533	LEU
2	G	1549	THR
2	G	1563	ILE
2	G	1567	ARG
2	G	1590	ARG
2	G	1602	SER
2	G	1605	VAL
2	G	1609	THR
2	G	1616	VAL
2	G	1624	THR
2	G	1627	GLN
2	G	1632	ILE
2	G	1637	LEU
2	G	1651	LEU
2	G	1672	GLN
2	G	1678	MET
2	G	1680	LEU
2	G	1683	THR
2	G	1712	ASN
2	G	1718	THR
2	G	1757	GLU
2	G	1775	GLN
2	G	1781	LEU
2	G	1784	MET
2	G	1825	GLU
2	G	1831	VAL
2	G	1834	ARG
2	G	1840	VAL
2	G	1844	ARG
2	G	1847	LEU
2	G	1857	ILE
2	G	1862	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	G	1886	VAL
2	G	1914	LEU
2	G	1936	VAL
2	G	1937	GLU
2	G	1941	PHE
2	G	1982	MET
2	G	2003	VAL
2	G	2042	ILE
2	G	2044	ASN
2	G	2047	LYS
2	G	2048	TYR
2	G	2050	GLN
2	H	6	THR
2	H	7	ARG
2	H	45	THR
2	H	46	GLU
2	H	48	PHE
2	H	56	THR
2	H	65	LEU
2	H	84	LEU
2	H	86	LEU
2	H	93	ASN
2	H	99	ASN
2	H	101	ILE
2	H	109	LEU
2	H	117	VAL
2	H	122	LEU
2	H	149	VAL
2	H	153	ASN
2	H	155	GLN
2	H	159	ILE
2	H	173	LEU
2	H	176	LEU
2	H	178	GLN
2	H	182	VAL
2	H	186	ASP
2	H	198	LEU
2	H	210	THR
2	H	227	ASP
2	H	236	ILE
2	H	240	LEU
2	H	246	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	H	281	VAL
2	H	286	THR
2	H	295	SER
2	H	297	ARG
2	H	300	ILE
2	H	315	PRO
2	H	319	LEU
2	H	339	LEU
2	H	340	SER
2	H	342	SER
2	H	344	LEU
2	H	353	VAL
2	H	371	VAL
2	H	376	ASN
2	H	389	LEU
2	H	392	THR
2	H	402	LEU
2	H	418	ASN
2	H	425	SER
2	H	431	LEU
2	H	448	VAL
2	H	455	ILE
2	H	462	THR
2	H	463	PHE
2	H	471	LEU
2	H	476	SER
2	H	478	ARG
2	H	482	CYS
2	H	492	THR
2	H	499	THR
2	H	545	GLN
2	H	553	ASN
2	H	562	LEU
2	H	572	ASN
2	H	574	SER
2	H	586	LEU
2	H	587	ILE
2	H	598	THR
2	H	607	VAL
2	H	611	THR
2	H	616	THR
2	H	653	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	H	665	LEU
2	H	669	LEU
2	H	670	ARG
2	H	676	ILE
2	H	693	GLU
2	H	714	SER
2	H	719	ILE
2	H	723	HIS
2	H	730	LEU
2	H	733	THR
2	H	736	ARG
2	H	741	HIS
2	H	751	LEU
2	H	762	ASN
2	H	767	PHE
2	H	775	ASP
2	H	777	THR
2	H	787	THR
2	H	794	MET
2	H	797	ASP
2	H	800	LEU
2	H	810	GLU
2	H	825	THR
2	H	832	TRP
2	H	835	THR
2	H	844	VAL
2	H	852	GLU
2	H	855	HIS
2	H	857	ILE
2	H	869	ASP
2	H	880	LEU
2	H	881	VAL
2	H	892	ILE
2	H	907	VAL
2	H	929	LEU
2	H	945	THR
2	H	952	ARG
2	H	953	ARG
2	H	964	LEU
2	H	971	SER
2	H	993	GLN
2	H	1015	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	H	1021	LEU
2	H	1024	ARG
2	H	1048	VAL
2	H	1066	ILE
2	H	1070	ILE
2	H	1082	ILE
2	H	1109	VAL
2	H	1123	ASP
2	H	1145	SER
2	H	1148	ASN
2	H	1160	THR
2	H	1171	ARG
2	H	1189	THR
2	H	1197	LEU
2	H	1211	LEU
2	H	1219	ILE
2	H	1227	ARG
2	H	1260	GLN
2	H	1265	MET
2	H	1284	VAL
2	H	1314	ARG
2	H	1318	THR
2	H	1328	VAL
2	H	1335	ILE
2	H	1348	LEU
2	H	1359	MET
2	H	1360	ILE
2	H	1378	ILE
2	H	1397	SER
2	H	1407	THR
2	H	1408	SER
2	H	1420	GLU
2	H	1434	HIS
2	H	1437	THR
2	H	1441	ILE
2	H	1443	VAL
2	H	1446	SER
2	H	1452	LEU
2	H	1463	THR
2	H	1468	THR
2	H	1470	THR
2	H	1472	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	H	1473	THR
2	H	1501	ILE
2	H	1511	SER
2	H	1526	THR
2	H	1527	LEU
2	H	1528	GLU
2	H	1533	LEU
2	H	1549	THR
2	H	1563	ILE
2	H	1567	ARG
2	H	1590	ARG
2	H	1602	SER
2	H	1605	VAL
2	H	1609	THR
2	H	1616	VAL
2	H	1624	THR
2	H	1627	GLN
2	H	1632	ILE
2	H	1637	LEU
2	H	1651	LEU
2	H	1672	GLN
2	H	1678	MET
2	H	1680	LEU
2	H	1683	THR
2	H	1693	ARG
2	H	1712	ASN
2	H	1718	THR
2	H	1757	GLU
2	H	1775	GLN
2	H	1781	LEU
2	H	1784	MET
2	H	1825	GLU
2	H	1831	VAL
2	H	1834	ARG
2	H	1840	VAL
2	H	1844	ARG
2	H	1847	LEU
2	H	1862	VAL
2	H	1886	VAL
2	H	1914	LEU
2	H	1936	VAL
2	H	1937	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	H	1982	MET
2	H	2003	VAL
2	H	2038	ILE
2	H	2042	ILE
2	H	2044	ASN
2	H	2047	LYS
2	H	2048	TYR
2	H	2050	GLN
2	I	6	THR
2	I	7	ARG
2	I	45	THR
2	I	46	GLU
2	I	48	PHE
2	I	56	THR
2	I	65	LEU
2	I	84	LEU
2	I	86	LEU
2	I	93	ASN
2	I	99	ASN
2	I	101	ILE
2	I	109	LEU
2	I	117	VAL
2	I	122	LEU
2	I	149	VAL
2	I	153	ASN
2	I	155	GLN
2	I	159	ILE
2	I	173	LEU
2	I	175	ASP
2	I	176	LEU
2	I	178	GLN
2	I	182	VAL
2	I	210	THR
2	I	227	ASP
2	I	236	ILE
2	I	240	LEU
2	I	246	LEU
2	I	281	VAL
2	I	286	THR
2	I	295	SER
2	I	297	ARG
2	I	300	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	I	303	LEU
2	I	319	LEU
2	I	339	LEU
2	I	340	SER
2	I	342	SER
2	I	344	LEU
2	I	353	VAL
2	I	371	VAL
2	I	376	ASN
2	I	389	LEU
2	I	392	THR
2	I	402	LEU
2	I	418	ASN
2	I	425	SER
2	I	431	LEU
2	I	444	VAL
2	I	448	VAL
2	I	455	ILE
2	I	462	THR
2	I	463	PHE
2	I	471	LEU
2	I	476	SER
2	I	478	ARG
2	I	479	ILE
2	I	482	CYS
2	I	492	THR
2	I	499	THR
2	I	539	ASP
2	I	545	GLN
2	I	553	ASN
2	I	562	LEU
2	I	572	ASN
2	I	574	SER
2	I	586	LEU
2	I	587	ILE
2	I	598	THR
2	I	607	VAL
2	I	611	THR
2	I	616	THR
2	I	653	TYR
2	I	665	LEU
2	I	669	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	I	670	ARG
2	I	676	ILE
2	I	680	THR
2	I	693	GLU
2	I	714	SER
2	I	719	ILE
2	I	723	HIS
2	I	730	LEU
2	I	733	THR
2	I	736	ARG
2	I	741	HIS
2	I	750	MET
2	I	751	LEU
2	I	762	ASN
2	I	767	PHE
2	I	775	ASP
2	I	777	THR
2	I	787	THR
2	I	794	MET
2	I	800	LEU
2	I	810	GLU
2	I	825	THR
2	I	832	TRP
2	I	835	THR
2	I	844	VAL
2	I	846	VAL
2	I	852	GLU
2	I	855	HIS
2	I	857	ILE
2	I	865	TRP
2	I	869	ASP
2	I	880	LEU
2	I	881	VAL
2	I	892	ILE
2	I	907	VAL
2	I	929	LEU
2	I	945	THR
2	I	952	ARG
2	I	953	ARG
2	I	964	LEU
2	I	971	SER
2	I	993	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	I	1015	VAL
2	I	1021	LEU
2	I	1024	ARG
2	I	1048	VAL
2	I	1066	ILE
2	I	1070	ILE
2	I	1082	ILE
2	I	1109	VAL
2	I	1123	ASP
2	I	1124	SER
2	I	1145	SER
2	I	1148	ASN
2	I	1160	THR
2	I	1171	ARG
2	I	1189	THR
2	I	1197	LEU
2	I	1211	LEU
2	I	1219	ILE
2	I	1227	ARG
2	I	1260	GLN
2	I	1265	MET
2	I	1284	VAL
2	I	1314	ARG
2	I	1318	THR
2	I	1328	VAL
2	I	1335	ILE
2	I	1348	LEU
2	I	1359	MET
2	I	1360	ILE
2	I	1378	ILE
2	I	1397	SER
2	I	1407	THR
2	I	1408	SER
2	I	1420	GLU
2	I	1434	HIS
2	I	1437	THR
2	I	1441	ILE
2	I	1443	VAL
2	I	1446	SER
2	I	1452	LEU
2	I	1463	THR
2	I	1468	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	I	1470	THR
2	I	1472	VAL
2	I	1473	THR
2	I	1501	ILE
2	I	1511	SER
2	I	1526	THR
2	I	1527	LEU
2	I	1528	GLU
2	I	1533	LEU
2	I	1549	THR
2	I	1563	ILE
2	I	1567	ARG
2	I	1590	ARG
2	I	1602	SER
2	I	1605	VAL
2	I	1609	THR
2	I	1616	VAL
2	I	1624	THR
2	I	1627	GLN
2	I	1632	ILE
2	I	1637	LEU
2	I	1651	LEU
2	I	1672	GLN
2	I	1678	MET
2	I	1680	LEU
2	I	1683	THR
2	I	1712	ASN
2	I	1718	THR
2	I	1757	GLU
2	I	1775	GLN
2	I	1781	LEU
2	I	1784	MET
2	I	1825	GLU
2	I	1831	VAL
2	I	1834	ARG
2	I	1844	ARG
2	I	1847	LEU
2	I	1862	VAL
2	I	1871	LEU
2	I	1886	VAL
2	I	1914	LEU
2	I	1936	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	I	1937	GLU
2	I	1982	MET
2	I	2003	VAL
2	I	2042	ILE
2	I	2044	ASN
2	I	2047	LYS
2	I	2048	TYR
2	I	2050	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (288) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	11	HIS
1	A	21	GLN
1	A	32	GLN
1	A	58	GLN
1	A	63	ASN
1	A	157	HIS
1	A	183	GLN
1	A	214	GLN
1	A	271	ASN
1	A	335	HIS
1	A	341	GLN
1	A	344	GLN
1	A	374	GLN
1	A	411	GLN
1	A	427	ASN
1	A	438	ASN
1	A	506	ASN
1	A	527	GLN
1	A	618	ASN
1	A	694	GLN
1	A	738	ASN
1	A	758	ASN
1	A	792	HIS
1	A	860	ASN
1	A	898	GLN
1	A	983	GLN
1	A	987	ASN
1	A	989	GLN
1	A	1000	GLN
1	A	1003	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1063	HIS
1	A	1064	ASN
1	A	1066	ASN
1	A	1146	HIS
1	A	1239	HIS
1	A	1385	GLN
1	A	1432	HIS
1	A	1433	HIS
1	A	1442	ASN
1	A	1458	GLN
1	A	1482	GLN
1	A	1495	ASN
1	A	1505	GLN
1	A	1510	ASN
1	A	1542	HIS
1	A	1549	ASN
1	A	1563	HIS
1	A	1577	GLN
1	A	1610	ASN
1	A	1652	GLN
1	A	1690	ASN
1	B	11	HIS
1	B	21	GLN
1	B	32	GLN
1	B	58	GLN
1	B	63	ASN
1	B	157	HIS
1	B	183	GLN
1	B	214	GLN
1	B	271	ASN
1	B	335	HIS
1	B	341	GLN
1	B	344	GLN
1	B	374	GLN
1	B	407	ASN
1	B	411	GLN
1	B	427	ASN
1	B	438	ASN
1	B	506	ASN
1	B	527	GLN
1	B	618	ASN
1	B	694	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	738	ASN
1	B	758	ASN
1	B	792	HIS
1	B	898	GLN
1	B	987	ASN
1	B	989	GLN
1	B	1000	GLN
1	B	1003	GLN
1	B	1063	HIS
1	B	1064	ASN
1	B	1066	ASN
1	B	1146	HIS
1	B	1239	HIS
1	B	1385	GLN
1	B	1432	HIS
1	B	1433	HIS
1	B	1442	ASN
1	B	1458	GLN
1	B	1482	GLN
1	B	1495	ASN
1	B	1505	GLN
1	B	1510	ASN
1	B	1542	HIS
1	B	1549	ASN
1	B	1563	HIS
1	B	1577	GLN
1	B	1610	ASN
1	B	1652	GLN
1	B	1690	ASN
1	C	11	HIS
1	C	21	GLN
1	C	32	GLN
1	C	58	GLN
1	C	63	ASN
1	C	157	HIS
1	C	183	GLN
1	C	214	GLN
1	C	271	ASN
1	C	335	HIS
1	C	341	GLN
1	C	344	GLN
1	C	374	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	411	GLN
1	C	427	ASN
1	C	438	ASN
1	C	506	ASN
1	C	527	GLN
1	C	618	ASN
1	C	694	GLN
1	C	738	ASN
1	C	758	ASN
1	C	792	HIS
1	C	860	ASN
1	C	898	GLN
1	C	987	ASN
1	C	989	GLN
1	C	1000	GLN
1	C	1003	GLN
1	C	1063	HIS
1	C	1064	ASN
1	C	1066	ASN
1	C	1146	HIS
1	C	1239	HIS
1	C	1385	GLN
1	C	1432	HIS
1	C	1433	HIS
1	C	1442	ASN
1	C	1458	GLN
1	C	1482	GLN
1	C	1495	ASN
1	C	1505	GLN
1	C	1510	ASN
1	C	1542	HIS
1	C	1549	ASN
1	C	1563	HIS
1	C	1577	GLN
1	C	1610	ASN
1	C	1652	GLN
1	C	1690	ASN
2	G	34	GLN
2	G	36	GLN
2	G	85	ASN
2	G	102	HIS
2	G	178	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	G	359	HIS
2	G	376	ASN
2	G	418	ASN
2	G	428	HIS
2	G	440	ASN
2	G	447	ASN
2	G	500	HIS
2	G	517	HIS
2	G	545	GLN
2	G	558	ASN
2	G	572	ASN
2	G	612	ASN
2	G	650	ASN
2	G	718	ASN
2	G	740	HIS
2	G	741	HIS
2	G	747	HIS
2	G	752	GLN
2	G	762	ASN
2	G	855	HIS
2	G	900	GLN
2	G	910	GLN
2	G	1046	GLN
2	G	1148	ASN
2	G	1217	ASN
2	G	1220	GLN
2	G	1260	GLN
2	G	1341	ASN
2	G	1352	HIS
2	G	1355	ASN
2	G	1367	GLN
2	G	1384	GLN
2	G	1595	ASN
2	G	1659	GLN
2	G	1669	GLN
2	G	1672	GLN
2	G	1697	HIS
2	G	1890	ASN
2	G	1896	GLN
2	G	1977	HIS
2	G	2013	ASN
2	G	2020	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	H	34	GLN
2	H	85	ASN
2	H	102	HIS
2	H	178	GLN
2	H	359	HIS
2	H	376	ASN
2	H	418	ASN
2	H	428	HIS
2	H	440	ASN
2	H	447	ASN
2	H	500	HIS
2	H	517	HIS
2	H	545	GLN
2	H	558	ASN
2	H	572	ASN
2	H	612	ASN
2	H	650	ASN
2	H	718	ASN
2	H	740	HIS
2	H	741	HIS
2	H	747	HIS
2	H	752	GLN
2	H	762	ASN
2	H	900	GLN
2	H	910	GLN
2	H	1039	HIS
2	H	1046	GLN
2	H	1148	ASN
2	H	1217	ASN
2	H	1220	GLN
2	H	1260	GLN
2	H	1341	ASN
2	H	1352	HIS
2	H	1355	ASN
2	H	1367	GLN
2	H	1659	GLN
2	H	1669	GLN
2	H	1672	GLN
2	H	1697	HIS
2	H	1890	ASN
2	H	1896	GLN
2	H	1977	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	H	2013	ASN
2	H	2020	GLN
2	I	34	GLN
2	I	36	GLN
2	I	85	ASN
2	I	102	HIS
2	I	178	GLN
2	I	359	HIS
2	I	376	ASN
2	I	418	ASN
2	I	428	HIS
2	I	440	ASN
2	I	447	ASN
2	I	500	HIS
2	I	517	HIS
2	I	545	GLN
2	I	558	ASN
2	I	572	ASN
2	I	612	ASN
2	I	718	ASN
2	I	740	HIS
2	I	741	HIS
2	I	747	HIS
2	I	752	GLN
2	I	762	ASN
2	I	855	HIS
2	I	900	GLN
2	I	910	GLN
2	I	1046	GLN
2	I	1055	HIS
2	I	1148	ASN
2	I	1217	ASN
2	I	1220	GLN
2	I	1260	GLN
2	I	1341	ASN
2	I	1352	HIS
2	I	1355	ASN
2	I	1367	GLN
2	I	1595	ASN
2	I	1669	GLN
2	I	1672	GLN
2	I	1697	HIS

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Mol	Chain	Res	Type
2	I	1868	GLN
2	I	1890	ASN
2	I	1896	GLN
2	I	1977	HIS
2	I	2013	ASN
2	I	2020	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FMN	G	3051	-	31,33,33	6.88	18 (58%)	40,50,50	1.96	7 (17%)
4	FMN	H	3051	-	31,33,33	6.73	18 (58%)	40,50,50	1.91	8 (20%)
3	CER	A	2748	1	10,11,15	4.19	3 (30%)	9,13,17	3.18	3 (33%)
3	CER	B	2748	1	10,11,15	4.19	3 (30%)	9,13,17	3.05	3 (33%)
4	FMN	I	3051	-	31,33,33	6.74	21 (67%)	40,50,50	1.81	7 (17%)
3	CER	C	2748	1	10,11,15	4.21	3 (30%)	9,13,17	3.18	3 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FMN	G	3051	-	-	5/18/18/18	0/3/3/3
4	FMN	H	3051	-	-	5/18/18/18	0/3/3/3
3	CER	A	2748	1	-	5/12/12/16	-
3	CER	B	2748	1	-	5/12/12/16	-
4	FMN	I	3051	-	-	5/18/18/18	0/3/3/3
3	CER	C	2748	1	-	5/12/12/16	-

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	3051	FMN	C4A-C10	16.06	1.54	1.38
4	H	3051	FMN	C4A-C10	15.15	1.53	1.38
4	I	3051	FMN	C4A-C10	14.86	1.53	1.38
4	G	3051	FMN	C4A-N5	12.70	1.51	1.33
4	I	3051	FMN	C4A-N5	12.26	1.50	1.33
4	H	3051	FMN	C4A-N5	12.20	1.50	1.33
3	C	2748	CER	O1-C4	11.69	1.41	1.21
3	A	2748	CER	O1-C4	11.67	1.41	1.21
3	B	2748	CER	O1-C4	11.63	1.41	1.21
4	G	3051	FMN	C10-N1	11.49	1.48	1.33
4	H	3051	FMN	C10-N1	11.35	1.47	1.33
4	I	3051	FMN	C6-C5A	11.06	1.59	1.41
4	I	3051	FMN	C10-N1	10.87	1.47	1.33
4	G	3051	FMN	C6-C5A	10.78	1.58	1.41
4	H	3051	FMN	C6-C5A	10.58	1.58	1.41
4	H	3051	FMN	C4-N3	10.22	1.50	1.33
4	I	3051	FMN	C5A-N5	9.86	1.51	1.35
4	G	3051	FMN	C4-N3	9.85	1.50	1.33
4	I	3051	FMN	C4-N3	9.83	1.50	1.33
4	G	3051	FMN	C5A-N5	9.70	1.51	1.35
4	H	3051	FMN	C5A-N5	9.56	1.51	1.35
4	G	3051	FMN	C9-C9A	9.45	1.59	1.40
4	H	3051	FMN	C9-C9A	9.33	1.59	1.40
4	I	3051	FMN	C9-C9A	9.29	1.59	1.40
4	G	3051	FMN	C9A-N10	8.68	1.50	1.38
4	H	3051	FMN	C9A-N10	8.32	1.49	1.38
4	I	3051	FMN	C9A-N10	8.27	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	3051	FMN	C6-C7	7.90	1.57	1.37
4	I	3051	FMN	C6-C7	7.71	1.57	1.37
4	G	3051	FMN	C2-N1	7.69	1.53	1.38
4	H	3051	FMN	C2-N3	7.68	1.53	1.38
4	H	3051	FMN	C6-C7	7.55	1.57	1.37
4	H	3051	FMN	C2-N1	7.51	1.53	1.38
4	I	3051	FMN	C2-N1	7.45	1.52	1.38
4	I	3051	FMN	C9-C8	7.33	1.56	1.37
4	I	3051	FMN	C8-C7	7.29	1.59	1.40
4	G	3051	FMN	C2-N3	7.27	1.52	1.38
4	G	3051	FMN	O4-C4	7.17	1.42	1.24
4	I	3051	FMN	C2-N3	7.10	1.52	1.38
4	G	3051	FMN	C9-C8	7.10	1.55	1.37
4	G	3051	FMN	C4-C4A	7.09	1.53	1.41
4	H	3051	FMN	O4-C4	7.08	1.42	1.24
4	H	3051	FMN	C9-C8	7.00	1.55	1.37
4	I	3051	FMN	O4-C4	6.94	1.42	1.24
4	G	3051	FMN	C8-C7	6.89	1.58	1.40
4	H	3051	FMN	C4-C4A	6.82	1.53	1.41
4	H	3051	FMN	C8-C7	6.72	1.57	1.40
4	I	3051	FMN	C4-C4A	6.61	1.52	1.41
4	I	3051	FMN	C9A-C5A	6.59	1.55	1.42
4	G	3051	FMN	C9A-C5A	6.31	1.55	1.42
4	H	3051	FMN	C9A-C5A	6.04	1.54	1.42
3	C	2748	CER	C1-N1	4.46	1.47	1.32
3	B	2748	CER	C1-N1	4.44	1.47	1.32
3	A	2748	CER	C1-N1	4.39	1.47	1.32
3	B	2748	CER	C5-C4	3.49	1.56	1.51
3	C	2748	CER	C5-C4	3.47	1.55	1.51
3	A	2748	CER	C5-C4	3.38	1.55	1.51
4	I	3051	FMN	P-O2P	3.04	1.66	1.54
4	H	3051	FMN	P-O2P	2.92	1.66	1.54
4	G	3051	FMN	P-O2P	2.89	1.66	1.54
4	I	3051	FMN	P-O3P	2.84	1.65	1.54
4	H	3051	FMN	P-O3P	2.81	1.65	1.54
4	G	3051	FMN	P-O3P	2.60	1.64	1.54
4	I	3051	FMN	C8M-C8	2.26	1.55	1.51
4	I	3051	FMN	C7M-C7	2.10	1.55	1.51
4	I	3051	FMN	C5'-C4'	2.04	1.54	1.51

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2748	CER	O1-C4-C5	-7.72	107.97	121.70
3	A	2748	CER	O1-C4-C5	-7.67	108.06	121.70
4	H	3051	FMN	C4-N3-C2	7.46	121.44	115.14
3	B	2748	CER	O1-C4-C5	-7.34	108.64	121.70
4	G	3051	FMN	C4-N3-C2	7.33	121.33	115.14
4	I	3051	FMN	C4-N3-C2	7.00	121.05	115.14
4	G	3051	FMN	C1'-N10-C9A	4.68	121.97	118.29
4	H	3051	FMN	C1'-N10-C9A	4.30	121.68	118.29
4	H	3051	FMN	C4A-C4-N3	-3.94	118.04	123.43
4	G	3051	FMN	C4A-C4-N3	-3.90	118.10	123.43
4	I	3051	FMN	C1'-N10-C9A	3.89	121.35	118.29
3	A	2748	CER	C5-C4-C3	-3.86	110.87	117.94
3	B	2748	CER	C5-C4-C3	-3.77	111.03	117.94
3	C	2748	CER	C5-C4-C3	-3.76	111.05	117.94
4	I	3051	FMN	C4A-C4-N3	-3.67	118.41	123.43
3	A	2748	CER	C6-C5-C4	-3.35	108.47	113.88
3	C	2748	CER	C6-C5-C4	-3.30	108.56	113.88
4	G	3051	FMN	C4A-N5-C5A	3.29	120.06	116.77
4	H	3051	FMN	C4A-N5-C5A	3.17	119.94	116.77
4	G	3051	FMN	C10-C4A-N5	-3.15	119.08	121.26
3	B	2748	CER	C6-C5-C4	-3.05	108.95	113.88
4	H	3051	FMN	C10-C4A-N5	-2.98	119.20	121.26
4	I	3051	FMN	C4A-N5-C5A	2.97	119.74	116.77
4	G	3051	FMN	C5A-C9A-N10	2.97	119.86	117.72
4	I	3051	FMN	C4'-C3'-C2'	-2.76	107.62	113.36
4	H	3051	FMN	C4'-C3'-C2'	-2.72	107.71	113.36
4	G	3051	FMN	C4'-C3'-C2'	-2.70	107.74	113.36
4	I	3051	FMN	C5A-C9A-N10	2.59	119.59	117.72
4	H	3051	FMN	C5A-C9A-N10	2.51	119.53	117.72
4	I	3051	FMN	C10-C4A-N5	-2.41	119.59	121.26
4	H	3051	FMN	O5'-C5'-C4'	-2.03	103.94	109.36

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	3051	FMN	C2'-C3'-C4'-C5'
4	G	3051	FMN	O3'-C3'-C4'-C5'
4	H	3051	FMN	C2'-C3'-C4'-C5'
4	H	3051	FMN	O3'-C3'-C4'-C5'
3	A	2748	CER	C2-C3-C4-O1
3	B	2748	CER	C2-C3-C4-O1
4	I	3051	FMN	C2'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
4	I	3051	FMN	O3'-C3'-C4'-C5'
3	C	2748	CER	C2-C3-C4-O1
4	H	3051	FMN	O3'-C3'-C4'-O4'
4	I	3051	FMN	O3'-C3'-C4'-O4'
4	I	3051	FMN	C2'-C3'-C4'-O4'
4	H	3051	FMN	C2'-C3'-C4'-O4'
3	A	2748	CER	O2-C1-C2-C3
3	B	2748	CER	O2-C1-C2-C3
3	C	2748	CER	O2-C1-C2-C3
4	G	3051	FMN	C2'-C3'-C4'-O4'
4	G	3051	FMN	O3'-C3'-C4'-O4'
3	A	2748	CER	N1-C1-C2-C3
3	B	2748	CER	N1-C1-C2-C3
3	C	2748	CER	N1-C1-C2-C3
3	C	2748	CER	C5-C6-C7-C8
3	A	2748	CER	O3-C3-C4-O1
3	B	2748	CER	O3-C3-C4-O1
3	C	2748	CER	O3-C3-C4-O1
3	A	2748	CER	C5-C6-C7-C8
3	B	2748	CER	C5-C6-C7-C8
4	G	3051	FMN	C4'-C5'-O5'-P
4	H	3051	FMN	C4'-C5'-O5'-P
4	I	3051	FMN	C4'-C5'-O5'-P

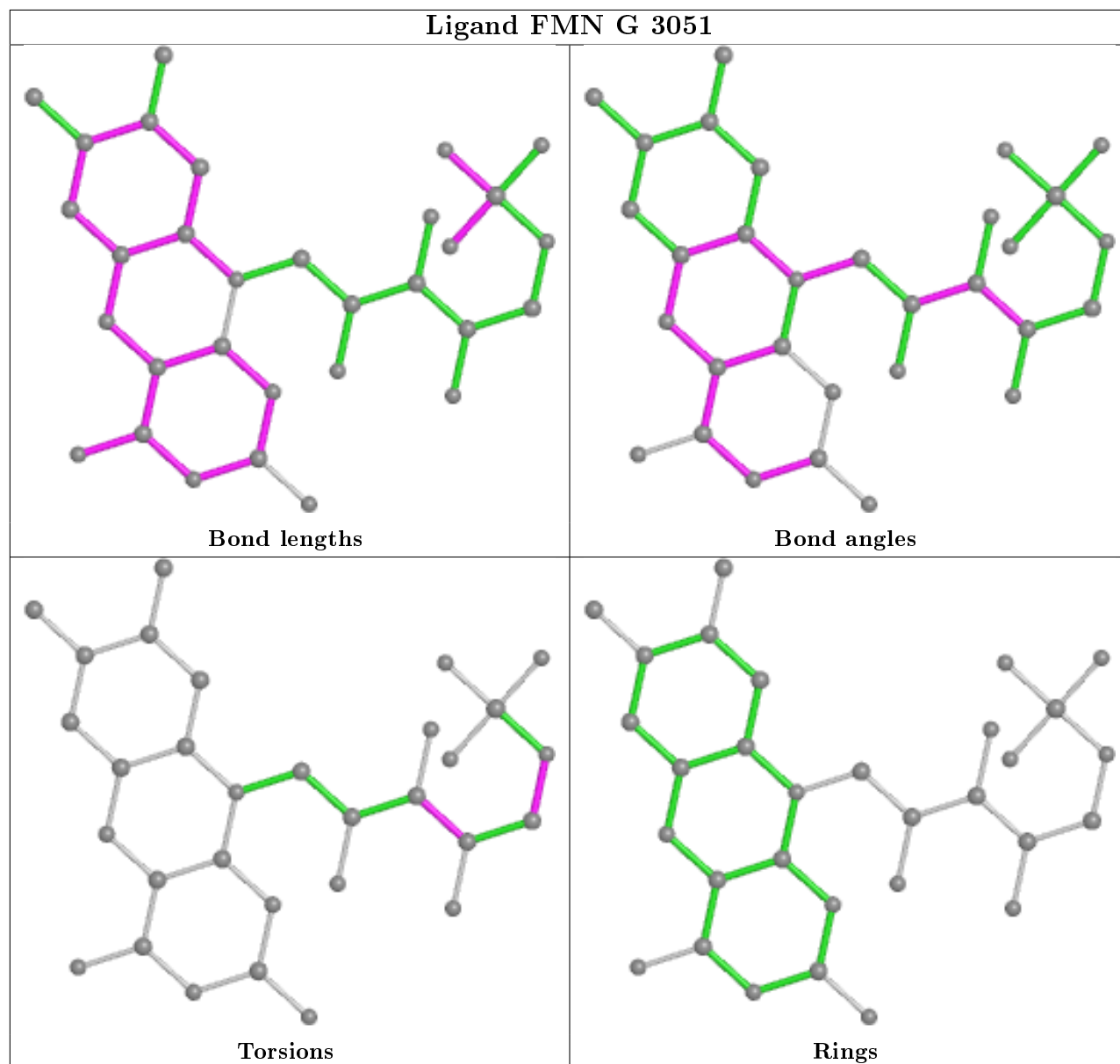
There are no ring outliers.

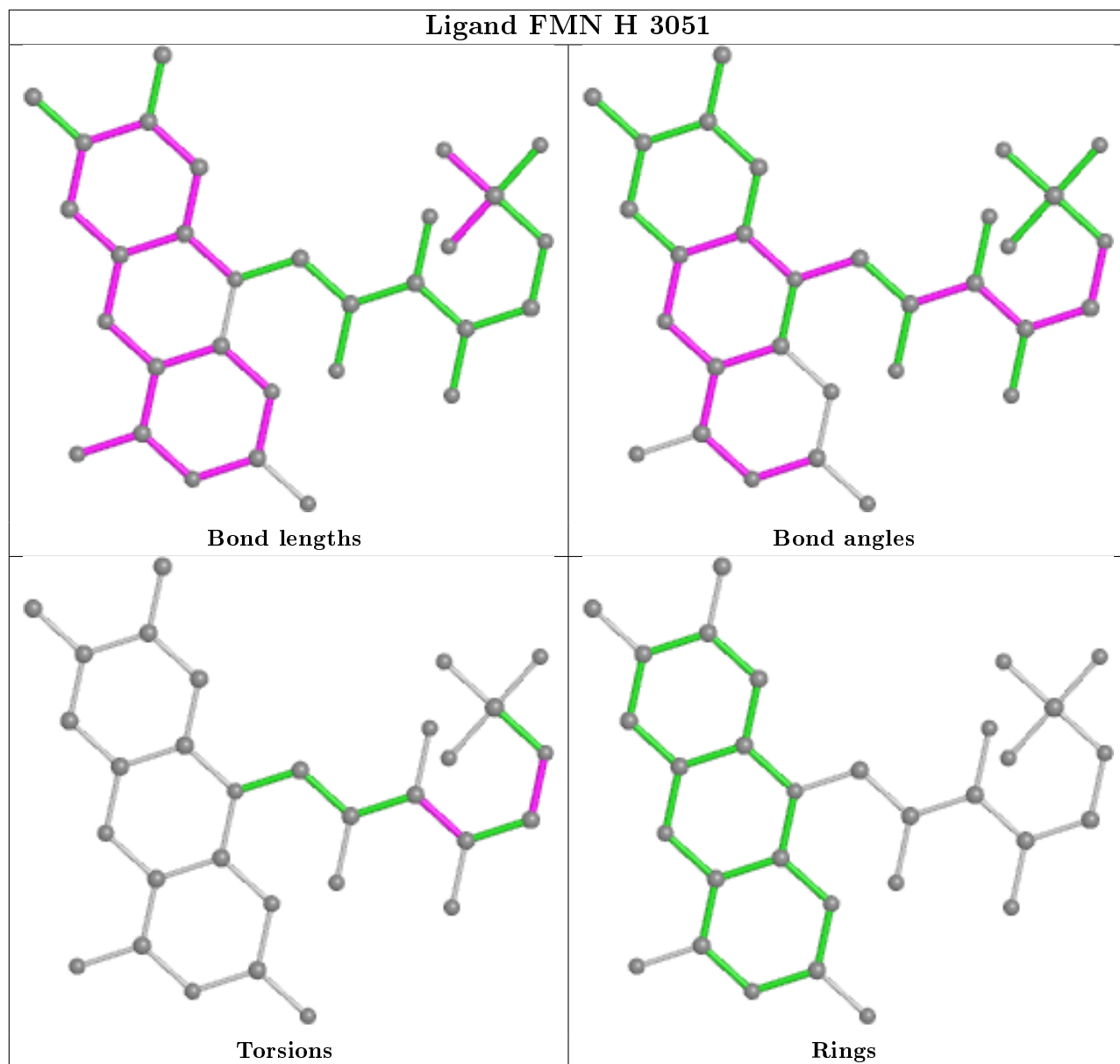
6 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	3051	FMN	7	0
4	H	3051	FMN	6	0
3	A	2748	CER	3	0
3	B	2748	CER	4	0
4	I	3051	FMN	8	0
3	C	2748	CER	4	0

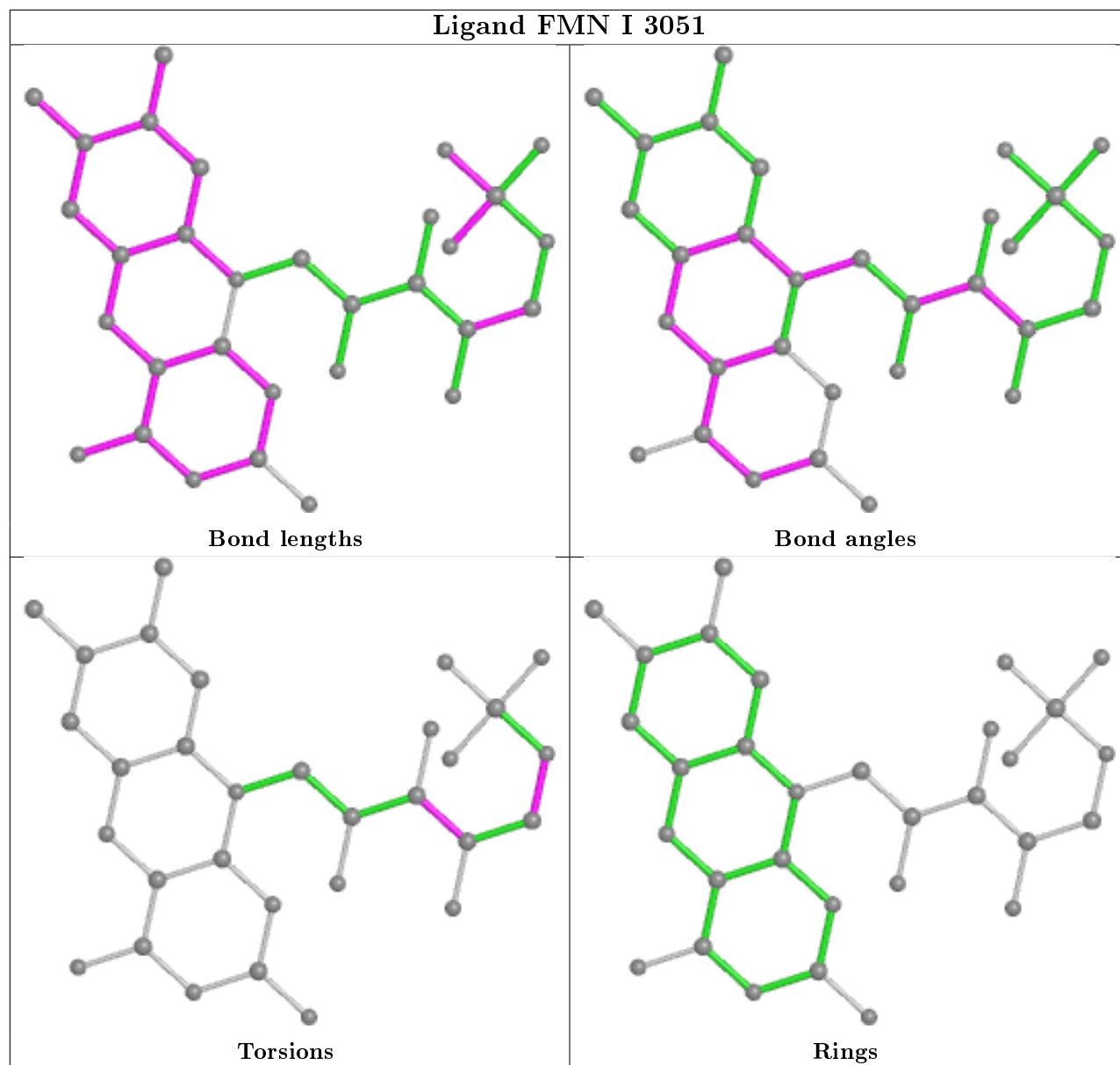
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	6
1	C	4
2	G	3

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Mol	Chain	Number of breaks
1	A	3
2	I	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	559:PRO	C	560:ASN	N	1.87
1	A	485:ASP	C	486:VAL	N	1.77
1	H	315:PRO	C	316:ASN	N	1.64
1	H	1530:LYS	C	1531:VAL	N	1.60
1	C	932:PHE	C	933:VAL	N	1.19
1	I	1529:GLN	C	1530:LYS	N	1.19
1	C	381:GLU	C	382:LEU	N	1.18
1	G	559:PRO	C	560:ASN	N	1.18
1	G	1422:THR	C	1423:PHE	N	1.18
1	I	1422:THR	C	1423:PHE	N	1.18
1	G	1841:ALA	C	1842:VAL	N	1.17
1	A	1118:LYS	C	1119:LYS	N	1.14
1	H	1529:GLN	C	1530:LYS	N	1.12
1	A	932:PHE	C	933:VAL	N	1.11
1	C	181:THR	C	182:VAL	N	1.05
1	H	1422:THR	C	1423:PHE	N	1.03
1	C	1430:ARG	C	1431:GLU	N	1.02
1	H	1657:ILE	C	1658:GLU	N	0.58

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1614/1887 (85%)	-0.42	11 (0%) 87 82	98, 134, 233, 288	0
1	B	1614/1887 (85%)	-0.42	10 (0%) 89 84	99, 133, 233, 296	0
1	C	1614/1887 (85%)	-0.41	14 (0%) 84 77	100, 135, 233, 294	0
2	G	2033/2051 (99%)	-0.42	6 (0%) 94 90	134, 172, 221, 270	0
2	H	2033/2051 (99%)	-0.31	11 (0%) 91 85	133, 173, 218, 268	0
2	I	2033/2051 (99%)	-0.39	6 (0%) 94 90	134, 173, 218, 264	0
All	All	10941/11814 (92%)	-0.39	58 (0%) 91 85	98, 164, 226, 296	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	539	SER	6.2
1	C	875	THR	5.8
1	B	875	THR	5.3
1	B	1747	ALA	5.3
1	A	540	GLN	4.1
2	G	1956	ARG	4.0
1	A	539	SER	4.0
1	B	540	GLN	3.8
2	H	1953	VAL	3.8
2	I	1928	GLN	3.7
1	C	540	GLN	3.7
1	C	539	SER	3.6
2	H	1671	SER	3.5
1	B	976	ALA	3.5
1	A	1747	ALA	3.5
1	A	208	GLU	3.4
2	H	1929	LYS	3.3
1	B	141	ALA	3.3
1	B	599	MET	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	140	ILE	3.1
1	A	974	ASP	3.1
1	C	204	THR	3.0
1	A	1476	GLU	3.0
1	B	1746	ASN	3.0
2	H	1964	PHE	2.9
2	H	2033	THR	2.9
2	H	408	PRO	2.9
1	A	1746	ASN	2.9
2	I	75	SER	2.8
1	C	201	PRO	2.8
1	C	198	PRO	2.7
1	C	141	ALA	2.7
1	A	975	ALA	2.7
1	C	202	GLU	2.7
1	A	875	THR	2.6
2	H	1959	LYS	2.6
1	C	199	GLU	2.6
2	I	648	GLY	2.5
1	C	200	LYS	2.4
1	C	260	ARG	2.4
2	G	1747	LYS	2.4
2	H	1853	GLY	2.3
1	B	600	ASP	2.3
2	I	74	PRO	2.3
2	I	1929	LYS	2.3
2	G	413	LYS	2.3
1	A	199	GLU	2.3
2	H	1740	THR	2.2
1	C	301	ASP	2.2
2	H	1956	ARG	2.2
2	G	1958	LEU	2.1
2	G	1806	GLY	2.1
2	G	333	GLY	2.1
2	H	406	ARG	2.1
2	I	1741	ILE	2.1
1	A	202	GLU	2.1
1	C	1475	GLU	2.1
1	C	302	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

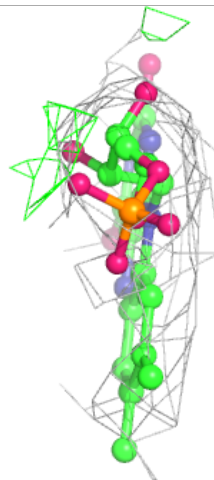
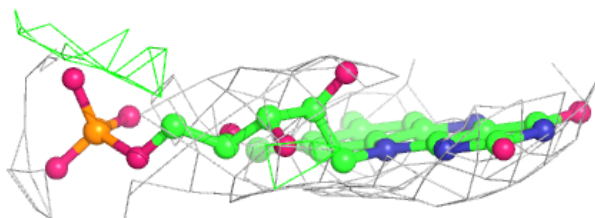
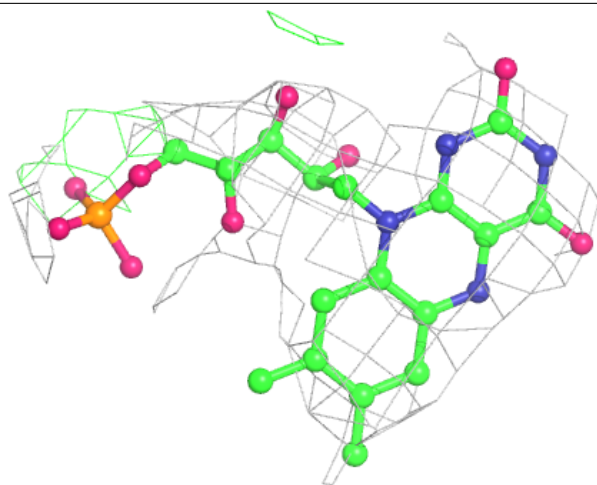
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CER	A	2748	12/16	0.81	0.32	70,134,243,252	0
4	FMN	I	3051	31/31	0.85	0.41	132,164,181,204	0
4	FMN	G	3051	31/31	0.87	0.33	137,161,187,206	0
4	FMN	H	3051	31/31	0.88	0.26	133,160,184,188	0
3	CER	C	2748	12/16	0.90	0.37	70,134,252,253	0
3	CER	B	2748	12/16	0.91	0.21	70,134,252,253	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

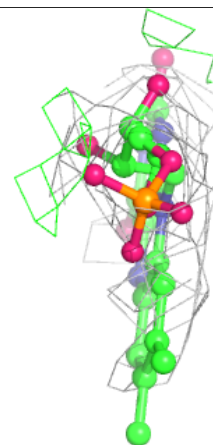
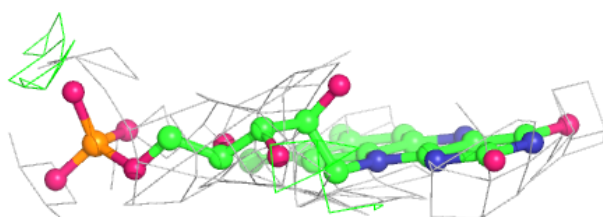
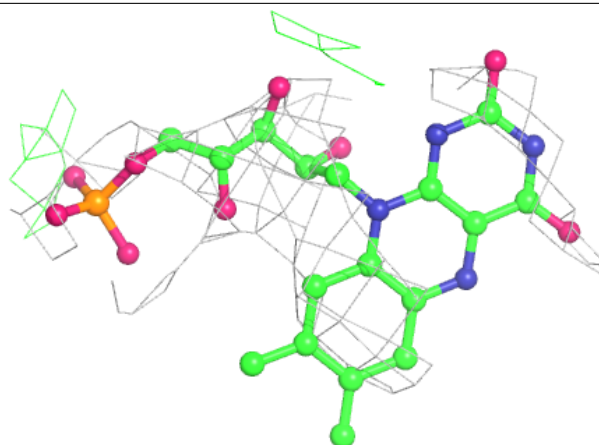
**Electron density around FMN I 3051:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

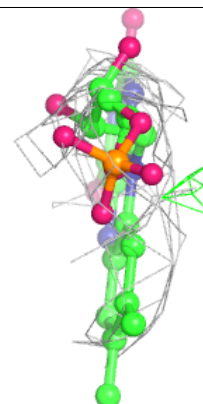
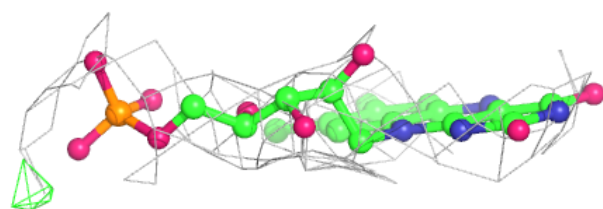
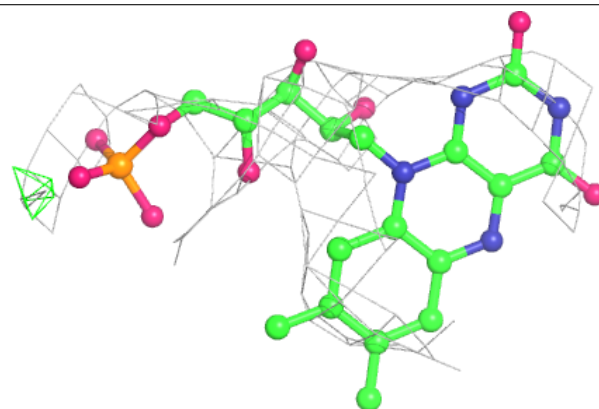


**Electron density around FMN G 3051:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around FMN H 3051:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers

There are no such residues in this entry.