



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2020 – 10:09 AM BST

PDB ID : 2UV8
Title : Crystal structure of yeast fatty acid synthase with stalled acyl carrier protein at 3.1 angstrom resolution
Authors : Leibundgut, M.; Jenni, S.; Frick, C.; Ban, N.
Deposited on : 2007-03-09
Resolution : 3.10 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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 : 2.13
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) : 2.13

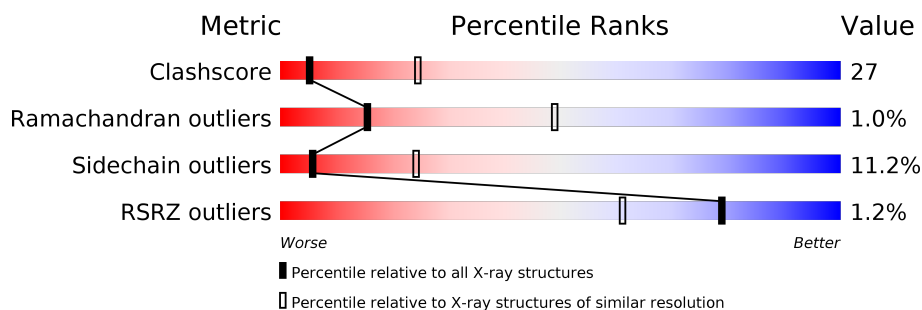
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 ≥ 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	<div> <div>2%</div> <div>50% 31% 5% 14%</div> </div>
1	B	1887	<div> <div>%</div> <div>51% 30% 5% 14%</div> </div>
1	C	1887	<div> <div>2%</div> <div>49% 31% 5% 14%</div> </div>
2	G	2051	<div> <div>%</div> <div>51% 41% 7%</div> </div>
2	H	2051	<div> <div>%</div> <div>52% 40% 7%</div> </div>
2	I	2051	<div> <div>%</div> <div>51% 41% 8%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 85962 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.

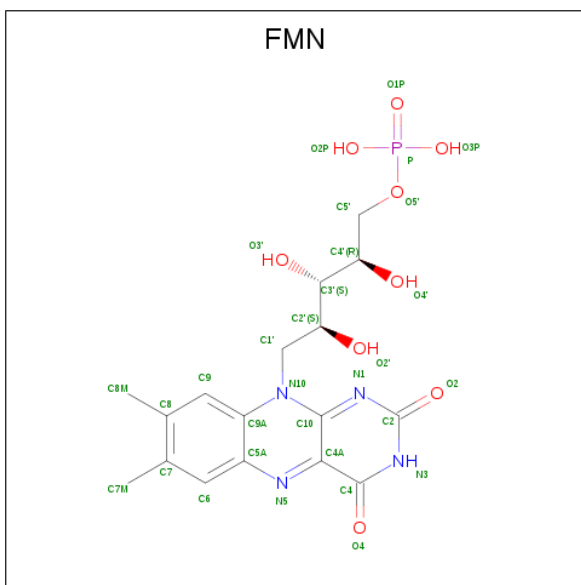
- Molecule 1 is a protein called FATTY ACID SYNTHASE SUBUNIT ALPHA (FAS2).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1614	Total	C	N	O	P	S	0	0	0
			12628	8003	2128	2448	1	48			
1	B	1614	Total	C	N	O	P	S	0	0	0
			12628	8003	2128	2448	1	48			
1	C	1614	Total	C	N	O	P	S	0	0	0
			12628	8003	2128	2448	1	48			

- Molecule 2 is a protein called FATTY ACID SYNTHASE SUBUNIT BETA (FAS1).

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

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).

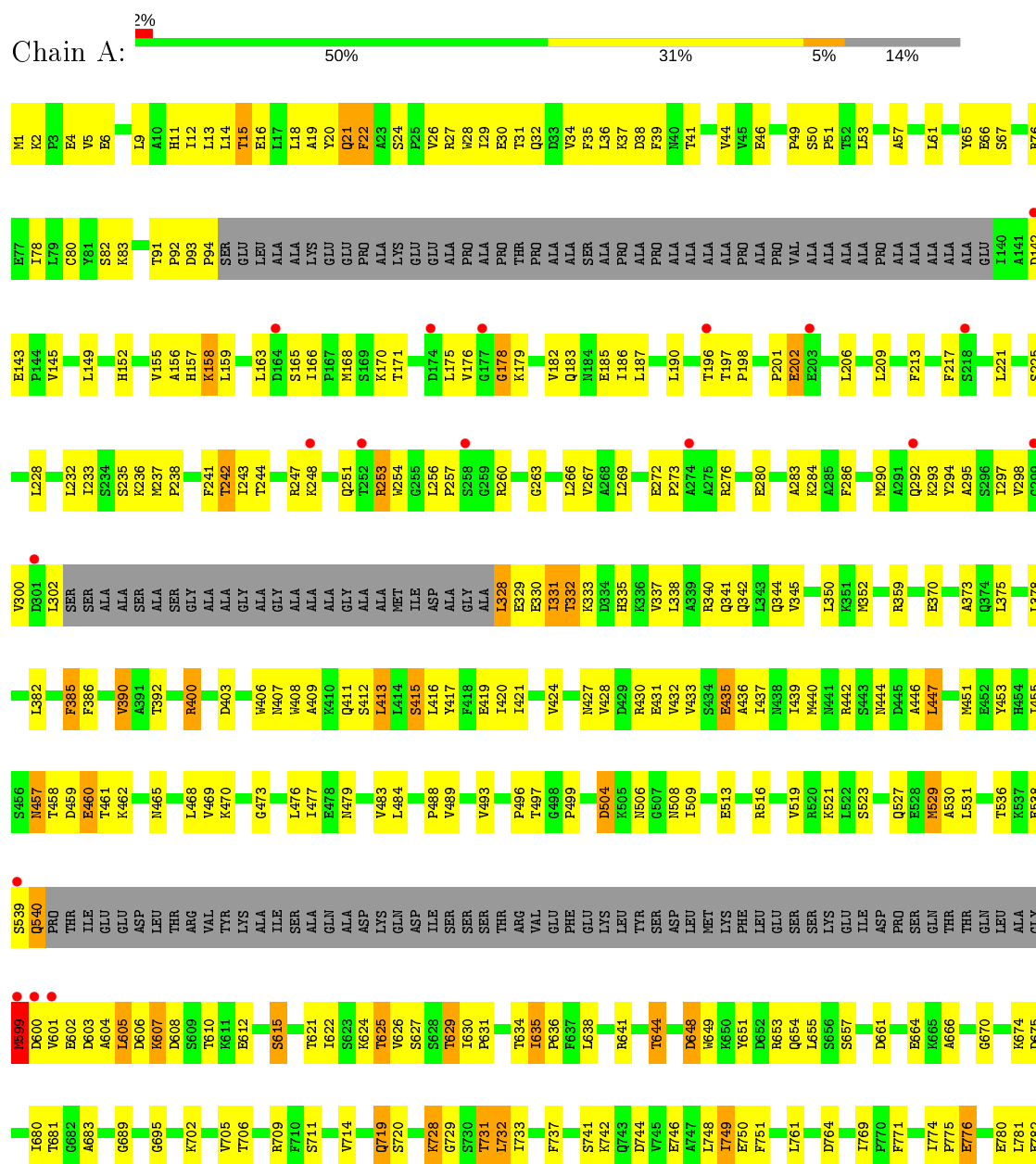


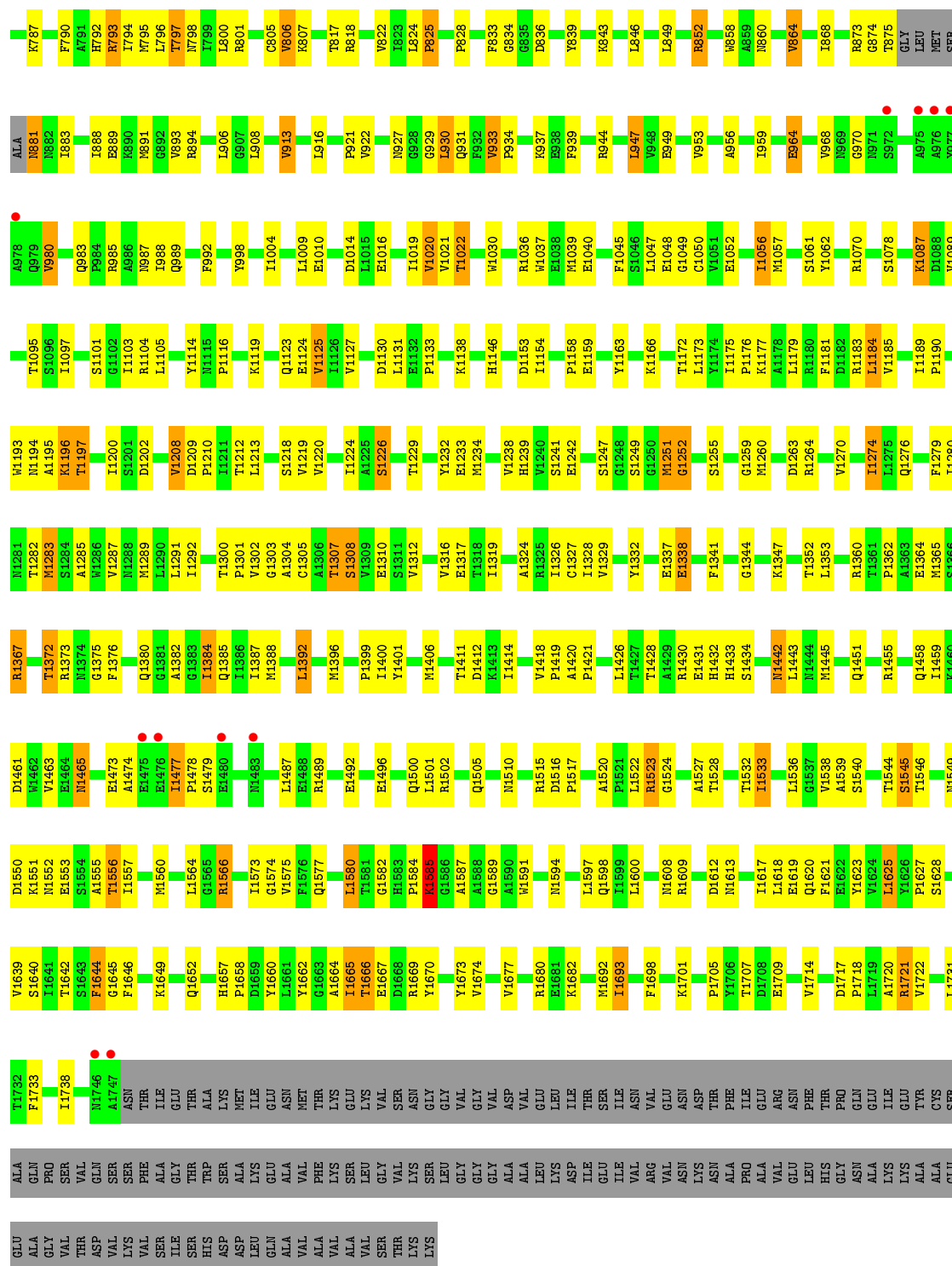
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total 31	C 17	N 4	O 9	P 1	0	0
3	H	1	Total 31	C 17	N 4	O 9	P 1	0	0
3	I	1	Total 31	C 17	N 4	O 9	P 1	0	0

3 Residue-property plots

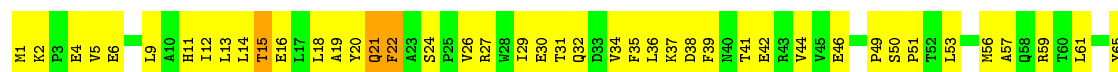
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 (FAS2)

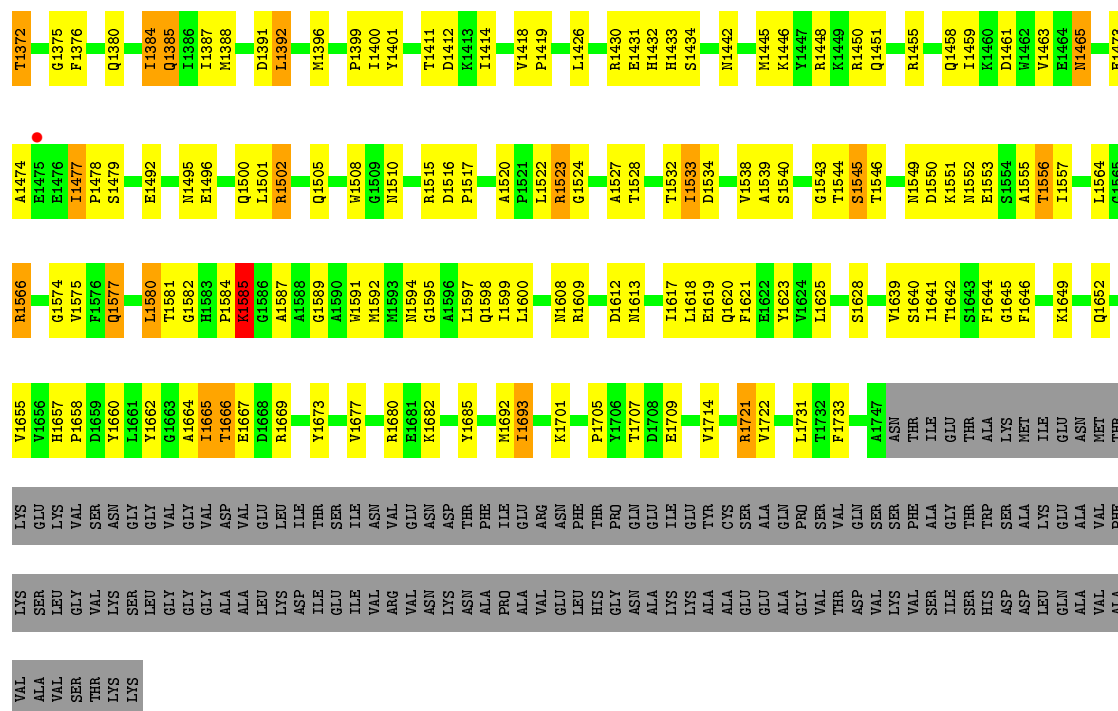




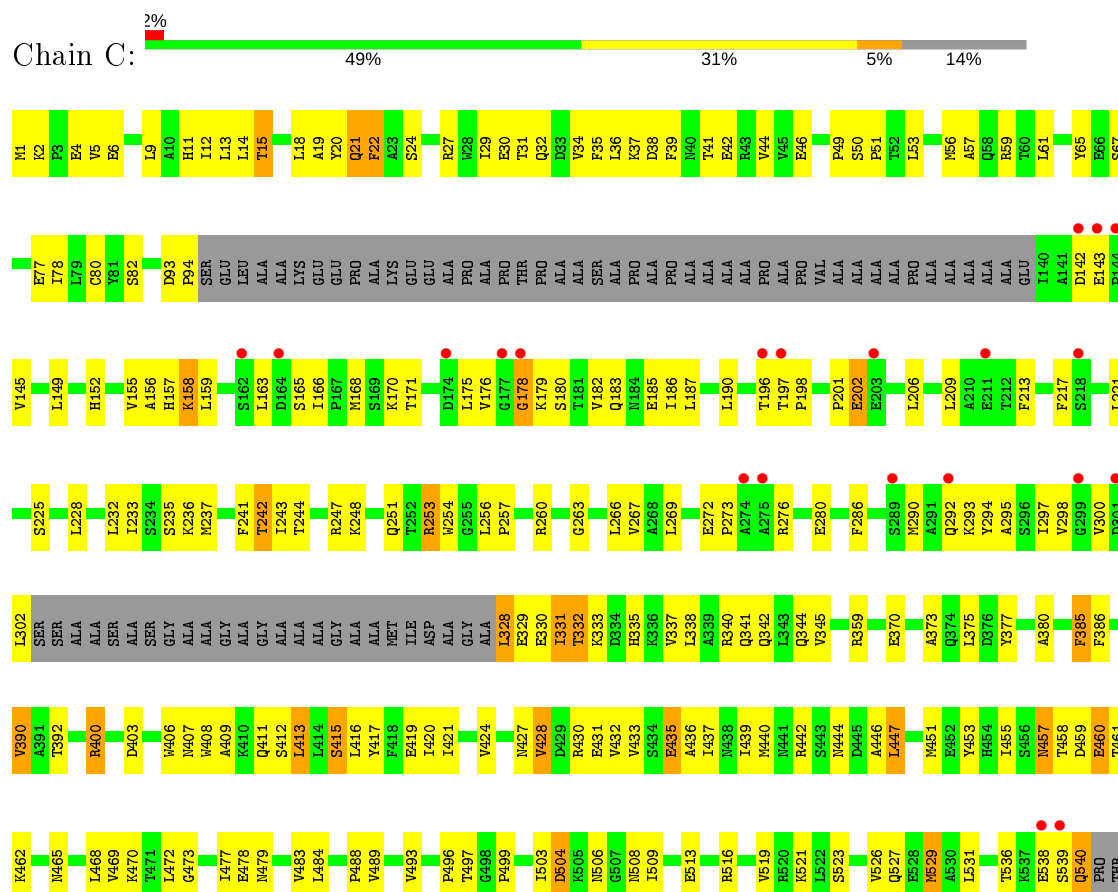
• Molecule 1: FATTY ACID SYNTHASE SUBUNIT ALPHA (FAS2)







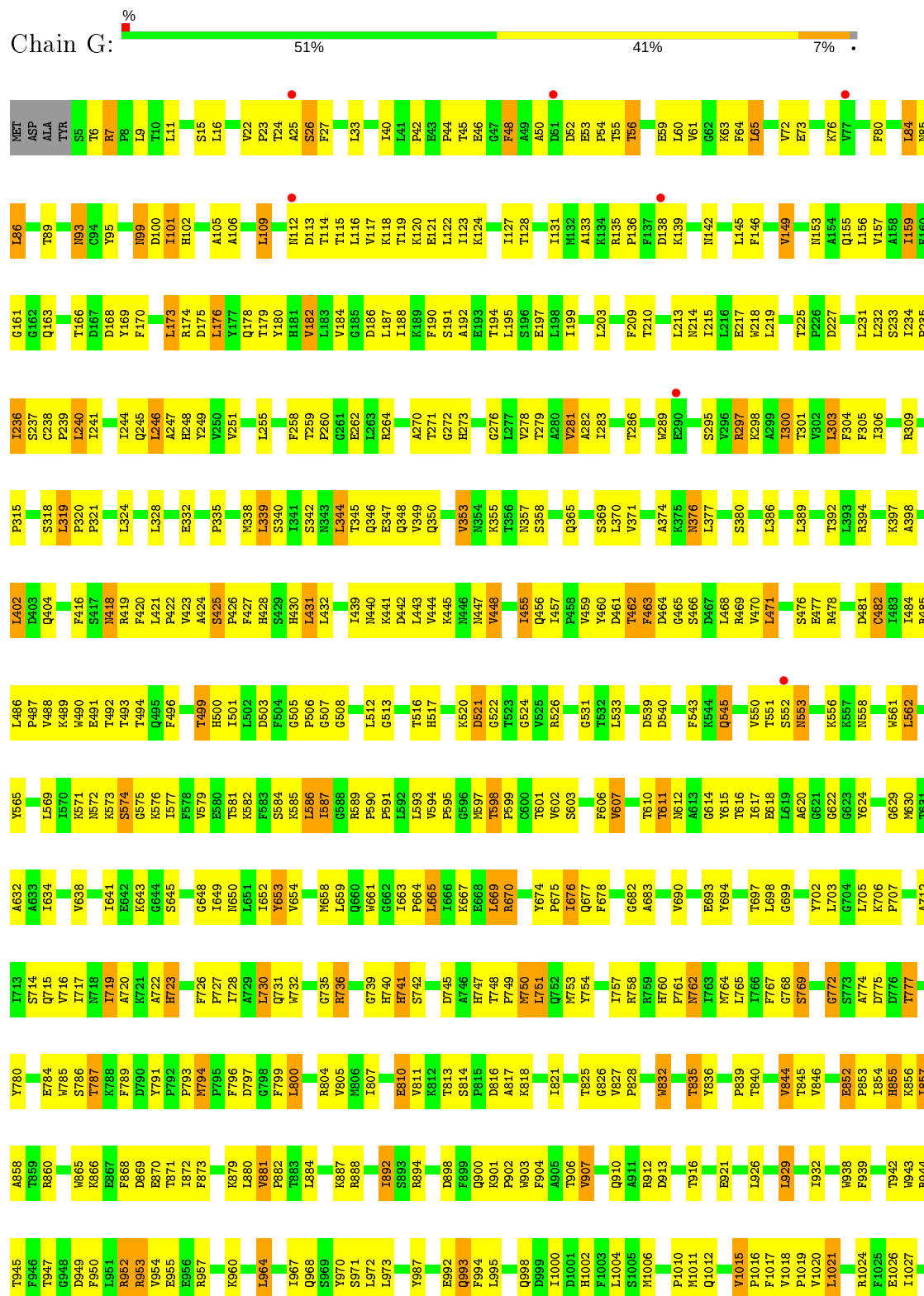
• Molecule 1: FATTY ACID SYNTHASE SUBUNIT ALPHA (FAS2)

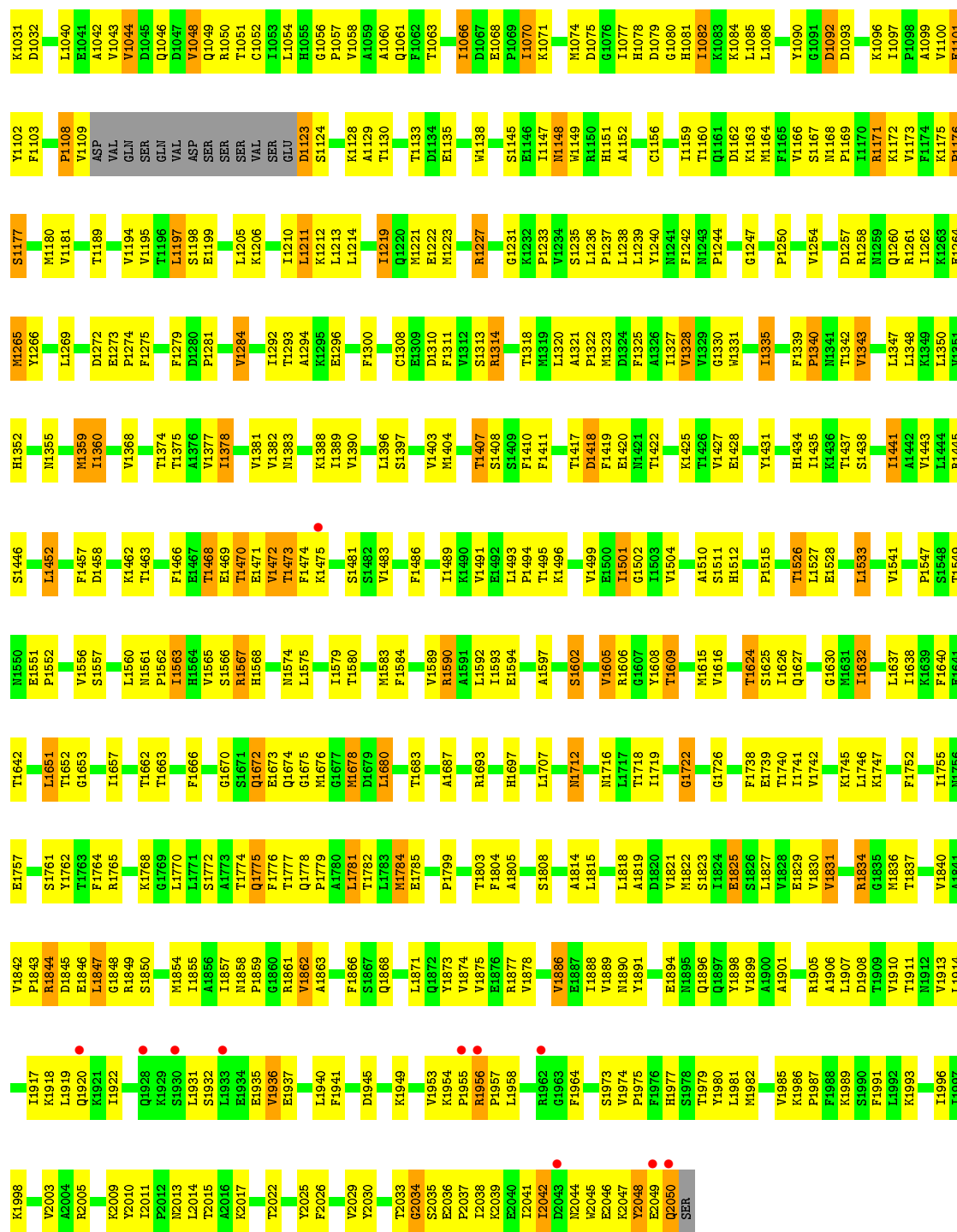




VAL	ASP	ASN	LYS	ASN	ALA	PRO	ALA	ALA	VAL	GLU	HIS	GLY	ASN	ALA	LYS	LYS	ALA	ALA	GLU	GLU	GLY	VAL	THR	ASP	VAL	LYS	VAL	SER	ILE	SER	HIS	ASP	ASP	LEU	GLN	ALA	VAL	ALA	VAL	ALA	VAL	SER	THR	LYS	LYS
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• Molecule 2: FATTY ACID SYNTHASE SUBUNIT BETA (FAS1)

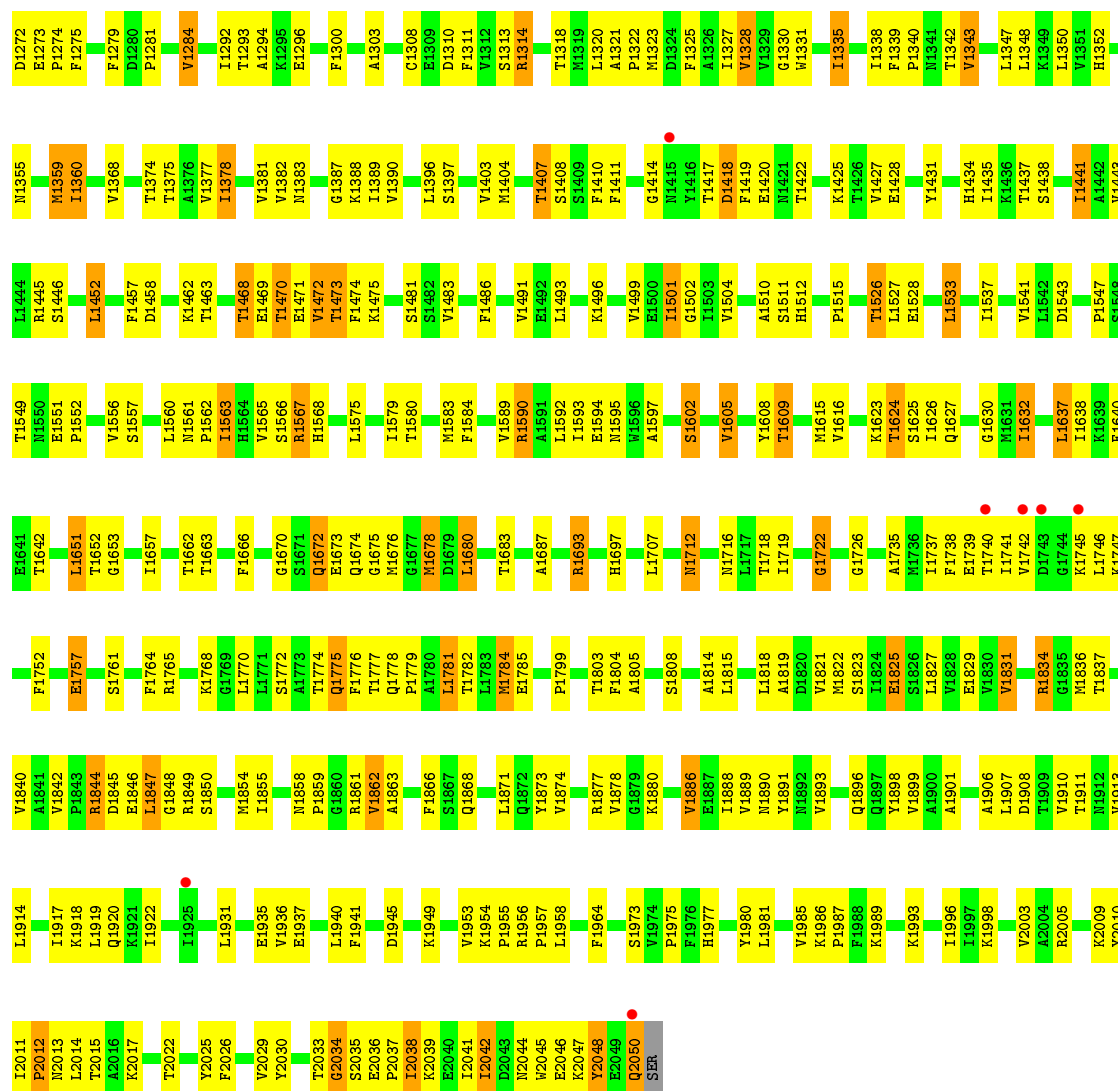




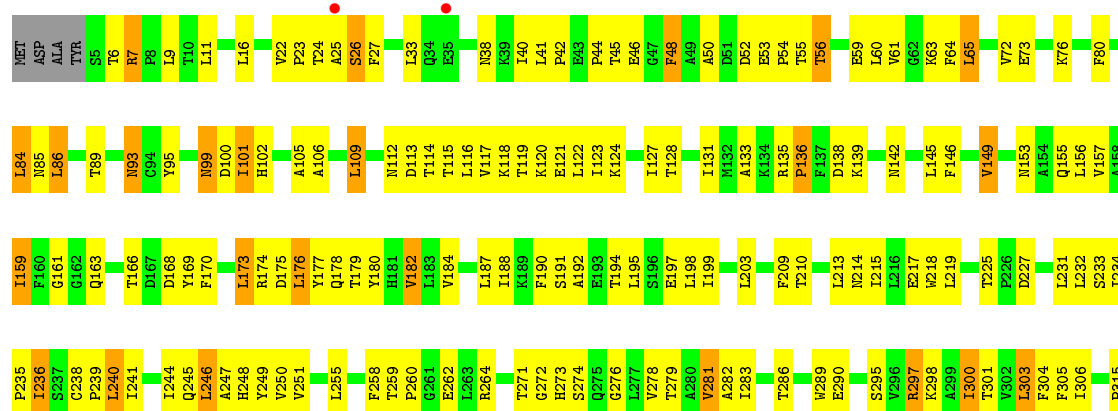
- Molecule 2: FATTY ACID SYNTHASE SUBUNIT BETA (FAS1)



V1195	V1196	L1197	S1198	E1199	L1205	K1206	L1210	L1211	L1212	L1213	L1214	M1217	L1218	Q1220	M1221	E1222	M1223	L1227	L1228	G1231	K1232	P1233	V1234	S1235	L1236	L1237	L1238	L1239	F1242	H1243	P1244	G1247	P1250	V1254	D1257	R1258	H1259	Q1260	R1261	L1262	K1263	E1264	M1265	Y1266	L1269	M1270	I1271				
ASP	VAL	GLN	SER	GLN	VAL	ASP	SER	SER	VAL	SER	GLU	D1123	K1128	A1129	T1130	T1133	E1135	M1138	S1145	E1146	D1147	M1148	M1149	R1150	H1151	C1156	I1159	T1160	Q1161	D1162	K1163	V1166	S1167	M1168	P1169	I1170	K1171	V1172	F1173	K1174	P1175	S1177	M1180	V1181	T1189	V1194					
P346	T947	G948	D949	P950	L951	R952	R953	R954	E955	R962	R963	L964	R967	Q968	S969	T970	S971	L972	R973	Y987	Q993	F994	L995	Q998	D999	I1000	H1002	H1003	L1004	S1005	M1006	P1010	M1011	Q1012	V1015	F1016	F1017	V1018	P1019	V1020	L1021	R1024	E1025	E1026	I1027	K1031	P1032				
L1040	E1041	A1042	V1043	V1044	D1045	Q1046	D1047	V1048	V1049	T1051	C1052	L1053	L1054	H1055	V1058	A1059	A1060	Q1061	F1062	T1063	I1066	D1067	A1068	P1069	L1070	K1071	M1074	I1077	H1078	D1079	G1080	H1081	I1082	K1083	K1084	L1085	L1086	Y1090	G1091	D1092	D1093	K1096	I1097	E1101	Y1102	F1103	P1108	V1109			
S785	S786	T787	K788	F789	D790	Y791	F792	M793	F794	I795	D796	G798	F799	L800	R804	V805	M806	I807	E810	V811	K812	T813	S814	H815	D816	A817	K818	I821	M822	A823	C824	T825	G826	V827	P828	M832	T835	P839	T840	I843	V844	T845	V846	E852	P853	I854	H855	R856	I857	A858	
T859	R860	M865	K866	E867	F868	D869	E870	T871	I872	F873	K879	L880	R881	P882	K887	R888	I889	S893	R894	I895	M896	A897	D898	F899	Q900	K901	P902	W903	F904	T906	V907	Q910	A911	R912	D913	T916	E921	L926	L929	I932	W938	F939	T942	W943	R944	T945					
P946	T947	G948	D949	P950	L951	R952	R953	R954	E955	R962	R963	L964	R967	Q968	S969	T970	S971	L972	R973	Y987	Q993	F994	L995	Q998	D999	I1000	H1002	H1003	L1004	S1005	M1006	P1010	M1011	Q1012	V1015	F1016	F1017	V1018	P1019	V1020	L1021	R1024	E1025	E1026	I1027	K1031	P1032				
L1040	E1041	A1042	V1043	V1044	D1045	Q1046	D1047	V1048	V1049	T1051	C1052	L1053	L1054	H1055	V1058	A1059	A1060	Q1061	F1062	T1063	I1066	D1067	A1068	P1069	L1070	K1071	M1074	I1077	H1078	D1079	G1080	H1081	I1082	K1083	K1084	L1085	L1086	Y1090	G1091	D1092	D1093	K1096	I1097	E1101	Y1102	F1103	P1108	V1109			
ASP	VAL	GLN	SER	GLN	VAL	ASP	SER	SER	VAL	SER	GLU	D1123	K1128	A1129	T1130	T1133	E1135	M1138	S1145	E1146	D1147	M1148	M1149	R1150	H1151	C1156	I1159	T1160	Q1161	D1162	K1163	V1166	S1167	M1168	P1169	I1170	K1171	V1172	F1173	K1174	P1175	S1177	M1180	V1181	T1189	V1194					
V1195	V1196	L1197	S1198	E1199	L1205	K1206	L1210	L1211	L1212	L1213	L1214	M1217	L1218	Q1220	M1221	E1222	M1223	L1227	L1228	G1231	K1232	P1233	V1234	S1235	L1236	L1237	L1238	L1239	F1242	H1243	P1244	G1247	P1250	V1254	D1257	R1258	H1259	Q1260	R1261	L1262	K1263	E1264	M1265	Y1266	L1269	M1270	I1271				
S75	K76	F80	L84	N85	L86	T89	N93	C94	Y95	N99	D100	I101	H102	A105	A106	L109	N112	D113	T114	T115	L116	V117	K118	T119	K120	E121	L122	I123	K124	T127	T128	I129	T131	K132	A133	R134	P135	P136	F137	D138	K139	N142	L145	F146	V149	N153					
A154	Q155	L156	V157	A158	L159	F160	G161	Q162	Q163	T166	D167	D168	Y169	F170	L173	R174	D175	L176	Y177	Q178	T179	Y180	H181	V182	L183	V184	G185	D186	L187	I188	K189	F190	S191	A192	E193	T194	S196	E197	L198	I199	L203	P209	T210	L213	M214	L216	E217	W218	L219	T225	P226
D227	L231	L232	S233	L234	P235	L236	S237	M238	P239	L240	L241	L244	Q245	L246	L247	H248	Y249	V250	V251	L255	F258	T259	P260	V184	E262	L263	R264	T271	G272	H273	S274	Q275	G276	L277	V278	T279	A280	V281	A282	L283	T286	D287	S288	W289	S295	L296	T297	K298	L299	I300	L303
F304	F305	L306	R309	P315	L319	M318	L324	S327	L328	E332	P335	L339	S340	L341	S342	L343	L344	T345	Q346	D347	Q348	V349	Q350	V353	N354	K355	N357	S358	H359	S369	L370	V371	A374	K375	N376	L377	S380	L389	N390	L391	T392	L393	R394	K397	L486						
S400	G401	L402	D403	Q404	F416	S417	M418	R419	V423	A424	S425	P426	F427	H428	L431	L432	V433	P434	T439	N443	M440	K441	D442	L443	V444	K445	M446	M447	V448	L455	Q456	V459	Y460	D461	F462	D463	G465	S466	R469	N470	L471	S476	E477	R478	L481	C482	E483	L484	R485	L486	
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V638	I641	E642	K643	G644	S645	G648	I649	N650	I651	I652	M653	V654	M658	Q660	M661	I662	P663	L665	I666	K667	E668	L669	R670	Y674	P675	R676	F677	F678	G682	A683	V690	E693	Y694	T697	L698	G699	Y702	L703	G704	D705	K706	P707	G709	A712	I713	S714	Q715	V716			
I717	M718	I719	A720	K721	G722	H723	F726	P727	I728	L729	Q731	W732	T733	R736	G739	H740	H741	P742	D745	A746	H747	T748	P749	M750	L751	Q752	M753	Y754	I757	R758	H759	H760	P761	N762	I763	M764	L765	I766	F767	G768	S769	G772	A773	D775	D776	T777	Y778	P779	Y780	E784	
W785	S786	T787	K788	F789	D790	Y791	F792	M793	F794	I795	D796	G798	F799	L800	R804	V805	M806	I807	E810	V811	K812	T813	S814	H815	D816	A817	K818	I821	M822	A823	C824	T825	G826	V827	P828	M832	T835	P839	T840	I843	V844	T845	V846	E852	P853	I854	H855	R856	I857	A858	
T859	R860	M865	K866	E867	F868	D869	E870	T871	I872	F873	K879	L880	R881	P882	K887	R888	I889	S893	R894	I895	M896	A897	D898	F899	Q900	K901	P902	W903	F904	T906	V907	Q910	A911	R912	D913	T916	E921	L926	L929	I932	W938	F939	T942	W943	R944	T945					
P946	T947	G948	D949	P950	L951	R952	R953	R954	E955	R962	R963	L964	R967	Q968	S969	T970	S971	L972	R973	Y987	Q993	F994	L995	Q998	D999	I1000	H1002	H1003	L1004	S1005	M1006	P1010	M1011	Q1012	V1015	F1016	F1017	V1018	P1019	V1020	L1021	R1024	E1025	E1026	I1027	K1031	P1032				
L1040	E1041	A1042	V1043	V1044	D1045	Q1046	D1047	V1048	V1049	T1051	C1052	L1053	L1054	H1055	V1058	A1059	A1060	Q1061	F1062	T1063	I1066	D1067	A1068	P1069	L1070	K1071	M1074	I1077	H1078	D1079	G1080	H1081	I1082	K1083	K1084	L1085	L1086	Y1090	G1091	D1092	D1093	K1096	I1097	E1101	Y1102	F1103	P1108	V1109			
ASP	VAL	GLN	SER	GLN	VAL	ASP	SER	SER	VAL	SER	GLU	D1123	K1128	A1129	T1130	T1133	E1135	M1138	S1145	E1146	D1147	M1148	M1149	R1150	H1151	C1156	I1159	T1160	Q1161	D1162	K1163	V1166	S1167	M1168	P1169	I1170	K1171	V1172	F1173	K1174	P1175	S1177	M1180	V1181	T1189	V1194					
V1195	V1196	L1197	S1198	E1199	L1205	K1206	L1210	L1211	L1212	L1213	L1214	M1217	L1218	Q1220	M1221	E1222	M1223	L1227	L1228	G1231	K1232	P1233	V1234	S1235	L1236	L1237	L1238	L1239	F1242	H1243	P1244	G1247	P1250	V1254	D1257	R1258	H1259	Q1260	R1261	L1262	K1263	E1264	M1265	Y1266	L1269	M1270	I1271				
S75	K76	F80	L84	N85	L86	T89	N93	C94	Y95	N99	D100	I101	H102	A105	A106	L109	N112	D113	T114	T115	L116	V117	K118	T119	K120	E121	L122	I123	K124	T127	T128	I129	T131	K132	A133	R134	P135	P136	F137	D138	K139	N142	L145	F146	V149	N153					
A154	Q155	L156	V157	A158	L159	F160	G161	Q162	Q163	T166	D167	D168	Y169	F170	L173	R174	D175	L176	Y177	Q178	T179	Y180	H181	V182	L183	V184	G185	D186	L187	I188	K189	F190	S191	A192	E193	T194	S196	E197	L198	I199	L203	P209	T210	L213	M214	L216	E217	W218	L219	T225	P226
D227	L231	L232	S233	L234	P235	L236	S237	M238	P239	L240	L241	L244	Q245	L246	L247	H248	Y249	V250	V251	L255	F258	T259	P260	V184	E262	L263	R264	T271	G272	H273	S274	Q275	G276	L277	V278	T279	A280	V281	A282	L283	T286	D287	S288	W289	S295	L296	T297	K298	L299	I300	L303
F304	F305	L306	R309	P315	L319	M318	L324	S327	L328	E332	P335	L339	S340	L341	S342	L343	L344	T345	Q346	D347	Q348	V349	Q350	V353	N354	K355	N357	S358	H359	S369	L370	V371	A374	K375	N376	L377	S380	L389	N390	L391	T392	L393	R394	K397	L486						
S400	G401	L402	D403	Q404	F416	S417	M418	R419	V423	A424	S425	P426	F427	H428	L431	L432	V433	P434	T439	N443	M440	K441	D442	L443	V444	K445	M446	M447	V448	L455	Q456	V459	Y460	D461	F462	D463	G465	S466	R469	N470	L471	S476	E477	R478	L481	C482	E483	L484	R485	L486	
P487	V488	K489	W490	E491																																															



• Molecule 2: FATTY ACID SYNTHASE SUBUNIT BETA (FAS1)





	K2009	I1917	T1837	K1745	T1642	S1548
	Y2010	K1918	M1838	L1746		T1549
	T2011	L1919		K1747	V1650	I1550
	P2012	Q1920	V1842		L1651	E1551
	N2013	K1921	P1843	F1752	T1652	P1552
	L2014	I1922	R1844	E1757	G1653	
	T2015	K1929	D1845		I1657	V1556
	T2016	S1930	E1846	S1761		S1557
	K2017	L1931	L1847	F1764	T1662	L1560
		S1932	R1849	R1765	T1663	N1561
	Q2020		S1850		F1666	P1562
	V2021	E1936	M1854	L1770		I1563
	T2022	V1936	I1855		G1670	H1564
		E1937		T1774	S1671	V1565
	Y2025	L1940	P1859	Q1775	Q1672	V1566
	F2026	F1941	G1860	F1776	E1673	R1567
			R1861	T1777	Q1674	H1568
	V2029	D1945	V1862	Q1778	Q1675	
	Y2030		A1863	P1779	M1676	L1575
		K1949		A1780	G1677	I1579
	T2033	V1953	F1866	L1781	M1678	T1580
	G2034	K1954	S1867	T1782	D1679	
	S2035	P1955	Q1868	L1783	L1680	M1583
	E2036	R1956		M1784	Y1681	F1584
	P2037	R1957	L1871	E1785	A1682	
	I2038	L1958	Q1872	Y1873	T1683	V1589
	K2039	K1959	Y1874	K1793	S1684	R1590
	E2040			I1798	A1687	A1591
	L2041	F1964	R1877	P1799	Q1688	L1592
	T2042	I1967	V1878	T1803		I1593
	D2043	P1968	V1886	F1804	R1693	E1594
	N2044		E1887	A1805	H1697	A1597
	W2045	S1973	I1888			
	E2046	V1974	V1889	S1808	L1707	S1602
	K2047	P1975	M1890	A1814		V1605
	Y2048	F1976	Y1891	L1815	M1712	Y1608
	E2049	H1977	M1892		N1716	T1609
	Q2050		V1893	L1818	N1717	Y1609
SER		Y1980		A1819	T1718	M1615
		L1981	Q1896	D1820	L1719	V1616
			Q1897	V1821		
		V1985	Y1898	M1822	G1722	T1624
		K1986	V1899	S1823		S1625
		P1987	A1900	I1824	G1726	I1626
		F1988	A1901	E1825		Q1627
		K1989		S1826	A1735	
			A1906	L1827	M1736	G1630
		K1993	L1907	V1828	I1737	M1631
			D1908	E1829	F1738	I1632
		I1996	T1909	V1830	E1739	
		I1997	V1910	V1831	T1740	L1637
		K1998	T1911		I1741	I1638
			H1912	R1834	V1742	F1640
		V2003	V1913	G1835	D1743	E1641
		A2004	L1914	M1836	G1744	
		R2005				

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	230.60 Å 230.60 Å 784.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.10 12.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	86.1 (12.00-3.10) 91.5 (12.00-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 3.09 Å)	Xtriage
Refinement program	PHENIX, PHENIX	Depositor
R, R_{free}	0.200 , 0.250 0.202 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	74.1	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	85962	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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

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	0.41	0/12848	0.59	2/17358 (0.0%)
1	B	0.42	0/12848	0.59	2/17358 (0.0%)
1	C	0.41	0/12848	0.59	2/17358 (0.0%)
2	G	0.37	0/16360	0.56	0/22198
2	H	0.37	0/16360	0.57	0/22198
2	I	0.37	0/16360	0.56	0/22198
All	All	0.39	0/87624	0.58	6/118668 (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	1
2	I	0	1
All	All	0	3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	599	MET	N-CA-C	-6.92	92.32	111.00
1	B	599	MET	N-CA-C	-6.91	92.36	111.00
1	C	599	MET	N-CA-C	-6.90	92.36	111.00
1	B	540	GLN	N-CA-C	-5.67	95.69	111.00
1	C	540	GLN	N-CA-C	-5.63	95.81	111.00
1	A	540	GLN	N-CA-C	-5.63	95.81	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	1108	PRO	Peptide
2	H	1108	PRO	Peptide
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	12628	0	12603	572	0
1	B	12628	0	12603	587	0
1	C	12628	0	12603	584	0
2	G	15995	0	15978	984	0
2	H	15995	0	15978	995	0
2	I	15995	0	15978	996	0
3	G	31	0	19	7	0
3	H	31	0	19	6	0
3	I	31	0	19	6	0
All	All	85962	0	85800	4562	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (4562) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1956:ARG:HB2	2:I:1957:PRO:HD3	1.23	1.21
2:G:499:THR:HB	2:G:500:HIS:HD2	1.07	1.16
2:G:1956:ARG:HB2	2:G:1957:PRO:HD3	1.23	1.14
2:H:490:TRP:HE1	2:H:516:THR:HG22	1.11	1.13
2:G:490:TRP:HE1	2:G:516:THR:HG22	1.12	1.13
1:B:253:ARG:HG3	1:B:254:TRP:HD1	1.17	1.10
2:I:499:THR:HB	2:I:500:HIS:HD2	1.07	1.09
2:H:1834:ARG:HH11	2:H:1834:ARG:HG2	1.06	1.09
2:H:601:THR:HG21	2:H:618:GLU:O	1.50	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1956:ARG:HB2	2:H:1957:PRO:HD3	1.24	1.09
2:I:601:THR:HG21	2:I:618:GLU:O	1.50	1.09
2:I:1834:ARG:HG2	2:I:1834:ARG:HH11	1.16	1.09
2:I:490:TRP:HE1	2:I:516:THR:HG22	1.10	1.09
2:G:1834:ARG:HG2	2:G:1834:ARG:HH11	1.16	1.08
2:G:1859:PRO:HG3	2:G:1871:LEU:HD12	1.29	1.08
2:H:499:THR:HB	2:H:500:HIS:HD2	1.10	1.08
1:A:1721:ARG:HG2	1:A:1721:ARG:HH11	1.16	1.08
2:I:297:ARG:HD3	2:I:447:ASN:HD21	1.15	1.07
2:G:601:THR:HG21	2:G:618:GLU:O	1.52	1.07
1:A:253:ARG:HG3	1:A:254:TRP:HD1	1.15	1.07
1:B:2:LYS:HD2	2:H:2050:GLN:HB3	1.36	1.07
1:C:253:ARG:HG3	1:C:254:TRP:HD1	1.15	1.06
1:C:852:ARG:HH11	1:C:852:ARG:HG2	1.14	1.06
2:I:1227:ARG:HH11	2:I:1227:ARG:HG3	1.18	1.06
2:H:1859:PRO:HG3	2:H:1871:LEU:HD12	1.38	1.05
1:B:1721:ARG:HH11	1:B:1721:ARG:HG2	1.20	1.05
1:B:1722:VAL:HG11	1:B:1731:LEU:HB3	1.37	1.05
1:C:1721:ARG:HG2	1:C:1721:ARG:HH11	1.20	1.05
1:A:1367:ARG:NH1	1:A:1372:THR:HB	1.72	1.05
2:H:1227:ARG:HG3	2:H:1227:ARG:HH11	1.19	1.05
2:G:7:ARG:HH21	2:G:27:PHE:HB3	1.22	1.04
1:C:1367:ARG:NH1	1:C:1372:THR:HB	1.71	1.04
2:H:7:ARG:HH21	2:H:27:PHE:HB3	1.22	1.04
2:H:297:ARG:HD3	2:H:447:ASN:HD21	1.16	1.03
1:A:1722:VAL:HG11	1:A:1731:LEU:HB3	1.41	1.03
1:C:1722:VAL:HG11	1:C:1731:LEU:HB3	1.37	1.02
1:B:1367:ARG:NH1	1:B:1372:THR:HB	1.73	1.02
2:G:1227:ARG:HH11	2:G:1227:ARG:HG3	1.18	1.02
1:A:852:ARG:HH11	1:A:852:ARG:HG2	1.23	1.02
1:A:599:MET:HB2	1:A:624:LYS:HD2	1.43	1.01
1:C:1303:GLY:HA2	1:C:1649:LYS:HE2	1.42	1.01
1:C:1219:VAL:HA	1:C:1384:ILE:HD11	1.40	1.01
2:G:297:ARG:HD3	2:G:447:ASN:HD21	1.18	1.01
2:I:762:ASN:HD22	2:I:762:ASN:H	1.08	1.01
1:B:852:ARG:HH11	1:B:852:ARG:HG2	1.20	1.01
2:G:835:THR:HG21	2:G:855:HIS:CD2	1.96	1.01
2:I:7:ARG:HH21	2:I:27:PHE:HB3	1.19	1.01
2:G:128:THR:HA	2:G:182:VAL:HG21	1.42	1.00
2:G:652:ILE:H	2:G:658:MET:HE3	1.20	1.00
2:G:499:THR:HB	2:G:500:HIS:CD2	1.97	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1739:GLU:HB2	2:I:1987:PRO:HB3	1.40	1.00
2:H:1739:GLU:HB2	2:H:1987:PRO:HB3	1.42	1.00
2:I:1859:PRO:HG3	2:I:1871:LEU:HD12	1.41	1.00
2:H:594:VAL:HB	2:H:617:ILE:HG13	1.44	0.99
1:A:2:LYS:HD2	2:G:2050:GLN:HB3	1.43	0.99
2:G:892:ILE:HD11	2:G:903:TRP:CE2	1.98	0.99
2:I:499:THR:HB	2:I:500:HIS:CD2	1.97	0.99
1:A:400:ARG:CG	1:A:400:ARG:HH11	1.76	0.99
2:H:1803:THR:HG22	2:H:2009:LYS:HA	1.45	0.99
1:A:1219:VAL:HA	1:A:1384:ILE:HD11	1.45	0.98
1:A:253:ARG:HG3	1:A:254:TRP:CD1	1.98	0.98
1:C:253:ARG:HG3	1:C:254:TRP:CD1	1.98	0.98
1:B:403:ASP:HB2	1:B:1613:ASN:HD21	1.29	0.98
2:G:1739:GLU:HB2	2:G:1987:PRO:HB3	1.43	0.98
2:H:499:THR:HB	2:H:500:HIS:CD2	1.99	0.97
2:G:1567:ARG:HG3	2:G:1567:ARG:HH11	1.29	0.97
2:H:1567:ARG:HG3	2:H:1567:ARG:HH11	1.27	0.97
1:B:1693:ILE:HD11	2:H:998:GLN:HB2	1.46	0.97
2:H:762:ASN:H	2:H:762:ASN:HD22	1.03	0.97
2:I:892:ILE:HD11	2:I:903:TRP:CE2	1.98	0.97
1:C:599:MET:HB2	1:C:624:LYS:HD2	1.43	0.97
2:G:762:ASN:H	2:G:762:ASN:HD22	1.03	0.97
1:A:198:PRO:HG3	1:A:209:LEU:HD21	1.47	0.97
2:I:490:TRP:NE1	2:I:516:THR:HG22	1.79	0.97
1:C:1693:ILE:HD11	2:I:998:GLN:HB2	1.42	0.97
1:B:599:MET:HB2	1:B:624:LYS:HD2	1.42	0.96
2:G:490:TRP:NE1	2:G:516:THR:HG22	1.81	0.96
2:I:835:THR:HG21	2:I:855:HIS:CD2	1.99	0.96
2:I:1567:ARG:HH11	2:I:1567:ARG:HG3	1.29	0.96
2:H:490:TRP:NE1	2:H:516:THR:HG22	1.81	0.96
2:I:594:VAL:HB	2:I:617:ILE:HG13	1.47	0.96
1:B:253:ARG:HG3	1:B:254:TRP:CD1	1.99	0.96
2:H:128:THR:HA	2:H:182:VAL:HG21	1.45	0.96
2:I:1567:ARG:HH11	2:I:1567:ARG:CG	1.78	0.96
1:B:1219:VAL:HA	1:B:1384:ILE:HD11	1.45	0.95
1:C:198:PRO:HG3	1:C:209:LEU:HD21	1.48	0.95
2:H:1567:ARG:HH11	2:H:1567:ARG:CG	1.78	0.95
2:I:932:ILE:HD11	2:I:1042:ALA:HB2	1.44	0.95
1:B:1303:GLY:HA2	1:B:1649:LYS:HE2	1.46	0.95
2:H:55:THR:HG22	2:H:56:THR:HG22	1.48	0.95
1:C:2:LYS:HD2	2:I:2050:GLN:HB3	1.47	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:652:ILE:H	2:I:658:MET:HE3	1.31	0.95
1:A:444:ASN:HB2	1:A:447:LEU:H	1.31	0.94
1:A:400:ARG:HG2	1:A:400:ARG:HH11	1.28	0.94
2:H:1314:ARG:HG3	2:H:1314:ARG:HH11	1.31	0.94
2:H:892:ILE:HD11	2:H:903:TRP:CE2	2.01	0.94
2:I:128:THR:HA	2:I:182:VAL:HG21	1.49	0.94
2:G:1878:VAL:HG11	2:G:1910:VAL:HG22	1.48	0.94
1:C:1523:ARG:HH11	1:C:1523:ARG:HG3	1.32	0.94
2:G:1567:ARG:CG	2:G:1567:ARG:HH11	1.80	0.94
2:G:1741:ILE:HD12	2:G:1986:LYS:HD2	1.47	0.94
1:C:400:ARG:HG2	1:C:400:ARG:HH11	1.33	0.94
2:I:1314:ARG:HG3	2:I:1314:ARG:HH11	1.32	0.94
1:B:444:ASN:HB2	1:B:447:LEU:H	1.31	0.94
2:G:1314:ARG:HH11	2:G:1314:ARG:HG3	1.32	0.94
1:B:529:MET:HE3	1:B:529:MET:HA	1.47	0.93
1:C:444:ASN:HB2	1:C:447:LEU:H	1.33	0.93
2:G:56:THR:HG23	2:G:59:GLU:HG3	1.50	0.93
2:H:1589:VAL:HA	2:H:1592:LEU:HD12	1.49	0.93
1:A:1303:GLY:HA2	1:A:1649:LYS:HE2	1.49	0.93
1:B:198:PRO:HG3	1:B:209:LEU:HD21	1.47	0.93
2:I:1878:VAL:HG11	2:I:1910:VAL:HG22	1.50	0.93
2:I:1741:ILE:HD12	2:I:1986:LYS:HD2	1.49	0.93
2:I:56:THR:HG23	2:I:59:GLU:HG3	1.49	0.93
2:G:594:VAL:HB	2:G:617:ILE:HG13	1.51	0.92
2:I:1589:VAL:HA	2:I:1592:LEU:HD12	1.51	0.92
2:H:1845:ASP:HB2	2:H:1849:ARG:H	1.34	0.92
1:B:400:ARG:HH11	1:B:400:ARG:CG	1.81	0.92
1:C:400:ARG:HH11	1:C:400:ARG:CG	1.81	0.92
1:C:793:ARG:HA	1:C:797:THR:HG23	1.52	0.92
2:G:1589:VAL:HA	2:G:1592:LEU:HD12	1.49	0.92
2:G:1803:THR:HG22	2:G:2009:LYS:HA	1.48	0.92
2:G:942:THR:HB	2:G:1012:GLN:HG2	1.50	0.92
1:C:1376:PHE:HB3	1:C:1544:THR:HG22	1.52	0.92
2:G:55:THR:HG22	2:G:56:THR:HG22	1.52	0.92
2:I:667:LYS:HD2	2:I:697:THR:HG22	1.51	0.92
1:C:152:HIS:CD2	1:C:163:LEU:HB2	2.05	0.92
2:I:55:THR:HG22	2:I:56:THR:HG22	1.51	0.91
2:I:942:THR:HB	2:I:1012:GLN:HG2	1.52	0.91
1:A:1523:ARG:HG3	1:A:1523:ARG:HH11	1.33	0.91
2:G:1845:ASP:HB2	2:G:1849:ARG:H	1.34	0.91
2:H:741:HIS:HE1	2:H:845:THR:CG2	1.82	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1352:HIS:HE1	2:H:1583:MET:HE2	1.34	0.91
2:I:707:PRO:HG3	2:I:716:VAL:HG21	1.52	0.91
1:A:1367:ARG:HH12	1:A:1372:THR:HB	1.35	0.91
1:A:403:ASP:HB2	1:A:1613:ASN:HD21	1.36	0.91
1:A:335:HIS:CE1	1:C:335:HIS:HE1	1.89	0.91
1:A:152:HIS:CD2	1:A:163:LEU:HB2	2.05	0.91
1:A:1279:PHE:HB2	1:A:1282:THR:HG23	1.52	0.90
1:A:1376:PHE:HB3	1:A:1544:THR:HG22	1.53	0.90
1:A:1721:ARG:CG	1:A:1721:ARG:HH11	1.84	0.90
1:B:1376:PHE:HB3	1:B:1544:THR:HG22	1.51	0.90
2:G:932:ILE:HD11	2:G:1042:ALA:HB2	1.51	0.90
1:B:1523:ARG:HH11	1:B:1523:ARG:HG3	1.36	0.90
2:H:942:THR:HB	2:H:1012:GLN:HG2	1.54	0.90
1:A:1693:ILE:HD11	2:G:998:GLN:HB2	1.51	0.90
2:H:1741:ILE:HD12	2:H:1986:LYS:HD2	1.54	0.90
2:H:903:TRP:O	2:H:906:THR:HG22	1.71	0.90
2:I:1441:ILE:HD11	2:I:1445:ARG:CZ	2.02	0.90
2:I:1803:THR:HG22	2:I:2009:LYS:HA	1.51	0.90
1:B:793:ARG:HA	1:B:797:THR:HG23	1.54	0.89
2:I:55:THR:HG21	2:I:113:ASP:HB2	1.53	0.89
1:A:793:ARG:HA	1:A:797:THR:HG23	1.53	0.89
1:C:403:ASP:HB2	1:C:1613:ASN:HD21	1.33	0.89
1:B:253:ARG:HE	1:B:254:TRP:HE1	1.21	0.89
1:C:253:ARG:HE	1:C:254:TRP:HE1	1.21	0.89
2:H:1878:VAL:HG11	2:H:1910:VAL:HG22	1.55	0.89
2:H:707:PRO:HG3	2:H:716:VAL:HG21	1.54	0.89
2:G:1352:HIS:HE1	2:G:1583:MET:HE2	1.36	0.89
1:B:1721:ARG:HH11	1:B:1721:ARG:CG	1.85	0.89
2:H:667:LYS:HD2	2:H:697:THR:HG22	1.55	0.89
2:I:1845:ASP:HB2	2:I:1849:ARG:H	1.38	0.89
1:B:152:HIS:CD2	1:B:163:LEU:HB2	2.08	0.89
1:B:260:ARG:HH12	1:B:300:VAL:HG21	1.38	0.89
1:A:529:MET:HA	1:A:529:MET:HE3	1.54	0.88
2:G:55:THR:HG21	2:G:113:ASP:HB2	1.52	0.88
2:H:1533:LEU:HD13	2:H:1630:GLY:HA2	1.56	0.88
2:G:1847:LEU:H	2:G:1847:LEU:HD12	1.37	0.88
2:G:741:HIS:HE1	2:G:845:THR:CG2	1.86	0.88
2:I:1352:HIS:HE1	2:I:1583:MET:HE2	1.36	0.88
2:G:1352:HIS:CE1	2:G:1583:MET:HE2	2.09	0.88
2:G:835:THR:HB	2:G:845:THR:HG23	1.55	0.88
2:G:903:TRP:O	2:G:906:THR:HG22	1.74	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:707:PRO:HG3	2:G:716:VAL:HG21	1.56	0.88
2:G:1441:ILE:HD11	2:G:1445:ARG:CZ	2.02	0.88
1:A:1584:PRO:HG3	1:A:1591:TRP:CZ3	2.09	0.88
2:G:667:LYS:HD2	2:G:697:THR:HG22	1.55	0.88
2:H:1441:ILE:HD11	2:H:1445:ARG:CZ	2.04	0.88
2:H:1847:LEU:H	2:H:1847:LEU:HD12	1.36	0.88
2:H:55:THR:HG21	2:H:113:ASP:HB2	1.53	0.87
1:C:1279:PHE:HB2	1:C:1282:THR:HG23	1.56	0.87
1:B:1584:PRO:HG3	1:B:1591:TRP:CZ3	2.08	0.87
2:G:369:SER:OG	2:G:380:SER:HB3	1.75	0.87
2:H:741:HIS:NE2	2:H:855:HIS:CE1	2.42	0.87
1:C:1721:ARG:CG	1:C:1721:ARG:HH11	1.87	0.87
1:A:340:ARG:NH1	1:A:344:GLN:HG2	1.88	0.87
1:C:1014:ASP:H	1:C:1510:ASN:HD21	1.23	0.87
1:B:893:VAL:HG11	1:B:930:LEU:HD23	1.55	0.87
2:G:741:HIS:HE1	2:G:845:THR:HG22	1.39	0.87
2:I:1227:ARG:HH11	2:I:1227:ARG:CG	1.87	0.86
1:A:1474:ALA:HA	1:A:1478:PRO:HG2	1.55	0.86
1:C:1367:ARG:HH12	1:C:1372:THR:HB	1.38	0.86
1:B:1367:ARG:HH12	1:B:1372:THR:HB	1.38	0.86
2:H:1739:GLU:HB3	2:H:1746:LEU:HD11	1.56	0.86
2:H:56:THR:HG23	2:H:59:GLU:HG3	1.54	0.86
2:I:1847:LEU:HD12	2:I:1847:LEU:H	1.40	0.86
2:I:298:LYS:HG2	2:I:448:VAL:HG22	1.56	0.86
1:A:253:ARG:HE	1:A:254:TRP:HE1	1.21	0.86
2:H:774:ALA:HB1	2:H:1081:HIS:HD2	1.41	0.86
2:H:1352:HIS:CE1	2:H:1583:MET:HE2	2.11	0.86
2:G:1425:LYS:HG2	2:G:1471:GLU:HG3	1.57	0.86
2:H:1844:ARG:HH11	2:H:1844:ARG:CG	1.89	0.86
2:H:835:THR:HG21	2:H:855:HIS:CD2	2.10	0.85
2:I:774:ALA:HB2	2:I:1077:ILE:HA	1.58	0.85
2:I:903:TRP:O	2:I:906:THR:HG22	1.76	0.85
1:B:1474:ALA:HA	1:B:1478:PRO:HG2	1.58	0.85
1:C:340:ARG:NH1	1:C:344:GLN:HG2	1.91	0.85
2:I:1352:HIS:CE1	2:I:1583:MET:HE2	2.10	0.85
1:B:340:ARG:NH1	1:B:344:GLN:HG2	1.91	0.85
1:A:893:VAL:HG11	1:A:930:LEU:HD23	1.58	0.85
1:C:529:MET:HA	1:C:529:MET:HE3	1.57	0.85
2:I:741:HIS:HE1	2:I:845:THR:CG2	1.88	0.85
1:A:335:HIS:CE1	1:C:335:HIS:CE1	2.64	0.85
2:H:741:HIS:CE1	2:H:845:THR:CG2	2.60	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1227:ARG:HH11	2:G:1227:ARG:CG	1.89	0.85
2:H:1672:GLN:HG2	2:H:1777:THR:HG23	1.59	0.85
2:H:1227:ARG:HH11	2:H:1227:ARG:CG	1.90	0.85
1:C:1474:ALA:HA	1:C:1478:PRO:HG2	1.57	0.84
1:C:893:VAL:HG11	1:C:930:LEU:HD23	1.59	0.84
2:G:1739:GLU:HB3	2:G:1746:LEU:HD11	1.59	0.84
2:H:777:THR:CG2	2:H:1081:HIS:NE2	2.40	0.84
2:H:297:ARG:HD3	2:H:447:ASN:ND2	1.91	0.84
1:C:31:THR:HG23	2:I:2011:ILE:HG21	1.58	0.84
1:B:1279:PHE:HB2	1:B:1282:THR:HG23	1.57	0.84
2:H:741:HIS:CE1	2:H:845:THR:HG22	2.11	0.84
2:I:297:ARG:HD3	2:I:447:ASN:ND2	1.92	0.84
1:B:400:ARG:HH11	1:B:400:ARG:HG2	1.40	0.84
1:C:1584:PRO:HG3	1:C:1591:TRP:CZ3	2.11	0.84
2:H:369:SER:OG	2:H:380:SER:HB3	1.78	0.84
2:I:369:SER:OG	2:I:380:SER:HB3	1.75	0.84
2:G:1834:ARG:HG2	2:G:1834:ARG:NH1	1.93	0.83
2:I:1834:ARG:HG2	2:I:1834:ARG:NH1	1.92	0.83
2:I:1844:ARG:HH11	2:I:1844:ARG:HG2	1.42	0.83
2:I:774:ALA:HB1	2:I:1081:HIS:HD2	1.43	0.83
2:H:995:LEU:HD23	2:H:1000:ILE:HD13	1.58	0.83
2:I:1739:GLU:HB3	2:I:1746:LEU:HD11	1.58	0.83
2:G:777:THR:CG2	2:G:1081:HIS:NE2	2.42	0.83
2:I:1533:LEU:HD13	2:I:1630:GLY:HA2	1.59	0.83
2:G:995:LEU:HD23	2:G:1000:ILE:HD13	1.60	0.83
2:H:932:ILE:HD11	2:H:1042:ALA:HB2	1.59	0.83
2:H:1425:LYS:HG2	2:H:1471:GLU:HG3	1.58	0.83
1:A:36:LEU:HD22	1:A:61:LEU:HD21	1.60	0.83
2:G:1533:LEU:HD13	2:G:1630:GLY:HA2	1.60	0.83
2:G:2038:ILE:HG22	2:G:2042:ILE:HD11	1.60	0.83
2:G:297:ARG:HD3	2:G:447:ASN:ND2	1.94	0.82
2:G:298:LYS:HG2	2:G:448:VAL:HG22	1.61	0.82
2:H:1844:ARG:HH11	2:H:1844:ARG:HG2	1.41	0.82
1:B:31:THR:HG23	2:H:2011:ILE:HG21	1.61	0.82
1:C:333:LYS:O	1:C:337:VAL:HG23	1.80	0.82
2:I:1931:LEU:HB3	2:I:1935:GLU:HG2	1.61	0.82
2:H:652:ILE:H	2:H:658:MET:HE3	1.42	0.82
2:I:124:LYS:HG2	2:I:179:THR:HA	1.62	0.82
2:I:1672:GLN:HG2	2:I:1777:THR:HG23	1.61	0.82
2:G:1284:VAL:HG13	2:G:1377:VAL:HG22	1.62	0.82
2:I:1425:LYS:HG2	2:I:1471:GLU:HG3	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1844:ARG:CG	2:I:1844:ARG:HH11	1.93	0.82
1:B:1189:ILE:HD12	1:B:1380:GLN:HG3	1.61	0.81
2:G:1931:LEU:HB3	2:G:1935:GLU:HG2	1.61	0.81
2:H:1931:LEU:HB3	2:H:1935:GLU:HG2	1.62	0.81
2:H:1159:ILE:HG12	2:H:1168:ASN:HA	1.61	0.81
2:G:652:ILE:N	2:G:658:MET:HE3	1.95	0.81
2:I:1242:PHE:HE2	2:I:1244:PRO:HG3	1.46	0.81
2:G:774:ALA:HB2	2:G:1077:ILE:HA	1.61	0.81
2:G:1293:THR:HG23	2:G:1296:GLU:H	1.44	0.81
2:I:598:THR:HG22	2:I:622:GLY:HA3	1.61	0.81
2:H:1149:TRP:HA	2:H:1242:PHE:CE1	2.15	0.81
2:H:543:PHE:HB2	2:H:545:GLN:HE22	1.45	0.81
2:I:2038:ILE:HG22	2:I:2042:ILE:HD11	1.61	0.81
2:I:345:THR:HG22	2:I:347:GLU:H	1.46	0.81
2:I:1693:ARG:HD2	2:I:1825:GLU:OE2	1.80	0.81
2:G:1678:MET:HE3	2:G:1707:LEU:HD22	1.62	0.81
2:H:85:ASN:HD22	2:H:135:ARG:HH11	1.26	0.81
2:I:741:HIS:HE1	2:I:845:THR:HG22	1.44	0.81
2:I:85:ASN:HD22	2:I:135:ARG:HH11	1.28	0.81
1:B:1014:ASP:H	1:B:1510:ASN:HD21	1.28	0.80
2:H:2038:ILE:HG22	2:H:2042:ILE:HD11	1.60	0.80
1:B:93:ASP:HB3	1:B:94:PRO:HD2	1.62	0.80
2:I:995:LEU:HD23	2:I:1000:ILE:HD13	1.60	0.80
2:H:741:HIS:HE1	2:H:845:THR:HG22	1.41	0.80
1:B:1030:TRP:CD1	1:B:1580:LEU:HD22	2.17	0.80
2:G:1352:HIS:HE1	2:G:1583:MET:CE	1.95	0.80
2:G:1672:GLN:HG2	2:G:1777:THR:HG23	1.61	0.80
1:A:1552:ASN:O	1:A:1556:THR:HG22	1.80	0.80
1:A:340:ARG:HH12	1:A:344:GLN:HG2	1.44	0.80
2:H:757:ILE:HG21	2:H:765:LEU:HD13	1.64	0.80
1:B:36:LEU:HD22	1:B:61:LEU:HD21	1.64	0.80
2:G:1314:ARG:CG	2:G:1314:ARG:HH11	1.95	0.80
2:G:85:ASN:HD22	2:G:135:ARG:HH11	1.28	0.80
2:G:1847:LEU:HD13	2:G:1849:ARG:HD2	1.62	0.80
2:G:634:ILE:HD11	2:G:649:ILE:HD11	1.63	0.80
2:I:777:THR:CG2	2:I:1081:HIS:NE2	2.43	0.80
1:A:333:LYS:O	1:A:337:VAL:HG23	1.81	0.80
1:C:852:ARG:HG2	1:C:852:ARG:NH1	1.93	0.80
2:G:131:ILE:HD12	2:G:182:VAL:HB	1.64	0.80
2:G:1956:ARG:CB	2:G:1957:PRO:HD3	2.10	0.80
1:A:400:ARG:HG2	1:A:400:ARG:NH1	1.91	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ASP:HB3	1:A:94:PRO:HD2	1.63	0.80
2:G:1844:ARG:CG	2:G:1844:ARG:HH11	1.94	0.80
2:H:741:HIS:CE1	2:H:855:HIS:CE1	2.69	0.80
2:H:907:VAL:HG21	2:H:921:GLU:HG2	1.64	0.80
2:I:1159:ILE:HG12	2:I:1168:ASN:HA	1.63	0.80
2:I:345:THR:HB	2:I:348:GLN:H	1.46	0.80
2:I:543:PHE:HB2	2:I:545:GLN:HE22	1.46	0.80
2:G:774:ALA:HB1	2:G:1081:HIS:HD2	1.47	0.79
2:I:455:ILE:HD11	2:I:469:ARG:HD3	1.63	0.79
2:I:584:SER:HB3	2:I:591:PRO:HG3	1.63	0.79
2:G:1693:ARG:HD2	2:G:1825:GLU:OE2	1.81	0.79
2:G:1844:ARG:HG2	2:G:1844:ARG:HH11	1.46	0.79
2:I:1847:LEU:HD13	2:I:1849:ARG:HD2	1.64	0.79
2:H:1847:LEU:HD13	2:H:1849:ARG:HD2	1.63	0.79
2:I:259:THR:HG22	2:I:262:GLU:HG3	1.64	0.79
2:I:907:VAL:HG21	2:I:921:GLU:HG2	1.65	0.79
2:H:774:ALA:HB2	2:H:1077:ILE:HA	1.65	0.79
2:I:732:TRP:CG	2:I:750:MET:HE1	2.17	0.79
1:B:333:LYS:O	1:B:337:VAL:HG23	1.81	0.79
2:G:907:VAL:HG21	2:G:921:GLU:HG2	1.65	0.79
2:H:1159:ILE:HG12	2:H:1169:PRO:HD3	1.64	0.79
2:H:598:THR:HG22	2:H:622:GLY:HA3	1.64	0.79
2:G:543:PHE:HB2	2:G:545:GLN:HE22	1.46	0.79
2:H:1693:ARG:HD2	2:H:1825:GLU:OE2	1.83	0.79
2:I:238:CYS:HB2	2:I:239:PRO:HD3	1.65	0.79
1:B:198:PRO:HG3	1:B:209:LEU:CD2	2.13	0.79
2:G:741:HIS:CE1	2:G:845:THR:HG22	2.17	0.79
2:I:1956:ARG:HB2	2:I:1957:PRO:CD	2.11	0.79
2:I:55:THR:CG2	2:I:113:ASP:HB2	2.12	0.79
2:H:455:ILE:HD11	2:H:469:ARG:HD3	1.64	0.79
2:H:298:LYS:HG2	2:H:448:VAL:HG22	1.64	0.78
1:B:260:ARG:NH1	1:B:300:VAL:HG21	1.97	0.78
1:C:400:ARG:HG2	1:C:400:ARG:NH1	1.94	0.78
2:H:55:THR:CG2	2:H:113:ASP:HB2	2.13	0.78
1:B:1665:ILE:HG13	1:B:1669:ARG:HD3	1.66	0.78
2:H:960:LYS:HA	2:H:960:LYS:HE2	1.65	0.78
2:I:1293:THR:HG23	2:I:1296:GLU:H	1.47	0.78
1:C:340:ARG:HH12	1:C:344:GLN:HG2	1.49	0.78
1:A:328:LEU:O	1:A:331:ILE:HG22	1.84	0.78
2:G:345:THR:HG22	2:G:347:GLU:H	1.47	0.78
2:H:124:LYS:HG2	2:H:179:THR:HA	1.62	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1834:ARG:NH1	2:H:1834:ARG:HG2	1.86	0.78
2:I:1149:TRP:HA	2:I:1242:PHE:CE1	2.19	0.78
2:I:192:ALA:HA	2:I:215:ILE:HD12	1.64	0.78
2:I:741:HIS:CE1	2:I:845:THR:HG22	2.18	0.78
1:B:1722:VAL:CG1	1:B:1731:LEU:HB3	2.13	0.78
1:C:328:LEU:O	1:C:331:ILE:HG22	1.84	0.78
2:H:105:ALA:HB1	2:H:119:THR:HG23	1.65	0.78
1:C:93:ASP:HB3	1:C:94:PRO:HD2	1.65	0.77
2:G:960:LYS:HE2	2:G:960:LYS:HA	1.67	0.77
2:I:131:ILE:HD12	2:I:182:VAL:HB	1.66	0.77
2:I:1956:ARG:CB	2:I:1957:PRO:HD3	2.09	0.77
2:I:741:HIS:NE2	2:I:855:HIS:CE1	2.52	0.77
1:C:1523:ARG:CG	1:C:1523:ARG:HH11	1.96	0.77
2:G:146:PHE:HA	2:G:149:VAL:CG1	2.15	0.77
2:G:1770:LEU:HD23	2:G:1776:PHE:CE2	2.20	0.77
2:G:55:THR:CG2	2:G:113:ASP:HB2	2.13	0.77
1:A:1030:TRP:NE1	1:A:1580:LEU:HD22	1.99	0.77
1:A:198:PRO:HG3	1:A:209:LEU:CD2	2.14	0.77
1:B:335:HIS:HE1	1:C:335:HIS:CE1	2.02	0.77
2:G:839:PRO:HA	2:G:844:VAL:HG13	1.64	0.77
2:H:345:THR:HB	2:H:348:GLN:H	1.48	0.77
1:C:968:VAL:O	2:I:1512:HIS:HB2	1.85	0.77
2:I:1770:LEU:HD23	2:I:1776:PHE:CE2	2.19	0.77
2:I:634:ILE:HD11	2:I:649:ILE:HD11	1.66	0.77
1:B:1239:HIS:HD2	1:B:1241:SER:OG	1.67	0.77
1:A:1523:ARG:CG	1:A:1523:ARG:HH11	1.97	0.77
1:A:31:THR:HG23	2:G:2011:ILE:HG21	1.66	0.77
2:G:757:ILE:HG21	2:G:765:LEU:HD13	1.67	0.77
2:I:105:ALA:HB1	2:I:119:THR:HG23	1.67	0.77
2:I:1422:THR:CG2	2:I:1474:PHE:HB2	2.15	0.77
2:G:192:ALA:HA	2:G:215:ILE:HD12	1.67	0.77
2:G:1956:ARG:HB2	2:G:1957:PRO:CD	2.11	0.76
2:H:355:LYS:O	2:H:358:SER:HB3	1.85	0.76
2:I:355:LYS:O	2:I:358:SER:HB3	1.85	0.76
1:A:1276:GLN:O	1:A:1282:THR:HG21	1.85	0.76
1:A:1665:ILE:HG13	1:A:1669:ARG:HD3	1.66	0.76
1:C:1030:TRP:CD1	1:C:1580:LEU:HD22	2.20	0.76
1:C:1722:VAL:CG1	1:C:1731:LEU:HB3	2.14	0.76
2:H:1314:ARG:HH11	2:H:1314:ARG:CG	1.97	0.76
1:A:881:ASN:HA	1:A:944:ARG:NH2	2.00	0.76
2:G:7:ARG:NH2	2:G:27:PHE:HB3	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:707:PRO:CG	2:I:716:VAL:HG21	2.15	0.76
1:B:1030:TRP:NE1	1:B:1580:LEU:HD22	2.00	0.76
1:C:1239:HIS:HD2	1:C:1241:SER:OG	1.68	0.76
1:C:1030:TRP:NE1	1:C:1580:LEU:HD22	2.00	0.76
2:G:964:LEU:H	2:G:964:LEU:HD23	1.50	0.76
1:A:1239:HIS:HD2	1:A:1241:SER:OG	1.69	0.76
1:B:340:ARG:HH12	1:B:344:GLN:HG2	1.48	0.76
2:I:1567:ARG:HG3	2:I:1567:ARG:NH1	2.00	0.76
2:I:741:HIS:CE1	2:I:845:THR:CG2	2.68	0.76
1:A:1189:ILE:HD12	1:A:1380:GLN:HG3	1.68	0.76
2:G:355:LYS:O	2:G:358:SER:HB3	1.84	0.76
2:G:835:THR:HG22	2:G:845:THR:N	2.01	0.76
2:H:7:ARG:NH2	2:H:27:PHE:HB3	1.99	0.76
2:H:579:VAL:HG23	2:H:1078:HIS:CD2	2.21	0.76
1:B:980:VAL:HG21	2:H:952:ARG:HH21	1.49	0.76
1:C:198:PRO:HG3	1:C:209:LEU:CD2	2.15	0.76
1:C:985:ARG:NH1	2:I:953:ARG:CZ	2.48	0.76
1:C:1693:ILE:CD1	2:I:998:GLN:HB2	2.15	0.76
2:H:1129:ALA:HB2	2:H:1138:TRP:CZ3	2.21	0.76
2:I:1314:ARG:CG	2:I:1314:ARG:HH11	1.98	0.76
2:I:7:ARG:NH2	2:I:27:PHE:HB3	1.97	0.75
1:B:1523:ARG:HH11	1:B:1523:ARG:CG	1.98	0.75
2:G:1149:TRP:HA	2:G:1242:PHE:CE1	2.21	0.75
2:I:1284:VAL:HG13	2:I:1377:VAL:HG22	1.68	0.75
1:A:1014:ASP:H	1:A:1510:ASN:HD21	1.34	0.75
2:G:741:HIS:CE1	2:G:845:THR:CG2	2.69	0.75
2:H:2015:THR:HG22	2:H:2017:LYS:H	1.51	0.75
2:H:259:THR:HG22	2:H:262:GLU:HG3	1.67	0.75
2:H:192:ALA:HA	2:H:215:ILE:HD12	1.68	0.75
1:B:1693:ILE:CD1	2:H:998:GLN:HB2	2.17	0.75
2:I:902:PRO:HG2	2:I:929:LEU:HD21	1.68	0.75
1:A:1310:GLU:OE1	1:A:1649:LYS:HE3	1.86	0.75
1:B:1208:VAL:HG13	1:B:1212:THR:HB	1.68	0.75
2:G:1159:ILE:HG12	2:G:1168:ASN:HA	1.67	0.75
2:G:598:THR:HG22	2:G:622:GLY:HA3	1.67	0.75
2:G:2015:THR:HG22	2:G:2017:LYS:H	1.51	0.75
2:G:345:THR:HB	2:G:348:GLN:H	1.50	0.75
2:H:1293:THR:HG23	2:H:1296:GLU:H	1.49	0.75
1:C:1665:ILE:HG13	1:C:1669:ARG:HD3	1.66	0.75
2:G:455:ILE:HD11	2:G:469:ARG:HD3	1.66	0.75
2:H:598:THR:OG1	2:H:599:PRO:HD3	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:943:TRP:CH2	2:I:1016:PRO:HG3	2.21	0.75
2:I:1310:ASP:OD2	2:I:1602:SER:HB3	1.87	0.75
2:I:1352:HIS:HE1	2:I:1583:MET:CE	1.99	0.75
1:A:427:ASN:HD21	1:A:610:THR:H	1.35	0.74
1:C:1189:ILE:HD12	1:C:1380:GLN:HG3	1.68	0.74
1:B:968:VAL:HG23	2:H:1515:PRO:HG3	1.67	0.74
2:I:2015:THR:HG22	2:I:2017:LYS:H	1.51	0.74
1:B:1552:ASN:O	1:B:1556:THR:HG22	1.88	0.74
1:A:1030:TRP:CD1	1:A:1580:LEU:HD22	2.21	0.74
2:G:572:ASN:HB3	2:G:576:LYS:H	1.52	0.74
2:H:943:TRP:CH2	2:H:1016:PRO:HG3	2.22	0.74
2:H:1770:LEU:HD23	2:H:1776:PHE:CE2	2.21	0.74
2:H:455:ILE:HD11	2:H:469:ARG:CD	2.17	0.74
2:I:138:ASP:O	2:I:139:LYS:HG3	1.87	0.74
2:I:1889:VAL:HG13	2:I:1977:HIS:HB2	1.70	0.74
2:H:1672:GLN:HA	2:H:1676:MET:CE	2.18	0.74
1:A:655:LEU:HD22	1:A:916:LEU:HD11	1.68	0.74
1:C:36:LEU:HD22	1:C:61:LEU:HD21	1.68	0.74
1:B:335:HIS:CE1	1:C:335:HIS:CE1	2.75	0.74
2:H:1284:VAL:HG13	2:H:1377:VAL:HG22	1.69	0.74
2:H:584:SER:HB3	2:H:591:PRO:HG3	1.67	0.74
2:I:960:LYS:HA	2:I:960:LYS:HE2	1.67	0.74
1:B:964:GLU:HG2	2:H:1515:PRO:HB3	1.69	0.74
2:I:741:HIS:CE1	2:I:855:HIS:CE1	2.76	0.74
1:C:260:ARG:HH12	1:C:300:VAL:HG21	1.52	0.74
2:G:259:THR:HG22	2:G:262:GLU:HG3	1.68	0.74
2:G:705:LEU:HD12	2:G:716:VAL:HG13	1.70	0.74
2:I:1159:ILE:HG12	2:I:1169:PRO:HD3	1.68	0.74
1:B:1551:LYS:HD2	1:B:1617:ILE:HG21	1.70	0.74
1:C:1552:ASN:O	1:C:1556:THR:HG22	1.88	0.74
2:H:1242:PHE:HE2	2:H:1244:PRO:HG3	1.51	0.74
2:H:1956:ARG:HB2	2:H:1957:PRO:CD	2.13	0.74
1:B:328:LEU:O	1:B:331:ILE:HG22	1.86	0.73
1:B:400:ARG:HG2	1:B:400:ARG:NH1	2.00	0.73
2:G:194:THR:HG23	2:G:300:ILE:HD11	1.70	0.73
2:G:584:SER:HB3	2:G:591:PRO:HG3	1.70	0.73
2:I:7:ARG:NH1	2:I:24:THR:HG23	2.03	0.73
2:I:757:ILE:HG21	2:I:765:LEU:HD13	1.69	0.73
1:B:1376:PHE:CB	1:B:1544:THR:HG22	2.18	0.73
2:G:777:THR:HG22	2:G:1081:HIS:NE2	2.03	0.73
2:H:579:VAL:HG23	2:H:1078:HIS:NE2	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1129:ALA:HB2	2:I:1138:TRP:CZ3	2.22	0.73
2:I:572:ASN:HB3	2:I:576:LYS:H	1.52	0.73
1:C:881:ASN:HA	1:C:944:ARG:NH2	2.01	0.73
2:H:1194:VAL:HG22	2:H:1212:LYS:HB3	1.70	0.73
2:H:1265:MET:HE1	2:H:1562:PRO:HG2	1.68	0.73
2:H:1331:TRP:CZ2	2:H:1335:ILE:HG13	2.23	0.73
2:H:84:LEU:HD13	2:H:133:ALA:HB2	1.69	0.73
2:G:124:LYS:HG2	2:G:179:THR:HA	1.70	0.73
2:I:1784:MET:HG3	2:I:1785:GLU:N	2.02	0.73
2:I:2035:SER:HB3	2:I:2038:ILE:HG13	1.70	0.73
2:H:345:THR:HG22	2:H:347:GLU:H	1.51	0.73
2:I:455:ILE:HD11	2:I:469:ARG:CD	2.19	0.73
2:G:7:ARG:NH1	2:G:24:THR:HG23	2.03	0.73
2:G:7:ARG:HH21	2:G:27:PHE:CB	2.01	0.73
1:A:44:VAL:CG1	1:A:78:ILE:HG12	2.18	0.73
1:B:749:ILE:HD13	1:B:806:VAL:HG12	1.71	0.73
1:C:1551:LYS:HD2	1:C:1617:ILE:HG21	1.70	0.73
2:G:105:ALA:HB1	2:G:119:THR:HG23	1.70	0.73
2:H:131:ILE:HD12	2:H:182:VAL:HB	1.71	0.73
1:A:1551:LYS:HD2	1:A:1617:ILE:HG21	1.70	0.73
2:G:1638:ILE:HD12	2:G:1657:ILE:HD12	1.71	0.73
2:G:1680:LEU:HD13	2:G:1687:ALA:HB2	1.71	0.73
1:C:67:SER:OG	2:H:359:HIS:HE1	1.70	0.73
2:H:572:ASN:HB3	2:H:576:LYS:H	1.54	0.73
1:B:1153:ASP:OD2	1:C:359:ARG:NH2	2.22	0.73
2:H:1956:ARG:CB	2:H:1957:PRO:HD3	2.11	0.73
1:A:335:HIS:HE1	1:B:335:HIS:CE1	2.06	0.72
1:C:749:ILE:HD13	1:C:806:VAL:HG12	1.70	0.72
2:H:194:THR:HG23	2:H:300:ILE:HD11	1.71	0.72
2:H:7:ARG:NH1	2:H:24:THR:HG23	2.03	0.72
2:I:777:THR:HG22	2:I:1081:HIS:NE2	2.04	0.72
2:I:835:THR:HB	2:I:845:THR:HG23	1.71	0.72
1:A:833:PHE:HA	1:A:937:LYS:HD2	1.71	0.72
2:H:1680:LEU:HD13	2:H:1687:ALA:HB2	1.71	0.72
2:H:238:CYS:HB2	2:H:239:PRO:HD3	1.71	0.72
2:I:84:LEU:HD13	2:I:133:ALA:HB2	1.71	0.72
1:A:1208:VAL:HG13	1:A:1212:THR:HB	1.70	0.72
1:C:1376:PHE:CB	1:C:1544:THR:HG22	2.19	0.72
2:G:598:THR:OG1	2:G:599:PRO:HD3	1.89	0.72
2:H:1784:MET:HG3	2:H:1785:GLU:N	2.03	0.72
2:H:856:LYS:HG2	2:H:1054:LEU:HD12	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1331:TRP:CZ2	2:I:1335:ILE:HG13	2.25	0.72
2:I:707:PRO:HG3	2:I:716:VAL:CG2	2.19	0.72
2:I:7:ARG:HH21	2:I:27:PHE:CB	1.99	0.72
1:B:473:GLY:O	1:B:477:ILE:HG13	1.89	0.72
1:C:655:LEU:HD22	1:C:916:LEU:HD11	1.71	0.72
2:H:705:LEU:HD12	2:H:716:VAL:HG13	1.70	0.72
2:I:1672:GLN:HA	2:I:1676:MET:CE	2.20	0.72
1:B:44:VAL:CG1	1:B:78:ILE:HG12	2.18	0.72
1:A:1279:PHE:HB2	1:A:1282:THR:CG2	2.19	0.72
2:G:1269:LEU:O	2:G:1560:LEU:HD23	1.90	0.72
1:A:411:GLN:HE22	1:A:1628:SER:H	1.34	0.72
1:C:473:GLY:O	1:C:477:ILE:HG13	1.88	0.72
1:C:733:ILE:HD13	1:C:761:LEU:HD11	1.72	0.72
1:C:427:ASN:HD21	1:C:610:THR:H	1.35	0.72
2:G:1310:ASP:OD2	2:G:1602:SER:HB3	1.90	0.72
2:G:238:CYS:HB2	2:G:239:PRO:HD3	1.71	0.72
2:G:707:PRO:CG	2:G:716:VAL:HG21	2.20	0.72
2:H:138:ASP:O	2:H:139:LYS:HG3	1.90	0.72
2:H:777:THR:HG22	2:H:1081:HIS:NE2	2.04	0.72
2:I:194:THR:HG23	2:I:300:ILE:HD11	1.70	0.72
1:B:254:TRP:CZ3	1:B:302:LEU:HD13	2.25	0.72
2:H:109:LEU:HD11	2:H:116:LEU:HD23	1.72	0.72
2:H:1355:ASN:HA	2:H:1407:THR:O	1.88	0.72
2:H:146:PHE:HA	2:H:149:VAL:CG1	2.18	0.72
1:B:852:ARG:NH1	1:B:852:ARG:HG2	1.98	0.71
2:H:1678:MET:HE3	2:H:1707:LEU:HD22	1.71	0.71
1:A:331:ILE:HD11	1:C:332:THR:HG22	1.71	0.71
1:A:733:ILE:HD13	1:A:761:LEU:HD11	1.71	0.71
1:B:1030:TRP:NE1	1:B:1580:LEU:CD2	2.54	0.71
2:G:1265:MET:HE1	2:G:1562:PRO:HG2	1.72	0.71
2:G:1917:ILE:HG23	2:G:1922:ILE:HB	1.72	0.71
2:H:455:ILE:CG1	2:H:469:ARG:HD3	2.20	0.71
2:H:634:ILE:HD11	2:H:649:ILE:HD11	1.70	0.71
2:I:1496:LYS:HE2	2:I:1693:ARG:HH21	1.55	0.71
1:A:1045:PHE:HB3	1:A:1049:GLY:HA3	1.71	0.71
1:B:1312:VAL:HG22	1:B:1329:VAL:HG11	1.73	0.71
2:G:751:LEU:HD23	2:G:791:TYR:CE2	2.25	0.71
2:I:146:PHE:HA	2:I:149:VAL:CG1	2.20	0.71
2:I:1680:LEU:HD13	2:I:1687:ALA:HB2	1.73	0.71
2:I:2036:GLU:HB2	2:I:2037:PRO:HD3	1.72	0.71
2:I:732:TRP:CG	2:I:750:MET:CE	2.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:CE	1:B:6:GLU:HA	2.20	0.71
1:C:1208:VAL:HG13	1:C:1212:THR:HB	1.71	0.71
2:H:1819:ALA:HA	2:H:2005:ARG:HH11	1.55	0.71
2:I:751:LEU:HD23	2:I:791:TYR:CE2	2.25	0.71
2:I:964:LEU:H	2:I:964:LEU:HD23	1.55	0.71
1:B:1232:TYR:CZ	1:B:1701:LYS:HD2	2.26	0.71
1:B:459:ASP:HB3	1:B:462:LYS:HG3	1.72	0.71
2:G:109:LEU:HD11	2:G:116:LEU:HD23	1.71	0.71
2:G:949:ASP:HB3	2:G:1006:MET:HE2	1.72	0.71
2:H:1173:VAL:HG21	2:H:1221:MET:HE1	1.73	0.71
2:H:1889:VAL:HG13	2:H:1977:HIS:HB2	1.72	0.71
2:I:579:VAL:HG23	2:I:1078:HIS:CD2	2.24	0.71
2:I:1770:LEU:HD23	2:I:1776:PHE:HE2	1.55	0.71
2:I:1862:VAL:HG11	2:I:1866:PHE:CD1	2.26	0.71
2:I:191:SER:HA	2:I:194:THR:HG22	1.72	0.71
1:C:27:ARG:HH21	2:I:2015:THR:HA	1.54	0.71
2:I:455:ILE:CG1	2:I:469:ARG:HD3	2.21	0.71
1:A:1:MET:CE	1:A:6:GLU:HA	2.21	0.71
1:B:655:LEU:HD22	1:B:916:LEU:HD11	1.72	0.71
2:G:1159:ILE:HG12	2:G:1169:PRO:HD3	1.71	0.71
2:H:1352:HIS:HE1	2:H:1583:MET:CE	2.02	0.71
2:H:455:ILE:CD1	2:H:469:ARG:HD3	2.20	0.71
2:H:499:THR:CB	2:H:500:HIS:HD2	1.99	0.71
1:B:1208:VAL:CG1	1:B:1212:THR:HB	2.20	0.71
2:G:1496:LYS:HE2	2:G:1693:ARG:HH21	1.54	0.71
2:H:1279:PHE:HD2	2:H:1340:PRO:HG3	1.55	0.71
2:I:234:ILE:HG13	2:I:235:PRO:HD3	1.73	0.71
2:I:856:LYS:HG2	2:I:1054:LEU:HD12	1.72	0.71
1:A:12:ILE:HA	1:A:15:THR:CG2	2.21	0.71
1:B:27:ARG:HH21	2:H:2015:THR:HA	1.56	0.71
2:H:1567:ARG:NH1	2:H:1567:ARG:HG3	1.99	0.71
2:I:1058:VAL:O	2:I:1061:GLN:HG2	1.90	0.71
2:I:652:ILE:N	2:I:658:MET:HE3	2.04	0.71
2:G:2036:GLU:HB2	2:G:2037:PRO:HD3	1.73	0.70
2:G:161:GLY:H	2:G:505:GLY:HA3	1.54	0.70
2:I:259:THR:HG22	2:I:262:GLU:CG	2.20	0.70
2:G:1889:VAL:HG13	2:G:1977:HIS:HB2	1.72	0.70
2:G:50:ALA:HB3	2:G:53:GLU:HG3	1.72	0.70
1:A:27:ARG:HH21	2:G:2015:THR:HA	1.56	0.70
2:H:7:ARG:HH21	2:H:27:PHE:CB	2.01	0.70
2:H:816:ASP:HB3	2:H:1048:VAL:HG21	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:968:VAL:O	2:H:1512:HIS:HB2	1.91	0.70
2:G:762:ASN:N	2:G:762:ASN:HD22	1.82	0.70
2:H:54:PRO:HG3	2:H:63:LYS:HG3	1.73	0.70
2:H:762:ASN:N	2:H:762:ASN:HD22	1.82	0.70
2:I:1242:PHE:CE2	2:I:1244:PRO:HG3	2.26	0.70
2:I:1279:PHE:HD2	2:I:1340:PRO:HG3	1.54	0.70
2:I:1419:PHE:O	2:I:1422:THR:HG22	1.90	0.70
2:H:1310:ASP:OD2	2:H:1602:SER:HB3	1.91	0.70
1:A:852:ARG:NH1	1:A:852:ARG:HG2	2.00	0.70
1:C:1219:VAL:HG22	1:C:1384:ILE:HD12	1.73	0.70
2:I:1917:ILE:HG23	2:I:1922:ILE:HB	1.74	0.70
1:A:1208:VAL:CG1	1:A:1212:THR:HB	2.21	0.70
1:A:1722:VAL:CG1	1:A:1731:LEU:HB3	2.19	0.70
1:B:881:ASN:HA	1:B:944:ARG:NH2	2.06	0.70
1:C:888:ILE:HD12	1:C:939:PHE:HE2	1.57	0.70
2:G:1331:TRP:CZ2	2:G:1335:ILE:HG13	2.26	0.70
2:H:2036:GLU:HB2	2:H:2037:PRO:HD3	1.72	0.70
1:A:254:TRP:CZ3	1:A:292:GLN:HG3	2.26	0.70
1:A:631:PRO:HB2	1:A:634:THR:OG1	1.92	0.70
1:C:833:PHE:HA	1:C:937:LYS:HD2	1.73	0.70
2:I:1086:LEU:HG	2:I:1092:ASP:HA	1.72	0.70
1:A:1312:VAL:HG22	1:A:1329:VAL:HG11	1.73	0.70
1:A:749:ILE:HD13	1:A:806:VAL:HG12	1.72	0.70
2:G:1194:VAL:HG22	2:G:1212:LYS:HB3	1.74	0.70
2:G:964:LEU:CD2	2:G:964:LEU:H	2.04	0.70
2:H:652:ILE:H	2:H:658:MET:CE	2.03	0.70
2:I:455:ILE:CD1	2:I:469:ARG:HD3	2.21	0.70
1:C:631:PRO:HB2	1:C:634:THR:OG1	1.92	0.70
2:G:1670:GLY:H	2:G:1672:GLN:HE21	1.40	0.70
2:G:652:ILE:H	2:G:658:MET:CE	2.01	0.70
2:H:707:PRO:CG	2:H:716:VAL:HG21	2.21	0.70
2:I:161:GLY:H	2:I:505:GLY:HA3	1.56	0.70
1:C:1045:PHE:HB3	1:C:1049:GLY:HA3	1.74	0.69
1:C:1276:GLN:O	1:C:1282:THR:HG21	1.92	0.69
2:G:1672:GLN:HA	2:G:1676:MET:CE	2.21	0.69
1:C:260:ARG:NH1	1:C:300:VAL:HG21	2.06	0.69
1:C:459:ASP:HB3	1:C:462:LYS:HG3	1.73	0.69
2:H:1889:VAL:HG13	2:H:1977:HIS:CB	2.22	0.69
2:I:768:GLY:HA3	2:I:800:LEU:HD21	1.75	0.69
1:A:1376:PHE:CB	1:A:1544:THR:HG22	2.19	0.69
2:G:1242:PHE:HE2	2:G:1244:PRO:HG3	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:707:PRO:HG3	2:G:716:VAL:CG2	2.22	0.69
2:H:259:THR:HG22	2:H:262:GLU:CG	2.22	0.69
2:I:109:LEU:HD11	2:I:116:LEU:HD23	1.73	0.69
1:C:1208:VAL:CG1	1:C:1212:THR:HB	2.23	0.69
1:C:1219:VAL:HA	1:C:1384:ILE:CD1	2.20	0.69
2:G:191:SER:HA	2:G:194:THR:HG22	1.74	0.69
2:H:1808:SER:OG	2:H:1977:HIS:HE1	1.74	0.69
2:H:964:LEU:HD23	2:H:964:LEU:H	1.56	0.69
2:G:732:TRP:CG	2:G:750:MET:HE1	2.27	0.69
2:H:1422:THR:CG2	2:H:1474:PHE:HB2	2.22	0.69
2:H:741:HIS:CE1	2:H:845:THR:HG21	2.27	0.69
1:B:1219:VAL:HG22	1:B:1384:ILE:HD12	1.75	0.69
1:B:888:ILE:HD12	1:B:939:PHE:HE2	1.57	0.69
2:G:187:LEU:HA	2:G:190:PHE:HB3	1.74	0.69
2:H:1670:GLY:H	2:H:1672:GLN:HE21	1.40	0.69
2:H:234:ILE:HG13	2:H:235:PRO:HD3	1.74	0.69
2:I:1264:GLU:HA	2:I:1275:PHE:CE1	2.27	0.69
1:A:1232:TYR:CZ	1:A:1701:LYS:HD2	2.27	0.69
1:B:254:TRP:CZ3	1:B:292:GLN:HG3	2.27	0.69
1:C:1310:GLU:OE1	1:C:1649:LYS:HE3	1.93	0.69
2:G:1355:ASN:HA	2:G:1407:THR:O	1.92	0.69
2:G:1676:MET:HE1	2:G:1781:LEU:HD21	1.73	0.69
2:G:455:ILE:HD11	2:G:469:ARG:CD	2.22	0.69
2:H:751:LEU:HD23	2:H:791:TYR:CE2	2.27	0.69
2:I:926:LEU:HD13	2:I:947:THR:HG22	1.73	0.69
1:A:504:ASP:HB3	1:A:508:ASN:H	1.56	0.69
1:A:888:ILE:HD12	1:A:939:PHE:HE2	1.57	0.69
2:G:259:THR:HG22	2:G:262:GLU:CG	2.22	0.69
2:H:663:ILE:HB	2:H:664:PRO:HD3	1.75	0.69
2:I:910:GLN:HE21	2:I:912:ARG:HH21	1.40	0.69
2:G:579:VAL:HG23	2:G:1078:HIS:CD2	2.27	0.69
2:G:455:ILE:CG1	2:G:469:ARG:HD3	2.23	0.69
2:I:1920:GLN:HG2	2:I:1922:ILE:HD11	1.75	0.69
2:I:949:ASP:HB3	2:I:1006:MET:HE2	1.74	0.69
1:A:1431:GLU:HG3	1:A:1433:HIS:CE1	2.28	0.69
2:H:2022:THR:HG23	2:H:2025:TYR:H	1.58	0.69
2:I:1265:MET:HE1	2:I:1562:PRO:HG2	1.74	0.69
2:G:490:TRP:HE1	2:G:516:THR:CG2	1.99	0.69
2:G:741:HIS:NE2	2:G:855:HIS:CE1	2.61	0.69
2:I:598:THR:CG2	2:I:622:GLY:HA3	2.23	0.69
1:C:44:VAL:CG1	1:C:78:ILE:HG12	2.24	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
1:B:985:ARG:NH1	2:H:953:ARG:CZ	2.55	0.68
2:I:1638:ILE:HD12	2:I:1657:ILE:HD12	1.75	0.68
2:I:652:ILE:H	2:I:658:MET:CE	2.04	0.68
2:H:187:LEU:HA	2:H:190:PHE:HB3	1.75	0.68
2:H:305:PHE:CE1	2:H:442:ASP:HB3	2.27	0.68
2:I:1739:GLU:CB	2:I:1987:PRO:HB3	2.20	0.68
2:I:663:ILE:HB	2:I:664:PRO:HD3	1.76	0.68
2:I:748:THR:HB	2:I:749:PRO:HD3	1.74	0.68
2:G:1264:GLU:HA	2:G:1275:PHE:CE1	2.28	0.68
2:G:84:LEU:HD13	2:G:133:ALA:HB2	1.75	0.68
2:I:594:VAL:HG21	2:I:610:THR:HG21	1.75	0.68
1:C:985:ARG:HH12	2:I:953:ARG:CZ	2.06	0.68
1:C:968:VAL:HG23	2:I:1515:PRO:HG3	1.75	0.68
2:G:732:TRP:CG	2:G:750:MET:CE	2.76	0.68
2:G:835:THR:HG21	2:G:855:HIS:HD2	1.51	0.68
2:H:1195:VAL:CG1	2:H:1211:LEU:HB3	2.23	0.68
2:H:1638:ILE:HD12	2:H:1657:ILE:HD12	1.76	0.68
2:I:1355:ASN:HB3	2:I:1583:MET:HE1	1.74	0.68
2:I:305:PHE:CE1	2:I:442:ASP:HB3	2.29	0.68
2:I:545:GLN:HE21	2:I:545:GLN:H	1.41	0.68
1:A:1056:ILE:HD13	1:A:1193:TRP:HD1	1.59	0.68
1:C:12:ILE:HA	1:C:15:THR:CG2	2.22	0.68
2:G:1770:LEU:HD23	2:G:1776:PHE:HE2	1.58	0.68
2:G:1784:MET:HG3	2:G:1785:GLU:N	2.07	0.68
2:G:663:ILE:HB	2:G:664:PRO:HD3	1.74	0.68
2:H:1381:VAL:HG13	2:H:1390:VAL:HG22	1.74	0.68
1:A:1721:ARG:NH1	1:A:1721:ARG:CG	2.52	0.68
2:G:1058:VAL:O	2:G:1061:GLN:HG2	1.93	0.68
2:G:2035:SER:HB3	2:G:2038:ILE:HG13	1.74	0.68
1:C:964:GLU:HG2	2:I:1515:PRO:HB3	1.76	0.68
1:C:11:HIS:ND1	2:I:1998:LYS:HA	2.08	0.68
2:I:163:GLN:HG2	2:I:423:VAL:HG12	1.76	0.68
1:B:427:ASN:HD21	1:B:610:THR:H	1.41	0.68
2:H:1058:VAL:O	2:H:1061:GLN:HG2	1.94	0.68
2:H:1419:PHE:O	2:H:1422:THR:HG22	1.93	0.68
1:A:1474:ALA:HA	1:A:1478:PRO:CG	2.24	0.68
1:B:1279:PHE:HB2	1:B:1282:THR:CG2	2.24	0.68
1:B:1310:GLU:OE1	1:B:1649:LYS:HE3	1.94	0.68
1:B:183:GLN:HE21	1:B:202:GLU:HG2	1.59	0.68
1:B:833:PHE:HA	1:B:937:LYS:HD2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:488:PRO:HG3	1:C:728:LYS:HG3	1.75	0.68
2:G:910:GLN:HE21	2:G:912:ARG:HH21	1.42	0.68
2:H:1264:GLU:HA	2:H:1275:PHE:CE1	2.29	0.68
1:A:1030:TRP:NE1	1:A:1580:LEU:CD2	2.57	0.68
2:H:902:PRO:HG2	2:H:929:LEU:HD21	1.75	0.68
2:I:1670:GLY:H	2:I:1672:GLN:HE21	1.38	0.68
2:I:187:LEU:HA	2:I:190:PHE:HB3	1.76	0.68
1:A:183:GLN:HE21	1:A:202:GLU:HG2	1.59	0.68
1:A:359:ARG:NH2	1:C:1153:ASP:OD2	2.27	0.68
2:G:1889:VAL:HG13	2:G:1977:HIS:CB	2.24	0.68
2:I:1269:LEU:O	2:I:1560:LEU:HD23	1.93	0.68
2:I:1675:GLY:O	2:I:1678:MET:HB2	1.94	0.68
2:I:499:THR:CB	2:I:500:HIS:HD2	1.95	0.68
1:A:1594:ASN:O	1:A:1598:GLN:HG3	1.94	0.67
1:B:1391:ASP:OD2	1:B:1502:ARG:NH2	2.27	0.67
2:H:1834:ARG:CG	2:H:1834:ARG:HH11	1.92	0.67
2:I:1673:GLU:H	2:I:1676:MET:HE3	1.58	0.67
2:I:703:LEU:HD21	2:I:705:LEU:HD21	1.76	0.67
1:A:328:LEU:O	1:A:328:LEU:HD22	1.94	0.67
1:A:459:ASP:HB3	1:A:462:LYS:HG3	1.76	0.67
1:C:257:PRO:HD2	1:C:260:ARG:HB2	1.76	0.67
2:H:1770:LEU:HD23	2:H:1776:PHE:HE2	1.59	0.67
2:H:762:ASN:H	2:H:762:ASN:ND2	1.85	0.67
2:I:1194:VAL:HG22	2:I:1212:LYS:HB3	1.75	0.67
1:C:1021:VAL:HG11	1:C:1597:LEU:HD11	1.74	0.67
2:H:1159:ILE:CG1	2:H:1169:PRO:HD3	2.25	0.67
2:I:1676:MET:HE1	2:I:1781:LEU:HD21	1.77	0.67
1:C:1232:TYR:CZ	1:C:1701:LYS:HD2	2.29	0.67
1:C:1279:PHE:HB2	1:C:1282:THR:CG2	2.23	0.67
1:C:254:TRP:CZ3	1:C:292:GLN:HG3	2.29	0.67
2:G:579:VAL:HG23	2:G:1078:HIS:NE2	2.10	0.67
2:G:1173:VAL:HG21	2:G:1221:MET:HE1	1.77	0.67
2:G:1808:SER:H	2:G:2013:ASN:ND2	1.93	0.67
2:G:54:PRO:HG3	2:G:63:LYS:HG3	1.76	0.67
2:G:768:GLY:HA3	2:G:800:LEU:HD21	1.76	0.67
2:H:1741:ILE:HG12	2:H:1746:LEU:HD13	1.76	0.67
2:H:1917:ILE:HG23	2:H:1922:ILE:HB	1.74	0.67
2:H:648:GLY:HA3	2:H:678:PHE:CE2	2.29	0.67
1:B:1045:PHE:HB3	1:B:1049:GLY:HA3	1.76	0.67
1:C:409:ALA:HB2	1:C:442:ARG:HD2	1.76	0.67
2:G:1176:PRO:O	2:G:1177:SER:HB3	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:499:THR:CB	2:G:500:HIS:HD2	1.97	0.67
2:H:1086:LEU:HG	2:H:1092:ASP:HA	1.76	0.67
2:H:1269:LEU:O	2:H:1560:LEU:HD23	1.94	0.67
2:I:1889:VAL:HG13	2:I:1977:HIS:CB	2.25	0.67
1:B:1276:GLN:O	1:B:1282:THR:HG21	1.95	0.67
2:G:816:ASP:HB3	2:G:1048:VAL:HG21	1.77	0.67
1:B:20:TYR:CE2	2:H:1985:VAL:HG11	2.29	0.67
2:I:1101:GLU:HB3	2:I:1147:ILE:HG22	1.75	0.67
1:B:1039:MET:O	1:B:1609:ARG:NH2	2.27	0.67
2:G:1475:LYS:CG	2:G:1481:SER:HB2	2.25	0.67
2:G:1227:ARG:HD2	2:G:1565:VAL:HG11	1.76	0.67
1:B:2:LYS:CD	2:H:2050:GLN:HB3	2.21	0.67
2:H:545:GLN:HE21	2:H:545:GLN:H	1.41	0.67
2:I:904:PHE:HB2	2:I:1017:PHE:CD1	2.28	0.67
1:A:1219:VAL:HA	1:A:1384:ILE:CD1	2.23	0.67
1:A:1360:ARG:HH11	1:A:1364:GLU:HG2	1.60	0.67
1:A:749:ILE:HD11	1:A:805:CYS:HB3	1.75	0.67
1:C:1030:TRP:NE1	1:C:1580:LEU:CD2	2.58	0.67
1:C:12:ILE:HD11	2:I:2041:ILE:HD12	1.76	0.67
2:H:826:GLY:HA3	2:H:1061:GLN:HB3	1.76	0.67
2:H:1242:PHE:CE2	2:H:1244:PRO:HG3	2.30	0.67
2:I:1195:VAL:CG1	2:I:1211:LEU:HB3	2.25	0.67
1:C:746:GLU:O	1:C:750:GLU:HG3	1.95	0.67
2:H:1054:LEU:HB2	3:H:3051:FMN:HM72	1.77	0.67
2:H:50:ALA:HB3	2:H:53:GLU:HG3	1.76	0.67
2:H:707:PRO:HG3	2:H:716:VAL:CG2	2.24	0.67
2:I:598:THR:OG1	2:I:599:PRO:HD3	1.94	0.67
1:A:257:PRO:HD2	1:A:260:ARG:HB2	1.76	0.66
1:C:1360:ARG:HH11	1:C:1364:GLU:HG2	1.60	0.66
1:C:1455:ARG:HH11	1:C:1458:GLN:HE21	1.42	0.66
1:A:836:ASP:HB3	1:A:839:TYR:HB3	1.76	0.66
1:B:504:ASP:HB3	1:B:508:ASN:H	1.60	0.66
1:C:328:LEU:HD22	1:C:328:LEU:O	1.95	0.66
2:G:1101:GLU:HB3	2:G:1147:ILE:HG22	1.76	0.66
2:G:904:PHE:HB2	2:G:1017:PHE:CD1	2.30	0.66
2:H:641:ILE:HG12	2:H:645:SER:HB2	1.76	0.66
2:H:910:GLN:HE21	2:H:912:ARG:HH21	1.43	0.66
2:I:705:LEU:HD12	2:I:716:VAL:HG13	1.76	0.66
1:A:1662:TYR:O	1:A:1665:ILE:HG22	1.95	0.66
1:B:12:ILE:HA	1:B:15:THR:CG2	2.25	0.66
1:C:294:TYR:CE1	1:C:298:VAL:HG21	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:504:ASP:HB3	1:C:508:ASN:H	1.60	0.66
2:G:1381:VAL:HG13	2:G:1390:VAL:HG22	1.78	0.66
2:I:1672:GLN:HA	2:I:1676:MET:HE1	1.76	0.66
1:C:183:GLN:HE21	1:C:202:GLU:HG2	1.60	0.66
2:G:1419:PHE:O	2:G:1422:THR:HG22	1.96	0.66
2:G:1739:GLU:CB	2:G:1987:PRO:HB3	2.23	0.66
2:H:1227:ARG:HD2	2:H:1565:VAL:HG11	1.77	0.66
2:I:1054:LEU:HB2	3:I:3051:FMN:HM72	1.78	0.66
1:B:328:LEU:O	1:B:328:LEU:HD22	1.95	0.66
1:B:883:ILE:HD12	1:B:947:LEU:HD12	1.77	0.66
1:B:864:VAL:HG22	1:B:921:PRO:HB3	1.77	0.66
1:C:836:ASP:HB3	1:C:839:TYR:HB3	1.77	0.66
2:H:1862:VAL:HG11	2:H:1866:PHE:CD1	2.30	0.66
1:A:1219:VAL:HG22	1:A:1384:ILE:HD12	1.77	0.66
1:A:473:GLY:O	1:A:477:ILE:HG13	1.95	0.66
1:C:32:GLN:HA	1:C:35:PHE:CE2	2.31	0.66
1:C:1:MET:CE	1:C:6:GLU:HA	2.25	0.66
2:G:1352:HIS:CD2	2:G:1410:PHE:CE2	2.84	0.66
2:G:1355:ASN:HB3	2:G:1583:MET:HE1	1.77	0.66
2:G:1862:VAL:HG11	2:G:1866:PHE:CD1	2.30	0.66
2:G:163:GLN:HG2	2:G:423:VAL:HG12	1.77	0.66
1:A:599:MET:HB2	1:A:624:LYS:CD	2.25	0.66
1:C:1721:ARG:HG2	1:C:1721:ARG:NH1	2.00	0.66
2:G:1129:ALA:HB2	2:G:1138:TRP:CZ3	2.30	0.66
2:G:353:VAL:HG23	2:G:357:ASN:ND2	2.10	0.66
2:G:736:ARG:NH1	2:G:769:SER:O	2.29	0.66
2:H:1676:MET:HE1	2:H:1781:LEU:HD21	1.78	0.66
2:I:1173:VAL:HG21	2:I:1221:MET:HE1	1.78	0.66
1:C:460:GLU:HG2	1:C:470:LYS:HD3	1.77	0.66
2:G:1457:PHE:CZ	2:G:1501:ILE:HD11	2.30	0.66
2:G:1920:GLN:HG2	2:G:1922:ILE:HD11	1.78	0.66
2:G:835:THR:HG22	2:G:844:VAL:C	2.17	0.66
2:G:902:PRO:HG2	2:G:929:LEU:HD21	1.76	0.66
2:H:161:GLY:H	2:H:505:GLY:HA3	1.59	0.66
2:H:594:VAL:HG21	2:H:610:THR:HG21	1.77	0.66
2:H:670:ARG:HD3	2:H:699:GLY:O	1.95	0.66
2:I:835:THR:HG21	2:I:855:HIS:HD2	1.59	0.66
1:C:435:GLU:O	1:C:439:ILE:HG13	1.96	0.66
2:G:670:ARG:HD3	2:G:699:GLY:O	1.95	0.66
2:G:748:THR:HB	2:G:749:PRO:HD3	1.78	0.66
2:H:1986:LYS:N	2:H:1987:PRO:HD2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:50:ALA:HB3	2:I:53:GLU:HG3	1.76	0.66
1:A:504:ASP:HB2	1:A:508:ASN:HB2	1.78	0.66
2:H:768:GLY:HA3	2:H:800:LEU:HD21	1.77	0.66
2:I:1176:PRO:O	2:I:1177:SER:HB3	1.95	0.66
2:I:54:PRO:HG3	2:I:63:LYS:HG3	1.75	0.66
1:A:254:TRP:CH2	1:A:292:GLN:HG3	2.31	0.65
1:B:460:GLU:HG2	1:B:470:LYS:HD3	1.78	0.65
1:B:529:MET:CG	1:B:638:LEU:HG	2.26	0.65
1:C:1056:ILE:HD13	1:C:1193:TRP:HD1	1.60	0.65
1:C:749:ILE:HD11	1:C:805:CYS:HB3	1.78	0.65
1:A:968:VAL:O	2:G:1512:HIS:HB2	1.96	0.65
2:I:251:VAL:O	2:I:255:LEU:HB2	1.96	0.65
2:I:61:VAL:O	2:I:65:LEU:HB2	1.96	0.65
2:I:750:MET:HG3	2:I:796:PHE:HZ	1.60	0.65
1:A:864:VAL:HG22	1:A:921:PRO:HB3	1.78	0.65
1:B:294:TYR:CE1	1:B:298:VAL:HG21	2.31	0.65
2:G:61:VAL:O	2:G:65:LEU:HB2	1.96	0.65
2:H:904:PHE:HB2	2:H:1017:PHE:CD1	2.30	0.65
2:I:816:ASP:HB3	2:I:1048:VAL:CG2	2.26	0.65
1:A:294:TYR:CE1	1:A:298:VAL:HG21	2.32	0.65
1:A:488:PRO:HG3	1:A:728:LYS:HG3	1.77	0.65
1:A:881:ASN:HA	1:A:944:ARG:HH21	1.60	0.65
2:G:1279:PHE:HD2	2:G:1340:PRO:HG3	1.62	0.65
2:G:234:ILE:HG13	2:G:235:PRO:HD3	1.77	0.65
2:G:33:LEU:HD11	2:G:80:PHE:HD2	1.61	0.65
2:H:816:ASP:HB3	2:H:1048:VAL:CG2	2.26	0.65
2:H:61:VAL:O	2:H:65:LEU:HB2	1.96	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	1.78	0.65
2:H:964:LEU:CD2	2:H:964:LEU:H	2.10	0.65
1:A:1305:CYS:HB2	1:A:1645:GLY:HA2	1.79	0.65
1:B:497:THR:OG1	1:B:513:GLU:HG2	1.95	0.65
1:C:497:THR:OG1	1:C:513:GLU:HG2	1.97	0.65
2:G:856:LYS:NZ	2:G:1052:CYS:SG	2.69	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:1739:GLU:O	2:I:1987:PRO:HG3	1.95	0.65
1:A:335:HIS:CE1	1:B:335:HIS:CE1	2.84	0.65
1:A:985:ARG:NH1	2:G:953:ARG:CZ	2.60	0.65
1:C:411:GLN:HE22	1:C:1628:SER:H	1.42	0.65
2:G:1242:PHE:CE2	2:G:1244:PRO:HG3	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2035:SER:HB3	2:H:2038:ILE:HG13	1.79	0.65
2:I:579:VAL:HG23	2:I:1078:HIS:NE2	2.10	0.65
2:I:1808:SER:H	2:I:2013:ASN:ND2	1.94	0.65
1:A:27:ARG:HD2	1:A:30:GLU:OE2	1.97	0.65
1:B:421:ILE:CG1	1:B:469:VAL:HG21	2.27	0.65
1:C:295:ALA:HB2	1:C:302:LEU:HD11	1.77	0.65
2:G:1567:ARG:HG3	2:G:1567:ARG:NH1	2.02	0.65
2:G:353:VAL:HG23	2:G:357:ASN:HD22	1.61	0.65
2:H:1739:GLU:CB	2:H:1987:PRO:HB3	2.21	0.65
1:A:1021:VAL:HG11	1:A:1597:LEU:HD11	1.79	0.65
1:B:1317:GLU:OE1	1:B:1317:GLU:HA	1.96	0.65
2:G:816:ASP:HB3	2:G:1048:VAL:CG2	2.26	0.65
2:G:1741:ILE:HG12	2:G:1746:LEU:HD13	1.77	0.65
2:G:1740:THR:HG22	2:G:1742:VAL:HG23	1.78	0.65
2:H:1740:THR:HG22	2:H:1742:VAL:HG23	1.79	0.65
2:H:703:LEU:HD21	2:H:705:LEU:HD21	1.79	0.65
2:I:1678:MET:HE3	2:I:1707:LEU:HD22	1.78	0.65
1:A:340:ARG:HH12	1:A:344:GLN:CG	2.09	0.65
1:B:257:PRO:HD2	1:B:260:ARG:HB2	1.78	0.65
1:C:1194:ASN:HB3	1:C:1197:THR:CG2	2.27	0.65
1:C:864:VAL:HG22	1:C:921:PRO:HB3	1.79	0.65
2:G:1265:MET:CE	2:G:1562:PRO:HG2	2.27	0.65
2:G:826:GLY:HA3	2:G:1061:GLN:HB3	1.78	0.65
2:H:1823:SER:OG	2:H:1825:GLU:HG2	1.96	0.65
2:I:1378:ILE:HD11	2:I:1381:VAL:HG21	1.79	0.65
1:B:746:GLU:O	1:B:750:GLU:HG3	1.97	0.65
2:H:1472:VAL:HG22	2:H:1483:VAL:HG22	1.79	0.65
1:A:497:THR:OG1	1:A:513:GLU:HG2	1.96	0.65
1:B:749:ILE:HD11	1:B:805:CYS:HB3	1.78	0.65
2:G:131:ILE:HB	2:G:182:VAL:HG11	1.78	0.65
2:G:305:PHE:CE1	2:G:442:ASP:HB3	2.32	0.65
2:H:191:SER:HA	2:H:194:THR:HG22	1.77	0.65
2:H:1808:SER:H	2:H:2013:ASN:ND2	1.95	0.65
2:H:163:GLN:HG2	2:H:423:VAL:HG12	1.79	0.65
2:I:1475:LYS:CG	2:I:1481:SER:HB2	2.27	0.65
1:A:1039:MET:O	1:A:1609:ARG:NH2	2.30	0.64
1:A:529:MET:CG	1:A:638:LEU:HG	2.27	0.64
1:B:1474:ALA:HA	1:B:1478:PRO:CG	2.27	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:1378:ILE:HD11	2:G:1381:VAL:HG21	1.76	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:259:THR:HG23	2:G:262:GLU:H	1.62	0.64
2:I:7:ARG:HE	2:I:27:PHE:HB2	1.62	0.64
1:C:1292:ILE:CD1	1:C:1328:ILE:HD11	2.27	0.64
1:C:408:TRP:CZ3	1:C:1628:SER:HB3	2.32	0.64
2:H:259:THR:CG2	2:H:262:GLU:H	2.10	0.64
2:I:1782:THR:HG22	2:I:1827:LEU:HD21	1.78	0.64
1:C:604:ALA:HB3	1:C:612:GLU:HG2	1.80	0.64
2:H:1205:LEU:O	2:H:1206:LYS:HG3	1.97	0.64
2:H:1719:ILE:O	2:H:1761:SER:HB2	1.97	0.64
2:I:1355:ASN:HA	2:I:1407:THR:O	1.96	0.64
1:A:746:GLU:O	1:A:750:GLU:HG3	1.97	0.64
1:B:254:TRP:CH2	1:B:292:GLN:HG3	2.32	0.64
2:G:1054:LEU:HB2	3:G:3051:FMN:HM72	1.78	0.64
2:I:1266:TYR:CB	2:I:1347:LEU:HD23	2.28	0.64
2:I:826:GLY:HA3	2:I:1061:GLN:HB3	1.79	0.64
1:A:1693:ILE:CD1	2:G:998:GLN:HB2	2.25	0.64
2:H:658:MET:HA	2:H:661:TRP:NE1	2.13	0.64
2:I:1741:ILE:HG12	2:I:1746:LEU:HD13	1.80	0.64
1:A:1022:THR:HG22	1:A:1226:SER:HB2	1.80	0.64
1:A:1317:GLU:OE1	1:A:1317:GLU:HA	1.96	0.64
1:A:330:GLU:HA	1:A:333:LYS:HD2	1.80	0.64
1:C:883:ILE:HD12	1:C:947:LEU:HD12	1.80	0.64
2:G:1086:LEU:HG	2:G:1092:ASP:HA	1.77	0.64
2:G:159:ILE:HD11	2:G:512:LEU:HG	1.80	0.64
2:G:1986:LYS:N	2:G:1987:PRO:HD2	2.12	0.64
2:H:598:THR:CG2	2:H:622:GLY:HA3	2.28	0.64
2:I:816:ASP:HB3	2:I:1048:VAL:HG21	1.79	0.64
1:C:1317:GLU:HA	1:C:1317:GLU:OE1	1.96	0.64
2:H:1457:PHE:CZ	2:H:1501:ILE:HD11	2.32	0.64
2:H:259:THR:HG23	2:H:262:GLU:H	1.63	0.64
2:H:871:THR:HB	2:H:872:ILE:HD12	1.80	0.64
2:I:259:THR:CG2	2:I:262:GLU:H	2.11	0.64
2:I:719:ILE:O	2:I:722:ALA:HB3	1.97	0.64
2:G:259:THR:CG2	2:G:262:GLU:H	2.10	0.64
2:H:1266:TYR:CB	2:H:1347:LEU:HD23	2.28	0.64
2:I:184:VAL:HG13	2:I:187:LEU:HD21	1.80	0.64
2:I:892:ILE:HD11	2:I:903:TRP:NE1	2.12	0.64
1:A:331:ILE:CD1	1:C:332:THR:HG22	2.28	0.64
2:G:1422:THR:CG2	2:G:1474:PHE:HB2	2.27	0.64
2:G:641:ILE:HG12	2:G:645:SER:HB2	1.80	0.64
2:I:648:GLY:HA3	2:I:678:PHE:CE2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:ASP:CB	1:A:508:ASN:H	2.10	0.64
1:B:733:ILE:HD13	1:B:761:LEU:HD11	1.78	0.64
1:B:980:VAL:H	2:H:968:GLN:HE22	1.45	0.64
1:C:436:ALA:O	1:C:440:MET:HG3	1.98	0.64
2:G:1205:LEU:O	2:G:1206:LYS:HG3	1.98	0.64
2:I:1103:PHE:O	2:I:1247:GLY:HA3	1.98	0.64
1:C:12:ILE:HD11	2:I:2041:ILE:CD1	2.27	0.64
1:C:1312:VAL:HG22	1:C:1329:VAL:HG11	1.78	0.63
1:C:1474:ALA:HA	1:C:1478:PRO:CG	2.27	0.63
2:G:1906:ALA:O	2:G:1910:VAL:HG23	1.97	0.63
2:G:259:THR:OG1	2:G:260:PRO:HD2	1.98	0.63
2:H:1352:HIS:CD2	2:H:1410:PHE:CE2	2.85	0.63
2:H:1874:VAL:O	2:H:1878:VAL:HG12	1.98	0.63
2:H:601:THR:CG2	2:H:618:GLU:O	2.38	0.63
2:H:732:TRP:CG	2:H:750:MET:HE1	2.32	0.63
2:I:1195:VAL:HG13	2:I:1211:LEU:HB3	1.79	0.63
2:I:1381:VAL:HG13	2:I:1390:VAL:HG22	1.79	0.63
2:I:1740:THR:HG22	2:I:1742:VAL:HG23	1.79	0.63
1:B:330:GLU:HA	1:B:333:LYS:HD2	1.80	0.63
1:B:529:MET:HG3	1:B:638:LEU:HG	1.80	0.63
2:H:85:ASN:ND2	2:H:135:ARG:HH11	1.96	0.63
2:H:1859:PRO:O	2:H:1862:VAL:HG13	1.98	0.63
2:H:232:LEU:O	2:H:232:LEU:HD23	1.98	0.63
2:H:667:LYS:HB2	2:H:698:LEU:HD23	1.79	0.63
2:I:1194:VAL:HG12	2:I:1194:VAL:O	1.99	0.63
2:I:1819:ALA:HA	2:I:2005:ARG:HH11	1.61	0.63
2:I:259:THR:OG1	2:I:260:PRO:HD2	1.98	0.63
2:I:490:TRP:HE1	2:I:516:THR:CG2	2.00	0.63
2:I:670:ARG:HD3	2:I:699:GLY:O	1.98	0.63
1:C:158:LYS:HD3	1:C:185:GLU:HB3	1.79	0.63
2:G:648:GLY:HA3	2:G:678:PHE:CE2	2.33	0.63
2:G:726:PHE:O	2:G:762:ASN:HB2	1.98	0.63
2:I:115:THR:HB	2:I:118:LYS:HB2	1.80	0.63
2:I:1859:PRO:O	2:I:1862:VAL:HG13	1.98	0.63
1:A:421:ILE:CG1	1:A:469:VAL:HG21	2.27	0.63
2:G:835:THR:CB	2:G:845:THR:HG23	2.28	0.63
2:H:1168:ASN:ND2	2:H:1171:ARG:HB2	2.14	0.63
2:H:353:VAL:HG23	2:H:357:ASN:ND2	2.13	0.63
2:I:964:LEU:CD2	2:I:964:LEU:H	2.11	0.63
1:A:1194:ASN:HB3	1:A:1197:THR:CG2	2.28	0.63
1:A:1308:SER:HB3	1:A:1589:GLY:HA3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1292:ILE:CD1	1:A:1328:ILE:HD11	2.28	0.63
1:A:436:ALA:O	1:A:440:MET:HG3	1.99	0.63
1:A:460:GLU:HG2	1:A:470:LYS:HD3	1.79	0.63
1:C:680:ILE:HG13	1:C:769:ILE:HB	1.80	0.63
2:H:131:ILE:HB	2:H:182:VAL:HG11	1.81	0.63
2:H:33:LEU:HD11	2:H:80:PHE:HD2	1.63	0.63
2:I:1159:ILE:CG1	2:I:1169:PRO:HD3	2.28	0.63
2:I:131:ILE:HB	2:I:182:VAL:HG11	1.79	0.63
2:I:56:THR:HG23	2:I:59:GLU:CG	2.28	0.63
1:B:488:PRO:HG3	1:B:728:LYS:HG3	1.78	0.63
1:C:1431:GLU:HG3	1:C:1433:HIS:CE1	2.33	0.63
2:G:1673:GLU:H	2:G:1676:MET:HE3	1.62	0.63
2:H:856:LYS:NZ	2:H:1052:CYS:SG	2.70	0.63
2:H:1176:PRO:O	2:H:1177:SER:HB3	1.97	0.63
1:A:1461:ASP:O	1:A:1465:ASN:HB2	1.99	0.63
1:B:1540:SER:HA	1:B:1575:VAL:HG22	1.81	0.63
1:C:1039:MET:O	1:C:1609:ARG:NH2	2.31	0.63
1:C:254:TRP:CH2	1:C:292:GLN:HG3	2.34	0.63
1:C:742:LYS:HD3	1:C:746:GLU:OE2	1.98	0.63
2:G:1266:TYR:CB	2:G:1347:LEU:HD23	2.29	0.63
2:G:138:ASP:O	2:G:139:LYS:HG3	1.99	0.63
1:A:11:HIS:ND1	2:G:1998:LYS:HA	2.13	0.63
2:G:1808:SER:H	2:G:2013:ASN:HD21	1.47	0.63
2:G:2022:THR:HG23	2:G:2025:TYR:H	1.63	0.63
2:G:99:ASN:HA	2:G:550:VAL:CG2	2.28	0.63
2:H:1004:LEU:HD21	2:H:1020:VAL:HG23	1.81	0.63
2:H:1931:LEU:HD22	2:H:1935:GLU:HG2	1.81	0.63
2:I:2022:THR:HG23	2:I:2025:TYR:H	1.63	0.63
1:B:1219:VAL:HA	1:B:1384:ILE:CD1	2.24	0.63
1:C:1292:ILE:HD11	1:C:1328:ILE:HD11	1.81	0.63
1:C:956:ALA:O	1:C:959:ILE:HG22	1.99	0.63
2:G:7:ARG:HE	2:G:27:PHE:HB2	1.63	0.63
2:G:545:GLN:H	2:G:545:GLN:HE21	1.46	0.63
2:H:100:ASP:OD2	2:H:102:HIS:HD2	1.82	0.63
2:H:1672:GLN:HA	2:H:1676:MET:HE1	1.79	0.63
2:I:259:THR:HG23	2:I:262:GLU:H	1.64	0.63
1:A:158:LYS:HD3	1:A:185:GLU:HB3	1.81	0.63
1:A:1721:ARG:NH1	1:A:1721:ARG:HG2	1.97	0.63
1:B:504:ASP:HB2	1:B:508:ASN:HB2	1.79	0.63
2:G:241:ILE:HG23	2:G:506:PRO:HG3	1.80	0.63
2:H:115:THR:HB	2:H:118:LYS:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1195:VAL:HG13	2:H:1211:LEU:HB3	1.79	0.63
2:H:1475:LYS:CG	2:H:1481:SER:HB2	2.29	0.63
2:I:1457:PHE:CZ	2:I:1501:ILE:HD11	2.33	0.63
2:I:1890:ASN:HB2	2:I:1899:VAL:HB	1.81	0.63
1:B:444:ASN:HB3	1:B:446:ALA:H	1.63	0.62
2:G:943:TRP:CH2	2:G:1016:PRO:HG3	2.34	0.62
2:G:1103:PHE:O	2:G:1247:GLY:HA3	1.99	0.62
2:H:1149:TRP:CD1	2:H:1213:LEU:HD12	2.34	0.62
2:H:1808:SER:H	2:H:2013:ASN:HD21	1.46	0.62
2:H:741:HIS:CB	2:H:853:PRO:HB2	2.29	0.62
2:H:750:MET:HG3	2:H:796:PHE:HZ	1.64	0.62
2:I:1808:SER:H	2:I:2013:ASN:HD21	1.47	0.62
1:B:836:ASP:HB3	1:B:839:TYR:HB3	1.79	0.62
1:C:330:GLU:HA	1:C:333:LYS:HD2	1.79	0.62
2:G:1672:GLN:HA	2:G:1676:MET:HE1	1.81	0.62
2:G:324:LEU:HD12	2:G:328:LEU:HG	1.81	0.62
2:H:1675:GLY:O	2:H:1678:MET:HB2	1.99	0.62
2:H:251:VAL:O	2:H:255:LEU:HB2	1.99	0.62
2:I:641:ILE:HG12	2:I:645:SER:HB2	1.79	0.62
1:A:1523:ARG:CG	1:A:1523:ARG:NH1	2.57	0.62
2:H:7:ARG:HE	2:H:27:PHE:HB2	1.64	0.62
1:B:1455:ARG:HH11	1:B:1458:GLN:HE21	1.47	0.62
1:C:985:ARG:HH12	2:I:953:ARG:NH2	1.97	0.62
2:G:490:TRP:O	2:G:494:THR:HG22	1.98	0.62
2:I:1472:VAL:HG22	2:I:1483:VAL:HG22	1.81	0.62
2:I:159:ILE:HD11	2:I:512:LEU:HG	1.80	0.62
2:I:1823:SER:OG	2:I:1825:GLU:HG2	2.00	0.62
2:I:1868:GLN:HG3	2:I:1898:TYR:OH	1.99	0.62
2:I:846:VAL:HG13	2:I:865:TRP:NE1	2.15	0.62
1:A:152:HIS:HD2	1:A:163:LEU:HB2	1.61	0.62
2:G:115:THR:HB	2:G:118:LYS:HB2	1.81	0.62
2:G:1819:ALA:HA	2:G:2005:ARG:HH11	1.65	0.62
2:H:1906:ALA:O	2:H:1910:VAL:HG23	1.98	0.62
1:C:1523:ARG:CG	1:C:1523:ARG:NH1	2.57	0.62
1:C:529:MET:CG	1:C:638:LEU:HG	2.30	0.62
1:C:824:LEU:HD12	1:C:846:LEU:HB3	1.82	0.62
2:G:251:VAL:O	2:G:255:LEU:HB2	1.99	0.62
2:H:159:ILE:HD11	2:H:512:LEU:HG	1.82	0.62
2:I:667:LYS:HB2	2:I:698:LEU:HD23	1.82	0.62
1:A:529:MET:HE1	1:A:894:ARG:HD2	1.80	0.62
1:B:1056:ILE:HD13	1:B:1193:TRP:HD1	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1721:ARG:NH1	1:B:1721:ARG:HG2	2.00	0.62
2:G:33:LEU:HD11	2:G:80:PHE:CD2	2.35	0.62
2:H:33:LEU:HD11	2:H:80:PHE:CD2	2.35	0.62
1:A:705:VAL:HG23	1:A:732:LEU:HD21	1.82	0.62
1:A:956:ALA:O	1:A:959:ILE:HG22	1.98	0.62
1:B:27:ARG:HD2	1:B:30:GLU:OE2	2.00	0.62
2:H:601:THR:O	2:H:601:THR:HG22	2.00	0.62
2:I:464:ASP:HB3	2:I:466:SER:HB3	1.80	0.62
1:B:1594:ASN:O	1:B:1598:GLN:HG3	2.00	0.62
2:G:1859:PRO:O	2:G:1862:VAL:HG13	1.99	0.62
2:H:1374:THR:HG23	2:H:1396:LEU:HD12	1.81	0.62
1:B:1292:ILE:HD11	1:B:1328:ILE:HD11	1.82	0.62
1:B:198:PRO:CG	1:B:209:LEU:HD21	2.26	0.62
2:G:1360:ILE:HG23	2:G:1403:VAL:O	1.99	0.62
2:G:607:VAL:HA	2:G:617:ILE:HD13	1.82	0.62
2:G:719:ILE:O	2:G:722:ALA:HB3	2.00	0.62
2:H:1673:GLU:H	2:H:1676:MET:HE3	1.63	0.62
1:A:1326:ILE:HG12	1:A:1388:MET:HG3	1.82	0.61
1:A:644:THR:HG23	1:A:648:ASP:H	1.65	0.61
1:A:749:ILE:CD1	1:A:805:CYS:HB3	2.29	0.61
1:A:824:LEU:HD12	1:A:846:LEU:HB3	1.80	0.61
1:B:340:ARG:HH12	1:B:344:GLN:CG	2.13	0.61
1:C:992:PHE:CE2	1:C:1399:PRO:HG3	2.36	0.61
1:C:644:THR:HG23	1:C:648:ASP:H	1.65	0.61
2:H:490:TRP:O	2:H:494:THR:HG22	2.00	0.61
2:H:589:ARG:HB3	2:H:590:PRO:HD2	1.82	0.61
2:H:892:ILE:HD11	2:H:903:TRP:NE1	2.14	0.61
1:B:604:ALA:HB3	1:B:612:GLU:HG2	1.82	0.61
1:C:504:ASP:CB	1:C:508:ASN:H	2.13	0.61
2:G:741:HIS:CE1	2:G:855:HIS:CE1	2.88	0.61
2:H:174:ARG:NH2	2:H:225:THR:OG1	2.33	0.61
2:I:1624:THR:HB	2:I:1642:THR:HG23	1.81	0.61
2:I:241:ILE:HG23	2:I:506:PRO:HG3	1.81	0.61
2:I:33:LEU:HD11	2:I:80:PHE:HD2	1.65	0.61
1:A:1455:ARG:HH11	1:A:1458:GLN:HE21	1.47	0.61
1:B:1292:ILE:CD1	1:B:1328:ILE:HD11	2.30	0.61
1:B:1555:ALA:HA	1:B:1621:PHE:CE1	2.36	0.61
1:C:233:ILE:HD13	1:C:237:MET:CE	2.30	0.61
1:C:529:MET:HG3	1:C:638:LEU:HG	1.83	0.61
1:C:881:ASN:HA	1:C:944:ARG:HH21	1.64	0.61
2:G:1719:ILE:O	2:G:1761:SER:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:745:ASP:HA	2:G:832:TRP:HH2	1.64	0.61
2:G:85:ASN:ND2	2:G:135:ARG:HH11	1.97	0.61
2:H:1086:LEU:HD12	2:H:1090:TYR:HB2	1.83	0.61
2:H:315:PRO:O	2:I:1314:ARG:NH2	2.33	0.61
2:H:353:VAL:HG23	2:H:357:ASN:HD22	1.65	0.61
1:C:24:SER:CB	2:I:2014:LEU:HD12	2.30	0.61
2:I:565:TYR:CZ	2:I:758:ARG:HD2	2.35	0.61
1:B:411:GLN:HE22	1:B:1628:SER:H	1.47	0.61
1:B:421:ILE:HG13	1:B:469:VAL:HG21	1.81	0.61
2:G:1004:LEU:HD21	2:G:1020:VAL:HG23	1.82	0.61
2:G:1359:MET:HA	2:G:1359:MET:HE3	1.81	0.61
2:G:1908:ASP:HB2	2:G:1958:LEU:HD21	1.81	0.61
2:H:1624:THR:HB	2:H:1642:THR:HG23	1.82	0.61
2:H:1496:LYS:HE2	2:H:1693:ARG:HH21	1.65	0.61
2:H:603:SER:O	2:H:607:VAL:HG12	2.01	0.61
2:I:1325:PHE:CZ	2:I:1328:VAL:HG11	2.36	0.61
1:A:232:LEU:HD22	1:A:269:LEU:HA	1.83	0.61
1:A:32:GLN:HA	1:A:35:PHE:CE2	2.35	0.61
1:A:822:VAL:HG12	1:A:824:LEU:HD22	1.82	0.61
2:G:1931:LEU:HD22	2:G:1935:GLU:HG2	1.82	0.61
2:I:835:THR:HG21	2:I:855:HIS:NE2	2.14	0.61
1:B:1194:ASN:HB3	1:B:1197:THR:CG2	2.30	0.61
2:G:174:ARG:NH2	2:G:225:THR:OG1	2.34	0.61
2:G:522:GLY:HA3	2:G:561:TRP:CZ3	2.35	0.61
2:I:1054:LEU:HB2	3:I:3051:FMN:C7M	2.30	0.61
1:A:1103:ILE:HD11	1:A:1582:GLY:N	2.16	0.61
1:B:1523:ARG:CG	1:B:1523:ARG:NH1	2.59	0.61
1:C:1540:SER:HA	1:C:1575:VAL:HG22	1.82	0.61
2:I:1906:ALA:O	2:I:1910:VAL:HG23	2.00	0.61
2:I:745:ASP:HA	2:I:832:TRP:HH2	1.65	0.61
1:A:1259:GLY:HA2	1:A:1263:ASP:HB2	1.81	0.61
1:B:1021:VAL:HG11	1:B:1597:LEU:HD11	1.83	0.61
1:B:400:ARG:HH11	1:B:400:ARG:HG3	1.64	0.61
1:C:1308:SER:HB3	1:C:1589:GLY:HA3	1.80	0.61
1:C:529:MET:CE	1:C:894:ARG:HD2	2.30	0.61
2:I:1101:GLU:HB2	2:I:1147:ILE:O	2.00	0.61
1:B:1052:GLU:O	1:B:1056:ILE:HG23	2.00	0.61
1:B:158:LYS:HD3	1:B:185:GLU:HB3	1.82	0.61
1:B:631:PRO:HB2	1:B:634:THR:OG1	2.00	0.61
2:G:1782:THR:HG22	2:G:1827:LEU:HD21	1.81	0.61
2:H:597:MET:HA	3:H:3051:FMN:N5	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1227:ARG:HD2	2:I:1565:VAL:HG11	1.81	0.61
2:I:1355:ASN:CB	2:I:1583:MET:HE1	2.31	0.61
2:I:1822:MET:HE2	2:I:1996:ILE:HG12	1.83	0.61
2:I:33:LEU:HD11	2:I:80:PHE:CD2	2.36	0.61
2:I:663:ILE:HG13	2:I:694:TYR:HE1	1.66	0.61
2:I:860:ARG:HB3	2:I:898:ASP:HB3	1.81	0.61
1:B:1431:GLU:HG3	1:B:1433:HIS:CE1	2.36	0.61
2:G:871:THR:HB	2:G:872:ILE:HD12	1.82	0.61
2:I:1086:LEU:HD12	2:I:1090:TYR:HB2	1.82	0.61
2:I:835:THR:HG22	2:I:845:THR:N	2.16	0.61
1:A:1292:ILE:HD11	1:A:1328:ILE:HD11	1.81	0.60
1:C:444:ASN:HB3	1:C:446:ALA:H	1.65	0.60
1:C:599:MET:HB2	1:C:624:LYS:CD	2.25	0.60
1:C:635:ILE:HG22	1:C:651:TYR:CG	2.36	0.60
2:G:601:THR:O	2:G:601:THR:HG22	2.01	0.60
2:H:260:PRO:HD3	2:H:289:TRP:CE2	2.36	0.60
1:B:644:THR:HG23	1:B:648:ASP:H	1.65	0.60
1:C:504:ASP:HB2	1:C:508:ASN:HB2	1.81	0.60
1:C:980:VAL:HG21	2:I:952:ARG:HH21	1.65	0.60
2:G:1378:ILE:HD11	2:G:1381:VAL:CG2	2.30	0.60
2:I:932:ILE:HD11	2:I:1042:ALA:CB	2.25	0.60
1:A:12:ILE:HD11	2:G:2041:ILE:CD1	2.30	0.60
1:B:1062:TYR:CD2	1:B:1693:ILE:HG23	2.36	0.60
1:C:1492:GLU:O	1:C:1496:GLU:HG3	2.01	0.60
1:C:340:ARG:HH12	1:C:344:GLN:CG	2.14	0.60
1:C:705:VAL:HG23	1:C:732:LEU:HD21	1.82	0.60
2:G:1086:LEU:HD12	2:G:1090:TYR:HB2	1.83	0.60
2:G:1123:ASP:N	2:G:1123:ASP:OD1	2.34	0.60
2:G:1805:ALA:HB2	2:G:2011:ILE:HB	1.84	0.60
2:G:598:THR:CG2	2:G:622:GLY:HA3	2.30	0.60
2:H:499:THR:CB	2:H:500:HIS:CD2	2.81	0.60
2:I:1805:ALA:HB2	2:I:2011:ILE:HB	1.82	0.60
2:I:741:HIS:CE1	2:I:845:THR:HG21	2.35	0.60
1:B:1184:LEU:HB2	1:B:1352:THR:HG21	1.83	0.60
1:B:956:ALA:O	1:B:959:ILE:HG22	2.02	0.60
1:C:1057:MET:SD	1:C:1097:ILE:HG23	2.40	0.60
2:G:1195:VAL:HG13	2:G:1211:LEU:HB3	1.84	0.60
2:G:1325:PHE:CZ	2:G:1328:VAL:HG11	2.37	0.60
2:G:1739:GLU:O	2:G:1987:PRO:HG3	2.00	0.60
2:G:271:THR:OG1	2:G:460:TYR:HB2	2.01	0.60
2:G:443:LEU:HD22	2:G:448:VAL:HG11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:526:ARG:HH11	2:G:558:ASN:HD21	1.49	0.60
2:I:1374:THR:HG23	2:I:1396:LEU:HD12	1.84	0.60
1:B:233:ILE:HD13	1:B:237:MET:HE2	1.83	0.60
1:C:1544:THR:O	1:C:1545:SER:HB3	2.02	0.60
1:C:198:PRO:CG	1:C:209:LEU:HD21	2.28	0.60
1:C:822:VAL:HG12	1:C:824:LEU:HD22	1.82	0.60
2:G:1472:VAL:HG22	2:G:1483:VAL:HG22	1.83	0.60
2:G:846:VAL:HG13	2:G:865:TRP:NE1	2.16	0.60
2:H:814:SER:HB2	2:H:1040:LEU:HD13	1.83	0.60
2:H:324:LEU:HD12	2:H:328:LEU:HG	1.84	0.60
2:H:455:ILE:HG13	2:H:469:ARG:HD3	1.83	0.60
2:H:241:ILE:HG23	2:H:506:PRO:HG3	1.83	0.60
2:I:100:ASP:OD2	2:I:102:HIS:HD2	1.83	0.60
2:I:1173:VAL:O	2:I:1567:ARG:NH2	2.35	0.60
2:I:1360:ILE:HG23	2:I:1403:VAL:O	2.01	0.60
2:I:324:LEU:HD12	2:I:328:LEU:HG	1.82	0.60
2:I:732:TRP:CD2	2:I:750:MET:CE	2.84	0.60
1:A:635:ILE:HG22	1:A:651:TYR:CG	2.36	0.60
1:B:221:LEU:O	1:B:225:SER:HB3	2.02	0.60
1:B:680:ILE:HG13	1:B:769:ILE:HB	1.83	0.60
1:B:80:CYS:SG	1:B:82:SER:HB3	2.42	0.60
2:G:1834:ARG:HH11	2:G:1834:ARG:CG	2.02	0.60
1:A:980:VAL:HG21	2:G:952:ARG:HH21	1.64	0.60
2:H:1219:ILE:HD11	2:H:1242:PHE:HB2	1.83	0.60
2:H:197:GLU:HA	2:H:197:GLU:OE1	2.02	0.60
2:H:1739:GLU:O	2:H:1987:PRO:HG3	2.02	0.60
2:H:565:TYR:CZ	2:H:758:ARG:HD2	2.35	0.60
2:H:745:ASP:HA	2:H:832:TRP:HH2	1.66	0.60
2:I:1198:SER:HB3	2:I:1205:LEU:HD21	1.82	0.60
2:I:1205:LEU:O	2:I:1206:LYS:HG3	2.00	0.60
1:A:1194:ASN:O	1:A:1197:THR:HG23	2.02	0.60
1:C:1194:ASN:O	1:C:1197:THR:HG23	2.01	0.60
2:G:1355:ASN:CB	2:G:1583:MET:HE1	2.32	0.60
2:G:184:VAL:HG13	2:G:187:LEU:HD21	1.84	0.60
2:G:907:VAL:O	2:G:910:GLN:HB3	2.02	0.60
2:I:1874:VAL:O	2:I:1878:VAL:HG12	2.02	0.60
1:B:992:PHE:CD2	1:B:1399:PRO:HG3	2.37	0.60
1:C:1009:LEU:HD13	1:C:1445:MET:HE1	1.83	0.60
1:C:1062:TYR:CD2	1:C:1693:ILE:HG23	2.37	0.60
1:C:221:LEU:O	1:C:225:SER:HB3	2.02	0.60
1:C:531:LEU:HD21	1:C:629:THR:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:100:ASP:OD2	2:G:102:HIS:HD2	1.85	0.60
2:G:61:VAL:HG21	2:G:95:TYR:HE1	1.67	0.60
2:H:1103:PHE:O	2:H:1247:GLY:HA3	2.02	0.60
2:H:1198:SER:HB3	2:H:1205:LEU:HD21	1.83	0.60
2:I:1986:LYS:N	2:I:1987:PRO:HD2	2.17	0.60
1:A:529:MET:HG3	1:A:638:LEU:HG	1.84	0.60
1:B:1259:GLY:HA2	1:B:1263:ASP:HB2	1.84	0.60
1:B:824:LEU:HD12	1:B:846:LEU:HB3	1.82	0.60
1:C:749:ILE:CD1	1:C:805:CYS:HB3	2.32	0.60
2:G:762:ASN:H	2:G:762:ASN:ND2	1.85	0.60
2:H:652:ILE:N	2:H:658:MET:HE3	2.13	0.60
2:H:663:ILE:HG13	2:H:694:TYR:HE1	1.67	0.60
2:H:817:ALA:O	2:H:821:ILE:HG13	2.02	0.60
2:H:860:ARG:HB3	2:H:898:ASP:HB3	1.83	0.60
2:I:1719:ILE:O	2:I:1761:SER:HB2	2.01	0.60
2:I:732:TRP:CD2	2:I:750:MET:HE1	2.37	0.60
1:C:1304:ALA:O	1:C:1307:THR:HG23	2.02	0.60
1:C:1662:TYR:O	1:C:1665:ILE:HG22	2.01	0.60
2:G:565:TYR:CZ	2:G:758:ARG:HD2	2.37	0.60
2:G:892:ILE:HD11	2:G:903:TRP:NE1	2.17	0.60
2:H:1805:ALA:HB2	2:H:2011:ILE:HB	1.82	0.60
2:H:1054:LEU:HB2	3:H:3051:FMN:C7M	2.31	0.60
2:H:490:TRP:HE1	2:H:516:THR:CG2	2.01	0.60
2:I:1123:ASP:OD1	2:I:1123:ASP:N	2.35	0.60
2:I:1149:TRP:CD1	2:I:1213:LEU:HD12	2.37	0.60
2:I:674:TYR:HB3	2:I:676:ILE:HG22	1.84	0.60
2:I:762:ASN:HD22	2:I:762:ASN:N	1.88	0.60
1:A:440:MET:HE3	1:A:483:VAL:HG21	1.84	0.59
1:B:1057:MET:SD	1:B:1097:ILE:HG23	2.42	0.59
1:C:80:CYS:SG	1:C:82:SER:HB3	2.42	0.59
2:H:846:VAL:HG13	2:H:865:TRP:NE1	2.17	0.59
2:I:402:LEU:HD13	2:I:402:LEU:O	2.02	0.59
2:I:817:ALA:O	2:I:821:ILE:HG13	2.01	0.59
1:B:1657:HIS:ND1	1:B:1658:PRO:HD2	2.17	0.59
2:G:747:HIS:HE1	2:G:780:TYR:OH	1.84	0.59
2:I:1004:LEU:HD21	2:I:1020:VAL:HG23	1.84	0.59
1:A:233:ILE:HD13	1:A:237:MET:CE	2.32	0.59
1:B:1360:ARG:HH11	1:B:1364:GLU:HG2	1.66	0.59
1:B:989:GLN:NE2	2:H:993:GLN:OE1	2.35	0.59
1:C:152:HIS:HD2	1:C:163:LEU:HB2	1.63	0.59
1:C:232:LEU:HD22	1:C:269:LEU:HA	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:750:MET:HG3	2:G:796:PHE:HZ	1.65	0.59
2:H:1378:ILE:HD11	2:H:1381:VAL:HG21	1.84	0.59
2:I:942:THR:HG21	2:I:1012:GLN:HA	1.85	0.59
2:I:1352:HIS:CD2	2:I:1410:PHE:CE2	2.89	0.59
2:I:601:THR:HG22	2:I:601:THR:O	2.02	0.59
2:I:658:MET:HA	2:I:661:TRP:NE1	2.17	0.59
1:A:1304:ALA:O	1:A:1307:THR:HG23	2.03	0.59
1:A:1524:GLY:O	1:A:1528:THR:HG23	2.03	0.59
1:A:251:GLN:HA	1:A:256:LEU:H	1.68	0.59
1:A:417:TYR:OH	1:A:458:THR:HG22	2.02	0.59
1:B:1392:LEU:HD22	1:B:1396:MET:HG3	1.84	0.59
1:C:980:VAL:HG23	2:I:968:GLN:OE1	2.02	0.59
2:G:1223:MET:HE3	2:G:1238:LEU:HD12	1.84	0.59
2:I:839:PRO:HA	2:I:844:VAL:HG13	1.83	0.59
1:A:50:SER:HB2	1:A:51:PRO:HD3	1.85	0.59
1:B:233:ILE:HD13	1:B:237:MET:CE	2.32	0.59
1:B:504:ASP:CB	1:B:508:ASN:H	2.15	0.59
1:C:421:ILE:CG1	1:C:469:VAL:HG21	2.32	0.59
2:G:2038:ILE:O	2:G:2042:ILE:HG12	2.02	0.59
2:G:597:MET:HA	3:G:3051:FMN:N5	2.17	0.59
2:G:732:TRP:CD2	2:G:750:MET:CE	2.85	0.59
2:G:926:LEU:HD13	2:G:947:THR:HG22	1.83	0.59
2:H:184:VAL:HG13	2:H:187:LEU:HD21	1.83	0.59
2:H:99:ASN:HA	2:H:550:VAL:CG2	2.32	0.59
2:I:1567:ARG:CG	2:I:1567:ARG:NH1	2.50	0.59
1:A:12:ILE:HD11	2:G:2041:ILE:HD12	1.82	0.59
1:A:37:LYS:HB2	1:A:65:TYR:HE1	1.67	0.59
1:A:989:GLN:NE2	2:G:993:GLN:OE1	2.36	0.59
1:B:1461:ASP:O	1:B:1465:ASN:HB2	2.03	0.59
1:B:1474:ALA:O	1:B:1478:PRO:HD2	2.03	0.59
1:C:1461:ASP:O	1:C:1465:ASN:HB2	2.02	0.59
1:C:1657:HIS:ND1	1:C:1658:PRO:HD2	2.17	0.59
1:C:1:MET:HE3	1:C:5:VAL:HG12	1.84	0.59
2:H:719:ILE:O	2:H:722:ALA:HB3	2.02	0.59
2:I:163:GLN:CG	2:I:423:VAL:HG12	2.32	0.59
2:I:490:TRP:O	2:I:494:THR:HG22	2.03	0.59
1:A:1432:HIS:CE1	1:A:1434:SER:OG	2.56	0.59
1:B:1119:LYS:HE2	1:B:1341:PHE:CG	2.38	0.59
1:C:1555:ALA:HA	1:C:1621:PHE:CE1	2.38	0.59
1:C:421:ILE:HG13	1:C:469:VAL:HG21	1.85	0.59
2:G:594:VAL:HG21	2:G:610:THR:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:163:GLN:CG	2:H:423:VAL:HG12	2.32	0.59
2:I:127:ILE:O	2:I:131:ILE:HG13	2.03	0.59
1:B:1308:SER:HB3	1:B:1589:GLY:HA3	1.83	0.59
2:G:232:LEU:HD23	2:G:232:LEU:O	2.03	0.59
2:G:754:TYR:CD2	2:G:794:MET:HG3	2.38	0.59
2:H:1265:MET:CE	2:H:1562:PRO:HG2	2.31	0.59
2:H:1844:ARG:CG	2:H:1844:ARG:NH1	2.58	0.59
2:H:2038:ILE:O	2:H:2042:ILE:HG12	2.03	0.59
2:H:726:PHE:O	2:H:762:ASN:HB2	2.03	0.59
2:I:1908:ASP:HB2	2:I:1958:LEU:HD21	1.83	0.59
2:I:589:ARG:HB3	2:I:590:PRO:HD2	1.83	0.59
1:B:32:GLN:HA	1:B:35:PHE:CE2	2.38	0.59
1:B:413:LEU:HD13	1:B:451:MET:HG2	1.85	0.59
1:A:2:LYS:CD	2:G:2050:GLN:HB3	2.24	0.59
2:G:402:LEU:HD13	2:G:402:LEU:O	2.03	0.59
2:I:1210:ILE:HB	2:I:1222:GLU:HB3	1.85	0.59
1:C:20:TYR:CE1	2:I:2035:SER:HB2	2.38	0.59
2:I:174:ARG:NH2	2:I:225:THR:OG1	2.36	0.59
2:I:762:ASN:ND2	2:I:762:ASN:H	1.88	0.59
2:G:1823:SER:OG	2:G:1825:GLU:HG2	2.03	0.59
2:H:1314:ARG:NH1	2:H:1314:ARG:CG	2.62	0.59
2:H:813:THR:HB	2:H:818:LYS:HE3	1.84	0.59
2:I:99:ASN:HA	2:I:550:VAL:CG2	2.33	0.59
2:I:601:THR:CG2	2:I:618:GLU:O	2.39	0.59
2:I:813:THR:HB	2:I:818:LYS:HE3	1.85	0.59
1:A:409:ALA:HB2	1:A:442:ARG:HD2	1.84	0.58
1:B:286:PHE:O	1:B:290:MET:HG2	2.03	0.58
1:B:417:TYR:OH	1:B:458:THR:HG22	2.03	0.58
1:C:1233:GLU:OE2	1:C:1680:ARG:NH2	2.36	0.58
1:C:408:TRP:CH2	1:C:1628:SER:HB3	2.38	0.58
1:C:733:ILE:HD12	1:C:761:LEU:HD21	1.85	0.58
2:H:1575:LEU:HD13	2:H:1579:ILE:HD12	1.85	0.58
1:B:980:VAL:HG23	2:H:968:GLN:OE1	2.02	0.58
2:I:1223:MET:HE3	2:I:1238:LEU:HD12	1.85	0.58
1:A:444:ASN:HB3	1:A:446:ALA:H	1.66	0.58
1:B:332:THR:HG22	1:C:331:ILE:CD1	2.33	0.58
2:G:1844:ARG:NH1	2:G:1844:ARG:CG	2.62	0.58
2:H:105:ALA:HB3	2:H:533:LEU:HD21	1.84	0.58
2:H:1149:TRP:CD1	2:H:1213:LEU:CD1	2.85	0.58
2:H:606:PHE:HZ	2:H:805:VAL:HG11	1.68	0.58
2:I:597:MET:HA	3:I:3051:FMN:N5	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1496:GLU:O	1:B:1500:GLN:HG3	2.03	0.58
1:C:1721:ARG:CG	1:C:1721:ARG:NH1	2.56	0.58
2:G:166:THR:HG22	2:G:168:ASP:N	2.19	0.58
2:H:259:THR:OG1	2:H:260:PRO:HD2	2.03	0.58
2:I:736:ARG:NH1	2:I:769:SER:O	2.36	0.58
1:B:1662:TYR:O	1:B:1665:ILE:HG22	2.04	0.58
1:B:599:MET:HB2	1:B:624:LYS:CD	2.24	0.58
1:B:705:VAL:HG23	1:B:732:LEU:HD21	1.85	0.58
1:C:1056:ILE:CD1	1:C:1193:TRP:HD1	2.17	0.58
1:C:989:GLN:NE2	2:I:993:GLN:OE1	2.36	0.58
2:G:1931:LEU:HB3	2:G:1935:GLU:CG	2.33	0.58
2:G:674:TYR:HB3	2:G:676:ILE:HG22	1.85	0.58
2:H:1130:THR:H	2:H:1133:THR:HG23	1.68	0.58
2:H:1101:GLU:HB3	2:H:1147:ILE:HG22	1.86	0.58
2:H:926:LEU:HD13	2:H:947:THR:HG22	1.85	0.58
1:B:985:ARG:HH12	2:H:953:ARG:CZ	2.15	0.58
2:I:856:LYS:NZ	2:I:1052:CYS:SG	2.70	0.58
2:I:1086:LEU:HD12	2:I:1090:TYR:CB	2.33	0.58
2:I:1989:LYS:O	2:I:1993:LYS:HG3	2.02	0.58
2:I:907:VAL:O	2:I:910:GLN:HB3	2.03	0.58
1:A:1544:THR:O	1:A:1545:SER:HB3	2.02	0.58
1:A:11:HIS:O	1:A:15:THR:HG22	2.04	0.58
1:A:232:LEU:HD13	1:A:272:GLU:HB2	1.84	0.58
1:A:435:GLU:O	1:A:439:ILE:HG13	2.02	0.58
1:A:1:MET:HE3	1:A:5:VAL:HG12	1.85	0.58
1:B:232:LEU:HD22	1:B:269:LEU:HA	1.85	0.58
1:B:531:LEU:HD21	1:B:629:THR:HG22	1.84	0.58
1:C:852:ARG:CG	1:C:852:ARG:HH11	2.00	0.58
2:G:1149:TRP:CD1	2:G:1213:LEU:CD1	2.87	0.58
2:G:1597:ALA:HB1	2:G:1638:ILE:CD1	2.33	0.58
2:G:603:SER:O	2:G:607:VAL:HG12	2.03	0.58
2:G:807:ILE:CG2	2:G:1066:ILE:HA	2.34	0.58
2:H:1223:MET:HE3	2:H:1238:LEU:HD12	1.84	0.58
2:H:1360:ILE:HG23	2:H:1403:VAL:O	2.04	0.58
2:H:1589:VAL:HG11	2:H:1640:PHE:CE1	2.39	0.58
2:I:1265:MET:CE	2:I:1562:PRO:HG2	2.33	0.58
2:I:455:ILE:HG13	2:I:469:ARG:HD3	1.85	0.58
2:I:105:ALA:HB3	2:I:533:LEU:HD21	1.84	0.58
1:A:529:MET:CE	1:A:894:ARG:HD2	2.34	0.58
1:B:419:GLU:HG2	1:B:424:VAL:HB	1.86	0.58
1:B:50:SER:HB2	1:B:51:PRO:HD3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:LEU:HD13	1:C:272:GLU:HB2	1.85	0.58
2:G:611:THR:CG2	2:G:641:ILE:HG13	2.34	0.58
2:G:638:VAL:HA	2:G:641:ILE:HG22	1.86	0.58
2:H:1210:ILE:HB	2:H:1222:GLU:HB3	1.85	0.58
2:I:1219:ILE:HD11	2:I:1242:PHE:HB2	1.83	0.58
2:I:145:LEU:O	2:I:149:VAL:HG12	2.03	0.58
2:G:1149:TRP:CD1	2:G:1213:LEU:HD12	2.38	0.58
2:G:634:ILE:HD11	2:G:649:ILE:CD1	2.34	0.58
2:G:835:THR:HG21	2:G:855:HIS:NE2	2.19	0.58
2:H:1871:LEU:HD22	2:H:1888:ILE:HD11	1.85	0.58
2:H:732:TRP:CD2	2:H:750:MET:CE	2.87	0.58
2:H:89:THR:O	2:H:93:ASN:HB2	2.04	0.58
1:A:260:ARG:HH12	1:A:300:VAL:HG21	1.68	0.58
1:B:37:LYS:HB2	1:B:65:TYR:HE1	1.69	0.58
1:B:980:VAL:H	2:H:968:GLN:NE2	2.00	0.58
2:G:1210:ILE:HB	2:G:1222:GLU:HB3	1.85	0.58
2:H:1331:TRP:CE2	2:H:1335:ILE:HG13	2.38	0.58
1:A:992:PHE:CE2	1:A:1399:PRO:HG3	2.39	0.58
1:B:1125:VAL:HG21	1:B:1175:ILE:HD12	1.86	0.58
1:C:1020:VAL:HG13	1:C:1400:ILE:HG23	1.85	0.58
1:C:1665:ILE:HD11	1:C:1669:ARG:HG2	1.85	0.58
2:G:146:PHE:HA	2:G:149:VAL:HG12	1.86	0.58
2:G:260:PRO:HD3	2:G:289:TRP:CE2	2.38	0.58
2:G:56:THR:HG23	2:G:59:GLU:CG	2.29	0.58
2:G:658:MET:HA	2:G:661:TRP:NE1	2.19	0.58
2:G:821:ILE:HA	2:G:857:ILE:HD11	1.84	0.58
2:G:741:HIS:CE1	2:G:845:THR:HG21	2.38	0.58
2:I:1822:MET:CE	2:I:1996:ILE:HG12	2.34	0.58
2:I:1931:LEU:HD22	2:I:1935:GLU:HG2	1.86	0.58
1:A:1062:TYR:CD2	1:A:1693:ILE:HG23	2.39	0.58
2:G:1778:GLN:HB3	2:G:1831:VAL:HG13	1.85	0.58
2:H:1093:ASP:HB3	2:H:1096:LYS:HG3	1.84	0.58
2:H:490:TRP:CH2	2:H:512:LEU:HD21	2.39	0.58
2:H:665:LEU:O	2:H:669:LEU:HB2	2.04	0.58
2:H:907:VAL:O	2:H:910:GLN:HB3	2.03	0.58
2:I:1004:LEU:CD2	2:I:1019:PRO:HB2	2.34	0.58
2:I:239:PRO:HG3	2:I:304:PHE:HA	1.86	0.58
1:A:828:PRO:HG3	1:A:868:ILE:HG22	1.86	0.57
1:B:749:ILE:CD1	1:B:805:CYS:HB3	2.33	0.57
1:C:1052:GLU:O	1:C:1056:ILE:HG23	2.04	0.57
2:G:1822:MET:HE2	2:G:1996:ILE:HG12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1054:LEU:HB2	3:G:3051:FMN:C7M	2.34	0.57
2:G:703:LEU:HD21	2:G:705:LEU:HD21	1.86	0.57
2:G:7:ARG:NH1	2:G:24:THR:HA	2.19	0.57
2:H:127:ILE:O	2:H:131:ILE:HG13	2.04	0.57
2:H:166:THR:HG22	2:H:168:ASP:N	2.19	0.57
1:A:419:GLU:HG2	1:A:424:VAL:HB	1.86	0.57
1:A:635:ILE:HG22	1:A:651:TYR:CD1	2.39	0.57
1:B:1009:LEU:HG	1:B:1664:ALA:HB2	1.87	0.57
1:B:1304:ALA:O	1:B:1307:THR:HG23	2.04	0.57
1:C:341:GLN:O	1:C:345:VAL:HG12	2.04	0.57
1:C:771:PHE:CD1	1:C:825:PRO:HG3	2.40	0.57
2:G:667:LYS:HB2	2:G:698:LEU:HD23	1.85	0.57
2:H:638:VAL:HA	2:H:641:ILE:HG22	1.86	0.57
2:I:1130:THR:H	2:I:1133:THR:HG23	1.69	0.57
2:I:353:VAL:HG23	2:I:357:ASN:ND2	2.19	0.57
2:I:376:ASN:HD22	2:I:377:LEU:N	2.01	0.57
1:B:436:ALA:O	1:B:440:MET:HG3	2.04	0.57
1:C:1184:LEU:HB2	1:C:1352:THR:HG21	1.85	0.57
2:G:1130:THR:H	2:G:1133:THR:HG23	1.70	0.57
2:G:1374:THR:HG23	2:G:1396:LEU:HD12	1.85	0.57
2:G:741:HIS:CB	2:G:853:PRO:HB2	2.34	0.57
2:H:443:LEU:HD22	2:H:448:VAL:HG11	1.86	0.57
2:H:736:ARG:NH1	2:H:769:SER:O	2.36	0.57
2:I:2030:TYR:CE1	2:I:2034:GLY:HA2	2.39	0.57
2:I:499:THR:CB	2:I:500:HIS:CD2	2.79	0.57
1:A:1056:ILE:CD1	1:A:1193:TRP:HD1	2.17	0.57
1:A:233:ILE:HD13	1:A:237:MET:HE2	1.87	0.57
1:A:604:ALA:HB3	1:A:612:GLU:HG2	1.86	0.57
1:B:232:LEU:HD13	1:B:272:GLU:HB2	1.87	0.57
1:C:1600:LEU:HD13	1:C:1657:HIS:HA	1.86	0.57
2:G:1624:THR:HB	2:G:1642:THR:HG23	1.86	0.57
2:G:601:THR:CG2	2:G:618:GLU:O	2.41	0.57
2:G:856:LYS:HG2	2:G:1054:LEU:HD12	1.86	0.57
2:I:726:PHE:O	2:I:762:ASN:HB2	2.04	0.57
1:A:1540:SER:HA	1:A:1575:VAL:HG22	1.86	0.57
1:A:1600:LEU:HD13	1:A:1657:HIS:HA	1.85	0.57
1:A:415:SER:O	1:A:419:GLU:HB2	2.05	0.57
1:A:421:ILE:HG12	1:A:469:VAL:HG21	1.85	0.57
1:A:985:ARG:HH12	2:G:953:ARG:NH2	2.03	0.57
1:B:11:HIS:ND1	2:H:1998:LYS:HA	2.19	0.57
1:B:1234:MET:HG2	1:B:1326:ILE:HD12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1159:ILE:CG1	2:G:1169:PRO:HD3	2.34	0.57
2:G:1293:THR:CG2	2:G:1296:GLU:H	2.14	0.57
2:G:817:ALA:O	2:G:821:ILE:HG13	2.04	0.57
2:H:1010:PRO:O	2:H:1011:MET:HB2	2.03	0.57
2:H:1231:GLY:O	2:H:1233:PRO:HD3	2.04	0.57
2:H:1355:ASN:HB3	2:H:1583:MET:HE1	1.86	0.57
2:H:601:THR:HG22	2:H:620:ALA:H	1.69	0.57
2:H:835:THR:HB	2:H:845:THR:HG23	1.85	0.57
2:H:835:THR:HG22	2:H:845:THR:N	2.20	0.57
1:B:1524:GLY:O	1:B:1528:THR:HG23	2.05	0.57
1:B:408:TRP:CZ3	1:B:1628:SER:HB3	2.40	0.57
1:B:1:MET:HE3	1:B:9:LEU:HD12	1.85	0.57
2:G:1010:PRO:O	2:G:1011:MET:HB2	2.05	0.57
2:G:163:GLN:CG	2:G:423:VAL:HG12	2.34	0.57
2:G:273:HIS:HB3	2:G:512:LEU:HD22	1.86	0.57
2:H:741:HIS:CE1	2:H:855:HIS:NE2	2.73	0.57
2:I:707:PRO:HG2	2:I:730:LEU:HD13	1.85	0.57
1:A:531:LEU:HD21	1:A:629:THR:HG22	1.87	0.57
2:G:1086:LEU:HD12	2:G:1090:TYR:CB	2.35	0.57
2:G:1194:VAL:HG12	2:G:1194:VAL:O	2.05	0.57
2:G:1775:GLN:HG2	2:G:1836:MET:SD	2.44	0.57
2:G:89:THR:O	2:G:93:ASN:HB2	2.05	0.57
2:H:1086:LEU:HD12	2:H:1090:TYR:CB	2.34	0.57
2:H:1123:ASP:OD1	2:H:1123:ASP:N	2.36	0.57
2:H:1782:THR:HG22	2:H:1827:LEU:HD21	1.86	0.57
2:H:543:PHE:CB	2:H:545:GLN:HE22	2.17	0.57
2:I:1931:LEU:HB3	2:I:1935:GLU:CG	2.35	0.57
2:I:2029:VAL:O	2:I:2033:THR:HG22	2.05	0.57
2:I:353:VAL:HG23	2:I:357:ASN:HD22	1.70	0.57
1:B:1022:THR:HG22	1:B:1226:SER:HB2	1.86	0.57
1:B:1538:VAL:HB	1:B:1639:VAL:HG22	1.87	0.57
1:B:440:MET:HE3	1:B:483:VAL:HG21	1.87	0.57
1:C:741:SER:HB3	1:C:744:ASP:HB2	1.86	0.57
2:G:1198:SER:HB3	2:G:1205:LEU:HD21	1.85	0.57
2:G:455:ILE:HG13	2:G:469:ARG:HD3	1.86	0.57
2:G:577:ILE:HD13	2:G:1097:ILE:CD1	2.35	0.57
2:H:273:HIS:HB3	2:H:512:LEU:HD22	1.85	0.57
2:H:517:HIS:CD2	2:H:517:HIS:C	2.78	0.57
2:H:722:ALA:HB1	2:H:723:HIS:CE1	2.38	0.57
1:B:980:VAL:HG21	2:H:952:ARG:NH2	2.19	0.57
2:H:99:ASN:HA	2:H:550:VAL:HG23	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1010:PRO:O	2:I:1011:MET:HB2	2.05	0.57
2:I:814:SER:HB2	2:I:1040:LEU:HD13	1.86	0.57
2:I:1575:LEU:HD13	2:I:1579:ILE:HD12	1.84	0.57
1:A:1057:MET:SD	1:A:1097:ILE:HG23	2.45	0.57
1:A:1474:ALA:O	1:A:1478:PRO:HD2	2.04	0.57
1:B:1431:GLU:HB3	1:B:1520:ALA:HB2	1.87	0.57
1:B:1473:GLU:O	1:B:1478:PRO:HD3	2.04	0.57
1:C:1474:ALA:O	1:C:1478:PRO:HD2	2.05	0.57
1:C:1305:CYS:HB2	1:C:1645:GLY:HA2	1.86	0.57
2:G:1954:LYS:HD3	2:G:1958:LEU:HD13	1.87	0.57
1:C:2:LYS:CD	2:I:2050:GLN:HB3	2.29	0.57
2:I:653:TYR:CD1	2:I:659:LEU:HD21	2.40	0.57
1:A:329:GLU:O	1:A:333:LYS:HG3	2.05	0.57
1:C:251:GLN:HA	1:C:256:LEU:H	1.70	0.57
1:C:433:VAL:O	1:C:437:ILE:HG13	2.04	0.57
2:G:942:THR:HG21	2:G:1012:GLN:HA	1.86	0.57
2:G:1266:TYR:CG	2:G:1347:LEU:HD23	2.40	0.57
2:G:1868:GLN:HG3	2:G:1898:TYR:OH	2.05	0.57
2:G:1989:LYS:O	2:G:1993:LYS:HG3	2.05	0.57
2:G:826:GLY:O	2:G:827:VAL:HG23	2.04	0.57
2:H:2029:VAL:O	2:H:2033:THR:HG22	2.05	0.57
2:H:271:THR:OG1	2:H:460:TYR:HB2	2.03	0.57
2:I:665:LEU:O	2:I:669:LEU:HB2	2.05	0.57
1:A:1538:VAL:HB	1:A:1639:VAL:HG22	1.86	0.56
1:A:400:ARG:HH11	1:A:400:ARG:HG3	1.67	0.56
1:B:251:GLN:HA	1:B:256:LEU:H	1.70	0.56
1:B:409:ALA:HB2	1:B:442:ARG:HD2	1.86	0.56
1:C:1524:GLY:O	1:C:1528:THR:HG23	2.05	0.56
2:G:1561:ASN:OD1	2:G:1563:ILE:HB	2.05	0.56
2:G:499:THR:CB	2:G:500:HIS:CD2	2.80	0.56
2:G:517:HIS:C	2:G:517:HIS:CD2	2.78	0.56
2:G:741:HIS:HE1	2:G:845:THR:HG21	1.69	0.56
2:H:1834:ARG:NH1	2:H:1834:ARG:CG	2.60	0.56
2:H:55:THR:CG2	2:H:56:THR:HG22	2.30	0.56
2:I:1300:PHE:HA	2:I:1556:VAL:HG11	1.87	0.56
2:I:273:HIS:HB3	2:I:512:LEU:HD22	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:634:ILE:HD11	2:I:649:ILE:CD1	2.35	0.56
2:I:741:HIS:CB	2:I:853:PRO:HB2	2.35	0.56
1:A:1285:ALA:O	1:A:1289:MET:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:CYS:SG	1:A:82:SER:HB3	2.45	0.56
1:A:883:ILE:HD12	1:A:947:LEU:HD12	1.86	0.56
1:B:1305:CYS:HB2	1:B:1645:GLY:HA2	1.86	0.56
1:B:742:LYS:HD3	1:B:746:GLU:OE2	2.05	0.56
1:C:1538:VAL:HB	1:C:1639:VAL:HG22	1.86	0.56
1:C:807:LYS:HG3	1:C:858:TRP:HB3	1.87	0.56
2:G:653:TYR:CD1	2:G:659:LEU:HD21	2.40	0.56
1:B:59:ARG:HH11	2:H:1896:GLN:NE2	2.03	0.56
2:H:1920:GLN:HG2	2:H:1922:ILE:HD11	1.87	0.56
2:H:1908:ASP:HB2	2:H:1958:LEU:HD21	1.86	0.56
2:I:777:THR:CG2	2:I:1081:HIS:CE1	2.88	0.56
2:I:1231:GLY:O	2:I:1233:PRO:HD3	2.05	0.56
2:I:1804:PHE:CZ	2:I:2010:TYR:HB2	2.40	0.56
2:I:7:ARG:NH1	2:I:24:THR:HA	2.20	0.56
2:I:463:PHE:HD1	2:I:486:LEU:HD13	1.70	0.56
1:C:1022:THR:HG22	1:C:1226:SER:HB2	1.87	0.56
1:C:625:THR:HG23	1:C:661:ASP:OD1	2.05	0.56
1:C:980:VAL:H	2:I:968:GLN:HE22	1.53	0.56
2:G:1874:VAL:O	2:G:1878:VAL:HG12	2.05	0.56
2:G:702:TYR:CB	2:G:727:PRO:HB2	2.35	0.56
2:G:732:TRP:CD2	2:G:750:MET:HE1	2.40	0.56
2:H:1223:MET:CE	2:H:1238:LEU:HD12	2.35	0.56
2:H:1266:TYR:CG	2:H:1347:LEU:HD23	2.40	0.56
2:H:653:TYR:CD1	2:H:659:LEU:HD21	2.40	0.56
2:I:1567:ARG:HH12	2:I:1568:HIS:HB3	1.70	0.56
2:I:89:THR:O	2:I:93:ASN:HB2	2.05	0.56
1:A:408:TRP:CZ3	1:A:1628:SER:HB3	2.40	0.56
1:B:1014:ASP:N	1:B:1510:ASN:HD21	2.01	0.56
1:C:1326:ILE:HG12	1:C:1388:MET:HG3	1.87	0.56
2:G:120:LYS:O	2:G:124:LYS:HG3	2.05	0.56
2:G:102:HIS:HE1	2:G:180:TYR:OH	1.88	0.56
2:G:376:ASN:HD22	2:G:377:LEU:N	2.02	0.56
2:G:543:PHE:CB	2:G:545:GLN:HE22	2.17	0.56
2:G:860:ARG:HB3	2:G:898:ASP:HB3	1.85	0.56
2:H:807:ILE:CG2	2:H:1066:ILE:HA	2.36	0.56
2:I:1314:ARG:CG	2:I:1314:ARG:NH1	2.63	0.56
2:I:1300:PHE:CA	2:I:1556:VAL:HG11	2.36	0.56
2:I:281:VAL:HG23	2:I:459:VAL:HG11	1.87	0.56
2:I:105:ALA:CB	2:I:533:LEU:HD21	2.34	0.56
1:A:411:GLN:NE2	1:A:1628:SER:H	2.01	0.56
1:B:635:ILE:HG22	1:B:651:TYR:CG	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:430:ARG:NH2	1:C:605:LEU:HD13	2.21	0.56
2:G:239:PRO:HG3	2:G:304:PHE:HA	1.88	0.56
2:I:120:LYS:O	2:I:124:LYS:HG3	2.06	0.56
2:I:1328:VAL:HG23	2:I:1557:SER:HA	1.88	0.56
2:I:2038:ILE:O	2:I:2042:ILE:HG12	2.04	0.56
2:I:603:SER:O	2:I:607:VAL:HG12	2.06	0.56
2:I:807:ILE:CG2	2:I:1066:ILE:HA	2.34	0.56
1:B:529:MET:HG2	1:B:638:LEU:CD1	2.35	0.56
1:C:419:GLU:HG2	1:C:424:VAL:HB	1.86	0.56
2:G:463:PHE:HD1	2:G:486:LEU:HD13	1.70	0.56
2:H:61:VAL:HG21	2:H:95:TYR:HE1	1.69	0.56
2:I:1149:TRP:CD1	2:I:1213:LEU:CD1	2.88	0.56
2:I:1292:ILE:O	2:I:1368:VAL:O	2.23	0.56
2:I:1378:ILE:HD11	2:I:1381:VAL:CG2	2.34	0.56
2:I:443:LEU:HD22	2:I:448:VAL:HG11	1.87	0.56
1:B:56:MET:HG3	2:H:1893:VAL:CG2	2.35	0.56
1:C:1259:GLY:HA2	1:C:1263:ASP:HB2	1.87	0.56
1:C:27:ARG:HD2	1:C:30:GLU:OE2	2.06	0.56
1:C:529:MET:HE1	1:C:894:ARG:HD2	1.88	0.56
2:G:1567:ARG:HG3	2:G:1568:HIS:N	2.20	0.56
2:G:1722:GLY:N	2:G:1726:GLY:HA3	2.21	0.56
2:G:584:SER:HA	2:G:587:ILE:HG23	1.87	0.56
2:H:1868:GLN:HG3	2:H:1898:TYR:OH	2.06	0.56
2:H:376:ASN:HD22	2:H:377:LEU:N	2.03	0.56
2:H:741:HIS:HB3	2:H:853:PRO:HB2	1.88	0.56
1:A:1665:ILE:HD11	1:A:1669:ARG:HG2	1.88	0.56
1:A:152:HIS:CE1	1:A:168:MET:HG3	2.41	0.56
1:A:295:ALA:HB2	1:A:302:LEU:HD11	1.87	0.56
1:A:742:LYS:HD3	1:A:746:GLU:OE2	2.05	0.56
1:B:1009:LEU:HD13	1:B:1445:MET:HE1	1.86	0.56
1:B:152:HIS:CE1	1:B:168:MET:HG3	2.41	0.56
1:C:1056:ILE:HD13	1:C:1193:TRP:CD1	2.41	0.56
1:C:1473:GLU:O	1:C:1478:PRO:HD3	2.05	0.56
2:H:777:THR:CG2	2:H:1081:HIS:CE1	2.88	0.56
2:H:1194:VAL:O	2:H:1194:VAL:HG12	2.05	0.56
2:H:16:LEU:HG	2:H:48:PHE:CZ	2.41	0.56
2:H:1890:ASN:HB2	2:H:1899:VAL:HB	1.88	0.56
2:H:1989:LYS:O	2:H:1993:LYS:HG3	2.06	0.56
2:I:1227:ARG:NH1	2:I:1227:ARG:HG3	2.00	0.56
2:I:232:LEU:HD23	2:I:232:LEU:O	2.06	0.56
1:B:644:THR:HG22	1:B:648:ASP:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1347:LYS:HD3	1:C:1347:LYS:O	2.05	0.56
2:G:1343:VAL:HG22	2:G:1343:VAL:O	2.06	0.56
2:G:1567:ARG:HH12	2:G:1568:HIS:HB3	1.71	0.56
2:G:1675:GLY:O	2:G:1678:MET:HB2	2.05	0.56
2:H:526:ARG:HH11	2:H:558:ASN:HD21	1.53	0.56
2:I:607:VAL:HA	2:I:617:ILE:HD13	1.86	0.56
2:I:774:ALA:HB1	2:I:1081:HIS:CD2	2.33	0.56
1:A:1052:GLU:O	1:A:1056:ILE:HG23	2.06	0.56
2:G:1101:GLU:HB2	2:G:1147:ILE:O	2.06	0.56
2:G:1428:GLU:HB2	2:G:1468:THR:HG22	1.88	0.56
2:G:589:ARG:HB3	2:G:590:PRO:HD2	1.87	0.56
2:G:654:VAL:HG23	2:G:683:ALA:HB1	1.87	0.56
2:G:663:ILE:HG13	2:G:694:TYR:HE1	1.70	0.56
2:G:964:LEU:CD2	2:G:964:LEU:N	2.68	0.56
2:H:1431:TYR:CE1	2:H:1526:THR:HG23	2.41	0.56
2:H:463:PHE:HD1	2:H:486:LEU:HD13	1.70	0.56
2:I:577:ILE:HD13	2:I:1097:ILE:CD1	2.35	0.56
2:I:1722:GLY:N	2:I:1726:GLY:HA3	2.20	0.56
1:A:1036:ARG:NH1	1:A:1040:GLU:OE1	2.39	0.56
1:A:1473:GLU:O	1:A:1478:PRO:HD3	2.06	0.56
1:A:864:VAL:CG2	1:A:921:PRO:HB3	2.36	0.56
1:B:2:LYS:HD2	2:H:2050:GLN:CB	2.26	0.56
1:C:417:TYR:OH	1:C:458:THR:HG22	2.06	0.56
1:C:50:SER:HB2	1:C:51:PRO:HD3	1.88	0.56
2:G:665:LEU:O	2:G:669:LEU:HB2	2.06	0.56
2:G:807:ILE:HG21	2:G:1066:ILE:HA	1.88	0.56
2:H:1166:VAL:HG12	2:H:1167:SER:N	2.21	0.56
1:A:1125:VAL:HG21	1:A:1175:ILE:HD12	1.88	0.55
1:A:1566:ARG:HB3	1:A:1623:TYR:CE1	2.42	0.55
1:A:221:LEU:O	1:A:225:SER:HB3	2.05	0.55
1:A:263:GLY:O	1:A:267:VAL:HG23	2.05	0.55
1:B:1665:ILE:HD11	1:B:1669:ARG:HG2	1.88	0.55
1:B:992:PHE:CE2	1:B:1399:PRO:HG3	2.41	0.55
1:C:12:ILE:HA	1:C:15:THR:HG23	1.87	0.55
1:C:254:TRP:CZ3	1:C:302:LEU:HD13	2.41	0.55
1:C:695:GLY:HA3	1:C:906:LEU:HD11	1.88	0.55
2:G:1168:ASN:ND2	2:G:1171:ARG:HB2	2.20	0.55
2:G:1475:LYS:HG3	2:G:1481:SER:HB2	1.88	0.55
2:G:1678:MET:CE	2:G:1707:LEU:HD22	2.35	0.55
2:G:1804:PHE:CZ	2:G:2010:TYR:HB2	2.40	0.55
2:G:1890:ASN:HB2	2:G:1899:VAL:HB	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:652:ILE:HB	2:G:658:MET:CE	2.36	0.55
2:G:99:ASN:HA	2:G:550:VAL:HG23	1.87	0.55
2:H:1475:LYS:HB2	2:H:1481:SER:HB2	1.88	0.55
2:I:1873:TYR:HE1	2:I:1877:ARG:HH21	1.54	0.55
2:I:601:THR:HG22	2:I:620:ALA:H	1.71	0.55
2:I:654:VAL:HG23	2:I:683:ALA:HB1	1.87	0.55
1:A:1238:VAL:HG12	1:A:1239:HIS:N	2.21	0.55
1:B:1233:GLU:OE2	1:B:1680:ARG:NH2	2.40	0.55
1:B:733:ILE:HD12	1:B:761:LEU:HD21	1.88	0.55
1:C:1496:GLU:O	1:C:1500:GLN:HG3	2.06	0.55
2:G:1227:ARG:CG	2:G:1227:ARG:NH1	2.56	0.55
2:G:1313:SER:O	2:G:1314:ARG:HD3	2.06	0.55
2:H:1567:ARG:HH12	2:H:1568:HIS:HB3	1.70	0.55
2:H:702:TYR:CB	2:H:727:PRO:HB2	2.36	0.55
2:I:1422:THR:HG21	2:I:1474:PHE:HB2	1.88	0.55
2:I:1778:GLN:HB3	2:I:1831:VAL:HG13	1.88	0.55
2:I:260:PRO:HD3	2:I:289:TRP:CE2	2.42	0.55
1:A:1657:HIS:ND1	1:A:1658:PRO:HD2	2.21	0.55
2:G:813:THR:HB	2:G:818:LYS:HE3	1.87	0.55
2:H:56:THR:HG23	2:H:59:GLU:CG	2.32	0.55
2:I:1382:VAL:HA	2:I:1422:THR:OG1	2.07	0.55
2:I:1589:VAL:HG11	2:I:1640:PHE:CE1	2.41	0.55
1:A:529:MET:HG2	1:A:638:LEU:CD1	2.36	0.55
1:A:680:ILE:HG13	1:A:769:ILE:HB	1.87	0.55
1:A:825:PRO:HB2	1:A:843:LYS:NZ	2.21	0.55
1:B:1584:PRO:HG3	1:B:1591:TRP:CH2	2.41	0.55
1:C:11:HIS:O	1:C:15:THR:HG22	2.06	0.55
2:H:120:LYS:O	2:H:124:LYS:HG3	2.06	0.55
2:I:197:GLU:OE1	2:I:197:GLU:HA	2.05	0.55
2:I:543:PHE:CB	2:I:545:GLN:HE22	2.17	0.55
1:A:1233:GLU:OE2	1:A:1680:ARG:NH2	2.40	0.55
1:B:1036:ARG:NH1	1:B:1040:GLU:OE1	2.40	0.55
1:B:49:PRO:O	1:B:82:SER:HB2	2.07	0.55
1:C:37:LYS:HB2	1:C:65:TYR:HE1	1.72	0.55
2:G:1004:LEU:CD2	2:G:1019:PRO:HB2	2.36	0.55
2:G:1359:MET:HE3	2:G:1404:MET:HB3	1.89	0.55
1:B:985:ARG:HH12	2:H:953:ARG:NH2	2.04	0.55
2:I:1093:ASP:HB3	2:I:1096:LYS:HG3	1.89	0.55
2:I:1331:TRP:CE2	2:I:1335:ILE:HG13	2.42	0.55
2:I:491:GLU:HA	2:I:494:THR:HG22	1.89	0.55
1:A:1524:GLY:HA2	1:A:1527:ALA:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1249:SER:HB3	1:C:1280:ILE:HG12	1.87	0.55
1:C:1014:ASP:N	1:C:1510:ASN:HD21	1.99	0.55
1:C:1585:LYS:HD3	1:C:1585:LYS:H	1.72	0.55
2:G:777:THR:CG2	2:G:1081:HIS:CE1	2.89	0.55
1:A:1555:ALA:HA	1:A:1621:PHE:CE1	2.42	0.55
1:A:733:ILE:CD1	1:A:761:LEU:HD11	2.37	0.55
1:B:1138:LYS:HG3	1:B:1163:TYR:CE1	2.41	0.55
1:B:1544:THR:O	1:B:1545:SER:HB3	2.06	0.55
2:H:1173:VAL:CG2	2:H:1221:MET:HE1	2.35	0.55
2:H:146:PHE:HA	2:H:149:VAL:HG12	1.89	0.55
2:H:7:ARG:NH1	2:H:24:THR:HA	2.21	0.55
2:H:839:PRO:HA	2:H:844:VAL:HG13	1.88	0.55
2:I:826:GLY:HA2	2:I:1060:ALA:HB3	1.88	0.55
2:I:85:ASN:ND2	2:I:135:ARG:HH11	1.99	0.55
2:I:1624:THR:HB	2:I:1642:THR:OG1	2.06	0.55
1:C:20:TYR:HE1	2:I:2035:SER:HB2	1.71	0.55
1:A:1455:ARG:NH2	1:A:1459:ILE:HG12	2.22	0.55
1:A:12:ILE:HA	1:A:15:THR:HG23	1.88	0.55
1:A:198:PRO:CG	1:A:209:LEU:HD21	2.28	0.55
1:A:824:LEU:HD11	1:A:849:LEU:HD12	1.89	0.55
1:A:771:PHE:CD1	1:A:825:PRO:HG3	2.42	0.55
1:B:328:LEU:C	1:B:328:LEU:HD22	2.27	0.55
1:B:433:VAL:O	1:B:437:ILE:HG13	2.07	0.55
1:B:529:MET:CE	1:B:894:ARG:HD2	2.37	0.55
1:B:771:PHE:CD1	1:B:825:PRO:HG3	2.42	0.55
1:C:329:GLU:O	1:C:333:LYS:HG3	2.06	0.55
1:C:335:HIS:HD2	1:C:335:HIS:O	1.89	0.55
2:G:197:GLU:OE1	2:G:197:GLU:HA	2.06	0.55
2:G:758:ARG:NH2	2:G:797:ASP:OD1	2.33	0.55
2:H:402:LEU:O	2:H:402:LEU:HD13	2.07	0.55
2:H:490:TRP:HA	2:H:493:THR:CG2	2.37	0.55
2:I:1452:LEU:HA	2:I:1502:GLY:HA3	1.88	0.55
2:I:145:LEU:HD21	2:I:156:LEU:HD21	1.89	0.55
2:I:166:THR:HG22	2:I:168:ASP:N	2.21	0.55
2:I:517:HIS:CD2	2:I:517:HIS:C	2.80	0.55
2:I:606:PHE:HZ	2:I:805:VAL:HG11	1.71	0.55
1:C:152:HIS:CE1	1:C:168:MET:HG3	2.42	0.55
2:G:1575:LEU:HD13	2:G:1579:ILE:HD12	1.89	0.55
2:H:1102:TYR:HB3	2:H:1244:PRO:HA	1.89	0.55
2:H:1359:MET:HE3	2:H:1359:MET:HA	1.88	0.55
2:H:1672:GLN:HA	2:H:1676:MET:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:264:ARG:NH1	2:H:456:GLN:HG3	2.22	0.55
2:I:702:TYR:CB	2:I:727:PRO:HB2	2.36	0.55
1:B:236:LYS:HE2	1:B:273:PRO:O	2.07	0.55
1:B:529:MET:HE1	1:B:894:ARG:HD2	1.89	0.55
1:C:286:PHE:O	1:C:290:MET:HG2	2.07	0.55
2:G:1859:PRO:CG	2:G:1871:LEU:HD12	2.21	0.55
2:H:1378:ILE:HD11	2:H:1381:VAL:CG2	2.37	0.55
2:H:1493:LEU:HD11	2:H:1499:VAL:CG2	2.36	0.55
2:H:2015:THR:HG22	2:H:2017:LYS:N	2.21	0.55
2:I:1382:VAL:HA	2:I:1422:THR:HG1	1.72	0.55
2:I:490:TRP:HA	2:I:493:THR:CG2	2.37	0.55
2:I:871:THR:HB	2:I:872:ILE:HD12	1.88	0.55
2:I:926:LEU:HB3	2:I:947:THR:HG22	1.88	0.55
1:A:20:TYR:CE2	2:G:1985:VAL:HG11	2.42	0.54
2:G:1227:ARG:HG3	2:G:1227:ARG:NH1	2.00	0.54
2:G:464:ASP:HB3	2:G:466:SER:HB3	1.88	0.54
2:H:1159:ILE:HG12	2:H:1169:PRO:CD	2.36	0.54
2:H:1325:PHE:CE1	2:H:1328:VAL:HG11	2.43	0.54
2:H:1778:GLN:HB3	2:H:1831:VAL:HG13	1.88	0.54
2:H:239:PRO:HG3	2:H:304:PHE:HA	1.88	0.54
2:H:464:ASP:HB3	2:H:466:SER:HB3	1.90	0.54
2:H:611:THR:CG2	2:H:641:ILE:HG13	2.38	0.54
2:H:826:GLY:O	2:H:827:VAL:HG23	2.07	0.54
2:I:1293:THR:HG22	2:I:1296:GLU:CD	2.27	0.54
2:I:584:SER:HA	2:I:587:ILE:HG23	1.89	0.54
2:I:611:THR:CG2	2:I:641:ILE:HG13	2.37	0.54
1:B:1492:GLU:O	1:B:1496:GLU:HG3	2.06	0.54
1:B:1:MET:HE3	1:B:5:VAL:HG12	1.89	0.54
2:G:1040:LEU:HD21	2:G:1048:VAL:HA	1.90	0.54
2:G:332:GLU:OE2	2:G:394:ARG:HD3	2.07	0.54
1:B:59:ARG:HH11	2:H:1896:GLN:HE22	1.54	0.54
2:H:584:SER:HA	2:H:587:ILE:HG23	1.89	0.54
2:H:607:VAL:HA	2:H:617:ILE:HD13	1.88	0.54
2:I:240:LEU:O	2:I:244:ILE:HG13	2.08	0.54
2:I:526:ARG:HH11	2:I:558:ASN:HD21	1.55	0.54
2:I:638:VAL:HA	2:I:641:ILE:HG22	1.88	0.54
1:A:1247:SER:HB2	1:A:1332:TYR:HE2	1.72	0.54
1:A:1392:LEU:HD22	1:A:1396:MET:HG3	1.89	0.54
1:A:1665:ILE:CG1	1:A:1669:ARG:HD3	2.36	0.54
1:C:1219:VAL:CA	1:C:1384:ILE:HD11	2.27	0.54
1:C:1477:ILE:H	1:C:1478:PRO:CD	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1231:GLY:O	2:G:1233:PRO:HD3	2.08	0.54
2:G:747:HIS:O	2:G:751:LEU:HB2	2.07	0.54
2:H:1343:VAL:HG22	2:H:1343:VAL:O	2.06	0.54
2:H:1822:MET:CE	2:H:1996:ILE:HG12	2.37	0.54
2:H:1697:HIS:CE1	2:H:1829:GLU:HG2	2.42	0.54
2:H:674:TYR:HB3	2:H:676:ILE:HG22	1.89	0.54
2:I:722:ALA:HB1	2:I:723:HIS:CE1	2.42	0.54
2:I:754:TYR:CD2	2:I:794:MET:HG3	2.43	0.54
1:B:529:MET:HE3	1:B:529:MET:CA	2.31	0.54
1:B:332:THR:HG22	1:C:331:ILE:HD11	1.88	0.54
2:G:722:ALA:HB1	2:G:723:HIS:CE1	2.42	0.54
2:H:1040:LEU:HD21	2:H:1048:VAL:HA	1.89	0.54
2:I:1475:LYS:HB2	2:I:1481:SER:HB2	1.89	0.54
2:I:1954:LYS:HD3	2:I:1958:LEU:HD13	1.89	0.54
2:I:61:VAL:HG21	2:I:95:TYR:HE1	1.72	0.54
1:A:1184:LEU:HB2	1:A:1352:THR:HG21	1.89	0.54
1:A:340:ARG:HH12	1:A:344:GLN:NE2	2.06	0.54
1:A:733:ILE:HD12	1:A:761:LEU:HD21	1.89	0.54
1:B:1285:ALA:O	1:B:1289:MET:HG3	2.07	0.54
1:C:1501:LEU:O	1:C:1505:GLN:HG3	2.07	0.54
1:C:236:LYS:HE2	1:C:273:PRO:O	2.08	0.54
2:G:127:ILE:O	2:G:131:ILE:HG13	2.07	0.54
2:G:1300:PHE:HA	2:G:1556:VAL:HG11	1.89	0.54
2:G:2036:GLU:O	2:G:2039:LYS:HG2	2.07	0.54
2:G:264:ARG:NH1	2:G:456:GLN:HG3	2.22	0.54
2:I:1427:VAL:HG12	2:I:1427:VAL:O	2.07	0.54
2:I:826:GLY:O	2:I:827:VAL:HG23	2.08	0.54
1:A:1234:MET:CE	1:A:1326:ILE:HG21	2.38	0.54
1:A:1584:PRO:HB2	1:A:1587:ALA:HB3	1.88	0.54
1:B:1432:HIS:CE1	1:B:1434:SER:OG	2.60	0.54
1:B:1566:ARG:HB3	1:B:1623:TYR:CE1	2.42	0.54
1:B:263:GLY:O	1:B:267:VAL:HG23	2.07	0.54
1:B:625:THR:HG23	1:B:661:ASP:OD1	2.07	0.54
1:C:1036:ARG:NH1	1:C:1040:GLU:OE1	2.41	0.54
1:C:1125:VAL:HG21	1:C:1175:ILE:HD12	1.88	0.54
2:G:344:LEU:HB3	2:G:349:VAL:HG23	1.90	0.54
2:G:462:THR:HB	2:G:482:CYS:SG	2.48	0.54
2:G:707:PRO:HG2	2:G:730:LEU:HD13	1.90	0.54
2:H:1239:LEU:O	2:H:1254:VAL:HG23	2.08	0.54
2:H:85:ASN:HD22	2:H:135:ARG:NH1	2.02	0.54
2:I:1227:ARG:NH1	2:I:1227:ARG:CG	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:545:GLN:NE2	2:I:545:GLN:H	2.06	0.54
1:A:1114:TYR:CD1	1:A:1337:GLU:HG3	2.41	0.54
1:A:1585:LYS:H	1:A:1585:LYS:HD3	1.71	0.54
1:A:529:MET:HG2	1:A:638:LEU:HG	1.89	0.54
1:B:12:ILE:HD11	2:H:2041:ILE:HD12	1.88	0.54
1:B:1501:LEU:O	1:B:1505:GLN:HG3	2.08	0.54
1:B:385:PHE:HD2	1:B:787:LYS:HA	1.73	0.54
1:C:1455:ARG:NH2	1:C:1459:ILE:HG12	2.22	0.54
1:C:479:ASN:O	1:C:483:VAL:HG23	2.07	0.54
2:G:1382:VAL:HA	2:G:1422:THR:OG1	2.08	0.54
2:G:346:GLN:HA	2:G:377:LEU:HD21	1.89	0.54
2:H:1293:THR:HG22	2:H:1296:GLU:CD	2.28	0.54
2:H:1279:PHE:CD2	2:H:1340:PRO:HG3	2.41	0.54
2:H:2036:GLU:O	2:H:2039:LYS:HG2	2.08	0.54
2:H:402:LEU:HD12	2:H:404:GLN:HG2	1.90	0.54
2:I:615:TYR:CZ	2:I:1074:MET:HB3	2.42	0.54
2:I:271:THR:OG1	2:I:460:TYR:HB2	2.08	0.54
1:A:1455:ARG:O	1:A:1459:ILE:HG13	2.08	0.54
1:B:1392:LEU:CD2	1:B:1396:MET:HG3	2.38	0.54
1:B:1600:LEU:HD13	1:B:1657:HIS:HA	1.90	0.54
1:C:411:GLN:NE2	1:C:1628:SER:H	2.05	0.54
2:G:1496:LYS:HE2	2:G:1693:ARG:NH2	2.22	0.54
2:H:1350:LEU:HD11	2:H:1410:PHE:HB3	1.89	0.54
2:H:1913:VAL:O	2:H:1917:ILE:HG13	2.08	0.54
2:H:173:LEU:HD13	2:H:219:LEU:HD21	1.90	0.54
1:A:1123:GLN:HB2	1:A:1177:LYS:HE2	1.90	0.54
1:A:1183:ARG:NH1	1:A:1344:GLY:HA2	2.23	0.54
1:A:236:LYS:HE2	1:A:273:PRO:O	2.07	0.54
1:B:1584:PRO:HB2	1:B:1587:ALA:HB3	1.90	0.54
1:A:24:SER:CB	2:G:2014:LEU:HD12	2.38	0.54
2:H:1173:VAL:O	2:H:1567:ARG:NH2	2.40	0.54
2:H:774:ALA:HB1	2:H:1081:HIS:CD2	2.32	0.54
2:I:1493:LEU:HD11	2:I:1499:VAL:CG2	2.37	0.54
2:I:2035:SER:HB3	2:I:2038:ILE:CG1	2.37	0.54
1:A:1194:ASN:HB3	1:A:1197:THR:HG22	1.88	0.54
1:A:183:GLN:O	1:A:187:LEU:HG	2.08	0.54
1:B:1123:GLN:HG3	1:B:1124:GLU:N	2.22	0.54
1:B:280:GLU:O	1:B:280:GLU:HG2	2.08	0.54
1:B:824:LEU:HD11	1:B:849:LEU:HD12	1.89	0.54
1:C:233:ILE:HD13	1:C:237:MET:HE2	1.88	0.54
1:C:263:GLY:O	1:C:267:VAL:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1378:ILE:O	2:G:1378:ILE:HG12	2.06	0.54
2:G:1822:MET:CE	2:G:1996:ILE:HG12	2.37	0.54
2:G:490:TRP:CH2	2:G:512:LEU:HD21	2.43	0.54
2:H:606:PHE:CE1	2:H:811:VAL:HG13	2.43	0.54
2:H:667:LYS:HD2	2:H:697:THR:CG2	2.35	0.54
2:H:707:PRO:HG2	2:H:730:LEU:HD13	1.89	0.54
2:I:652:ILE:HB	2:I:658:MET:CE	2.38	0.54
2:I:99:ASN:HA	2:I:550:VAL:HG23	1.90	0.54
1:A:1020:VAL:HG13	1:A:1400:ILE:HG23	1.90	0.53
1:A:421:ILE:HG13	1:A:469:VAL:HG21	1.89	0.53
1:B:1401:TYR:C	1:B:1658:PRO:HG3	2.28	0.53
1:B:329:GLU:O	1:B:333:LYS:HG3	2.08	0.53
1:C:1285:ALA:O	1:C:1289:MET:HG3	2.09	0.53
2:G:1166:VAL:HG12	2:G:1167:SER:N	2.23	0.53
2:G:1173:VAL:CG2	2:G:1221:MET:HE1	2.38	0.53
2:H:1313:SER:O	2:H:1314:ARG:HD3	2.08	0.53
2:I:868:PHE:HB3	2:I:873:PHE:CE2	2.43	0.53
1:B:11:HIS:O	1:B:15:THR:HG22	2.06	0.53
1:B:751:PHE:CZ	1:B:761:LEU:HD13	2.42	0.53
1:C:1123:GLN:HG3	1:C:1124:GLU:N	2.23	0.53
2:G:750:MET:CG	2:G:796:PHE:HZ	2.21	0.53
2:H:964:LEU:N	2:H:964:LEU:CD2	2.70	0.53
2:I:1168:ASN:ND2	2:I:1171:ARG:HB2	2.22	0.53
2:I:1266:TYR:CG	2:I:1347:LEU:HD23	2.43	0.53
1:A:1392:LEU:CD2	1:A:1396:MET:HG3	2.38	0.53
1:A:625:THR:HG23	1:A:661:ASP:OD1	2.08	0.53
1:B:1010:GLU:HA	1:B:1664:ALA:HA	1.89	0.53
2:G:1093:ASP:HB3	2:G:1096:LYS:HG3	1.91	0.53
2:H:1804:PHE:CZ	2:H:2010:TYR:HB2	2.44	0.53
2:H:545:GLN:NE2	2:H:545:GLN:H	2.07	0.53
2:I:873:PHE:CD1	2:I:1026:GLU:HB2	2.43	0.53
1:A:1496:GLU:O	1:A:1500:GLN:HG3	2.07	0.53
1:A:1584:PRO:HG3	1:A:1591:TRP:CH2	2.42	0.53
1:A:1665:ILE:HG12	1:A:1666:THR:N	2.23	0.53
1:B:807:LYS:HG3	1:B:858:TRP:HB3	1.90	0.53
2:G:1697:HIS:CE1	2:G:1829:GLU:HG2	2.43	0.53
2:H:615:TYR:CZ	2:H:1074:MET:HB3	2.43	0.53
2:H:1177:SER:O	2:H:1180:MET:HG2	2.08	0.53
2:H:346:GLN:HA	2:H:377:LEU:HD21	1.91	0.53
2:H:123:ILE:HD11	2:H:533:LEU:CD2	2.38	0.53
2:H:652:ILE:HB	2:H:658:MET:CE	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:892:ILE:HG12	2:I:903:TRP:CG	2.44	0.53
2:I:964:LEU:CD2	2:I:964:LEU:N	2.72	0.53
1:A:1310:GLU:OE1	1:A:1649:LYS:CE	2.57	0.53
1:B:1247:SER:HB2	1:B:1332:TYR:HE2	1.74	0.53
2:G:1292:ILE:O	2:G:1368:VAL:O	2.26	0.53
2:G:2030:TYR:CE1	2:G:2034:GLY:HA2	2.43	0.53
2:H:1931:LEU:HB3	2:H:1935:GLU:CG	2.36	0.53
2:I:1861:ARG:HD2	2:I:1964:PHE:O	2.08	0.53
2:I:835:THR:HG22	2:I:844:VAL:C	2.29	0.53
1:A:1477:ILE:H	1:A:1478:PRO:CD	2.21	0.53
1:A:998:TYR:CE2	1:A:1667:GLU:HB2	2.44	0.53
1:A:328:LEU:C	1:A:328:LEU:HD22	2.28	0.53
1:B:408:TRP:CH2	1:B:1628:SER:HB3	2.44	0.53
1:C:1194:ASN:HB3	1:C:1197:THR:HG22	1.90	0.53
2:G:1672:GLN:HA	2:G:1676:MET:HE3	1.90	0.53
2:G:176:LEU:HD22	2:G:247:ALA:HB1	1.90	0.53
2:G:1808:SER:OG	2:G:1977:HIS:HE1	1.91	0.53
2:G:606:PHE:HZ	2:G:805:VAL:HG11	1.74	0.53
2:G:839:PRO:CA	2:G:844:VAL:HG13	2.35	0.53
2:G:892:ILE:HG12	2:G:903:TRP:CG	2.44	0.53
2:H:835:THR:HG21	2:H:855:HIS:NE2	2.23	0.53
2:I:1040:LEU:HD21	2:I:1048:VAL:HA	1.90	0.53
1:C:24:SER:HB3	2:I:2014:LEU:HD12	1.90	0.53
2:I:2036:GLU:O	2:I:2039:LYS:HG2	2.09	0.53
1:A:1138:LYS:HG3	1:A:1163:TYR:CE1	2.43	0.53
1:A:1492:GLU:O	1:A:1496:GLU:HG3	2.09	0.53
1:B:12:ILE:HA	1:B:15:THR:HG23	1.90	0.53
2:G:1475:LYS:HB2	2:G:1481:SER:HB2	1.89	0.53
2:H:1292:ILE:O	2:H:1368:VAL:O	2.27	0.53
2:H:194:THR:CG2	2:H:300:ILE:HD11	2.39	0.53
1:B:980:VAL:N	2:H:968:GLN:HE22	2.07	0.53
2:I:102:HIS:HE1	2:I:180:TYR:OH	1.91	0.53
2:I:2046:GLU:C	2:I:2048:TYR:H	2.11	0.53
2:I:161:GLY:N	2:I:505:GLY:HA3	2.24	0.53
1:A:341:GLN:O	1:A:345:VAL:HG12	2.09	0.53
1:B:1194:ASN:O	1:B:1197:THR:HG23	2.08	0.53
1:B:1665:ILE:CG1	1:B:1669:ARG:HD3	2.35	0.53
2:G:1427:VAL:HG12	2:G:1427:VAL:O	2.09	0.53
2:G:1475:LYS:CB	2:G:1481:SER:HB2	2.39	0.53
2:G:1697:HIS:HE1	2:G:1829:GLU:HG2	1.74	0.53
2:G:85:ASN:HD22	2:G:135:ARG:NH1	2.03	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1227:ARG:CG	2:H:1227:ARG:NH1	2.57	0.53
2:H:1954:LYS:HD3	2:H:1958:LEU:HD13	1.91	0.53
2:I:1279:PHE:CD2	2:I:1340:PRO:HG3	2.40	0.53
2:I:1343:VAL:HG22	2:I:1343:VAL:O	2.09	0.53
2:I:1441:ILE:HD11	2:I:1445:ARG:NH2	2.23	0.53
2:I:2036:GLU:HG2	2:I:2039:LYS:NZ	2.24	0.53
2:I:465:GLY:HA2	2:I:493:THR:HA	1.91	0.53
2:I:606:PHE:CE1	2:I:811:VAL:HG13	2.44	0.53
1:A:644:THR:HG22	1:A:648:ASP:O	2.08	0.53
1:B:340:ARG:HH12	1:B:344:GLN:NE2	2.07	0.53
1:B:607:LYS:HG2	1:B:608:ASP:N	2.23	0.53
1:B:881:ASN:HA	1:B:944:ARG:HH21	1.73	0.53
1:C:825:PRO:HB2	1:C:843:LYS:NZ	2.24	0.53
1:C:992:PHE:CD2	1:C:1399:PRO:HG3	2.44	0.53
2:G:1314:ARG:CG	2:G:1314:ARG:NH1	2.61	0.53
2:H:654:VAL:HG23	2:H:683:ALA:HB1	1.91	0.53
2:I:1166:VAL:HG12	2:I:1167:SER:N	2.23	0.53
2:I:1350:LEU:HD11	2:I:1410:PHE:HB3	1.91	0.53
2:I:332:GLU:OE2	2:I:394:ARG:HD3	2.08	0.53
1:A:807:LYS:HG3	1:A:858:TRP:HB3	1.90	0.53
1:B:1304:ALA:N	1:B:1307:THR:HG22	2.24	0.53
1:B:1312:VAL:CG2	1:B:1329:VAL:HG11	2.39	0.53
1:C:529:MET:HG2	1:C:638:LEU:CD1	2.39	0.53
2:G:1236:LEU:HD11	2:G:1262:ILE:HG12	1.91	0.53
2:G:121:GLU:HA	2:G:124:LYS:HD2	1.91	0.53
2:G:1359:MET:CE	2:G:1404:MET:HB3	2.39	0.53
2:G:1422:THR:HG21	2:G:1474:PHE:HB2	1.91	0.53
1:A:964:GLU:HG2	2:G:1515:PRO:HB3	1.91	0.53
2:G:376:ASN:C	2:G:376:ASN:HD22	2.13	0.53
2:G:913:ASP:H	2:G:916:THR:CG2	2.22	0.53
2:H:1382:VAL:HA	2:H:1422:THR:OG1	2.09	0.53
2:H:1567:ARG:HG3	2:H:1568:HIS:N	2.23	0.53
2:H:281:VAL:HG23	2:H:459:VAL:HG11	1.90	0.53
2:I:1040:LEU:O	2:I:1046:GLN:HG3	2.09	0.53
2:I:1177:SER:O	2:I:1180:MET:HG2	2.09	0.53
2:I:1438:SER:O	2:I:1441:ILE:HG23	2.08	0.53
1:B:1056:ILE:CD1	1:B:1193:TRP:HD1	2.22	0.52
1:B:152:HIS:HD2	1:B:163:LEU:HB2	1.66	0.52
1:B:695:GLY:HA3	1:B:906:LEU:HD11	1.90	0.52
1:C:1103:ILE:HD11	1:C:1582:GLY:N	2.24	0.52
1:C:1401:TYR:C	1:C:1658:PRO:HG3	2.29	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:G:663:ILE:HB	2:G:664:PRO:CD	2.40	0.52
2:H:2026:PHE:CD2	2:H:2045:TRP:HZ3	2.27	0.52
2:H:455:ILE:HG12	2:H:469:ARG:HG2	1.91	0.52
2:H:768:GLY:HA3	2:H:800:LEU:CD2	2.39	0.52
1:A:1249:SER:HB3	1:A:1280:ILE:HG12	1.92	0.52
1:B:1194:ASN:HB3	1:B:1197:THR:HG22	1.91	0.52
1:C:1524:GLY:HA2	1:C:1527:ALA:HB3	1.91	0.52
1:C:824:LEU:HD11	1:C:849:LEU:HD12	1.90	0.52
2:G:1331:TRP:CE2	2:G:1335:ILE:HG13	2.43	0.52
2:G:1774:THR:HA	2:G:1777:THR:HB	1.91	0.52
2:G:161:GLY:N	2:G:505:GLY:HA3	2.23	0.52
2:H:145:LEU:O	2:H:149:VAL:HG12	2.10	0.52
2:H:577:ILE:HD13	2:H:1097:ILE:CD1	2.40	0.52
2:I:1567:ARG:HH11	2:I:1567:ARG:HG2	1.70	0.52
2:I:234:ILE:CG1	2:I:235:PRO:HD3	2.38	0.52
2:I:747:HIS:O	2:I:751:LEU:HB2	2.10	0.52
1:A:1303:GLY:H	1:A:1307:THR:HG22	1.74	0.52
1:A:1119:LYS:HE2	1:A:1341:PHE:CG	2.44	0.52
1:A:156:ALA:HA	1:A:166:ILE:CD1	2.39	0.52
1:A:385:PHE:HD2	1:A:787:LYS:HA	1.74	0.52
1:A:705:VAL:CG2	1:A:732:LEU:HD21	2.39	0.52
1:C:864:VAL:CG2	1:C:921:PRO:HB3	2.39	0.52
2:G:871:THR:HG21	2:G:887:LYS:NZ	2.25	0.52
2:G:955:GLU:HG2	2:G:987:TYR:CE2	2.45	0.52
2:H:1427:VAL:O	2:H:1427:VAL:HG12	2.08	0.52
2:H:1452:LEU:HA	2:H:1502:GLY:HA3	1.90	0.52
2:H:1300:PHE:HA	2:H:1556:VAL:HG11	1.92	0.52
2:H:732:TRP:CD2	2:H:750:MET:HE1	2.44	0.52
2:H:754:TYR:CD2	2:H:794:MET:HG3	2.45	0.52
2:I:1293:THR:CG2	2:I:1296:GLU:H	2.20	0.52
2:I:1566:SER:HB3	2:I:1568:HIS:CE1	2.45	0.52
2:I:2026:PHE:CD2	2:I:2045:TRP:HZ3	2.27	0.52
1:A:988:ILE:HD13	1:A:1048:GLU:HB3	1.91	0.52
1:B:1326:ILE:HG12	1:B:1388:MET:HG3	1.91	0.52
1:C:1411:THR:HG22	1:C:1412:ASP:N	2.24	0.52
1:C:1577:GLN:HE22	1:C:1591:TRP:C	2.13	0.52
1:C:607:LYS:HG2	1:C:608:ASP:N	2.24	0.52
1:C:630:ILE:O	1:C:653:ARG:NH2	2.42	0.52
2:G:1328:VAL:HG23	2:G:1557:SER:HA	1.91	0.52
2:G:926:LEU:HB3	2:G:947:THR:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1359:MET:HE3	2:H:1404:MET:HB3	1.90	0.52
1:B:12:ILE:HD11	2:H:2041:ILE:CD1	2.38	0.52
2:H:814:SER:CB	2:H:1040:LEU:HD13	2.40	0.52
2:I:1597:ALA:HB1	2:I:1638:ILE:CD1	2.39	0.52
2:I:598:THR:O	2:I:602:VAL:HB	2.09	0.52
2:I:652:ILE:HD12	2:I:652:ILE:N	2.25	0.52
2:I:871:THR:HG21	2:I:887:LYS:NZ	2.25	0.52
1:A:741:SER:HB3	1:A:744:ASP:HB2	1.89	0.52
1:A:655:LEU:CD2	1:A:916:LEU:HD11	2.38	0.52
1:B:1158:PRO:HD2	1:B:1159:GLU:OE2	2.10	0.52
1:B:1577:GLN:HE22	1:B:1591:TRP:C	2.12	0.52
1:C:1037:TRP:HB2	1:C:1598:GLN:OE1	2.09	0.52
1:C:385:PHE:HD2	1:C:787:LYS:HA	1.73	0.52
2:G:1745:LYS:HD3	2:G:1747:LYS:HE2	1.91	0.52
2:G:1986:LYS:HA	2:G:1989:LYS:HB3	1.92	0.52
2:G:2026:PHE:CD2	2:G:2045:TRP:HZ3	2.27	0.52
2:H:1491:VAL:HB	2:H:1501:ILE:HD12	1.92	0.52
2:H:1776:PHE:O	2:H:1779:PRO:HD2	2.09	0.52
2:I:1293:THR:HG22	2:I:1296:GLU:CG	2.39	0.52
2:I:1868:GLN:HG3	2:I:1898:TYR:CZ	2.45	0.52
2:I:418:ASN:HD22	2:I:418:ASN:N	2.07	0.52
2:I:582:LYS:HE2	2:I:1108:PRO:HB3	1.91	0.52
1:A:13:LEU:HB2	2:G:2026:PHE:CE1	2.45	0.52
1:A:1411:THR:HG22	1:A:1412:ASP:N	2.25	0.52
1:A:674:LYS:O	1:A:675:ASP:HB2	2.09	0.52
1:B:341:GLN:O	1:B:345:VAL:HG12	2.10	0.52
1:B:415:SER:O	1:B:419:GLU:HB2	2.10	0.52
2:H:1745:LYS:HE2	2:H:1747:LYS:HG2	1.91	0.52
2:I:1475:LYS:HG3	2:I:1481:SER:HB2	1.92	0.52
2:I:2015:THR:HG22	2:I:2017:LYS:N	2.21	0.52
2:I:702:TYR:HB2	2:I:727:PRO:HB2	1.92	0.52
1:A:335:HIS:HD2	1:A:335:HIS:O	1.92	0.52
1:B:1234:MET:CE	1:B:1326:ILE:HG21	2.40	0.52
1:B:1721:ARG:CG	1:B:1721:ARG:NH1	2.55	0.52
1:B:655:LEU:CD2	1:B:916:LEU:HD11	2.38	0.52
2:G:278:VAL:HG11	2:G:303:LEU:HD13	1.92	0.52
2:G:490:TRP:HA	2:G:493:THR:CG2	2.40	0.52
2:G:768:GLY:HA3	2:G:800:LEU:CD2	2.38	0.52
2:H:1159:ILE:CG1	2:H:1169:PRO:CD	2.87	0.52
2:H:2038:ILE:HG22	2:H:2042:ILE:CD1	2.36	0.52
2:I:264:ARG:NH1	2:I:456:GLN:HG3	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:751:LEU:HD23	2:I:791:TYR:CZ	2.44	0.52
2:I:821:ILE:HA	2:I:857:ILE:HD11	1.92	0.52
2:I:949:ASP:CB	2:I:1006:MET:HE2	2.39	0.52
1:A:1123:GLN:HG3	1:A:1124:GLU:N	2.24	0.52
1:B:1020:VAL:HG13	1:B:1400:ILE:HG23	1.91	0.52
1:B:1411:THR:HG22	1:B:1412:ASP:H	1.75	0.52
1:B:338:LEU:O	1:B:342:GLN:HG3	2.10	0.52
1:B:784:ILE:HG23	1:B:788:SER:HB2	1.92	0.52
1:C:1247:SER:HB2	1:C:1332:TYR:HE2	1.75	0.52
1:C:328:LEU:HD22	1:C:328:LEU:C	2.30	0.52
1:C:635:ILE:HG22	1:C:651:TYR:CD1	2.45	0.52
2:G:1589:VAL:HG11	2:G:1640:PHE:CE1	2.45	0.52
2:G:234:ILE:CG1	2:G:235:PRO:HD3	2.40	0.52
2:H:1227:ARG:HG3	2:H:1227:ARG:NH1	2.01	0.52
2:I:1173:VAL:CG2	2:I:1221:MET:HE1	2.39	0.52
2:I:1567:ARG:HG3	2:I:1568:HIS:N	2.22	0.52
2:I:715:GLN:O	2:I:719:ILE:HG12	2.10	0.52
1:A:50:SER:HB2	1:A:51:PRO:CD	2.39	0.52
1:A:36:LEU:CD2	1:A:61:LEU:HD21	2.37	0.52
1:B:1665:ILE:HG12	1:B:1666:THR:N	2.25	0.52
1:B:335:HIS:HD2	1:B:335:HIS:O	1.93	0.52
1:B:529:MET:HG2	1:B:638:LEU:HG	1.92	0.52
1:C:1238:VAL:HG12	1:C:1239:HIS:N	2.25	0.52
2:G:1223:MET:CE	2:G:1238:LEU:HD12	2.40	0.52
2:G:1678:MET:HE3	2:G:1707:LEU:CD2	2.38	0.52
2:H:1081:HIS:O	2:H:1085:LEU:HB2	2.10	0.52
2:H:1422:THR:HG21	2:H:1474:PHE:HB2	1.91	0.52
2:H:1561:ASN:OD1	2:H:1563:ILE:HB	2.10	0.52
2:I:1871:LEU:HD22	2:I:1888:ILE:HD11	1.92	0.52
1:B:1123:GLN:HB2	1:B:1177:LYS:HE2	1.91	0.52
1:B:1238:VAL:HG12	1:B:1239:HIS:N	2.25	0.52
1:B:864:VAL:CG2	1:B:921:PRO:HB3	2.40	0.52
1:C:1665:ILE:CG1	1:C:1669:ARG:HD3	2.36	0.52
1:C:156:ALA:HA	1:C:166:ILE:CD1	2.40	0.52
2:G:1493:LEU:HD11	2:G:1499:VAL:CG2	2.40	0.52
2:H:1148:ASN:ND2	2:H:1151:HIS:H	2.08	0.52
2:H:1475:LYS:CB	2:H:1481:SER:HB2	2.40	0.52
2:H:1722:GLY:N	2:H:1726:GLY:HA3	2.24	0.52
2:H:2046:GLU:C	2:H:2048:TYR:H	2.14	0.52
2:I:1486:PHE:HA	2:I:1504:VAL:O	2.10	0.52
2:I:1745:LYS:HE2	2:I:1747:LYS:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1776:PHE:O	2:I:1779:PRO:HD2	2.09	0.52
2:I:273:HIS:CB	2:I:512:LEU:HD22	2.40	0.52
2:I:346:GLN:HA	2:I:377:LEU:HD21	1.92	0.52
1:B:1477:ILE:H	1:B:1478:PRO:CD	2.23	0.51
1:B:1524:GLY:HA2	1:B:1527:ALA:HB3	1.93	0.51
1:B:50:SER:HB2	1:B:51:PRO:CD	2.40	0.51
1:C:440:MET:HE3	1:C:483:VAL:HG21	1.92	0.51
1:C:465:ASN:O	1:C:469:VAL:HG23	2.09	0.51
2:G:654:VAL:HG12	2:G:654:VAL:O	2.09	0.51
2:H:1004:LEU:CD2	2:H:1019:PRO:HB2	2.40	0.51
2:H:747:HIS:O	2:H:751:LEU:HB2	2.10	0.51
2:I:1223:MET:CE	2:I:1238:LEU:HD12	2.40	0.51
2:I:281:VAL:HG12	2:I:282:ALA:N	2.26	0.51
2:I:913:ASP:H	2:I:916:THR:CG2	2.23	0.51
1:A:411:GLN:HE22	1:A:1628:SER:N	2.06	0.51
1:A:607:LYS:HG2	1:A:608:ASP:N	2.25	0.51
1:B:386:PHE:O	1:B:390:VAL:HB	2.10	0.51
1:C:157:HIS:HE1	1:C:228:LEU:HD22	1.75	0.51
2:H:807:ILE:HG21	2:H:1066:ILE:HA	1.92	0.51
2:H:1775:GLN:HG2	2:H:1836:MET:SD	2.50	0.51
2:H:234:ILE:CG1	2:H:235:PRO:HD3	2.40	0.51
2:I:55:THR:CG2	2:I:56:THR:HG22	2.33	0.51
2:I:786:SER:CB	2:I:794:MET:HE2	2.40	0.51
1:A:1056:ILE:HD13	1:A:1193:TRP:CD1	2.42	0.51
1:B:1682:LYS:HB3	2:H:994:PHE:CE2	2.45	0.51
1:C:1303:GLY:H	1:C:1307:THR:HG22	1.75	0.51
1:C:1411:THR:HG22	1:C:1412:ASP:H	1.75	0.51
2:G:1177:SER:O	2:G:1180:MET:HG2	2.09	0.51
2:G:1438:SER:O	2:G:1441:ILE:HG23	2.09	0.51
2:G:145:LEU:HD21	2:G:156:LEU:HD21	1.91	0.51
2:H:1378:ILE:HG12	2:H:1378:ILE:O	2.10	0.51
2:H:1493:LEU:HD11	2:H:1499:VAL:HG21	1.93	0.51
2:H:1697:HIS:HE1	2:H:1829:GLU:CG	2.23	0.51
2:H:55:THR:HB	2:H:59:GLU:OE2	2.10	0.51
2:H:892:ILE:HG12	2:H:903:TRP:CG	2.45	0.51
1:B:852:ARG:CG	1:B:852:ARG:HH11	2.06	0.51
1:C:1431:GLU:HB3	1:C:1520:ALA:HB2	1.92	0.51
2:G:105:ALA:CB	2:G:533:LEU:HD21	2.40	0.51
2:G:1081:HIS:O	2:G:1085:LEU:HB2	2.10	0.51
2:G:1579:ILE:HD11	2:G:1615:MET:SD	2.51	0.51
2:G:16:LEU:HG	2:G:48:PHE:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1764:PHE:HB2	2:G:1770:LEU:HD21	1.93	0.51
2:G:489:LYS:O	2:G:493:THR:HG22	2.10	0.51
2:H:1435:ILE:HG22	2:H:1435:ILE:O	2.10	0.51
1:B:1585:LYS:H	1:B:1585:LYS:HD3	1.76	0.51
1:C:644:THR:HG22	1:C:648:ASP:O	2.10	0.51
2:G:1431:TYR:CE1	2:G:1526:THR:HG23	2.45	0.51
2:G:1861:ARG:HD2	2:G:1964:PHE:O	2.10	0.51
1:A:20:TYR:CE1	2:G:2035:SER:HB2	2.45	0.51
2:H:1697:HIS:HE1	2:H:1829:GLU:HG2	1.74	0.51
2:H:278:VAL:HG11	2:H:303:LEU:HD13	1.92	0.51
2:H:835:THR:HG22	2:H:844:VAL:C	2.31	0.51
2:H:949:ASP:CB	2:H:1006:MET:HE2	2.40	0.51
2:I:376:ASN:C	2:I:376:ASN:HD22	2.13	0.51
1:A:630:ILE:O	1:A:653:ARG:NH2	2.42	0.51
1:B:1189:ILE:CD1	1:B:1380:GLN:HG3	2.38	0.51
1:B:430:ARG:NH2	1:B:605:LEU:HD13	2.26	0.51
1:C:1584:PRO:HB2	1:C:1587:ALA:HB3	1.92	0.51
1:C:46:GLU:OE1	1:C:53:LEU:HB2	2.10	0.51
2:G:1389:ILE:HG13	2:G:1411:PHE:HD1	1.75	0.51
2:G:1932:SER:O	2:G:1936:VAL:HG22	2.10	0.51
2:G:786:SER:CB	2:G:794:MET:HE2	2.41	0.51
2:G:99:ASN:HA	2:G:550:VAL:HG21	1.92	0.51
2:H:105:ALA:CB	2:H:533:LEU:HD21	2.40	0.51
2:H:332:GLU:OE2	2:H:394:ARG:HD3	2.10	0.51
2:I:1697:HIS:CE1	2:I:1829:GLU:HG2	2.45	0.51
2:I:1716:ASN:OD1	2:I:1765:ARG:HA	2.11	0.51
2:I:1953:VAL:HG12	2:I:1953:VAL:O	2.11	0.51
2:I:2038:ILE:HG22	2:I:2042:ILE:CD1	2.37	0.51
2:I:306:ILE:HA	2:I:439:ILE:CD1	2.40	0.51
2:I:522:GLY:HA3	2:I:561:TRP:CZ3	2.46	0.51
1:A:1577:GLN:HE22	1:A:1591:TRP:C	2.13	0.51
1:A:286:PHE:O	1:A:290:MET:HG2	2.10	0.51
1:B:170:LYS:HD3	1:B:175:LEU:HD23	1.92	0.51
2:G:443:LEU:HD22	2:G:448:VAL:CG1	2.41	0.51
2:G:868:PHE:HB3	2:G:873:PHE:CE2	2.46	0.51
2:H:1389:ILE:HG13	2:H:1411:PHE:HD1	1.76	0.51
2:H:1673:GLU:N	2:H:1676:MET:HE3	2.26	0.51
2:H:598:THR:O	2:H:602:VAL:HB	2.11	0.51
2:H:955:GLU:HG2	2:H:987:TYR:CE2	2.45	0.51
2:I:675:PRO:HG3	2:I:1163:LYS:O	2.11	0.51
2:I:1159:ILE:HG12	2:I:1169:PRO:CD	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:259:THR:HG22	2:I:262:GLU:CB	2.41	0.51
1:A:1004:ILE:HG22	1:A:1660:TYR:CE2	2.46	0.51
1:A:1533:ILE:HD11	1:A:1564:LEU:HD13	1.93	0.51
1:A:34:VAL:O	1:A:38:ASP:HB2	2.10	0.51
1:A:465:ASN:O	1:A:469:VAL:HG23	2.11	0.51
1:B:1104:ARG:O	1:B:1185:VAL:HG13	2.11	0.51
1:B:1303:GLY:H	1:B:1307:THR:HG22	1.76	0.51
1:B:421:ILE:HG12	1:B:469:VAL:HG21	1.93	0.51
1:C:1705:PRO:HB2	1:C:1733:PHE:CE1	2.46	0.51
1:C:260:ARG:HH12	1:C:300:VAL:CG2	2.22	0.51
1:C:340:ARG:HH12	1:C:344:GLN:NE2	2.08	0.51
1:C:411:GLN:HE22	1:C:1628:SER:N	2.09	0.51
2:G:1159:ILE:HG12	2:G:1169:PRO:CD	2.39	0.51
1:A:29:ILE:HG13	2:G:1891:TYR:O	2.10	0.51
2:G:2015:THR:HG22	2:G:2017:LYS:N	2.22	0.51
2:G:281:VAL:HG23	2:G:459:VAL:HG11	1.91	0.51
2:H:1162:ASP:O	2:H:1163:LYS:HB2	2.11	0.51
2:H:1293:THR:HG22	2:H:1296:GLU:CG	2.41	0.51
2:H:1382:VAL:HA	2:H:1422:THR:HG1	1.74	0.51
2:H:1716:ASN:OD1	2:H:1765:ARG:HA	2.11	0.51
2:H:1774:THR:HA	2:H:1777:THR:HB	1.93	0.51
2:I:1313:SER:O	2:I:1314:ARG:HD3	2.11	0.51
2:I:2035:SER:HB3	2:I:2038:ILE:CD1	2.40	0.51
1:A:1105:LEU:HD23	1:A:1185:VAL:HG22	1.93	0.51
1:A:254:TRP:HZ3	1:A:292:GLN:HG3	1.75	0.51
1:B:822:VAL:HG12	1:B:824:LEU:HD22	1.93	0.51
1:B:983:GLN:NE2	2:H:962:LYS:HD2	2.26	0.51
1:C:705:VAL:CG2	1:C:732:LEU:HD21	2.40	0.51
2:G:1452:LEU:HA	2:G:1502:GLY:HA3	1.92	0.51
2:G:145:LEU:O	2:G:149:VAL:HG12	2.10	0.51
2:G:55:THR:CG2	2:G:56:THR:HG22	2.33	0.51
2:H:1845:ASP:HB2	2:H:1849:ARG:N	2.15	0.51
2:H:2026:PHE:HD2	2:H:2045:TRP:HZ3	1.59	0.51
2:H:2030:TYR:CE1	2:H:2034:GLY:HA2	2.46	0.51
2:I:1015:VAL:HG11	2:I:1017:PHE:CE1	2.45	0.51
1:A:1304:ALA:N	1:A:1307:THR:HG22	2.26	0.51
1:A:1181:PHE:CZ	1:A:1341:PHE:HA	2.46	0.51
1:B:1196:LYS:HE3	1:B:1202:ASP:CG	2.31	0.51
1:B:764:ASP:OD2	1:B:818:ARG:HD3	2.11	0.51
1:C:1304:ALA:N	1:C:1307:THR:HG22	2.26	0.51
1:C:1009:LEU:HG	1:C:1664:ALA:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:213:LEU:HG	2:G:213:LEU:O	2.11	0.51
2:G:784:GLU:O	2:G:787:THR:HB	2.11	0.51
2:G:7:ARG:HE	2:G:27:PHE:CB	2.24	0.51
2:H:273:HIS:CB	2:H:512:LEU:HD22	2.41	0.51
2:H:281:VAL:HG12	2:H:282:ALA:N	2.25	0.51
2:H:463:PHE:CE1	2:H:486:LEU:HD22	2.46	0.51
2:H:533:LEU:HD13	2:H:545:GLN:HG3	1.92	0.51
2:I:1359:MET:HE3	2:I:1404:MET:HB3	1.93	0.51
2:I:1918:LYS:HG2	2:I:1919:LEU:HD23	1.92	0.51
2:I:60:LEU:O	2:I:63:LYS:HB2	2.11	0.51
2:I:955:GLU:HG2	2:I:987:TYR:CE2	2.46	0.51
1:A:1347:LYS:HD3	1:A:1347:LYS:O	2.11	0.50
1:B:1411:THR:HG22	1:B:1412:ASP:N	2.26	0.50
1:C:280:GLU:O	1:C:280:GLU:HG2	2.11	0.50
2:G:1272:ASP:O	2:G:1273:GLU:HG3	2.11	0.50
2:G:2035:SER:HB3	2:G:2038:ILE:CG1	2.41	0.50
2:G:732:TRP:CG	2:G:750:MET:HE3	2.46	0.50
2:G:7:ARG:CZ	2:G:24:THR:HA	2.41	0.50
2:G:932:ILE:HD11	2:G:1042:ALA:CB	2.33	0.50
2:H:1475:LYS:HG3	2:H:1481:SER:HB2	1.93	0.50
2:H:2036:GLU:HG2	2:H:2039:LYS:NZ	2.26	0.50
2:H:418:ASN:HD22	2:H:418:ASN:N	2.08	0.50
2:I:157:VAL:HG11	2:I:496:PHE:CZ	2.46	0.50
2:I:1945:ASP:O	2:I:1949:LYS:HG3	2.11	0.50
2:I:1986:LYS:HA	2:I:1989:LYS:HB3	1.93	0.50
2:I:455:ILE:HG12	2:I:469:ARG:HG2	1.92	0.50
1:A:156:ALA:HA	1:A:166:ILE:HD12	1.93	0.50
1:B:635:ILE:HG22	1:B:651:TYR:CD1	2.46	0.50
1:C:1566:ARG:HB3	1:C:1623:TYR:CE1	2.46	0.50
1:C:702:LYS:HE2	1:C:729:GLY:O	2.11	0.50
2:G:440:ASN:ND2	2:G:477:GLU:HG2	2.26	0.50
2:G:601:THR:HG22	2:G:620:ALA:H	1.75	0.50
2:G:611:THR:HA	2:G:615:TYR:O	2.11	0.50
2:G:702:TYR:HB2	2:G:727:PRO:HB2	1.93	0.50
2:H:871:THR:HG21	2:H:887:LYS:NZ	2.26	0.50
1:A:1411:THR:HG22	1:A:1412:ASP:H	1.76	0.50
1:B:1642:THR:HG22	1:B:1652:GLN:HG3	1.93	0.50
1:B:411:GLN:NE2	1:B:1628:SER:H	2.09	0.50
1:B:435:GLU:O	1:B:439:ILE:HG13	2.11	0.50
1:B:674:LYS:O	1:B:675:ASP:HB2	2.11	0.50
1:C:1116:PRO:HB2	1:C:1184:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1455:ARG:O	1:C:1459:ILE:HG13	2.12	0.50
1:C:1584:PRO:O	1:C:1585:LYS:C	2.50	0.50
1:C:157:HIS:CE1	1:C:228:LEU:HD22	2.47	0.50
2:G:1293:THR:HG22	2:G:1296:GLU:CG	2.40	0.50
2:G:1716:ASN:OD1	2:G:1765:ARG:HA	2.12	0.50
2:H:1597:ALA:HB1	2:H:1638:ILE:CD1	2.41	0.50
2:H:432:LEU:HB3	2:H:484:ILE:HG23	1.92	0.50
2:H:732:TRP:CG	2:H:750:MET:HE3	2.47	0.50
2:I:1431:TYR:CE1	2:I:1526:THR:HG23	2.46	0.50
2:I:1678:MET:CE	2:I:1707:LEU:HD22	2.41	0.50
2:I:650:ASN:HD21	3:I:3051:FMN:HN3	1.58	0.50
1:A:142:ASP:CG	1:A:257:PRO:HB2	2.32	0.50
1:A:1474:ALA:HA	1:A:1478:PRO:CD	2.41	0.50
1:A:280:GLU:O	1:A:280:GLU:HG2	2.10	0.50
1:B:1347:LYS:O	1:B:1347:LYS:HD3	2.11	0.50
2:G:1135:GLU:OE2	2:G:1175:LYS:HE3	2.11	0.50
2:G:1873:TYR:CE1	2:G:1877:ARG:NE	2.75	0.50
2:G:1918:LYS:HG2	2:G:1919:LEU:HD23	1.93	0.50
2:H:1428:GLU:HB2	2:H:1468:THR:HG22	1.94	0.50
2:H:1873:TYR:HE1	2:H:1877:ARG:HH21	1.59	0.50
2:H:260:PRO:HD3	2:H:289:TRP:CZ2	2.46	0.50
2:H:344:LEU:HB3	2:H:349:VAL:HG23	1.94	0.50
2:H:750:MET:CG	2:H:796:PHE:HZ	2.25	0.50
2:I:1308:CYS:HB3	2:I:1311:PHE:CD2	2.46	0.50
2:I:344:LEU:HB3	2:I:349:VAL:HG23	1.93	0.50
2:I:460:TYR:HA	2:I:466:SER:O	2.10	0.50
2:I:161:GLY:HA3	2:I:506:PRO:HD2	1.94	0.50
1:B:1600:LEU:HD11	1:B:1655:VAL:HG12	1.94	0.50
1:B:1685:TYR:CE1	2:H:993:GLN:OE1	2.64	0.50
1:C:1392:LEU:HD22	1:C:1396:MET:HG3	1.93	0.50
2:G:105:ALA:HB3	2:G:533:LEU:HD21	1.94	0.50
2:G:1493:LEU:HD11	2:G:1499:VAL:HG21	1.93	0.50
2:G:741:HIS:HB3	2:G:853:PRO:HB2	1.94	0.50
2:H:582:LYS:HE2	2:H:1108:PRO:HB3	1.92	0.50
2:H:1678:MET:CE	2:H:1707:LEU:HD22	2.40	0.50
2:H:1861:ARG:HD2	2:H:1964:PHE:O	2.11	0.50
2:I:1359:MET:HA	2:I:1359:MET:HE3	1.94	0.50
2:I:1475:LYS:CB	2:I:1481:SER:HB2	2.41	0.50
1:C:20:TYR:CG	2:I:2033:THR:OG1	2.65	0.50
1:A:433:VAL:O	1:A:437:ILE:HG13	2.12	0.50
1:A:889:GLU:HG3	1:A:893:VAL:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1105:LEU:HD23	1:B:1185:VAL:HG22	1.93	0.50
1:B:254:TRP:HZ3	1:B:292:GLN:HG3	1.76	0.50
1:C:156:ALA:HA	1:C:166:ILE:HD12	1.92	0.50
1:C:328:LEU:HD13	1:C:329:GLU:N	2.27	0.50
1:C:674:LYS:O	1:C:675:ASP:HB2	2.11	0.50
1:C:702:LYS:HD3	1:C:731:THR:CG2	2.41	0.50
2:G:2046:GLU:C	2:G:2048:TYR:H	2.15	0.50
2:G:24:THR:O	2:G:26:SER:N	2.44	0.50
2:G:281:VAL:HG12	2:G:282:ALA:N	2.26	0.50
2:G:418:ASN:N	2:G:418:ASN:HD22	2.08	0.50
2:G:533:LEU:HD13	2:G:545:GLN:HG3	1.94	0.50
2:G:606:PHE:CE1	2:G:811:VAL:HG13	2.47	0.50
2:H:1822:MET:HE2	2:H:1996:ILE:HG12	1.92	0.50
2:H:491:GLU:HA	2:H:494:THR:HG22	1.93	0.50
2:H:702:TYR:HB2	2:H:727:PRO:HB2	1.94	0.50
2:I:1673:GLU:N	2:I:1676:MET:HE3	2.25	0.50
1:C:29:ILE:HG13	2:I:1891:TYR:O	2.12	0.50
1:A:1234:MET:HG2	1:A:1326:ILE:HD12	1.93	0.50
1:B:1234:MET:HE3	1:B:1326:ILE:HG21	1.92	0.50
1:B:1705:PRO:HB2	1:B:1733:PHE:CE1	2.46	0.50
1:C:1264:ARG:NH1	1:C:1270:VAL:HB	2.27	0.50
1:C:1474:ALA:HA	1:C:1478:PRO:CD	2.42	0.50
1:C:335:HIS:O	1:C:335:HIS:CD2	2.65	0.50
1:C:627:SER:HB2	1:C:657:SER:CB	2.41	0.50
1:C:828:PRO:HG3	1:C:868:ILE:HG22	1.94	0.50
2:G:814:SER:HB2	2:G:1040:LEU:HD13	1.93	0.50
2:G:1593:ILE:HD13	2:G:1626:ILE:HD13	1.92	0.50
2:G:1697:HIS:HE1	2:G:1829:GLU:CG	2.25	0.50
2:G:2035:SER:HB3	2:G:2038:ILE:CD1	2.42	0.50
2:G:751:LEU:HD23	2:G:791:TYR:CZ	2.46	0.50
2:G:949:ASP:CB	2:G:1006:MET:HE2	2.40	0.50
2:H:1148:ASN:HD22	2:H:1151:HIS:H	1.60	0.50
2:H:1889:VAL:HG13	2:H:1977:HIS:HB3	1.93	0.50
2:I:1428:GLU:HB2	2:I:1468:THR:HG22	1.93	0.50
2:I:1774:THR:HA	2:I:1777:THR:HB	1.92	0.50
1:B:1362:PRO:HA	1:B:1365:MET:HG3	1.94	0.50
1:B:1451:GLN:OE1	1:B:1451:GLN:HA	2.12	0.50
1:C:888:ILE:HD12	1:C:939:PHE:CE2	2.44	0.50
2:G:1871:LEU:HD22	2:G:1888:ILE:HD11	1.93	0.50
2:G:1913:VAL:O	2:G:1917:ILE:HG13	2.12	0.50
2:G:732:TRP:CD1	2:G:750:MET:HE3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:836:TYR:HA	2:G:845:THR:OG1	2.11	0.50
2:H:1308:CYS:HB3	2:H:1311:PHE:CD2	2.47	0.50
2:H:1593:ILE:O	2:H:1597:ALA:HB3	2.12	0.50
2:H:161:GLY:N	2:H:505:GLY:HA3	2.25	0.50
2:H:233:SER:HA	2:H:424:ALA:CB	2.41	0.50
2:H:638:VAL:HG22	2:H:675:PRO:HG2	1.94	0.50
2:I:1027:ILE:O	2:I:1031:LYS:HB2	2.11	0.50
2:I:238:CYS:CB	2:I:239:PRO:HD3	2.40	0.50
2:I:324:LEU:HD12	2:I:324:LEU:O	2.12	0.50
2:I:807:ILE:HG21	2:I:1066:ILE:HA	1.92	0.50
1:A:1104:ARG:O	1:A:1185:VAL:HG13	2.12	0.50
1:A:408:TRP:CH2	1:A:1628:SER:HB3	2.47	0.50
1:B:156:ALA:HA	1:B:166:ILE:CD1	2.41	0.50
1:C:1105:LEU:HD23	1:C:1185:VAL:HG22	1.94	0.50
1:C:1123:GLN:HB2	1:C:1177:LYS:HE2	1.93	0.50
1:C:267:VAL:HG12	1:C:290:MET:CE	2.42	0.50
2:G:1382:VAL:HA	2:G:1422:THR:HG1	1.76	0.50
2:G:1552:PRO:O	2:G:1556:VAL:HG23	2.12	0.50
2:G:60:LEU:O	2:G:63:LYS:HB2	2.12	0.50
2:H:121:GLU:HA	2:H:124:LYS:HD2	1.93	0.50
2:H:455:ILE:HD11	2:H:469:ARG:NE	2.27	0.50
2:H:835:THR:HG21	2:H:855:HIS:HD2	1.70	0.50
2:H:995:LEU:HB3	2:H:1000:ILE:HD11	1.94	0.50
2:I:1435:ILE:O	2:I:1435:ILE:HG22	2.12	0.50
2:I:1493:LEU:HD11	2:I:1499:VAL:HG21	1.93	0.50
2:I:173:LEU:HD13	2:I:219:LEU:HD21	1.93	0.50
1:A:1125:VAL:HG21	1:A:1175:ILE:CD1	2.42	0.49
1:A:1451:GLN:OE1	1:A:1451:GLN:HA	2.12	0.49
1:A:1459:ILE:O	1:A:1463:VAL:HG23	2.12	0.49
1:A:157:HIS:HE1	1:A:228:LEU:HD22	1.76	0.49
1:A:328:LEU:HD13	1:A:329:GLU:N	2.27	0.49
1:B:157:HIS:HE1	1:B:228:LEU:HD22	1.77	0.49
1:B:413:LEU:HB2	1:B:439:ILE:HD13	1.94	0.49
1:B:790:PHE:CE2	1:B:794:ILE:HD11	2.47	0.49
2:G:369:SER:HG	2:G:380:SER:HB3	1.73	0.49
2:H:102:HIS:HE1	2:H:180:TYR:OH	1.95	0.49
2:H:214:ASN:ND2	2:H:217:GLU:HB2	2.27	0.49
2:H:460:TYR:HA	2:H:466:SER:O	2.12	0.49
2:H:7:ARG:CZ	2:H:24:THR:HA	2.42	0.49
2:H:868:PHE:HB3	2:H:873:PHE:CE2	2.47	0.49
2:I:1378:ILE:O	2:I:1378:ILE:HG12	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1873:TYR:CE2	2:I:1940:LEU:HD21	2.47	0.49
2:I:7:ARG:CZ	2:I:24:THR:HA	2.42	0.49
2:I:194:THR:CG2	2:I:300:ILE:HD11	2.40	0.49
2:I:402:LEU:HD12	2:I:404:GLN:HG2	1.94	0.49
2:I:611:THR:HA	2:I:615:TYR:O	2.11	0.49
1:B:156:ALA:HA	1:B:166:ILE:HD12	1.93	0.49
1:B:465:ASN:O	1:B:469:VAL:HG23	2.12	0.49
1:C:1665:ILE:HG12	1:C:1666:THR:N	2.27	0.49
1:C:176:VAL:HG12	1:C:178:GLY:H	1.77	0.49
1:C:233:ILE:HD13	1:C:237:MET:HE3	1.94	0.49
1:C:56:MET:HG3	2:I:1893:VAL:CG2	2.42	0.49
1:C:655:LEU:CD2	1:C:916:LEU:HD11	2.39	0.49
2:G:463:PHE:CE1	2:G:486:LEU:HD22	2.47	0.49
2:G:491:GLU:HA	2:G:494:THR:HG22	1.95	0.49
2:G:597:MET:H	2:G:601:THR:HB	1.77	0.49
2:G:677:GLN:O	2:G:678:PHE:HB3	2.13	0.49
2:G:740:HIS:HA	2:G:854:ILE:HD13	1.94	0.49
2:H:1745:LYS:HD3	2:H:1747:LYS:HE2	1.94	0.49
2:H:2035:SER:HB3	2:H:2038:ILE:CD1	2.42	0.49
2:H:461:ASP:HB3	2:H:464:ASP:HB2	1.93	0.49
2:I:24:THR:O	2:I:26:SER:N	2.45	0.49
2:I:274:SER:OG	2:I:428:HIS:HE1	1.96	0.49
2:I:573:LYS:HE3	2:I:1101:GLU:OE1	2.12	0.49
2:I:712:ALA:O	2:I:715:GLN:HB3	2.12	0.49
1:A:1419:PRO:HB3	1:A:1646:PHE:CE2	2.48	0.49
1:A:1401:TYR:C	1:A:1658:PRO:HG3	2.33	0.49
1:B:1474:ALA:HA	1:B:1478:PRO:CD	2.41	0.49
1:B:1584:PRO:O	1:B:1585:LYS:C	2.50	0.49
1:C:1050:CYS:HB3	1:C:1089:VAL:HG12	1.93	0.49
1:C:790:PHE:CE2	1:C:794:ILE:HD11	2.48	0.49
1:C:889:GLU:HG3	1:C:893:VAL:O	2.13	0.49
2:G:1441:ILE:HD11	2:G:1445:ARG:NH2	2.25	0.49
2:G:157:VAL:HG11	2:G:496:PHE:CZ	2.47	0.49
2:G:1666:PHE:CD1	2:G:1814:ALA:HA	2.47	0.49
2:G:1845:ASP:HB2	2:G:1849:ARG:N	2.15	0.49
1:A:980:VAL:HG23	2:G:968:GLN:OE1	2.12	0.49
2:H:1567:ARG:NH1	2:H:1567:ARG:CG	2.50	0.49
2:H:7:ARG:HE	2:H:27:PHE:CB	2.25	0.49
2:H:306:ILE:HA	2:H:439:ILE:CD1	2.43	0.49
2:H:634:ILE:HD11	2:H:649:ILE:CD1	2.40	0.49
2:I:950:PHE:O	2:I:954:VAL:HG23	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ILE:HD13	1:B:255:GLY:O	2.11	0.49
1:C:34:VAL:O	1:C:38:ASP:HB2	2.11	0.49
1:C:415:SER:O	1:C:419:GLU:HB2	2.12	0.49
1:C:764:ASP:OD2	1:C:818:ARG:HD3	2.12	0.49
2:G:1350:LEU:HD11	2:G:1410:PHE:HB3	1.93	0.49
2:G:1428:GLU:HG2	2:G:1470:THR:HG22	1.94	0.49
2:G:194:THR:CG2	2:G:300:ILE:HD11	2.41	0.49
2:G:306:ILE:HA	2:G:439:ILE:CD1	2.42	0.49
2:G:676:ILE:HG12	2:G:676:ILE:O	2.11	0.49
1:B:11:HIS:HE1	2:H:1996:ILE:O	1.94	0.49
2:H:259:THR:HG22	2:H:262:GLU:CB	2.42	0.49
2:H:777:THR:HG23	2:H:1081:HIS:CE1	2.47	0.49
2:I:72:VAL:HG12	2:I:73:GLU:N	2.28	0.49
2:I:7:ARG:HE	2:I:27:PHE:CB	2.25	0.49
2:I:866:LYS:O	2:I:870:GLU:HG3	2.12	0.49
1:A:1312:VAL:CG2	1:A:1329:VAL:HG11	2.41	0.49
1:B:1419:PRO:HB3	1:B:1646:PHE:CE2	2.48	0.49
1:B:1455:ARG:NH2	1:B:1459:ILE:HG12	2.26	0.49
1:B:1533:ILE:HG13	1:B:1564:LEU:HB3	1.94	0.49
1:B:46:GLU:OE1	1:B:53:LEU:HB2	2.12	0.49
1:C:1020:VAL:CG1	1:C:1400:ILE:HG23	2.42	0.49
1:C:254:TRP:HZ3	1:C:292:GLN:HG3	1.77	0.49
2:G:1776:PHE:O	2:G:1779:PRO:HD2	2.12	0.49
2:H:173:LEU:O	2:H:173:LEU:HD22	2.13	0.49
2:H:732:TRP:CD2	2:H:750:MET:HE3	2.48	0.49
2:I:777:THR:HG23	2:I:1081:HIS:CE1	2.47	0.49
2:I:1135:GLU:OE2	2:I:1175:LYS:HE3	2.12	0.49
2:I:1844:ARG:NH1	2:I:1844:ARG:CG	2.61	0.49
2:I:1850:SER:HB2	2:I:1973:SER:HB2	1.95	0.49
2:I:2026:PHE:HD2	2:I:2045:TRP:HZ3	1.60	0.49
2:I:629:GLY:O	2:I:632:ALA:HB3	2.12	0.49
2:I:682:GLY:O	2:I:683:ALA:HB3	2.13	0.49
1:A:1009:LEU:HD13	1:A:1445:MET:HE1	1.94	0.49
1:A:427:ASN:ND2	1:A:610:THR:H	2.05	0.49
1:B:9:LEU:HD23	2:H:2041:ILE:HD13	1.95	0.49
1:C:256:LEU:HD22	1:C:260:ARG:HB3	1.95	0.49
2:G:1547:PRO:HD3	2:G:1584:PHE:CE2	2.47	0.49
2:G:1567:ARG:CG	2:G:1567:ARG:NH1	2.51	0.49
2:G:2029:VAL:O	2:G:2033:THR:HG22	2.13	0.49
2:G:273:HIS:CB	2:G:512:LEU:HD22	2.43	0.49
2:G:774:ALA:HB1	2:G:1081:HIS:CD2	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:860:ARG:HB2	2:H:1049:GLN:HG3	1.94	0.49
2:H:369:SER:O	2:H:370:LEU:HD23	2.13	0.49
2:H:758:ARG:NH2	2:H:797:ASP:OD1	2.35	0.49
2:I:1130:THR:H	2:I:1133:THR:CG2	2.25	0.49
2:I:1491:VAL:HB	2:I:1501:ILE:HD12	1.93	0.49
1:A:1523:ARG:NH2	1:A:1564:LEU:O	2.45	0.49
1:A:1705:PRO:HB2	1:A:1733:PHE:CE1	2.47	0.49
1:B:328:LEU:N	1:B:330:GLU:H	2.11	0.49
1:C:267:VAL:O	1:C:290:MET:HE1	2.13	0.49
1:C:733:ILE:CD1	1:C:761:LEU:HD11	2.40	0.49
2:G:706:LYS:HE2	2:G:731:GLN:OE1	2.13	0.49
2:H:1040:LEU:O	2:H:1046:GLN:HG3	2.13	0.49
2:H:826:GLY:HA2	2:H:1060:ALA:HB3	1.94	0.49
2:H:1323:MET:CE	2:H:1605:VAL:HG22	2.42	0.49
2:H:1632:ILE:O	2:H:1632:ILE:HG23	2.13	0.49
2:H:747:HIS:HE1	2:H:780:TYR:OH	1.95	0.49
2:I:345:THR:HG22	2:I:347:GLU:N	2.23	0.49
2:I:768:GLY:HA3	2:I:800:LEU:CD2	2.41	0.49
2:I:995:LEU:HB3	2:I:1000:ILE:HD11	1.95	0.49
1:A:1477:ILE:H	1:A:1478:PRO:HD3	1.78	0.49
1:A:430:ARG:NH2	1:A:605:LEU:HD13	2.27	0.49
1:A:927:ASN:O	1:A:929:GLY:N	2.41	0.49
1:B:1056:ILE:HD13	1:B:1193:TRP:CD1	2.45	0.49
1:B:182:VAL:O	1:B:186:ILE:HG13	2.12	0.49
2:G:1130:THR:H	2:G:1133:THR:CG2	2.26	0.49
2:G:1425:LYS:HG2	2:G:1471:GLU:CG	2.37	0.49
2:G:1300:PHE:CA	2:G:1556:VAL:HG11	2.42	0.49
2:G:1673:GLU:N	2:G:1676:MET:HE3	2.26	0.49
2:G:11:LEU:HD11	2:G:64:PHE:CD2	2.48	0.49
2:H:597:MET:H	2:H:601:THR:HB	1.78	0.49
2:H:682:GLY:O	2:H:683:ALA:HB3	2.13	0.49
2:I:814:SER:CB	2:I:1040:LEU:HD13	2.42	0.49
2:I:1266:TYR:HB2	2:I:1347:LEU:HD23	1.95	0.49
2:I:1697:HIS:HE1	2:I:1829:GLU:CG	2.26	0.49
2:I:1745:LYS:HD3	2:I:1747:LYS:HE2	1.93	0.49
2:I:306:ILE:HA	2:I:439:ILE:HD13	1.94	0.49
1:A:400:ARG:CG	1:A:400:ARG:NH1	2.47	0.49
1:A:67:SER:OG	2:I:359:HIS:HE1	1.95	0.49
1:B:1009:LEU:HA	1:B:1445:MET:HE2	1.95	0.49
1:B:1014:ASP:H	1:B:1510:ASN:ND2	2.06	0.49
1:B:187:LEU:HD22	1:B:201:PRO:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1584:PRO:HG3	1:C:1591:TRP:CH2	2.47	0.49
1:C:983:GLN:NE2	2:I:962:LYS:HD2	2.27	0.49
2:G:1486:PHE:HA	2:G:1504:VAL:O	2.12	0.49
2:G:1567:ARG:NH1	2:G:1568:HIS:HB3	2.28	0.49
2:G:463:PHE:O	2:G:463:PHE:HD2	1.95	0.49
2:H:569:LEU:HD12	2:H:1090:TYR:CD1	2.48	0.49
2:H:489:LYS:O	2:H:493:THR:HG22	2.13	0.49
2:I:569:LEU:HD12	2:I:1090:TYR:CD1	2.48	0.49
2:I:1632:ILE:HG23	2:I:1632:ILE:O	2.12	0.49
2:I:926:LEU:HB3	2:I:947:THR:CG2	2.43	0.49
1:B:825:PRO:HB2	1:B:843:LYS:NZ	2.27	0.49
1:C:1419:PRO:HB3	1:C:1646:PHE:CE2	2.47	0.49
1:C:427:ASN:HB2	1:C:468:LEU:HD21	1.95	0.49
2:G:569:LEU:HD12	2:G:1090:TYR:CD1	2.48	0.49
2:G:2026:PHE:HD2	2:G:2045:TRP:HZ3	1.60	0.49
2:G:455:ILE:HG12	2:G:469:ARG:HG2	1.94	0.49
2:H:1441:ILE:HD11	2:H:1445:ARG:NH2	2.27	0.49
2:H:22:VAL:HG11	2:H:27:PHE:HA	1.94	0.49
2:H:950:PHE:O	2:H:954:VAL:HG23	2.13	0.49
2:I:1697:HIS:HE1	2:I:1829:GLU:HG2	1.77	0.49
2:I:1738:PHE:CE1	2:I:1837:THR:HG23	2.48	0.49
2:I:249:TYR:CD2	2:I:283:ILE:HD11	2.48	0.49
2:I:428:HIS:HD2	2:I:486:LEU:O	1.95	0.49
2:I:55:THR:HB	2:I:59:GLU:OE2	2.13	0.49
2:I:900:GLN:NE2	2:I:1051:THR:HA	2.28	0.49
1:A:1264:ARG:NH1	1:A:1270:VAL:HB	2.28	0.48
1:A:46:GLU:OE1	1:A:53:LEU:HB2	2.12	0.48
1:A:987:ASN:HD22	2:G:957:ARG:HD2	1.77	0.48
1:B:1183:ARG:NH1	1:B:1344:GLY:HA2	2.28	0.48
1:B:243:ILE:O	1:B:247:ARG:HG3	2.13	0.48
1:C:1119:LYS:HE2	1:C:1341:PHE:CG	2.48	0.48
1:C:420:ILE:HG22	1:C:469:VAL:HG22	1.96	0.48
2:G:1325:PHE:CE1	2:G:1328:VAL:HG11	2.48	0.48
2:G:1427:VAL:HG22	2:G:1469:GLU:HG2	1.94	0.48
2:G:2038:ILE:HG22	2:G:2042:ILE:CD1	2.37	0.48
2:G:463:PHE:CD1	2:G:486:LEU:HD22	2.48	0.48
2:G:682:GLY:O	2:G:683:ALA:HB3	2.12	0.48
2:H:1272:ASP:O	2:H:1273:GLU:HG3	2.13	0.48
2:H:1438:SER:O	2:H:1441:ILE:HG23	2.13	0.48
2:H:176:LEU:HD22	2:H:247:ALA:HB1	1.95	0.48
2:H:522:GLY:O	2:H:560:ASN:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:705:VAL:CG2	1:B:732:LEU:HD21	2.43	0.48
1:C:1114:TYR:CD1	1:C:1337:GLU:HG3	2.48	0.48
1:C:1392:LEU:CD2	1:C:1396:MET:HG3	2.43	0.48
1:C:1523:ARG:NH2	1:C:1564:LEU:O	2.46	0.48
1:C:331:ILE:HG23	1:C:332:THR:N	2.28	0.48
1:C:386:PHE:O	1:C:390:VAL:HB	2.14	0.48
1:C:430:ARG:CZ	1:C:605:LEU:HD13	2.43	0.48
2:G:1266:TYR:HB2	2:G:1347:LEU:HD23	1.95	0.48
2:G:1330:GLY:HA2	2:G:1374:THR:HG21	1.94	0.48
2:G:653:TYR:HD1	2:G:659:LEU:HD21	1.78	0.48
2:G:618:GLU:HG2	2:G:678:PHE:CZ	2.48	0.48
2:H:901:LYS:NZ	2:H:1031:LYS:O	2.46	0.48
2:H:1624:THR:HB	2:H:1642:THR:OG1	2.14	0.48
2:H:1842:VAL:HG21	2:H:1975:PRO:HD3	1.95	0.48
2:H:397:LYS:HB3	2:H:416:PHE:CE2	2.48	0.48
2:H:232:LEU:HD21	2:H:423:VAL:HA	1.95	0.48
2:H:465:GLY:HA2	2:H:493:THR:HA	1.95	0.48
2:I:1325:PHE:CE1	2:I:1328:VAL:HG11	2.48	0.48
2:I:1579:ILE:HD11	2:I:1615:MET:SD	2.54	0.48
2:I:562:LEU:HG	2:I:793:PRO:CB	2.44	0.48
2:I:881:VAL:N	2:I:882:PRO:CD	2.76	0.48
1:A:1362:PRO:HA	1:A:1365:MET:HG3	1.94	0.48
1:A:340:ARG:HH12	1:A:344:GLN:HE21	1.60	0.48
1:B:256:LEU:HD22	1:B:260:ARG:HB3	1.95	0.48
1:B:328:LEU:HD13	1:B:329:GLU:N	2.28	0.48
1:B:413:LEU:C	1:B:415:SER:H	2.17	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:1010:GLU:HA	1:C:1664:ALA:HA	1.95	0.48
1:C:237:MET:HG3	1:C:241:PHE:HB3	1.95	0.48
2:G:109:LEU:HD11	2:G:116:LEU:CD2	2.41	0.48
2:G:428:HIS:CD2	2:G:488:VAL:HG23	2.47	0.48
2:G:741:HIS:HB2	2:G:853:PRO:O	2.13	0.48
2:I:11:LEU:HD11	2:I:64:PHE:CD2	2.47	0.48
2:I:750:MET:CG	2:I:796:PHE:HZ	2.24	0.48
2:I:741:HIS:HB3	2:I:853:PRO:HB2	1.95	0.48
1:A:1037:TRP:HB2	1:A:1598:GLN:OE1	2.13	0.48
1:A:695:GLY:HA3	1:A:906:LEU:HD11	1.94	0.48
1:B:1116:PRO:HB2	1:B:1184:LEU:HD12	1.95	0.48
1:B:1125:VAL:HG21	1:B:1175:ILE:CD1	2.42	0.48
1:C:1019:ILE:HG21	1:C:1316:VAL:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HE3	1:C:9:LEU:HD12	1.94	0.48
2:G:1148:ASN:ND2	2:G:1151:HIS:H	2.11	0.48
2:G:1213:LEU:O	2:G:1214:LEU:HD23	2.12	0.48
2:G:1868:GLN:HG3	2:G:1898:TYR:CZ	2.48	0.48
2:G:545:GLN:NE2	2:G:545:GLN:H	2.09	0.48
2:G:598:THR:O	2:G:602:VAL:HB	2.13	0.48
2:G:715:GLN:O	2:G:719:ILE:HG12	2.13	0.48
2:G:950:PHE:O	2:G:954:VAL:HG23	2.13	0.48
2:H:169:TYR:CG	2:H:170:PHE:N	2.81	0.48
2:H:1986:LYS:HA	2:H:1989:LYS:HB3	1.95	0.48
2:H:441:LYS:O	2:H:444:VAL:HG12	2.12	0.48
2:H:715:GLN:O	2:H:719:ILE:HG12	2.13	0.48
2:H:932:ILE:HD12	2:H:939:PHE:HD1	1.78	0.48
2:I:1081:HIS:O	2:I:1085:LEU:HB2	2.13	0.48
2:I:1159:ILE:HG22	2:I:1160:THR:N	2.28	0.48
2:I:1169:PRO:O	2:I:1173:VAL:HG23	2.13	0.48
2:I:173:LEU:O	2:I:173:LEU:HD22	2.13	0.48
2:I:1784:MET:HE2	2:I:1784:MET:O	2.13	0.48
2:I:1834:ARG:NH1	2:I:1834:ARG:CG	2.66	0.48
1:A:1:MET:HE3	1:A:9:LEU:HD12	1.95	0.48
1:A:335:HIS:O	1:A:338:LEU:HB3	2.12	0.48
1:A:683:ALA:HA	1:A:689:GLY:HA3	1.95	0.48
1:B:683:ALA:HA	1:B:689:GLY:HA3	1.96	0.48
2:G:593:LEU:HD21	2:G:800:LEU:HB3	1.96	0.48
2:G:720:ALA:HA	2:G:728:ILE:CD1	2.43	0.48
2:H:1323:MET:HE3	2:H:1605:VAL:HG22	1.96	0.48
2:H:1566:SER:HB3	2:H:1568:HIS:CE1	2.47	0.48
2:H:1674:GLN:OE1	2:H:1712:ASN:HA	2.12	0.48
2:H:455:ILE:HG13	2:H:455:ILE:O	2.14	0.48
2:H:428:HIS:CD2	2:H:488:VAL:HG23	2.49	0.48
2:I:16:LEU:HG	2:I:48:PHE:CZ	2.48	0.48
2:I:663:ILE:HB	2:I:664:PRO:CD	2.42	0.48
2:I:871:THR:HG21	2:I:887:LYS:HZ2	1.78	0.48
2:I:970:TYR:O	2:I:973:LEU:HB2	2.13	0.48
1:A:1116:PRO:HB2	1:A:1184:LEU:HD12	1.94	0.48
1:A:1189:ILE:HG23	1:A:1190:PRO:HD2	1.94	0.48
1:A:182:VAL:O	1:A:186:ILE:HG13	2.14	0.48
1:B:186:ILE:O	1:B:190:LEU:HG	2.13	0.48
1:C:50:SER:HB2	1:C:51:PRO:CD	2.43	0.48
2:G:1745:LYS:HE2	2:G:1747:LYS:HG2	1.95	0.48
2:G:259:THR:HG22	2:G:262:GLU:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:145:LEU:HD21	2:H:156:LEU:HD21	1.95	0.48
2:H:1868:GLN:HG3	2:H:1898:TYR:CZ	2.48	0.48
2:H:1918:LYS:HG2	2:H:1919:LEU:HD23	1.96	0.48
2:I:1015:VAL:HG13	2:I:1017:PHE:CE2	2.48	0.48
2:I:455:ILE:O	2:I:455:ILE:HG13	2.13	0.48
2:I:747:HIS:HE1	2:I:780:TYR:OH	1.97	0.48
2:I:758:ARG:NH2	2:I:797:ASP:OD1	2.38	0.48
2:I:85:ASN:HD22	2:I:135:ARG:NH1	2.04	0.48
1:A:1061:SER:HB2	1:A:1078:SER:HB3	1.96	0.48
1:A:1584:PRO:O	1:A:1585:LYS:C	2.51	0.48
1:A:985:ARG:HH12	2:G:953:ARG:CZ	2.26	0.48
1:B:438:ASN:HD21	1:B:698:GLN:HE21	1.61	0.48
1:C:852:ARG:CG	1:C:852:ARG:NH1	2.66	0.48
2:G:1493:LEU:HB3	2:G:1494:PRO:HD2	1.96	0.48
2:G:1590:ARG:HG3	2:G:1608:TYR:CD2	2.48	0.48
2:G:173:LEU:HD13	2:G:219:LEU:HD21	1.94	0.48
2:G:1666:PHE:CD1	2:G:1814:ALA:HB2	2.49	0.48
2:G:55:THR:HB	2:G:59:GLU:OE2	2.14	0.48
2:H:1953:VAL:O	2:H:1953:VAL:HG12	2.13	0.48
2:H:40:ILE:O	2:H:42:PRO:HD3	2.13	0.48
2:H:161:GLY:HA3	2:H:506:PRO:HD2	1.94	0.48
2:H:967:ILE:HD12	2:H:972:LEU:HD22	1.96	0.48
2:I:1674:GLN:OE1	2:I:1712:ASN:HA	2.13	0.48
2:I:593:LEU:HD21	2:I:800:LEU:HB3	1.95	0.48
2:I:753:MET:O	2:I:757:ILE:HG13	2.14	0.48
1:A:256:LEU:HD22	1:A:260:ARG:HB3	1.94	0.48
1:A:908:LEU:HA	1:A:913:VAL:HG21	1.96	0.48
1:B:34:VAL:O	1:B:38:ASP:HB2	2.14	0.48
1:C:1617:ILE:O	1:C:1620:GLN:HG2	2.13	0.48
1:C:335:HIS:O	1:C:338:LEU:HB3	2.14	0.48
1:C:400:ARG:HH11	1:C:400:ARG:HG3	1.72	0.48
2:G:1180:MET:HB2	2:G:1197:LEU:HD21	1.95	0.48
2:G:1651:LEU:O	2:G:1652:THR:HG23	2.14	0.48
2:G:376:ASN:C	2:G:376:ASN:ND2	2.67	0.48
2:G:754:TYR:CE2	2:G:794:MET:HG3	2.48	0.48
2:H:739:GLY:HA2	2:H:1054:LEU:HG	1.95	0.48
2:G:318:SER:HB3	2:H:1595:ASN:HD21	1.78	0.48
2:H:1873:TYR:CE1	2:H:1877:ARG:NE	2.78	0.48
2:H:7:ARG:HH11	2:H:24:THR:HG23	1.75	0.48
2:H:428:HIS:HD2	2:H:486:LEU:O	1.96	0.48
2:H:463:PHE:CD1	2:H:486:LEU:HD22	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:955:GLU:HG2	2:H:987:TYR:HE2	1.78	0.48
1:A:1319:ILE:HA	1:A:1324:ALA:O	2.14	0.48
1:B:157:HIS:CE1	1:B:228:LEU:HD22	2.49	0.48
2:G:1148:ASN:HD22	2:G:1148:ASN:C	2.17	0.48
2:G:173:LEU:HD22	2:G:173:LEU:O	2.13	0.48
2:G:40:ILE:O	2:G:42:PRO:HD3	2.14	0.48
2:G:465:GLY:HA2	2:G:493:THR:HA	1.95	0.48
2:H:1130:THR:H	2:H:1133:THR:CG2	2.27	0.48
2:H:238:CYS:CB	2:H:239:PRO:HD3	2.43	0.48
2:H:376:ASN:C	2:H:376:ASN:HD22	2.18	0.48
2:H:786:SER:CB	2:H:794:MET:HE2	2.43	0.48
2:I:1567:ARG:NH1	2:I:1568:HIS:HB3	2.28	0.48
2:I:233:SER:HA	2:I:424:ALA:CB	2.44	0.48
2:I:551:THR:HG22	2:I:552:SER:N	2.29	0.48
2:I:835:THR:CB	2:I:845:THR:HG23	2.42	0.48
2:I:894:ARG:NH1	2:I:898:ASP:OD2	2.42	0.48
1:A:1501:LEU:O	1:A:1505:GLN:HG3	2.14	0.48
1:A:176:VAL:HG12	1:A:178:GLY:H	1.79	0.48
1:A:157:HIS:CE1	1:A:228:LEU:HD22	2.48	0.48
1:A:427:ASN:HB2	1:A:468:LEU:HD21	1.95	0.48
1:A:852:ARG:NH1	1:A:852:ARG:CG	2.73	0.48
1:B:2:LYS:HE2	1:B:4:GLU:CD	2.34	0.48
1:C:1738:ILE:O	1:C:1739:GLN:HB2	2.14	0.48
1:C:751:PHE:CZ	1:C:761:LEU:HD13	2.49	0.48
2:G:240:LEU:O	2:G:244:ILE:HG13	2.13	0.48
2:G:455:ILE:O	2:G:455:ILE:HG13	2.14	0.48
2:G:72:VAL:HG12	2:G:73:GLU:N	2.28	0.48
2:G:807:ILE:HD12	2:G:1063:THR:HG23	1.95	0.48
2:I:675:PRO:HD3	2:I:1164:MET:HE2	1.95	0.48
2:I:131:ILE:HD12	2:I:182:VAL:CB	2.42	0.48
2:I:1496:LYS:HE2	2:I:1693:ARG:NH2	2.25	0.48
2:I:1804:PHE:CD2	2:I:1818:LEU:HD22	2.49	0.48
2:I:278:VAL:HG11	2:I:303:LEU:HD13	1.95	0.48
2:I:455:ILE:HD11	2:I:469:ARG:NE	2.29	0.48
1:A:1158:PRO:HD2	1:A:1159:GLU:OE2	2.14	0.47
1:A:1682:LYS:HB3	2:G:994:PHE:CE2	2.49	0.47
1:A:19:ALA:O	1:A:22:PHE:HB2	2.14	0.47
1:A:243:ILE:O	1:A:247:ARG:HG3	2.14	0.47
1:A:332:THR:HG22	1:B:331:ILE:HD11	1.96	0.47
1:C:186:ILE:O	1:C:190:LEU:HG	2.14	0.47
1:C:370:GLU:O	1:C:373:ALA:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1873:TYR:CE2	2:G:1940:LEU:HD21	2.49	0.47
2:G:732:TRP:CD2	2:G:750:MET:HE3	2.48	0.47
2:H:1417:THR:C	2:H:1419:PHE:H	2.18	0.47
2:H:1425:LYS:HG2	2:H:1471:GLU:CG	2.38	0.47
2:H:1590:ARG:NH2	2:H:1594:GLU:OE2	2.47	0.47
2:H:463:PHE:O	2:H:463:PHE:HD2	1.96	0.47
1:B:983:GLN:NE2	2:H:962:LYS:HB2	2.28	0.47
2:I:1764:PHE:HB2	2:I:1770:LEU:HD21	1.96	0.47
2:I:489:LYS:O	2:I:493:THR:HG22	2.13	0.47
2:I:533:LEU:HG	2:I:533:LEU:O	2.13	0.47
1:A:1021:VAL:HG22	1:A:1387:ILE:HG22	1.95	0.47
1:A:20:TYR:HE1	2:G:2035:SER:HB2	1.79	0.47
1:A:529:MET:HE3	1:A:529:MET:CA	2.36	0.47
1:B:1319:ILE:HA	1:B:1324:ALA:O	2.13	0.47
1:B:1310:GLU:OE1	1:B:1649:LYS:CE	2.62	0.47
1:B:335:HIS:O	1:B:338:LEU:HB3	2.14	0.47
1:B:741:SER:HB3	1:B:744:ASP:HB2	1.97	0.47
2:G:1566:SER:HB3	2:G:1568:HIS:CE1	2.49	0.47
2:G:1676:MET:HE1	2:G:1781:LEU:CD2	2.43	0.47
2:G:461:ASP:HB3	2:G:464:ASP:HB2	1.96	0.47
2:G:995:LEU:HB3	2:G:1000:ILE:HD11	1.95	0.47
2:H:1427:VAL:HG22	2:H:1469:GLU:HG2	1.96	0.47
2:H:157:VAL:HG11	2:H:496:PHE:CZ	2.49	0.47
2:H:33:LEU:HD21	2:H:80:PHE:CE2	2.49	0.47
2:H:740:HIS:HA	2:H:854:ILE:HD13	1.96	0.47
2:I:146:PHE:HA	2:I:149:VAL:HG12	1.93	0.47
2:I:214:ASN:ND2	2:I:217:GLU:HB2	2.28	0.47
2:I:845:THR:HG22	2:I:855:HIS:CD2	2.49	0.47
1:A:1238:VAL:CG1	1:A:1242:GLU:HB2	2.44	0.47
1:B:889:GLU:HG3	1:B:893:VAL:O	2.15	0.47
1:C:1133:PRO:HG3	1:C:1166:LYS:HG3	1.97	0.47
1:C:1312:VAL:CG2	1:C:1329:VAL:HG11	2.44	0.47
1:C:1477:ILE:H	1:C:1478:PRO:HD3	1.78	0.47
1:C:998:TYR:CE2	1:C:1667:GLU:HB2	2.49	0.47
1:C:328:LEU:N	1:C:330:GLU:H	2.13	0.47
1:C:32:GLN:NE2	1:C:57:ALA:HA	2.28	0.47
2:G:123:ILE:HD11	2:G:533:LEU:CD2	2.44	0.47
2:G:1308:CYS:HB3	2:G:1311:PHE:CD2	2.49	0.47
2:G:1624:THR:HB	2:G:1642:THR:OG1	2.15	0.47
1:A:980:VAL:HG21	2:G:952:ARG:NH2	2.28	0.47
2:H:1355:ASN:CB	2:H:1583:MET:HE1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1486:PHE:HA	2:H:1504:VAL:O	2.14	0.47
2:H:1300:PHE:CA	2:H:1556:VAL:HG11	2.44	0.47
2:I:1071:LYS:HE3	2:I:1075:ASP:OD2	2.14	0.47
2:I:109:LEU:HD11	2:I:116:LEU:CD2	2.43	0.47
2:I:109:LEU:HD22	2:I:114:THR:HG23	1.96	0.47
2:I:1389:ILE:HG13	2:I:1411:PHE:HD1	1.80	0.47
2:I:176:LEU:HD22	2:I:247:ALA:HB1	1.96	0.47
2:I:741:HIS:CE1	2:I:855:HIS:NE2	2.82	0.47
1:A:1639:VAL:HG12	1:A:1640:SER:N	2.28	0.47
1:A:186:ILE:O	1:A:190:LEU:HG	2.14	0.47
1:A:702:LYS:HD3	1:A:731:THR:CG2	2.44	0.47
1:B:32:GLN:NE2	1:B:57:ALA:HA	2.30	0.47
1:C:142:ASP:CG	1:C:257:PRO:HB2	2.34	0.47
2:G:777:THR:HG23	2:G:1081:HIS:CE1	2.50	0.47
2:G:1842:VAL:HG21	2:G:1975:PRO:HD3	1.96	0.47
2:G:2036:GLU:HG2	2:G:2039:LYS:NZ	2.28	0.47
2:G:33:LEU:HD21	2:G:80:PHE:CE2	2.50	0.47
2:G:804:ARG:NH2	2:G:1068:GLU:OE1	2.48	0.47
2:H:1666:PHE:CD1	2:H:1814:ALA:HA	2.48	0.47
2:H:1666:PHE:CD1	2:H:1814:ALA:HB2	2.49	0.47
2:H:598:THR:CB	2:H:599:PRO:HD3	2.44	0.47
2:H:751:LEU:HD23	2:H:791:TYR:CZ	2.49	0.47
2:I:1913:VAL:O	2:I:1917:ILE:HG13	2.15	0.47
2:I:376:ASN:C	2:I:376:ASN:ND2	2.68	0.47
2:I:461:ASP:HB3	2:I:464:ASP:HB2	1.95	0.47
1:A:1714:VAL:HG22	1:A:1738:ILE:HD11	1.96	0.47
1:B:260:ARG:HH12	1:B:300:VAL:CG2	2.20	0.47
1:B:702:LYS:HD3	1:B:731:THR:CG2	2.44	0.47
1:C:1138:LYS:HG3	1:C:1163:TYR:CE1	2.49	0.47
1:C:1004:ILE:HG22	1:C:1660:TYR:CE2	2.49	0.47
1:C:908:LEU:HA	1:C:913:VAL:HG21	1.96	0.47
2:G:1227:ARG:CZ	2:G:1565:VAL:HG12	2.44	0.47
2:G:1850:SER:HB2	2:G:1973:SER:HB2	1.96	0.47
2:G:2042:ILE:HG12	2:G:2042:ILE:H	1.39	0.47
2:G:22:VAL:HG11	2:G:27:PHE:HA	1.96	0.47
2:G:428:HIS:HD2	2:G:486:LEU:O	1.97	0.47
2:H:807:ILE:HD12	2:H:1063:THR:HG23	1.95	0.47
2:H:1567:ARG:NH1	2:H:1568:HIS:HB3	2.29	0.47
2:H:551:THR:HG22	2:H:552:SER:N	2.30	0.47
2:H:677:GLN:O	2:H:678:PHE:HB3	2.15	0.47
2:I:597:MET:H	2:I:601:THR:HB	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:772:GLY:O	2:I:804:ARG:HD3	2.14	0.47
1:B:1477:ILE:H	1:B:1478:PRO:HD3	1.79	0.47
1:B:998:TYR:CE2	1:B:1667:GLU:HB2	2.49	0.47
1:C:1642:THR:HG22	1:C:1652:GLN:HG3	1.96	0.47
1:C:1709:GLU:H	1:C:1709:GLU:HG3	1.42	0.47
1:C:460:GLU:HG3	1:C:460:GLU:H	1.27	0.47
1:C:499:PRO:HD3	1:C:516:ARG:HH21	1.80	0.47
1:C:539:SER:O	1:C:540:GLN:C	2.52	0.47
2:G:369:SER:O	2:G:370:LEU:HD23	2.15	0.47
2:G:402:LEU:HD12	2:G:404:GLN:HG2	1.95	0.47
2:G:481:ASP:OD2	2:G:485:ARG:NH1	2.47	0.47
2:H:579:VAL:CG2	2:H:1078:HIS:CD2	2.95	0.47
2:H:490:TRP:HA	2:H:493:THR:HG22	1.96	0.47
2:H:706:LYS:HE2	2:H:731:GLN:OE1	2.14	0.47
2:I:1547:PRO:HD3	2:I:1584:PHE:CE2	2.49	0.47
1:C:13:LEU:HB2	2:I:2026:PHE:CE1	2.50	0.47
2:I:490:TRP:HA	2:I:493:THR:HG22	1.96	0.47
1:A:232:LEU:HD13	1:A:272:GLU:CB	2.44	0.47
1:A:516:ARG:NH1	1:A:894:ARG:CZ	2.78	0.47
1:B:1308:SER:HB3	1:B:1589:GLY:CA	2.45	0.47
1:B:1114:TYR:CD1	1:B:1337:GLU:HG3	2.50	0.47
1:C:1125:VAL:HG21	1:C:1175:ILE:CD1	2.43	0.47
1:C:1319:ILE:HA	1:C:1324:ALA:O	2.14	0.47
1:C:1332:TYR:HB3	1:C:1382:ALA:CB	2.44	0.47
2:G:279:THR:O	2:G:283:ILE:HB	2.15	0.47
2:G:512:LEU:O	2:G:516:THR:HG23	2.15	0.47
2:G:652:ILE:HD12	2:G:652:ILE:N	2.29	0.47
2:G:7:ARG:HH11	2:G:24:THR:HG23	1.76	0.47
2:H:1002:HIS:NE2	2:H:1006:MET:HE3	2.29	0.47
2:H:942:THR:HG21	2:H:1012:GLN:HA	1.95	0.47
2:H:1227:ARG:CZ	2:H:1565:VAL:HG12	2.45	0.47
2:H:1804:PHE:CD2	2:H:1818:LEU:HD22	2.50	0.47
2:H:559:PRO:HB3	2:H:564:GLU:HG3	1.97	0.47
2:H:784:GLU:O	2:H:787:THR:HB	2.13	0.47
2:H:751:LEU:HD23	2:H:791:TYR:CD2	2.50	0.47
2:H:860:ARG:H	2:H:1049:GLN:HG3	1.80	0.47
2:I:1159:ILE:CG1	2:I:1169:PRO:CD	2.91	0.47
2:I:740:HIS:HA	2:I:854:ILE:HD13	1.97	0.47
1:A:1238:VAL:CG1	1:A:1239:HIS:N	2.78	0.47
1:A:1487:LEU:C	1:A:1487:LEU:HD23	2.35	0.47
1:A:413:LEU:C	1:A:415:SER:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:331:ILE:HG23	1:B:332:THR:N	2.29	0.47
1:B:66:GLU:HA	1:B:66:GLU:OE1	2.15	0.47
1:C:427:ASN:ND2	1:C:610:THR:H	2.08	0.47
1:C:636:PRO:HB2	1:C:638:LEU:O	2.15	0.47
2:G:1027:ILE:O	2:G:1031:LYS:HB2	2.14	0.47
2:G:1100:VAL:HG21	2:G:1147:ILE:CD1	2.45	0.47
2:G:169:TYR:CG	2:G:170:PHE:N	2.83	0.47
2:G:1784:MET:HE2	2:G:1784:MET:O	2.14	0.47
2:G:232:LEU:HD21	2:G:423:VAL:HA	1.97	0.47
2:G:730:LEU:C	2:G:730:LEU:HD12	2.35	0.47
2:G:852:GLU:HG3	2:G:852:GLU:H	1.40	0.47
2:H:943:TRP:CZ2	2:H:1016:PRO:HG3	2.49	0.47
2:H:1854:MET:CG	2:H:1901:ALA:HB2	2.45	0.47
2:H:213:LEU:HG	2:H:213:LEU:O	2.14	0.47
2:H:652:ILE:N	2:H:652:ILE:HD12	2.30	0.47
1:A:1009:LEU:HG	1:A:1664:ALA:HB2	1.95	0.47
1:A:1208:VAL:HG11	1:A:1212:THR:HB	1.96	0.47
1:A:1533:ILE:HG13	1:A:1564:LEU:HB3	1.97	0.47
1:A:406:TRP:CE3	1:A:1619:GLU:HG3	2.50	0.47
1:A:1557:ILE:HD11	1:A:1642:THR:HG21	1.97	0.47
1:A:187:LEU:HD22	1:A:201:PRO:HB2	1.96	0.47
1:B:142:ASP:CG	1:B:257:PRO:HB2	2.35	0.47
1:B:916:LEU:HD22	1:B:922:VAL:HG22	1.95	0.47
1:C:529:MET:HG2	1:C:638:LEU:HG	1.95	0.47
1:C:930:LEU:HD23	1:C:930:LEU:HA	1.68	0.47
2:G:1002:HIS:NE2	2:G:1006:MET:HE3	2.30	0.47
2:G:1417:THR:C	2:G:1419:PHE:H	2.18	0.47
1:A:18:LEU:HD21	2:G:1815:LEU:HD12	1.97	0.47
2:G:650:ASN:HD21	3:G:3051:FMN:HN3	1.63	0.47
2:G:306:ILE:HA	2:G:439:ILE:HD13	1.96	0.47
2:G:355:LYS:HE2	2:G:355:LYS:HB3	1.64	0.47
2:H:873:PHE:CD1	2:H:1026:GLU:HB2	2.49	0.47
2:H:1195:VAL:HG13	2:H:1211:LEU:CB	2.44	0.47
2:H:1273:GLU:HB3	2:H:1274:PRO:CD	2.45	0.47
2:H:159:ILE:CG2	2:H:501:ILE:HG22	2.44	0.47
2:H:894:ARG:NH1	2:H:898:ASP:OD2	2.41	0.47
2:I:1590:ARG:NH2	2:I:1594:GLU:OE2	2.48	0.47
2:I:1593:ILE:HD13	2:I:1626:ILE:HD13	1.97	0.47
2:I:7:ARG:HH11	2:I:24:THR:HG23	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:589:ARG:HB3	2:I:590:PRO:CD	2.44	0.47
2:I:706:LYS:HE2	2:I:731:GLN:OE1	2.15	0.47
2:I:955:GLU:HG2	2:I:987:TYR:HE2	1.79	0.47
1:A:1251:MET:O	1:A:1252:GLY:O	2.33	0.47
1:A:1430:ARG:O	1:A:1430:ARG:HG2	2.15	0.47
1:A:1617:ILE:O	1:A:1620:GLN:HG2	2.15	0.47
1:B:1219:VAL:CA	1:B:1384:ILE:HD11	2.31	0.47
1:B:513:GLU:OE2	1:B:873:ARG:NH1	2.45	0.47
1:C:1577:GLN:NE2	1:C:1591:TRP:HB3	2.30	0.47
1:C:187:LEU:HD22	1:C:201:PRO:HB2	1.96	0.47
1:C:338:LEU:O	1:C:342:GLN:HG3	2.15	0.47
1:C:2:LYS:HE2	1:C:4:GLU:CD	2.35	0.47
2:G:249:TYR:CD2	2:G:283:ILE:HD11	2.50	0.47
2:G:309:ARG:HA	2:G:309:ARG:HD3	1.65	0.47
2:G:732:TRP:CE2	2:G:750:MET:HE3	2.50	0.47
2:H:1135:GLU:OE2	2:H:1175:LYS:HE3	2.15	0.47
2:H:1258:ARG:O	2:H:1262:ILE:HG13	2.15	0.47
2:H:1738:PHE:CE1	2:H:1837:THR:HG23	2.50	0.47
2:H:7:ARG:NH2	2:H:24:THR:O	2.48	0.47
2:H:306:ILE:HA	2:H:439:ILE:HD13	1.96	0.47
2:H:741:HIS:HE1	2:H:845:THR:HG21	1.65	0.47
2:H:751:LEU:HA	2:H:794:MET:HE3	1.97	0.47
2:I:1180:MET:HB2	2:I:1197:LEU:HD21	1.97	0.47
2:I:121:GLU:HA	2:I:124:LYS:HD2	1.96	0.47
2:I:42:PRO:HG2	2:I:52:ASP:CG	2.35	0.47
2:I:732:TRP:CD1	2:I:750:MET:HE3	2.49	0.47
2:I:844:VAL:HG22	2:I:858:ALA:HB2	1.97	0.47
1:A:1114:TYR:CE1	1:A:1337:GLU:HG3	2.50	0.47
1:A:1010:GLU:HA	1:A:1664:ALA:HA	1.97	0.47
1:A:2:LYS:HD2	2:G:2050:GLN:CB	2.30	0.47
1:A:852:ARG:HB3	1:A:858:TRP:HZ2	1.80	0.47
1:B:979:GLN:HB3	2:H:968:GLN:NE2	2.29	0.47
1:C:1533:ILE:HD11	1:C:1564:LEU:HD13	1.97	0.47
2:G:1327:ILE:HD12	2:G:1327:ILE:HA	1.79	0.47
2:G:1886:VAL:HG22	2:G:1906:ALA:HB1	1.97	0.47
2:G:214:ASN:ND2	2:G:217:GLU:HB2	2.30	0.47
2:G:432:LEU:HB3	2:G:484:ILE:HG23	1.96	0.47
2:G:7:ARG:NH2	2:G:24:THR:O	2.48	0.47
2:G:772:GLY:O	2:G:804:ARG:HD3	2.15	0.47
2:G:860:ARG:HB2	2:G:1049:GLN:HG3	1.97	0.47
2:H:109:LEU:HD11	2:H:116:LEU:CD2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1491:VAL:HB	2:H:1501:ILE:CD1	2.45	0.47
2:H:481:ASP:OD2	2:H:485:ARG:NH1	2.48	0.47
2:H:11:LEU:HD11	2:H:64:PHE:CD2	2.50	0.47
2:H:720:ALA:HA	2:H:728:ILE:CD1	2.45	0.47
2:I:586:LEU:HD12	2:I:764:MET:SD	2.54	0.47
2:I:584:SER:CB	2:I:591:PRO:HG3	2.41	0.47
1:A:170:LYS:HD3	1:A:175:LEU:HD23	1.97	0.46
1:A:636:PRO:HB2	1:A:638:LEU:O	2.15	0.46
1:B:1133:PRO:HG3	1:B:1166:LYS:HG3	1.97	0.46
1:B:1239:HIS:CD2	1:B:1241:SER:H	2.33	0.46
1:C:1189:ILE:HG23	1:C:1190:PRO:HD2	1.97	0.46
2:G:1148:ASN:HD22	2:G:1151:HIS:H	1.63	0.46
2:G:1273:GLU:HB3	2:G:1274:PRO:CD	2.45	0.46
2:H:1266:TYR:HB2	2:H:1347:LEU:HD23	1.97	0.46
2:H:440:ASN:ND2	2:H:477:GLU:HG2	2.30	0.46
2:H:573:LYS:HE3	2:H:1101:GLU:OE1	2.15	0.46
1:C:59:ARG:HH11	2:I:1896:GLN:HE22	1.62	0.46
2:I:350:GLN:HA	2:I:353:VAL:HG13	1.97	0.46
1:A:11:HIS:HE1	2:G:1996:ILE:O	1.98	0.46
1:A:1639:VAL:CG1	1:A:1640:SER:N	2.78	0.46
1:B:340:ARG:HH12	1:B:344:GLN:HE21	1.64	0.46
1:B:702:LYS:HE2	1:B:729:GLY:O	2.15	0.46
1:C:11:HIS:C	1:C:11:HIS:CD2	2.89	0.46
1:C:1183:ARG:NH1	1:C:1344:GLY:HA2	2.30	0.46
1:C:293:LYS:O	1:C:297:ILE:HG13	2.15	0.46
2:G:1199:GLU:OE2	2:G:1567:ARG:NH1	2.47	0.46
2:G:247:ALA:O	2:G:251:VAL:HG13	2.15	0.46
2:G:894:ARG:NH1	2:G:898:ASP:OD2	2.42	0.46
2:H:1945:ASP:O	2:H:1949:LYS:HG3	2.15	0.46
2:H:42:PRO:HG2	2:H:52:ASP:CG	2.36	0.46
2:H:586:LEU:HD12	2:H:764:MET:SD	2.55	0.46
2:H:589:ARG:HB3	2:H:590:PRO:CD	2.43	0.46
2:H:702:TYR:HB3	2:H:727:PRO:HB2	1.97	0.46
2:I:873:PHE:CE1	2:I:1026:GLU:HB2	2.49	0.46
2:I:817:ALA:HA	2:I:1048:VAL:HG11	1.97	0.46
2:I:1080:GLY:O	2:I:1084:LYS:HG3	2.15	0.46
2:I:1100:VAL:HG21	2:I:1147:ILE:CD1	2.46	0.46
2:I:1148:ASN:HD22	2:I:1148:ASN:C	2.19	0.46
2:I:1609:THR:O	2:I:1653:GLY:HA3	2.15	0.46
2:I:1873:TYR:CE1	2:I:1877:ARG:NH2	2.81	0.46
2:I:443:LEU:HD22	2:I:448:VAL:CG1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:553:ASN:O	2:I:556:LYS:HE3	2.15	0.46
2:I:736:ARG:HG3	2:I:736:ARG:H	1.57	0.46
1:A:1270:VAL:HG11	1:A:1274:ILE:HD13	1.97	0.46
1:A:328:LEU:N	1:A:330:GLU:H	2.12	0.46
1:A:539:SER:O	1:A:540:GLN:C	2.52	0.46
1:A:709:ARG:O	1:A:714:VAL:HG21	2.16	0.46
1:B:1375:GLY:HA2	1:B:1546:THR:HG22	1.97	0.46
1:B:1618:LEU:HD23	1:B:1621:PHE:CE2	2.50	0.46
1:B:19:ALA:O	1:B:22:PHE:HB2	2.15	0.46
1:C:59:ARG:HH11	2:I:1896:GLN:NE2	2.14	0.46
1:C:893:VAL:HG11	1:C:930:LEU:CD2	2.40	0.46
2:G:1015:VAL:HG11	2:G:1017:PHE:CE1	2.50	0.46
2:G:873:PHE:CD1	2:G:1026:GLU:HB2	2.50	0.46
2:G:1173:VAL:O	2:G:1567:ARG:NH2	2.48	0.46
2:G:1949:LYS:O	2:G:1953:VAL:HG23	2.15	0.46
2:G:233:SER:HA	2:G:424:ALA:CB	2.46	0.46
2:G:785:TRP:CG	2:G:786:SER:N	2.83	0.46
2:G:955:GLU:HG2	2:G:987:TYR:HE2	1.80	0.46
2:H:1593:ILE:HD13	2:H:1626:ILE:HD13	1.97	0.46
2:H:1666:PHE:CE1	2:H:1814:ALA:HA	2.50	0.46
1:C:67:SER:CB	2:H:359:HIS:HE1	2.29	0.46
2:H:606:PHE:HZ	2:H:805:VAL:CG1	2.28	0.46
2:H:881:VAL:N	2:H:882:PRO:CD	2.79	0.46
2:H:926:LEU:HB3	2:H:947:THR:HG22	1.97	0.46
2:I:1021:LEU:HD22	2:I:1021:LEU:HA	1.61	0.46
2:I:1842:VAL:HG21	2:I:1975:PRO:HD3	1.97	0.46
2:I:1873:TYR:CE1	2:I:1877:ARG:NE	2.77	0.46
2:G:1314:ARG:NH2	2:I:315:PRO:O	2.48	0.46
2:I:606:PHE:HZ	2:I:805:VAL:CG1	2.28	0.46
2:I:751:LEU:HD11	2:I:789:PHE:CD1	2.51	0.46
1:A:1308:SER:HB3	1:A:1589:GLY:CA	2.45	0.46
1:A:37:LYS:HB2	1:A:65:TYR:CE1	2.48	0.46
1:A:479:ASN:O	1:A:483:VAL:HG23	2.15	0.46
1:B:1019:ILE:HG21	1:B:1316:VAL:HG22	1.98	0.46
1:B:733:ILE:CD1	1:B:761:LEU:HD11	2.46	0.46
1:C:1238:VAL:CG1	1:C:1242:GLU:HB2	2.45	0.46
1:C:1300:THR:HA	1:C:1301:PRO:HD3	1.67	0.46
2:G:1004:LEU:HD21	2:G:1019:PRO:HB2	1.98	0.46
2:G:101:ILE:HG13	2:G:101:ILE:H	1.31	0.46
2:G:1314:ARG:HA	2:G:1314:ARG:HD3	1.63	0.46
2:G:1435:ILE:O	2:G:1435:ILE:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1666:PHE:CE1	2:G:1814:ALA:HA	2.50	0.46
2:G:1980:TYR:HD1	2:G:1981:LEU:HD12	1.80	0.46
2:G:629:GLY:O	2:G:632:ALA:HB3	2.15	0.46
2:G:745:ASP:HA	2:G:832:TRP:CH2	2.48	0.46
2:H:1169:PRO:O	2:H:1173:VAL:HG23	2.15	0.46
2:H:1359:MET:CE	2:H:1404:MET:HB3	2.44	0.46
2:H:553:ASN:O	2:H:556:LYS:HE3	2.16	0.46
2:I:1752:PHE:HZ	2:I:1836:MET:HE3	1.80	0.46
2:I:213:LEU:HG	2:I:213:LEU:O	2.16	0.46
2:I:391:LEU:CD2	2:I:394:ARG:NH2	2.78	0.46
2:I:732:TRP:CG	2:I:750:MET:HE3	2.50	0.46
2:I:99:ASN:HA	2:I:550:VAL:HG21	1.98	0.46
1:B:1595:GLY:O	1:B:1599:ILE:HG13	2.15	0.46
1:B:2:LYS:HE2	1:B:4:GLU:OE1	2.15	0.46
1:C:1021:VAL:HG11	1:C:1597:LEU:CD1	2.44	0.46
1:C:421:ILE:HG12	1:C:469:VAL:HG21	1.98	0.46
2:G:1567:ARG:HG2	2:G:1567:ARG:HH11	1.73	0.46
2:G:159:ILE:CG2	2:G:501:ILE:HG22	2.46	0.46
2:G:739:GLY:HA2	2:G:1054:LEU:HG	1.97	0.46
2:G:826:GLY:HA3	2:G:1061:GLN:CB	2.45	0.46
2:H:1328:VAL:HG23	2:H:1557:SER:HA	1.98	0.46
1:B:29:ILE:HG13	2:H:1891:TYR:O	2.15	0.46
2:I:123:ILE:HD11	2:I:533:LEU:CD2	2.46	0.46
1:A:1056:ILE:HG13	1:A:1057:MET:N	2.30	0.46
1:A:293:LYS:O	1:A:297:ILE:HG13	2.16	0.46
1:B:1251:MET:O	1:B:1252:GLY:O	2.33	0.46
1:C:243:ILE:O	1:C:247:ARG:HG3	2.16	0.46
1:C:143:GLU:H	1:C:260:ARG:HG2	1.81	0.46
2:G:1738:PHE:CE1	2:G:1837:THR:HG23	2.50	0.46
2:G:441:LYS:O	2:G:444:VAL:HG12	2.15	0.46
2:G:807:ILE:HA	2:G:818:LYS:HG2	1.97	0.46
2:H:1624:THR:HB	2:H:1642:THR:CG2	2.45	0.46
2:H:1850:SER:HB2	2:H:1973:SER:HB2	1.97	0.46
2:H:1908:ASP:HA	2:H:1911:THR:HG22	1.97	0.46
2:H:2037:PRO:O	2:H:2041:ILE:HG13	2.15	0.46
2:H:350:GLN:HA	2:H:353:VAL:HG13	1.97	0.46
2:I:1148:ASN:HD22	2:I:1151:HIS:H	1.63	0.46
2:I:1561:ASN:OD1	2:I:1563:ILE:HB	2.16	0.46
2:I:1651:LEU:HA	2:I:1651:LEU:HD23	1.73	0.46
2:I:2037:PRO:O	2:I:2041:ILE:HG13	2.14	0.46
2:I:573:LYS:C	2:I:575:GLY:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:THR:HG22	1:A:1226:SER:CB	2.43	0.46
1:A:1234:MET:HE3	1:A:1326:ILE:HG21	1.97	0.46
1:A:420:ILE:HG22	1:A:469:VAL:HG22	1.96	0.46
1:B:11:HIS:C	1:B:11:HIS:CD2	2.89	0.46
1:B:776:GLU:OE1	1:B:795:MET:HE1	2.16	0.46
1:B:792:HIS:CE1	1:B:796:LEU:HD23	2.51	0.46
1:C:1040:GLU:HB2	1:C:1580:LEU:HD12	1.98	0.46
1:C:182:VAL:O	1:C:186:ILE:HG13	2.15	0.46
2:G:218:TRP:HB3	2:G:225:THR:OG1	2.16	0.46
2:H:1764:PHE:HB2	2:H:1770:LEU:HD21	1.97	0.46
2:H:599:PRO:HD2	3:H:3051:FMN:H6	1.98	0.46
2:H:72:VAL:HG12	2:H:73:GLU:N	2.31	0.46
2:I:106:ALA:HB2	2:I:545:GLN:HG2	1.98	0.46
2:I:1272:ASP:O	2:I:1273:GLU:HG3	2.15	0.46
2:I:860:ARG:H	2:I:1049:GLN:HG3	1.80	0.46
1:A:1196:LYS:HE3	1:A:1202:ASP:CG	2.36	0.46
1:A:225:SER:OG	1:A:266:LEU:HD21	2.16	0.46
1:A:338:LEU:O	1:A:342:GLN:HG3	2.16	0.46
1:A:825:PRO:HB2	1:A:843:LYS:HZ2	1.79	0.46
1:B:143:GLU:H	1:B:260:ARG:HG2	1.81	0.46
1:C:1308:SER:HB3	1:C:1589:GLY:CA	2.44	0.46
1:C:1459:ILE:O	1:C:1463:VAL:HG23	2.16	0.46
1:C:1673:TYR:CZ	1:C:1677:VAL:HG21	2.51	0.46
1:C:41:THR:HG21	2:I:1663:THR:HB	1.97	0.46
2:G:2037:PRO:O	2:G:2041:ILE:HG13	2.16	0.46
2:G:751:LEU:HA	2:G:794:MET:HE3	1.97	0.46
2:I:1102:TYR:HB3	2:I:1244:PRO:HA	1.98	0.46
2:I:1148:ASN:ND2	2:I:1151:HIS:H	2.13	0.46
2:I:1666:PHE:CD1	2:I:1814:ALA:HA	2.51	0.46
2:I:1782:THR:CG2	2:I:1827:LEU:HD21	2.45	0.46
2:I:232:LEU:HD21	2:I:423:VAL:HA	1.98	0.46
2:I:807:ILE:HD12	2:I:1063:THR:HG23	1.98	0.46
1:A:702:LYS:HE2	1:A:729:GLY:O	2.15	0.46
1:B:1639:VAL:HG12	1:B:1640:SER:N	2.30	0.46
1:B:601:VAL:O	1:B:602:GLU:C	2.54	0.46
1:C:1367:ARG:HH12	1:C:1372:THR:CB	2.20	0.46
1:C:1682:LYS:HB3	2:I:994:PHE:CE2	2.50	0.46
2:G:675:PRO:HD3	2:G:1164:MET:HE2	1.97	0.46
2:G:1159:ILE:CG1	2:G:1169:PRO:CD	2.93	0.46
2:G:1873:TYR:HE1	2:G:1877:ARG:HH21	1.60	0.46
2:G:1889:VAL:HG13	2:G:1977:HIS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:9:LEU:HB2	2:G:27:PHE:HE1	1.81	0.46
2:G:490:TRP:HA	2:G:493:THR:HG22	1.98	0.46
2:H:1552:PRO:O	2:H:1556:VAL:HG23	2.15	0.46
2:H:1567:ARG:HH11	2:H:1567:ARG:HG2	1.72	0.46
2:H:324:LEU:HD12	2:H:324:LEU:O	2.16	0.46
2:H:821:ILE:HA	2:H:857:ILE:HD11	1.97	0.46
2:I:1417:THR:C	2:I:1419:PHE:H	2.18	0.46
2:I:1624:THR:HB	2:I:1642:THR:CG2	2.43	0.46
2:I:1932:SER:O	2:I:1936:VAL:HG22	2.16	0.46
1:A:1353:LEU:HA	1:A:1353:LEU:HD23	1.62	0.46
1:B:1639:VAL:CG1	1:B:1640:SER:N	2.79	0.46
1:B:719:GLN:HG3	1:B:720:SER:N	2.31	0.46
1:C:1196:LYS:HE3	1:C:1202:ASP:CG	2.37	0.46
1:C:776:GLU:OE1	1:C:795:MET:HE1	2.15	0.46
2:G:131:ILE:HD12	2:G:182:VAL:CB	2.42	0.46
2:G:551:THR:HG22	2:G:552:SER:N	2.31	0.46
2:G:582:LYS:HE2	2:G:1108:PRO:HB3	1.97	0.46
2:G:702:TYR:HB3	2:G:727:PRO:HB2	1.97	0.46
2:H:1015:VAL:HG11	2:H:1017:PHE:CE1	2.50	0.46
1:B:13:LEU:HB2	2:H:2026:PHE:CE1	2.51	0.46
2:H:218:TRP:HB3	2:H:225:THR:OG1	2.16	0.46
2:H:345:THR:HG22	2:H:347:GLU:N	2.25	0.46
2:H:650:ASN:HD21	3:H:3051:FMN:HN3	1.64	0.46
2:H:730:LEU:HD12	2:H:730:LEU:C	2.36	0.46
2:H:845:THR:HG22	2:H:855:HIS:CD2	2.51	0.46
2:I:1031:LYS:O	2:I:1032:ASP:C	2.54	0.46
2:I:1776:PHE:C	2:I:1779:PRO:HD2	2.37	0.46
2:I:1886:VAL:HG22	2:I:1906:ALA:HB1	1.98	0.46
2:I:231:LEU:HA	2:I:236:ILE:HD12	1.98	0.46
2:I:618:GLU:HG2	2:I:678:PHE:CZ	2.51	0.46
2:I:785:TRP:CG	2:I:786:SER:N	2.84	0.46
1:A:792:HIS:CE1	1:A:796:LEU:HD23	2.52	0.45
1:A:893:VAL:HG11	1:A:930:LEU:CD2	2.37	0.45
1:B:479:ASN:O	1:B:483:VAL:HG23	2.16	0.45
1:C:406:TRP:CE3	1:C:1619:GLU:HG3	2.51	0.45
1:C:225:SER:OG	1:C:266:LEU:HD21	2.16	0.45
2:G:826:GLY:HA2	2:G:1060:ALA:HB3	1.97	0.45
2:G:845:THR:HG22	2:G:855:HIS:CD2	2.50	0.45
2:G:970:TYR:O	2:G:973:LEU:HB2	2.16	0.45
2:H:1031:LYS:O	2:H:1032:ASP:C	2.54	0.45
2:H:817:ALA:HA	2:H:1048:VAL:HG11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1079:ASP:O	2:H:1082:ILE:HG22	2.16	0.45
2:H:1327:ILE:HA	2:H:1327:ILE:HD12	1.76	0.45
2:H:1428:GLU:HG2	2:H:1470:THR:HG22	1.97	0.45
2:H:319:LEU:HA	2:H:319:LEU:HD22	1.68	0.45
2:I:1236:LEU:HA	2:I:1237:PRO:HD3	1.74	0.45
2:I:1239:LEU:O	2:I:1254:VAL:HG23	2.15	0.45
2:I:22:VAL:HG11	2:I:27:PHE:HA	1.97	0.45
2:I:745:ASP:HA	2:I:832:TRP:CH2	2.49	0.45
2:I:23:PRO:HG2	2:I:86:LEU:HD11	1.98	0.45
1:A:988:ILE:HD13	1:A:1048:GLU:CB	2.47	0.45
1:A:168:MET:HA	1:A:206:LEU:HB2	1.98	0.45
1:A:764:ASP:OD2	1:A:818:ARG:HD3	2.17	0.45
1:B:183:GLN:O	1:B:187:LEU:HG	2.17	0.45
1:B:196:THR:O	1:B:213:PHE:HE2	2.00	0.45
1:B:460:GLU:H	1:B:460:GLU:HG3	1.34	0.45
1:B:9:LEU:CD2	2:H:2041:ILE:HD13	2.47	0.45
2:G:1222:GLU:HG3	2:G:1235:SER:OG	2.17	0.45
2:G:1609:THR:O	2:G:1653:GLY:HA3	2.16	0.45
2:G:209:PHE:CE2	2:G:213:LEU:HD22	2.51	0.45
2:G:712:ALA:O	2:G:715:GLN:HB3	2.16	0.45
2:G:817:ALA:HA	2:G:1048:VAL:HG11	1.98	0.45
2:G:881:VAL:N	2:G:882:PRO:CD	2.78	0.45
2:H:1330:GLY:HA2	2:H:1374:THR:HG21	1.98	0.45
2:H:1417:THR:O	2:H:1419:PHE:N	2.45	0.45
2:H:1388:LYS:HE3	2:H:1418:ASP:OD2	2.16	0.45
2:H:1858:ASN:HA	2:H:1896:GLN:O	2.16	0.45
2:H:913:ASP:H	2:H:916:THR:CG2	2.29	0.45
2:I:1323:MET:CE	2:I:1605:VAL:HG22	2.45	0.45
2:I:1589:VAL:HG21	2:I:1651:LEU:HD12	1.99	0.45
2:I:2026:PHE:HB3	2:I:2042:ILE:HD13	1.98	0.45
2:I:490:TRP:CZ2	2:I:512:LEU:HD21	2.51	0.45
2:I:739:GLY:HA2	2:I:1054:LEU:HG	1.97	0.45
1:A:335:HIS:CD2	1:A:335:HIS:O	2.69	0.45
1:A:460:GLU:H	1:A:460:GLU:HG3	1.34	0.45
1:A:49:PRO:O	1:A:82:SER:HB2	2.16	0.45
1:C:290:MET:HB3	1:C:290:MET:HE2	1.92	0.45
2:G:1472:VAL:CG2	2:G:1483:VAL:HG22	2.46	0.45
2:G:1491:VAL:HB	2:G:1501:ILE:HD12	1.98	0.45
2:G:624:TYR:HB2	2:G:630:MET:HE3	1.98	0.45
2:H:1027:ILE:O	2:H:1031:LYS:HB2	2.16	0.45
2:H:1223:MET:HE3	2:H:1238:LEU:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1473:THR:O	2:H:1481:SER:HB3	2.15	0.45
2:H:1579:ILE:HG22	2:H:1580:THR:O	2.16	0.45
2:H:1590:ARG:HG3	2:H:1608:TYR:CD2	2.51	0.45
2:H:597:MET:HA	3:H:3051:FMN:C5A	2.46	0.45
2:H:490:TRP:CZ2	2:H:512:LEU:HD21	2.51	0.45
2:H:611:THR:HA	2:H:615:TYR:O	2.16	0.45
2:I:1156:CYS:SG	2:I:1250:PRO:HD2	2.56	0.45
2:I:1846:GLU:C	2:I:1848:GLY:H	2.20	0.45
2:I:355:LYS:HE2	2:I:355:LYS:HB3	1.70	0.45
2:I:463:PHE:CE1	2:I:486:LEU:HD22	2.51	0.45
1:A:776:GLU:OE1	1:A:795:MET:HE1	2.15	0.45
1:B:1061:SER:HB2	1:B:1078:SER:HB3	1.98	0.45
1:B:183:GLN:NE2	1:B:202:GLU:HG2	2.29	0.45
1:B:237:MET:HG3	1:B:241:PHE:HB3	1.97	0.45
1:B:825:PRO:HB2	1:B:843:LYS:HZ2	1.81	0.45
1:C:1208:VAL:HG11	1:C:1212:THR:HB	1.98	0.45
1:C:1375:GLY:HA2	1:C:1546:THR:HG22	1.98	0.45
1:C:1670:TYR:O	1:C:1674:VAL:HG23	2.17	0.45
1:C:183:GLN:O	1:C:187:LEU:HG	2.16	0.45
2:G:1080:GLY:O	2:G:1084:LYS:HG3	2.16	0.45
2:G:675:PRO:HG3	2:G:1163:LYS:O	2.15	0.45
2:G:1102:TYR:HB3	2:G:1244:PRO:HA	1.98	0.45
2:G:1293:THR:HG22	2:G:1296:GLU:CD	2.35	0.45
2:G:1854:MET:CG	2:G:1901:ALA:HB2	2.46	0.45
2:G:1953:VAL:O	2:G:1953:VAL:HG12	2.16	0.45
2:G:315:PRO:O	2:H:1314:ARG:NH2	2.49	0.45
2:G:463:PHE:C	2:G:463:PHE:CD2	2.90	0.45
2:H:1472:VAL:CG2	2:H:1483:VAL:HG22	2.43	0.45
2:H:1651:LEU:O	2:H:1652:THR:HG23	2.16	0.45
2:H:1735:ALA:O	2:H:1737:ILE:HG13	2.16	0.45
2:H:1697:HIS:CE1	2:H:1829:GLU:CG	3.00	0.45
2:I:1775:GLN:HG2	2:I:1836:MET:SD	2.57	0.45
2:I:533:LEU:HD13	2:I:545:GLN:HG3	1.97	0.45
2:I:938:TRP:CD1	2:I:944:ARG:HG3	2.52	0.45
1:A:1373:ARG:NE	1:A:1550:ASP:HB2	2.32	0.45
1:A:2:LYS:HE2	1:A:4:GLU:CD	2.36	0.45
1:B:1021:VAL:HG22	1:B:1387:ILE:HG22	1.98	0.45
1:C:1234:MET:HG2	1:C:1326:ILE:HD12	1.98	0.45
1:C:1233:GLU:CD	1:C:1680:ARG:HH21	2.19	0.45
1:C:170:LYS:HD3	1:C:175:LEU:HD23	1.97	0.45
2:G:460:TYR:HA	2:G:466:SER:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:161:GLY:HA3	2:G:506:PRO:HD2	1.98	0.45
2:G:553:ASN:O	2:G:556:LYS:HE3	2.16	0.45
2:H:843:ILE:HD11	2:H:1055:HIS:HB3	1.98	0.45
2:H:161:GLY:H	2:H:505:GLY:CA	2.29	0.45
2:I:1002:HIS:NE2	2:I:1006:MET:CE	2.80	0.45
2:I:1949:LYS:O	2:I:1953:VAL:HG23	2.17	0.45
2:I:653:TYR:HD1	2:I:659:LEU:HD21	1.79	0.45
2:I:786:SER:HB2	2:I:794:MET:HE2	1.99	0.45
2:I:751:LEU:HA	2:I:794:MET:HE3	1.98	0.45
1:A:143:GLU:H	1:A:260:ARG:HG2	1.81	0.45
1:A:35:PHE:HA	1:A:39:PHE:HD2	1.81	0.45
1:B:1617:ILE:O	1:B:1620:GLN:HG2	2.17	0.45
1:B:378:LEU:HA	1:B:378:LEU:HD12	1.75	0.45
1:B:427:ASN:ND2	1:B:610:THR:H	2.12	0.45
1:B:612:GLU:O	1:B:615:SER:HB3	2.17	0.45
1:C:1056:ILE:CD1	1:C:1193:TRP:CD1	2.99	0.45
1:C:1022:THR:HG22	1:C:1226:SER:CB	2.47	0.45
1:C:1362:PRO:HA	1:C:1365:MET:HG3	1.97	0.45
1:C:1533:ILE:HG13	1:C:1564:LEU:HB3	1.98	0.45
1:C:1720:ALA:O	1:C:1721:ARG:HG2	2.17	0.45
1:C:709:ARG:O	1:C:714:VAL:HG21	2.16	0.45
2:H:1776:PHE:C	2:H:1779:PRO:HD2	2.37	0.45
2:H:427:PHE:HB3	2:H:428:HIS:ND1	2.32	0.45
2:I:860:ARG:HB2	2:I:1049:GLN:HG3	1.97	0.45
2:I:1162:ASP:O	2:I:1163:LYS:HB2	2.16	0.45
2:I:1491:VAL:HB	2:I:1501:ILE:CD1	2.47	0.45
2:I:440:ASN:ND2	2:I:477:GLU:HG2	2.31	0.45
2:I:601:THR:HB	2:I:620:ALA:HB2	1.98	0.45
2:I:677:GLN:O	2:I:678:PHE:HB3	2.17	0.45
2:I:720:ALA:HA	2:I:728:ILE:CD1	2.47	0.45
1:A:1644:PHE:CD1	1:A:1644:PHE:N	2.85	0.45
1:A:242:THR:HG22	1:A:243:ILE:H	1.81	0.45
1:A:256:LEU:HA	1:A:257:PRO:HD3	1.73	0.45
1:A:331:ILE:HG23	1:A:332:THR:N	2.31	0.45
1:B:1020:VAL:CG1	1:B:1400:ILE:HG23	2.45	0.45
1:B:32:GLN:NE2	1:B:57:ALA:CA	2.80	0.45
1:C:1431:GLU:OE2	1:C:1433:HIS:HE1	2.00	0.45
1:C:197:THR:HG22	1:C:198:PRO:O	2.16	0.45
2:G:1281:PRO:O	2:G:1378:ILE:HG23	2.17	0.45
2:G:1632:ILE:O	2:G:1632:ILE:HG23	2.16	0.45
2:G:1858:ASN:ND2	2:G:1861:ARG:HG3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:597:MET:HA	3:G:3051:FMN:C5A	2.47	0.45
2:G:350:GLN:HA	2:G:353:VAL:HG13	1.97	0.45
2:G:357:ASN:OD1	2:G:365:GLN:HB3	2.16	0.45
2:G:835:THR:CG2	2:G:845:THR:HG23	2.46	0.45
2:G:960:LYS:CE	2:G:960:LYS:HA	2.44	0.45
2:H:1311:PHE:HD1	2:H:1320:LEU:O	1.99	0.45
2:H:1325:PHE:O	2:H:1328:VAL:HG12	2.16	0.45
2:H:1680:LEU:HD13	2:H:1687:ALA:CB	2.45	0.45
2:H:2035:SER:HB3	2:H:2038:ILE:CG1	2.44	0.45
2:H:60:LEU:O	2:H:63:LYS:HB2	2.16	0.45
2:H:618:GLU:HG2	2:H:678:PHE:CZ	2.52	0.45
2:I:624:TYR:HB2	2:I:630:MET:HE3	1.99	0.45
2:I:659:LEU:HD12	2:I:659:LEU:HA	1.84	0.45
1:A:1133:PRO:HG3	1:A:1166:LYS:HG3	1.99	0.45
1:A:1300:THR:HA	1:A:1301:PRO:HD3	1.70	0.45
1:A:625:THR:HG23	1:A:627:SER:H	1.82	0.45
1:B:1234:MET:HG2	1:B:1326:ILE:CD1	2.46	0.45
1:B:235:SER:HA	1:B:276:ARG:NH2	2.32	0.45
1:B:930:LEU:HD23	1:B:930:LEU:HA	1.67	0.45
1:C:1432:HIS:CE1	1:C:1434:SER:OG	2.69	0.45
1:C:1573:ILE:HG23	1:C:1627:PRO:HG3	1.98	0.45
1:C:774:ILE:HA	1:C:775:PRO:HD3	1.74	0.45
2:G:1662:THR:HB	2:G:1799:PRO:HG2	1.99	0.45
2:G:598:THR:CB	2:G:599:PRO:HD3	2.46	0.45
2:G:754:TYR:CG	2:G:794:MET:HG2	2.51	0.45
2:G:844:VAL:HG22	2:G:858:ALA:HB2	1.98	0.45
2:H:1175:LYS:HA	2:H:1176:PRO:HD3	1.84	0.45
2:H:443:LEU:HD22	2:H:448:VAL:CG1	2.46	0.45
2:H:732:TRP:CD1	2:H:750:MET:HE3	2.51	0.45
2:I:1428:GLU:HG2	2:I:1470:THR:HG22	1.99	0.45
2:I:441:LYS:O	2:I:444:VAL:HG12	2.17	0.45
1:A:413:LEU:HD13	1:A:451:MET:HG2	1.97	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:1592:MET:HE2	1:B:1641:ILE:HG23	1.99	0.45
1:B:420:ILE:HG22	1:B:469:VAL:HG22	1.99	0.45
1:C:1238:VAL:CG1	1:C:1239:HIS:N	2.80	0.45
1:C:253:ARG:O	1:C:254:TRP:CD1	2.70	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:CE	2.79	0.45
2:G:1015:VAL:HG13	2:G:1017:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1945:ASP:O	2:G:1949:LYS:HG3	2.17	0.45
2:G:573:LYS:C	2:G:575:GLY:H	2.21	0.45
2:G:595:PRO:HD3	2:G:800:LEU:HB2	1.99	0.45
2:G:665:LEU:O	2:G:665:LEU:HD22	2.17	0.45
2:G:871:THR:HG21	2:G:887:LYS:HZ2	1.82	0.45
2:G:932:ILE:HD12	2:G:939:PHE:HD1	1.82	0.45
2:H:249:TYR:CD2	2:H:283:ILE:HD11	2.52	0.45
2:H:785:TRP:CG	2:H:786:SER:N	2.84	0.45
2:H:99:ASN:HA	2:H:550:VAL:HG21	1.99	0.45
2:I:1228:THR:HG21	2:I:1234:VAL:HG23	1.98	0.45
2:I:1422:THR:HG23	2:I:1474:PHE:HB2	1.94	0.45
2:I:159:ILE:CG2	2:I:501:ILE:HG22	2.47	0.45
2:I:1854:MET:CG	2:I:1901:ALA:HB2	2.47	0.45
2:I:901:LYS:NZ	2:I:1031:LYS:O	2.50	0.45
1:A:1020:VAL:CG1	1:A:1400:ILE:HG23	2.47	0.45
1:A:1431:GLU:HB3	1:A:1520:ALA:HB2	1.99	0.45
1:A:386:PHE:O	1:A:390:VAL:HB	2.16	0.45
1:A:798:ASN:HA	1:A:801:ARG:HB2	1.98	0.45
1:B:1533:ILE:HD11	1:B:1564:LEU:HD13	1.98	0.45
1:B:1239:HIS:HE1	1:B:1714:VAL:O	2.00	0.45
1:C:24:SER:O	2:I:1977:HIS:HD2	2.00	0.45
1:C:784:ILE:HG23	1:C:788:SER:HB2	1.98	0.45
2:G:1311:PHE:HD1	2:G:1320:LEU:O	1.99	0.45
2:G:1417:THR:O	2:G:1419:PHE:N	2.46	0.45
2:G:245:GLN:HG2	2:G:505:GLY:HA2	1.99	0.45
2:H:1389:ILE:HG13	2:H:1411:PHE:CD1	2.52	0.45
2:H:1547:PRO:HD3	2:H:1584:PHE:CE2	2.52	0.45
2:H:2026:PHE:HB3	2:H:2042:ILE:HD13	1.98	0.45
2:H:209:PHE:CE2	2:H:213:LEU:HD22	2.52	0.45
2:H:24:THR:O	2:H:26:SER:N	2.49	0.45
2:H:376:ASN:C	2:H:376:ASN:ND2	2.70	0.45
2:H:439:ILE:HD12	2:H:484:ILE:HD11	1.99	0.45
2:H:562:LEU:HG	2:H:793:PRO:CB	2.47	0.45
2:H:938:TRP:CE2	2:H:944:ARG:HG3	2.52	0.45
2:I:184:VAL:HG12	2:I:188:ILE:HG12	1.99	0.45
2:I:784:GLU:O	2:I:787:THR:HB	2.17	0.45
2:I:9:LEU:HB2	2:I:27:PHE:HE1	1.82	0.45
1:A:1516:ASP:HA	1:A:1517:PRO:HD3	1.61	0.44
1:B:335:HIS:HE1	1:C:335:HIS:ND1	2.16	0.44
1:C:1181:PHE:CZ	1:C:1341:PHE:HA	2.52	0.44
1:C:1263:ASP:HB2	1:C:1270:VAL:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1431:GLU:CG	1:C:1433:HIS:CE1	3.00	0.44
1:C:248:LYS:HB2	1:C:248:LYS:HE3	1.84	0.44
1:C:37:LYS:HB2	1:C:65:TYR:CE1	2.52	0.44
1:C:641:ARG:HD3	1:C:649:TRP:O	2.17	0.44
1:C:627:SER:HB2	1:C:657:SER:HB3	1.99	0.44
2:G:1071:LYS:HE3	2:G:1075:ASP:OD2	2.16	0.44
2:G:615:TYR:CE2	2:G:1074:MET:HB3	2.52	0.44
2:G:1219:ILE:HD11	2:G:1242:PHE:HB2	1.98	0.44
2:G:1579:ILE:HG22	2:G:1580:THR:O	2.16	0.44
2:G:297:ARG:O	2:G:301:THR:HG22	2.16	0.44
2:G:900:GLN:NE2	2:G:1051:THR:HA	2.32	0.44
2:H:1159:ILE:HG22	2:H:1160:THR:N	2.32	0.44
2:H:1768:LYS:HE2	2:H:1772:SER:HB3	1.98	0.44
2:H:1784:MET:HB2	2:H:1784:MET:HE2	1.79	0.44
2:H:1846:GLU:C	2:H:1848:GLY:H	2.19	0.44
2:I:1222:GLU:HG3	2:I:1235:SER:OG	2.16	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:780:TYR:HB2	2:I:799:PHE:CE2	2.53	0.44
1:A:413:LEU:HG	1:A:413:LEU:O	2.17	0.44
1:B:1103:ILE:HD11	1:B:1582:GLY:N	2.31	0.44
1:B:1029:PRO:HA	1:B:1188:GLN:O	2.17	0.44
1:B:1248:GLY:HA3	1:B:1301:PRO:HD2	1.99	0.44
1:B:330:GLU:O	1:B:330:GLU:HG2	2.16	0.44
1:B:444:ASN:HB2	1:B:447:LEU:N	2.15	0.44
1:B:893:VAL:HG11	1:B:930:LEU:CD2	2.36	0.44
1:B:931:GLN:H	1:B:931:GLN:HG3	1.32	0.44
2:G:1804:PHE:CD2	2:G:1818:LEU:HD22	2.53	0.44
2:G:240:LEU:HD12	2:G:240:LEU:HA	1.83	0.44
2:G:319:LEU:HA	2:G:319:LEU:HD22	1.62	0.44
2:G:419:ARG:HG3	2:G:420:PHE:N	2.33	0.44
2:H:109:LEU:HD22	2:H:114:THR:HG23	1.99	0.44
2:H:369:SER:C	2:H:370:LEU:HD23	2.38	0.44
2:H:663:ILE:HB	2:H:664:PRO:CD	2.44	0.44
2:I:1175:LYS:HA	2:I:1176:PRO:HD3	1.84	0.44
2:I:161:GLY:H	2:I:505:GLY:CA	2.28	0.44
2:I:478:ARG:O	2:I:482:CYS:HB2	2.17	0.44
1:A:1375:GLY:HA2	1:A:1546:THR:HG22	1.99	0.44
1:A:1420:ALA:HA	1:A:1421:PRO:HD3	1.75	0.44
1:A:183:GLN:NE2	1:A:202:GLU:HG2	2.29	0.44
1:A:233:ILE:HD13	1:A:237:MET:HE3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:VAL:HG13	2:G:2013:ASN:ND2	2.33	0.44
1:A:635:ILE:CG2	1:A:651:TYR:CG	3.00	0.44
1:A:44:VAL:HG11	1:A:78:ILE:HG12	1.96	0.44
1:B:1239:HIS:CD2	1:B:1241:SER:OG	2.59	0.44
1:B:1181:PHE:CZ	1:B:1341:PHE:HA	2.53	0.44
1:B:1455:ARG:O	1:B:1459:ILE:HG13	2.17	0.44
1:B:1040:GLU:OE2	1:B:1577:GLN:HB2	2.18	0.44
1:B:267:VAL:O	1:B:290:MET:HE1	2.17	0.44
1:C:625:THR:HG23	1:C:627:SER:H	1.82	0.44
2:G:1908:ASP:HA	2:G:1911:THR:HG22	1.99	0.44
2:G:156:LEU:HD23	2:G:500:HIS:HB2	2.00	0.44
2:G:589:ARG:HB3	2:G:590:PRO:CD	2.48	0.44
2:H:1180:MET:HB2	2:H:1197:LEU:HD21	1.98	0.44
2:H:512:LEU:O	2:H:516:THR:HG23	2.17	0.44
2:H:653:TYR:HD1	2:H:659:LEU:HD21	1.80	0.44
2:H:670:ARG:HD2	2:H:676:ILE:O	2.18	0.44
2:H:676:ILE:O	2:H:676:ILE:HG12	2.17	0.44
2:I:1258:ARG:O	2:I:1262:ILE:HG13	2.17	0.44
2:I:1637:LEU:HD23	2:I:1637:LEU:HA	1.79	0.44
2:I:432:LEU:HB3	2:I:484:ILE:HG23	1.99	0.44
2:I:732:TRP:CD2	2:I:750:MET:HE3	2.52	0.44
2:I:748:THR:CB	2:I:749:PRO:HD3	2.44	0.44
2:I:892:ILE:HD11	2:I:903:TRP:CD2	2.50	0.44
1:A:1050:CYS:HB3	1:A:1089:VAL:HG12	1.98	0.44
1:A:774:ILE:HA	1:A:775:PRO:HD3	1.76	0.44
1:A:790:PHE:CE2	1:A:794:ILE:HD11	2.53	0.44
1:B:1208:VAL:HG11	1:B:1212:THR:HB	1.97	0.44
1:B:1300:THR:HA	1:B:1301:PRO:HD3	1.69	0.44
1:B:232:LEU:HD13	1:B:272:GLU:CB	2.47	0.44
1:B:427:ASN:HB2	1:B:468:LEU:HD21	1.99	0.44
1:C:980:VAL:H	2:I:968:GLN:NE2	2.15	0.44
2:G:1172:LYS:HE3	2:G:1574:ASN:OD1	2.18	0.44
2:G:1294:ALA:HA	2:G:1368:VAL:CG2	2.47	0.44
2:G:1466:PHE:HE2	2:G:1489:ILE:HD13	1.81	0.44
2:G:1590:ARG:NH2	2:G:1594:GLU:OE2	2.50	0.44
2:G:298:LYS:HG2	2:G:448:VAL:CG2	2.40	0.44
2:G:717:ILE:O	2:G:720:ALA:HB3	2.18	0.44
2:G:786:SER:HB2	2:G:794:MET:HE2	2.00	0.44
2:H:1236:LEU:HA	2:H:1237:PRO:HD3	1.79	0.44
2:H:582:LYS:HE2	2:H:761:PRO:O	2.16	0.44
2:H:772:GLY:O	2:H:804:ARG:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:943:TRP:CZ2	2:I:1016:PRO:HG3	2.52	0.44
2:I:1004:LEU:HD21	2:I:1019:PRO:HB2	1.99	0.44
2:I:670:ARG:HD2	2:I:676:ILE:O	2.16	0.44
2:I:653:TYR:OH	2:I:690:VAL:HG11	2.17	0.44
2:I:826:GLY:HA3	2:I:1061:GLN:CB	2.46	0.44
1:A:1022:THR:CG2	1:A:1226:SER:OG	2.66	0.44
1:A:1283:MET:O	1:A:1287:VAL:HG23	2.17	0.44
1:A:641:ARG:HD3	1:A:649:TRP:O	2.18	0.44
1:A:627:SER:HB2	1:A:657:SER:CB	2.48	0.44
1:B:1249:SER:HB3	1:B:1280:ILE:HG12	1.99	0.44
1:B:1263:ASP:HB2	1:B:1270:VAL:HG21	2.00	0.44
1:B:1303:GLY:C	1:B:1307:THR:HG22	2.38	0.44
1:B:1431:GLU:OE2	1:B:1433:HIS:HE1	1.99	0.44
1:B:32:GLN:HE21	1:B:57:ALA:HB2	1.82	0.44
2:G:1236:LEU:HA	2:G:1237:PRO:HD3	1.76	0.44
2:G:1325:PHE:O	2:G:1328:VAL:HG12	2.17	0.44
2:G:669:LEU:HD12	2:G:669:LEU:HA	1.63	0.44
2:H:234:ILE:HG13	2:H:235:PRO:CD	2.47	0.44
2:H:612:ASN:HD21	2:H:641:ILE:HA	1.81	0.44
2:H:641:ILE:HG12	2:H:645:SER:CB	2.46	0.44
2:I:369:SER:O	2:I:370:LEU:HD23	2.17	0.44
2:I:468:LEU:O	2:I:471:LEU:HB2	2.18	0.44
2:I:517:HIS:CE1	2:I:540:ASP:O	2.71	0.44
2:I:654:VAL:O	2:I:654:VAL:HG12	2.17	0.44
2:I:665:LEU:HD22	2:I:665:LEU:O	2.17	0.44
1:A:1239:HIS:CD2	1:A:1241:SER:H	2.35	0.44
1:A:267:VAL:HG12	1:A:290:MET:CE	2.47	0.44
1:A:451:MET:HE3	1:A:476:LEU:HG	1.98	0.44
1:A:751:PHE:CZ	1:A:761:LEU:HD13	2.51	0.44
1:A:933:VAL:HA	1:A:934:PRO:HD3	1.65	0.44
1:B:1516:ASP:HA	1:B:1517:PRO:HD3	1.65	0.44
1:B:168:MET:HA	1:B:206:LEU:HB2	2.00	0.44
1:C:1104:ARG:O	1:C:1185:VAL:HG13	2.17	0.44
1:C:1270:VAL:HG11	1:C:1274:ILE:HD13	1.99	0.44
1:C:1557:ILE:HD11	1:C:1642:THR:HG21	2.00	0.44
1:C:1657:HIS:CG	1:C:1658:PRO:HD2	2.53	0.44
1:C:521:LYS:HB3	1:C:523:SER:HB3	1.99	0.44
1:C:67:SER:OG	2:H:359:HIS:CE1	2.61	0.44
2:G:1493:LEU:HB3	2:G:1494:PRO:CD	2.48	0.44
2:G:1846:GLU:C	2:G:1848:GLY:H	2.21	0.44
2:G:324:LEU:O	2:G:324:LEU:HD12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:459:VAL:HG12	2:G:468:LEU:HD12	2.00	0.44
2:G:860:ARG:H	2:G:1049:GLN:HG3	1.83	0.44
2:G:926:LEU:HB3	2:G:947:THR:CG2	2.46	0.44
2:H:1347:LEU:HA	2:H:1347:LEU:HD12	1.86	0.44
2:H:1561:ASN:HA	2:H:1562:PRO:HD3	1.83	0.44
2:H:455:ILE:C	2:H:455:ILE:HD12	2.38	0.44
2:H:594:VAL:CG2	2:H:610:THR:HG21	2.46	0.44
2:H:607:VAL:O	2:H:611:THR:HB	2.17	0.44
2:I:101:ILE:HG13	2:I:101:ILE:H	1.30	0.44
2:I:1180:MET:HB3	2:I:1199:GLU:HG2	1.98	0.44
2:I:938:TRP:CE2	2:I:944:ARG:HG3	2.52	0.44
1:A:1443:LEU:HA	1:A:1443:LEU:HD23	1.75	0.44
1:B:1385:GLN:HE21	1:B:1385:GLN:HB3	1.66	0.44
1:B:335:HIS:CD2	1:B:335:HIS:O	2.70	0.44
1:C:1158:PRO:HD2	1:C:1159:GLU:OE2	2.18	0.44
1:C:1243:VAL:O	1:C:1296:GLY:HA3	2.18	0.44
1:C:1487:LEU:C	1:C:1487:LEU:HD23	2.38	0.44
1:C:196:THR:O	1:C:213:PHE:HE2	2.01	0.44
1:C:235:SER:HA	1:C:276:ARG:NH2	2.33	0.44
1:C:340:ARG:HH12	1:C:344:GLN:HE21	1.65	0.44
1:C:413:LEU:C	1:C:415:SER:H	2.21	0.44
1:C:639:HIS:HB2	1:C:656:SER:OG	2.18	0.44
2:G:120:LYS:HB3	2:G:124:LYS:HE3	1.99	0.44
2:G:1321:ALA:HA	2:G:1322:PRO:HD3	1.86	0.44
2:G:142:ASN:HB2	2:G:550:VAL:HG13	1.99	0.44
2:G:231:LEU:HA	2:G:236:ILE:HD12	2.00	0.44
2:G:272:GLY:HA3	2:G:276:GLY:C	2.38	0.44
2:G:754:TYR:CD2	2:G:794:MET:CG	3.01	0.44
2:H:1222:GLU:HG3	2:H:1235:SER:OG	2.17	0.44
1:B:18:LEU:HD21	2:H:1815:LEU:HD12	1.99	0.44
2:H:463:PHE:CD2	2:H:463:PHE:C	2.90	0.44
2:H:601:THR:O	2:H:601:THR:CG2	2.65	0.44
2:H:826:GLY:HA3	2:H:1061:GLN:CB	2.44	0.44
2:H:938:TRP:CD1	2:H:944:ARG:HG3	2.53	0.44
2:I:1102:TYR:CE2	2:I:1152:ALA:HB2	2.53	0.44
2:I:1168:ASN:HA	2:I:1169:PRO:HD3	1.84	0.44
2:I:1210:ILE:O	2:I:1210:ILE:HG22	2.18	0.44
2:I:1236:LEU:HB2	2:I:1265:MET:SD	2.57	0.44
2:I:1493:LEU:HB3	2:I:1494:PRO:CD	2.48	0.44
2:I:1579:ILE:HG22	2:I:1580:THR:O	2.18	0.44
2:I:1676:MET:HE1	2:I:1781:LEU:CD2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:719:ILE:H	2:I:719:ILE:HG12	1.58	0.44
1:A:1431:GLU:CG	1:A:1433:HIS:CE1	3.00	0.44
1:A:1670:TYR:O	1:A:1674:VAL:HG23	2.18	0.44
1:A:254:TRP:CZ3	1:A:302:LEU:HD13	2.53	0.44
1:B:225:SER:OG	1:B:266:LEU:HD21	2.18	0.44
1:B:26:VAL:HG13	2:H:2013:ASN:ND2	2.33	0.44
1:C:295:ALA:HB1	1:C:300:VAL:O	2.18	0.44
1:C:478:GLU:OE1	1:C:478:GLU:HA	2.18	0.44
1:C:601:VAL:O	1:C:602:GLU:C	2.56	0.44
1:C:852:ARG:HB3	1:C:858:TRP:HZ2	1.83	0.44
2:G:1257:ASP:O	2:G:1261:ARG:HG3	2.17	0.44
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:1855:ILE:HB	2:G:1907:LEU:HD12	2.00	0.44
1:A:24:SER:HB3	2:G:2014:LEU:HD12	1.98	0.44
2:G:967:ILE:HD12	2:G:972:LEU:HD22	1.99	0.44
2:H:856:LYS:CE	2:H:1052:CYS:SG	3.06	0.44
2:H:120:LYS:HB3	2:H:124:LYS:HE3	1.99	0.44
2:H:439:ILE:HD12	2:H:484:ILE:CD1	2.47	0.44
2:H:73:GLU:OE2	2:H:76:LYS:HD2	2.18	0.44
2:H:852:GLU:H	2:H:852:GLU:HG3	1.37	0.44
2:I:1590:ARG:HG3	2:I:1608:TYR:CD2	2.53	0.44
2:I:1778:GLN:HB2	2:I:1779:PRO:HD3	2.00	0.44
2:I:1494:PRO:HB2	2:I:1823:SER:HB2	1.99	0.44
2:I:209:PHE:CE2	2:I:213:LEU:HD22	2.53	0.44
2:I:439:ILE:HD12	2:I:484:ILE:CD1	2.48	0.44
2:I:760:HIS:HA	2:I:761:PRO:HD3	1.82	0.44
1:B:1037:TRP:HB2	1:B:1598:GLN:OE1	2.18	0.44
1:B:1244:GLY:C	1:B:1327:CYS:HB2	2.38	0.44
1:B:176:VAL:HG12	1:B:178:GLY:H	1.83	0.44
1:B:267:VAL:HG12	1:B:290:MET:CE	2.48	0.44
1:B:32:GLN:HE22	1:B:57:ALA:N	2.15	0.44
1:B:496:PRO:HB2	1:B:519:VAL:HG12	1.99	0.44
1:C:1234:MET:CE	1:C:1326:ILE:HG21	2.48	0.44
1:C:1373:ARG:NE	1:C:1550:ASP:HB2	2.33	0.44
1:C:655:LEU:HD23	1:C:655:LEU:HA	1.79	0.44
2:G:455:ILE:HD11	2:G:469:ARG:NE	2.32	0.44
2:G:753:MET:O	2:G:757:ILE:HG13	2.18	0.44
2:H:1101:GLU:HB2	2:H:1147:ILE:O	2.17	0.44
2:H:1551:GLU:HB2	2:H:1552:PRO:HD3	2.00	0.44
2:H:272:GLY:HA3	2:H:276:GLY:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:391:LEU:CD2	2:H:394:ARG:NH2	2.80	0.44
2:H:572:ASN:CB	2:H:576:LYS:H	2.28	0.44
2:H:653:TYR:OH	2:H:690:VAL:HG11	2.18	0.44
2:I:1236:LEU:HD22	2:I:1238:LEU:HG	1.99	0.44
2:I:1330:GLY:HA2	2:I:1374:THR:HG21	1.99	0.44
2:I:272:GLY:HA3	2:I:276:GLY:C	2.37	0.44
2:I:297:ARG:O	2:I:301:THR:HG22	2.18	0.44
2:I:427:PHE:HB3	2:I:428:HIS:ND1	2.33	0.44
1:A:1291:LEU:HD21	1:A:1698:PHE:CE1	2.53	0.43
1:A:1539:ALA:O	1:A:1574:GLY:HA2	2.18	0.43
1:A:1666:THR:HG23	1:A:1669:ARG:CB	2.47	0.43
1:A:1717:ASP:HA	1:A:1718:PRO:HD3	1.83	0.43
1:B:42:GLU:O	1:B:77:GLU:N	2.47	0.43
1:B:833:PHE:O	1:B:834:GLY:O	2.35	0.43
2:G:1016:PRO:HD2	2:G:1017:PHE:CE2	2.53	0.43
2:G:1551:GLU:HB2	2:G:1552:PRO:HD3	2.00	0.43
2:G:1674:GLN:OE1	2:G:1712:ASN:HA	2.18	0.43
2:G:1776:PHE:C	2:G:1779:PRO:HD2	2.38	0.43
2:G:522:GLY:HA3	2:G:561:TRP:CH2	2.53	0.43
2:G:653:TYR:OH	2:G:690:VAL:HG11	2.17	0.43
2:G:719:ILE:H	2:G:719:ILE:HG12	1.57	0.43
2:H:1148:ASN:HD22	2:H:1148:ASN:C	2.21	0.43
2:H:15:SER:H	2:H:48:PHE:HE2	1.66	0.43
2:H:573:LYS:C	2:H:575:GLY:H	2.21	0.43
2:H:871:THR:HG21	2:H:887:LYS:HZ2	1.83	0.43
2:I:1159:ILE:CG2	2:I:1160:THR:N	2.81	0.43
2:I:1651:LEU:O	2:I:1652:THR:HG23	2.17	0.43
1:C:21:GLN:O	2:I:1977:HIS:CD2	2.71	0.43
2:I:218:TRP:HB3	2:I:225:THR:OG1	2.18	0.43
2:I:425:SER:HA	2:I:426:PRO:HD3	1.78	0.43
2:I:751:LEU:HD23	2:I:791:TYR:CD2	2.53	0.43
1:A:11:HIS:CD2	1:A:11:HIS:C	2.92	0.43
1:A:1556:THR:O	1:A:1560:MET:HG2	2.18	0.43
1:A:235:SER:HA	1:A:276:ARG:NH2	2.32	0.43
1:B:1022:THR:HG22	1:B:1226:SER:CB	2.48	0.43
1:B:1644:PHE:CD1	1:B:1644:PHE:N	2.86	0.43
1:C:1009:LEU:HA	1:C:1445:MET:HE2	1.99	0.43
1:C:406:TRP:CE3	1:C:407:ASN:HB2	2.53	0.43
1:C:833:PHE:O	1:C:834:GLY:O	2.36	0.43
2:G:184:VAL:HG12	2:G:188:ILE:HG12	2.00	0.43
2:G:397:LYS:HB2	2:G:398:ALA:H	1.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:674:TYR:HA	2:G:675:PRO:HD3	1.71	0.43
2:G:901:LYS:NZ	2:G:1031:LYS:O	2.50	0.43
2:H:1294:ALA:HA	2:H:1368:VAL:CG2	2.48	0.43
2:H:590:PRO:HA	2:H:591:PRO:HD3	1.82	0.43
2:H:778:TYR:N	2:H:779:PRO:CD	2.80	0.43
2:I:1257:ASP:O	2:I:1261:ARG:HG3	2.18	0.43
2:I:1735:ALA:O	2:I:1737:ILE:HG13	2.17	0.43
2:I:1662:THR:HB	2:I:1799:PRO:HG2	2.00	0.43
2:I:1808:SER:OG	2:I:1977:HIS:HE1	2.01	0.43
2:I:597:MET:HA	3:I:3051:FMN:C5A	2.47	0.43
2:I:397:LYS:HB3	2:I:416:PHE:CE2	2.53	0.43
2:I:732:TRP:CE2	2:I:750:MET:HE3	2.53	0.43
1:A:1442:ASN:HA	1:A:1442:ASN:HD22	1.62	0.43
1:A:451:MET:HE2	1:A:451:MET:HB3	1.79	0.43
1:B:242:THR:HG22	1:B:243:ILE:H	1.83	0.43
1:B:335:HIS:C	1:B:335:HIS:CD2	2.92	0.43
1:B:807:LYS:HD3	1:B:807:LYS:C	2.39	0.43
1:B:852:ARG:HB3	1:B:858:TRP:HZ2	1.83	0.43
1:C:1021:VAL:HG22	1:C:1387:ILE:HG22	2.01	0.43
1:C:1303:GLY:C	1:C:1307:THR:HG22	2.38	0.43
1:C:1291:LEU:HD21	1:C:1698:PHE:CE1	2.53	0.43
2:G:1102:TYR:CE2	2:G:1152:ALA:HB2	2.53	0.43
2:G:1175:LYS:HG3	2:G:1176:PRO:HD2	2.01	0.43
2:G:195:LEU:O	2:G:199:ILE:HG13	2.18	0.43
2:G:42:PRO:HG2	2:G:52:ASP:CG	2.38	0.43
2:G:751:LEU:HD23	2:G:791:TYR:CD2	2.53	0.43
2:H:1149:TRP:HA	2:H:1242:PHE:CD1	2.54	0.43
2:H:666:ILE:HG22	2:H:698:LEU:HD22	2.00	0.43
2:I:674:TYR:HA	2:I:675:PRO:HD3	1.69	0.43
2:I:754:TYR:CG	2:I:794:MET:HG2	2.53	0.43
1:A:1194:ASN:OD1	1:A:1196:LYS:HB2	2.18	0.43
1:A:335:HIS:CD2	1:A:335:HIS:C	2.92	0.43
1:A:458:THR:OG1	1:A:470:LYS:HD2	2.18	0.43
1:A:32:GLN:NE2	1:A:57:ALA:HA	2.33	0.43
1:B:1238:VAL:CG1	1:B:1239:HIS:N	2.81	0.43
1:B:908:LEU:HA	1:B:913:VAL:HG21	2.00	0.43
1:B:987:ASN:HD21	2:H:993:GLN:HE22	1.66	0.43
1:B:990:LEU:HD23	1:B:990:LEU:HA	1.77	0.43
1:C:825:PRO:HB2	1:C:843:LYS:HZ2	1.83	0.43
2:G:1040:LEU:O	2:G:1046:GLN:HG3	2.18	0.43
2:G:1180:MET:HB3	2:G:1199:GLU:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1589:VAL:HG21	2:G:1651:LEU:HD12	1.99	0.43
2:G:1782:THR:CG2	2:G:1827:LEU:HD21	2.48	0.43
2:G:397:LYS:HB3	2:G:416:PHE:CE2	2.53	0.43
2:G:581:THR:O	2:G:585:LYS:HB2	2.18	0.43
2:G:599:PRO:HD2	3:G:3051:FMN:H6	2.00	0.43
2:G:659:LEU:HD12	2:G:659:LEU:HA	1.81	0.43
2:H:1015:VAL:HG13	2:H:1017:PHE:CE2	2.53	0.43
2:H:1021:LEU:HA	2:H:1021:LEU:HD22	1.58	0.43
2:H:1228:THR:HG21	2:H:1234:VAL:HG23	2.00	0.43
2:H:1458:ASP:O	2:H:1462:LYS:HE3	2.19	0.43
2:H:1637:LEU:HA	2:H:1637:LEU:HD23	1.76	0.43
2:H:551:THR:C	2:H:553:ASN:H	2.21	0.43
2:H:654:VAL:HG12	2:H:654:VAL:O	2.18	0.43
2:H:652:ILE:CD1	2:H:658:MET:HE3	2.47	0.43
2:H:807:ILE:HA	2:H:818:LYS:HG2	1.98	0.43
2:H:854:ILE:HG22	2:H:856:LYS:HG3	1.99	0.43
1:B:1685:TYR:CZ	2:H:993:GLN:OE1	2.72	0.43
2:I:430:HIS:CE1	2:I:431:LEU:HD13	2.54	0.43
2:I:428:HIS:CD2	2:I:488:VAL:HG23	2.53	0.43
1:A:32:GLN:HE22	1:A:57:ALA:N	2.16	0.43
1:A:985:ARG:NH1	2:G:953:ARG:NH2	2.65	0.43
1:B:1050:CYS:HB3	1:B:1089:VAL:HG12	2.00	0.43
1:B:1430:ARG:HG2	1:B:1430:ARG:O	2.18	0.43
1:C:49:PRO:O	1:C:82:SER:HB2	2.19	0.43
2:G:1162:ASP:O	2:G:1163:LYS:HB2	2.19	0.43
2:G:1219:ILE:HB	2:G:1240:TYR:HB2	2.01	0.43
2:G:1496:LYS:CE	2:G:1693:ARG:HH21	2.26	0.43
2:H:1383:ASN:HD21	2:H:1418:ASP:CB	2.30	0.43
1:B:20:TYR:CD2	2:H:1985:VAL:HG21	2.54	0.43
2:H:245:GLN:HG2	2:H:505:GLY:HA2	2.01	0.43
2:H:246:LEU:HD12	2:H:246:LEU:HA	1.85	0.43
2:H:309:ARG:HD3	2:H:309:ARG:HA	1.63	0.43
2:H:160:PHE:CE2	2:H:504:PHE:HB2	2.54	0.43
2:H:643:LYS:HA	2:H:1163:LYS:HG2	1.99	0.43
2:I:1175:LYS:HG3	2:I:1176:PRO:HD2	2.00	0.43
2:I:1311:PHE:HD1	2:I:1320:LEU:O	2.02	0.43
2:I:319:LEU:HA	2:I:319:LEU:HD22	1.67	0.43
2:I:607:VAL:O	2:I:611:THR:HB	2.18	0.43
2:I:73:GLU:OE2	2:I:76:LYS:HD2	2.18	0.43
2:I:754:TYR:CE2	2:I:794:MET:HG3	2.53	0.43
2:I:856:LYS:CE	2:I:1052:CYS:SG	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1195:ALA:HB1	1:B:1200:ILE:HD12	1.99	0.43
1:A:332:THR:HG22	1:B:331:ILE:CD1	2.48	0.43
1:B:526:VAL:HG12	1:B:626:VAL:HG11	1.99	0.43
1:C:1310:GLU:OE1	1:C:1649:LYS:CE	2.65	0.43
1:C:1491:ARG:NH1	1:C:1744:TYR:O	2.51	0.43
1:C:1553:GLU:HA	1:C:1556:THR:HG23	2.00	0.43
1:C:1539:ALA:O	1:C:1574:GLY:HA2	2.18	0.43
1:C:1592:MET:HE2	1:C:1641:ILE:HG23	2.01	0.43
1:C:232:LEU:HD13	1:C:272:GLU:CB	2.48	0.43
2:G:562:LEU:HG	2:G:793:PRO:CB	2.48	0.43
2:G:23:PRO:HG2	2:G:86:LEU:HD11	2.00	0.43
2:H:745:ASP:HA	2:H:832:TRP:CH2	2.51	0.43
2:H:754:TYR:CE2	2:H:794:MET:HG3	2.52	0.43
2:I:1561:ASN:HA	2:I:1562:PRO:HD3	1.80	0.43
2:I:159:ILE:HG12	2:I:512:LEU:HD23	2.00	0.43
2:I:191:SER:HA	2:I:194:THR:CG2	2.43	0.43
2:I:240:LEU:HA	2:I:240:LEU:HD12	1.80	0.43
2:I:439:ILE:HD12	2:I:484:ILE:HD11	1.99	0.43
2:I:44:PRO:HA	2:I:53:GLU:OE2	2.19	0.43
2:I:594:VAL:CG2	2:I:610:THR:HG21	2.44	0.43
2:I:810:GLU:OE2	2:I:1070:ILE:N	2.43	0.43
1:A:1673:TYR:CZ	1:A:1677:VAL:HG21	2.53	0.43
1:B:1189:ILE:HG23	1:B:1190:PRO:HD2	2.00	0.43
1:B:256:LEU:HA	1:B:257:PRO:HD3	1.73	0.43
1:B:774:ILE:HA	1:B:775:PRO:HD3	1.74	0.43
1:C:1220:VAL:O	1:C:1224:ILE:HG12	2.19	0.43
1:C:1248:GLY:HA3	1:C:1301:PRO:HD2	2.01	0.43
1:C:1625:LEU:O	1:C:1627:PRO:HD3	2.18	0.43
2:G:1858:ASN:HA	2:G:1896:GLN:O	2.18	0.43
2:G:441:LYS:O	2:G:445:LYS:HG3	2.18	0.43
2:G:751:LEU:HD11	2:G:789:PHE:CD1	2.53	0.43
2:G:810:GLU:OE2	2:G:1070:ILE:N	2.44	0.43
2:G:835:THR:HG22	2:G:844:VAL:CA	2.49	0.43
2:H:1199:GLU:OE2	2:H:1567:ARG:NH1	2.52	0.43
2:H:536:ASN:HD21	2:H:540:ASP:HB3	1.84	0.43
2:H:595:PRO:HD3	2:H:800:LEU:HB2	2.00	0.43
2:H:705:LEU:HD23	2:H:705:LEU:HA	1.78	0.43
2:H:758:ARG:HD3	2:H:758:ARG:HA	1.88	0.43
2:I:914:LEU:HD21	2:I:1003:PHE:CD2	2.53	0.43
2:I:142:ASN:HB2	2:I:550:VAL:HG13	1.99	0.43
2:I:1427:VAL:HG22	2:I:1469:GLU:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:246:LEU:O	2:I:250:VAL:HG23	2.18	0.43
2:I:572:ASN:CB	2:I:576:LYS:H	2.27	0.43
2:I:703:LEU:HD21	2:I:705:LEU:CD2	2.45	0.43
2:I:33:LEU:HD21	2:I:80:PHE:CE2	2.54	0.43
2:I:972:LEU:HD23	2:I:979:ALA:HB2	2.00	0.43
1:A:1019:ILE:HG13	1:A:1316:VAL:HG13	2.01	0.43
1:A:411:GLN:O	1:A:415:SER:HB2	2.19	0.43
1:A:430:ARG:CZ	1:A:605:LEU:HD13	2.49	0.43
1:A:521:LYS:HB3	1:A:523:SER:HB3	2.01	0.43
1:A:888:ILE:HD12	1:A:939:PHE:CE2	2.45	0.43
1:B:1131:LEU:HA	1:B:1131:LEU:HD12	1.73	0.43
1:B:681:THR:HA	1:B:706:THR:OG1	2.19	0.43
1:B:828:PRO:HG3	1:B:868:ILE:HG22	2.00	0.43
1:C:1047:LEU:O	1:C:1051:VAL:HG23	2.19	0.43
1:C:330:GLU:O	1:C:330:GLU:HG2	2.18	0.43
2:G:109:LEU:HD22	2:G:114:THR:HG23	2.00	0.43
2:G:1768:LYS:HE2	2:G:1772:SER:HB3	2.00	0.43
2:G:938:TRP:CE2	2:G:944:ARG:HG3	2.54	0.43
2:H:1070:ILE:CD1	2:H:1074:MET:HG2	2.49	0.43
2:H:1156:CYS:SG	2:H:1250:PRO:HD2	2.59	0.43
2:H:184:VAL:HG12	2:H:188:ILE:HG12	2.00	0.43
2:H:305:PHE:CD1	2:H:442:ASP:HB3	2.53	0.43
2:H:786:SER:HB2	2:H:794:MET:HE2	2.01	0.43
2:H:780:TYR:HB2	2:H:799:PHE:CE2	2.53	0.43
2:I:1417:THR:O	2:I:1419:PHE:N	2.45	0.43
2:I:1684:SER:O	2:I:1688:GLN:HG3	2.18	0.43
2:I:2030:TYR:CD1	2:I:2034:GLY:HA2	2.54	0.43
2:I:279:THR:O	2:I:283:ILE:HB	2.19	0.43
2:I:245:GLN:HG2	2:I:505:GLY:HA2	2.00	0.43
2:I:503:ASP:O	2:I:530:ALA:HB3	2.19	0.43
2:I:778:TYR:N	2:I:779:PRO:CD	2.82	0.43
2:I:786:SER:HB3	2:I:794:MET:HE2	2.00	0.43
2:I:932:ILE:HD12	2:I:939:PHE:HD1	1.83	0.43
1:A:1219:VAL:CA	1:A:1384:ILE:HD11	2.32	0.43
1:A:1618:LEU:HD23	1:A:1621:PHE:CE2	2.54	0.43
1:A:248:LYS:HB2	1:A:248:LYS:HE3	1.82	0.43
1:A:66:GLU:HA	1:A:66:GLU:OE1	2.18	0.43
1:B:1283:MET:O	1:B:1287:VAL:HG23	2.18	0.43
1:B:370:GLU:O	1:B:373:ALA:HB3	2.19	0.43
1:B:35:PHE:HA	1:B:39:PHE:HD2	1.83	0.43
1:C:256:LEU:HA	1:C:257:PRO:HD3	1.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:884:LEU:HD22	2:G:1021:LEU:CD1	2.49	0.43
2:G:1021:LEU:HA	2:G:1021:LEU:HD22	1.60	0.43
2:G:1195:VAL:HG13	2:G:1211:LEU:CB	2.48	0.43
2:G:1651:LEU:HA	2:G:1651:LEU:HD23	1.73	0.43
2:G:184:VAL:O	2:G:184:VAL:HG12	2.19	0.43
2:G:607:VAL:O	2:G:611:THR:HB	2.17	0.43
2:G:866:LYS:O	2:G:870:GLU:HG3	2.18	0.43
2:H:1374:THR:HG23	2:H:1396:LEU:CD1	2.46	0.43
2:H:1889:VAL:HG22	2:H:1977:HIS:O	2.19	0.43
2:H:900:GLN:NE2	2:H:1051:THR:HA	2.34	0.43
2:I:7:ARG:CG	2:I:22:VAL:O	2.67	0.43
2:I:551:THR:C	2:I:553:ASN:H	2.22	0.43
2:I:562:LEU:HD23	2:I:562:LEU:HA	1.80	0.43
1:A:1019:ILE:HG21	1:A:1316:VAL:HG22	2.01	0.43
1:A:1332:TYR:HB3	1:A:1382:ALA:CB	2.49	0.43
1:A:242:THR:HB	1:A:244:THR:HB	2.00	0.43
1:A:267:VAL:O	1:A:290:MET:HE1	2.19	0.43
1:B:1270:VAL:HG11	1:B:1274:ILE:HD13	2.00	0.43
1:B:242:THR:HB	1:B:244:THR:HB	2.01	0.43
1:B:350:LEU:HB2	1:B:352:MET:HG2	2.01	0.43
1:B:411:GLN:O	1:B:415:SER:HB2	2.18	0.43
1:B:625:THR:HG23	1:B:627:SER:H	1.84	0.43
1:C:335:HIS:C	1:C:335:HIS:CD2	2.91	0.43
1:C:616:LEU:HB2	1:C:617:PRO:HD3	2.01	0.43
2:G:1494:PRO:HB2	2:G:1823:SER:HB2	2.00	0.43
2:G:2026:PHE:HB3	2:G:2042:ILE:HD13	2.00	0.43
2:H:1080:GLY:O	2:H:1084:LYS:HG3	2.19	0.43
2:H:1642:THR:HB	2:H:1651:LEU:HB2	2.01	0.43
2:H:1896:GLN:HE21	2:H:1896:GLN:HB3	1.60	0.43
2:H:258:PHE:CD1	2:H:258:PHE:N	2.87	0.43
2:H:629:GLY:O	2:H:632:ALA:HB3	2.18	0.43
2:H:748:THR:CB	2:H:749:PRO:HD3	2.46	0.43
2:H:732:TRP:CH2	2:H:749:PRO:HG2	2.53	0.43
2:I:615:TYR:CE2	2:I:1074:MET:HB3	2.53	0.43
2:I:198:LEU:HD13	2:I:198:LEU:HA	1.93	0.43
2:I:573:LYS:C	2:I:575:GLY:N	2.72	0.43
2:I:993:GLN:HB3	2:I:993:GLN:HE21	1.61	0.43
1:A:155:VAL:O	1:A:159:LEU:HG	2.19	0.42
1:A:1396:MET:O	1:A:1680:ARG:NH1	2.52	0.42
1:A:521:LYS:HE2	1:A:605:LEU:HD11	2.01	0.42
1:A:44:VAL:HG13	1:A:78:ILE:HG12	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1233:GLU:CD	1:B:1680:ARG:HH21	2.22	0.42
1:B:335:HIS:CE1	1:C:335:HIS:ND1	2.87	0.42
1:B:980:VAL:H	2:H:968:GLN:CD	2.22	0.42
1:C:706:THR:HB	1:C:737:PHE:HB3	2.00	0.42
2:G:427:PHE:HB3	2:G:428:HIS:ND1	2.34	0.42
2:G:455:ILE:C	2:G:455:ILE:HD12	2.39	0.42
2:G:551:THR:C	2:G:553:ASN:H	2.20	0.42
2:H:1579:ILE:HD11	2:H:1615:MET:SD	2.58	0.42
2:H:1651:LEU:HD23	2:H:1651:LEU:HA	1.79	0.42
2:H:1757:GLU:HG3	2:H:1757:GLU:H	1.51	0.42
2:H:960:LYS:CE	2:H:960:LYS:HA	2.44	0.42
2:I:1551:GLU:HB2	2:I:1552:PRO:HD3	2.00	0.42
2:I:1980:TYR:HD1	2:I:1981:LEU:HD12	1.83	0.42
2:I:702:TYR:HB3	2:I:727:PRO:HB2	1.99	0.42
2:I:583:PHE:CD2	2:I:764:MET:HE3	2.54	0.42
1:A:1009:LEU:HA	1:A:1445:MET:HE2	2.01	0.42
1:A:1056:ILE:CD1	1:A:1193:TRP:CD1	3.00	0.42
1:A:1195:ALA:CB	1:A:1213:LEU:HD13	2.49	0.42
1:A:1553:GLU:HA	1:A:1556:THR:HG23	2.01	0.42
1:A:340:ARG:NH1	1:A:344:GLN:CG	2.70	0.42
1:B:1238:VAL:CG1	1:B:1242:GLU:HB2	2.49	0.42
1:B:1280:ILE:HD13	1:B:1302:VAL:HG22	2.01	0.42
1:B:1553:GLU:HA	1:B:1556:THR:HG23	2.00	0.42
1:C:406:TRP:CD2	1:C:1619:GLU:HG3	2.55	0.42
1:C:451:MET:HE2	1:C:451:MET:HB3	1.73	0.42
1:C:949:GLU:O	1:C:953:VAL:CG1	2.67	0.42
2:G:1339:PHE:N	2:G:1340:PRO:CD	2.82	0.42
2:G:1458:ASP:O	2:G:1462:LYS:HE3	2.19	0.42
2:G:238:CYS:CB	2:G:239:PRO:HD3	2.45	0.42
2:H:240:LEU:O	2:H:244:ILE:HG13	2.19	0.42
2:H:274:SER:OG	2:H:428:HIS:HE1	2.02	0.42
2:H:543:PHE:CB	2:H:545:GLN:NE2	2.82	0.42
2:H:601:THR:HB	2:H:620:ALA:HB2	2.01	0.42
2:H:703:LEU:HD21	2:H:705:LEU:CD2	2.49	0.42
2:I:1666:PHE:CE1	2:I:1814:ALA:HA	2.53	0.42
1:C:18:LEU:HD21	2:I:1815:LEU:HD12	2.00	0.42
2:I:814:SER:HB2	2:I:1040:LEU:CD1	2.48	0.42
1:A:1175:ILE:HA	1:A:1176:PRO:HD3	1.86	0.42
1:A:499:PRO:HD3	1:A:516:ARG:HH21	1.83	0.42
1:B:1446:LYS:O	1:B:1450:ARG:HG3	2.19	0.42
1:B:24:SER:CB	2:H:2014:LEU:HD12	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:LYS:HB2	1:B:65:TYR:CE1	2.51	0.42
1:C:1061:SER:HB2	1:C:1078:SER:HB3	1.99	0.42
1:C:1446:LYS:O	1:C:1450:ARG:HG3	2.18	0.42
1:C:377:TYR:O	1:C:380:ALA:HB3	2.19	0.42
2:G:1389:ILE:HG13	2:G:1411:PHE:CD1	2.52	0.42
2:G:1473:THR:O	2:G:1481:SER:HB3	2.18	0.42
2:G:258:PHE:N	2:G:258:PHE:CD1	2.87	0.42
2:H:1980:TYR:HD1	2:H:1981:LEU:HD12	1.84	0.42
2:H:9:LEU:HB2	2:H:27:PHE:HE1	1.83	0.42
2:H:717:ILE:HG23	2:H:760:HIS:CE1	2.54	0.42
2:I:1308:CYS:HB3	2:I:1311:PHE:CE2	2.54	0.42
2:I:1325:PHE:O	2:I:1328:VAL:HG12	2.18	0.42
2:I:1845:ASP:HB2	2:I:1849:ARG:N	2.20	0.42
2:I:298:LYS:HA	2:I:448:VAL:CG2	2.50	0.42
1:A:1220:VAL:O	1:A:1224:ILE:HG12	2.18	0.42
1:B:1244:GLY:O	1:B:1327:CYS:HB2	2.19	0.42
1:B:1455:ARG:HD2	1:B:1455:ARG:HA	1.86	0.42
1:B:1618:LEU:HD23	1:B:1621:PHE:HE2	1.85	0.42
1:B:458:THR:OG1	1:B:470:LYS:HD2	2.20	0.42
1:C:1105:LEU:HA	1:C:1105:LEU:HD23	1.85	0.42
1:C:1114:TYR:CE1	1:C:1337:GLU:HG3	2.55	0.42
1:C:168:MET:HA	1:C:206:LEU:HB2	2.00	0.42
1:C:27:ARG:HB2	2:I:2016:ALA:HB2	2.00	0.42
1:C:32:GLN:NE2	1:C:57:ALA:CA	2.82	0.42
1:C:428:VAL:HG12	1:C:606:ASP:O	2.20	0.42
1:C:798:ASN:HA	1:C:801:ARG:HB2	2.01	0.42
1:C:852:ARG:NH1	1:C:856:GLU:OE1	2.52	0.42
2:G:579:VAL:CG2	2:G:1078:HIS:CD2	3.01	0.42
2:G:1156:CYS:SG	2:G:1250:PRO:HD2	2.60	0.42
2:G:1323:MET:CE	2:G:1605:VAL:HG22	2.49	0.42
2:G:1979:THR:O	2:G:1982:MET:HB2	2.19	0.42
2:G:339:LEU:HD23	2:G:419:ARG:O	2.19	0.42
2:H:1002:HIS:NE2	2:H:1006:MET:CE	2.82	0.42
2:H:1159:ILE:CG2	2:H:1160:THR:N	2.83	0.42
2:H:1149:TRP:NE1	2:H:1213:LEU:HD12	2.34	0.42
2:H:1427:VAL:HG22	2:H:1469:GLU:CG	2.49	0.42
2:H:1862:VAL:HG22	2:H:1863:ALA:N	2.34	0.42
2:H:478:ARG:O	2:H:482:CYS:HB2	2.20	0.42
2:H:652:ILE:HD13	2:H:658:MET:HE3	2.02	0.42
2:H:665:LEU:HD22	2:H:665:LEU:O	2.19	0.42
2:H:827:VAL:HG12	2:H:828:PRO:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:835:THR:HG23	2:H:843:ILE:O	2.18	0.42
2:H:950:PHE:O	2:H:953:ARG:HB3	2.19	0.42
2:I:579:VAL:CG2	2:I:1078:HIS:CD2	3.01	0.42
2:I:1101:GLU:HG2	2:I:1148:ASN:HA	2.01	0.42
2:I:1541:VAL:HG22	2:I:1625:SER:HB2	2.01	0.42
2:I:1672:GLN:HA	2:I:1676:MET:HE3	1.95	0.42
2:I:169:TYR:CG	2:I:170:PHE:N	2.86	0.42
2:I:2036:GLU:HG2	2:I:2039:LYS:HZ3	1.83	0.42
2:I:298:LYS:HG2	2:I:448:VAL:CG2	2.38	0.42
2:I:538:ASP:HB2	2:I:540:ASP:HB2	2.01	0.42
2:I:732:TRP:CH2	2:I:749:PRO:HG2	2.55	0.42
1:A:1431:GLU:OE2	1:A:1433:HIS:HE1	2.02	0.42
1:A:12:ILE:O	1:A:15:THR:HG23	2.19	0.42
1:B:1145:LYS:HD3	1:B:1154:ILE:HG12	2.02	0.42
1:B:1657:HIS:CG	1:B:1658:PRO:HD2	2.55	0.42
1:B:1682:LYS:O	2:H:994:PHE:HD2	2.02	0.42
1:C:20:TYR:CE2	2:I:1985:VAL:HG11	2.54	0.42
1:C:44:VAL:HG13	1:C:78:ILE:HG12	1.98	0.42
2:G:1015:VAL:HA	2:G:1016:PRO:HD3	1.78	0.42
2:G:1135:GLU:HG2	2:G:1176:PRO:HG2	2.02	0.42
2:G:1223:MET:HE3	2:G:1238:LEU:CD1	2.49	0.42
2:G:1279:PHE:CD2	2:G:1340:PRO:HG3	2.48	0.42
2:G:1495:THR:O	2:G:1496:LYS:HB2	2.19	0.42
2:G:246:LEU:HD12	2:G:246:LEU:HA	1.82	0.42
2:G:324:LEU:O	2:G:328:LEU:HG	2.18	0.42
2:G:667:LYS:HD2	2:G:697:THR:CG2	2.38	0.42
2:H:1159:ILE:HG13	2:H:1169:PRO:CD	2.50	0.42
2:H:176:LEU:CD2	2:H:184:VAL:HG21	2.50	0.42
2:H:520:LYS:O	2:H:521:ASP:C	2.58	0.42
2:H:970:TYR:O	2:H:973:LEU:HB2	2.18	0.42
2:I:1101:GLU:CB	2:I:1147:ILE:O	2.68	0.42
2:I:1214:LEU:HD11	2:I:1220:GLN:NE2	2.35	0.42
2:I:1347:LEU:HA	2:I:1347:LEU:HD12	1.91	0.42
2:I:1359:MET:CE	2:I:1404:MET:HB3	2.50	0.42
2:I:339:LEU:HD23	2:I:419:ARG:O	2.20	0.42
2:I:441:LYS:O	2:I:445:LYS:HG3	2.20	0.42
2:I:612:ASN:HD21	2:I:641:ILE:HA	1.84	0.42
2:I:7:ARG:NH2	2:I:24:THR:O	2.52	0.42
2:I:967:ILE:HD12	2:I:972:LEU:HD22	2.00	0.42
1:C:1682:LYS:O	2:I:994:PHE:HD2	2.03	0.42
1:A:12:ILE:O	1:A:16:GLU:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:THR:O	1:A:213:PHE:HE2	2.01	0.42
1:A:406:TRP:CD2	1:A:1619:GLU:HG3	2.55	0.42
1:A:406:TRP:CE3	1:A:407:ASN:HB2	2.54	0.42
1:A:444:ASN:HB2	1:A:447:LEU:N	2.14	0.42
1:B:1534:ASP:OD1	1:B:1566:ARG:HD3	2.19	0.42
1:B:155:VAL:HG22	1:B:186:ILE:CG2	2.50	0.42
1:B:706:THR:HB	1:B:737:PHE:HB3	2.01	0.42
1:B:874:GLY:O	1:B:875:THR:C	2.58	0.42
1:C:1338:GLU:HG2	1:C:1338:GLU:H	1.57	0.42
1:C:1516:ASP:HA	1:C:1517:PRO:HD3	1.66	0.42
1:C:242:THR:HB	1:C:244:THR:HB	2.02	0.42
2:G:1044:VAL:HG21	2:G:1050:ARG:NE	2.34	0.42
2:G:1056:GLY:HA2	2:G:1057:PRO:HD3	1.92	0.42
2:G:1210:ILE:O	2:G:1210:ILE:HG22	2.20	0.42
2:G:1383:ASN:OD1	2:G:1388:LYS:HG3	2.20	0.42
2:G:1697:HIS:CE1	2:G:1829:GLU:CG	3.02	0.42
2:G:439:ILE:HD12	2:G:484:ILE:HD11	2.00	0.42
2:G:15:SER:H	2:G:48:PHE:HE2	1.67	0.42
2:G:638:VAL:HG22	2:G:675:PRO:HG2	2.02	0.42
2:G:854:ILE:HG22	2:G:856:LYS:HG3	2.01	0.42
2:H:1015:VAL:HA	2:H:1016:PRO:HD3	1.79	0.42
2:H:1303:ALA:HB2	2:H:1556:VAL:HG21	2.01	0.42
2:H:1335:ILE:O	2:H:1338:ILE:HG12	2.19	0.42
2:H:142:ASN:HB2	2:H:550:VAL:HG13	2.01	0.42
1:B:59:ARG:NH1	2:H:1896:GLN:HE22	2.17	0.42
2:H:726:PHE:HA	2:H:727:PRO:HD3	1.88	0.42
2:H:963:THR:HB	2:H:964:LEU:H	1.72	0.42
2:H:967:ILE:CD1	2:H:972:LEU:HD22	2.50	0.42
2:I:804:ARG:NH2	2:I:1068:GLU:OE1	2.53	0.42
2:I:1666:PHE:CD1	2:I:1814:ALA:HB2	2.54	0.42
2:I:463:PHE:CD1	2:I:486:LEU:HD22	2.54	0.42
2:I:592:LEU:O	2:I:616:THR:HG23	2.19	0.42
1:A:382:LEU:HA	1:A:382:LEU:HD23	1.79	0.42
1:A:666:ALA:O	1:A:670:GLY:HA2	2.19	0.42
1:B:1705:PRO:HB2	1:B:1733:PHE:CD1	2.55	0.42
1:B:20:TYR:CE1	2:H:2035:SER:HB2	2.55	0.42
1:B:411:GLN:HE22	1:B:1628:SER:N	2.16	0.42
1:C:1219:VAL:CA	1:C:1384:ILE:CD1	2.94	0.42
1:C:1239:HIS:HE1	1:C:1714:VAL:O	2.02	0.42
1:C:626:VAL:HG23	1:C:664:GLU:OE2	2.20	0.42
1:C:719:GLN:HG3	1:C:720:SER:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:814:SER:CB	2:G:1040:LEU:HD13	2.50	0.42
2:G:543:PHE:CB	2:G:545:GLN:NE2	2.81	0.42
2:G:827:VAL:HG21	2:G:840:THR:CG2	2.49	0.42
2:G:879:LYS:HA	2:G:879:LYS:HD3	1.68	0.42
2:H:1180:MET:HB3	2:H:1199:GLU:HG2	2.02	0.42
2:H:1293:THR:CG2	2:H:1296:GLU:H	2.24	0.42
1:B:90:TYR:O	2:H:1537:ILE:HD11	2.20	0.42
2:H:1781:LEU:HA	2:H:1781:LEU:HD22	1.83	0.42
2:H:581:THR:O	2:H:585:LYS:HB2	2.20	0.42
2:I:896:ASN:O	2:I:1050:ARG:NH2	2.52	0.42
2:I:1552:PRO:O	2:I:1556:VAL:HG23	2.19	0.42
2:I:1838:MET:O	2:I:1974:VAL:HG21	2.20	0.42
2:I:1959:LYS:HG2	2:I:1959:LYS:O	2.19	0.42
2:I:258:PHE:N	2:I:258:PHE:CD1	2.87	0.42
2:I:730:LEU:C	2:I:730:LEU:HD12	2.40	0.42
2:I:950:PHE:O	2:I:953:ARG:HB3	2.19	0.42
1:A:28:TRP:CE2	1:A:53:LEU:HD22	2.55	0.42
1:A:496:PRO:HB2	1:A:519:VAL:HG12	2.01	0.42
1:A:32:GLN:NE2	1:A:57:ALA:CA	2.83	0.42
1:B:1008:GLU:HG2	1:B:1446:LYS:HA	2.02	0.42
1:B:280:GLU:O	1:B:284:LYS:HG3	2.20	0.42
1:B:290:MET:HE2	1:B:290:MET:HB3	1.95	0.42
1:B:451:MET:HE2	1:B:451:MET:HB3	1.74	0.42
1:B:888:ILE:HD12	1:B:939:PHE:CE2	2.45	0.42
1:B:949:GLU:O	1:B:953:VAL:CG1	2.68	0.42
1:C:1420:ALA:HA	1:C:1421:PRO:HD3	1.78	0.42
1:C:1618:LEU:HD23	1:C:1621:PHE:CE2	2.55	0.42
1:C:183:GLN:NE2	1:C:202:GLU:HG2	2.31	0.42
1:C:455:ILE:HD13	1:C:455:ILE:HA	1.85	0.42
1:C:827:SER:HA	1:C:828:PRO:HD3	1.70	0.42
2:G:106:ALA:HB2	2:G:545:GLN:HG2	2.02	0.42
2:G:1666:PHE:CD1	2:G:1814:ALA:CB	3.02	0.42
2:G:1875:VAL:HG22	2:G:1910:VAL:HG11	2.01	0.42
2:G:191:SER:HA	2:G:194:THR:CG2	2.46	0.42
2:G:2036:GLU:HB2	2:G:2037:PRO:CD	2.47	0.42
2:G:586:LEU:HD12	2:G:764:MET:SD	2.59	0.42
2:G:584:SER:CB	2:G:591:PRO:HG3	2.47	0.42
2:G:892:ILE:HD11	2:G:903:TRP:CD2	2.51	0.42
2:H:1339:PHE:N	2:H:1340:PRO:CD	2.83	0.42
2:H:1541:VAL:HG22	2:H:1625:SER:HB2	2.01	0.42
2:H:1676:MET:HE1	2:H:1781:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1752:PHE:HZ	2:H:1836:MET:HE3	1.84	0.42
2:H:1855:ILE:HB	2:H:1907:LEU:HD12	2.01	0.42
2:H:1940:LEU:HD12	2:H:1941:PHE:N	2.34	0.42
2:I:1590:ARG:HG3	2:I:1608:TYR:CG	2.54	0.42
2:I:190:PHE:O	2:I:194:THR:HG22	2.19	0.42
2:I:581:THR:O	2:I:585:LYS:HB2	2.20	0.42
1:A:1303:GLY:C	1:A:1307:THR:HG22	2.40	0.42
1:A:1657:HIS:CG	1:A:1658:PRO:HD2	2.55	0.42
1:A:998:TYR:CD2	1:A:1667:GLU:HG3	2.55	0.42
1:B:1119:LYS:HE2	1:B:1341:PHE:CD1	2.54	0.42
1:B:400:ARG:CG	1:B:400:ARG:NH1	2.51	0.42
1:B:36:LEU:CD2	1:B:61:LEU:HD21	2.42	0.42
1:B:44:VAL:HG13	1:B:78:ILE:HG12	1.98	0.42
1:C:1076:VAL:CG1	1:C:1081:LYS:HA	2.50	0.42
1:C:1304:ALA:O	1:C:1307:THR:CG2	2.68	0.42
1:C:1418:VAL:N	1:C:1419:PRO:CD	2.83	0.42
1:C:1600:LEU:HD11	1:C:1655:VAL:HG12	2.01	0.42
1:C:155:VAL:HG22	1:C:186:ILE:CG2	2.50	0.42
1:C:19:ALA:O	1:C:22:PHE:HB2	2.19	0.42
1:C:453:TYR:O	1:C:457:ASN:HB2	2.19	0.42
1:C:792:HIS:CE1	1:C:796:LEU:HD23	2.55	0.42
2:G:856:LYS:CE	2:G:1052:CYS:SG	3.07	0.42
2:G:571:LYS:HB2	2:G:1099:ALA:HB2	2.02	0.42
2:G:237:SER:O	2:G:241:ILE:HG13	2.20	0.42
2:G:298:LYS:HA	2:G:448:VAL:CG2	2.50	0.42
2:G:468:LEU:O	2:G:471:LEU:HB2	2.20	0.42
2:G:490:TRP:CZ2	2:G:512:LEU:HD21	2.55	0.42
2:I:1457:PHE:CD2	2:I:1459:LEU:HD23	2.55	0.42
2:I:258:PHE:HD1	2:I:258:PHE:N	2.18	0.42
2:I:524:GLY:HA2	2:I:558:ASN:O	2.20	0.42
2:I:740:HIS:CE1	2:I:852:GLU:OE1	2.73	0.42
1:B:1264:ARG:NH1	1:B:1270:VAL:HB	2.34	0.42
1:B:1338:GLU:HG2	1:B:1338:GLU:H	1.58	0.42
1:B:1665:ILE:HD11	1:B:1669:ARG:CG	2.50	0.42
1:B:238:PRO:CG	1:B:283:ALA:HB2	2.50	0.42
1:B:539:SER:O	1:B:540:GLN:C	2.54	0.42
1:C:1029:PRO:HG2	1:C:1581:THR:O	2.20	0.42
1:C:1430:ARG:O	1:C:1430:ARG:HG2	2.19	0.42
1:C:1639:VAL:HG12	1:C:1640:SER:N	2.35	0.42
1:C:1657:HIS:CE1	1:C:1658:PRO:HD2	2.54	0.42
1:C:42:GLU:O	1:C:77:GLU:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:683:ALA:HA	1:C:689:GLY:HA3	2.02	0.42
2:G:1541:VAL:HG22	2:G:1625:SER:HB2	2.02	0.42
2:G:1989:LYS:NZ	2:G:2037:PRO:HG2	2.35	0.42
2:G:507:GLY:O	2:G:508:GLY:C	2.58	0.42
2:G:601:THR:O	2:G:601:THR:CG2	2.66	0.42
2:G:670:ARG:HD2	2:G:676:ILE:O	2.20	0.42
2:G:732:TRP:CH2	2:G:749:PRO:HG2	2.55	0.42
2:H:1321:ALA:HA	2:H:1322:PRO:HD3	1.84	0.42
2:H:1819:ALA:CA	2:H:2005:ARG:HH11	2.26	0.42
2:H:279:THR:O	2:H:283:ILE:HB	2.19	0.42
2:H:712:ALA:O	2:H:715:GLN:HB3	2.20	0.42
2:I:1079:ASP:O	2:I:1082:ILE:HG22	2.19	0.42
2:I:1195:VAL:HG13	2:I:1211:LEU:CB	2.46	0.42
2:I:1738:PHE:HE1	2:I:1837:THR:HG23	1.85	0.42
2:I:248:HIS:CE1	2:I:531:GLY:HA2	2.55	0.42
2:I:156:LEU:HD23	2:I:500:HIS:HB2	2.02	0.42
2:I:703:LEU:CD2	2:I:705:LEU:HG	2.50	0.42
1:A:1260:MET:HB2	1:A:1274:ILE:HD12	2.02	0.41
1:A:1263:ASP:HB2	1:A:1270:VAL:HG21	2.01	0.41
1:A:530:ALA:HA	1:A:636:PRO:HB3	2.01	0.41
1:A:91:THR:HA	1:A:92:PRO:HD3	1.81	0.41
1:A:93:ASP:CB	1:A:94:PRO:HD2	2.37	0.41
1:B:1543:GLY:HA2	1:B:1550:ASP:OD1	2.20	0.41
1:B:1666:THR:HG23	1:B:1669:ARG:CB	2.49	0.41
1:B:82:SER:OG	1:B:83:LYS:HG3	2.20	0.41
1:B:988:ILE:H	1:B:988:ILE:HG12	1.69	0.41
1:C:1154:ILE:O	1:C:1154:ILE:HG13	2.20	0.41
1:C:1644:PHE:CD1	1:C:1644:PHE:N	2.88	0.41
2:G:995:LEU:HB3	2:G:1000:ILE:CD1	2.50	0.41
2:G:1079:ASP:O	2:G:1082:ILE:HG22	2.19	0.41
2:G:1169:PRO:O	2:G:1173:VAL:HG23	2.20	0.41
2:G:1579:ILE:CD1	2:G:1615:MET:SD	3.08	0.41
2:G:1778:GLN:HB2	2:G:1779:PRO:HD3	2.02	0.41
2:G:258:PHE:HD1	2:G:258:PHE:N	2.18	0.41
2:G:520:LYS:O	2:G:521:ASP:C	2.58	0.41
2:G:786:SER:HB3	2:G:794:MET:HE2	2.01	0.41
2:H:712:ALA:O	2:H:716:VAL:HG23	2.20	0.41
2:H:754:TYR:CG	2:H:794:MET:HG2	2.55	0.41
2:H:810:GLU:OE2	2:H:1070:ILE:N	2.45	0.41
2:I:1002:HIS:NE2	2:I:1006:MET:HE3	2.35	0.41
2:I:1593:ILE:O	2:I:1597:ALA:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1842:VAL:HA	2:I:1843:PRO:HD2	1.80	0.41
2:I:1862:VAL:HG22	2:I:1863:ALA:N	2.35	0.41
2:I:1940:LEU:HD12	2:I:1941:PHE:N	2.35	0.41
2:I:1989:LYS:NZ	2:I:2037:PRO:HG2	2.35	0.41
2:I:360:LEU:HA	2:I:361:PRO:HD3	1.89	0.41
2:I:659:LEU:O	2:I:663:ILE:HG12	2.20	0.41
1:A:1154:ILE:O	1:A:1154:ILE:HG13	2.19	0.41
1:A:1406:MET:HE1	1:A:1428:THR:HB	2.03	0.41
1:A:21:GLN:O	2:G:1977:HIS:CD2	2.74	0.41
1:A:237:MET:HG3	1:A:241:PHE:HB3	2.00	0.41
1:A:370:GLU:O	1:A:373:ALA:HB3	2.20	0.41
1:A:453:TYR:O	1:A:457:ASN:HB2	2.20	0.41
1:A:2:LYS:HE2	1:A:4:GLU:OE1	2.19	0.41
1:B:1056:ILE:HG13	1:B:1057:MET:N	2.35	0.41
1:B:157:HIS:CE1	1:B:269:LEU:HD11	2.55	0.41
1:C:1280:ILE:HD13	1:C:1302:VAL:HG22	2.02	0.41
1:C:1639:VAL:CG1	1:C:1640:SER:N	2.82	0.41
1:C:444:ASN:HB2	1:C:447:LEU:N	2.17	0.41
1:C:927:ASN:O	1:C:929:GLY:N	2.41	0.41
2:G:1352:HIS:HD2	2:G:1410:PHE:CD2	2.38	0.41
2:G:1383:ASN:HD21	2:G:1418:ASP:CB	2.33	0.41
1:A:29:ILE:HD13	2:G:1894:GLU:HA	2.02	0.41
2:G:1986:LYS:N	2:G:1987:PRO:CD	2.82	0.41
2:G:260:PRO:HD3	2:G:289:TRP:CZ2	2.55	0.41
2:G:345:THR:HG22	2:G:347:GLU:N	2.25	0.41
2:G:601:THR:HB	2:G:620:ALA:HB2	2.02	0.41
2:G:612:ASN:HD21	2:G:641:ILE:HA	1.84	0.41
2:H:1257:ASP:O	2:H:1261:ARG:HG3	2.19	0.41
2:H:1590:ARG:HG3	2:H:1608:TYR:CG	2.55	0.41
2:H:1593:ILE:HD13	2:H:1626:ILE:CD1	2.51	0.41
2:H:2039:LYS:HA	2:H:2042:ILE:HG13	2.03	0.41
2:H:38:ASN:HA	2:H:41:LEU:HD12	2.02	0.41
2:I:1135:GLU:HG2	2:I:1176:PRO:HG2	2.02	0.41
2:I:120:LYS:HB3	2:I:124:LYS:HE3	2.00	0.41
2:I:717:ILE:O	2:I:720:ALA:HB3	2.20	0.41
2:I:732:TRP:CB	2:I:750:MET:HE1	2.49	0.41
2:I:827:VAL:HG12	2:I:828:PRO:O	2.20	0.41
1:A:1195:ALA:HB1	1:A:1200:ILE:HD12	2.02	0.41
1:A:1239:HIS:HE1	1:A:1714:VAL:O	2.04	0.41
1:A:529:MET:HG2	1:A:638:LEU:CG	2.50	0.41
1:A:807:LYS:C	1:A:807:LYS:HD3	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:931:GLN:H	1:A:931:GLN:HG3	1.30	0.41
1:B:44:VAL:HG11	1:B:78:ILE:HG12	2.00	0.41
1:C:1257:LEU:HA	1:C:1257:LEU:HD23	1.84	0.41
1:C:12:ILE:HD11	2:I:2041:ILE:HD11	2.01	0.41
1:C:1370:THR:HG22	1:C:1371:THR:N	2.35	0.41
1:C:155:VAL:O	1:C:159:LEU:HG	2.19	0.41
1:C:2:LYS:HE2	1:C:4:GLU:OE1	2.19	0.41
1:C:413:LEU:HD13	1:C:451:MET:HG2	2.03	0.41
1:C:635:ILE:CG2	1:C:651:TYR:CG	3.01	0.41
2:G:1258:ARG:O	2:G:1262:ILE:HG13	2.20	0.41
2:G:455:ILE:HD13	2:G:457:ILE:O	2.20	0.41
2:G:638:VAL:HA	2:G:641:ILE:CG2	2.50	0.41
2:G:717:ILE:HG23	2:G:760:HIS:CE1	2.56	0.41
2:H:1128:LYS:HG2	2:H:1181:VAL:HG22	2.02	0.41
2:H:1223:MET:HE2	2:H:1223:MET:HB2	1.99	0.41
1:B:41:THR:HG21	2:H:1663:THR:HB	2.01	0.41
2:H:455:ILE:HG12	2:H:469:ARG:CG	2.49	0.41
2:H:705:LEU:CD1	2:H:716:VAL:HG13	2.46	0.41
2:H:732:TRP:CE2	2:H:750:MET:HE3	2.55	0.41
2:H:812:LYS:HA	2:H:812:LYS:HD3	1.82	0.41
2:H:844:VAL:HG22	2:H:858:ALA:HB2	2.01	0.41
2:I:1273:GLU:HB3	2:I:1274:PRO:CD	2.50	0.41
2:I:1493:LEU:HB3	2:I:1494:PRO:HD2	2.02	0.41
2:I:1680:LEU:HD13	2:I:1687:ALA:CB	2.48	0.41
2:I:38:ASN:HA	2:I:41:LEU:HD12	2.02	0.41
1:A:1720:ALA:O	1:A:1721:ARG:HG2	2.21	0.41
1:A:916:LEU:HD22	1:A:922:VAL:HG22	2.02	0.41
1:B:1257:LEU:HD23	1:B:1257:LEU:HA	1.76	0.41
1:B:1396:MET:O	1:B:1680:ARG:NH1	2.52	0.41
1:B:406:TRP:CE3	1:B:1619:GLU:HG3	2.55	0.41
1:B:293:LYS:O	1:B:297:ILE:HG13	2.21	0.41
1:B:444:ASN:CB	1:B:446:ALA:H	2.31	0.41
1:B:780:GLU:O	1:B:781:LEU:C	2.58	0.41
1:C:1215:VAL:O	1:C:1219:VAL:HG23	2.20	0.41
1:C:1477:ILE:N	1:C:1478:PRO:CD	2.83	0.41
1:C:294:TYR:CZ	1:C:298:VAL:HG21	2.55	0.41
1:C:931:GLN:HG3	1:C:931:GLN:H	1.31	0.41
1:C:949:GLU:O	1:C:953:VAL:HG12	2.21	0.41
2:G:1842:VAL:HA	2:G:1843:PRO:HD2	1.86	0.41
2:G:421:LEU:HA	2:G:422:PRO:HD3	1.81	0.41
2:G:638:VAL:O	2:G:641:ILE:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:73:GLU:OE2	2:G:76:LYS:HD2	2.20	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:1175:LYS:HG3	2:H:1176:PRO:HD2	2.02	0.41
2:H:60:LEU:HD23	2:H:60:LEU:O	2.20	0.41
2:H:827:VAL:HG21	2:H:840:THR:CG2	2.51	0.41
2:I:1458:ASP:O	2:I:1462:LYS:HE3	2.21	0.41
2:I:2020:GLN:NE2	2:I:2020:GLN:HA	2.36	0.41
2:I:599:PRO:HD2	3:I:3051:FMN:H6	2.02	0.41
2:I:397:LYS:HB2	2:I:398:ALA:H	1.68	0.41
2:I:516:THR:O	2:I:519:ASN:HB2	2.19	0.41
2:I:559:PRO:HB3	2:I:564:GLU:HG3	2.02	0.41
2:I:566:HIS:ND1	2:I:567:PRO:HD2	2.35	0.41
2:I:601:THR:O	2:I:601:THR:CG2	2.68	0.41
2:I:846:VAL:CG1	2:I:865:TRP:NE1	2.82	0.41
1:A:1625:LEU:O	1:A:1627:PRO:HD3	2.21	0.41
1:A:155:VAL:HG22	1:A:186:ILE:CG2	2.50	0.41
1:A:350:LEU:HB2	1:A:352:MET:HG2	2.03	0.41
1:B:1244:GLY:HA3	1:B:1297:PRO:HD2	2.03	0.41
1:B:12:ILE:O	1:B:16:GLU:HG2	2.20	0.41
1:B:1418:VAL:N	1:B:1419:PRO:CD	2.83	0.41
1:B:187:LEU:CD2	1:B:201:PRO:HB2	2.51	0.41
1:B:495:LYS:HA	1:B:496:PRO:HD3	1.88	0.41
1:C:1029:PRO:HA	1:C:1188:GLN:O	2.20	0.41
1:C:1239:HIS:CD2	1:C:1241:SER:H	2.38	0.41
1:C:400:ARG:NH1	1:C:400:ARG:CG	2.51	0.41
1:C:413:LEU:O	1:C:413:LEU:HG	2.19	0.41
1:C:503:ILE:HD11	1:C:947:LEU:HD22	2.03	0.41
2:G:1815:LEU:O	2:G:1821:VAL:HG23	2.20	0.41
2:G:1862:VAL:HG22	2:G:1863:ALA:N	2.36	0.41
2:G:517:HIS:CE1	2:G:540:ASP:O	2.73	0.41
2:G:612:ASN:C	2:G:614:GLY:H	2.24	0.41
2:G:938:TRP:CD1	2:G:944:ARG:HG3	2.56	0.41
2:H:1213:LEU:O	2:H:1214:LEU:HD23	2.19	0.41
2:H:1320:LEU:HA	2:H:1320:LEU:HD12	1.85	0.41
2:H:1281:PRO:O	2:H:1378:ILE:HG23	2.20	0.41
2:H:1383:ASN:HD21	2:H:1418:ASP:HB3	1.84	0.41
2:H:1666:PHE:CD1	2:H:1814:ALA:CB	3.03	0.41
2:H:503:ASP:OD2	2:H:513:GLY:N	2.52	0.41
2:H:601:THR:HG22	2:H:620:ALA:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1388:LYS:HE3	2:I:1418:ASP:OD2	2.21	0.41
2:I:195:LEU:O	2:I:199:ILE:HG13	2.21	0.41
2:I:463:PHE:CD2	2:I:463:PHE:C	2.94	0.41
2:I:712:ALA:O	2:I:716:VAL:HG23	2.21	0.41
1:A:1338:GLU:H	1:A:1338:GLU:HG2	1.55	0.41
1:A:1666:THR:HG23	1:A:1669:ARG:HB2	2.01	0.41
1:B:1009:LEU:CD1	1:B:1445:MET:HE1	2.51	0.41
1:B:197:THR:HG22	1:B:198:PRO:O	2.20	0.41
1:B:50:SER:CB	1:B:51:PRO:CD	2.99	0.41
1:B:644:THR:HG23	1:B:648:ASP:N	2.35	0.41
1:B:798:ASN:HA	1:B:801:ARG:HB2	2.02	0.41
1:C:1208:VAL:HG13	1:C:1209:ASP:O	2.21	0.41
1:C:1391:ASP:OD2	1:C:1502:ARG:NH2	2.54	0.41
1:C:1543:GLY:HA2	1:C:1550:ASP:OD1	2.21	0.41
1:C:1599:ILE:HD11	1:C:1606:PRO:HD2	2.01	0.41
1:C:427:ASN:HB2	1:C:468:LEU:CD2	2.51	0.41
2:G:1624:THR:HB	2:G:1642:THR:CG2	2.50	0.41
2:G:1642:THR:HB	2:G:1651:LEU:HB2	2.02	0.41
2:H:896:ASN:O	2:H:1050:ARG:NH2	2.53	0.41
2:H:1949:LYS:O	2:H:1953:VAL:HG23	2.21	0.41
2:H:195:LEU:O	2:H:199:ILE:HG13	2.20	0.41
2:H:1986:LYS:N	2:H:1987:PRO:CD	2.82	0.41
2:H:231:LEU:HA	2:H:236:ILE:HD12	2.03	0.41
2:H:23:PRO:HG2	2:H:86:LEU:HD11	2.01	0.41
2:H:33:LEU:HD13	2:H:68:VAL:HG22	2.02	0.41
2:H:433:VAL:N	2:H:434:PRO:CD	2.83	0.41
2:H:106:ALA:HB2	2:H:545:GLN:HG2	2.01	0.41
2:H:641:ILE:CD1	2:H:645:SER:HB2	2.50	0.41
2:H:719:ILE:HG12	2:H:719:ILE:H	1.62	0.41
2:H:740:HIS:CE1	2:H:852:GLU:OE1	2.74	0.41
2:H:995:LEU:HB3	2:H:1000:ILE:CD1	2.50	0.41
2:I:1213:LEU:O	2:I:1214:LEU:HD23	2.20	0.41
2:I:1357:TYR:HD1	2:I:1406:VAL:HG22	1.85	0.41
2:I:1173:VAL:HG13	2:I:1568:HIS:HB2	2.02	0.41
2:I:1855:ILE:HB	2:I:1907:LEU:HD12	2.02	0.41
2:I:507:GLY:O	2:I:508:GLY:C	2.59	0.41
2:I:590:PRO:HA	2:I:591:PRO:HD3	1.79	0.41
2:I:846:VAL:CG2	2:I:866:LYS:HB2	2.51	0.41
1:C:1685:TYR:CE1	2:I:993:GLN:OE1	2.73	0.41
1:A:1573:ILE:HG23	1:A:1627:PRO:HG3	2.03	0.41
1:A:1233:GLU:CD	1:A:1680:ARG:HH21	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:GLU:O	1:A:284:LYS:HG3	2.21	0.41
1:A:36:LEU:O	1:A:76:ARG:NH1	2.53	0.41
1:A:50:SER:CB	1:A:51:PRO:CD	2.97	0.41
1:A:28:TRP:CZ2	1:A:53:LEU:HD22	2.56	0.41
1:A:612:GLU:O	1:A:615:SER:HB3	2.21	0.41
1:B:1431:GLU:CG	1:B:1433:HIS:CE1	3.02	0.41
1:B:1029:PRO:HG2	1:B:1581:THR:O	2.20	0.41
1:B:1673:TYR:CZ	1:B:1677:VAL:HG21	2.55	0.41
1:B:709:ARG:O	1:B:714:VAL:HG21	2.21	0.41
1:B:906:LEU:HD23	1:B:906:LEU:HA	1.88	0.41
1:C:1244:GLY:C	1:C:1327:CYS:HB2	2.41	0.41
1:C:12:ILE:O	1:C:15:THR:HG23	2.20	0.41
2:G:1173:VAL:HG13	2:G:1568:HIS:HB2	2.02	0.41
2:G:1149:TRP:NE1	2:G:1213:LEU:HD12	2.35	0.41
2:G:1388:LYS:HE3	2:G:1418:ASP:OD2	2.20	0.41
2:G:2035:SER:OG	2:G:2037:PRO:HD2	2.21	0.41
2:G:339:LEU:HB2	2:G:386:LEU:HD22	2.03	0.41
2:G:441:LYS:HG2	2:G:445:LYS:HE3	2.02	0.41
2:H:1085:LEU:HD12	2:H:1085:LEU:HA	1.85	0.41
2:H:1214:LEU:HD11	2:H:1220:GLN:NE2	2.36	0.41
2:H:258:PHE:N	2:H:258:PHE:HD1	2.18	0.41
2:H:339:LEU:HD23	2:H:419:ARG:O	2.20	0.41
2:I:1107:SER:HA	2:I:1108:PRO:HD3	1.96	0.41
2:I:118:LYS:O	2:I:121:GLU:HB2	2.20	0.41
2:I:1348:LEU:HD12	2:I:1348:LEU:HA	1.86	0.41
2:I:1503:ILE:HG22	2:I:1504:VAL:C	2.41	0.41
2:I:1819:ALA:CA	2:I:2005:ARG:HH11	2.33	0.41
2:I:654:VAL:CG2	2:I:683:ALA:HB1	2.50	0.41
2:I:758:ARG:HA	2:I:758:ARG:HD3	1.86	0.41
1:A:1209:ASP:OD1	1:A:1210:PRO:HD2	2.21	0.41
1:A:413:LEU:HB2	1:A:439:ILE:HD13	2.03	0.41
1:A:681:THR:HA	1:A:706:THR:OG1	2.21	0.41
1:A:706:THR:HB	1:A:737:PHE:HB3	2.02	0.41
1:B:1066:ASN:HD22	1:B:1071:PRO:HA	1.86	0.41
1:B:1304:ALA:O	1:B:1307:THR:CG2	2.69	0.41
1:B:140:ILE:CG2	1:B:141:ALA:N	2.83	0.41
1:B:1495:ASN:HA	1:B:1495:ASN:HD22	1.65	0.41
1:B:32:GLN:HE22	1:B:57:ALA:CA	2.34	0.41
1:B:620:SER:HB2	1:B:668:PHE:HB3	2.02	0.41
1:B:91:THR:HA	1:B:92:PRO:HD3	1.81	0.41
1:C:11:HIS:HE1	2:I:1996:ILE:O	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:496:PRO:HB2	1:C:519:VAL:HG12	2.02	0.41
2:G:1031:LYS:O	2:G:1032:ASP:C	2.57	0.41
2:G:1070:ILE:O	2:G:1070:ILE:HD13	2.21	0.41
2:G:1383:ASN:HD21	2:G:1418:ASP:HB3	1.85	0.41
2:G:270:ALA:O	2:G:459:VAL:HA	2.21	0.41
2:G:425:SER:HA	2:G:426:PRO:HD3	1.79	0.41
2:G:159:ILE:HG12	2:G:512:LEU:HD23	2.03	0.41
2:H:1217:ASN:HA	2:H:1217:ASN:HD22	1.66	0.41
2:H:159:ILE:HG12	2:H:512:LEU:HD23	2.02	0.41
2:H:1815:LEU:O	2:H:1821:VAL:HG23	2.21	0.41
2:H:1873:TYR:CE2	2:H:1940:LEU:HD21	2.56	0.41
2:H:2010:TYR:O	2:H:2012:PRO:HD3	2.20	0.41
2:I:1335:ILE:O	2:I:1338:ILE:HG12	2.20	0.41
2:I:1868:GLN:HG3	2:I:1898:TYR:HH	1.85	0.41
2:I:1889:VAL:HG13	2:I:1977:HIS:HB3	2.00	0.41
2:I:1908:ASP:HA	2:I:1911:THR:HG22	2.03	0.41
2:I:463:PHE:O	2:I:463:PHE:HD2	2.04	0.41
2:I:582:LYS:HE2	2:I:761:PRO:O	2.21	0.41
1:A:238:PRO:CG	1:A:283:ALA:HB2	2.51	0.41
1:A:427:ASN:HB2	1:A:468:LEU:CD2	2.51	0.41
1:B:1047:LEU:O	1:B:1051:VAL:HG23	2.21	0.41
1:B:1539:ALA:O	1:B:1574:GLY:HA2	2.20	0.41
1:B:403:ASP:HB2	1:B:1613:ASN:ND2	2.14	0.41
1:B:949:GLU:O	1:B:953:VAL:HG12	2.21	0.41
1:B:979:GLN:HA	2:H:968:GLN:OE1	2.21	0.41
1:C:933:VAL:HA	1:C:934:PRO:HD3	1.65	0.41
2:G:643:LYS:HA	2:G:1163:LYS:HG2	2.03	0.41
2:G:1239:LEU:O	2:G:1254:VAL:HG23	2.20	0.41
2:G:486:LEU:HA	2:G:487:PRO:HD3	1.91	0.41
2:G:754:TYR:CG	2:G:794:MET:CG	3.04	0.41
2:G:992:GLU:HA	2:G:992:GLU:OE1	2.20	0.41
2:H:873:PHE:CE1	2:H:1026:GLU:HB2	2.56	0.41
2:H:1431:TYR:CE1	2:H:1526:THR:CG2	3.04	0.41
2:H:1739:GLU:HB2	2:H:1987:PRO:CB	2.30	0.41
2:H:1778:GLN:CB	2:H:1831:VAL:HG13	2.51	0.41
2:H:236:ILE:C	2:H:236:ILE:HD13	2.41	0.41
2:H:355:LYS:HB3	2:H:355:LYS:HE2	1.65	0.41
2:H:624:TYR:HB2	2:H:630:MET:HE3	2.02	0.41
2:H:641:ILE:CG1	2:H:645:SER:HB2	2.45	0.41
2:H:669:LEU:HD12	2:H:669:LEU:HA	1.66	0.41
2:H:717:ILE:CG2	2:H:760:HIS:CE1	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:846:VAL:HG13	2:H:865:TRP:CD1	2.56	0.41
2:I:1327:ILE:O	2:I:1331:TRP:HB2	2.21	0.41
2:I:1579:ILE:CD1	2:I:1615:MET:SD	3.09	0.41
2:I:807:ILE:HA	2:I:818:LYS:HG2	2.02	0.41
1:A:1146:HIS:O	1:A:1146:HIS:HD2	2.04	0.41
1:A:197:THR:HG22	1:A:198:PRO:O	2.21	0.41
1:A:330:GLU:O	1:A:330:GLU:HG2	2.20	0.41
1:A:41:THR:HG21	2:G:1663:THR:HB	2.02	0.41
1:A:983:GLN:OE1	1:A:1087:LYS:HD3	2.21	0.41
1:B:1019:ILE:HG13	1:B:1316:VAL:HG13	2.03	0.41
1:C:526:VAL:HG12	1:C:626:VAL:HG11	2.03	0.41
1:C:889:GLU:C	1:C:891:MET:H	2.23	0.41
1:C:906:LEU:HD23	1:C:906:LEU:HA	1.91	0.41
1:C:988:ILE:H	1:C:988:ILE:HG12	1.73	0.41
2:G:1501:ILE:HD13	2:G:1501:ILE:HG21	1.79	0.41
2:G:503:ASP:OD2	2:G:513:GLY:N	2.51	0.41
2:G:705:LEU:HA	2:G:705:LEU:HD23	1.72	0.41
2:G:735:GLY:O	2:G:741:HIS:CD2	2.73	0.41
2:G:888:ARG:O	2:G:892:ILE:HB	2.20	0.41
2:H:1004:LEU:HD21	2:H:1019:PRO:HB2	2.03	0.41
2:H:1543:ASP:OD1	2:H:1623:LYS:HG2	2.21	0.41
2:H:1662:THR:HB	2:H:1799:PRO:HG2	2.02	0.41
2:H:1989:LYS:HZ1	2:H:2037:PRO:HG2	1.86	0.41
2:H:462:THR:HB	2:H:482:CYS:SG	2.61	0.41
2:I:1219:ILE:H	2:I:1219:ILE:HG12	1.63	0.41
2:I:369:SER:C	2:I:370:LEU:HD23	2.41	0.41
2:I:421:LEU:HA	2:I:422:PRO:HD3	1.79	0.41
2:I:643:LYS:HA	2:I:1163:LYS:HG2	2.01	0.41
2:I:666:ILE:HG22	2:I:698:LEU:HD22	2.03	0.41
2:I:667:LYS:HD2	2:I:697:THR:CG2	2.35	0.41
2:I:754:TYR:CD1	2:I:794:MET:HG2	2.56	0.41
1:A:253:ARG:O	1:A:254:TRP:CD1	2.74	0.41
1:A:32:GLN:O	1:A:36:LEU:HB2	2.21	0.41
1:A:455:ILE:HA	1:A:455:ILE:HD13	1.84	0.41
1:A:601:VAL:O	1:A:602:GLU:C	2.59	0.41
1:A:780:GLU:O	1:A:781:LEU:C	2.59	0.41
1:B:1194:ASN:OD1	1:B:1196:LYS:HB2	2.21	0.41
1:B:982:ILE:HD11	2:H:955:GLU:OE2	2.21	0.41
1:B:998:TYR:CD2	1:B:1667:GLU:HG3	2.56	0.41
1:C:1244:GLY:HA3	1:C:1297:PRO:HD2	2.02	0.41
1:C:1443:LEU:HA	1:C:1443:LEU:HD23	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:ILE:CD1	1:C:472:LEU:HD23	2.51	0.41
1:C:658:LEU:HD13	1:C:916:LEU:HD12	2.03	0.41
2:G:1830:VAL:HA	2:G:1991:PHE:HE2	1.86	0.41
2:G:1834:ARG:CG	2:G:1834:ARG:NH1	2.68	0.41
2:G:1890:ASN:HA	2:G:1890:ASN:HD22	1.69	0.41
2:G:748:THR:CB	2:G:749:PRO:HD3	2.47	0.41
2:G:7:ARG:NH1	2:G:24:THR:CG2	2.79	0.41
2:H:1063:THR:HG22	2:H:1063:THR:O	2.21	0.41
2:H:538:ASP:HB2	2:H:540:ASP:HB2	2.03	0.41
2:H:603:SER:HA	2:H:604:PRO:HD2	1.95	0.41
2:H:879:LYS:HA	2:H:879:LYS:HD3	1.71	0.41
2:I:1129:ALA:HB2	2:I:1138:TRP:CH2	2.55	0.41
2:I:1624:THR:CB	2:I:1642:THR:HG23	2.48	0.41
2:I:177:TYR:CD1	2:I:188:ILE:HG21	2.56	0.41
2:I:2035:SER:OG	2:I:2037:PRO:HD2	2.21	0.41
2:I:2046:GLU:C	2:I:2048:TYR:N	2.73	0.41
2:I:512:LEU:O	2:I:516:THR:HG23	2.20	0.41
2:I:587:ILE:HD11	2:I:589:ARG:HB2	2.03	0.41
2:I:7:ARG:NH1	2:I:24:THR:CG2	2.80	0.41
1:A:232:LEU:O	1:A:236:LYS:HB2	2.21	0.40
1:A:32:GLN:HE21	1:A:57:ALA:HB2	1.85	0.40
1:A:930:LEU:HD23	1:A:930:LEU:HA	1.70	0.40
1:B:1274:ILE:H	1:B:1274:ILE:HG13	1.55	0.40
1:B:483:VAL:O	1:B:483:VAL:HG12	2.21	0.40
1:B:827:SER:HA	1:B:828:PRO:HD3	1.73	0.40
1:C:1131:LEU:HA	1:C:1131:LEU:HD12	1.69	0.40
1:C:1194:ASN:OD1	1:C:1196:LYS:HB2	2.21	0.40
1:C:1353:LEU:HD23	1:C:1353:LEU:HA	1.62	0.40
2:G:1878:VAL:CG1	2:G:1910:VAL:HG22	2.33	0.40
1:A:24:SER:O	2:G:1977:HIS:HD2	2.04	0.40
2:G:248:HIS:CE1	2:G:531:GLY:HA2	2.56	0.40
2:G:439:ILE:HD12	2:G:484:ILE:CD1	2.50	0.40
2:G:524:GLY:HA2	2:G:558:ASN:O	2.22	0.40
2:H:1168:ASN:HA	2:H:1169:PRO:HD3	1.79	0.40
2:H:1173:VAL:HG13	2:H:1568:HIS:HB2	2.03	0.40
2:H:1270:TRP:HZ3	2:H:1347:LEU:HD21	1.85	0.40
2:H:1387:GLY:HA2	2:H:1414:GLY:O	2.21	0.40
2:H:1886:VAL:HG22	2:H:1906:ALA:HB1	2.02	0.40
2:H:44:PRO:HA	2:H:53:GLU:OE2	2.21	0.40
2:H:751:LEU:HD11	2:H:789:PHE:CD1	2.55	0.40
2:H:805:VAL:HG12	2:H:805:VAL:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:866:LYS:O	2:H:870:GLU:HG3	2.19	0.40
2:H:888:ARG:O	2:H:892:ILE:HB	2.21	0.40
2:I:1219:ILE:HB	2:I:1240:TYR:HB2	2.03	0.40
2:I:1339:PHE:N	2:I:1340:PRO:CD	2.85	0.40
2:I:1642:THR:HB	2:I:1651:LEU:HB2	2.03	0.40
2:I:1815:LEU:O	2:I:1821:VAL:HG23	2.20	0.40
2:I:2042:ILE:HG12	2:I:2042:ILE:H	1.36	0.40
2:I:641:ILE:HG12	2:I:645:SER:CB	2.49	0.40
2:I:595:PRO:HD3	2:I:800:LEU:HB2	2.02	0.40
2:I:800:LEU:H	2:I:800:LEU:HD23	1.85	0.40
2:I:827:VAL:HG21	2:I:840:THR:CG2	2.51	0.40
1:A:800:LEU:HA	1:A:800:LEU:HD23	1.84	0.40
1:A:874:GLY:O	1:A:875:THR:C	2.60	0.40
1:A:908:LEU:O	1:A:913:VAL:HG22	2.21	0.40
1:B:1126:ILE:CD1	1:B:1172:THR:HG22	2.51	0.40
1:B:1557:ILE:HD11	1:B:1642:THR:HG21	2.03	0.40
1:C:1050:CYS:HB3	1:C:1089:VAL:CG1	2.51	0.40
1:C:1408:ALA:O	1:C:1651:GLY:HA2	2.21	0.40
1:C:1585:LYS:H	1:C:1585:LYS:CD	2.34	0.40
1:C:1717:ASP:HA	1:C:1718:PRO:HD3	1.85	0.40
2:G:1018:VAL:HA	2:G:1019:PRO:HD3	1.92	0.40
2:G:1043:VAL:O	2:G:1044:VAL:C	2.60	0.40
2:G:1491:VAL:HB	2:G:1501:ILE:CD1	2.51	0.40
2:G:159:ILE:HD11	2:G:512:LEU:CD2	2.52	0.40
2:G:1905:ARG:HA	2:G:1958:LEU:CD2	2.51	0.40
2:G:1974:VAL:HA	2:G:1975:PRO:HD3	1.92	0.40
2:G:2049:GLU:O	2:G:2050:GLN:C	2.60	0.40
2:G:44:PRO:HA	2:G:53:GLU:OE2	2.21	0.40
2:G:582:LYS:HE2	2:G:761:PRO:O	2.22	0.40
2:G:827:VAL:HG12	2:G:828:PRO:O	2.21	0.40
2:H:1044:VAL:HG21	2:H:1050:ARG:NE	2.37	0.40
2:H:585:LYS:HD2	2:H:585:LYS:HA	1.88	0.40
2:I:1495:THR:O	2:I:1496:LYS:HB2	2.20	0.40
2:I:259:THR:HG22	2:I:262:GLU:H	1.85	0.40
1:A:460:GLU:CG	1:A:470:LYS:HD3	2.49	0.40
1:B:1154:ILE:HG13	1:B:1154:ILE:O	2.22	0.40
1:C:822:VAL:HG12	1:C:824:LEU:CD2	2.49	0.40
2:G:1100:VAL:HG21	2:G:1147:ILE:HD13	2.04	0.40
2:G:1428:GLU:CG	2:G:1468:THR:HG22	2.51	0.40
2:G:780:TYR:HB2	2:G:799:PHE:CE2	2.56	0.40
2:H:1589:VAL:HG21	2:H:1651:LEU:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:259:THR:HG22	2:H:262:GLU:H	1.85	0.40
2:H:517:HIS:CE1	2:H:540:ASP:O	2.74	0.40
2:H:720:ALA:HA	2:H:728:ILE:HD11	2.04	0.40
2:H:753:MET:O	2:H:757:ILE:HG13	2.21	0.40
2:I:135:ARG:N	2:I:136:PRO:HD3	2.36	0.40
2:I:1383:ASN:HD21	2:I:1418:ASP:CB	2.34	0.40
2:I:1616:VAL:HG22	2:I:1650:VAL:HG11	2.03	0.40
2:I:1847:LEU:CD1	2:I:1847:LEU:H	2.14	0.40
2:I:2039:LYS:HA	2:I:2042:ILE:HG13	2.03	0.40
2:I:441:LYS:HG2	2:I:445:LYS:HE3	2.02	0.40
1:A:1418:VAL:N	1:A:1419:PRO:CD	2.84	0.40
1:A:157:HIS:CE1	1:A:269:LEU:HD11	2.57	0.40
1:A:16:GLU:OE2	1:A:16:GLU:HA	2.21	0.40
1:A:1705:PRO:HB2	1:A:1733:PHE:CD1	2.56	0.40
1:A:719:GLN:HG3	1:A:720:SER:N	2.36	0.40
1:B:1448:ARG:HD2	1:B:1508:TRP:O	2.21	0.40
1:B:20:TYR:HE1	2:H:2035:SER:HB2	1.87	0.40
1:A:1153:ASP:OD2	1:B:359:ARG:NH2	2.55	0.40
1:B:453:TYR:O	1:B:457:ASN:HB2	2.21	0.40
1:C:1014:ASP:H	1:C:1510:ASN:ND2	2.03	0.40
1:C:1705:PRO:HB2	1:C:1733:PHE:CD1	2.56	0.40
1:C:35:PHE:HA	1:C:39:PHE:HD2	1.86	0.40
2:G:119:THR:HG22	2:G:120:LYS:N	2.36	0.40
2:G:1352:HIS:CD2	2:G:1410:PHE:CD2	3.09	0.40
2:G:1359:MET:HB3	2:G:1606:ARG:NH2	2.36	0.40
2:G:1755:ILE:HD11	2:G:1762:TYR:HB2	2.02	0.40
2:G:430:HIS:CE1	2:G:431:LEU:HD13	2.57	0.40
2:G:827:VAL:HG21	2:G:840:THR:HG22	2.04	0.40
2:H:1270:TRP:C	2:H:1271:ILE:HD13	2.42	0.40
2:H:1609:THR:O	2:H:1653:GLY:HA3	2.21	0.40
2:H:1775:GLN:HG3	2:H:1775:GLN:H	1.68	0.40
2:H:1873:TYR:CE1	2:H:1877:ARG:NH2	2.83	0.40
1:B:21:GLN:O	2:H:1977:HIS:CD2	2.75	0.40
2:H:2036:GLU:HB2	2:H:2037:PRO:CD	2.47	0.40
2:H:184:VAL:HG11	2:H:247:ALA:HB1	2.04	0.40
2:H:298:LYS:HG2	2:H:448:VAL:CG2	2.45	0.40
2:H:499:THR:CG2	2:H:500:HIS:CD2	3.05	0.40
2:H:624:TYR:CD1	2:H:630:MET:HE2	2.56	0.40
2:H:804:ARG:NH2	2:H:1068:GLU:OE1	2.54	0.40
2:H:7:ARG:HA	2:H:8:PRO:HD3	1.91	0.40
2:I:1085:LEU:HD12	2:I:1085:LEU:HA	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1271:ILE:HG22	2:I:1273:GLU:HB2	2.03	0.40
2:I:1793:LYS:HA	2:I:1798:ILE:HG12	2.04	0.40
2:I:1889:VAL:HG21	2:I:1901:ALA:HB3	2.04	0.40
2:I:1967:ILE:HA	2:I:1968:PRO:HD3	1.94	0.40
2:I:499:THR:CG2	2:I:500:HIS:CD2	3.05	0.40
2:I:638:VAL:HG22	2:I:675:PRO:HG2	2.03	0.40
2:I:912:ARG:HB2	2:I:916:THR:HG23	2.04	0.40
1:A:1280:ILE:HD13	1:A:1302:VAL:HG22	2.03	0.40
1:A:1406:MET:CE	1:A:1428:THR:HB	2.51	0.40
1:A:1642:THR:HG22	1:A:1652:GLN:HG3	2.03	0.40
1:A:1657:HIS:HA	1:A:1658:PRO:HD3	1.92	0.40
1:A:626:VAL:HG23	1:A:664:GLU:OE2	2.21	0.40
1:A:82:SER:OG	1:A:83:LYS:HG3	2.20	0.40
1:B:1232:TYR:CE2	1:B:1701:LYS:HD2	2.56	0.40
1:B:294:TYR:CZ	1:B:298:VAL:HG21	2.57	0.40
1:B:413:LEU:HG	1:B:413:LEU:O	2.21	0.40
1:B:636:PRO:HB2	1:B:638:LEU:O	2.21	0.40
1:C:1195:ALA:CB	1:C:1213:LEU:HD13	2.51	0.40
1:C:32:GLN:HE22	1:C:57:ALA:N	2.19	0.40
2:G:1128:LYS:HG2	2:G:1181:VAL:HG22	2.03	0.40
2:G:1427:VAL:HG22	2:G:1469:GLU:CG	2.51	0.40
2:G:142:ASN:CB	2:G:550:VAL:HG13	2.52	0.40
2:G:236:ILE:HG12	2:G:240:LEU:HD22	2.02	0.40
2:G:320:PRO:HA	2:G:321:PRO:HD3	1.90	0.40
2:G:338:MET:HG3	2:G:423:VAL:HG21	2.04	0.40
2:G:682:GLY:HA3	3:G:3051:FMN:O2	2.20	0.40
2:G:751:LEU:HD11	2:G:789:PHE:CG	2.57	0.40
2:H:1880:LYS:HE3	2:H:1880:LYS:HB2	1.92	0.40
2:H:389:LEU:HD22	2:H:393:LEU:HG	2.03	0.40
2:H:441:LYS:O	2:H:445:LYS:HG3	2.22	0.40
2:H:57:PRO:O	2:H:61:VAL:HG23	2.22	0.40
2:H:723:HIS:ND1	2:H:723:HIS:N	2.70	0.40
2:H:949:ASP:HB3	2:H:1006:MET:CE	2.47	0.40
2:I:1100:VAL:HG21	2:I:1147:ILE:HD12	2.03	0.40
2:I:1352:HIS:CE1	2:I:1583:MET:CE	2.86	0.40
2:I:2026:PHE:HD2	2:I:2045:TRP:CZ3	2.39	0.40
2:I:246:LEU:HA	2:I:246:LEU:HD12	1.78	0.40
2:I:247:ALA:O	2:I:251:VAL:HG13	2.21	0.40
2:I:283:ILE:HD12	2:I:283:ILE:HA	1.94	0.40
2:I:290:GLU:OE1	2:I:290:GLU:N	2.41	0.40
2:I:543:PHE:CB	2:I:545:GLN:NE2	2.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:598:THR:CB	2:I:599:PRO:HD3	2.52	0.40
2:I:732:TRP:HB2	2:I:750:MET:HE1	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1603/1887 (85%)	1498 (93%)	91 (6%)	14 (1%)	17	52
1	B	1603/1887 (85%)	1495 (93%)	95 (6%)	13 (1%)	19	54
1	C	1603/1887 (85%)	1498 (93%)	90 (6%)	15 (1%)	17	52
2	G	2029/2051 (99%)	1841 (91%)	163 (8%)	25 (1%)	13	44
2	H	2029/2051 (99%)	1841 (91%)	166 (8%)	22 (1%)	14	46
2	I	2029/2051 (99%)	1837 (90%)	168 (8%)	24 (1%)	13	44
All	All	10896/11814 (92%)	10010 (92%)	773 (7%)	113 (1%)	15	49

All (113) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	504	ASP
1	A	538	GLU
1	A	605	LEU
1	A	834	GLY
1	A	1252	GLY
1	A	1585	LYS
1	B	504	ASP
1	B	538	GLU
1	B	605	LEU
1	B	834	GLY

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Mol	Chain	Res	Type
1	B	1252	GLY
1	B	1585	LYS
1	C	504	ASP
1	C	538	GLU
1	C	605	LEU
1	C	834	GLY
1	C	1252	GLY
1	C	1585	LYS
2	G	521	ASP
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	179	LYS
1	A	1608	ASN
1	B	179	LYS
1	B	1608	ASN
1	C	179	LYS
1	C	1608	ASN
2	G	203	LEU
2	G	1044	VAL
2	G	1177	SER
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	B	1545	SER
2	G	112	ASN
2	G	1101	GLU
2	G	2034	GLY
2	H	112	ASN
2	H	1101	GLU
2	I	374	ALA

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Mol	Chain	Res	Type
2	I	1092	ASP
2	I	1101	GLU
2	I	2034	GLY
1	A	1545	SER
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
1	C	1545	SER
2	H	769	SER
2	H	1092	ASP
2	I	25	ALA
2	I	769	SER
2	I	823	ALA
2	I	1510	ALA
1	A	970	GLY
1	C	970	GLY
1	C	1536	LEU
2	G	574	SER
2	G	1340	PRO
2	H	136	PRO
2	I	136	PRO
2	I	574	SER
1	A	178	GLY

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Mol	Chain	Res	Type
1	B	178	GLY
1	C	178	GLY
2	G	136	PRO
2	G	335	PRO
2	H	335	PRO
2	G	1956	ARG
2	H	772	GLY
1	C	1240	VAL
2	G	772	GLY
2	I	772	GLY
2	I	1340	PRO
2	I	1956	ARG
1	B	726	GLY
1	C	726	GLY
2	G	470	VAL
2	G	1176	PRO
2	H	470	VAL
2	H	2012	PRO
2	I	335	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	1366/1565 (87%)	1220 (89%)	146 (11%)	6	26
1	B	1366/1565 (87%)	1222 (90%)	144 (10%)	7	26
1	C	1366/1565 (87%)	1224 (90%)	142 (10%)	7	27
2	G	1772/1789 (99%)	1564 (88%)	208 (12%)	5	22
2	H	1772/1789 (99%)	1564 (88%)	208 (12%)	5	22
2	I	1772/1789 (99%)	1562 (88%)	210 (12%)	5	20
All	All	9414/10062 (94%)	8356 (89%)	1058 (11%)	6	24

All (1058) 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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	1251	MET
1	A	1255	SER
1	A	1274	ILE
1	A	1283	MET
1	A	1307	THR
1	A	1308	SER
1	A	1327	CYS
1	A	1338	GLU
1	A	1367	ARG
1	A	1372	THR
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

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Mol	Chain	Res	Type
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	1644	PHE
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	1251	MET
1	B	1255	SER

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Mol	Chain	Res	Type
1	B	1274	ILE
1	B	1283	MET
1	B	1307	THR
1	B	1308	SER
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	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
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

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Mol	Chain	Res	Type
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	1251	MET
1	C	1255	SER
1	C	1274	ILE
1	C	1283	MET
1	C	1307	THR
1	C	1308	SER
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
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

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Mol	Chain	Res	Type
1	C	1585	LYS
1	C	1612	ASP
1	C	1625	LEU
1	C	1644	PHE
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	186	ASP
2	G	210	THR
2	G	227	ASP
2	G	236	ILE
2	G	240	LEU
2	G	246	LEU
2	G	281	VAL

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Mol	Chain	Res	Type
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
2	G	607	VAL
2	G	611	THR
2	G	616	THR
2	G	653	TYR
2	G	665	LEU

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Mol	Chain	Res	Type
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
2	G	971	SER
2	G	993	GLN
2	G	1015	VAL
2	G	1021	LEU
2	G	1024	ARG

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Mol	Chain	Res	Type
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	1342	THR
2	G	1343	VAL
2	G	1348	LEU
2	G	1359	MET
2	G	1360	ILE
2	G	1375	THR
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
2	G	1463	THR
2	G	1468	THR

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Mol	Chain	Res	Type
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
2	G	1886	VAL
2	G	1914	LEU

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Mol	Chain	Res	Type
2	G	1936	VAL
2	G	1937	GLU
2	G	1941	PHE
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
2	H	281	VAL
2	H	286	THR
2	H	295	SER

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Mol	Chain	Res	Type
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
2	H	665	LEU
2	H	669	LEU
2	H	670	ARG

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Mol	Chain	Res	Type
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
2	H	1021	LEU
2	H	1024	ARG
2	H	1048	VAL

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Mol	Chain	Res	Type
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	1342	THR
2	H	1343	VAL
2	H	1348	LEU
2	H	1359	MET
2	H	1360	ILE
2	H	1375	THR
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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Mol	Chain	Res	Type
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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Mol	Chain	Res	Type
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
2	I	303	LEU

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Mol	Chain	Res	Type
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	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
2	I	670	ARG
2	I	676	ILE

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Mol	Chain	Res	Type
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	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
2	I	1015	VAL
2	I	1021	LEU
2	I	1024	ARG

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Mol	Chain	Res	Type
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	1342	THR
2	I	1343	VAL
2	I	1348	LEU
2	I	1359	MET
2	I	1360	ILE
2	I	1375	THR
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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Mol	Chain	Res	Type
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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Mol	Chain	Res	Type
2	I	1937	GLU
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 (276) such sidechains are listed below:

Mol	Chain	Res	Type
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	987	ASN
1	A	989	GLN
1	A	1000	GLN
1	A	1003	GLN
1	A	1063	HIS
1	A	1064	ASN

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Mol	Chain	Res	Type
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	1510	ASN
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
1	B	738	ASN
1	B	758	ASN
1	B	792	HIS
1	B	898	GLN

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Mol	Chain	Res	Type
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	1510	ASN
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
1	C	407	ASN
1	C	411	GLN
1	C	427	ASN
1	C	438	ASN
1	C	506	ASN
1	C	527	GLN

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Mol	Chain	Res	Type
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	1510	ASN
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	359	HIS
2	G	376	ASN
2	G	418	ASN
2	G	428	HIS
2	G	430	HIS
2	G	440	ASN
2	G	447	ASN
2	G	500	HIS

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Mol	Chain	Res	Type
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	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	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
2	H	34	GLN
2	H	85	ASN
2	H	102	HIS
2	H	359	HIS
2	H	376	ASN
2	H	418	ASN
2	H	428	HIS
2	H	430	HIS
2	H	440	ASN

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Mol	Chain	Res	Type
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	1352	HIS
2	H	1355	ASN
2	H	1367	GLN
2	H	1595	ASN
2	H	1672	GLN
2	H	1697	HIS
2	H	1890	ASN
2	H	1896	GLN
2	H	1977	HIS
2	H	2013	ASN
2	H	2020	GLN
2	I	34	GLN
2	I	85	ASN
2	I	102	HIS
2	I	359	HIS
2	I	376	ASN
2	I	418	ASN
2	I	428	HIS
2	I	430	HIS
2	I	440	ASN
2	I	447	ASN

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Mol	Chain	Res	Type
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	650	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	900	GLN
2	I	910	GLN
2	I	1046	GLN
2	I	1055	HIS
2	I	1148	ASN
2	I	1151	HIS
2	I	1217	ASN
2	I	1220	GLN
2	I	1260	GLN
2	I	1352	HIS
2	I	1355	ASN
2	I	1367	GLN
2	I	1384	GLN
2	I	1595	ASN
2	I	1669	GLN
2	I	1672	GLN
2	I	1697	HIS
2	I	1890	ASN
2	I	1896	GLN
2	I	1977	HIS
2	I	2013	ASN
2	I	2020	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	GVL	C	180	1	15,18,19	0.77	0	20,26,28	0.98	1 (5%)
1	GVL	B	180	1	15,18,19	0.70	0	20,26,28	0.86	1 (5%)
1	GVL	A	180	1	15,18,19	0.73	0	20,26,28	0.81	0

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
1	GVL	C	180	1	-	6/21/25/27	-
1	GVL	B	180	1	-	6/21/25/27	-
1	GVL	A	180	1	-	6/21/25/27	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	180	GVL	C30-C29-C32	2.47	113.10	108.82
1	B	180	GVL	O35-C34-C32	2.20	121.15	119.04

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	180	GVL	CB-O25-P24-O23
1	C	180	GVL	CB-O25-P24-O27
1	C	180	GVL	C28-O27-P24-O26
1	B	180	GVL	CB-O25-P24-O23

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Mol	Chain	Res	Type	Atoms
1	B	180	GVL	CB-O25-P24-O27
1	B	180	GVL	C28-O27-P24-O26
1	A	180	GVL	CB-O25-P24-O23
1	A	180	GVL	CB-O25-P24-O27
1	A	180	GVL	C28-O27-P24-O26
1	C	180	GVL	C28-O27-P24-O25
1	B	180	GVL	C28-O27-P24-O25
1	A	180	GVL	C28-O27-P24-O25
1	C	180	GVL	CB-O25-P24-O26
1	C	180	GVL	C28-O27-P24-O23
1	B	180	GVL	CB-O25-P24-O26
1	A	180	GVL	CB-O25-P24-O26
1	A	180	GVL	C28-O27-P24-O23
1	B	180	GVL	C28-O27-P24-O23

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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$
3	FMN	H	3051	-	31,33,33	6.72	18 (58%)	40,50,50	1.90	8 (20%)
3	FMN	I	3051	-	31,33,33	6.75	20 (64%)	40,50,50	1.82	7 (17%)
3	FMN	G	3051	-	31,33,33	6.89	18 (58%)	40,50,50	1.95	7 (17%)

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
3	FMN	H	3051	-	-	5/18/18/18	0/3/3/3
3	FMN	I	3051	-	-	5/18/18/18	0/3/3/3
3	FMN	G	3051	-	-	5/18/18/18	0/3/3/3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	3051	FMN	C4A-C10	16.15	1.55	1.38
3	H	3051	FMN	C4A-C10	15.08	1.53	1.38
3	I	3051	FMN	C4A-C10	14.93	1.53	1.38
3	G	3051	FMN	C4A-N5	12.72	1.51	1.33
3	I	3051	FMN	C4A-N5	12.29	1.50	1.33
3	H	3051	FMN	C4A-N5	12.27	1.50	1.33
3	G	3051	FMN	C10-N1	11.33	1.47	1.33
3	H	3051	FMN	C10-N1	11.31	1.47	1.33
3	I	3051	FMN	C10-N1	10.99	1.47	1.33
3	I	3051	FMN	C6-C5A	10.94	1.58	1.41
3	G	3051	FMN	C6-C5A	10.87	1.58	1.41
3	H	3051	FMN	C6-C5A	10.60	1.58	1.41
3	H	3051	FMN	C4-N3	10.16	1.50	1.33
3	G	3051	FMN	C4-N3	9.95	1.50	1.33
3	I	3051	FMN	C5A-N5	9.88	1.51	1.35
3	I	3051	FMN	C4-N3	9.84	1.50	1.33
3	G	3051	FMN	C5A-N5	9.68	1.51	1.35
3	H	3051	FMN	C5A-N5	9.58	1.51	1.35
3	G	3051	FMN	C9-C9A	9.46	1.59	1.40
3	I	3051	FMN	C9-C9A	9.30	1.59	1.40
3	H	3051	FMN	C9-C9A	9.29	1.59	1.40
3	G	3051	FMN	C9A-N10	8.66	1.50	1.38
3	I	3051	FMN	C9A-N10	8.30	1.49	1.38
3	H	3051	FMN	C9A-N10	8.28	1.49	1.38
3	G	3051	FMN	C6-C7	7.91	1.57	1.37
3	G	3051	FMN	C2-N1	7.74	1.53	1.38
3	I	3051	FMN	C6-C7	7.70	1.57	1.37
3	H	3051	FMN	C2-N3	7.65	1.53	1.38
3	H	3051	FMN	C6-C7	7.57	1.57	1.37
3	H	3051	FMN	C2-N1	7.56	1.53	1.38
3	I	3051	FMN	C2-N1	7.47	1.53	1.38
3	I	3051	FMN	C9-C8	7.39	1.56	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	3051	FMN	C2-N3	7.29	1.52	1.38
3	I	3051	FMN	C8-C7	7.26	1.59	1.40
3	I	3051	FMN	C2-N3	7.15	1.52	1.38
3	G	3051	FMN	O4-C4	7.14	1.42	1.24
3	G	3051	FMN	C9-C8	7.09	1.55	1.37
3	H	3051	FMN	O4-C4	7.08	1.42	1.24
3	G	3051	FMN	C4-C4A	7.06	1.53	1.41
3	H	3051	FMN	C9-C8	7.01	1.55	1.37
3	I	3051	FMN	O4-C4	6.96	1.42	1.24
3	G	3051	FMN	C8-C7	6.90	1.58	1.40
3	H	3051	FMN	C4-C4A	6.85	1.53	1.41
3	H	3051	FMN	C8-C7	6.66	1.57	1.40
3	I	3051	FMN	C9A-C5A	6.61	1.55	1.42
3	I	3051	FMN	C4-C4A	6.55	1.52	1.41
3	G	3051	FMN	C9A-C5A	6.29	1.55	1.42
3	H	3051	FMN	C9A-C5A	6.05	1.54	1.42
3	I	3051	FMN	P-O2P	3.01	1.66	1.54
3	H	3051	FMN	P-O2P	2.92	1.66	1.54
3	G	3051	FMN	P-O2P	2.91	1.66	1.54
3	I	3051	FMN	P-O3P	2.86	1.65	1.54
3	H	3051	FMN	P-O3P	2.78	1.65	1.54
3	G	3051	FMN	P-O3P	2.60	1.64	1.54
3	I	3051	FMN	C8M-C8	2.26	1.55	1.51
3	I	3051	FMN	C7M-C7	2.09	1.55	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	3051	FMN	C4-N3-C2	7.49	121.47	115.14
3	G	3051	FMN	C4-N3-C2	7.30	121.30	115.14
3	I	3051	FMN	C4-N3-C2	6.98	121.03	115.14
3	G	3051	FMN	C1'-N10-C9A	4.66	121.96	118.29
3	H	3051	FMN	C1'-N10-C9A	4.18	121.58	118.29
3	H	3051	FMN	C4A-C4-N3	-3.94	118.04	123.43
3	G	3051	FMN	C4A-C4-N3	-3.90	118.10	123.43
3	I	3051	FMN	C1'-N10-C9A	3.86	121.33	118.29
3	I	3051	FMN	C4A-C4-N3	-3.63	118.47	123.43
3	G	3051	FMN	C4A-N5-C5A	3.23	120.00	116.77
3	H	3051	FMN	C4A-N5-C5A	3.13	119.90	116.77
3	G	3051	FMN	C10-C4A-N5	-3.06	119.14	121.26
3	I	3051	FMN	C4A-N5-C5A	3.01	119.78	116.77
3	G	3051	FMN	C5A-C9A-N10	2.93	119.84	117.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	3051	FMN	C10-C4A-N5	-2.91	119.25	121.26
3	H	3051	FMN	C4'-C3'-C2'	-2.76	107.62	113.36
3	G	3051	FMN	C4'-C3'-C2'	-2.75	107.65	113.36
3	I	3051	FMN	C4'-C3'-C2'	-2.73	107.68	113.36
3	I	3051	FMN	C5A-C9A-N10	2.65	119.63	117.72
3	I	3051	FMN	C10-C4A-N5	-2.54	119.50	121.26
3	H	3051	FMN	C5A-C9A-N10	2.48	119.51	117.72
3	H	3051	FMN	O5'-C5'-C4'	-2.02	103.96	109.36

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	3051	FMN	C2'-C3'-C4'-C5'
3	H	3051	FMN	O3'-C3'-C4'-C5'
3	I	3051	FMN	C2'-C3'-C4'-C5'
3	I	3051	FMN	O3'-C3'-C4'-C5'
3	G	3051	FMN	C2'-C3'-C4'-C5'
3	G	3051	FMN	O3'-C3'-C4'-C5'
3	H	3051	FMN	O3'-C3'-C4'-O4'
3	I	3051	FMN	O3'-C3'-C4'-O4'
3	I	3051	FMN	C2'-C3'-C4'-O4'
3	H	3051	FMN	C2'-C3'-C4'-O4'
3	G	3051	FMN	C2'-C3'-C4'-O4'
3	G	3051	FMN	O3'-C3'-C4'-O4'
3	H	3051	FMN	C4'-C5'-O5'-P
3	G	3051	FMN	C4'-C5'-O5'-P
3	I	3051	FMN	C4'-C5'-O5'-P

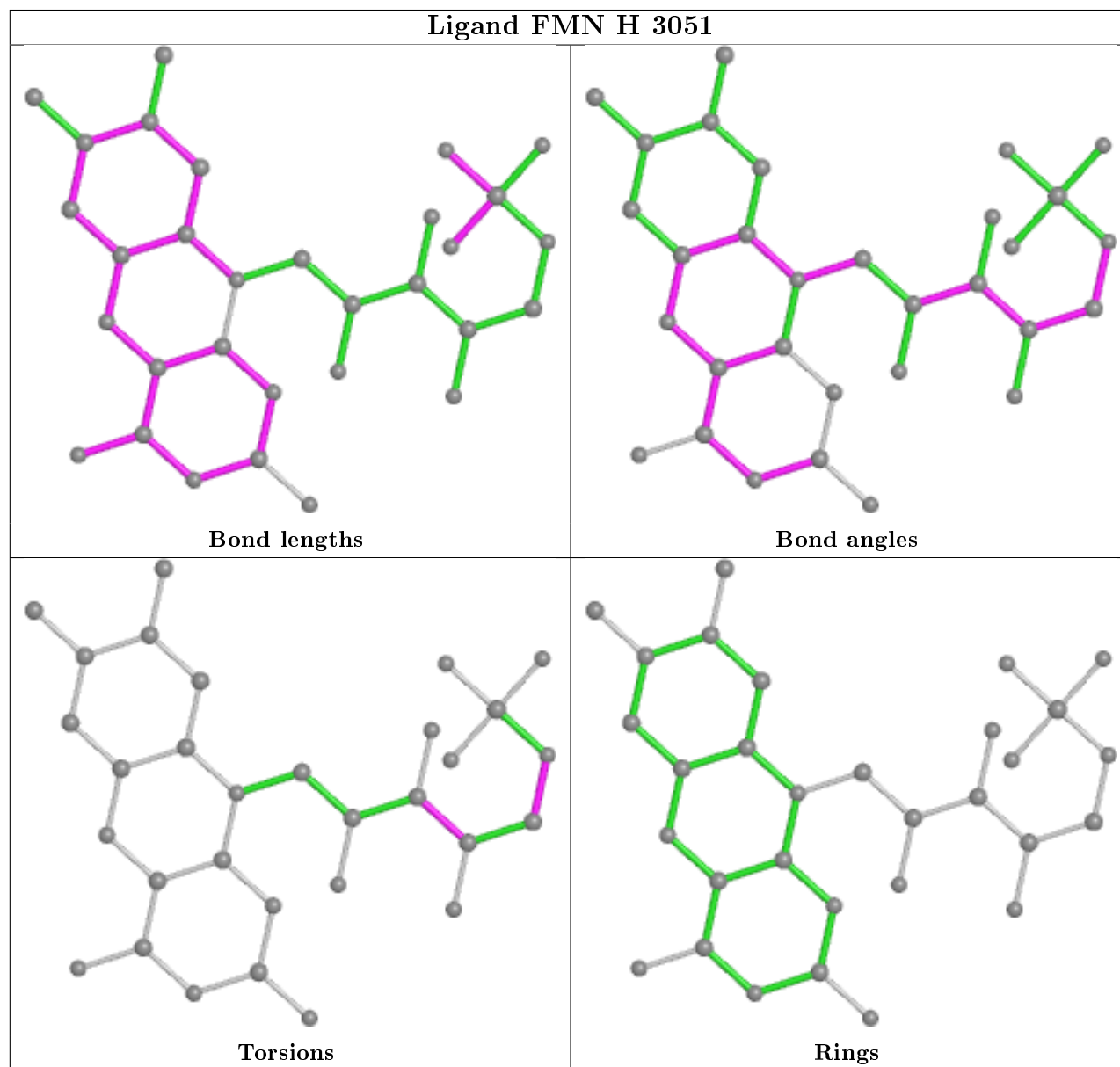
There are no ring outliers.

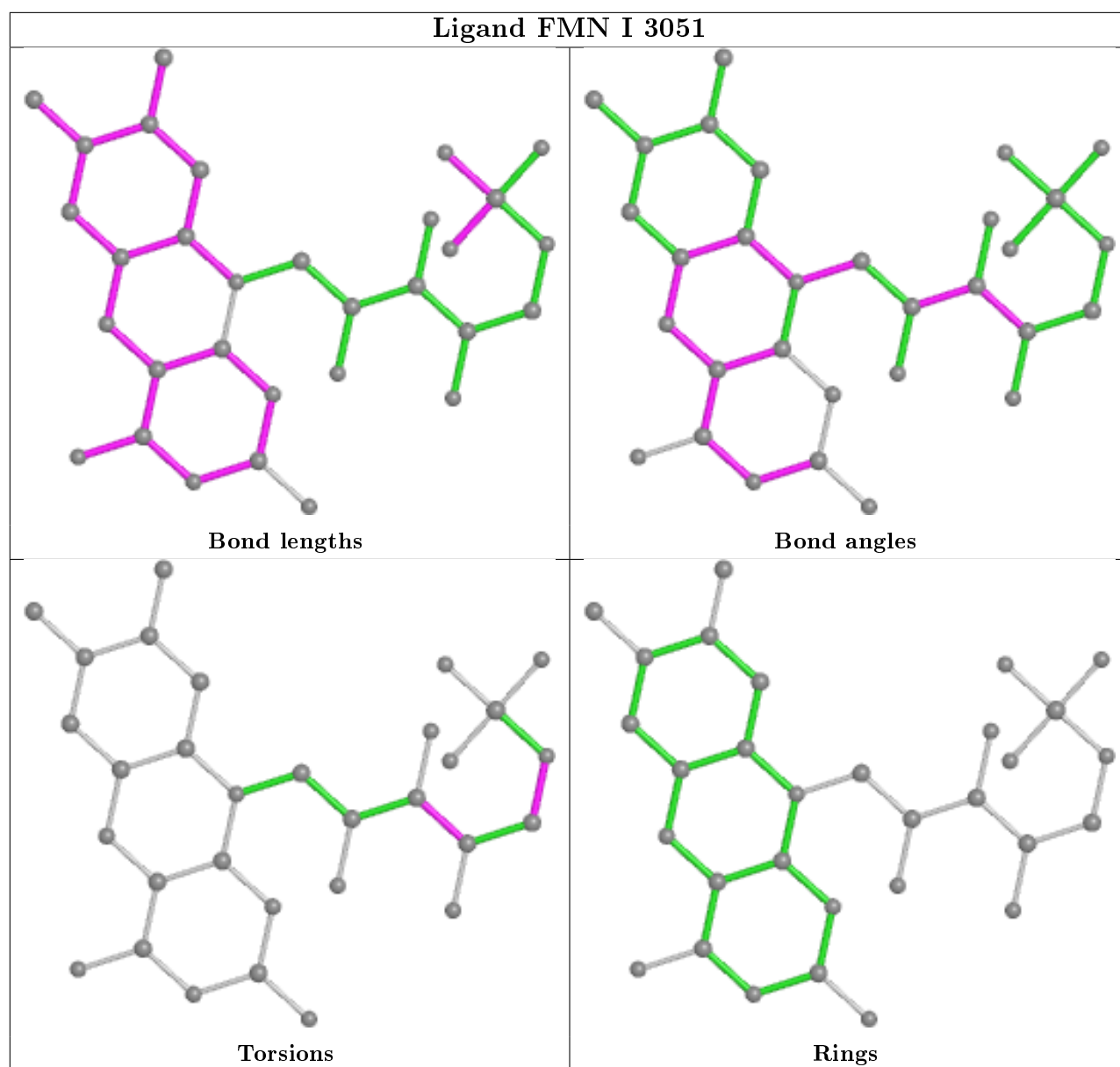
3 monomers are involved in 19 short contacts:

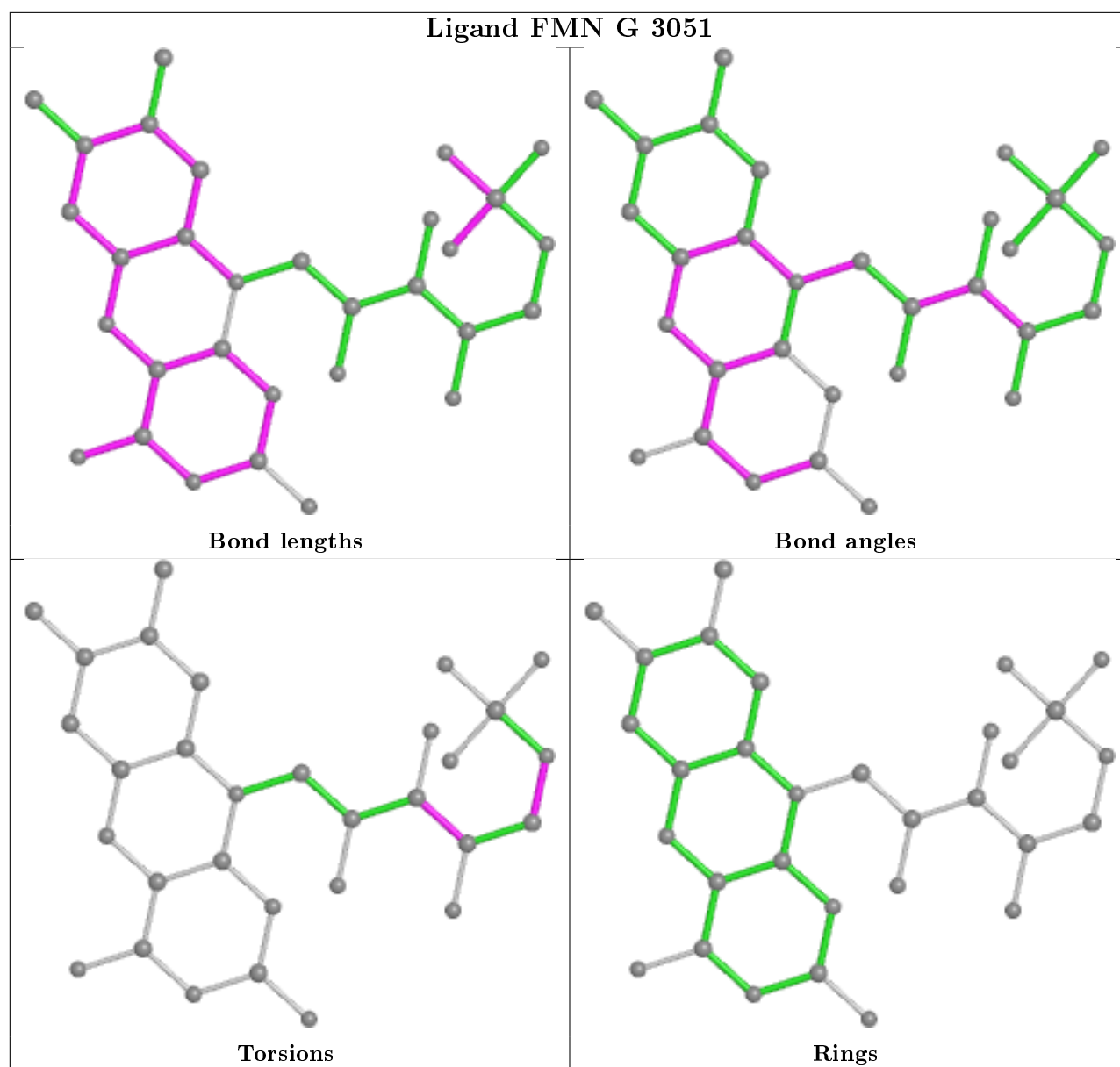
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	3051	FMN	6	0
3	I	3051	FMN	6	0
3	G	3051	FMN	7	0

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](#)

There are no chain breaks in this entry.

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, 95th 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 ²)	Q<0.9
1	A	1613/1887 (85%)	-0.60	29 (1%)	68	47	28, 59, 126, 166	0
1	B	1613/1887 (85%)	-0.59	26 (1%)	72	51	30, 59, 127, 170	0
1	C	1613/1887 (85%)	-0.59	31 (1%)	66	46	29, 61, 126, 170	0
2	G	2033/2051 (99%)	-0.52	18 (0%)	84	69	39, 73, 114, 151	0
2	H	2033/2051 (99%)	-0.54	17 (0%)	86	72	41, 73, 113, 152	0
2	I	2033/2051 (99%)	-0.53	14 (0%)	87	75	42, 74, 113, 150	0
All	All	10938/11814 (92%)	-0.56	135 (1%)	79	61	28, 69, 119, 170	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	977	TYR	5.6
1	C	976	ALA	5.2
2	H	35	GLU	5.2
1	C	975	ALA	5.2
1	C	1475	GLU	4.7
2	H	2050	GLN	4.6
1	A	978	ALA	4.4
2	I	1929	LYS	4.4
1	C	972	SER	4.3
2	H	25	ALA	4.2
1	B	977	TYR	4.0
1	B	177	GLY	3.9
1	A	1476	GLU	3.8
1	C	1480	GLU	3.8
1	B	976	ALA	3.8
1	A	1483	ASN	3.7
2	G	2043	ASP	3.7
1	A	977	TYR	3.7
1	C	218	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	1746	ASN	3.6
1	A	600	ASP	3.5
1	B	196	THR	3.4
1	A	976	ALA	3.4
1	A	975	ALA	3.4
1	A	164	ASP	3.4
1	A	292	GLN	3.4
2	G	1930	SER	3.4
1	C	1476	GLU	3.4
1	C	971	ASN	3.3
1	A	258	SER	3.3
2	H	75	SER	3.3
1	A	539	SER	3.3
1	A	1746	ASN	3.2
1	B	164	ASP	3.2
1	A	299	GLY	3.2
2	I	1930	SER	3.2
2	I	2050	GLN	3.1
1	A	248	LYS	3.1
2	H	1745	LYS	3.1
1	C	142	ASP	3.0
1	A	1480	GLU	3.0
2	I	1740	THR	3.0
1	C	203	GLU	3.0
2	G	2050	GLN	3.0
2	G	25	ALA	3.0
1	B	972	SER	3.0
1	C	539	SER	2.9
2	G	1956	ARG	2.9
1	A	599	MET	2.9
1	B	537	LYS	2.9
1	A	274	ALA	2.9
1	B	169	SER	2.9
1	B	178	GLY	2.9
2	G	1933	LEU	2.9
2	I	25	ALA	2.9
1	A	196	THR	2.9
2	I	35	GLU	2.8
2	H	1742	VAL	2.8
1	A	252	THR	2.7
1	A	601	VAL	2.7
1	A	177	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
2	I	1956	ARG	2.7
2	H	1925	ILE	2.7
1	C	174	ASP	2.7
1	B	143	GLU	2.7
1	A	972	SER	2.6
1	C	1068	LYS	2.6
1	B	188	GLY	2.6
1	B	539	SER	2.6
2	H	1740	THR	2.6
1	C	143	GLU	2.6
1	B	274	ALA	2.6
2	G	1955	PRO	2.6
1	C	289	SER	2.5
2	G	2049	GLU	2.5
2	G	1962	ARG	2.5
2	H	1743	ASP	2.5
1	C	538	GLU	2.5
2	H	327	SER	2.5
1	C	177	GLY	2.4
1	A	203	GLU	2.4
1	B	301	ASP	2.4
1	B	538	GLU	2.4
1	B	600	ASP	2.4
1	B	296	SER	2.4
1	A	218	SER	2.4
1	C	292	GLN	2.4
1	C	162	SER	2.3
2	G	290	GLU	2.3
2	H	76	LYS	2.3
1	C	196	THR	2.3
1	A	174	ASP	2.3
1	A	1475	GLU	2.3
1	B	973	ALA	2.3
1	B	208	GLU	2.3
2	G	51	ASP	2.3
1	C	274	ALA	2.3
1	C	301	ASP	2.3
1	C	178	GLY	2.3
1	B	1068	LYS	2.3
2	G	1475	LYS	2.3
2	G	138	ASP	2.3
2	H	93	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	198	PRO	2.3
2	H	138	ASP	2.2
2	H	287	ASP	2.2
1	C	144	PRO	2.2
2	G	77	VAL	2.2
1	C	299	GLY	2.2
2	G	552	SER	2.2
2	I	1400	GLY	2.2
2	G	1928	GLN	2.2
1	A	301	ASP	2.2
2	G	1920	GLN	2.2
1	A	142	ASP	2.2
1	C	197	THR	2.2
1	B	1475	GLU	2.1
1	C	164	ASP	2.1
2	I	1475	LYS	2.1
1	A	1747	ALA	2.1
1	C	211	GLU	2.1
1	B	192	LYS	2.1
1	B	240	GLY	2.1
2	I	1744	GLY	2.1
1	C	275	ALA	2.1
2	I	2043	ASP	2.1
2	I	552	SER	2.1
2	I	1682	LYS	2.0
2	H	1415	ASN	2.0
2	H	142	ASN	2.0
2	I	1415	ASN	2.0
2	G	112	ASN	2.0
1	B	215	ASP	2.0
2	H	400	SER	2.0
1	B	251	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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(Å ²)	Q<0.9
1	GVL	C	180	19/20	0.76	0.38	49,130,161,187	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	GVL	B	180	19/20	0.82	0.30	48,119,172,190	0
1	GVL	A	180	19/20	0.86	0.26	44,125,164,189	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

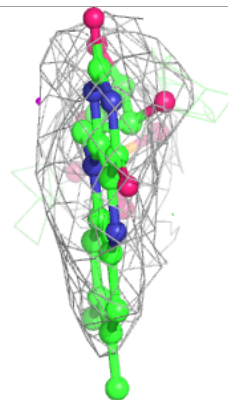
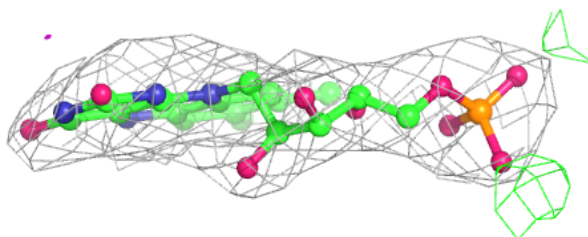
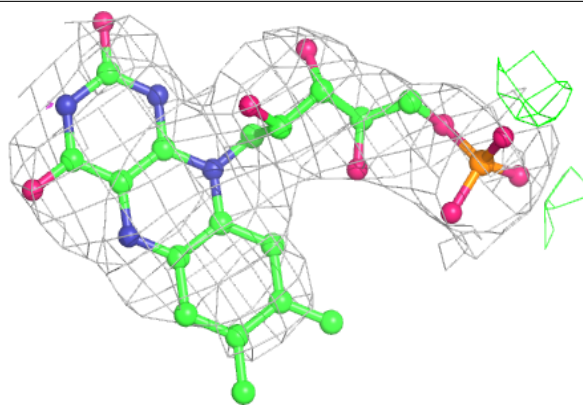
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FMN	I	3051	31/31	0.96	0.13	26,57,75,97	0
3	FMN	G	3051	31/31	0.96	0.14	31,55,81,100	0
3	FMN	H	3051	31/31	0.97	0.14	27,54,78,82	0

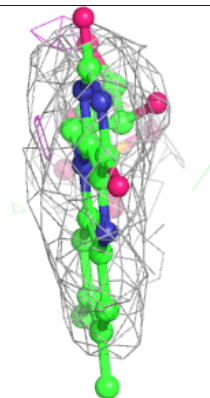
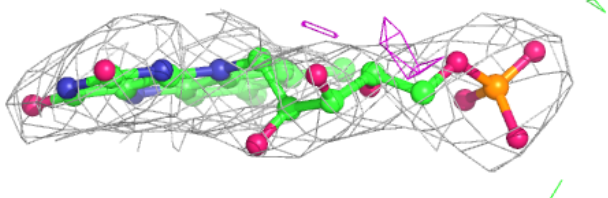
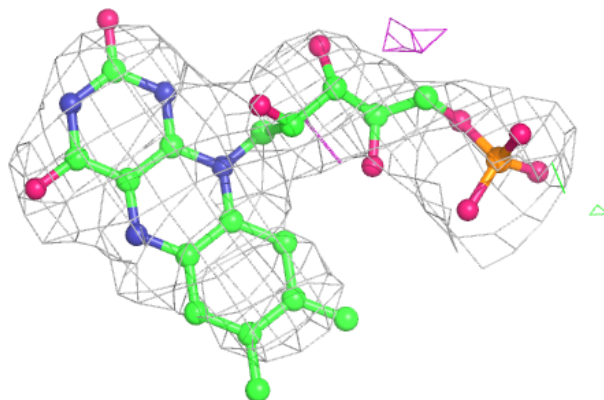
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

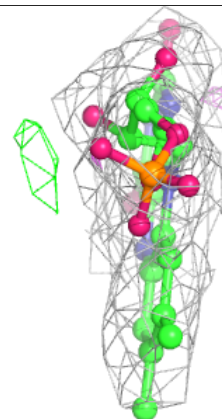
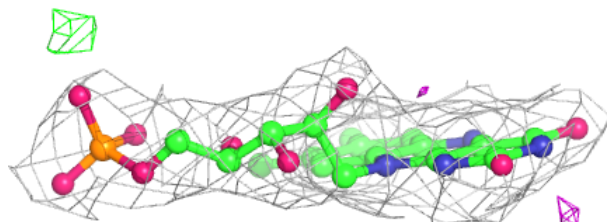
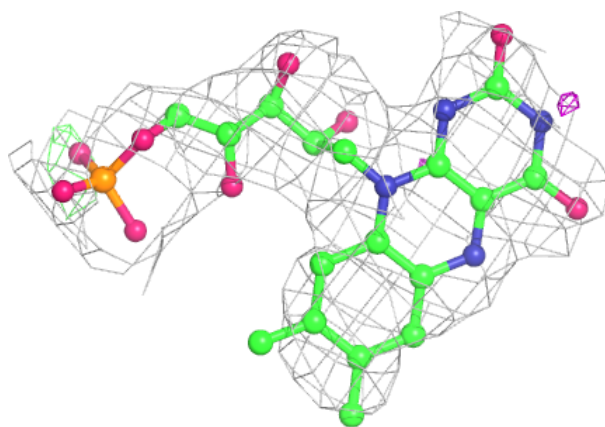
**Electron density around FMN G 3051:**

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.