



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 12:55 am BST

PDB ID : 3HMJ  
Title : Saccharomyces cerevisiae FAS type I  
Authors : Johansson, P.; Mulinacci, B.; Koestler, C.; Vollrath, R.; Oesterhelt, D.; Grininger, M.  
Deposited on : 2009-05-29  
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

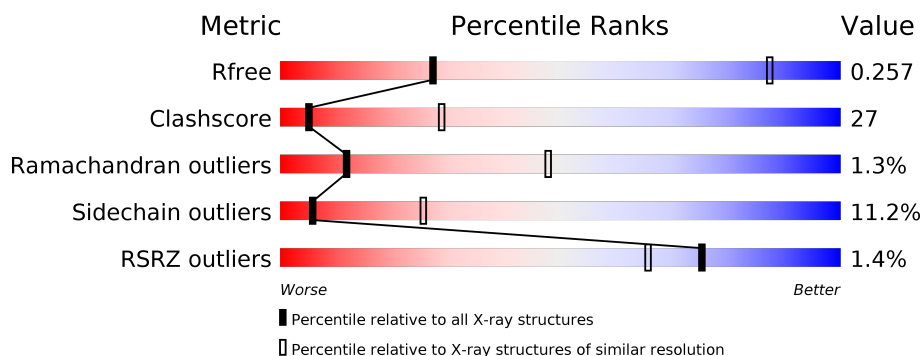
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1887	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>32%</div> <div>5%</div> <div>7%</div> </div> </div>
1	B	1887	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>32%</div> <div>5%</div> <div>7%</div> </div> </div>
1	C	1887	<div> <div>3%</div> <div> <div></div> <div>54%</div> <div>33%</div> <div>5%</div> <div>7%</div> </div> </div>
2	G	2051	<div> <div></div> <div> <div>51%</div> <div>40%</div> <div>8%</div> </div> </div>
2	H	2051	<div> <div></div> <div> <div>51%</div> <div>40%</div> <div>8%</div> </div> </div>
2	I	2051	<div> <div></div> <div> <div>51%</div> <div>40%</div> <div>8%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 88830 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

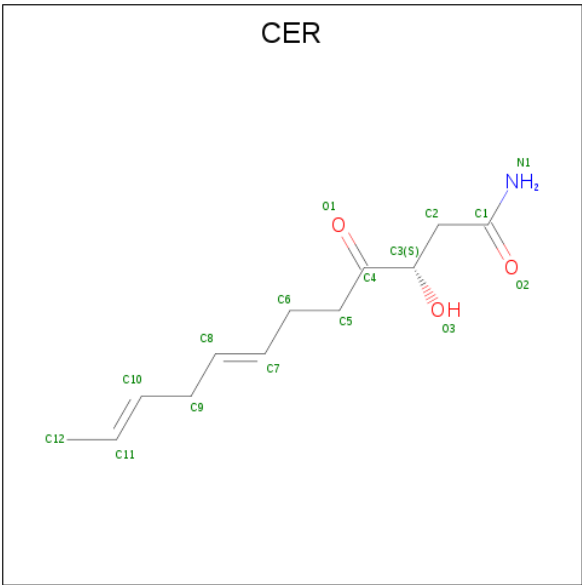
- Molecule 1 is a protein called Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1750	Total	C	N	O	S	0	0	0
			13572	8594	2292	2637	49			
1	B	1750	Total	C	N	O	S	0	0	0
			13572	8594	2292	2637	49			
1	C	1750	Total	C	N	O	S	0	0	0
			13572	8594	2292	2637	49			

- Molecule 2 is a protein called Fatty acid synthase subunit beta.

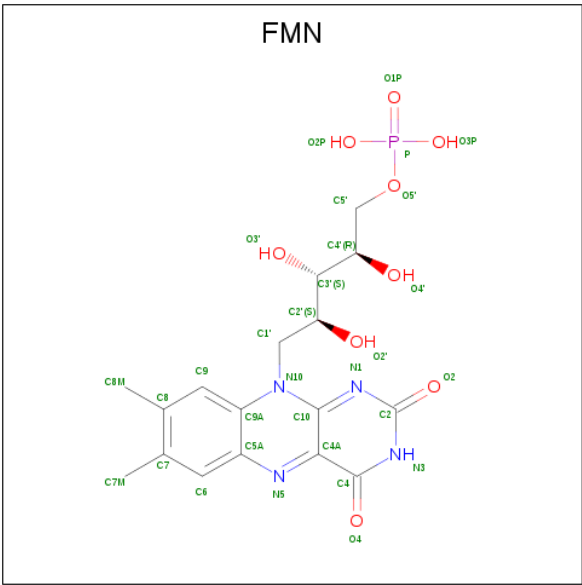
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	2033	Total	C	N	O	S	0	0	0
			15995	10253	2660	3026	56			
2	H	2033	Total	C	N	O	S	0	0	0
			15995	10253	2660	3026	56			
2	I	2033	Total	C	N	O	S	0	0	0
			15995	10253	2660	3026	56			

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



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

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



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

Continued on next page...

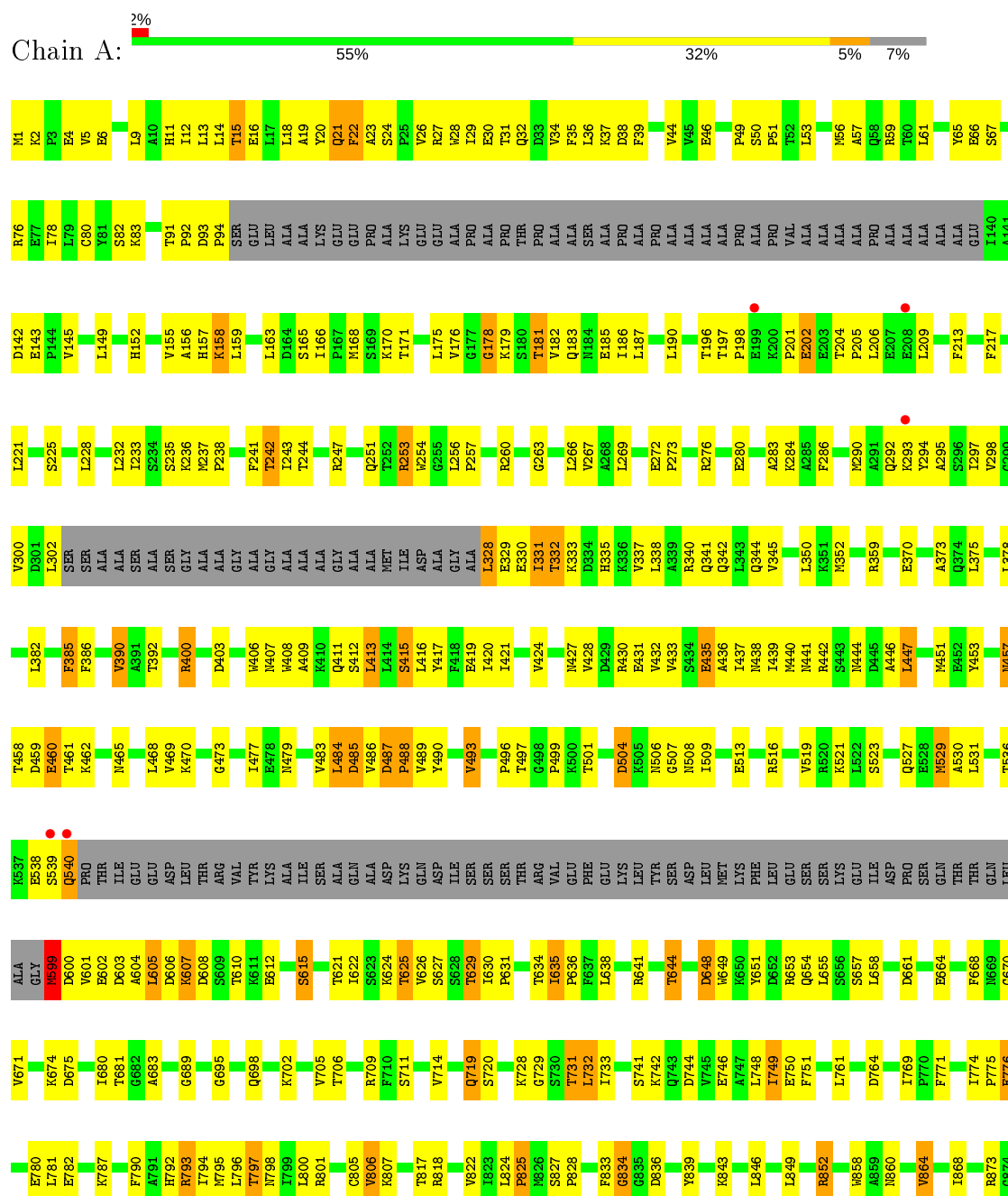
*Continued from previous page...*

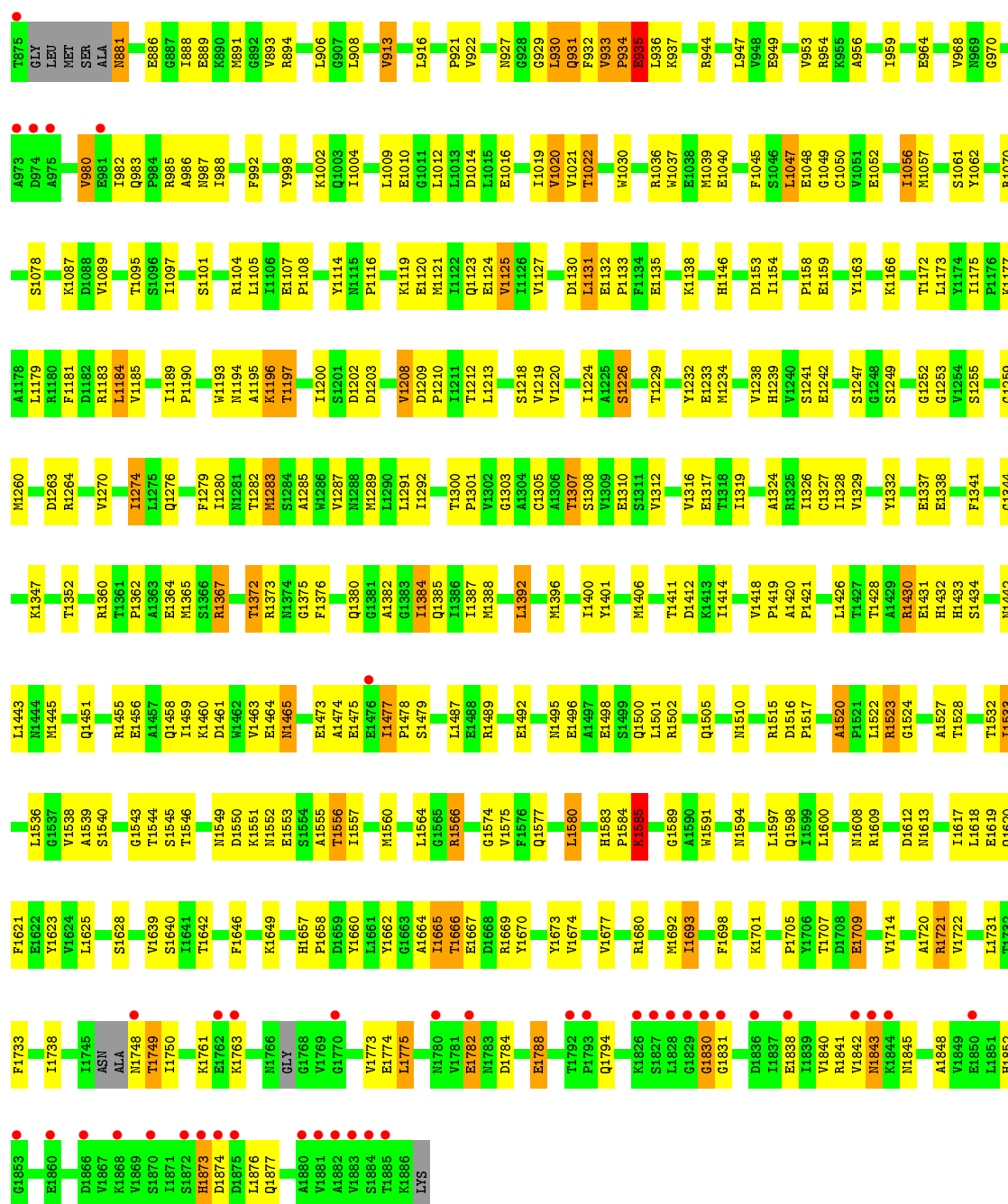
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	I	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

### 3 Residue-property plots

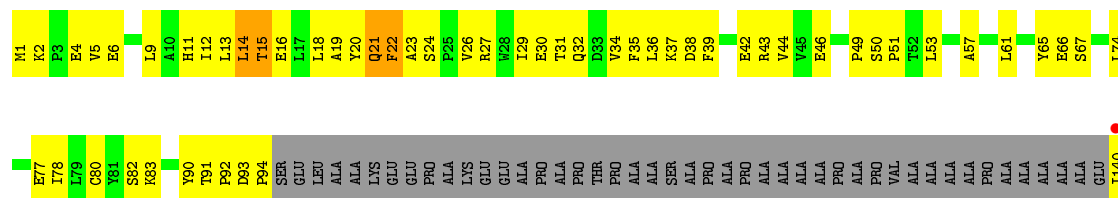
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Fatty acid synthase subunit alpha



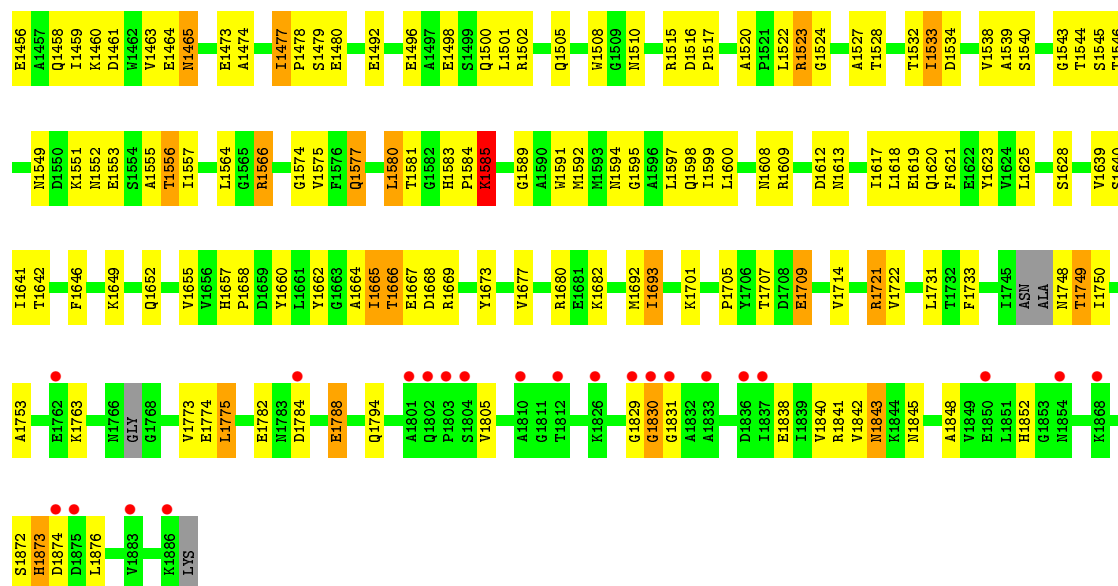


• Molecule 1: Fatty acid synthase subunit alpha

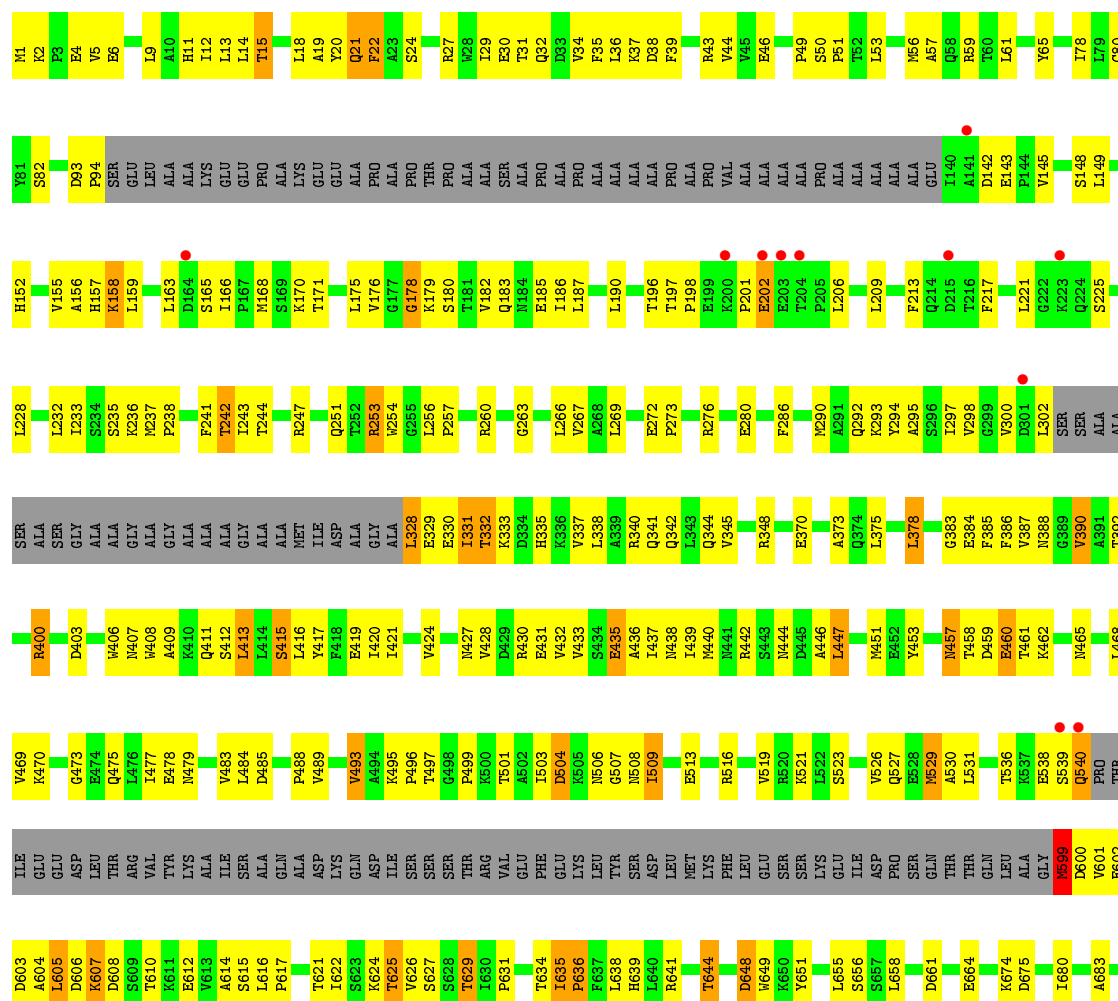


S1366	I1280	W1193	K1087	I982	SER	K787	G889	GLY	E533	D459	F386	L302	S225	A141
R1367	M1281	N1194	D1088	R985	ALA	S788	G695	R699	S539	E460	V390	SER	S226	D142
T1370	M1282	A1195	V1089	R988	R881	S789	G696	V601	P940	T461	A391	SER	L228	E143
T1371	S1284	K1196	T1095	I988	R882	A790	Q698	E602	THR	K462	T392	ALA	L232	V145
T1372	K1285	T1197	S1096	Q989	I883	F791	K702	D603	ILE	N465	R400	SER	L233	L149
R1373	H286	T1200	I1097	F992	E886	H792	K703	A804	GLU	L468	T401	ALA	S234	L232
H1374	V1287	S1201	S1101	Y998	G887	R793	V705	L605	ASP	V469	F402	SER	S235	H152
F1375	M1288	D1202	R1104	Y998	R888	M795	T706	K607	LEU	K470	D403	ALA	K236	V155
F1376	M1289	R1104	R1104	I1004	R890	L796	T706	D608	THR	G473	D406	ALA	K237	A156
Q1380	I1292	V1208	L1105	I1004	M891	T797	R709	S609	ARG	G473	H406	GLY	P238	H157
I1384	D1209	D1209	N798	I1004	G892	F710	F710	T610	VAL	I477	H407	ALA	F241	K158
Q1385	T1212	T1212	R801	L1009	E812	S711	S711	E812	TTR	I477	H408	GLY	T242	K158
T1386	M1115	E1010	R801	E1010	E812	V714	V714	E812	LYS	H408	A409	ALA	T243	L163
T1387	P1301	G1011	C805	L1012	G907	Q719	Q719	S615	ILE	H409	K410	ALA	T244	D164
M1388	V1302	L1013	R806	L1013	G907	S720	S720	T621	ALA	R410	Q411	ALA	R247	S165
L1392	G1303	S1218	K807	D1014	L908	G726	G726	I622	GLN	V483	S412	GLY	Q251	I166
A1304	A1304	E1015	R818	L1015	V913	A727	A727	S623	ALA	L484	I414	ALA	R251	F167
M1396	C1305	S1226	E1124	E1016	L916	K728	K728	G624	MET	S415	S415	MET	Q252	M168
T1397	T1307	T1229	V1125	I1019	L916	G729	G729	T625	ASP	V489	Y417	ILE	R253	S169
S1308	T1307	T1229	V1125	I1019	L916	G729	G729	T625	LYS	V489	Y417	ILE	W254	K170
P1309	T1307	T1229	V1125	I1019	L916	G729	G729	T625	LYS	V489	Y417	ILE	G255	T171
E1310	T1307	T1229	V1125	I1019	L916	G729	G729	T625	LYS	V489	Y417	ILE	L256	L175
E1310	T1307	T1229	V1125	I1019	L916	G729	G729	T625	LYS	V489	Y417	ILE	P257	V176
S1311	T1307	T1229	V1125	I1019	L916	G729	G729	T625	LYS	V489	Y417	ILE	R260	G177
V1312	T1307	T1229	V1125	I1019	L916	G729	G729	T625	LYS	V489	Y417	ILE	G263	K178
V1312	T1307	T1229	V1125	I1019	L916	G729	G729	T625	LYS	V489	Y417	ILE	L266	S180
V1312	T1307	T1229	V1125	I1019	L916	G729	G729	T625	LYS	V489	Y417	ILE	V267	T181
V1312	T1307	T1229	V1125	I1019	L916	G729	G729	T625	LYS	V489	Y417	ILE	Q183	V182
V1312	T1307	T1229	V1125	I1019	L916	G729	G729	T625	LYS	V489	Y417	ILE	N184	K183
V1312	T1307	T1229	V1125	I1019	L916	G729	G729	T625	LYS	V489	Y417	ILE	L269	E185
V1312	T1307	T1229	V1125	I1019	L916	G729	G729	T625	LYS	V489	Y417	ILE	E272	I186
V1312	T1307	T1229	V1125	I1019	L916	G729	G729	T625	LYS	V489	Y417	ILE	P273	L187
V1312	T1307	T1229	V1125	I1019	L916	G729	G729	T625	LYS	V489	Y417	ILE	R276	L190
V1312	T1307	T1229	V1125	I1019	L916	G729	G729	T625	LYS	V489	Y417	ILE	E280	G195
V1312	T1307	T1229	V1125	I1019	L916	G729	G729	T625	LYS	V489	Y417	ILE	A283	T196
V1312	T1307	T1229	V1125	I1019	L916	G729	G729	T625	LYS	V489	Y417	ILE	K284	P197
V1312	T1307	T1229	V1125	I1019	L916	G729	G729	T625	LYS	V489	Y417	ILE	P201	P198
V1312	T1307	T1229	V1125	I1019	L916	G729	G729	T625	LYS	V489	Y417	ILE	E202	P201
V1312	T1307	T1229	V1125	I1019	L916	G729	G729	T625	LYS	V489	Y417	ILE	P286	E202
V1312	T1307	T1229	V1125	I1019	L916	G729	G729	T625	LYS	V489	Y417	ILE	M290	L206
V1312	T1307	T1229	V1125	I1019	L916	G729	G729	T625	LYS	V489	Y417	ILE	A291	L206
V1312	T1307	T1229	V1125	I1019	L916	G729	G729	T625	LYS	V489	Y417	ILE	Q292	L209
V1312	T1307	T1229	V1125	I1019	L916	G729	G729	T625	LYS	V489	Y417	ILE	Y294	L209
V1312	T1307	T1229	V1125	I1019	L916	G729	G729	T625	LYS	V489	Y417	ILE	F213	F213
V1312	T1307	T1229	V1125	I1019	L916	G729	G729	T625	LYS	V489	Y417	ILE	I297	F217
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V1312	T1307	T1229	V1125	I1019	L916	G729	G729	T625	LYS	V489	Y417	ILE	D301	L221
V1312	T1307	T1229	V1125	I1019	L916	G729	G729	T625	LYS	V489	Y417	ILE	F385	L221





• Molecule 1: Fatty acid synthase subunit alpha





WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

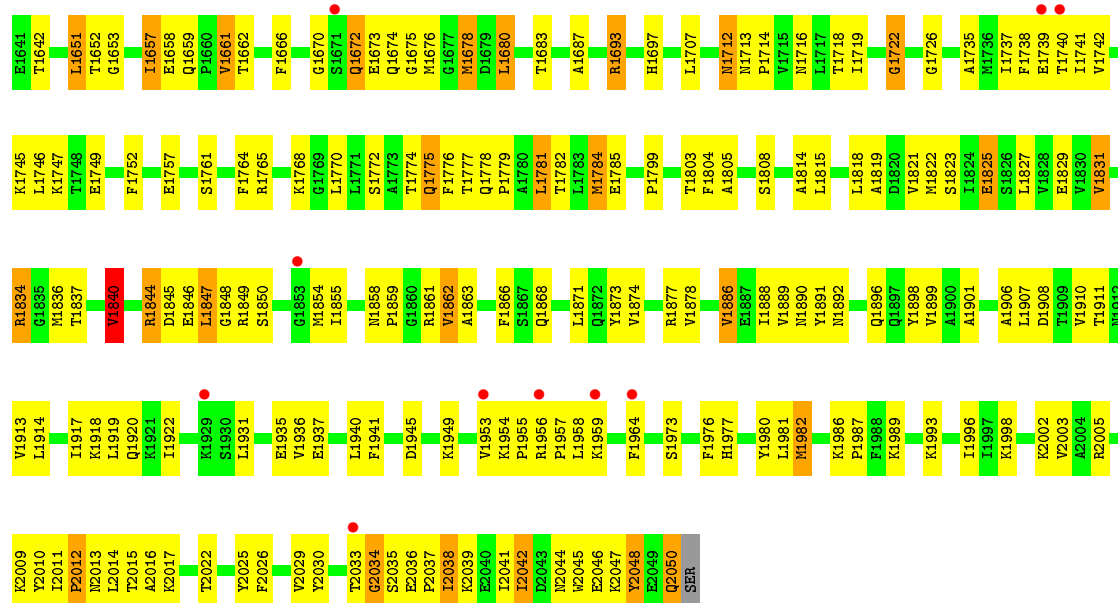
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P1274	T1374	T1463	M1561	G1653	S1761	V1842	V1913	K2009
F1275			P1562		I1657	P1843	L1914	Y2010
	V1377	F1466	M1563		T1763	D1844	I1917	I2011
F1279	L1378	F1467	H1564	T1662	F1764	E1846	K1918	P2012
V1284	E1379	T1468	V1565	F1666	A1765	L1847	L1919	N2013
	S1380	O1469	V1566		K1768	G1848	Q1920	L2014
I1292	V1381	T1470	H1568	F1666	F1768	R1849	T2015	T2015
T1293	N1383	E1471	H1568	G1670	L1770	S1850	I1922	A2016
A1294		T1472	M1574	S1671	L1771	M1854	L1931	K2017
K1295	K1388	T1473	L1575	Q1672	S1772	I1855	S1932	T2022
E1296	I1389	F1474	L1575	Q1673	A1773	I1856	E1935	Y2025
	V1390	K1475	I1579	Q1674	T1774	I1857	V1936	F2026
F1300			T1580	M1676	F1776	M1858	E1937	Y2029
A1303	S1397	S1481	M1583	M1677	T1777	P1859	E1937	V2029
C1308	V1403	V1483	F1584	D1678	Q1778	R1861	L1940	Y2030
E1309	M1404	F1486	S1585	L1680	P1779	V1862	F1941	T2033
D1310			S1586	T1683	L1781	A1863	D1945	G2034
F1311	T1407	I1489	V1589	A1687	T1782	F1866	S2035	S2035
V1312	S1408	K1490	R1590	A1687	L1783	S1867	E2036	E2036
S1313	S1409	V1491	A1591	R1693	M1784	Q1868	P2037	P2037
R1314	F1410	E1492	A1592		E1785		V1953	I2038
	F1411	L1493	L1593	H1697	P1799	L1871	K1954	K2039
T1318	Y1416	P1494	E1594			Y1873	P1955	I2041
M1319	T1417	T1495	A1597	I1706	T1803	V1874	P1957	I2042
L1320	T1417	K1496		L1707	A1804	V1875	L1958	D2043
	D1413				A1805	E1876	F1964	N2044
F1325	F1419	V1499	S1602	I1711	S1808	L1877	S1973	Y2047
A1326	E1420	E1500	M1605	M1716	A1814	V1884	V1974	K2048
N1327	N1421	I1501	R1606	L1717	L1815	L1885	P1975	E2049
V1328	T1422	G1502	G1607	I1718	L1818	V1886	F1976	E2049
V1329	Q1423	I1503	G1607	I1719	A1819	E1887	H1977	Q2050
G1330	Q1424	V1504	V1608		V1820	I1888	S1978	SER
V1331	K1425	A1504	T1609		V1821	V1889	T1979	
	T1426	S1511	M1615	G1722	M1822	M1890	Y1980	
I1335	V1427	H1512	V1616	G1726	S1823	Y1891	L1981	
	E1428				I1824	N1892	M1982	
F1339	Y1431	T1526	K1623		E1825	V1893	K1986	
P1340	H1434	L1527	T1624	F1738	S1826	E1894	P1987	
V1343	I1435	E1528	S1625	I1739	I1827	M1895	F1988	
D1344	K1436	Q1529	Q1627	T1740	V1741	Q1896	K1989	
L1347	T1437	L1533		V1742		Q1897	S1990	
L1348	S1438	D1543	G1630		K1745	Y1898	L1992	
K1349			M1631		L1746	A1900	F1991	
L1350	I1441	P1547	I1632	K1748	V1831	A1901	K1993	
V1351	A1442	S1548	T1637	E1749	R1834	A1906	I1996	
H1352	L1443	T1549	I1638		E1748	L1907	I1997	
	R1445	N1550	K1639		E1749	D1908	K1998	
N1355	S1446	P1551	F1640		F1752	T1909	V2003	
M1359		P1552	T1641		T1755	V1910		
L1360	L1452	Y1553						
P1361		V1556						
	F1457							

• Molecule 2: Fatty acid synthase subunit beta

Chain H:  51% 40% 8%

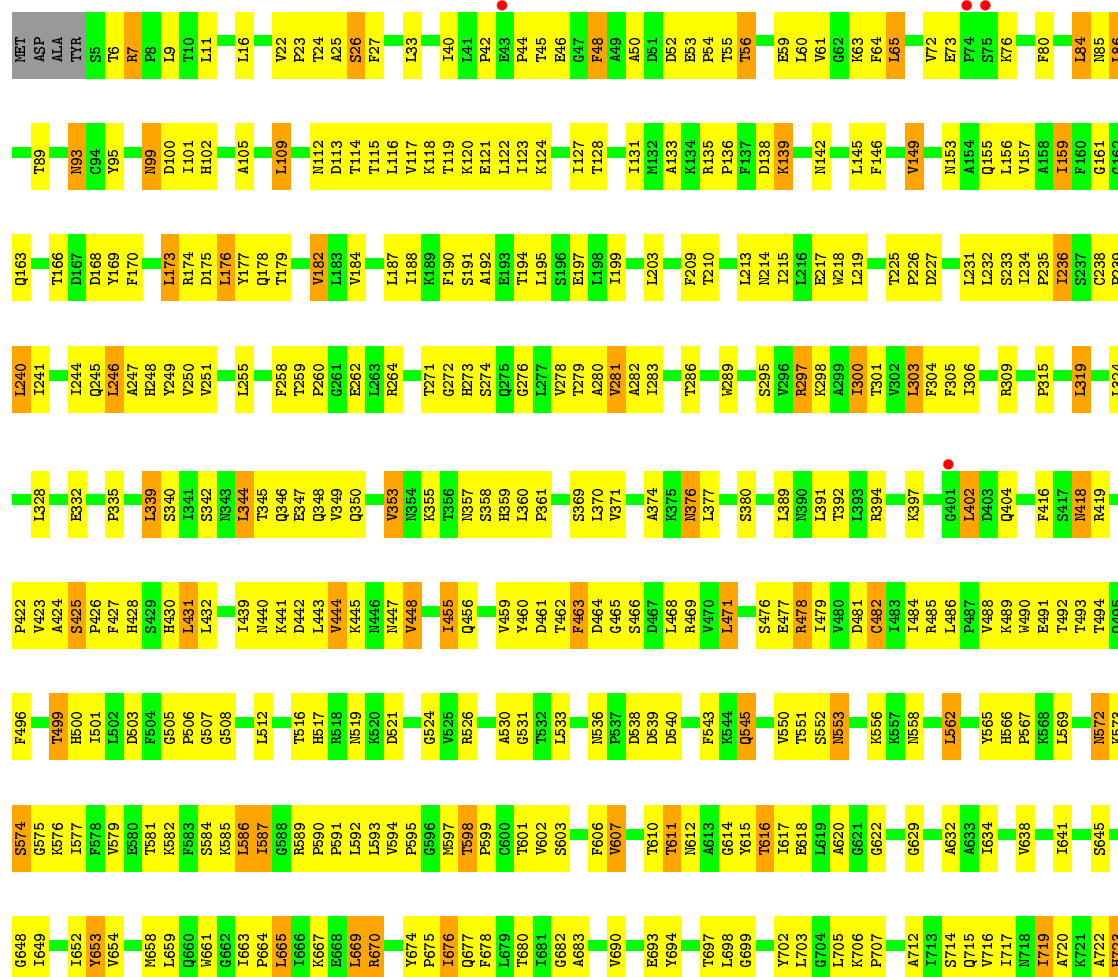
MET	L84	I159	T234	P315
ASP	M85	F160	P235	M316
ALA	L86	G161	I236	T317
TYR	S5	Q163	S237	S318
	T89	T166	C238	L319
T6	R7	D167	L240	P320
P8	M93	D168	I241	P321
	G94	Y169	T244	L324
L9	Y95	F170	Q245	L328
T10			A247	E322
L11	M99	L173	E248	P335
	D100	A174	V249	M338
S15	I101	D175	V251	L339
L16	H102	Y177	L255	S340
V22	A105	T178	F258	S342
P23	L109	T179	T259	S343
P23	M112	V180	P260	T344
T24	D113	V182	G261	T345
A25	T114	L183	E262	Q346
S26	T115	G185	L263	E347
F27	L116	D186	R264	Q348
F28	V117	L187		Q350
L33	K118	I188	T271	V353
M38	K120	K189	G272	R354
A39	K121	S191	H273	K355
L41	L122	I192	S274	N357
P42	I123	E193	Q275	S358
	K124	T194	L276	R359
T45		L195	L277	L360
E46	I127	G196	T278	P361
Q47	T128	E197	V279	S369
F48	I131	L198	A280	L370
A49	M132	I199	V281	V371
D51	A133	L203	A282	A374
D52	R134	P209	T286	R375
P54	R135	T210	E289	R376
T55	P136	L213	E290	L377
	F137	N214	S295	S380
E59	D138	I215	V296	L389
L60	K139	E217	K298	R390
V61	N142	L218	A299	T392
G62	L145	F146	I300	L393
K63	V149		L303	R394
F64	M153		F304	
L65	Q155		P305	
	E156		L306	
V68	V157		R309	
V72	A158			
E73				
K76				
F80				

V1556	D1458	T1374	F1279	L1197	VAL	L1040	T945	A858	E784	I717	P567	I483
S1557	K1462	V1374	D1280	S1198	GLN	E1041	F946	T859	W785	H718	K568	I484
L1560	T1463	I1377	P1281	E1199	GLN	A1042	T947	R860	S786	I719	L569	R485
M1561		V1378				V1043	G948			A720		Q404
P1562	T1468	I1378	V1284	L1205	VAL	D1044	D949	W865	K787	K721	N572	P487
T1563	E1469	V1381	I1292	K1206	ASP	D1045	F950	K866	F789	A722	K573	V488
H1564	T1470	V1382	T1293	L1210	SER	Q1046	L951	E867	D790	H723	S574	K489
S1565	E1471	N1383	A1294	R952	SER	D1047	R953	F868	Y791	F726	S575	W490
S1566	V1472	V1383	K1295	K1212	VAL	Q1048	V954	D869	P792	P727	K576	E491
S1567	T1473	SER	E1296	L1213	VAL	R1050	E955	T871	M794	T728	I577	T492
H1568	F1474	GLU	L1214	L1214	SER	T1051	E956	R872	T795	I729	F578	T493
	K1388				GLU	C1052			F796	A729	W579	R419
	I1389					T1051		F873	D797	L730	E580	Q495
N1574	V1390		F1300	I1219	D1123	I1053	K960		D797	Q731	T581	F496
L1575	S1481		A1303	Q1220	K1128	L1054	L964	K879	G798	W732	K582	L421
I1579	S1482	M1221	M1221	M1221	A1129			L880	F799	T733	F583	T499
T1580	V1483	T1130	M1223	M1223	T1130	V1058	I967	V881	L800		K585	A424
	F1486					A1059		P882	R804	R736	L586	S425
M1583	V1403	T1133	D1310	D1310	T1133	A1060	Y970	K887	R805	G739	W661	F504
F1584	M1404	D1134	F1311	T1227	D1134	Q1061	Y971	R888	W806	H740	G662	G505
S1585	T1407	E1135	V1312	T1228	E1135	F1062	S971		R807	H741	I663	P506
S1586	S1408		R1313	G1231		T1063	L972	I892	I807	S742	P664	P590
	S1409	W1138	R1314	G1231			L973				P664	P590
T1485	F1410	S1145	T1318	K1232	S1145	I1066	Y987	R894	R811	D745	I666	V433
K1486	F1411	E1146	H1319	V1234	E1146	D1067	Q993	L895	K812	A746	K667	T516
E1492	G1414	T1147	L1320	S1235	T1147	P1069	Q993	R896	T813	H747	E668	H517
L1493	T1498	N1148	A1321	L1236	N1148	I1070	F994	A897	L669	T748	G596	N440
P1494	V1415	W1149	P1322	P1237	W1149	K1071	L995	D898	D816	P749	M597	K520
T1495	E1500	R1160	L1238	L1238	R1160	M1074	Q998	F899	A817	M750	T598	D821
G1502	T1417	H1151	F1325	N1241	H1151	D1075	D999	Q900	K818	L751	P599	G822
I1503	F1419	A1152	A1386	F1242	A1152	G1076	P999	K901		Q752	G600	V827
V1504	E1420	I1159	V1329	P1243	I1159	I1077	D1001	P902	I821	Y754	T601	N443
D1505	T1421	Q1161	G1330	M1421	Q1161	H1078	H1002	W903	A822		V602	V444
V1506	T1422	D1162	W1331	G1247	D1162	D1079	F1003	A805	G824		F678	N446
						G1080	L1004	T906	T825	I757		N447
A1510	T1425	K1163			K1163	H1081	S1005	V907	G826	R758	V607	N636
S1511	T1426	V1166	I1385	S1262	V1166	I1082	M1006		P828	H759		P537
H1512	V1427	E1256	I1388	D1257	E1256	K1084	P1010	A911	W832	N762	T610	D538
P1515	E1428	N1167	F1339	D1258	N1167	L1085	M1011	R912	E333	M764	N612	D539
	Y1431	P1169	P1340	W1259	P1169	L1086	Q1012	D913	Q834	L765	Y694	D540
T1526	H1434	I1170	V1343	Q1260	I1170	Y1090	V1015	T916	Q834	L765	Y694	
L1527	I1435	K1172	D1344	R1261	K1172	G1091	P1016		T835	T697	T616	K544
S1825	F1436	V1173	L1347	I1262	V1173	D1092	F1017	E921	Y836	F767	I617	Q645
I626	T1437	F1174	L1347	K1263	F1174	D1093	V1018		P839	G768	E618	V550
Q1627	S1438	K1175	L1348	E1264	K1175	K1096	P1019	L926	T840	S769	L619	T551
		P1176	K1350	M1265	P1176	I1097	V1020			Y702	A620	S552
L1533	I1441	S1177	L1350	Y1266	S1177		L1021	L929	W844	G772	G621	N653
D1543	A1442	M1180	V1351		M1180				T845	L705	G622	K556
P1547	V1443	V1181	H1352	L1269	V1181	E1100	R1024	I932	A774	K706	Y624	
R1634	T1444	M1181	N1355	M1270	M1181	F1025	F1025		D775	P707		
K1635	R1445	T1189	N1355	I1271	T1189	Y1026	I1026	W938	E852	T777	G629	N660
T1549	S1446		D1272	I1271		F1103	I1027	P939	P853	Y778	M630	W661
M1550	L1452	V1189	E1273	E1273	V1189	P1108	K1031	T942	I854	I743	T631	E563
L1637		V1195	F1274	F1275	V1194	P1108	K1031	R944	R855	W714	A632	E564
L1638						V1109	D1032	W943	R855	Y780	K453	Y565
F1640						ASP			T852	L781	I634	C482



• Molecule 2: Fatty acid synthase subunit beta

Chain I: 51% 40% 8%



[illegible]

Y2029	Y2030
T2033	G2034
S2035	E2036
P2037	I2038
K2039	E2040
I2041	I2042
D2043	I2044
E2045	K2047
Y2048	Q2049
Q2050	SER



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	231.88Å 231.88Å 756.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.00 20.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	97.3 (20.00-4.00) 97.3 (20.00-4.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 3.94Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.266 , 0.267 0.257 , 0.257	Depositor DCC
$R_{free}$ test set	8521 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	130.2	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 74.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	88830	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	168.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.43	5/13822 (0.0%)	0.59	6/18682 (0.0%)
1	B	0.43	3/13822 (0.0%)	0.61	9/18682 (0.0%)
1	C	0.43	4/13822 (0.0%)	0.59	4/18682 (0.0%)
2	G	0.41	7/16360 (0.0%)	0.58	6/22198 (0.0%)
2	H	0.40	7/16360 (0.0%)	0.57	3/22198 (0.0%)
2	I	0.40	5/16360 (0.0%)	0.58	10/22198 (0.0%)
All	All	0.42	31/90546 (0.0%)	0.59	38/122640 (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	2
2	I	0	1
All	All	0	4

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	992	PHE	C-N	13.35	1.59	1.34
1	C	992	PHE	C-N	13.18	1.59	1.34
2	I	842	GLY	C-N	11.12	1.59	1.34
2	G	315	PRO	C-N	10.45	1.58	1.34
1	C	485	ASP	C-N	9.61	1.56	1.34
2	H	1256	GLU	C-N	9.35	1.55	1.34
2	H	138	ASP	C-N	9.07	1.54	1.34
2	H	1840	VAL	C-N	8.47	1.53	1.34
2	G	1657	ILE	C-N	8.15	1.52	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	315	PRO	C-N	7.84	1.52	1.34
1	A	668	PHE	C-N	7.73	1.51	1.34
2	I	1980	TYR	C-N	7.70	1.51	1.34
1	A	181	THR	C-N	7.05	1.50	1.34
2	G	422	PRO	C-N	6.97	1.50	1.34
2	I	1018	VAL	C-N	-6.57	1.21	1.34
2	G	1256	GLU	C-N	6.43	1.48	1.34
1	C	1520	ALA	C-N	-6.36	1.22	1.34
2	I	903	TRP	C-N	6.33	1.48	1.34
2	H	1053	ILE	C-N	6.30	1.48	1.34
2	H	422	PRO	C-N	6.29	1.48	1.34
2	G	842	GLY	C-N	6.06	1.48	1.34
2	H	137	PHE	C-N	5.95	1.47	1.34
1	A	1520	ALA	C-N	5.79	1.45	1.34
2	H	1982	MET	C-N	5.67	1.47	1.34
1	B	181	THR	C-N	-5.65	1.21	1.34
2	G	1529	GLN	C-N	-5.50	1.21	1.34
2	G	1980	TYR	C-N	5.38	1.46	1.34
1	C	636	PRO	C-N	-5.29	1.21	1.34
1	B	668	PHE	C-N	5.29	1.46	1.34
1	B	1430	ARG	C-N	-5.19	1.22	1.34
1	A	1181	PHE	C-N	5.13	1.45	1.34

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1116	PRO	O-C-N	-11.67	104.02	122.70
2	I	1982	MET	O-C-N	-9.44	107.59	122.70
2	G	842	GLY	O-C-N	-8.86	108.52	122.70
2	G	1053	ILE	O-C-N	-8.58	108.97	122.70
1	B	992	PHE	O-C-N	8.47	137.19	121.10
2	I	422	PRO	O-C-N	-8.30	109.42	122.70
1	B	992	PHE	C-N-CD	8.15	145.52	128.40
2	I	1982	MET	C-N-CA	8.08	141.89	121.70
1	B	1116	PRO	CA-C-N	8.00	134.79	117.20
2	I	1657	ILE	O-C-N	-7.47	110.75	122.70
1	C	1520	ALA	O-C-N	7.43	135.22	121.10
1	A	1430	ARG	O-C-N	-7.40	110.85	122.70
1	B	1116	PRO	C-N-CA	7.29	139.94	121.70
1	B	599	MET	N-CA-C	-6.93	92.27	111.00
1	C	599	MET	N-CA-C	-6.92	92.32	111.00
1	A	599	MET	N-CA-C	-6.90	92.37	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	992	PHE	C-N-CD	6.65	142.37	128.40
2	I	422	PRO	CA-C-N	6.52	131.55	117.20
2	H	1840	VAL	O-C-N	-6.51	112.29	122.70
2	I	1982	MET	CA-C-N	6.50	131.50	117.20
1	C	1116	PRO	O-C-N	-6.36	112.52	122.70
1	B	992	PHE	CA-C-N	-6.11	100.00	117.10
2	G	1053	ILE	CA-C-N	6.05	130.50	117.20
1	A	992	PHE	O-C-N	5.97	132.45	121.10
2	I	315	PRO	O-C-N	-5.75	113.50	122.70
1	B	540	GLN	N-CA-C	-5.65	95.74	111.00
1	A	540	GLN	N-CA-C	-5.64	95.77	111.00
1	C	540	GLN	N-CA-C	-5.63	95.80	111.00
1	B	178	GLY	O-C-N	5.57	131.61	122.70
2	I	422	PRO	C-N-CA	5.52	135.50	121.70
2	G	138	ASP	O-C-N	-5.44	113.99	122.70
1	A	1520	ALA	O-C-N	5.44	131.44	121.10
2	H	1256	GLU	CA-C-N	-5.39	105.35	117.20
2	I	1657	ILE	CA-C-N	5.34	128.95	117.20
2	G	842	GLY	CA-C-N	5.30	128.86	117.20
2	H	138	ASP	O-C-N	-5.08	114.56	122.70
2	G	138	ASP	C-N-CA	5.05	134.32	121.70
2	I	1657	ILE	C-N-CA	5.03	134.27	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

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

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13572	0	13489	663	15

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	13572	0	13490	618	6
1	C	13572	0	13490	638	22
2	G	15995	0	15978	1026	32
2	H	15995	0	15978	1023	7
2	I	15995	0	15977	983	26
3	A	12	0	10	3	0
3	B	12	0	10	4	0
3	C	12	0	10	4	0
4	G	31	0	19	7	0
4	H	31	0	19	6	0
4	I	31	0	19	8	0
All	All	88830	0	88489	4773	54

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 (4773) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1749:THR:CB	1:A:1874:ASP:HB3	1.53	1.37
1:B:1749:THR:CB	1:B:1874:ASP:HB3	1.56	1.34
1:B:1749:THR:CB	1:B:1873:HIS:O	1.75	1.32
1:A:1464:GLU:HG3	1:A:1773:VAL:CG1	1.58	1.32
1:C:1749:THR:CB	1:C:1874:ASP:HB3	1.62	1.29
1:A:1464:GLU:CG	1:A:1773:VAL:HG12	1.65	1.26
1:A:1749:THR:CB	1:A:1873:HIS:O	1.88	1.21
1:C:1749:THR:CB	1:C:1874:ASP:CA	2.20	1.19
2:H:1956:ARG:HB2	2:H:1957:PRO:HD3	1.24	1.18
1:C:1749:THR:CB	1:C:1874:ASP:CB	2.22	1.16
2:G:28:PHE:CE2	2:H:7:ARG:HD2	1.80	1.16
1:C:1464:GLU:CG	1:C:1773:VAL:HG12	1.75	1.16
2:G:1859:PRO:HG3	2:G:1871:LEU:HD12	1.29	1.15
2:H:1834:ARG:HH11	2:H:1834:ARG:HG2	1.06	1.15
1:C:1501:LEU:CD1	1:C:1775:LEU:HD21	1.75	1.15
1:C:1460:LYS:NZ	1:C:1774:GLU:OE2	1.80	1.15
1:C:1498:GLU:HG3	1:C:1876:LEU:HD13	1.19	1.14
2:H:490:TRP:HE1	2:H:516:THR:HG22	1.12	1.14
1:C:1464:GLU:HG3	1:C:1773:VAL:CG1	1.77	1.14
2:H:499:THR:HB	2:H:500:HIS:HD2	1.10	1.12
2:I:490:TRP:HE1	2:I:516:THR:HG22	1.10	1.12
2:G:1956:ARG:HB2	2:G:1957:PRO:HD3	1.23	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:131:ILE:HD12	2:G:182:VAL:HB	1.18	1.12
2:H:131:ILE:HD12	2:H:182:VAL:CB	1.79	1.11
2:I:601:THR:HG21	2:I:618:GLU:O	1.50	1.11
2:I:1956:ARG:HB2	2:I:1957:PRO:HD3	1.23	1.11
1:A:253:ARG:HG3	1:A:254:TRP:HD1	1.15	1.10
1:A:1721:ARG:HG2	1:A:1721:ARG:HH11	1.16	1.10
2:H:601:THR:HG21	2:H:618:GLU:O	1.50	1.10
2:G:601:THR:HG21	2:G:618:GLU:O	1.52	1.10
1:B:1464:GLU:HG3	1:B:1773:VAL:HG12	1.31	1.09
2:G:499:THR:HB	2:G:500:HIS:HD2	1.08	1.09
2:H:131:ILE:CB	2:H:182:VAL:HG11	1.82	1.09
2:I:297:ARG:HD3	2:I:447:ASN:HD21	1.15	1.09
2:G:131:ILE:HB	2:G:182:VAL:HG11	1.31	1.09
2:I:499:THR:HB	2:I:500:HIS:HD2	1.07	1.08
2:G:490:TRP:HE1	2:G:516:THR:HG22	1.12	1.08
1:B:1460:LYS:NZ	1:B:1774:GLU:OE2	1.85	1.08
1:B:1749:THR:CB	1:B:1874:ASP:CB	2.32	1.08
1:A:1749:THR:CB	1:A:1874:ASP:CB	2.31	1.08
1:C:852:ARG:HG2	1:C:852:ARG:HH11	1.14	1.08
1:C:1498:GLU:CG	1:C:1876:LEU:HD13	1.84	1.07
2:H:131:ILE:HG21	2:H:182:VAL:HG12	1.35	1.07
2:H:128:THR:HA	2:H:182:VAL:HG21	1.31	1.07
2:I:1227:ARG:HH11	2:I:1227:ARG:HG3	1.18	1.07
2:G:297:ARG:HD3	2:G:447:ASN:HD21	1.17	1.06
2:G:28:PHE:CZ	2:H:7:ARG:HD2	1.91	1.06
2:I:1834:ARG:HG2	2:I:1834:ARG:HH11	1.16	1.06
1:C:1367:ARG:NH1	1:C:1372:THR:HB	1.71	1.06
2:G:903:TRP:O	2:G:906:THR:HG22	1.57	1.05
1:C:1721:ARG:HG2	1:C:1721:ARG:HH11	1.19	1.05
2:G:1834:ARG:HG2	2:G:1834:ARG:HH11	1.16	1.05
2:I:7:ARG:HH21	2:I:27:PHE:HB3	1.20	1.05
1:B:253:ARG:HG3	1:B:254:TRP:HD1	1.17	1.04
1:A:1367:ARG:NH1	1:A:1372:THR:HB	1.72	1.04
1:C:253:ARG:HG3	1:C:254:TRP:HD1	1.15	1.04
2:G:932:ILE:HD11	2:G:1042:ALA:HB2	1.36	1.04
2:I:1739:GLU:HB2	2:I:1987:PRO:HB3	1.40	1.04
1:B:1367:ARG:NH1	1:B:1372:THR:HB	1.73	1.04
2:H:1227:ARG:HG3	2:H:1227:ARG:HH11	1.19	1.03
2:G:1227:ARG:HH11	2:G:1227:ARG:HG3	1.18	1.03
2:H:297:ARG:HD3	2:H:447:ASN:HD21	1.16	1.03
1:B:1721:ARG:HH11	1:B:1721:ARG:HG2	1.21	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1722:VAL:HG11	1:B:1731:LEU:HB3	1.37	1.03
1:C:1722:VAL:HG11	1:C:1731:LEU:HB3	1.37	1.02
2:G:7:ARG:HH21	2:G:27:PHE:HB3	1.22	1.02
1:B:599:MET:HB2	1:B:624:LYS:HD2	1.42	1.02
2:H:7:ARG:HH21	2:H:27:PHE:HB3	1.22	1.02
1:B:852:ARG:HH11	1:B:852:ARG:HG2	1.20	1.02
1:A:852:ARG:HH11	1:A:852:ARG:HG2	1.23	1.02
1:C:1498:GLU:HG3	1:C:1876:LEU:CD1	1.84	1.02
1:C:1501:LEU:HD12	1:C:1775:LEU:HD21	1.38	1.02
2:H:1739:GLU:HB2	2:H:1987:PRO:HB3	1.42	1.02
2:H:1859:PRO:HG3	2:H:1871:LEU:HD12	1.37	1.01
2:I:1859:PRO:HG3	2:I:1871:LEU:HD12	1.41	1.01
2:H:131:ILE:HB	2:H:182:VAL:CG1	1.89	1.01
1:C:1219:VAL:HA	1:C:1384:ILE:HD11	1.40	1.01
2:H:131:ILE:CD1	2:H:182:VAL:HB	1.91	1.00
1:C:1014:ASP:H	1:C:1510:ASN:HD21	1.03	1.00
2:H:903:TRP:O	2:H:906:THR:HG22	1.59	1.00
1:A:1722:VAL:HG11	1:A:1731:LEU:HB3	1.40	1.00
2:I:741:HIS:NE2	2:I:855:HIS:CE1	2.30	1.00
1:A:599:MET:HB2	1:A:624:LYS:HD2	1.43	0.99
2:H:1567:ARG:HG3	2:H:1567:ARG:HH11	1.27	0.99
1:C:1749:THR:CB	1:C:1874:ASP:HA	1.90	0.99
1:C:599:MET:HB2	1:C:624:LYS:HD2	1.43	0.99
1:C:253:ARG:HG3	1:C:254:TRP:CD1	1.98	0.99
2:G:499:THR:HB	2:G:500:HIS:CD2	1.97	0.98
2:I:892:ILE:HD11	2:I:903:TRP:CE2	1.98	0.98
1:A:253:ARG:HG3	1:A:254:TRP:CD1	1.98	0.98
1:B:1219:VAL:HA	1:B:1384:ILE:HD11	1.45	0.98
1:C:1460:LYS:HE3	1:C:1774:GLU:CD	1.83	0.98
2:H:1803:THR:HG22	2:H:2009:LYS:HA	1.45	0.98
2:H:762:ASN:H	2:H:762:ASN:HD22	1.03	0.98
2:H:131:ILE:HB	2:H:182:VAL:HG11	1.00	0.98
2:I:499:THR:HB	2:I:500:HIS:CD2	1.97	0.98
2:I:903:TRP:O	2:I:906:THR:HG22	1.63	0.98
2:G:1844:ARG:HG2	2:G:1844:ARG:HH11	1.26	0.97
1:A:400:ARG:HG2	1:A:400:ARG:HH11	1.28	0.97
2:G:892:ILE:HD11	2:G:903:TRP:CE2	1.98	0.97
1:A:400:ARG:CG	1:A:400:ARG:HH11	1.76	0.97
2:H:499:THR:HB	2:H:500:HIS:CD2	1.99	0.97
2:H:1172:LYS:HE3	2:H:1574:ASN:OD1	1.64	0.97
1:B:198:PRO:HG3	1:B:209:LEU:HD21	1.47	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ARG:HG3	1:B:254:TRP:CD1	1.99	0.96
2:H:594:VAL:HB	2:H:617:ILE:HG13	1.44	0.96
2:I:490:TRP:NE1	2:I:516:THR:HG22	1.79	0.96
2:I:762:ASN:HD22	2:I:762:ASN:H	1.08	0.96
1:A:1014:ASP:H	1:A:1510:ASN:HD21	1.10	0.96
2:H:490:TRP:NE1	2:H:516:THR:HG22	1.81	0.96
2:H:131:ILE:HD12	2:H:182:VAL:HB	0.96	0.96
1:A:12:ILE:HD11	2:G:2041:ILE:HD12	1.47	0.95
1:C:198:PRO:HG3	1:C:209:LEU:HD21	1.48	0.95
2:G:490:TRP:NE1	2:G:516:THR:HG22	1.81	0.95
2:H:1567:ARG:HH11	2:H:1567:ARG:CG	1.79	0.95
2:H:892:ILE:HD11	2:H:903:TRP:CE2	2.01	0.95
2:G:1803:THR:HG22	2:G:2009:LYS:HA	1.48	0.95
1:B:1460:LYS:CE	1:B:1773:VAL:O	2.15	0.95
2:I:1567:ARG:HH11	2:I:1567:ARG:HG3	1.29	0.95
2:I:594:VAL:HB	2:I:617:ILE:HG13	1.46	0.95
2:I:1567:ARG:HH11	2:I:1567:ARG:CG	1.79	0.95
2:H:1199:GLU:OE2	2:H:1567:ARG:NH1	2.00	0.95
2:G:1878:VAL:HG11	2:G:1910:VAL:HG22	1.48	0.95
2:G:1741:ILE:HD12	2:G:1986:LYS:HD2	1.47	0.95
1:A:198:PRO:HG3	1:A:209:LEU:HD21	1.47	0.95
2:I:741:HIS:CE1	2:I:855:HIS:CE1	2.55	0.95
2:G:1567:ARG:CG	2:G:1567:ARG:HH11	1.80	0.95
1:A:444:ASN:HB2	1:A:447:LEU:H	1.31	0.95
1:B:1464:GLU:HG3	1:B:1773:VAL:CG1	1.95	0.95
2:H:741:HIS:HE1	2:H:845:THR:CG2	1.80	0.95
2:H:835:THR:HG21	2:H:855:HIS:CD2	1.99	0.94
2:G:1739:GLU:HB2	2:G:1987:PRO:HB3	1.43	0.94
2:G:1589:VAL:HA	2:G:1592:LEU:HD12	1.49	0.94
1:B:1460:LYS:HE3	1:B:1773:VAL:O	1.68	0.94
2:H:55:THR:HG22	2:H:56:THR:HG22	1.48	0.94
1:B:444:ASN:HB2	1:B:447:LEU:H	1.31	0.94
1:C:1498:GLU:OE2	1:C:1876:LEU:HA	1.65	0.94
2:I:1741:ILE:HD12	2:I:1986:LYS:HD2	1.49	0.94
1:C:400:ARG:HG2	1:C:400:ARG:HH11	1.33	0.94
1:C:2:LYS:HD2	2:I:2050:GLN:HB3	1.50	0.94
2:I:1878:VAL:HG11	2:I:1910:VAL:HG22	1.50	0.94
2:H:1314:ARG:HH11	2:H:1314:ARG:HG3	1.31	0.94
2:G:762:ASN:H	2:G:762:ASN:HD22	1.03	0.93
2:G:942:THR:HB	2:G:1012:GLN:HG2	1.50	0.93
1:A:1219:VAL:HA	1:A:1384:ILE:HD11	1.45	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:MET:HE3	1:B:529:MET:HA	1.47	0.93
1:A:1501:LEU:CD1	1:A:1775:LEU:HD21	1.98	0.93
2:I:741:HIS:HE1	2:I:845:THR:CG2	1.81	0.93
2:H:1845:ASP:HB2	2:H:1849:ARG:H	1.34	0.93
2:H:652:ILE:H	2:H:658:MET:HE3	1.30	0.93
1:B:400:ARG:HH11	1:B:400:ARG:CG	1.81	0.93
2:H:1589:VAL:HA	2:H:1592:LEU:HD12	1.49	0.93
2:G:565:TYR:CZ	2:G:758:ARG:HD2	2.04	0.93
2:I:1314:ARG:HG3	2:I:1314:ARG:HH11	1.32	0.93
1:A:12:ILE:HD11	2:G:2041:ILE:CD1	1.99	0.93
2:I:56:THR:HG23	2:I:59:GLU:HG3	1.49	0.93
1:C:1501:LEU:HD11	1:C:1775:LEU:CD2	1.99	0.93
2:G:1567:ARG:HG3	2:G:1567:ARG:HH11	1.30	0.93
2:G:128:THR:HA	2:G:182:VAL:HG21	1.51	0.92
1:A:1523:ARG:HG3	1:A:1523:ARG:HH11	1.33	0.92
1:C:1523:ARG:HH11	1:C:1523:ARG:HG3	1.32	0.92
1:C:1501:LEU:CD1	1:C:1775:LEU:CD2	2.47	0.92
2:I:741:HIS:CE1	2:I:845:THR:CG2	2.52	0.92
2:G:55:THR:HG21	2:G:113:ASP:HB2	1.52	0.92
1:A:1460:LYS:CE	1:A:1773:VAL:O	2.17	0.92
1:A:152:HIS:CD2	1:A:163:LEU:HB2	2.05	0.92
2:G:741:HIS:NE2	2:G:855:HIS:CE1	2.38	0.92
1:B:1749:THR:CB	1:B:1873:HIS:C	2.37	0.92
2:G:1844:ARG:CG	2:G:1844:ARG:HH11	1.82	0.92
2:I:55:THR:HG22	2:I:56:THR:HG22	1.51	0.91
2:I:667:LYS:HD2	2:I:697:THR:HG22	1.51	0.91
2:I:741:HIS:CE1	2:I:845:THR:HG22	2.04	0.91
1:A:1721:ARG:CG	1:A:1721:ARG:HH11	1.84	0.91
1:C:400:ARG:HH11	1:C:400:ARG:CG	1.81	0.91
2:G:1314:ARG:HH11	2:G:1314:ARG:HG3	1.32	0.91
1:C:152:HIS:CD2	1:C:163:LEU:HB2	2.05	0.91
2:G:56:THR:HG23	2:G:59:GLU:HG3	1.50	0.91
2:G:741:HIS:CE1	2:G:855:HIS:CE1	2.57	0.91
2:I:1803:THR:HG22	2:I:2009:LYS:HA	1.51	0.91
2:I:707:PRO:HG3	2:I:716:VAL:HG21	1.52	0.91
1:A:1693:ILE:HD11	2:G:998:GLN:HB2	1.51	0.91
1:B:1523:ARG:HH11	1:B:1523:ARG:HG3	1.36	0.91
1:C:1464:GLU:HG3	1:C:1773:VAL:HG12	0.91	0.91
1:C:793:ARG:HA	1:C:797:THR:HG23	1.52	0.90
2:H:1741:ILE:HD12	2:H:1986:LYS:HD2	1.54	0.90
2:I:942:THR:HB	2:I:1012:GLN:HG2	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:707:PRO:HG3	2:H:716:VAL:HG21	1.54	0.90
1:C:1498:GLU:HG3	1:C:1876:LEU:HB3	1.53	0.90
2:I:1441:ILE:HD11	2:I:1445:ARG:CZ	2.02	0.90
2:I:652:ILE:H	2:I:658:MET:HE3	1.36	0.90
1:C:1498:GLU:CG	1:C:1876:LEU:HB3	2.02	0.90
2:G:55:THR:HG22	2:G:56:THR:HG22	1.52	0.90
2:H:565:TYR:CZ	2:H:758:ARG:HD2	2.06	0.90
1:B:1456:GLU:OE1	1:B:1775:LEU:HD23	1.71	0.89
2:G:131:ILE:HD12	2:G:182:VAL:CB	2.01	0.89
1:C:1431:GLU:HG3	1:C:1433:HIS:CE1	2.07	0.89
2:G:1847:LEU:H	2:G:1847:LEU:HD12	1.37	0.89
1:C:444:ASN:HB2	1:C:447:LEU:H	1.33	0.89
2:G:594:VAL:HB	2:G:617:ILE:HG13	1.52	0.89
1:B:1721:ARG:HH11	1:B:1721:ARG:CG	1.85	0.89
1:B:793:ARG:HA	1:B:797:THR:HG23	1.54	0.89
2:I:1589:VAL:HA	2:I:1592:LEU:HD12	1.51	0.89
1:A:253:ARG:HE	1:A:254:TRP:HE1	1.21	0.89
2:G:1441:ILE:HD11	2:G:1445:ARG:CZ	2.02	0.89
2:H:1847:LEU:H	2:H:1847:LEU:HD12	1.37	0.89
2:H:55:THR:HG21	2:H:113:ASP:HB2	1.53	0.89
1:A:529:MET:HA	1:A:529:MET:HE3	1.53	0.89
2:H:56:THR:HG23	2:H:59:GLU:HG3	1.54	0.89
1:A:1474:ALA:HA	1:A:1478:PRO:HG2	1.54	0.88
1:B:1749:THR:CB	1:B:1874:ASP:CA	2.51	0.88
2:G:667:LYS:HD2	2:G:697:THR:HG22	1.55	0.88
1:A:1501:LEU:HD11	1:A:1775:LEU:CD2	2.01	0.88
2:H:667:LYS:HD2	2:H:697:THR:HG22	1.55	0.88
1:A:1367:ARG:HH12	1:A:1372:THR:HB	1.35	0.88
1:A:403:ASP:HB2	1:A:1613:ASN:HD21	1.38	0.88
1:B:31:THR:HG23	2:H:2011:ILE:HG21	1.56	0.88
2:H:942:THR:HB	2:H:1012:GLN:HG2	1.54	0.88
2:I:55:THR:HG21	2:I:113:ASP:HB2	1.53	0.88
1:B:1367:ARG:HH12	1:B:1372:THR:HB	1.38	0.88
1:B:152:HIS:CD2	1:B:163:LEU:HB2	2.09	0.88
1:B:1464:GLU:CG	1:B:1773:VAL:HG12	2.01	0.88
2:I:1227:ARG:HH11	2:I:1227:ARG:CG	1.87	0.88
1:C:1721:ARG:CG	1:C:1721:ARG:HH11	1.87	0.87
2:G:707:PRO:HG3	2:G:716:VAL:HG21	1.56	0.87
2:H:1441:ILE:HD11	2:H:1445:ARG:CZ	2.04	0.87
2:I:131:ILE:HD12	2:I:182:VAL:HB	1.55	0.87
1:B:1501:LEU:HD11	1:B:1775:LEU:HD21	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1422:THR:CG2	2:G:1474:PHE:HB2	2.05	0.87
1:A:793:ARG:HA	1:A:797:THR:HG23	1.53	0.87
1:C:59:ARG:HH11	2:I:1896:GLN:NE2	1.71	0.87
2:I:369:SER:OG	2:I:380:SER:HB3	1.74	0.87
2:I:298:LYS:HG2	2:I:448:VAL:HG22	1.56	0.87
1:C:1498:GLU:OE2	1:C:1876:LEU:CA	2.12	0.87
1:C:529:MET:HA	1:C:529:MET:HE3	1.57	0.87
2:H:131:ILE:CG2	2:H:182:VAL:HG12	2.04	0.87
2:I:1845:ASP:HB2	2:I:1849:ARG:H	1.38	0.87
1:B:260:ARG:HH12	1:B:300:VAL:HG21	1.38	0.87
2:I:932:ILE:HD11	2:I:1042:ALA:HB2	1.57	0.87
1:C:253:ARG:HE	1:C:254:TRP:HE1	1.21	0.87
1:A:1119:LYS:HD3	1:A:1121:MET:HE2	1.55	0.87
1:A:340:ARG:NH1	1:A:344:GLN:HG2	1.88	0.87
1:B:893:VAL:HG11	1:B:930:LEU:HD23	1.55	0.87
2:H:1422:THR:CG2	2:H:1474:PHE:HB2	2.04	0.86
2:H:741:HIS:HE1	2:H:845:THR:HG22	1.38	0.86
1:C:1474:ALA:HA	1:C:1478:PRO:HG2	1.57	0.86
2:H:1878:VAL:HG11	2:H:1910:VAL:HG22	1.55	0.86
2:I:1739:GLU:HB3	2:I:1746:LEU:HD11	1.58	0.86
1:B:1474:ALA:HA	1:B:1478:PRO:HG2	1.58	0.86
2:G:741:HIS:HE1	2:G:845:THR:CG2	1.88	0.86
2:H:1533:LEU:HD13	2:H:1630:GLY:HA2	1.55	0.86
1:B:400:ARG:HH11	1:B:400:ARG:HG2	1.41	0.85
2:H:1739:GLU:HB3	2:H:1746:LEU:HD11	1.56	0.85
2:G:741:HIS:CE1	2:G:845:THR:CG2	2.59	0.85
2:I:1533:LEU:HD13	2:I:1630:GLY:HA2	1.59	0.85
2:I:1422:THR:HG23	2:I:1422:THR:O	1.77	0.85
1:A:1749:THR:CB	1:A:1874:ASP:CA	2.55	0.85
2:H:774:ALA:HB1	2:H:1081:HIS:HD2	1.41	0.85
2:I:1847:LEU:HD12	2:I:1847:LEU:H	1.40	0.85
1:B:340:ARG:NH1	1:B:344:GLN:HG2	1.91	0.85
2:G:28:PHE:HE2	2:H:7:ARG:HD2	1.36	0.85
2:H:1844:ARG:HH11	2:H:1844:ARG:CG	1.89	0.85
1:A:1119:LYS:HD3	1:A:1121:MET:CE	2.07	0.85
2:H:1844:ARG:HH11	2:H:1844:ARG:HG2	1.41	0.85
2:G:28:PHE:CZ	2:H:7:ARG:CD	2.59	0.85
2:H:932:ILE:HD11	2:H:1042:ALA:HB2	1.58	0.84
2:H:297:ARG:HD3	2:H:447:ASN:ND2	1.91	0.84
2:G:369:SER:OG	2:G:380:SER:HB3	1.75	0.84
2:H:777:THR:CG2	2:H:1081:HIS:NE2	2.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:131:ILE:HG21	2:G:182:VAL:HG12	1.57	0.84
1:C:340:ARG:NH1	1:C:344:GLN:HG2	1.91	0.84
2:I:297:ARG:HD3	2:I:447:ASN:ND2	1.92	0.84
2:G:1054:LEU:HB2	4:G:3051:FMN:HM72	1.60	0.84
2:G:652:ILE:H	2:G:658:MET:HE3	1.42	0.84
2:H:2038:ILE:HG22	2:H:2042:ILE:HD11	1.60	0.84
2:H:369:SER:OG	2:H:380:SER:HB3	1.78	0.84
1:C:852:ARG:HG2	1:C:852:ARG:NH1	1.93	0.84
2:I:774:ALA:HB2	2:I:1077:ILE:HA	1.58	0.84
1:B:11:HIS:ND1	2:H:1998:LYS:HA	1.93	0.84
1:C:1303:GLY:HA2	1:C:1649:LYS:HE2	1.58	0.84
2:I:995:LEU:HD23	2:I:1000:ILE:HD13	1.60	0.84
2:H:741:HIS:CE1	2:H:845:THR:HG22	2.12	0.84
1:C:31:THR:HG23	2:I:2011:ILE:HG21	1.59	0.84
2:G:1425:LYS:HG2	2:G:1471:GLU:HG3	1.58	0.83
2:G:1533:LEU:HD13	2:G:1630:GLY:HA2	1.60	0.83
2:G:774:ALA:HB2	2:G:1077:ILE:HA	1.61	0.83
1:A:980:VAL:HG23	2:G:968:GLN:OE1	1.78	0.83
1:B:253:ARG:HE	1:B:254:TRP:HE1	1.21	0.83
2:G:1227:ARG:HH11	2:G:1227:ARG:CG	1.89	0.83
2:I:774:ALA:HB1	2:I:1081:HIS:HD2	1.43	0.83
2:H:1227:ARG:HH11	2:H:1227:ARG:CG	1.90	0.83
2:H:1672:GLN:HG2	2:H:1777:THR:HG23	1.59	0.83
2:H:741:HIS:CE1	2:H:845:THR:CG2	2.60	0.83
2:I:1844:ARG:HH11	2:I:1844:ARG:HG2	1.43	0.83
2:G:1293:THR:HG23	2:G:1296:GLU:H	1.44	0.83
2:I:598:THR:HG22	2:I:622:GLY:HA3	1.61	0.83
1:B:403:ASP:HB2	1:B:1613:ASN:HD21	1.44	0.82
2:G:777:THR:CG2	2:G:1081:HIS:NE2	2.41	0.82
1:A:20:TYR:CG	2:G:2033:THR:OG1	2.32	0.82
2:G:297:ARG:HD3	2:G:447:ASN:ND2	1.94	0.82
2:H:85:ASN:HD22	2:H:135:ARG:HH11	1.26	0.82
1:C:1367:ARG:HH12	1:C:1372:THR:HB	1.37	0.82
2:G:1739:GLU:HB3	2:G:1746:LEU:HD11	1.60	0.82
2:G:131:ILE:CB	2:G:182:VAL:HG11	2.07	0.82
2:G:298:LYS:HG2	2:G:448:VAL:HG22	1.61	0.82
2:I:1672:GLN:HG2	2:I:1777:THR:HG23	1.61	0.82
1:A:1249:SER:HB3	1:A:1280:ILE:HG23	1.62	0.82
1:A:36:LEU:HD22	1:A:61:LEU:HD21	1.60	0.82
1:B:1014:ASP:H	1:B:1510:ASN:HD21	1.28	0.82
2:H:995:LEU:HD23	2:H:1000:ILE:HD13	1.58	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1931:LEU:HB3	2:I:1935:GLU:HG2	1.62	0.82
2:I:2038:ILE:HG22	2:I:2042:ILE:HD11	1.61	0.82
1:A:335:HIS:HE1	1:B:335:HIS:CE1	1.98	0.82
1:B:12:ILE:HD11	2:H:2041:ILE:CD1	2.10	0.82
1:C:333:LYS:O	1:C:337:VAL:HG23	1.80	0.81
2:G:995:LEU:HD23	2:G:1000:ILE:HD13	1.60	0.81
2:G:1847:LEU:HD13	2:G:1849:ARG:HD2	1.62	0.81
2:I:128:THR:HA	2:I:182:VAL:HG21	1.62	0.81
1:A:1501:LEU:HD11	1:A:1775:LEU:HD21	1.61	0.81
2:H:1159:ILE:HG12	2:H:1168:ASN:HA	1.61	0.81
2:H:543:PHE:HB2	2:H:545:GLN:HE22	1.45	0.81
2:I:1844:ARG:CG	2:I:1844:ARG:HH11	1.93	0.81
1:A:1464:GLU:HG3	1:A:1773:VAL:HG12	0.85	0.81
2:I:1054:LEU:HB2	4:I:3051:FMN:C7M	2.11	0.81
1:B:1249:SER:HB3	1:B:1280:ILE:HG23	1.62	0.81
2:G:543:PHE:HB2	2:G:545:GLN:HE22	1.46	0.81
2:I:777:THR:CG2	2:I:1081:HIS:NE2	2.43	0.81
2:I:345:THR:HG22	2:I:347:GLU:H	1.46	0.81
2:G:1931:LEU:HB3	2:G:1935:GLU:HG2	1.61	0.81
1:A:1460:LYS:HE2	1:A:1773:VAL:O	1.80	0.81
2:H:1149:TRP:HA	2:H:1242:PHE:CE1	2.15	0.81
1:C:59:ARG:HH11	2:I:1896:GLN:HE22	1.25	0.81
1:B:881:ASN:HA	1:B:944:ARG:NH2	1.96	0.81
1:B:93:ASP:HB3	1:B:94:PRO:HD2	1.62	0.81
1:A:1203:ASP:HB3	1:B:179:LYS:NZ	1.95	0.81
2:G:2038:ILE:HG22	2:G:2042:ILE:HD11	1.60	0.81
1:A:335:HIS:CE1	1:C:335:HIS:HE1	1.98	0.81
2:I:345:THR:HB	2:I:348:GLN:H	1.46	0.81
1:A:93:ASP:HB3	1:A:94:PRO:HD2	1.63	0.81
2:I:1159:ILE:HG12	2:I:1168:ASN:HA	1.63	0.81
1:A:400:ARG:HG2	1:A:400:ARG:NH1	1.91	0.80
2:I:1693:ARG:HD2	2:I:1825:GLU:OE2	1.80	0.80
1:A:1552:ASN:O	1:A:1556:THR:HG22	1.80	0.80
1:A:333:LYS:O	1:A:337:VAL:HG23	1.82	0.80
2:G:1693:ARG:HD2	2:G:1825:GLU:OE2	1.81	0.80
2:I:584:SER:HB3	2:I:591:PRO:HG3	1.63	0.80
1:B:1030:TRP:CD1	1:B:1580:LEU:HD22	2.17	0.80
2:H:1931:LEU:HB3	2:H:1935:GLU:HG2	1.62	0.80
2:H:298:LYS:HG2	2:H:448:VAL:HG22	1.63	0.80
1:A:340:ARG:HH12	1:A:344:GLN:HG2	1.45	0.80
1:A:20:TYR:CE1	2:G:2035:SER:HB2	2.17	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:259:THR:HG22	2:I:262:GLU:HG3	1.63	0.80
2:G:1672:GLN:HG2	2:G:1777:THR:HG23	1.61	0.80
1:B:36:LEU:HD22	1:B:61:LEU:HD21	1.64	0.80
2:H:1159:ILE:HG12	2:H:1169:PRO:HD3	1.63	0.80
1:B:24:SER:CB	2:H:2014:LEU:HD12	2.11	0.80
2:G:741:HIS:CE1	2:G:845:THR:HG22	2.17	0.80
2:H:1847:LEU:HD13	2:H:1849:ARG:HD2	1.63	0.80
2:I:192:ALA:HA	2:I:215:ILE:HD12	1.64	0.80
1:C:1249:SER:HB3	1:C:1280:ILE:HG23	1.63	0.80
1:C:1460:LYS:CE	1:C:1774:GLU:OE2	2.29	0.80
2:I:1242:PHE:HE2	2:I:1244:PRO:HG3	1.46	0.80
1:A:1501:LEU:HD12	1:A:1775:LEU:HD21	1.63	0.79
1:A:484:LEU:O	1:A:485:ASP:HB2	1.82	0.79
2:H:598:THR:HG22	2:H:622:GLY:HA3	1.64	0.79
2:H:907:VAL:HG21	2:H:921:GLU:HG2	1.64	0.79
2:I:455:ILE:HD11	2:I:469:ARG:HD3	1.63	0.79
1:C:1460:LYS:CE	1:C:1774:GLU:CD	2.50	0.79
2:I:1293:THR:HG23	2:I:1296:GLU:H	1.47	0.79
2:H:1199:GLU:OE2	2:H:1567:ARG:CZ	2.31	0.79
2:I:55:THR:CG2	2:I:113:ASP:HB2	2.12	0.79
1:C:1501:LEU:HD11	1:C:1775:LEU:HD21	1.55	0.79
1:A:31:THR:HG23	2:G:2011:ILE:HG21	1.64	0.79
2:I:1310:ASP:OD2	2:I:1602:SER:HB3	1.82	0.79
2:H:774:ALA:HB2	2:H:1077:ILE:HA	1.64	0.79
2:H:1636:LYS:N	2:H:1657:ILE:O	2.14	0.79
2:H:455:ILE:HD11	2:H:469:ARG:HD3	1.63	0.79
2:I:238:CYS:HB2	2:I:239:PRO:HD3	1.64	0.79
2:I:543:PHE:HB2	2:I:545:GLN:HE22	1.46	0.79
2:G:634:ILE:HD11	2:G:649:ILE:HD11	1.63	0.79
2:I:907:VAL:HG21	2:I:921:GLU:HG2	1.65	0.79
2:G:1314:ARG:CG	2:G:1314:ARG:HH11	1.95	0.79
1:B:260:ARG:NH1	1:B:300:VAL:HG21	1.97	0.79
1:C:403:ASP:HB2	1:C:1613:ASN:HD21	1.46	0.79
2:G:774:ALA:HB1	2:G:1081:HIS:HD2	1.47	0.79
1:B:1303:GLY:HA2	1:B:1649:LYS:HE2	1.63	0.79
2:G:55:THR:CG2	2:G:113:ASP:HB2	2.13	0.79
2:H:105:ALA:HB1	2:H:119:THR:HG23	1.65	0.79
2:H:757:ILE:HG21	2:H:765:LEU:HD13	1.64	0.79
2:I:1847:LEU:HD13	2:I:1849:ARG:HD2	1.64	0.79
1:B:1722:VAL:CG1	1:B:1731:LEU:HB3	2.13	0.78
1:C:1523:ARG:CG	1:C:1523:ARG:HH11	1.96	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:85:ASN:HD22	2:G:135:ARG:HH11	1.28	0.78
2:I:1149:TRP:HA	2:I:1242:PHE:CE1	2.19	0.78
1:C:328:LEU:O	1:C:331:ILE:HG22	1.84	0.78
2:H:1567:ARG:NH1	2:H:1567:ARG:HG3	1.98	0.78
2:H:345:THR:HB	2:H:348:GLN:H	1.48	0.78
2:H:960:LYS:HA	2:H:960:LYS:HE2	1.65	0.78
2:I:85:ASN:HD22	2:I:135:ARG:HH11	1.28	0.78
1:B:12:ILE:HD11	2:H:2041:ILE:HD12	1.63	0.78
2:G:7:ARG:NH2	2:G:27:PHE:HB3	1.99	0.78
2:H:131:ILE:CB	2:H:182:VAL:CG1	2.53	0.78
1:A:328:LEU:O	1:A:331:ILE:HG22	1.84	0.78
1:B:333:LYS:O	1:B:337:VAL:HG23	1.81	0.78
2:I:741:HIS:HE1	2:I:845:THR:HG22	1.41	0.78
1:C:1014:ASP:N	1:C:1510:ASN:HD21	1.82	0.78
2:I:138:ASP:O	2:I:139:LYS:HG3	1.83	0.78
2:I:1770:LEU:HD23	2:I:1776:PHE:CE2	2.19	0.78
1:A:2:LYS:HD2	2:G:2050:GLN:HB3	1.66	0.78
1:B:198:PRO:HG3	1:B:209:LEU:CD2	2.13	0.78
1:B:24:SER:O	2:H:1977:HIS:HD2	1.67	0.78
2:H:55:THR:CG2	2:H:113:ASP:HB2	2.13	0.78
1:C:1498:GLU:CG	1:C:1876:LEU:CD1	2.51	0.78
2:I:7:ARG:NH2	2:I:27:PHE:HB3	1.97	0.78
2:I:634:ILE:HD11	2:I:649:ILE:HD11	1.66	0.78
2:G:1227:ARG:HD2	2:G:1565:VAL:HG11	1.66	0.77
2:G:1770:LEU:HD23	2:G:1776:PHE:CE2	2.20	0.77
2:H:1693:ARG:HD2	2:H:1825:GLU:OE2	1.83	0.77
1:A:335:HIS:CE1	1:C:335:HIS:CE1	2.72	0.77
1:C:1463:VAL:HG11	1:C:1877:GLN:HE22	1.48	0.77
2:H:1293:THR:HG23	2:H:1296:GLU:H	1.49	0.77
1:C:1665:ILE:HG13	1:C:1669:ARG:HD3	1.66	0.77
2:G:455:ILE:HD11	2:G:469:ARG:HD3	1.66	0.77
2:G:355:LYS:O	2:G:358:SER:HB3	1.84	0.77
2:H:131:ILE:CG2	2:H:182:VAL:CG1	2.63	0.77
2:G:28:PHE:HZ	2:H:7:ARG:CD	1.97	0.77
2:I:741:HIS:CE1	2:I:855:HIS:NE2	2.52	0.77
1:A:1523:ARG:CG	1:A:1523:ARG:HH11	1.97	0.77
2:H:1310:ASP:OD2	2:H:1602:SER:HB3	1.82	0.77
1:A:24:SER:HB3	2:G:2014:LEU:HD12	1.64	0.77
1:B:1239:HIS:HD2	1:B:1241:SER:OG	1.67	0.77
2:I:1314:ARG:CG	2:I:1314:ARG:HH11	1.98	0.77
2:I:1423:PHE:H	2:I:1423:PHE:HD1	1.30	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1030:TRP:CD1	1:C:1580:LEU:HD22	2.20	0.77
2:G:1284:VAL:HG13	2:G:1377:VAL:HG22	1.65	0.77
2:G:345:THR:HG22	2:G:347:GLU:H	1.47	0.77
2:G:598:THR:HG22	2:G:622:GLY:HA3	1.67	0.77
1:C:1693:ILE:HD11	2:I:998:GLN:HB2	1.67	0.77
1:C:93:ASP:HB3	1:C:94:PRO:HD2	1.65	0.77
1:B:29:ILE:HG13	2:H:1891:TYR:O	1.85	0.77
1:C:1030:TRP:NE1	1:C:1580:LEU:HD22	2.00	0.77
1:C:12:ILE:HD11	2:I:2041:ILE:HD12	1.67	0.77
1:C:340:ARG:HH12	1:C:344:GLN:HG2	1.49	0.77
2:G:907:VAL:HG21	2:G:921:GLU:HG2	1.65	0.77
1:A:1665:ILE:HG13	1:A:1669:ARG:HD3	1.66	0.76
2:H:1834:ARG:NH1	2:H:1834:ARG:HG2	1.86	0.76
2:I:1567:ARG:HG3	2:I:1567:ARG:NH1	2.00	0.76
2:I:1834:ARG:NH1	2:I:1834:ARG:HG2	1.93	0.76
2:I:1956:ARG:CB	2:I:1957:PRO:HD3	2.09	0.76
1:A:1030:TRP:NE1	1:A:1580:LEU:HD22	1.99	0.76
1:B:1030:TRP:NE1	1:B:1580:LEU:HD22	2.00	0.76
1:A:198:PRO:HG3	1:A:209:LEU:CD2	2.14	0.76
1:C:198:PRO:HG3	1:C:209:LEU:CD2	2.15	0.76
2:G:1678:MET:HE3	2:G:1707:LEU:HD22	1.66	0.76
1:C:400:ARG:HG2	1:C:400:ARG:NH1	1.94	0.76
2:H:762:ASN:N	2:H:762:ASN:HD22	1.82	0.76
2:G:146:PHE:HA	2:G:149:VAL:CG1	2.15	0.76
2:G:345:THR:HB	2:G:348:GLN:H	1.50	0.76
2:I:355:LYS:O	2:I:358:SER:HB3	1.85	0.76
1:A:1030:TRP:CD1	1:A:1580:LEU:HD22	2.21	0.76
2:G:1149:TRP:HA	2:G:1242:PHE:CE1	2.20	0.76
2:G:964:LEU:H	2:G:964:LEU:HD23	1.50	0.76
2:H:598:THR:OG1	2:H:599:PRO:HD3	1.86	0.76
2:I:2015:THR:HG22	2:I:2017:LYS:H	1.51	0.76
1:C:1722:VAL:CG1	1:C:1731:LEU:HB3	2.14	0.76
1:C:24:SER:O	2:I:1977:HIS:HD2	1.68	0.76
2:H:1638:ILE:HD12	2:H:1657:ILE:HG13	1.67	0.76
2:H:1956:ARG:HB2	2:H:1957:PRO:CD	2.12	0.76
1:C:1239:HIS:HD2	1:C:1241:SER:OG	1.68	0.76
2:H:584:SER:HB3	2:H:591:PRO:HG3	1.67	0.76
1:A:988:ILE:HD13	1:A:1048:GLU:CB	2.15	0.75
1:B:1501:LEU:CD1	1:B:1775:LEU:HD21	2.16	0.75
2:G:2015:THR:HG22	2:G:2017:LYS:H	1.51	0.75
2:H:1314:ARG:HH11	2:H:1314:ARG:CG	1.97	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:317:THR:HG21	2:I:1309:GLU:HG3	1.67	0.75
2:I:707:PRO:CG	2:I:716:VAL:HG21	2.15	0.75
1:B:1523:ARG:HH11	1:B:1523:ARG:CG	1.98	0.75
1:B:340:ARG:HH12	1:B:344:GLN:HG2	1.48	0.75
2:H:192:ALA:HA	2:H:215:ILE:HD12	1.68	0.75
2:I:1054:LEU:HB2	4:I:3051:FMN:HM72	1.66	0.75
1:B:1665:ILE:HG13	1:B:1669:ARG:HD3	1.66	0.75
2:G:1159:ILE:HG12	2:G:1168:ASN:HA	1.67	0.75
2:G:1956:ARG:HB2	2:G:1957:PRO:CD	2.11	0.75
2:H:7:ARG:NH2	2:H:27:PHE:HB3	1.99	0.75
2:I:856:LYS:HG2	2:I:1054:LEU:HD12	1.68	0.75
1:A:1460:LYS:HE3	1:A:1773:VAL:O	1.86	0.75
2:G:960:LYS:HE2	2:G:960:LYS:HA	1.67	0.75
2:H:355:LYS:O	2:H:358:SER:HB3	1.85	0.75
2:H:84:LEU:HD13	2:H:133:ALA:HB2	1.69	0.75
1:B:328:LEU:O	1:B:331:ILE:HG22	1.86	0.75
2:H:1770:LEU:HD23	2:H:1776:PHE:CE2	2.22	0.75
2:H:259:THR:HG22	2:H:262:GLU:HG3	1.68	0.75
1:A:1498:GLU:HB2	1:A:1876:LEU:HD13	1.67	0.75
1:B:1460:LYS:HE2	1:B:1773:VAL:O	1.86	0.75
1:B:1208:VAL:HG13	1:B:1212:THR:HB	1.68	0.75
2:H:2015:THR:HG22	2:H:2017:LYS:H	1.51	0.75
2:H:579:VAL:HG23	2:H:1078:HIS:CD2	2.21	0.75
1:A:1303:GLY:HA2	1:A:1649:LYS:HE2	1.68	0.75
1:A:1310:GLU:OE1	1:A:1649:LYS:HE3	1.86	0.75
2:G:192:ALA:HA	2:G:215:ILE:HD12	1.67	0.75
2:G:572:ASN:HB3	2:G:576:LYS:H	1.52	0.75
2:H:455:ILE:HD11	2:H:469:ARG:CD	2.17	0.75
2:H:741:HIS:CB	2:H:853:PRO:HB2	2.16	0.75
2:I:960:LYS:HA	2:I:960:LYS:HE2	1.67	0.75
2:I:1129:ALA:HB2	2:I:1138:TRP:CZ3	2.22	0.75
2:I:1956:ARG:HB2	2:I:1957:PRO:CD	2.11	0.75
2:I:572:ASN:HB3	2:I:576:LYS:H	1.52	0.75
2:I:757:ILE:HG21	2:I:765:LEU:HD13	1.69	0.75
2:H:943:TRP:CH2	2:H:1016:PRO:HG3	2.22	0.74
2:H:1834:ARG:CG	2:H:1834:ARG:HH11	1.92	0.74
2:I:1159:ILE:HG12	2:I:1169:PRO:HD3	1.67	0.74
2:I:1284:VAL:HG13	2:I:1377:VAL:HG22	1.69	0.74
1:A:427:ASN:HD21	1:A:610:THR:H	1.33	0.74
1:B:1552:ASN:O	1:B:1556:THR:HG22	1.88	0.74
2:H:1678:MET:HE3	2:H:1707:LEU:HD22	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:TYR:CD2	2:G:2033:THR:OG1	2.40	0.74
2:H:1242:PHE:HE2	2:H:1244:PRO:HG3	1.51	0.74
2:H:1672:GLN:HA	2:H:1676:MET:HE1	1.68	0.74
2:I:943:TRP:CH2	2:I:1016:PRO:HG3	2.21	0.74
2:H:1784:MET:HG3	2:H:1785:GLU:N	2.03	0.74
1:A:1239:HIS:HD2	1:A:1241:SER:OG	1.69	0.74
1:A:335:HIS:CE1	1:B:335:HIS:CE1	2.74	0.74
1:B:335:HIS:HE1	1:C:335:HIS:CE1	2.06	0.74
1:C:749:ILE:HD13	1:C:806:VAL:HG12	1.70	0.74
2:H:1129:ALA:HB2	2:H:1138:TRP:CZ3	2.21	0.74
2:H:1672:GLN:HA	2:H:1676:MET:CE	2.18	0.74
2:H:1956:ARG:CB	2:H:1957:PRO:HD3	2.11	0.74
2:I:105:ALA:HB1	2:I:119:THR:HG23	1.67	0.74
2:I:131:ILE:HB	2:I:182:VAL:HG11	1.69	0.74
1:A:1749:THR:CB	1:A:1873:HIS:C	2.56	0.74
1:C:1552:ASN:O	1:C:1556:THR:HG22	1.88	0.74
2:G:1310:ASP:OD2	2:G:1602:SER:HB3	1.88	0.74
2:I:2035:SER:HB3	2:I:2038:ILE:HG13	1.69	0.74
2:I:835:THR:HG21	2:I:855:HIS:CD2	2.23	0.74
1:B:1551:LYS:HD2	1:B:1617:ILE:HG21	1.70	0.74
2:G:705:LEU:HD12	2:G:716:VAL:HG13	1.70	0.74
2:I:741:HIS:CE1	2:I:845:THR:HG21	2.22	0.74
1:A:1456:GLU:OE1	1:A:1775:LEU:HD23	1.87	0.74
2:G:757:ILE:HG21	2:G:765:LEU:HD13	1.67	0.74
1:B:18:LEU:HD21	2:H:1815:LEU:HD12	1.70	0.74
2:I:1889:VAL:HG13	2:I:1977:HIS:HB2	1.69	0.74
1:A:44:VAL:CG1	1:A:78:ILE:HG12	2.18	0.73
1:B:833:PHE:HA	1:B:937:LYS:HD2	1.69	0.73
2:H:1194:VAL:HG22	2:H:1212:LYS:HB3	1.70	0.73
2:H:7:ARG:NH1	2:H:24:THR:HG23	2.03	0.73
2:H:1004:LEU:HD21	2:H:1020:VAL:HG23	1.70	0.73
1:C:36:LEU:HD22	1:C:61:LEU:HD21	1.68	0.73
2:G:1159:ILE:HG12	2:G:1169:PRO:HD3	1.71	0.73
1:A:982:ILE:HD11	2:G:965:SER:HB2	1.69	0.73
2:H:705:LEU:HD12	2:H:716:VAL:HG13	1.70	0.73
1:C:888:ILE:HD11	1:C:930:LEU:HD21	1.71	0.73
2:H:1680:LEU:HD13	2:H:1687:ALA:HB2	1.71	0.73
2:I:1784:MET:HG3	2:I:1785:GLU:N	2.02	0.73
2:G:105:ALA:HB1	2:G:119:THR:HG23	1.70	0.73
2:G:7:ARG:NH1	2:G:24:THR:HG23	2.03	0.73
2:I:455:ILE:HD11	2:I:469:ARG:CD	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:749:ILE:HD13	1:B:806:VAL:HG12	1.70	0.73
1:C:1431:GLU:CG	1:C:1433:HIS:CE1	2.72	0.73
2:G:259:THR:HG22	2:G:262:GLU:HG3	1.68	0.73
2:G:777:THR:HG22	2:G:1081:HIS:NE2	2.03	0.73
2:I:7:ARG:NH1	2:I:24:THR:HG23	2.03	0.73
1:A:1551:LYS:HD2	1:A:1617:ILE:HG21	1.70	0.73
2:G:194:THR:HG23	2:G:300:ILE:HD11	1.70	0.73
2:H:1422:THR:HG21	2:H:1474:PHE:HB2	1.70	0.73
2:H:1300:PHE:CA	2:H:1556:VAL:HG11	2.19	0.73
2:H:345:THR:HG22	2:H:347:GLU:H	1.51	0.73
1:C:260:ARG:HH12	1:C:300:VAL:HG21	1.52	0.73
2:G:562:LEU:HG	2:G:793:PRO:HG2	1.71	0.73
2:G:652:ILE:H	2:G:658:MET:CE	2.01	0.73
2:H:1331:TRP:CZ2	2:H:1335:ILE:HG13	2.23	0.73
2:H:1355:ASN:HA	2:H:1407:THR:O	1.88	0.73
2:H:194:THR:HG23	2:H:300:ILE:HD11	1.71	0.73
2:H:146:PHE:HA	2:H:149:VAL:CG1	2.18	0.73
2:H:1300:PHE:HA	2:H:1556:VAL:HG11	1.70	0.73
2:H:7:ARG:HH21	2:H:27:PHE:CB	2.01	0.73
1:B:44:VAL:CG1	1:B:78:ILE:HG12	2.18	0.72
2:H:1284:VAL:HG13	2:H:1377:VAL:HG22	1.71	0.72
2:H:579:VAL:HG23	2:H:1078:HIS:NE2	2.03	0.72
2:I:707:PRO:HG3	2:I:716:VAL:CG2	2.18	0.72
2:G:762:ASN:N	2:G:762:ASN:HD22	1.82	0.72
2:I:579:VAL:HG23	2:I:1078:HIS:CD2	2.24	0.72
1:A:1045:PHE:HB3	1:A:1049:GLY:HA3	1.71	0.72
1:A:655:LEU:HD22	1:A:916:LEU:HD11	1.71	0.72
1:C:1208:VAL:HG13	1:C:1212:THR:HB	1.71	0.72
1:C:1551:LYS:HD2	1:C:1617:ILE:HG21	1.70	0.72
2:G:1889:VAL:HG13	2:G:1977:HIS:HB2	1.72	0.72
2:H:128:THR:HA	2:H:182:VAL:CG2	2.16	0.72
2:H:634:ILE:HD11	2:H:649:ILE:HD11	1.71	0.72
2:I:1672:GLN:HA	2:I:1676:MET:HE1	1.70	0.72
1:A:1722:VAL:CG1	1:A:1731:LEU:HB3	2.19	0.72
1:C:473:GLY:O	1:C:477:ILE:HG13	1.88	0.72
2:I:191:SER:HA	2:I:194:THR:HG22	1.71	0.72
2:I:194:THR:HG23	2:I:300:ILE:HD11	1.70	0.72
1:C:427:ASN:HD21	1:C:610:THR:H	1.38	0.72
1:A:24:SER:CB	2:G:2014:LEU:HD12	2.19	0.72
2:H:109:LEU:HD11	2:H:116:LEU:HD23	1.72	0.72
1:A:1208:VAL:HG13	1:A:1212:THR:HB	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1668:ASP:OD2	1:B:1805:VAL:HB	1.90	0.72
1:B:254:TRP:CZ3	1:B:302:LEU:HD13	2.24	0.72
2:I:1672:GLN:HA	2:I:1676:MET:CE	2.20	0.72
2:I:777:THR:HG22	2:I:1081:HIS:NE2	2.04	0.72
2:I:7:ARG:HH21	2:I:27:PHE:CB	1.99	0.72
1:B:24:SER:HB3	2:H:2014:LEU:HD12	1.69	0.72
2:G:584:SER:HB3	2:G:591:PRO:HG3	1.70	0.72
2:H:455:ILE:CD1	2:H:469:ARG:HD3	2.20	0.72
2:H:455:ILE:CG1	2:H:469:ARG:HD3	2.20	0.72
2:I:259:THR:HG22	2:I:262:GLU:CG	2.20	0.72
1:B:473:GLY:O	1:B:477:ILE:HG13	1.89	0.72
2:G:1680:LEU:HD13	2:G:1687:ALA:HB2	1.71	0.72
2:G:598:THR:OG1	2:G:599:PRO:HD3	1.89	0.72
2:H:572:ASN:HB3	2:H:576:LYS:H	1.54	0.72
2:G:131:ILE:CD1	2:G:182:VAL:HB	2.09	0.72
2:H:777:THR:HG22	2:H:1081:HIS:NE2	2.04	0.72
2:G:751:LEU:HD23	2:G:791:TYR:CE2	2.25	0.72
2:G:741:HIS:CE1	2:G:845:THR:HG21	2.24	0.72
2:G:741:HIS:CE1	2:G:855:HIS:NE2	2.58	0.72
2:I:1086:LEU:HG	2:I:1092:ASP:HA	1.72	0.72
2:I:84:LEU:HD13	2:I:133:ALA:HB2	1.71	0.72
1:B:1232:TYR:CZ	1:B:1701:LYS:HD2	2.26	0.71
2:G:1567:ARG:HG3	2:G:1567:ARG:NH1	2.02	0.71
2:G:161:GLY:H	2:G:505:GLY:HA3	1.54	0.71
2:I:2036:GLU:HB2	2:I:2037:PRO:HD3	1.72	0.71
1:A:1501:LEU:CD1	1:A:1775:LEU:CD2	2.62	0.71
1:B:888:ILE:HD12	1:B:939:PHE:HE2	1.55	0.71
1:C:59:ARG:NH1	2:I:1896:GLN:NE2	2.38	0.71
2:H:652:ILE:H	2:H:658:MET:CE	2.03	0.71
2:H:741:HIS:NE2	2:H:855:HIS:CE1	2.58	0.71
2:I:1673:GLU:H	2:I:1676:MET:HE3	1.55	0.71
1:B:1030:TRP:NE1	1:B:1580:LEU:CD2	2.54	0.71
2:G:1638:ILE:HD12	2:G:1657:ILE:HD12	1.71	0.71
2:G:762:ASN:H	2:G:762:ASN:ND2	1.85	0.71
2:H:1227:ARG:HD2	2:H:1565:VAL:HG11	1.71	0.71
2:I:1670:GLY:H	2:I:1672:GLN:HE21	1.38	0.71
1:A:733:ILE:HD13	1:A:761:LEU:HD11	1.71	0.71
1:A:982:ILE:HD11	2:G:965:SER:CB	2.21	0.71
2:G:2036:GLU:HB2	2:G:2037:PRO:HD3	1.73	0.71
2:G:50:ALA:HB3	2:G:53:GLU:HG3	1.72	0.71
1:A:983:GLN:NE2	2:G:962:LYS:HD2	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1819:ALA:HA	2:H:2005:ARG:HH11	1.55	0.71
1:B:2:LYS:HD2	2:H:2050:GLN:HB3	1.72	0.71
2:I:1331:TRP:CZ2	2:I:1335:ILE:HG13	2.25	0.71
2:I:455:ILE:CG1	2:I:469:ARG:HD3	2.21	0.71
1:C:733:ILE:HD13	1:C:761:LEU:HD11	1.72	0.71
2:H:1054:LEU:HB2	4:H:3051:FMN:C7M	2.21	0.71
2:I:732:TRP:CG	2:I:750:MET:CE	2.73	0.71
1:A:1208:VAL:CG1	1:A:1212:THR:HB	2.21	0.71
1:C:1219:VAL:HG22	1:C:1384:ILE:HD12	1.73	0.71
2:G:1199:GLU:OE2	2:G:1567:ARG:NH1	2.23	0.71
2:G:1672:GLN:HA	2:G:1676:MET:HE1	1.72	0.71
2:G:1917:ILE:HG23	2:G:1922:ILE:HB	1.72	0.71
2:G:238:CYS:HB2	2:G:239:PRO:HD3	1.71	0.71
2:G:949:ASP:HB3	2:G:1006:MET:HE2	1.71	0.71
2:H:238:CYS:HB2	2:H:239:PRO:HD3	1.71	0.71
2:I:1058:VAL:O	2:I:1061:GLN:HG2	1.90	0.71
2:G:109:LEU:HD11	2:G:116:LEU:HD23	1.71	0.71
1:B:18:LEU:HD21	2:H:1815:LEU:CD1	2.20	0.71
1:B:655:LEU:HD22	1:B:916:LEU:HD11	1.72	0.71
1:C:1498:GLU:CB	1:C:1876:LEU:HD13	2.21	0.71
2:G:707:PRO:CG	2:G:716:VAL:HG21	2.20	0.71
2:H:964:LEU:HD23	2:H:964:LEU:H	1.56	0.71
1:C:1498:GLU:HG3	1:C:1876:LEU:CB	2.09	0.70
1:C:459:ASP:HB3	1:C:462:LYS:HG3	1.73	0.70
2:I:1242:PHE:CE2	2:I:1244:PRO:HG3	2.26	0.70
1:C:59:ARG:NH1	2:I:1896:GLN:HE22	1.88	0.70
2:I:751:LEU:HD23	2:I:791:TYR:CE2	2.25	0.70
1:A:1119:LYS:HE2	1:A:1341:PHE:CD1	2.27	0.70
1:B:1721:ARG:NH1	1:B:1721:ARG:HG2	2.00	0.70
2:H:562:LEU:O	2:H:566:HIS:HB2	1.90	0.70
2:H:707:PRO:CG	2:H:716:VAL:HG21	2.21	0.70
1:A:1:MET:CE	1:A:6:GLU:HA	2.21	0.70
1:B:1460:LYS:HZ1	1:B:1774:GLU:CD	1.92	0.70
1:C:631:PRO:HB2	1:C:634:THR:OG1	1.91	0.70
2:G:1672:GLN:HA	2:G:1676:MET:CE	2.21	0.70
1:C:12:ILE:HD11	2:I:2041:ILE:CD1	2.21	0.70
2:I:964:LEU:H	2:I:964:LEU:HD23	1.56	0.70
1:C:881:ASN:HA	1:C:944:ARG:NH2	2.06	0.70
2:G:650:ASN:HD21	4:G:3051:FMN:HN3	1.40	0.70
2:I:1680:LEU:HD13	2:I:1687:ALA:HB2	1.72	0.70
2:I:732:TRP:CG	2:I:750:MET:HE1	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1208:VAL:CG1	1:B:1212:THR:HB	2.20	0.70
1:B:1501:LEU:HD11	1:B:1775:LEU:CD2	2.22	0.70
2:G:579:VAL:HG23	2:G:1078:HIS:CD2	2.27	0.70
2:G:123:ILE:HD11	2:G:533:LEU:CD2	2.21	0.70
1:B:90:TYR:HE2	2:H:1659:GLN:OE1	1.73	0.70
2:I:455:ILE:CD1	2:I:469:ARG:HD3	2.20	0.70
2:I:748:THR:HB	2:I:749:PRO:HD3	1.74	0.70
1:B:459:ASP:HB3	1:B:462:LYS:HG3	1.73	0.70
2:G:1956:ARG:CB	2:G:1957:PRO:HD3	2.10	0.70
2:G:707:PRO:HG3	2:G:716:VAL:CG2	2.22	0.70
2:G:732:TRP:CG	2:G:750:MET:HE1	2.27	0.70
2:I:146:PHE:HA	2:I:149:VAL:CG1	2.20	0.70
1:A:1312:VAL:HG22	1:A:1329:VAL:HG11	1.73	0.70
1:B:1:MET:CE	1:B:6:GLU:HA	2.21	0.70
2:G:1242:PHE:HE2	2:G:1244:PRO:HG3	1.55	0.70
1:B:968:VAL:HG23	2:H:1515:PRO:HG3	1.74	0.70
1:C:260:ARG:NH1	1:C:300:VAL:HG21	2.06	0.70
2:G:1355:ASN:HA	2:G:1407:THR:O	1.92	0.70
2:H:234:ILE:HG13	2:H:235:PRO:HD3	1.73	0.70
2:I:1264:GLU:HA	2:I:1275:PHE:CE1	2.27	0.70
1:C:655:LEU:HD22	1:C:916:LEU:HD11	1.74	0.70
2:G:455:ILE:HD11	2:G:469:ARG:CD	2.22	0.70
2:H:741:HIS:CE1	2:H:845:THR:HG21	2.26	0.70
1:A:12:ILE:HA	1:A:15:THR:CG2	2.21	0.70
2:G:1331:TRP:CZ2	2:G:1335:ILE:HG13	2.26	0.70
2:G:1673:GLU:H	2:G:1676:MET:HE3	1.57	0.70
2:H:2036:GLU:HB2	2:H:2037:PRO:HD3	1.72	0.70
1:A:1232:TYR:CZ	1:A:1701:LYS:HD2	2.27	0.69
2:G:7:ARG:HH21	2:G:27:PHE:CB	2.01	0.69
2:H:1673:GLU:H	2:H:1676:MET:HE3	1.57	0.69
2:H:499:THR:CB	2:H:500:HIS:HD2	1.99	0.69
2:H:835:THR:HB	2:H:845:THR:HG23	1.73	0.69
2:I:926:LEU:HD13	2:I:947:THR:HG22	1.73	0.69
1:B:427:ASN:HD21	1:B:610:THR:H	1.40	0.69
2:G:1194:VAL:HG22	2:G:1212:LYS:HB3	1.74	0.69
2:G:1422:THR:HG21	2:G:1474:PHE:HB2	1.72	0.69
2:H:1670:GLY:H	2:H:1672:GLN:HE21	1.40	0.69
2:I:1862:VAL:HG11	2:I:1866:PHE:CD1	2.26	0.69
1:A:749:ILE:HD13	1:A:806:VAL:HG12	1.72	0.69
1:C:12:ILE:HA	1:C:15:THR:CG2	2.22	0.69
1:C:852:ARG:CG	1:C:852:ARG:HH11	2.00	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1054:LEU:HB2	4:G:3051:FMN:C7M	2.22	0.69
2:H:1195:VAL:CG1	2:H:1211:LEU:HB3	2.23	0.69
2:H:1381:VAL:HG13	2:H:1390:VAL:HG22	1.74	0.69
2:H:567:PRO:HG3	2:H:781:LEU:CD1	2.22	0.69
2:I:652:ILE:H	2:I:658:MET:CE	2.04	0.69
1:A:254:TRP:CZ3	1:A:292:GLN:HG3	2.26	0.69
1:B:254:TRP:CZ3	1:B:292:GLN:HG3	2.27	0.69
2:I:1770:LEU:HD23	2:I:1776:PHE:HE2	1.55	0.69
2:G:84:LEU:HD13	2:G:133:ALA:HB2	1.75	0.69
2:G:964:LEU:CD2	2:G:964:LEU:H	2.05	0.69
2:I:1678:MET:HE3	2:I:1707:LEU:HD22	1.75	0.69
1:C:1208:VAL:CG1	1:C:1212:THR:HB	2.23	0.69
2:G:856:LYS:HG2	2:G:1054:LEU:HD12	1.73	0.69
2:H:1917:ILE:HG23	2:H:1922:ILE:HB	1.74	0.69
2:H:1889:VAL:HG13	2:H:1977:HIS:CB	2.22	0.69
1:A:1721:ARG:NH1	1:A:1721:ARG:HG2	1.97	0.69
1:A:749:ILE:HD11	1:A:805:CYS:HB3	1.75	0.69
1:B:1376:PHE:HB3	1:B:1544:THR:HG22	1.74	0.69
2:G:191:SER:HA	2:G:194:THR:HG22	1.74	0.69
2:I:109:LEU:HD11	2:I:116:LEU:HD23	1.73	0.69
2:I:1194:VAL:HG22	2:I:1212:LYS:HB3	1.75	0.69
1:A:479:ASN:O	1:A:483:VAL:HG23	1.91	0.69
2:G:1172:LYS:HE3	2:G:1574:ASN:OD1	1.92	0.69
2:G:1670:GLY:H	2:G:1672:GLN:HE21	1.39	0.69
2:H:1889:VAL:HG13	2:H:1977:HIS:HB2	1.72	0.69
2:H:2022:THR:HG23	2:H:2025:TYR:H	1.58	0.69
1:A:1693:ILE:CD1	2:G:998:GLN:HB2	2.23	0.69
2:H:663:ILE:HB	2:H:664:PRO:HD3	1.75	0.69
2:H:751:LEU:HD23	2:H:791:TYR:CE2	2.27	0.69
2:I:652:ILE:N	2:I:658:MET:HE3	2.08	0.69
1:A:631:PRO:HB2	1:A:634:THR:OG1	1.92	0.69
1:C:1838:GLU:OE1	1:C:1852:HIS:HE1	1.76	0.69
2:G:1264:GLU:HA	2:G:1275:PHE:CE1	2.28	0.69
2:G:1496:LYS:HE2	2:G:1693:ARG:HH21	1.57	0.69
2:H:1172:LYS:CE	2:H:1574:ASN:OD1	2.40	0.69
2:H:1739:GLU:CB	2:H:1987:PRO:HB3	2.21	0.69
2:H:305:PHE:CE1	2:H:442:ASP:HB3	2.28	0.69
2:I:1739:GLU:CB	2:I:1987:PRO:HB3	2.20	0.69
2:I:663:ILE:HB	2:I:664:PRO:HD3	1.75	0.69
2:I:768:GLY:HA3	2:I:800:LEU:HD21	1.74	0.69
1:A:1376:PHE:HB3	1:A:1544:THR:HG22	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:PRO:HD2	1:A:260:ARG:HB2	1.75	0.69
1:C:1219:VAL:HA	1:C:1384:ILE:CD1	2.20	0.69
1:C:1431:GLU:OE2	1:C:1433:HIS:HE1	1.76	0.69
1:C:1021:VAL:HG11	1:C:1597:LEU:HD11	1.74	0.69
2:G:663:ILE:HB	2:G:664:PRO:HD3	1.74	0.69
2:H:54:PRO:HG3	2:H:63:LYS:HG3	1.72	0.69
2:H:652:ILE:N	2:H:658:MET:HE3	2.05	0.69
2:I:1917:ILE:HG23	2:I:1922:ILE:HB	1.74	0.69
2:I:499:THR:CB	2:I:500:HIS:HD2	1.95	0.69
1:A:1838:GLU:OE1	1:A:1852:HIS:HE1	1.75	0.68
2:H:259:THR:HG22	2:H:262:GLU:CG	2.22	0.68
2:I:234:ILE:HG13	2:I:235:PRO:HD3	1.73	0.68
1:A:1203:ASP:HB3	1:B:179:LYS:HZ3	1.58	0.68
2:G:1058:VAL:O	2:G:1061:GLN:HG2	1.93	0.68
1:A:1431:GLU:HG3	1:A:1433:HIS:CE1	2.28	0.68
1:C:1045:PHE:HB3	1:C:1049:GLY:HA3	1.74	0.68
2:G:2035:SER:HB3	2:G:2038:ILE:HG13	1.74	0.68
2:H:1101:GLU:HB3	2:H:1147:ILE:HG22	1.76	0.68
2:H:161:GLY:H	2:H:505:GLY:HA3	1.59	0.68
1:C:1376:PHE:HB3	1:C:1544:THR:HG22	1.74	0.68
2:G:1834:ARG:HG2	2:G:1834:ARG:NH1	1.93	0.68
2:I:1227:ARG:NH1	2:I:1227:ARG:HG3	2.00	0.68
2:I:598:THR:CG2	2:I:622:GLY:HA3	2.23	0.68
1:A:888:ILE:HD11	1:A:930:LEU:HD21	1.75	0.68
1:B:1312:VAL:HG22	1:B:1329:VAL:HG11	1.73	0.68
1:B:400:ARG:HG2	1:B:400:ARG:NH1	2.00	0.68
2:I:187:LEU:HA	2:I:190:PHE:HB3	1.76	0.68
2:I:161:GLY:H	2:I:505:GLY:HA3	1.56	0.68
1:C:985:ARG:NH1	2:I:953:ARG:CZ	2.57	0.68
1:C:1014:ASP:H	1:C:1510:ASN:ND2	1.84	0.68
2:G:1784:MET:HG3	2:G:1785:GLU:N	2.07	0.68
2:G:259:THR:HG22	2:G:262:GLU:CG	2.22	0.68
2:G:54:PRO:HG3	2:G:63:LYS:HG3	1.76	0.68
2:G:732:TRP:CG	2:G:750:MET:CE	2.76	0.68
1:B:90:TYR:CE2	2:H:1659:GLN:OE1	2.47	0.68
2:I:1638:ILE:HD12	2:I:1657:ILE:HD12	1.75	0.68
2:I:594:VAL:HG21	2:I:610:THR:HG21	1.75	0.68
1:A:1474:ALA:HA	1:A:1478:PRO:CG	2.24	0.68
1:C:987:ASN:HD22	2:I:957:ARG:HD2	1.58	0.68
2:H:648:GLY:HA3	2:H:678:PHE:CE2	2.29	0.68
1:A:504:ASP:HB3	1:A:508:ASN:H	1.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:THR:HG22	1:B:331:ILE:HD11	1.76	0.68
1:C:1460:LYS:HE3	1:C:1774:GLU:OE1	1.92	0.68
2:G:455:ILE:CG1	2:G:469:ARG:HD3	2.23	0.68
2:H:187:LEU:HA	2:H:190:PHE:HB3	1.75	0.68
2:I:305:PHE:CE1	2:I:442:ASP:HB3	2.28	0.68
1:B:1219:VAL:HG22	1:B:1384:ILE:HD12	1.75	0.68
1:C:1310:GLU:OE1	1:C:1649:LYS:HE3	1.93	0.68
2:G:455:ILE:CD1	2:G:469:ARG:HD3	2.24	0.68
2:H:641:ILE:HG12	2:H:645:SER:HB2	1.76	0.68
1:A:1056:ILE:HD13	1:A:1193:TRP:HD1	1.59	0.68
1:B:1838:GLU:OE1	1:B:1852:HIS:HE1	1.76	0.68
2:G:1176:PRO:O	2:G:1177:SER:HB3	1.93	0.68
2:H:1058:VAL:O	2:H:1061:GLN:HG2	1.94	0.68
1:A:1303:GLY:H	1:A:1307:THR:HG22	1.59	0.67
1:A:1594:ASN:O	1:A:1598:GLN:HG3	1.94	0.67
1:B:183:GLN:HE21	1:B:202:GLU:HG2	1.59	0.67
1:C:1303:GLY:H	1:C:1307:THR:HG22	1.60	0.67
1:C:254:TRP:CZ3	1:C:292:GLN:HG3	2.29	0.67
1:C:44:VAL:CG1	1:C:78:ILE:HG12	2.24	0.67
2:G:1475:LYS:CG	2:G:1481:SER:HB2	2.24	0.67
2:G:187:LEU:HA	2:G:190:PHE:HB3	1.74	0.67
2:H:1054:LEU:HB2	4:H:3051:FMN:HM72	1.76	0.67
2:H:707:PRO:HG3	2:H:716:VAL:CG2	2.24	0.67
2:H:191:SER:HA	2:H:194:THR:HG22	1.77	0.67
1:C:1232:TYR:CZ	1:C:1701:LYS:HD2	2.29	0.67
1:C:1455:ARG:HH11	1:C:1458:GLN:HE21	1.42	0.67
2:G:1889:VAL:HG13	2:G:1977:HIS:CB	2.24	0.67
2:G:163:GLN:HG2	2:G:423:VAL:HG12	1.77	0.67
2:H:50:ALA:HB3	2:H:53:GLU:HG3	1.76	0.67
2:I:579:VAL:HG23	2:I:1078:HIS:NE2	2.10	0.67
1:C:504:ASP:HB3	1:C:508:ASN:H	1.60	0.67
2:G:1129:ALA:HB2	2:G:1138:TRP:CZ3	2.30	0.67
2:I:598:THR:OG1	2:I:599:PRO:HD3	1.94	0.67
1:A:459:ASP:HB3	1:A:462:LYS:HG3	1.76	0.67
1:B:1303:GLY:H	1:B:1307:THR:HG22	1.59	0.67
1:C:1056:ILE:HD13	1:C:1193:TRP:HD1	1.60	0.67
1:C:1523:ARG:CG	1:C:1523:ARG:NH1	2.57	0.67
1:C:409:ALA:HB2	1:C:442:ARG:HD2	1.76	0.67
2:G:768:GLY:HA3	2:G:800:LEU:HD21	1.76	0.67
2:G:910:GLN:HE21	2:G:912:ARG:HH21	1.42	0.67
2:H:902:PRO:HG2	2:H:929:LEU:HD21	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:904:PHE:HB2	2:I:1017:PHE:CD1	2.28	0.67
2:I:910:GLN:HE21	2:I:912:ARG:HH21	1.40	0.67
1:A:1360:ARG:HH11	1:A:1364:GLU:HG2	1.60	0.67
1:B:1039:MET:O	1:B:1609:ARG:NH2	2.27	0.67
2:G:1741:ILE:HG12	2:G:1746:LEU:HD13	1.77	0.67
1:B:1310:GLU:OE1	1:B:1649:LYS:HE3	1.94	0.67
2:I:1675:GLY:O	2:I:1678:MET:HB2	1.94	0.67
1:A:328:LEU:O	1:A:328:LEU:HD22	1.94	0.67
1:C:746:GLU:O	1:C:750:GLU:HG3	1.95	0.67
2:H:545:GLN:HE21	2:H:545:GLN:H	1.41	0.67
2:H:594:VAL:HG21	2:H:610:THR:HG21	1.77	0.67
2:H:768:GLY:HA3	2:H:800:LEU:HD21	1.77	0.67
2:I:54:PRO:HG3	2:I:63:LYS:HG3	1.75	0.67
2:G:1004:LEU:HD21	2:G:1020:VAL:HG23	1.77	0.67
2:G:1676:MET:HE1	2:G:1781:LEU:HD21	1.76	0.67
2:G:1770:LEU:HD23	2:G:1776:PHE:HE2	1.58	0.67
2:H:1086:LEU:HG	2:H:1092:ASP:HA	1.77	0.67
2:H:1242:PHE:CE2	2:H:1244:PRO:HG3	2.30	0.67
2:H:1264:GLU:HA	2:H:1275:PHE:CE1	2.29	0.67
2:H:315:PRO:O	2:I:1314:ARG:NH2	2.28	0.67
2:I:703:LEU:HD21	2:I:705:LEU:HD21	1.76	0.67
2:G:353:VAL:HG23	2:G:357:ASN:ND2	2.10	0.67
2:H:1256:GLU:O	2:H:1257:ASP:HB2	1.93	0.67
2:I:1889:VAL:HG13	2:I:1977:HIS:CB	2.24	0.67
2:I:949:ASP:HB3	2:I:1006:MET:HE2	1.77	0.67
1:A:1030:TRP:NE1	1:A:1580:LEU:CD2	2.57	0.66
1:C:257:PRO:HD2	1:C:260:ARG:HB2	1.76	0.66
1:C:888:ILE:HD12	1:C:939:PHE:HE2	1.60	0.66
2:G:670:ARG:HD3	2:G:699:GLY:O	1.95	0.66
2:H:1159:ILE:CG1	2:H:1169:PRO:HD3	2.24	0.66
2:H:1862:VAL:HG11	2:H:1866:PHE:CD1	2.30	0.66
2:I:1227:ARG:HD2	2:I:1565:VAL:HG11	1.77	0.66
2:I:163:GLN:HG2	2:I:423:VAL:HG12	1.76	0.66
2:I:50:ALA:HB3	2:I:53:GLU:HG3	1.76	0.66
1:A:1662:TYR:O	1:A:1665:ILE:HG22	1.95	0.66
1:A:473:GLY:O	1:A:477:ILE:HG13	1.95	0.66
1:B:328:LEU:O	1:B:328:LEU:HD22	1.95	0.66
1:B:335:HIS:CE1	1:C:335:HIS:CE1	2.82	0.66
1:C:1430:ARG:O	1:C:1430:ARG:HG2	1.94	0.66
1:C:294:TYR:CE1	1:C:298:VAL:HG21	2.29	0.66
1:C:328:LEU:HD22	1:C:328:LEU:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:670:ARG:HD3	2:H:699:GLY:O	1.95	0.66
2:I:1920:GLN:HG2	2:I:1922:ILE:HD11	1.75	0.66
2:I:1739:GLU:O	2:I:1987:PRO:HG3	1.95	0.66
1:A:183:GLN:HE21	1:A:202:GLU:HG2	1.59	0.66
1:B:1045:PHE:HB3	1:B:1049:GLY:HA3	1.76	0.66
1:B:27:ARG:HB2	2:H:2016:ALA:HB2	1.76	0.66
1:C:1030:TRP:NE1	1:C:1580:LEU:CD2	2.58	0.66
1:C:460:GLU:HG2	1:C:470:LYS:HD3	1.77	0.66
1:C:507:GLY:N	1:C:954:ARG:HG2	2.11	0.66
2:H:910:GLN:HE21	2:H:912:ARG:HH21	1.43	0.66
2:I:762:ASN:ND2	2:I:762:ASN:H	1.88	0.66
2:I:750:MET:HG3	2:I:796:PHE:HZ	1.60	0.66
1:A:864:VAL:HG22	1:A:921:PRO:HB3	1.78	0.66
1:B:12:ILE:HA	1:B:15:THR:CG2	2.25	0.66
2:I:705:LEU:HD12	2:I:716:VAL:HG13	1.75	0.66
1:B:504:ASP:HB3	1:B:508:ASN:H	1.60	0.66
1:C:934:PRO:O	1:C:935:GLU:C	2.34	0.66
2:G:1300:PHE:HA	2:G:1556:VAL:HG11	1.77	0.66
2:G:1862:VAL:HG11	2:G:1866:PHE:CD1	2.30	0.66
2:G:560:ASN:O	2:G:561:TRP:C	2.34	0.66
2:G:61:VAL:O	2:G:65:LEU:HB2	1.96	0.66
2:H:826:GLY:HA3	2:H:1061:GLN:HB3	1.75	0.66
2:H:835:THR:HG21	2:H:855:HIS:HD2	1.59	0.66
2:H:741:HIS:CE1	2:H:855:HIS:CE1	2.84	0.66
1:A:988:ILE:HD13	1:A:1048:GLU:HB3	1.76	0.66
1:B:1749:THR:CB	1:B:1874:ASP:N	2.58	0.66
2:G:579:VAL:HG23	2:G:1078:HIS:NE2	2.10	0.66
2:H:1173:VAL:HG21	2:H:1221:MET:HE1	1.77	0.66
2:H:1986:LYS:N	2:H:1987:PRO:HD2	2.11	0.66
1:A:836:ASP:HB3	1:A:839:TYR:HB3	1.76	0.66
1:B:1540:SER:HA	1:B:1575:VAL:HG22	1.78	0.66
1:B:497:THR:OG1	1:B:513:GLU:HG2	1.95	0.66
1:C:1431:GLU:OE2	1:C:1433:HIS:CE1	2.48	0.66
2:G:1920:GLN:HG2	2:G:1922:ILE:HD11	1.78	0.66
2:H:904:PHE:HB2	2:H:1017:PHE:CD1	2.30	0.66
2:H:1741:ILE:HG12	2:H:1746:LEU:HD13	1.76	0.66
2:H:61:VAL:O	2:H:65:LEU:HB2	1.96	0.66
1:B:733:ILE:HD13	1:B:761:LEU:HD11	1.78	0.66
2:G:1457:PHE:CZ	2:G:1501:ILE:HD11	2.30	0.66
2:G:1808:SER:H	2:G:2013:ASN:ND2	1.93	0.66
2:H:131:ILE:HG21	2:H:182:VAL:CG1	2.18	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1173:VAL:HG21	2:I:1221:MET:HE1	1.77	0.66
2:I:1195:VAL:CG1	2:I:1211:LEU:HB3	2.25	0.66
1:A:254:TRP:CH2	1:A:292:GLN:HG3	2.31	0.66
1:B:1219:VAL:HA	1:B:1384:ILE:CD1	2.24	0.66
1:C:295:ALA:HB2	1:C:302:LEU:HD11	1.77	0.66
2:H:1770:LEU:HD23	2:H:1776:PHE:HE2	1.59	0.66
2:H:560:ASN:O	2:H:561:TRP:C	2.33	0.66
2:I:1381:VAL:HG13	2:I:1390:VAL:HG22	1.78	0.66
2:I:1808:SER:H	2:I:2013:ASN:ND2	1.94	0.66
1:B:501:THR:N	1:B:886:GLU:OE1	2.21	0.66
1:C:1360:ARG:HH11	1:C:1364:GLU:HG2	1.60	0.66
2:G:843:ILE:HD11	2:G:1055:HIS:HB3	1.78	0.66
2:G:1352:HIS:CD2	2:G:1410:PHE:CE2	2.84	0.66
2:G:33:LEU:HD11	2:G:80:PHE:HD2	1.61	0.66
2:G:904:PHE:HB2	2:G:1017:PHE:CD1	2.30	0.66
2:I:1819:ALA:HA	2:I:2005:ARG:HH11	1.61	0.66
1:A:497:THR:OG1	1:A:513:GLU:HG2	1.96	0.65
1:B:529:MET:CG	1:B:638:LEU:HG	2.26	0.65
1:C:1317:GLU:HA	1:C:1317:GLU:OE1	1.96	0.65
1:C:1:MET:CE	1:C:6:GLU:HA	2.25	0.65
2:G:1976:PHE:HA	2:G:1981:LEU:HD22	1.78	0.65
2:G:652:ILE:N	2:G:658:MET:HE3	2.11	0.65
2:H:2035:SER:HB3	2:H:2038:ILE:HG13	1.78	0.65
1:B:836:ASP:HB3	1:B:839:TYR:HB3	1.79	0.65
1:C:1312:VAL:HG22	1:C:1329:VAL:HG11	1.78	0.65
1:C:330:GLU:HA	1:C:333:LYS:HD2	1.79	0.65
1:C:836:ASP:HB3	1:C:839:TYR:HB3	1.77	0.65
2:G:1352:HIS:HE1	2:G:1583:MET:HE1	1.60	0.65
2:G:1986:LYS:N	2:G:1987:PRO:HD2	2.12	0.65
2:H:1325:PHE:CZ	2:H:1328:VAL:HG11	2.32	0.65
2:H:732:TRP:CG	2:H:750:MET:CE	2.79	0.65
2:I:1782:THR:HG22	2:I:1827:LEU:HD21	1.78	0.65
1:A:27:ARG:HB2	2:G:2016:ALA:HB2	1.77	0.65
1:A:934:PRO:O	1:A:935:GLU:C	2.35	0.65
2:G:597:MET:HA	4:G:3051:FMN:N5	2.10	0.65
1:A:27:ARG:HD2	1:A:30:GLU:OE2	1.97	0.65
1:A:331:ILE:HD11	1:C:332:THR:HG22	1.79	0.65
1:B:1317:GLU:OE1	1:B:1317:GLU:HA	1.96	0.65
1:B:460:GLU:HG2	1:B:470:LYS:HD3	1.78	0.65
1:C:32:GLN:HA	1:C:35:PHE:CE2	2.31	0.65
2:G:1086:LEU:HG	2:G:1092:ASP:HA	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:234:ILE:HG13	2:G:235:PRO:HD3	1.77	0.65
2:G:259:THR:HG23	2:G:262:GLU:H	1.62	0.65
2:G:902:PRO:HG2	2:G:929:LEU:HD21	1.79	0.65
2:H:1719:ILE:O	2:H:1761:SER:HB2	1.97	0.65
2:I:251:VAL:O	2:I:255:LEU:HB2	1.96	0.65
1:B:257:PRO:HD2	1:B:260:ARG:HB2	1.78	0.65
1:B:749:ILE:HD11	1:B:805:CYS:HB3	1.77	0.65
2:G:736:ARG:NH1	2:G:769:SER:O	2.29	0.65
1:A:1219:VAL:HG22	1:A:1384:ILE:HD12	1.77	0.65
1:A:331:ILE:CD1	1:C:332:THR:HG22	2.26	0.65
2:G:131:ILE:HG21	2:G:182:VAL:CG1	2.26	0.65
2:I:545:GLN:HE21	2:I:545:GLN:H	1.42	0.65
1:C:435:GLU:O	1:C:439:ILE:HG13	1.96	0.65
2:G:1381:VAL:HG13	2:G:1390:VAL:HG22	1.77	0.65
1:A:968:VAL:O	2:G:1512:HIS:HB2	1.97	0.65
2:G:1740:THR:HG22	2:G:1742:VAL:HG23	1.78	0.65
1:B:294:TYR:CE1	1:B:298:VAL:HG21	2.32	0.65
1:C:497:THR:OG1	1:C:513:GLU:HG2	1.97	0.65
2:G:826:GLY:HA3	2:G:1061:GLN:HB3	1.77	0.65
2:H:667:LYS:HB2	2:H:698:LEU:HD23	1.79	0.65
2:H:748:THR:HB	2:H:749:PRO:HD3	1.78	0.65
2:H:949:ASP:HB3	2:H:1006:MET:HE2	1.79	0.65
1:A:1219:VAL:HA	1:A:1384:ILE:CD1	2.23	0.65
1:A:340:ARG:HH12	1:A:344:GLN:CG	2.09	0.65
1:A:529:MET:CG	1:A:638:LEU:HG	2.27	0.65
2:G:1242:PHE:CE2	2:G:1244:PRO:HG3	2.31	0.65
2:G:1418:ASP:O	2:G:1420:GLU:N	2.30	0.65
2:G:259:THR:CG2	2:G:262:GLU:H	2.10	0.65
2:H:567:PRO:HG3	2:H:781:LEU:HD12	1.77	0.65
1:A:294:TYR:CE1	1:A:298:VAL:HG21	2.32	0.65
1:C:1292:ILE:CD1	1:C:1328:ILE:HD11	2.27	0.65
2:I:1176:PRO:O	2:I:1177:SER:HB3	1.95	0.65
1:C:11:HIS:ND1	2:I:1998:LYS:HA	2.12	0.65
1:B:254:TRP:CH2	1:B:292:GLN:HG3	2.32	0.64
2:G:1841:ALA:O	2:G:1842:VAL:HG23	1.97	0.64
2:H:1195:VAL:HG13	2:H:1211:LEU:HB3	1.80	0.64
2:H:741:HIS:HB3	2:H:853:PRO:HB2	1.77	0.64
2:I:1475:LYS:CG	2:I:1481:SER:HB2	2.27	0.64
2:I:490:TRP:HE1	2:I:516:THR:CG2	2.00	0.64
1:B:599:MET:HB2	1:B:624:LYS:CD	2.24	0.64
1:C:1721:ARG:CG	1:C:1721:ARG:NH1	2.56	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1906:ALA:O	2:G:1910:VAL:HG23	1.97	0.64
2:G:353:VAL:HG23	2:G:357:ASN:HD22	1.61	0.64
2:H:1859:PRO:O	2:H:1862:VAL:HG13	1.98	0.64
2:I:1355:ASN:HA	2:I:1407:THR:O	1.97	0.64
2:I:719:ILE:O	2:I:722:ALA:HB3	1.97	0.64
1:A:421:ILE:CG1	1:A:469:VAL:HG21	2.28	0.64
1:A:893:VAL:HG11	1:A:930:LEU:HD23	1.80	0.64
1:B:864:VAL:HG22	1:B:921:PRO:HB3	1.77	0.64
1:C:749:ILE:HD11	1:C:805:CYS:HB3	1.78	0.64
2:H:115:THR:HB	2:H:118:LYS:HB2	1.80	0.64
2:H:1635:ARG:HG2	2:H:1658:GLU:CD	2.18	0.64
1:C:604:ALA:HB3	1:C:612:GLU:HG2	1.80	0.64
2:G:138:ASP:O	2:G:139:LYS:HG3	1.97	0.64
2:H:1352:HIS:CD2	2:H:1410:PHE:CE2	2.85	0.64
2:H:1906:ALA:O	2:H:1910:VAL:HG23	1.98	0.64
2:H:259:THR:HG23	2:H:262:GLU:H	1.63	0.64
2:I:1265:MET:HE1	2:I:1562:PRO:HG2	1.78	0.64
1:A:1039:MET:O	1:A:1609:ARG:NH2	2.30	0.64
1:B:746:GLU:O	1:B:750:GLU:HG3	1.97	0.64
2:G:1359:MET:HE3	2:G:1404:MET:HB3	1.79	0.64
2:G:490:TRP:HE1	2:G:516:THR:CG2	1.99	0.64
2:H:1823:SER:OG	2:H:1825:GLU:HG2	1.96	0.64
2:H:259:THR:CG2	2:H:262:GLU:H	2.10	0.64
2:H:658:MET:HA	2:H:661:TRP:NE1	2.13	0.64
1:B:504:ASP:HB2	1:B:508:ASN:HB2	1.79	0.64
1:C:1540:SER:HA	1:C:1575:VAL:HG22	1.79	0.64
1:C:1594:ASN:O	1:C:1598:GLN:HG3	1.97	0.64
2:G:1195:VAL:CG1	2:G:1211:LEU:HB3	2.27	0.64
2:G:1103:PHE:O	2:G:1247:GLY:HA3	1.97	0.64
2:G:1840:VAL:O	2:G:1840:VAL:CG1	2.44	0.64
2:I:61:VAL:O	2:I:65:LEU:HB2	1.96	0.64
2:I:826:GLY:HA3	2:I:1061:GLN:HB3	1.78	0.64
1:A:1022:THR:HG22	1:A:1226:SER:HB2	1.80	0.64
1:A:504:ASP:HB2	1:A:508:ASN:HB2	1.78	0.64
1:A:746:GLU:O	1:A:750:GLU:HG3	1.97	0.64
1:C:1460:LYS:NZ	1:C:1774:GLU:CD	2.51	0.64
1:C:833:PHE:HA	1:C:937:LYS:HD2	1.78	0.64
2:G:499:THR:CB	2:G:500:HIS:HD2	1.97	0.64
2:H:1808:SER:H	2:H:2013:ASN:HD21	1.46	0.64
2:I:1457:PHE:CZ	2:I:1501:ILE:HD11	2.33	0.64
2:I:7:ARG:HE	2:I:27:PHE:HB2	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:GLU:HA	1:B:333:LYS:HD2	1.80	0.64
1:B:852:ARG:NH1	1:B:852:ARG:HG2	1.98	0.64
1:C:1194:ASN:HB3	1:C:1197:THR:CG2	2.27	0.64
2:G:1838:MET:O	2:G:1974:VAL:HG21	1.98	0.64
2:G:1739:GLU:CB	2:G:1987:PRO:HB3	2.23	0.64
2:H:1457:PHE:CZ	2:H:1501:ILE:HD11	2.32	0.64
2:H:232:LEU:O	2:H:232:LEU:HD23	1.98	0.64
2:I:1676:MET:HE1	2:I:1781:LEU:HD21	1.79	0.64
2:I:2022:THR:HG23	2:I:2025:TYR:H	1.63	0.64
2:I:648:GLY:HA3	2:I:678:PHE:CE2	2.32	0.64
1:A:1317:GLU:OE1	1:A:1317:GLU:HA	1.96	0.64
1:B:421:ILE:CG1	1:B:469:VAL:HG21	2.27	0.64
2:G:545:GLN:H	2:G:545:GLN:HE21	1.46	0.64
2:H:1205:LEU:O	2:H:1206:LYS:HG3	1.97	0.64
2:H:1676:MET:HE1	2:H:1781:LEU:HD21	1.80	0.64
2:I:892:ILE:HD11	2:I:903:TRP:NE1	2.12	0.64
2:I:964:LEU:CD2	2:I:964:LEU:H	2.11	0.64
1:B:1474:ALA:HA	1:B:1478:PRO:CG	2.27	0.64
2:G:305:PHE:CE1	2:G:442:ASP:HB3	2.32	0.64
2:H:163:GLN:HG2	2:H:423:VAL:HG12	1.79	0.64
2:H:703:LEU:HD21	2:H:705:LEU:HD21	1.79	0.64
2:I:670:ARG:HD3	2:I:699:GLY:O	1.98	0.64
1:A:1021:VAL:HG11	1:A:1597:LEU:HD11	1.79	0.63
1:A:152:HIS:HD2	1:A:163:LEU:HB2	1.61	0.63
1:C:1474:ALA:HA	1:C:1478:PRO:CG	2.27	0.63
1:C:934:PRO:O	1:C:936:LEU:N	2.30	0.63
2:G:648:GLY:HA3	2:G:678:PHE:CE2	2.33	0.63
2:H:1176:PRO:O	2:H:1177:SER:HB3	1.97	0.63
2:H:1266:TYR:CB	2:H:1347:LEU:HD23	2.28	0.63
2:H:964:LEU:CD2	2:H:964:LEU:H	2.09	0.63
1:C:24:SER:CB	2:I:2014:LEU:HD12	2.27	0.63
2:I:641:ILE:HG12	2:I:645:SER:HB2	1.79	0.63
1:A:504:ASP:CB	1:A:508:ASN:H	2.10	0.63
1:B:438:ASN:HD21	1:B:698:GLN:HE21	1.46	0.63
1:C:436:ALA:O	1:C:440:MET:HG3	1.98	0.63
1:C:504:ASP:HB2	1:C:508:ASN:HB2	1.80	0.63
1:C:989:GLN:NE2	2:I:993:GLN:OE1	2.32	0.63
2:G:1205:LEU:O	2:G:1206:LYS:HG3	1.98	0.63
2:G:2022:THR:HG23	2:G:2025:TYR:H	1.63	0.63
2:H:1227:ARG:CG	2:H:1227:ARG:NH1	2.57	0.63
2:H:1808:SER:H	2:H:2013:ASN:ND2	1.95	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1279:PHE:HB2	2:I:1340:PRO:HG3	1.79	0.63
2:I:1266:TYR:CB	2:I:1347:LEU:HD23	2.28	0.63
2:I:1378:ILE:HD11	2:I:1381:VAL:CG2	2.28	0.63
2:I:902:PRO:HG2	2:I:929:LEU:HD21	1.79	0.63
1:A:1292:ILE:CD1	1:A:1328:ILE:HD11	2.28	0.63
1:A:1461:ASP:O	1:A:1465:ASN:HB2	1.99	0.63
1:A:956:ALA:O	1:A:959:ILE:HG22	1.98	0.63
1:B:992:PHE:CE2	1:B:1399:PRO:HG3	2.34	0.63
1:C:1721:ARG:HG2	1:C:1721:ARG:NH1	2.00	0.63
2:G:259:THR:OG1	2:G:260:PRO:HD2	1.97	0.63
2:G:7:ARG:HE	2:G:27:PHE:HB2	1.63	0.63
2:G:745:ASP:HA	2:G:832:TRP:HH2	1.64	0.63
2:H:353:VAL:HG23	2:H:357:ASN:ND2	2.13	0.63
2:I:1890:ASN:HB2	2:I:1899:VAL:HB	1.81	0.63
2:I:1976:PHE:HA	2:I:1981:LEU:HD22	1.81	0.63
1:A:824:LEU:HD12	1:A:846:LEU:HB3	1.80	0.63
1:A:852:ARG:NH1	1:A:852:ARG:HG2	2.00	0.63
1:B:881:ASN:HA	1:B:944:ARG:HH21	1.63	0.63
1:C:599:MET:HB2	1:C:624:LYS:CD	2.25	0.63
1:C:680:ILE:HG13	1:C:769:ILE:HB	1.80	0.63
2:G:1266:TYR:CB	2:G:1347:LEU:HD23	2.29	0.63
2:G:835:THR:HG21	2:G:855:HIS:CD2	2.33	0.63
2:H:1740:THR:HG22	2:H:1742:VAL:HG23	1.79	0.63
2:I:1159:ILE:CG1	2:I:1169:PRO:HD3	2.28	0.63
1:B:421:ILE:HG13	1:B:469:VAL:HG21	1.81	0.63
2:G:1738:PHE:CE1	2:G:1837:THR:HG23	2.34	0.63
2:G:1859:PRO:O	2:G:1862:VAL:HG13	1.99	0.63
2:H:598:THR:CG2	2:H:622:GLY:HA3	2.28	0.63
2:I:1195:VAL:HG13	2:I:1211:LEU:HB3	1.79	0.63
2:I:159:ILE:HD11	2:I:512:LEU:HG	1.80	0.63
1:A:330:GLU:HA	1:A:333:LYS:HD2	1.80	0.63
1:A:484:LEU:O	1:A:485:ASP:CB	2.47	0.63
1:B:1721:ARG:CG	1:B:1721:ARG:NH1	2.55	0.63
1:B:444:ASN:HB3	1:B:446:ALA:H	1.63	0.63
1:B:1:MET:HE3	1:B:5:VAL:HG12	1.81	0.63
2:G:115:THR:HB	2:G:118:LYS:HB2	1.80	0.63
2:G:251:VAL:O	2:G:255:LEU:HB2	1.99	0.63
2:H:1475:LYS:CG	2:H:1481:SER:HB2	2.29	0.63
2:H:601:THR:CG2	2:H:618:GLU:O	2.38	0.63
2:H:835:THR:HG22	2:H:845:THR:N	2.14	0.63
2:I:1741:ILE:HG12	2:I:1746:LEU:HD13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1859:PRO:O	2:I:1862:VAL:HG13	1.98	0.63
1:A:1194:ASN:HB3	1:A:1197:THR:CG2	2.28	0.63
1:A:233:ILE:HD13	1:A:237:MET:HE2	1.81	0.63
1:A:436:ALA:O	1:A:440:MET:HG3	1.99	0.63
2:I:241:ILE:HG23	2:I:506:PRO:HG3	1.81	0.63
1:B:27:ARG:HH21	2:H:2015:THR:HA	1.64	0.63
1:C:864:VAL:HG22	1:C:921:PRO:HB3	1.79	0.63
2:G:1360:ILE:HG23	2:G:1403:VAL:O	1.99	0.63
2:G:748:THR:HB	2:G:749:PRO:HD3	1.78	0.63
2:H:892:ILE:HD11	2:H:903:TRP:NE1	2.14	0.63
2:I:1194:VAL:HG12	2:I:1194:VAL:O	1.99	0.63
1:A:460:GLU:HG2	1:A:470:LYS:HD3	1.79	0.63
1:C:742:LYS:HD3	1:C:746:GLU:OE2	1.98	0.63
2:G:490:TRP:O	2:G:494:THR:HG22	1.99	0.63
2:I:115:THR:HB	2:I:118:LYS:HB2	1.80	0.63
2:I:259:THR:HG23	2:I:262:GLU:H	1.64	0.63
2:I:259:THR:OG1	2:I:260:PRO:HD2	1.98	0.63
1:A:411:GLN:HE22	1:A:1628:SER:H	1.47	0.62
1:B:1056:ILE:HD13	1:B:1193:TRP:HD1	1.64	0.62
1:C:1753:ALA:HB2	1:C:1872:SER:OG	1.98	0.62
1:C:956:ALA:O	1:C:959:ILE:HG22	1.98	0.62
2:G:1227:ARG:HG3	2:G:1227:ARG:NH1	2.00	0.62
2:H:1874:VAL:O	2:H:1878:VAL:HG12	1.98	0.62
2:H:33:LEU:HD11	2:H:80:PHE:HD2	1.63	0.62
1:A:13:LEU:HB2	2:G:2026:PHE:CE1	2.34	0.62
1:A:158:LYS:HD3	1:A:185:GLU:HB3	1.81	0.62
1:B:529:MET:HG3	1:B:638:LEU:HG	1.80	0.62
2:G:943:TRP:CH2	2:G:1016:PRO:HG3	2.34	0.62
2:G:1173:VAL:HG21	2:G:1221:MET:HE1	1.80	0.62
2:G:1378:ILE:HD11	2:G:1381:VAL:CG2	2.29	0.62
2:G:85:ASN:ND2	2:G:135:ARG:HH11	1.97	0.62
2:H:1374:THR:HG23	2:H:1396:LEU:HD12	1.81	0.62
2:H:1931:LEU:HD22	2:H:1935:GLU:HG2	1.81	0.62
2:H:251:VAL:O	2:H:255:LEU:HB2	1.99	0.62
1:A:1259:GLY:HA2	1:A:1263:ASP:HB2	1.81	0.62
1:C:254:TRP:CH2	1:C:292:GLN:HG3	2.34	0.62
1:C:529:MET:CG	1:C:638:LEU:HG	2.30	0.62
2:G:726:PHE:O	2:G:762:ASN:HB2	1.98	0.62
2:H:750:MET:HG3	2:H:796:PHE:HZ	1.64	0.62
2:H:856:LYS:HG2	2:H:1054:LEU:HD12	1.81	0.62
2:I:1472:VAL:HG22	2:I:1483:VAL:HG22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1624:THR:HB	2:I:1642:THR:HG23	1.81	0.62
2:I:324:LEU:HD12	2:I:328:LEU:HG	1.82	0.62
2:H:1472:VAL:HG22	2:H:1483:VAL:HG22	1.79	0.62
2:H:871:THR:HB	2:H:872:ILE:HD12	1.80	0.62
2:I:1868:GLN:HG3	2:I:1898:TYR:OH	1.99	0.62
2:I:1906:ALA:O	2:I:1910:VAL:HG23	2.00	0.62
1:A:1292:ILE:HD11	1:A:1328:ILE:HD11	1.81	0.62
1:A:1455:ARG:HH11	1:A:1458:GLN:HE21	1.46	0.62
1:B:1584:PRO:HG3	1:B:1591:TRP:CZ3	2.35	0.62
1:B:507:GLY:N	1:B:954:ARG:HG2	2.15	0.62
1:C:1039:MET:O	1:C:1609:ARG:NH2	2.31	0.62
2:G:1102:TYR:HB3	2:G:1244:PRO:HA	1.80	0.62
2:G:1782:THR:HG22	2:G:1827:LEU:HD21	1.81	0.62
2:G:1819:ALA:HA	2:G:2005:ARG:HH11	1.65	0.62
2:H:601:THR:O	2:H:601:THR:HG22	2.00	0.62
1:B:1455:ARG:HH11	1:B:1458:GLN:HE21	1.47	0.62
1:C:822:VAL:HG12	1:C:824:LEU:HD22	1.82	0.62
2:H:1168:ASN:ND2	2:H:1171:ARG:HB2	2.14	0.62
2:I:1740:THR:HG22	2:I:1742:VAL:HG23	1.79	0.62
2:I:464:ASP:HB3	2:I:466:SER:HB3	1.80	0.62
2:I:846:VAL:HG13	2:I:865:TRP:NE1	2.15	0.62
1:A:1540:SER:HA	1:A:1575:VAL:HG22	1.81	0.62
1:A:749:ILE:CD1	1:A:805:CYS:HB3	2.29	0.62
1:C:233:ILE:HD13	1:C:237:MET:CE	2.30	0.62
2:G:1908:ASP:HB2	2:G:1958:LEU:HD21	1.81	0.62
2:G:241:ILE:HG23	2:G:506:PRO:HG3	1.80	0.62
2:G:871:THR:HB	2:G:872:ILE:HD12	1.82	0.62
2:H:131:ILE:HD12	2:H:182:VAL:CG1	2.29	0.62
2:I:184:VAL:HG13	2:I:187:LEU:HD21	1.80	0.62
2:I:259:THR:CG2	2:I:262:GLU:H	2.11	0.62
1:C:444:ASN:HB3	1:C:446:ALA:H	1.65	0.62
2:G:1300:PHE:CA	2:G:1556:VAL:HG11	2.29	0.62
2:G:159:ILE:HD11	2:G:512:LEU:HG	1.80	0.62
2:G:641:ILE:HG12	2:G:645:SER:HB2	1.80	0.62
2:H:85:ASN:ND2	2:H:135:ARG:HH11	1.96	0.62
2:I:1805:ALA:HB2	2:I:2011:ILE:HB	1.82	0.62
1:A:1523:ARG:CG	1:A:1523:ARG:NH1	2.57	0.62
1:A:20:TYR:HE1	2:G:2035:SER:HB2	1.60	0.62
1:B:27:ARG:HD2	1:B:30:GLU:OE2	2.00	0.62
1:C:501:THR:N	1:C:886:GLU:OE1	2.21	0.62
2:G:750:MET:HG3	2:G:796:PHE:HZ	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:490:TRP:O	2:H:494:THR:HG22	2.00	0.62
1:A:1326:ILE:HG12	1:A:1388:MET:HG3	1.82	0.62
2:G:1719:ILE:O	2:G:1761:SER:HB2	2.00	0.62
2:G:1931:LEU:HD22	2:G:1935:GLU:HG2	1.82	0.62
2:H:1149:TRP:CD1	2:H:1213:LEU:HD12	2.34	0.62
2:I:1086:LEU:HD12	2:I:1090:TYR:HB2	1.82	0.62
2:I:1823:SER:OG	2:I:1825:GLU:HG2	2.00	0.62
2:I:745:ASP:HA	2:I:832:TRP:HH2	1.65	0.62
1:C:1057:MET:SD	1:C:1097:ILE:HG23	2.40	0.61
1:C:233:ILE:HD13	1:C:237:MET:HE2	1.80	0.61
1:C:509:ILE:HG12	1:C:951:SER:HB2	1.82	0.61
2:G:1199:GLU:OE2	2:G:1567:ARG:CZ	2.46	0.61
2:G:719:ILE:O	2:G:722:ALA:HB3	2.00	0.61
2:H:100:ASP:OD2	2:H:102:HIS:HD2	1.82	0.61
2:H:159:ILE:HD11	2:H:512:LEU:HG	1.82	0.61
2:H:1675:GLY:O	2:H:1678:MET:HB2	1.99	0.61
1:A:934:PRO:O	1:A:936:LEU:N	2.33	0.61
1:B:1292:ILE:CD1	1:B:1328:ILE:HD11	2.30	0.61
1:B:631:PRO:HB2	1:B:634:THR:OG1	2.00	0.61
2:H:7:ARG:HE	2:H:27:PHE:HB2	1.64	0.61
2:H:353:VAL:HG23	2:H:357:ASN:HD22	1.65	0.61
1:B:158:LYS:HD3	1:B:185:GLU:HB3	1.82	0.61
1:B:340:ARG:HH12	1:B:344:GLN:CG	2.13	0.61
1:B:824:LEU:HD12	1:B:846:LEU:HB3	1.82	0.61
1:C:1498:GLU:HB2	1:C:1876:LEU:HD13	1.82	0.61
2:H:856:LYS:NZ	2:H:1052:CYS:SG	2.70	0.61
2:H:1528:GLU:O	2:H:1530:LYS:N	2.30	0.61
2:H:589:ARG:HB3	2:H:590:PRO:HD2	1.82	0.61
2:I:1054:LEU:HB2	4:I:3051:FMN:HM71	1.82	0.61
2:I:860:ARG:HB3	2:I:898:ASP:HB3	1.81	0.61
1:A:1721:ARG:NH1	1:A:1721:ARG:CG	2.52	0.61
1:B:1555:ALA:HA	1:B:1621:PHE:CE1	2.36	0.61
2:G:1739:GLU:O	2:G:1987:PRO:HG3	2.00	0.61
2:H:1378:ILE:HD11	2:H:1381:VAL:CG2	2.31	0.61
2:H:835:THR:HG21	2:H:855:HIS:NE2	2.14	0.61
2:I:100:ASP:OD2	2:I:102:HIS:HD2	1.83	0.61
2:I:1808:SER:H	2:I:2013:ASN:HD21	1.47	0.61
1:C:20:TYR:CE1	2:I:2035:SER:HB2	2.35	0.61
1:A:24:SER:O	2:G:1977:HIS:HD2	1.84	0.61
1:B:20:TYR:CE1	2:H:2035:SER:HB2	2.35	0.61
1:B:644:THR:HG23	1:B:648:ASP:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1292:ILE:HD11	1:C:1328:ILE:HD11	1.81	0.61
2:G:324:LEU:HD12	2:G:328:LEU:HG	1.81	0.61
2:H:1086:LEU:HD12	2:H:1090:TYR:HB2	1.83	0.61
2:H:1279:PHE:HB2	2:H:1340:PRO:HG3	1.81	0.61
2:H:1419:PHE:O	2:H:1421:ASN:N	2.33	0.61
2:H:174:ARG:NH2	2:H:225:THR:OG1	2.33	0.61
2:H:33:LEU:HD11	2:H:80:PHE:CD2	2.35	0.61
1:C:20:TYR:CG	2:I:2033:THR:OG1	2.53	0.61
2:I:56:THR:HG23	2:I:59:GLU:CG	2.28	0.61
1:A:705:VAL:HG23	1:A:732:LEU:HD21	1.82	0.61
1:B:1431:GLU:HG3	1:B:1433:HIS:CE1	2.36	0.61
1:B:1693:ILE:HD11	2:H:998:GLN:HB2	1.83	0.61
1:B:24:SER:O	2:H:1977:HIS:CD2	2.53	0.61
2:H:603:SER:O	2:H:607:VAL:HG12	2.00	0.61
1:A:644:THR:HG23	1:A:648:ASP:H	1.65	0.61
1:A:822:VAL:HG12	1:A:824:LEU:HD22	1.82	0.61
1:B:1194:ASN:HB3	1:B:1197:THR:CG2	2.30	0.61
1:C:824:LEU:HD12	1:C:846:LEU:HB3	1.82	0.61
2:I:1325:PHE:CZ	2:I:1328:VAL:HG11	2.36	0.61
2:I:1352:HIS:HE1	2:I:1583:MET:HE1	1.65	0.61
1:C:24:SER:HB3	2:I:2014:LEU:HD12	1.82	0.61
2:I:663:ILE:HG13	2:I:694:TYR:HE1	1.66	0.61
1:B:1052:GLU:O	1:B:1056:ILE:HG23	2.01	0.61
1:B:1594:ASN:O	1:B:1598:GLN:HG3	2.00	0.61
1:A:599:MET:HB2	1:A:624:LYS:CD	2.25	0.61
1:B:1292:ILE:HD11	1:B:1328:ILE:HD11	1.82	0.61
1:B:1360:ARG:HH11	1:B:1364:GLU:HG2	1.66	0.61
2:G:1123:ASP:N	2:G:1123:ASP:OD1	2.34	0.61
2:G:1976:PHE:HB3	2:G:1981:LEU:HD21	1.82	0.61
1:A:11:HIS:ND1	2:G:1998:LYS:HA	2.15	0.61
2:G:601:THR:O	2:G:601:THR:HG22	2.01	0.61
2:H:260:PRO:HD3	2:H:289:TRP:CE2	2.36	0.61
1:A:1:MET:HE3	1:A:5:VAL:HG12	1.82	0.61
1:C:1501:LEU:HD11	1:C:1775:LEU:HD23	1.79	0.61
2:G:856:LYS:NZ	2:G:1052:CYS:SG	2.69	0.61
2:G:1472:VAL:HG22	2:G:1483:VAL:HG22	1.83	0.61
2:H:1805:ALA:HB2	2:H:2011:ILE:HB	1.83	0.61
2:H:184:VAL:HG13	2:H:187:LEU:HD21	1.83	0.61
2:I:1219:ILE:HD11	2:I:1242:PHE:HB2	1.83	0.61
1:C:504:ASP:CB	1:C:508:ASN:H	2.14	0.60
2:G:1417:THR:C	2:G:1419:PHE:H	2.04	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:846:VAL:HG13	2:H:865:TRP:NE1	2.16	0.60
2:I:565:TYR:CZ	2:I:758:ARG:HD2	2.35	0.60
1:A:32:GLN:HA	1:A:35:PHE:CE2	2.35	0.60
1:B:233:ILE:HD13	1:B:237:MET:HE2	1.82	0.60
2:G:174:ARG:NH2	2:G:225:THR:OG1	2.34	0.60
2:G:33:LEU:HD11	2:G:80:PHE:CD2	2.35	0.60
2:I:856:LYS:NZ	2:I:1052:CYS:SG	2.70	0.60
2:I:1300:PHE:HA	2:I:1556:VAL:HG11	1.84	0.60
1:C:2:LYS:CD	2:I:2050:GLN:HB3	2.30	0.60
2:I:33:LEU:HD11	2:I:80:PHE:CD2	2.36	0.60
1:A:232:LEU:HD22	1:A:269:LEU:HA	1.83	0.60
2:G:1844:ARG:NH1	2:G:1844:ARG:CG	2.49	0.60
2:G:1808:SER:H	2:G:2013:ASN:HD21	1.47	0.60
2:G:607:VAL:HA	2:G:617:ILE:HD13	1.82	0.60
2:G:747:HIS:HE1	2:G:780:TYR:OH	1.84	0.60
2:I:1198:SER:HB3	2:I:1205:LEU:HD21	1.82	0.60
2:I:1908:ASP:HB2	2:I:1958:LEU:HD21	1.83	0.60
1:A:1842:VAL:O	1:A:1845:ASN:HB2	2.02	0.60
1:B:400:ARG:HH11	1:B:400:ARG:HG3	1.64	0.60
1:A:20:TYR:OH	2:G:2035:SER:HB2	2.01	0.60
2:G:846:VAL:HG13	2:G:865:TRP:NE1	2.16	0.60
2:H:1198:SER:HB3	2:H:1205:LEU:HD21	1.83	0.60
2:H:1219:ILE:HD11	2:H:1242:PHE:HB2	1.83	0.60
2:H:324:LEU:HD12	2:H:328:LEU:HG	1.84	0.60
2:I:1352:HIS:CD2	2:I:1410:PHE:CE2	2.90	0.60
2:I:1360:ILE:HG23	2:I:1403:VAL:O	2.01	0.60
2:I:674:TYR:HB3	2:I:676:ILE:HG22	1.84	0.60
1:B:1523:ARG:NH1	1:B:1523:ARG:CG	2.59	0.60
1:B:509:ILE:HG12	1:B:951:SER:HB2	1.82	0.60
1:C:221:LEU:O	1:C:225:SER:HB3	2.02	0.60
2:G:1325:PHE:CZ	2:G:1328:VAL:HG11	2.37	0.60
2:G:499:THR:CB	2:G:500:HIS:CD2	2.80	0.60
2:G:61:VAL:HG21	2:G:95:TYR:HE1	1.67	0.60
2:G:926:LEU:HD13	2:G:947:THR:HG22	1.84	0.60
2:H:745:ASP:HA	2:H:832:TRP:HH2	1.66	0.60
2:I:1123:ASP:OD1	2:I:1123:ASP:N	2.35	0.60
2:I:1205:LEU:O	2:I:1206:LYS:HG3	2.00	0.60
2:I:667:LYS:HB2	2:I:698:LEU:HD23	1.82	0.60
2:I:817:ALA:O	2:I:821:ILE:HG13	2.01	0.60
1:C:644:THR:HG23	1:C:648:ASP:H	1.65	0.60
2:G:1822:MET:HE2	2:G:1996:ILE:HG12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:561:TRP:O	2:G:562:LEU:C	2.39	0.60
2:G:816:ASP:HB3	2:G:1048:VAL:HG21	1.83	0.60
2:H:1624:THR:HB	2:H:1642:THR:HG23	1.82	0.60
2:I:1976:PHE:HB3	2:I:1981:LEU:HD21	1.83	0.60
2:I:589:ARG:HB3	2:I:590:PRO:HD2	1.83	0.60
1:A:1194:ASN:O	1:A:1197:THR:HG23	2.02	0.60
1:A:529:MET:HG3	1:A:638:LEU:HG	1.84	0.60
1:B:513:GLU:OE2	1:B:873:ARG:NH1	2.33	0.60
2:G:184:VAL:HG13	2:G:187:LEU:HD21	1.84	0.60
2:G:271:THR:OG1	2:G:460:TYR:HB2	2.01	0.60
2:I:33:LEU:HD11	2:I:80:PHE:HD2	1.65	0.60
1:A:233:ILE:HD13	1:A:237:MET:CE	2.32	0.60
1:C:1062:TYR:CD2	1:C:1693:ILE:HG23	2.36	0.60
2:H:1149:TRP:CD1	2:H:1213:LEU:CD1	2.85	0.60
2:H:1739:GLU:O	2:H:1987:PRO:HG3	2.02	0.60
2:I:1986:LYS:N	2:I:1987:PRO:HD2	2.16	0.60
1:B:1657:HIS:ND1	1:B:1658:PRO:HD2	2.17	0.60
1:B:604:ALA:HB3	1:B:612:GLU:HG2	1.82	0.60
1:C:529:MET:HG3	1:C:638:LEU:HG	1.82	0.60
2:G:732:TRP:CD2	2:G:750:MET:CE	2.85	0.60
2:G:892:ILE:HD11	2:G:903:TRP:NE1	2.17	0.60
2:H:719:ILE:O	2:H:722:ALA:HB3	2.02	0.60
1:B:1021:VAL:HG11	1:B:1597:LEU:HD11	1.83	0.60
1:B:1057:MET:SD	1:B:1097:ILE:HG23	2.42	0.60
1:C:1662:TYR:O	1:C:1665:ILE:HG22	2.01	0.60
1:C:1842:VAL:O	1:C:1845:ASN:HB2	2.02	0.60
2:H:1093:ASP:HB3	2:H:1096:LYS:HG3	1.84	0.60
2:I:1874:VAL:O	2:I:1878:VAL:HG12	2.02	0.60
2:I:1989:LYS:O	2:I:1993:LYS:HG3	2.02	0.60
2:I:601:THR:HG22	2:I:601:THR:O	2.02	0.60
2:I:741:HIS:CB	2:I:853:PRO:HB2	2.32	0.60
1:A:1119:LYS:HE2	1:A:1341:PHE:CG	2.37	0.59
1:B:1189:ILE:HD12	1:B:1380:GLN:HG3	1.82	0.59
1:C:1461:ASP:O	1:C:1465:ASN:HB2	2.02	0.59
1:C:1585:LYS:HB3	3:C:2748:CER:H52	1.84	0.59
2:G:100:ASP:OD2	2:G:102:HIS:HD2	1.85	0.59
2:G:1417:THR:HG22	2:G:1419:PHE:CE2	2.37	0.59
2:G:1425:LYS:HG2	2:G:1471:GLU:CG	2.30	0.59
2:G:598:THR:CG2	2:G:622:GLY:HA3	2.30	0.59
2:H:1494:PRO:HB2	2:H:1823:SER:HB2	1.84	0.59
2:I:732:TRP:CD2	2:I:750:MET:CE	2.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1475:GLU:CG	1:A:1761:LYS:O	2.50	0.59
1:A:37:LYS:HB2	1:A:65:TYR:HE1	1.67	0.59
1:A:67:SER:OG	2:I:359:HIS:HE1	1.85	0.59
1:B:1062:TYR:CD2	1:B:1693:ILE:HG23	2.36	0.59
1:B:1184:LEU:HB2	1:B:1352:THR:HG21	1.83	0.59
1:B:80:CYS:SG	1:B:82:SER:HB3	2.42	0.59
2:H:813:THR:HB	2:H:818:LYS:HE3	1.84	0.59
2:I:1378:ILE:HD11	2:I:1381:VAL:HG21	1.84	0.59
2:I:163:GLN:CG	2:I:423:VAL:HG12	2.32	0.59
1:A:435:GLU:O	1:A:439:ILE:HG13	2.03	0.59
1:B:1460:LYS:NZ	1:B:1774:GLU:CD	2.51	0.59
1:B:32:GLN:HA	1:B:35:PHE:CE2	2.38	0.59
1:B:680:ILE:HG13	1:B:769:ILE:HB	1.83	0.59
1:C:705:VAL:HG23	1:C:732:LEU:HD21	1.83	0.59
2:G:594:VAL:HG21	2:G:610:THR:HG21	1.84	0.59
2:H:1314:ARG:NH1	2:H:1314:ARG:CG	2.62	0.59
2:I:1575:LEU:HD13	2:I:1579:ILE:HD12	1.84	0.59
1:A:1584:PRO:HG3	1:A:1591:TRP:CZ3	2.37	0.59
1:B:1259:GLY:HA2	1:B:1263:ASP:HB2	1.84	0.59
1:B:221:LEU:O	1:B:225:SER:HB3	2.02	0.59
1:C:421:ILE:CG1	1:C:469:VAL:HG21	2.32	0.59
1:C:56:MET:HG3	2:I:1893:VAL:CG2	2.32	0.59
2:G:2038:ILE:O	2:G:2042:ILE:HG12	2.02	0.59
2:G:754:TYR:CD2	2:G:794:MET:HG3	2.38	0.59
2:H:1223:MET:HE3	2:H:1238:LEU:HD12	1.84	0.59
2:H:409:PHE:HB3	2:H:833:GLU:OE1	2.02	0.59
2:H:241:ILE:HG23	2:H:506:PRO:HG3	1.83	0.59
2:H:860:ARG:HB3	2:H:898:ASP:HB3	1.83	0.59
2:I:658:MET:HA	2:I:661:TRP:NE1	2.17	0.59
1:A:1432:HIS:CE1	1:A:1434:SER:OG	2.55	0.59
1:A:1749:THR:CB	1:A:1874:ASP:HA	2.31	0.59
1:B:1842:VAL:O	1:B:1845:ASN:HB2	2.02	0.59
1:B:233:ILE:HD13	1:B:237:MET:CE	2.32	0.59
1:B:956:ALA:O	1:B:959:ILE:HG22	2.02	0.59
1:C:1194:ASN:O	1:C:1197:THR:HG23	2.02	0.59
1:C:1492:GLU:O	1:C:1496:GLU:HG3	2.01	0.59
2:G:1805:ALA:HB2	2:G:2011:ILE:HB	1.84	0.59
2:G:443:LEU:HD22	2:G:448:VAL:HG11	1.84	0.59
2:I:1149:TRP:CD1	2:I:1213:LEU:HD12	2.37	0.59
2:I:85:ASN:ND2	2:I:135:ARG:HH11	1.99	0.59
2:I:402:LEU:HD13	2:I:402:LEU:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:ASP:CB	1:B:508:ASN:H	2.15	0.59
1:C:1584:PRO:HG3	1:C:1591:TRP:CZ3	2.38	0.59
2:G:1195:VAL:HG13	2:G:1211:LEU:HB3	1.84	0.59
2:G:603:SER:O	2:G:607:VAL:HG12	2.03	0.59
2:G:932:ILE:HD11	2:G:1042:ALA:CB	2.24	0.59
2:H:817:ALA:O	2:H:821:ILE:HG13	2.02	0.59
2:I:1422:THR:CG2	2:I:1422:THR:O	2.49	0.59
1:A:417:TYR:OH	1:A:458:THR:HG22	2.02	0.59
1:A:516:ARG:NH2	1:A:889:GLU:OE1	2.35	0.59
1:B:1585:LYS:HB3	3:B:2748:CER:H52	1.85	0.59
1:C:733:ILE:HD12	1:C:761:LEU:HD21	1.85	0.59
2:G:1417:THR:O	2:G:1419:PHE:N	2.30	0.59
2:H:663:ILE:HG13	2:H:694:TYR:HE1	1.66	0.59
2:H:726:PHE:O	2:H:762:ASN:HB2	2.03	0.59
2:I:1086:LEU:HD12	2:I:1090:TYR:CB	2.33	0.59
2:I:1496:LYS:HE2	2:I:1693:ARG:HH21	1.67	0.59
2:I:99:ASN:HA	2:I:550:VAL:CG2	2.32	0.59
1:A:409:ALA:HB2	1:A:442:ARG:HD2	1.84	0.59
2:G:131:ILE:CG2	2:G:182:VAL:CG1	2.80	0.59
2:G:1417:THR:HG22	2:G:1419:PHE:CD2	2.37	0.59
2:H:197:GLU:HA	2:H:197:GLU:OE1	2.02	0.59
2:H:455:ILE:HG13	2:H:469:ARG:HD3	1.83	0.59
1:A:1002:LYS:NZ	1:A:1782:GLU:HG2	2.17	0.59
1:A:50:SER:HB2	1:A:51:PRO:HD3	1.85	0.59
1:C:1555:ALA:HA	1:C:1621:PHE:CE1	2.38	0.59
2:G:1086:LEU:HD12	2:G:1090:TYR:HB2	1.84	0.59
2:G:402:LEU:HD13	2:G:402:LEU:O	2.03	0.59
2:H:2038:ILE:O	2:H:2042:ILE:HG12	2.03	0.59
1:A:440:MET:HB3	1:A:483:VAL:HG21	1.85	0.59
1:B:1474:ALA:O	1:B:1478:PRO:HD2	2.03	0.59
1:B:417:TYR:OH	1:B:458:THR:HG22	2.03	0.59
2:G:1210:ILE:HB	2:G:1222:GLU:HB3	1.85	0.59
2:G:1293:THR:CG2	2:G:1296:GLU:H	2.14	0.59
2:G:1374:THR:HG23	2:G:1396:LEU:HD12	1.85	0.59
2:H:1130:THR:H	2:H:1133:THR:HG23	1.68	0.59
2:H:259:THR:OG1	2:H:260:PRO:HD2	2.03	0.59
2:I:174:ARG:NH2	2:I:225:THR:OG1	2.36	0.59
2:I:353:VAL:HG23	2:I:357:ASN:ND2	2.18	0.59
2:I:490:TRP:O	2:I:494:THR:HG22	2.03	0.59
1:A:1524:GLY:O	1:A:1528:THR:HG23	2.03	0.58
1:A:1585:LYS:HB3	3:A:2748:CER:H52	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1234:MET:HG2	1:B:1326:ILE:HD12	1.85	0.58
1:C:488:PRO:HG3	1:C:728:LYS:HG3	1.83	0.58
2:G:1198:SER:HB3	2:G:1205:LEU:HD21	1.85	0.58
2:G:1279:PHE:HB2	2:G:1340:PRO:HG3	1.85	0.58
2:G:1378:ILE:HD11	2:G:1381:VAL:HG21	1.85	0.58
2:H:273:HIS:HB3	2:H:512:LEU:HD22	1.85	0.58
2:I:455:ILE:HG13	2:I:469:ARG:HD3	1.85	0.58
1:A:421:ILE:HG12	1:A:469:VAL:HG21	1.85	0.58
1:A:531:LEU:HD21	1:A:629:THR:HG22	1.85	0.58
1:B:1392:LEU:HD22	1:B:1396:MET:HG3	1.84	0.58
1:C:1657:HIS:ND1	1:C:1658:PRO:HD2	2.17	0.58
1:C:749:ILE:CD1	1:C:805:CYS:HB3	2.32	0.58
1:C:80:CYS:SG	1:C:82:SER:HB3	2.42	0.58
2:G:1149:TRP:CD1	2:G:1213:LEU:HD12	2.38	0.58
2:H:1010:PRO:O	2:H:1011:MET:HB2	2.03	0.58
2:H:665:LEU:O	2:H:669:LEU:HB2	2.04	0.58
2:I:1822:MET:CE	2:I:1996:ILE:HG12	2.34	0.58
2:I:499:THR:CB	2:I:500:HIS:CD2	2.79	0.58
2:I:907:VAL:O	2:I:910:GLN:HB3	2.03	0.58
1:A:1463:VAL:HG11	1:A:1877:GLN:HE22	1.68	0.58
1:B:37:LYS:HB2	1:B:65:TYR:HE1	1.69	0.58
2:G:166:THR:HG22	2:G:168:ASP:N	2.19	0.58
2:G:28:PHE:CZ	2:H:7:ARG:NE	2.70	0.58
2:I:1227:ARG:NH1	2:I:1227:ARG:CG	2.55	0.58
2:I:1374:THR:HG23	2:I:1396:LEU:HD12	1.83	0.58
2:I:601:THR:CG2	2:I:618:GLU:O	2.39	0.58
1:A:260:ARG:HH12	1:A:300:VAL:HG21	1.68	0.58
1:A:444:ASN:HB3	1:A:446:ALA:H	1.66	0.58
1:B:409:ALA:HB2	1:B:442:ARG:HD2	1.86	0.58
1:C:1233:GLU:OE2	1:C:1680:ARG:NH2	2.36	0.58
1:C:24:SER:O	2:I:1977:HIS:CD2	2.54	0.58
2:H:1103:PHE:O	2:H:1247:GLY:HA3	2.03	0.58
2:H:1360:ILE:HG23	2:H:1403:VAL:O	2.04	0.58
2:I:127:ILE:O	2:I:131:ILE:HG13	2.03	0.58
2:I:736:ARG:NH1	2:I:769:SER:O	2.36	0.58
1:B:436:ALA:O	1:B:440:MET:HG3	2.04	0.58
1:C:1009:LEU:HA	1:C:1445:MET:HE2	1.85	0.58
1:C:232:LEU:HD22	1:C:269:LEU:HA	1.83	0.58
2:G:1597:ALA:HB1	2:G:1638:ILE:CD1	2.33	0.58
2:G:1823:SER:OG	2:G:1825:GLU:HG2	2.03	0.58
2:G:807:ILE:CG2	2:G:1066:ILE:HA	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:271:THR:OG1	2:H:460:TYR:HB2	2.03	0.58
2:H:499:THR:CB	2:H:500:HIS:CD2	2.81	0.58
2:H:762:ASN:H	2:H:762:ASN:ND2	1.85	0.58
2:I:1269:LEU:O	2:I:1560:LEU:HD23	2.03	0.58
1:A:986:ALA:HB2	1:A:1047:LEU:HD13	1.85	0.58
1:B:1461:ASP:O	1:B:1465:ASN:HB2	2.03	0.58
1:C:1665:ILE:HD11	1:C:1669:ARG:HG2	1.85	0.58
1:C:232:LEU:HD13	1:C:272:GLU:HB2	1.85	0.58
1:C:340:ARG:HH12	1:C:344:GLN:CG	2.13	0.58
1:C:421:ILE:HG13	1:C:469:VAL:HG21	1.84	0.58
2:G:1223:MET:HE3	2:G:1238:LEU:HD12	1.85	0.58
2:G:131:ILE:CG2	2:G:182:VAL:HG12	2.33	0.58
2:G:907:VAL:O	2:G:910:GLN:HB3	2.02	0.58
2:I:707:PRO:HG2	2:I:730:LEU:HD13	1.85	0.58
1:A:1600:LEU:HD13	1:A:1657:HIS:HA	1.85	0.58
1:C:419:GLU:HG2	1:C:424:VAL:HB	1.86	0.58
2:G:1159:ILE:CG1	2:G:1169:PRO:HD3	2.33	0.58
2:G:260:PRO:HD3	2:G:289:TRP:CE2	2.38	0.58
2:G:674:TYR:HB3	2:G:676:ILE:HG22	1.85	0.58
2:G:565:TYR:OH	2:G:758:ARG:HD2	2.02	0.58
1:B:29:ILE:HG13	2:H:1891:TYR:C	2.23	0.58
2:H:490:TRP:CH2	2:H:512:LEU:HD21	2.39	0.58
2:H:543:PHE:CB	2:H:545:GLN:HE22	2.17	0.58
2:I:942:THR:HG21	2:I:1012:GLN:HA	1.85	0.58
1:C:968:VAL:O	2:I:1512:HIS:HB2	2.04	0.58
2:I:1719:ILE:O	2:I:1761:SER:HB2	2.01	0.58
1:B:198:PRO:CG	1:B:209:LEU:HD21	2.26	0.58
1:B:286:PHE:O	1:B:290:MET:HG2	2.03	0.58
1:C:1020:VAL:HG13	1:C:1400:ILE:HG23	1.84	0.58
2:G:638:VAL:HA	2:G:641:ILE:HG22	1.86	0.58
2:H:163:GLN:CG	2:H:423:VAL:HG12	2.32	0.58
2:I:1822:MET:HE2	2:I:1996:ILE:HG12	1.86	0.58
1:A:198:PRO:CG	1:A:209:LEU:HD21	2.28	0.58
1:A:987:ASN:HD22	2:G:957:ARG:HD2	1.68	0.58
1:B:1473:GLU:O	1:B:1478:PRO:HD3	2.04	0.58
1:B:1662:TYR:O	1:B:1665:ILE:HG22	2.04	0.58
1:B:232:LEU:HD22	1:B:269:LEU:HA	1.85	0.58
1:B:749:ILE:CD1	1:B:805:CYS:HB3	2.33	0.58
1:C:1247:SER:HB2	1:C:1332:TYR:HE2	1.68	0.58
2:G:1359:MET:HA	2:G:1359:MET:HE3	1.86	0.58
1:A:20:TYR:CZ	2:G:2035:SER:HB2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:232:LEU:HD23	2:G:232:LEU:O	2.03	0.58
2:G:273:HIS:HB3	2:G:512:LEU:HD22	1.86	0.58
2:G:611:THR:CG2	2:G:641:ILE:HG13	2.34	0.58
2:G:817:ALA:O	2:G:821:ILE:HG13	2.04	0.58
2:G:860:ARG:HB3	2:G:898:ASP:HB3	1.85	0.58
2:H:1210:ILE:HB	2:H:1222:GLU:HB3	1.85	0.58
1:C:27:ARG:HH21	2:I:2015:THR:HA	1.68	0.58
1:A:1062:TYR:CD2	1:A:1693:ILE:HG23	2.39	0.57
1:A:1189:ILE:HD12	1:A:1380:GLN:HG3	1.86	0.57
1:A:1419:PRO:HB3	1:A:1646:PHE:CZ	2.39	0.57
1:A:329:GLU:O	1:A:333:LYS:HG3	2.04	0.57
1:B:1247:SER:HB2	1:B:1332:TYR:HE2	1.69	0.57
1:B:419:GLU:HG2	1:B:424:VAL:HB	1.86	0.57
1:C:1219:VAL:CA	1:C:1384:ILE:HD11	2.27	0.57
1:C:433:VAL:O	1:C:437:ILE:HG13	2.04	0.57
2:G:146:PHE:HA	2:G:149:VAL:HG12	1.86	0.57
2:G:376:ASN:HD22	2:G:377:LEU:N	2.02	0.57
2:G:56:THR:HG23	2:G:59:GLU:CG	2.29	0.57
2:G:7:ARG:NH1	2:G:24:THR:HA	2.19	0.57
2:I:239:PRO:HG3	2:I:304:PHE:HA	1.86	0.57
2:I:376:ASN:HD22	2:I:377:LEU:N	2.02	0.57
1:A:1056:ILE:CD1	1:A:1193:TRP:HD1	2.17	0.57
1:A:1203:ASP:HB3	1:B:179:LYS:HZ1	1.68	0.57
1:A:1247:SER:HB2	1:A:1332:TYR:HE2	1.66	0.57
1:A:11:HIS:O	1:A:15:THR:HG22	2.04	0.57
1:A:1464:GLU:CD	1:A:1773:VAL:HG12	2.23	0.57
1:B:1496:GLU:O	1:B:1500:GLN:HG3	2.03	0.57
1:B:232:LEU:HD13	1:B:272:GLU:HB2	1.87	0.57
1:C:1052:GLU:O	1:C:1056:ILE:HG23	2.04	0.57
1:C:1431:GLU:CD	1:C:1433:HIS:HE1	2.08	0.57
2:G:1149:TRP:CD1	2:G:1213:LEU:CD1	2.87	0.57
2:G:658:MET:HA	2:G:661:TRP:NE1	2.19	0.57
2:H:1331:TRP:CE2	2:H:1335:ILE:HG13	2.38	0.57
2:H:722:ALA:HB1	2:H:723:HIS:CE1	2.38	0.57
2:I:726:PHE:O	2:I:762:ASN:HB2	2.04	0.57
1:A:1538:VAL:HB	1:A:1639:VAL:HG22	1.86	0.57
1:B:1022:THR:HG22	1:B:1226:SER:HB2	1.87	0.57
1:B:1125:VAL:HG21	1:B:1175:ILE:HD12	1.86	0.57
1:B:50:SER:HB2	1:B:51:PRO:HD3	1.86	0.57
1:C:1056:ILE:CD1	1:C:1193:TRP:HD1	2.16	0.57
2:G:942:THR:HG21	2:G:1012:GLN:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:826:GLY:O	2:G:827:VAL:HG23	2.03	0.57
2:H:124:LYS:HG2	2:H:179:THR:HA	1.86	0.57
1:B:413:LEU:HD13	1:B:451:MET:HG2	1.85	0.57
1:B:705:VAL:HG23	1:B:732:LEU:HD21	1.85	0.57
1:C:183:GLN:HE21	1:C:202:GLU:HG2	1.69	0.57
2:G:163:GLN:CG	2:G:423:VAL:HG12	2.33	0.57
2:H:1086:LEU:HD12	2:H:1090:TYR:CB	2.34	0.57
2:H:1231:GLY:O	2:H:1233:PRO:HD3	2.04	0.57
2:H:1567:ARG:HH12	2:H:1568:HIS:HB3	1.70	0.57
2:H:1908:ASP:HB2	2:H:1958:LEU:HD21	1.86	0.57
2:H:601:THR:HG22	2:H:620:ALA:H	1.69	0.57
2:H:732:TRP:CG	2:H:750:MET:HE3	2.39	0.57
2:H:907:VAL:O	2:H:910:GLN:HB3	2.03	0.57
2:I:145:LEU:O	2:I:149:VAL:HG12	2.03	0.57
2:I:654:VAL:HG23	2:I:683:ALA:HB1	1.87	0.57
1:A:232:LEU:HD13	1:A:272:GLU:HB2	1.85	0.57
1:C:1189:ILE:HD12	1:C:1380:GLN:HG3	1.86	0.57
1:C:1600:LEU:HD13	1:C:1657:HIS:HA	1.87	0.57
1:C:198:PRO:CG	1:C:209:LEU:HD21	2.28	0.57
1:C:771:PHE:CD1	1:C:825:PRO:HG3	2.40	0.57
2:G:1010:PRO:O	2:G:1011:MET:HB2	2.05	0.57
2:G:932:ILE:CD1	2:G:1042:ALA:HB2	2.24	0.57
2:G:562:LEU:O	2:G:566:HIS:HB2	2.05	0.57
2:H:736:ARG:NH1	2:H:769:SER:O	2.36	0.57
2:H:89:THR:O	2:H:93:ASN:HB2	2.04	0.57
2:I:1130:THR:H	2:I:1133:THR:HG23	1.69	0.57
1:A:604:ALA:HB3	1:A:612:GLU:HG2	1.86	0.57
1:A:828:PRO:HG3	1:A:868:ILE:HG22	1.86	0.57
1:B:980:VAL:HG21	2:H:952:ARG:HH21	1.70	0.57
1:C:1184:LEU:HB2	1:C:1352:THR:HG21	1.85	0.57
1:C:1473:GLU:O	1:C:1478:PRO:HD3	2.05	0.57
1:C:251:GLN:HA	1:C:256:LEU:H	1.69	0.57
2:G:1314:ARG:CG	2:G:1314:ARG:NH1	2.61	0.57
2:G:1954:LYS:HD3	2:G:1958:LEU:HD13	1.86	0.57
2:G:517:HIS:C	2:G:517:HIS:CD2	2.78	0.57
2:H:1782:THR:HG22	2:H:1827:LEU:HD21	1.86	0.57
2:H:732:TRP:CG	2:H:750:MET:HE1	2.40	0.57
2:I:2038:ILE:O	2:I:2042:ILE:HG12	2.04	0.57
2:I:813:THR:HB	2:I:818:LYS:HE3	1.85	0.57
1:A:988:ILE:HA	1:A:1048:GLU:HG2	1.84	0.57
1:A:655:LEU:CD2	1:A:916:LEU:HD11	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1775:GLN:HG2	2:G:1836:MET:SD	2.44	0.57
2:G:1778:GLN:HB3	2:G:1831:VAL:HG13	1.85	0.57
2:G:1890:ASN:HB2	2:G:1899:VAL:HB	1.86	0.57
2:G:741:HIS:HE1	2:G:845:THR:HG22	1.58	0.57
2:H:166:THR:HG22	2:H:168:ASP:N	2.19	0.57
2:H:61:VAL:HG21	2:H:95:TYR:HE1	1.69	0.57
2:H:561:TRP:CD1	2:H:754:TYR:HE2	2.22	0.57
2:I:665:LEU:O	2:I:669:LEU:HB2	2.05	0.57
1:A:1285:ALA:O	1:A:1289:MET:HG3	2.04	0.57
1:A:1474:ALA:O	1:A:1478:PRO:HD2	2.04	0.57
1:A:680:ILE:HG13	1:A:769:ILE:HB	1.87	0.57
1:B:140:ILE:HD13	1:B:255:GLY:O	2.05	0.57
1:B:440:MET:HE3	1:B:483:VAL:HG21	1.87	0.57
2:G:1266:TYR:CG	2:G:1347:LEU:HD23	2.40	0.57
2:G:703:LEU:HD21	2:G:705:LEU:HD21	1.86	0.57
2:H:1123:ASP:OD1	2:H:1123:ASP:N	2.36	0.57
2:H:1100:VAL:HG21	2:H:1147:ILE:CD1	2.34	0.57
2:H:1575:LEU:HD13	2:H:1579:ILE:HD12	1.85	0.57
2:H:2029:VAL:O	2:H:2033:THR:HG22	2.05	0.57
2:H:732:TRP:CD2	2:H:750:MET:CE	2.87	0.57
2:I:1292:ILE:O	2:I:1368:VAL:O	2.23	0.57
2:I:273:HIS:HB3	2:I:512:LEU:HD22	1.87	0.57
2:I:353:VAL:HG23	2:I:357:ASN:HD22	1.69	0.57
1:A:415:SER:O	1:A:419:GLU:HB2	2.05	0.57
1:A:80:CYS:SG	1:A:82:SER:HB3	2.45	0.57
1:C:1474:ALA:O	1:C:1478:PRO:HD2	2.04	0.57
2:G:1168:ASN:ND2	2:G:1171:ARG:HB2	2.20	0.57
2:G:1547:PRO:HD3	2:G:1584:PHE:CE2	2.40	0.57
2:G:463:PHE:HD1	2:G:486:LEU:HD13	1.70	0.57
2:G:455:ILE:HG13	2:G:469:ARG:HD3	1.86	0.57
2:G:584:SER:HA	2:G:587:ILE:HG23	1.87	0.57
2:G:667:LYS:HB2	2:G:698:LEU:HD23	1.85	0.57
2:G:89:THR:O	2:G:93:ASN:HB2	2.05	0.57
2:H:777:THR:CG2	2:H:1081:HIS:CE1	2.88	0.57
2:H:127:ILE:O	2:H:131:ILE:HG13	2.04	0.57
2:H:1589:VAL:HG11	2:H:1640:PHE:CE1	2.39	0.57
2:I:777:THR:CG2	2:I:1081:HIS:CE1	2.88	0.57
2:I:1199:GLU:OE2	2:I:1567:ARG:NH1	2.37	0.57
2:I:463:PHE:HD1	2:I:486:LEU:HD13	1.70	0.57
2:I:807:ILE:CG2	2:I:1066:ILE:HA	2.35	0.57
1:B:1431:GLU:HB3	1:B:1520:ALA:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:MET:HE3	1:B:529:MET:CA	2.31	0.57
1:B:742:LYS:HD3	1:B:746:GLU:OE2	2.05	0.57
1:C:341:GLN:O	1:C:345:VAL:HG12	2.05	0.57
2:G:1675:GLY:O	2:G:1678:MET:HB2	2.05	0.57
2:H:1266:TYR:CG	2:H:1347:LEU:HD23	2.40	0.57
2:H:1871:LEU:HD22	2:H:1888:ILE:HD11	1.85	0.57
2:H:1976:PHE:HA	2:H:1981:LEU:HD22	1.86	0.57
2:H:565:TYR:OH	2:H:758:ARG:HD2	2.04	0.57
2:I:1210:ILE:HB	2:I:1222:GLU:HB3	1.85	0.57
2:I:1231:GLY:O	2:I:1233:PRO:HD3	2.05	0.57
2:I:2029:VAL:O	2:I:2033:THR:HG22	2.05	0.57
2:I:607:VAL:HA	2:I:617:ILE:HD13	1.86	0.57
1:A:263:GLY:O	1:A:267:VAL:HG23	2.05	0.56
1:A:742:LYS:HD3	1:A:746:GLU:OE2	2.05	0.56
1:B:1524:GLY:O	1:B:1528:THR:HG23	2.05	0.56
1:B:152:HIS:HD2	1:B:163:LEU:HB2	1.66	0.56
1:B:251:GLN:HA	1:B:256:LEU:H	1.70	0.56
1:C:893:VAL:HG11	1:C:930:LEU:HD23	1.87	0.56
2:G:1868:GLN:HG3	2:G:1898:TYR:OH	2.04	0.56
2:G:653:TYR:CD1	2:G:659:LEU:HD21	2.39	0.56
1:B:964:GLU:HG2	2:H:1515:PRO:HB3	1.86	0.56
2:H:517:HIS:CD2	2:H:517:HIS:C	2.78	0.56
2:H:56:THR:HG23	2:H:59:GLU:CG	2.32	0.56
2:H:653:TYR:CD1	2:H:659:LEU:HD21	2.40	0.56
2:H:740:HIS:CE1	2:H:852:GLU:OE1	2.58	0.56
2:I:120:LYS:O	2:I:124:LYS:HG3	2.05	0.56
2:I:2030:TYR:CE1	2:I:2034:GLY:HA2	2.39	0.56
1:A:419:GLU:HG2	1:A:424:VAL:HB	1.86	0.56
1:C:1326:ILE:HG12	1:C:1388:MET:HG3	1.86	0.56
1:C:1524:GLY:O	1:C:1528:THR:HG23	2.05	0.56
1:C:1538:VAL:HB	1:C:1639:VAL:HG22	1.86	0.56
1:C:626:VAL:HG23	1:C:664:GLU:OE2	2.05	0.56
2:G:1567:ARG:HG3	2:G:1568:HIS:N	2.20	0.56
2:G:1804:PHE:CZ	2:G:2010:TYR:HB2	2.40	0.56
2:G:654:VAL:HG23	2:G:683:ALA:HB1	1.87	0.56
2:H:1352:HIS:HE1	2:H:1583:MET:HE1	1.69	0.56
2:H:638:VAL:HA	2:H:641:ILE:HG22	1.86	0.56
2:G:28:PHE:HZ	2:H:7:ARG:NE	2.02	0.56
2:H:839:PRO:HA	2:H:844:VAL:HG13	1.86	0.56
2:H:926:LEU:HD13	2:H:947:THR:HG22	1.86	0.56
2:I:1223:MET:HE3	2:I:1238:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:197:GLU:OE1	2:I:197:GLU:HA	2.05	0.56
1:C:20:TYR:HE1	2:I:2035:SER:HB2	1.69	0.56
2:I:281:VAL:HG23	2:I:459:VAL:HG11	1.87	0.56
2:I:741:HIS:HB3	2:I:853:PRO:HB2	1.86	0.56
2:I:89:THR:O	2:I:93:ASN:HB2	2.05	0.56
1:A:1014:ASP:N	1:A:1510:ASN:HD21	1.92	0.56
1:B:152:HIS:CE1	1:B:168:MET:HG3	2.40	0.56
2:G:1194:VAL:HG12	2:G:1194:VAL:O	2.05	0.56
2:G:1989:LYS:O	2:G:1993:LYS:HG3	2.05	0.56
2:G:1086:LEU:HD12	2:G:1090:TYR:CB	2.35	0.56
2:G:663:ILE:HG13	2:G:694:TYR:HE1	1.70	0.56
2:H:522:GLY:HA3	2:H:561:TRP:CZ3	2.40	0.56
2:H:561:TRP:O	2:H:562:LEU:C	2.42	0.56
2:H:702:TYR:CB	2:H:727:PRO:HB2	2.36	0.56
2:I:1149:TRP:CD1	2:I:1213:LEU:CD1	2.88	0.56
2:I:443:LEU:HD22	2:I:448:VAL:HG11	1.87	0.56
2:I:481:ASP:OD2	2:I:485:ARG:NH1	2.38	0.56
2:I:490:TRP:CH2	2:I:512:LEU:HD21	2.40	0.56
2:I:543:PHE:CB	2:I:545:GLN:HE22	2.17	0.56
1:B:488:PRO:HG3	1:B:728:LYS:HG3	1.87	0.56
1:C:635:ILE:HG22	1:C:651:TYR:CD1	2.41	0.56
2:G:813:THR:HB	2:G:818:LYS:HE3	1.87	0.56
2:H:1223:MET:CE	2:H:1238:LEU:HD12	2.35	0.56
2:H:1834:ARG:NH1	2:H:1834:ARG:CG	2.60	0.56
2:H:376:ASN:HD22	2:H:377:LEU:N	2.03	0.56
2:H:835:THR:HG22	2:H:844:VAL:C	2.26	0.56
2:I:1722:GLY:N	2:I:1726:GLY:HA3	2.21	0.56
2:I:1804:PHE:CZ	2:I:2010:TYR:HB2	2.40	0.56
1:A:1009:LEU:HA	1:A:1445:MET:HE2	1.87	0.56
1:A:21:GLN:O	2:G:1977:HIS:CD2	2.59	0.56
1:B:411:GLN:HE22	1:B:1628:SER:H	1.52	0.56
1:C:152:HIS:HD2	1:C:163:LEU:HB2	1.63	0.56
2:G:1834:ARG:HH11	2:G:1834:ARG:CG	2.03	0.56
2:G:543:PHE:CB	2:G:545:GLN:HE22	2.17	0.56
2:G:758:ARG:NH2	2:G:797:ASP:OD1	2.33	0.56
2:H:120:LYS:O	2:H:124:LYS:HG3	2.06	0.56
2:H:606:PHE:HZ	2:H:805:VAL:HG11	1.68	0.56
1:A:1057:MET:SD	1:A:1097:ILE:HG23	2.45	0.56
1:A:221:LEU:O	1:A:225:SER:HB3	2.05	0.56
1:B:1419:PRO:HB3	1:B:1646:PHE:CZ	2.40	0.56
1:C:1022:THR:HG22	1:C:1226:SER:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:741:SER:HB3	1:C:744:ASP:HB2	1.86	0.56
2:H:1920:GLN:HG2	2:H:1922:ILE:HD11	1.87	0.56
1:B:1009:LEU:HG	1:B:1664:ALA:HB2	1.87	0.56
1:C:695:GLY:HA3	1:C:906:LEU:HD11	1.88	0.56
2:G:1722:GLY:N	2:G:1726:GLY:HA3	2.21	0.56
2:G:634:ILE:HD11	2:G:649:ILE:CD1	2.34	0.56
2:H:1890:ASN:HB2	2:H:1899:VAL:HB	1.88	0.56
2:H:443:LEU:HD22	2:H:448:VAL:HG11	1.86	0.56
2:H:463:PHE:HD1	2:H:486:LEU:HD13	1.71	0.56
2:I:1567:ARG:HH12	2:I:1568:HIS:HB3	1.71	0.56
2:I:835:THR:HG23	2:I:843:ILE:O	2.05	0.56
1:A:1036:ARG:NH1	1:A:1040:GLU:OE1	2.39	0.56
1:A:152:HIS:CE1	1:A:168:MET:HG3	2.41	0.56
1:A:251:GLN:HA	1:A:256:LEU:H	1.68	0.56
1:B:1138:LYS:HG3	1:B:1163:TYR:CE1	2.41	0.56
1:B:1492:GLU:O	1:B:1496:GLU:HG3	2.06	0.56
1:B:644:THR:HG22	1:B:648:ASP:O	2.06	0.56
2:G:577:ILE:HD13	2:G:1097:ILE:CD1	2.35	0.56
2:G:589:ARG:HB3	2:G:590:PRO:HD2	1.87	0.56
2:G:599:PRO:HD2	4:G:3051:FMN:H6	1.88	0.56
2:H:1868:GLN:HG3	2:H:1898:TYR:OH	2.05	0.56
2:H:607:VAL:HA	2:H:617:ILE:HD13	1.88	0.56
2:I:601:THR:HG22	2:I:620:ALA:H	1.71	0.56
2:I:702:TYR:CB	2:I:727:PRO:HB2	2.36	0.56
2:I:732:TRP:CG	2:I:750:MET:HE3	2.39	0.56
2:I:774:ALA:HB1	2:I:1081:HIS:CD2	2.33	0.56
2:I:871:THR:HB	2:I:872:ILE:HD12	1.88	0.56
1:B:529:MET:HG2	1:B:638:LEU:CD1	2.35	0.56
1:C:1259:GLY:HA2	1:C:1263:ASP:HB2	1.87	0.56
1:C:329:GLU:O	1:C:333:LYS:HG3	2.06	0.56
1:C:531:LEU:HD21	1:C:629:THR:HG22	1.88	0.56
1:C:881:ASN:HA	1:C:944:ARG:HH21	1.70	0.56
2:G:1130:THR:H	2:G:1133:THR:HG23	1.70	0.56
2:G:1567:ARG:HH12	2:G:1568:HIS:HB3	1.71	0.56
2:G:702:TYR:CB	2:G:727:PRO:HB2	2.35	0.56
2:H:1100:VAL:HG21	2:H:1147:ILE:HD13	1.88	0.56
2:H:1194:VAL:O	2:H:1194:VAL:HG12	2.05	0.56
2:H:1778:GLN:HB3	2:H:1831:VAL:HG13	1.88	0.56
2:H:1989:LYS:O	2:H:1993:LYS:HG3	2.06	0.56
2:H:553:ASN:O	2:H:556:LYS:HE3	2.06	0.56
2:I:1931:LEU:HD22	2:I:1935:GLU:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1052:GLU:O	1:A:1056:ILE:HG23	2.06	0.56
1:A:1665:ILE:CG1	1:A:1669:ARG:HD3	2.36	0.56
1:A:1498:GLU:CB	1:A:1876:LEU:HD13	1.83	0.56
1:C:1419:PRO:HB3	1:C:1646:PHE:CZ	2.41	0.56
1:C:1749:THR:CA	1:C:1874:ASP:HB3	2.32	0.56
2:G:120:LYS:O	2:G:124:LYS:HG3	2.05	0.56
2:G:1308:CYS:HB3	2:G:1311:PHE:CD2	2.41	0.56
2:G:1874:VAL:O	2:G:1878:VAL:HG12	2.05	0.56
2:H:1308:CYS:HB3	2:H:1311:PHE:CD2	2.41	0.56
2:H:1328:VAL:HG23	2:H:1557:SER:HA	1.88	0.56
2:I:826:GLY:HA2	2:I:1060:ALA:HB3	1.88	0.56
2:I:577:ILE:HD13	2:I:1097:ILE:CD1	2.36	0.56
2:I:1589:VAL:HG11	2:I:1640:PHE:CE1	2.41	0.56
2:I:732:TRP:CD1	2:I:750:MET:HE3	2.40	0.56
1:A:1524:GLY:HA2	1:A:1527:ALA:HB3	1.89	0.55
1:A:295:ALA:HB2	1:A:302:LEU:HD11	1.87	0.55
1:B:11:HIS:O	1:B:15:THR:HG22	2.06	0.55
1:B:1233:GLU:OE2	1:B:1680:ARG:NH2	2.40	0.55
1:C:1496:GLU:O	1:C:1500:GLN:HG3	2.06	0.55
2:G:1475:LYS:HG3	2:G:1481:SER:HB2	1.88	0.55
2:G:1561:ASN:OD1	2:G:1563:ILE:HB	2.05	0.55
2:G:732:TRP:CD2	2:G:750:MET:HE1	2.41	0.55
2:H:1493:LEU:HD11	2:H:1499:VAL:CG2	2.36	0.55
2:H:16:LEU:HG	2:H:48:PHE:CZ	2.40	0.55
2:H:239:PRO:HG3	2:H:304:PHE:HA	1.88	0.55
2:I:1308:CYS:HB3	2:I:1311:PHE:CD2	2.40	0.55
1:C:29:ILE:HG13	2:I:1891:TYR:O	2.06	0.55
2:I:7:ARG:NH1	2:I:24:THR:HA	2.20	0.55
2:I:653:TYR:CD1	2:I:659:LEU:HD21	2.40	0.55
1:A:1114:TYR:CD1	1:A:1337:GLU:HG3	2.41	0.55
1:A:1555:ALA:HA	1:A:1621:PHE:CE1	2.41	0.55
1:A:864:VAL:CG2	1:A:921:PRO:HB3	2.36	0.55
1:B:1538:VAL:HB	1:B:1639:VAL:HG22	1.87	0.55
1:B:733:ILE:HD12	1:B:761:LEU:HD21	1.88	0.55
1:B:988:ILE:HD13	1:B:1048:GLU:HB3	1.89	0.55
1:C:335:HIS:HD2	1:C:335:HIS:O	1.89	0.55
2:G:652:ILE:HB	2:G:658:MET:CE	2.36	0.55
2:H:7:ARG:NH1	2:H:24:THR:HA	2.21	0.55
2:I:1931:LEU:HB3	2:I:1935:GLU:CG	2.35	0.55
2:I:232:LEU:HD23	2:I:232:LEU:O	2.06	0.55
1:A:1665:ILE:HD11	1:A:1669:ARG:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1665:ILE:HD11	1:B:1669:ARG:HG2	1.88	0.55
1:B:433:VAL:O	1:B:437:ILE:HG13	2.07	0.55
1:C:12:ILE:HA	1:C:15:THR:HG23	1.88	0.55
1:C:417:TYR:OH	1:C:458:THR:HG22	2.06	0.55
2:G:1931:LEU:HB3	2:G:1935:GLU:CG	2.33	0.55
2:G:2036:GLU:O	2:G:2039:LYS:HG2	2.06	0.55
2:G:722:ALA:HB1	2:G:723:HIS:CE1	2.42	0.55
2:H:1822:MET:HE2	2:H:1996:ILE:HG12	1.89	0.55
2:H:490:TRP:HA	2:H:493:THR:CG2	2.36	0.55
2:I:124:LYS:HG2	2:I:179:THR:HA	1.87	0.55
2:I:634:ILE:HD11	2:I:649:ILE:CD1	2.35	0.55
1:A:825:PRO:HB2	1:A:843:LYS:NZ	2.21	0.55
1:B:1036:ARG:NH1	1:B:1040:GLU:OE1	2.40	0.55
1:C:1347:LYS:HD3	1:C:1347:LYS:O	2.05	0.55
1:C:1:MET:HE3	1:C:9:LEU:HD12	1.89	0.55
2:G:1678:MET:CE	2:G:1707:LEU:HD22	2.35	0.55
2:G:665:LEU:O	2:G:669:LEU:HB2	2.06	0.55
2:H:1431:TYR:CE1	2:H:1526:THR:HG23	2.41	0.55
1:C:1498:GLU:CG	1:C:1876:LEU:CB	2.64	0.55
1:C:254:TRP:CZ3	1:C:302:LEU:HD13	2.41	0.55
1:C:27:ARG:HD2	1:C:30:GLU:OE2	2.06	0.55
1:C:807:LYS:HG3	1:C:858:TRP:HB3	1.87	0.55
2:G:1475:LYS:HB2	2:G:1481:SER:HB2	1.89	0.55
2:H:1166:VAL:HG12	2:H:1167:SER:N	2.21	0.55
2:H:2038:ILE:HG22	2:H:2042:ILE:CD1	2.36	0.55
2:I:166:THR:HG22	2:I:168:ASP:N	2.21	0.55
2:I:638:VAL:HA	2:I:641:ILE:HG22	1.88	0.55
2:I:926:LEU:HB3	2:I:947:THR:HG22	1.88	0.55
2:I:61:VAL:HG21	2:I:95:TYR:HE1	1.72	0.55
1:A:1238:VAL:HG12	1:A:1239:HIS:N	2.21	0.55
1:A:1498:GLU:CB	1:A:1876:LEU:CD1	2.63	0.55
1:C:1125:VAL:HG21	1:C:1175:ILE:HD12	1.88	0.55
1:C:152:HIS:CE1	1:C:168:MET:HG3	2.41	0.55
1:C:11:HIS:O	1:C:15:THR:HG22	2.06	0.55
1:C:383:GLY:O	1:C:387:VAL:HG23	2.07	0.55
2:G:1496:LYS:HE2	2:G:1693:ARG:NH2	2.20	0.55
2:G:197:GLU:OE1	2:G:197:GLU:HA	2.06	0.55
2:H:807:ILE:CG2	2:H:1066:ILE:HA	2.36	0.55
2:H:1359:MET:HE3	2:H:1359:MET:HA	1.88	0.55
2:I:2015:THR:HG22	2:I:2017:LYS:N	2.21	0.55
1:A:1056:ILE:HD13	1:A:1193:TRP:CD1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1233:GLU:OE2	1:A:1680:ARG:NH2	2.40	0.55
1:A:12:ILE:HD11	2:G:2041:ILE:HD11	1.83	0.55
1:A:1473:GLU:O	1:A:1478:PRO:HD3	2.06	0.55
1:A:529:MET:HG2	1:A:638:LEU:CD1	2.36	0.55
1:A:771:PHE:CD1	1:A:825:PRO:HG3	2.42	0.55
1:B:1285:ALA:O	1:B:1289:MET:HG3	2.07	0.55
1:B:1432:HIS:CE1	1:B:1434:SER:OG	2.60	0.55
1:B:328:LEU:C	1:B:328:LEU:HD22	2.28	0.55
1:A:332:THR:HG22	1:B:331:ILE:CD1	2.36	0.55
1:C:883:ILE:HD12	1:C:947:LEU:HD12	1.88	0.55
2:G:239:PRO:HG3	2:G:304:PHE:HA	1.88	0.55
2:H:584:SER:HA	2:H:587:ILE:HG23	1.89	0.55
2:H:707:PRO:HG2	2:H:730:LEU:HD13	1.89	0.55
2:I:1432:GLN:HB2	2:I:1527:LEU:HD12	1.88	0.55
2:I:1873:TYR:HE1	2:I:1877:ARG:HH21	1.54	0.55
2:I:603:SER:O	2:I:607:VAL:HG12	2.06	0.55
1:C:635:ILE:HG22	1:C:651:TYR:CG	2.42	0.55
2:G:777:THR:CG2	2:G:1081:HIS:CE1	2.89	0.55
2:G:1822:MET:CE	2:G:1996:ILE:HG12	2.37	0.55
2:H:1173:VAL:CG2	2:H:1221:MET:HE1	2.35	0.55
2:H:1822:MET:CE	2:H:1996:ILE:HG12	2.37	0.55
2:H:264:ARG:NH1	2:H:456:GLN:HG3	2.22	0.55
2:H:740:HIS:HA	2:H:854:ILE:HD13	1.89	0.55
2:I:1427:VAL:HG12	2:I:1427:VAL:O	2.07	0.55
2:I:741:HIS:CE1	2:I:855:HIS:CD2	2.95	0.55
1:A:56:MET:HG3	2:G:1893:VAL:CG2	2.37	0.55
1:A:982:ILE:HG13	2:G:965:SER:N	2.22	0.55
1:C:176:VAL:HG12	1:C:178:GLY:H	1.72	0.55
1:C:50:SER:HB2	1:C:51:PRO:HD3	1.88	0.55
2:G:127:ILE:O	2:G:131:ILE:HG13	2.07	0.55
2:G:1624:THR:HB	2:G:1642:THR:HG23	1.86	0.55
2:G:747:HIS:O	2:G:751:LEU:HB2	2.07	0.55
2:G:835:THR:HG23	2:G:843:ILE:O	2.06	0.55
2:H:1350:LEU:HD11	2:H:1410:PHE:HB3	1.89	0.55
2:H:1567:ARG:NH1	2:H:1567:ARG:CG	2.50	0.55
2:H:1697:HIS:CE1	2:H:1829:GLU:HG2	2.42	0.55
2:H:1844:ARG:CG	2:H:1844:ARG:NH1	2.58	0.55
2:H:402:LEU:O	2:H:402:LEU:HD13	2.07	0.55
2:I:1010:PRO:O	2:I:1011:MET:HB2	2.05	0.55
2:I:1168:ASN:ND2	2:I:1171:ARG:HB2	2.22	0.55
1:A:1392:LEU:HD22	1:A:1396:MET:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1123:GLN:HG3	1:B:1124:GLU:N	2.22	0.55
1:B:1566:ARG:HB3	1:B:1623:TYR:CE1	2.42	0.55
1:B:49:PRO:O	1:B:82:SER:HB2	2.07	0.55
1:C:1009:LEU:HD13	1:C:1445:MET:HE1	1.89	0.55
1:C:1455:ARG:NH2	1:C:1459:ILE:HG12	2.22	0.55
2:G:264:ARG:NH1	2:G:456:GLN:HG3	2.22	0.55
2:H:1475:LYS:HB2	2:H:1481:SER:HB2	1.88	0.55
2:H:2036:GLU:O	2:H:2039:LYS:HG2	2.07	0.55
2:I:1293:THR:HG22	2:I:1296:GLU:CD	2.28	0.55
2:I:1624:THR:HB	2:I:1642:THR:OG1	2.06	0.55
2:I:260:PRO:HD3	2:I:289:TRP:CE2	2.42	0.55
1:A:1194:ASN:HB3	1:A:1197:THR:HG22	1.88	0.54
1:B:1373:ARG:HB2	1:B:1545:SER:O	2.07	0.54
1:C:1501:LEU:O	1:C:1505:GLN:HG3	2.07	0.54
1:C:1:MET:HE3	1:C:5:VAL:HG12	1.88	0.54
2:G:1227:ARG:CG	2:G:1227:ARG:NH1	2.56	0.54
2:G:1313:SER:O	2:G:1314:ARG:HD3	2.07	0.54
2:G:598:THR:HG23	4:G:3051:FMN:O4	2.06	0.54
2:H:1159:ILE:HG12	2:H:1169:PRO:CD	2.36	0.54
2:I:1493:LEU:HD11	2:I:1499:VAL:CG2	2.37	0.54
1:A:1455:ARG:NH2	1:A:1459:ILE:HG12	2.22	0.54
1:A:236:LYS:HE2	1:A:273:PRO:O	2.07	0.54
1:A:733:ILE:CD1	1:A:761:LEU:HD11	2.37	0.54
1:A:741:SER:HB3	1:A:744:ASP:HB2	1.89	0.54
1:B:263:GLY:O	1:B:267:VAL:HG23	2.07	0.54
1:B:771:PHE:CD1	1:B:825:PRO:HG3	2.42	0.54
1:C:1373:ARG:HB2	1:C:1545:SER:O	2.07	0.54
1:C:286:PHE:O	1:C:290:MET:HG2	2.07	0.54
2:G:1859:PRO:CG	2:G:1871:LEU:HD12	2.20	0.54
2:G:464:ASP:HB3	2:G:466:SER:HB3	1.88	0.54
2:H:1293:THR:HG22	2:H:1296:GLU:CD	2.28	0.54
2:H:1976:PHE:HB3	2:H:1981:LEU:HD21	1.89	0.54
2:I:131:ILE:HD12	2:I:182:VAL:CB	2.33	0.54
2:I:1331:TRP:CE2	2:I:1335:ILE:HG13	2.42	0.54
2:I:145:LEU:HD21	2:I:156:LEU:HD21	1.89	0.54
2:I:606:PHE:HZ	2:I:805:VAL:HG11	1.71	0.54
1:A:430:ARG:NH2	1:A:605:LEU:HD13	2.23	0.54
2:G:1292:ILE:O	2:G:1368:VAL:O	2.25	0.54
2:G:332:GLU:OE2	2:G:394:ARG:HD3	2.07	0.54
2:G:462:THR:HB	2:G:482:CYS:SG	2.48	0.54
2:H:1497:GLU:OE1	2:H:2002:LYS:HE3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2015:THR:HG22	2:H:2017:LYS:N	2.21	0.54
2:H:732:TRP:CD2	2:H:750:MET:HE3	2.43	0.54
2:I:1567:ARG:CG	2:I:1567:ARG:NH1	2.50	0.54
2:I:517:HIS:CD2	2:I:517:HIS:C	2.80	0.54
1:A:1475:GLU:HG2	1:A:1761:LYS:O	2.06	0.54
1:A:1748:ASN:C	1:A:1750:ILE:H	2.11	0.54
1:A:733:ILE:HD12	1:A:761:LEU:HD21	1.89	0.54
1:A:20:TYR:CD1	2:G:2033:THR:HG21	2.42	0.54
2:H:1102:TYR:HB3	2:H:1244:PRO:HA	1.90	0.54
2:H:490:TRP:HE1	2:H:516:THR:CG2	2.01	0.54
2:H:611:THR:CG2	2:H:641:ILE:HG13	2.38	0.54
2:I:1093:ASP:HB3	2:I:1096:LYS:HG3	1.89	0.54
2:I:1166:VAL:HG12	2:I:1167:SER:N	2.23	0.54
2:I:490:TRP:HA	2:I:493:THR:CG2	2.38	0.54
1:A:1501:LEU:CD1	1:A:1775:LEU:CG	2.86	0.54
1:A:1657:HIS:ND1	1:A:1658:PRO:HD2	2.21	0.54
1:A:183:GLN:O	1:A:187:LEU:HG	2.08	0.54
1:B:1501:LEU:O	1:B:1505:GLN:HG3	2.08	0.54
1:B:1401:TYR:C	1:B:1658:PRO:HG3	2.27	0.54
1:B:1749:THR:CB	1:B:1874:ASP:HA	2.33	0.54
1:C:479:ASN:O	1:C:483:VAL:HG23	2.07	0.54
2:G:1575:LEU:HD13	2:G:1579:ILE:HD12	1.89	0.54
2:G:344:LEU:HB3	2:G:349:VAL:HG23	1.90	0.54
2:H:85:ASN:HD22	2:H:135:ARG:NH1	2.02	0.54
2:I:1475:LYS:HB2	2:I:1481:SER:HB2	1.89	0.54
2:I:1547:PRO:HD3	2:I:1584:PHE:CE2	2.43	0.54
2:I:2046:GLU:C	2:I:2048:TYR:H	2.11	0.54
2:I:584:SER:HA	2:I:587:ILE:HG23	1.89	0.54
1:A:1234:MET:CE	1:A:1326:ILE:HG21	2.38	0.54
1:A:328:LEU:C	1:A:328:LEU:HD22	2.28	0.54
1:B:385:PHE:HD2	1:B:787:LYS:HA	1.73	0.54
1:B:824:LEU:HD11	1:B:849:LEU:HD12	1.89	0.54
1:C:1123:GLN:HG3	1:C:1124:GLU:N	2.23	0.54
2:G:1697:HIS:CE1	2:G:1829:GLU:HG2	2.43	0.54
2:G:2030:TYR:CE1	2:G:2034:GLY:HA2	2.43	0.54
2:G:807:ILE:HG21	2:G:1066:ILE:HA	1.88	0.54
2:H:1547:PRO:HD3	2:H:1584:PHE:CE2	2.42	0.54
2:H:464:ASP:HB3	2:H:466:SER:HB3	1.90	0.54
2:I:1417:THR:O	2:I:1419:PHE:N	2.30	0.54
2:I:1778:GLN:HB3	2:I:1831:VAL:HG13	1.88	0.54
2:I:123:ILE:HD11	2:I:533:LEU:CD2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:611:THR:CG2	2:I:641:ILE:HG13	2.37	0.54
2:I:652:ILE:HB	2:I:658:MET:CE	2.37	0.54
1:A:1184:LEU:HB2	1:A:1352:THR:HG21	1.89	0.54
1:B:23:ALA:O	2:H:1977:HIS:HA	2.07	0.54
2:G:1428:GLU:HB2	2:G:1468:THR:HG22	1.88	0.54
2:G:1749:GLU:OE2	2:G:1840:VAL:CG1	2.56	0.54
1:B:236:LYS:HE2	1:B:273:PRO:O	2.07	0.54
1:B:280:GLU:O	1:B:280:GLU:HG2	2.08	0.54
1:B:655:LEU:CD2	1:B:916:LEU:HD11	2.38	0.54
1:C:1748:ASN:C	1:C:1750:ILE:H	2.12	0.54
2:G:601:THR:CG2	2:G:618:GLU:O	2.41	0.54
2:H:1378:ILE:HD11	2:H:1381:VAL:HG21	1.90	0.54
2:H:964:LEU:N	2:H:964:LEU:CD2	2.70	0.54
2:I:1452:LEU:HA	2:I:1502:GLY:HA3	1.88	0.54
2:I:545:GLN:NE2	2:I:545:GLN:H	2.06	0.54
2:I:722:ALA:HB1	2:I:723:HIS:CE1	2.42	0.54
2:I:99:ASN:HA	2:I:550:VAL:HG21	1.90	0.54
1:A:1496:GLU:O	1:A:1500:GLN:HG3	2.07	0.54
1:B:695:GLY:HA3	1:B:906:LEU:HD11	1.90	0.54
1:C:1477:ILE:H	1:C:1478:PRO:CD	2.20	0.54
1:C:37:LYS:HB2	1:C:65:TYR:HE1	1.72	0.54
2:I:826:GLY:O	2:I:827:VAL:HG23	2.07	0.54
1:A:1138:LYS:HG3	1:A:1163:TYR:CE1	2.43	0.54
1:A:340:ARG:HH12	1:A:344:GLN:NE2	2.06	0.54
1:A:644:THR:HG22	1:A:648:ASP:O	2.08	0.54
1:A:625:THR:HG23	1:A:661:ASP:OD1	2.08	0.54
1:B:1600:LEU:HD13	1:B:1657:HIS:HA	1.90	0.54
1:B:635:ILE:HG22	1:B:651:TYR:CG	2.43	0.54
1:C:1682:LYS:HB3	2:I:994:PHE:CE2	2.43	0.54
1:C:516:ARG:NH2	1:C:889:GLU:OE1	2.41	0.54
2:G:1231:GLY:O	2:G:1233:PRO:HD3	2.08	0.54
2:I:1054:LEU:CB	4:I:3051:FMN:C7M	2.85	0.54
2:I:1172:LYS:HE3	2:I:1574:ASN:OD1	2.08	0.54
2:I:332:GLU:OE2	2:I:394:ARG:HD3	2.08	0.54
2:I:868:PHE:HB3	2:I:873:PHE:CE2	2.43	0.54
1:A:1125:VAL:HG21	1:A:1175:ILE:HD12	1.88	0.53
1:B:1010:GLU:HA	1:B:1664:ALA:HA	1.89	0.53
1:C:1194:ASN:HB3	1:C:1197:THR:HG22	1.89	0.53
1:C:529:MET:HG2	1:C:638:LEU:CD1	2.39	0.53
2:H:1313:SER:O	2:H:1314:ARG:HD3	2.09	0.53
2:H:1325:PHE:CE1	2:H:1328:VAL:HG11	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:146:PHE:HA	2:H:149:VAL:HG12	1.89	0.53
2:I:754:TYR:CD2	2:I:794:MET:HG3	2.42	0.53
1:A:1120:GLU:O	1:A:1121:MET:CG	2.56	0.53
1:A:1566:ARG:HB3	1:A:1623:TYR:CE1	2.42	0.53
1:B:807:LYS:HG3	1:B:858:TRP:HB3	1.90	0.53
1:C:825:PRO:HB2	1:C:843:LYS:NZ	2.24	0.53
2:G:1331:TRP:CE2	2:G:1335:ILE:HG13	2.43	0.53
2:H:1177:SER:O	2:H:1180:MET:HG2	2.08	0.53
2:H:606:PHE:CE1	2:H:811:VAL:HG13	2.43	0.53
2:I:615:TYR:CZ	2:I:1074:MET:HB3	2.42	0.53
2:I:1844:ARG:CG	2:I:1844:ARG:NH1	2.61	0.53
2:I:1954:LYS:HD3	2:I:1958:LEU:HD13	1.89	0.53
1:A:1153:ASP:OD2	1:B:359:ARG:NH2	2.41	0.53
1:A:1123:GLN:HB2	1:A:1177:LYS:HE2	1.90	0.53
1:A:1392:LEU:CD2	1:A:1396:MET:HG3	2.38	0.53
1:B:1194:ASN:O	1:B:1197:THR:HG23	2.08	0.53
1:C:236:LYS:HE2	1:C:273:PRO:O	2.08	0.53
2:G:1269:LEU:O	2:G:1560:LEU:HD23	2.08	0.53
2:H:281:VAL:HG23	2:H:459:VAL:HG11	1.90	0.53
2:H:674:TYR:HB3	2:H:676:ILE:HG22	1.88	0.53
2:H:826:GLY:O	2:H:827:VAL:HG23	2.07	0.53
2:I:873:PHE:CD1	2:I:1026:GLU:HB2	2.43	0.53
2:I:234:ILE:CG1	2:I:235:PRO:HD3	2.38	0.53
2:I:491:GLU:HA	2:I:494:THR:HG22	1.89	0.53
2:I:582:LYS:HE2	2:I:1108:PRO:HB3	1.91	0.53
1:A:1373:ARG:HB2	1:A:1545:SER:O	2.08	0.53
1:A:807:LYS:HG3	1:A:858:TRP:HB3	1.91	0.53
1:B:1392:LEU:CD2	1:B:1396:MET:HG3	2.38	0.53
1:B:1020:VAL:HG13	1:B:1400:ILE:HG23	1.91	0.53
1:C:263:GLY:O	1:C:267:VAL:HG23	2.08	0.53
1:C:824:LEU:HD11	1:C:849:LEU:HD12	1.90	0.53
2:G:741:HIS:CB	2:G:853:PRO:HB2	2.38	0.53
2:G:892:ILE:HG12	2:G:903:TRP:CG	2.43	0.53
2:G:964:LEU:CD2	2:G:964:LEU:N	2.68	0.53
2:H:55:THR:CG2	2:H:56:THR:HG22	2.30	0.53
2:I:1745:LYS:HE2	2:I:1747:LYS:HG2	1.91	0.53
2:I:271:THR:OG1	2:I:460:TYR:HB2	2.08	0.53
1:A:421:ILE:HG13	1:A:469:VAL:HG21	1.89	0.53
1:B:1665:ILE:CG1	1:B:1669:ARG:HD3	2.36	0.53
1:B:607:LYS:HG2	1:B:608:ASP:N	2.23	0.53
1:B:751:PHE:CZ	1:B:761:LEU:HD13	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:LYS:HD3	1:C:185:GLU:HB3	1.91	0.53
1:C:1401:TYR:C	1:C:1658:PRO:HG3	2.29	0.53
2:G:707:PRO:HG2	2:G:730:LEU:HD13	1.90	0.53
2:H:1804:PHE:CZ	2:H:2010:TYR:HB2	2.44	0.53
2:H:173:LEU:HD13	2:H:219:LEU:HD21	1.90	0.53
2:H:816:ASP:HB3	2:H:1048:VAL:HG21	1.91	0.53
2:I:1102:TYR:HB3	2:I:1244:PRO:HA	1.91	0.53
2:I:1177:SER:O	2:I:1180:MET:HG2	2.09	0.53
2:I:1314:ARG:CG	2:I:1314:ARG:NH1	2.63	0.53
2:I:1431:TYR:CE1	2:I:1526:THR:HG22	2.44	0.53
2:I:1567:ARG:HG3	2:I:1568:HIS:N	2.22	0.53
2:I:526:ARG:HH11	2:I:558:ASN:HD21	1.55	0.53
1:C:985:ARG:HH12	2:I:953:ARG:CZ	2.21	0.53
1:A:1020:VAL:HG13	1:A:1400:ILE:HG23	1.90	0.53
1:A:1665:ILE:HG12	1:A:1666:THR:N	2.23	0.53
1:A:50:SER:HB2	1:A:51:PRO:CD	2.39	0.53
1:A:635:ILE:HG22	1:A:651:TYR:CG	2.43	0.53
1:A:529:MET:CE	1:A:894:ARG:HD2	2.38	0.53
1:C:825:PRO:HB2	1:C:843:LYS:HZ2	1.73	0.53
2:G:2015:THR:HG22	2:G:2017:LYS:N	2.22	0.53
2:G:913:ASP:H	2:G:916:THR:CG2	2.22	0.53
2:H:1567:ARG:HG3	2:H:1568:HIS:N	2.23	0.53
2:H:652:ILE:HB	2:H:658:MET:CE	2.39	0.53
2:I:1173:VAL:CG2	2:I:1221:MET:HE1	2.39	0.53
2:I:1293:THR:HG22	2:I:1296:GLU:CG	2.39	0.53
2:I:2036:GLU:HG2	2:I:2039:LYS:NZ	2.23	0.53
1:A:1492:GLU:O	1:A:1496:GLU:HG3	2.09	0.53
1:B:1123:GLN:HB2	1:B:1177:LYS:HE2	1.91	0.53
1:B:1577:GLN:HE22	1:B:1591:TRP:C	2.12	0.53
1:C:1012:LEU:HD23	1:C:1445:MET:CE	2.39	0.53
1:C:1037:TRP:HB2	1:C:1598:GLN:OE1	2.09	0.53
2:G:1166:VAL:HG12	2:G:1167:SER:N	2.23	0.53
2:G:346:GLN:HA	2:G:377:LEU:HD21	1.89	0.53
2:G:606:PHE:HZ	2:G:805:VAL:HG11	1.74	0.53
2:H:1913:VAL:O	2:H:1917:ILE:HG13	2.08	0.53
2:H:402:LEU:HD12	2:H:404:GLN:HG2	1.90	0.53
2:H:774:ALA:HB1	2:H:1081:HIS:CD2	2.32	0.53
2:I:1327:ILE:HG12	2:I:1583:MET:HE3	1.91	0.53
1:A:1014:ASP:H	1:A:1510:ASN:ND2	1.93	0.53
1:A:385:PHE:HD2	1:A:787:LYS:HA	1.74	0.53
1:A:483:VAL:O	1:A:486:VAL:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:ILE:HA	1:B:15:THR:HG23	1.90	0.53
1:C:1524:GLY:HA2	1:C:1527:ALA:HB3	1.91	0.53
2:G:490:TRP:CH2	2:G:512:LEU:HD21	2.43	0.53
2:G:750:MET:CG	2:G:796:PHE:HZ	2.21	0.53
2:G:85:ASN:HD22	2:G:135:ARG:NH1	2.03	0.53
2:H:1040:LEU:HD21	2:H:1048:VAL:HA	1.89	0.53
2:H:1452:LEU:HA	2:H:1502:GLY:HA3	1.90	0.53
2:H:1954:LYS:HD3	2:H:1958:LEU:HD13	1.90	0.53
2:H:346:GLN:HA	2:H:377:LEU:HD21	1.91	0.53
2:I:1040:LEU:HD21	2:I:1048:VAL:HA	1.90	0.53
2:I:1441:ILE:HD11	2:I:1445:ARG:NH2	2.23	0.53
2:I:1861:ARG:HD2	2:I:1964:PHE:O	2.08	0.53
2:I:2038:ILE:HG22	2:I:2042:ILE:CD1	2.37	0.53
2:I:892:ILE:HG12	2:I:903:TRP:CG	2.44	0.53
1:A:1455:ARG:O	1:A:1459:ILE:HG13	2.08	0.53
1:A:12:ILE:HA	1:A:15:THR:HG23	1.88	0.53
1:C:1036:ARG:NH1	1:C:1040:GLU:OE1	2.41	0.53
2:G:1040:LEU:HD21	2:G:1048:VAL:HA	1.90	0.53
2:G:2038:ILE:HG22	2:G:2042:ILE:CD1	2.37	0.53
2:G:281:VAL:HG23	2:G:459:VAL:HG11	1.91	0.53
2:H:1745:LYS:HE2	2:H:1747:LYS:HG2	1.91	0.53
2:I:1266:TYR:CG	2:I:1347:LEU:HD23	2.43	0.53
2:I:2035:SER:HB3	2:I:2038:ILE:CG1	2.37	0.53
2:I:240:LEU:O	2:I:244:ILE:HG13	2.08	0.53
2:I:871:THR:HG21	2:I:887:LYS:NZ	2.24	0.53
1:B:1326:ILE:HG12	1:B:1388:MET:HG3	1.91	0.53
1:C:1285:ALA:O	1:C:1289:MET:HG3	2.09	0.53
1:C:625:THR:HG23	1:C:661:ASP:OD1	2.09	0.53
2:G:1173:VAL:CG2	2:G:1221:MET:HE1	2.38	0.53
2:G:102:HIS:HE1	2:G:180:TYR:OH	1.92	0.53
2:G:1861:ARG:HD2	2:G:1964:PHE:O	2.09	0.53
2:H:1101:GLU:HB2	2:H:1147:ILE:O	2.09	0.53
2:H:1697:HIS:HE1	2:H:1829:GLU:HG2	1.74	0.53
2:H:234:ILE:CG1	2:H:235:PRO:HD3	2.39	0.53
2:H:455:ILE:HG12	2:H:469:ARG:HG2	1.91	0.53
2:I:264:ARG:NH1	2:I:456:GLN:HG3	2.24	0.53
1:A:529:MET:HG2	1:A:638:LEU:HG	1.89	0.52
1:B:340:ARG:HH12	1:B:344:GLN:NE2	2.08	0.52
1:C:864:VAL:CG2	1:C:921:PRO:HB3	2.39	0.52
1:C:929:GLY:C	1:C:931:GLN:H	2.13	0.52
2:G:1418:ASP:C	2:G:1420:GLU:N	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:55:THR:CG2	2:G:56:THR:HG22	2.33	0.52
2:H:1418:ASP:O	2:H:1419:PHE:C	2.46	0.52
2:I:1040:LEU:O	2:I:1046:GLN:HG3	2.09	0.52
2:I:606:PHE:CE1	2:I:811:VAL:HG13	2.44	0.52
1:A:156:ALA:HA	1:A:166:ILE:CD1	2.39	0.52
1:A:341:GLN:O	1:A:345:VAL:HG12	2.09	0.52
1:A:986:ALA:CA	1:A:1047:LEU:HD13	2.39	0.52
1:B:12:ILE:HD11	2:H:2041:ILE:HD11	1.89	0.52
1:B:1234:MET:CE	1:B:1326:ILE:HG21	2.40	0.52
1:C:1749:THR:C	1:C:1874:ASP:HB3	2.29	0.52
2:H:1159:ILE:CG1	2:H:1169:PRO:CD	2.87	0.52
2:H:1427:VAL:O	2:H:1427:VAL:HG12	2.08	0.52
2:H:145:LEU:O	2:H:149:VAL:HG12	2.10	0.52
2:H:1697:HIS:HE1	2:H:1829:GLU:CG	2.22	0.52
2:H:2026:PHE:CD2	2:H:2045:TRP:HZ3	2.27	0.52
2:I:2036:GLU:O	2:I:2039:LYS:HG2	2.09	0.52
2:I:465:GLY:HA2	2:I:493:THR:HA	1.91	0.52
2:I:598:THR:O	2:I:602:VAL:HB	2.09	0.52
1:B:784:ILE:HG23	1:B:788:SER:HB2	1.92	0.52
1:C:1056:ILE:HD13	1:C:1193:TRP:CD1	2.41	0.52
1:C:1305:CYS:SG	1:C:1583:HIS:NE2	2.82	0.52
2:G:615:TYR:CZ	2:G:1074:MET:HB3	2.44	0.52
2:H:194:THR:CG2	2:H:300:ILE:HD11	2.39	0.52
2:H:768:GLY:HA3	2:H:800:LEU:CD2	2.39	0.52
1:B:980:VAL:HG21	2:H:952:ARG:NH2	2.24	0.52
2:I:418:ASN:HD22	2:I:418:ASN:N	2.07	0.52
1:A:335:HIS:HD2	1:A:335:HIS:O	1.92	0.52
1:A:824:LEU:HD11	1:A:849:LEU:HD12	1.89	0.52
1:B:329:GLU:O	1:B:333:LYS:HG3	2.08	0.52
1:C:1411:THR:HG22	1:C:1412:ASP:N	2.24	0.52
1:C:260:ARG:HH12	1:C:300:VAL:CG2	2.22	0.52
1:C:530:ALA:HA	1:C:636:PRO:HB3	1.91	0.52
2:G:1159:ILE:HG12	2:G:1169:PRO:CD	2.39	0.52
2:G:1359:MET:CE	2:G:1404:MET:HB3	2.39	0.52
2:G:1438:SER:O	2:G:1441:ILE:HG23	2.09	0.52
2:G:490:TRP:HA	2:G:493:THR:CG2	2.40	0.52
2:H:955:GLU:HG2	2:H:987:TYR:CE2	2.45	0.52
2:I:1486:PHE:HA	2:I:1504:VAL:O	2.10	0.52
1:A:988:ILE:HD13	1:A:1048:GLU:CA	2.39	0.52
1:C:406:TRP:CE3	1:C:1619:GLU:HG3	2.44	0.52
1:C:465:ASN:O	1:C:469:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1389:ILE:HG13	2:G:1411:PHE:HD1	1.75	0.52
2:G:145:LEU:HD21	2:G:156:LEU:HD21	1.91	0.52
2:G:871:THR:HG21	2:G:887:LYS:NZ	2.25	0.52
2:H:1722:GLY:N	2:H:1726:GLY:HA3	2.24	0.52
2:H:754:TYR:CD2	2:H:794:MET:HG3	2.44	0.52
2:I:1350:LEU:HD11	2:I:1410:PHE:HB3	1.91	0.52
2:I:1438:SER:O	2:I:1441:ILE:HG23	2.08	0.52
2:I:1475:LYS:HG3	2:I:1481:SER:HB2	1.92	0.52
2:I:1300:PHE:CA	2:I:1556:VAL:HG11	2.40	0.52
2:I:1774:THR:HA	2:I:1777:THR:HB	1.92	0.52
2:I:741:HIS:HE1	2:I:855:HIS:NE2	2.06	0.52
1:A:1477:ILE:H	1:A:1478:PRO:CD	2.21	0.52
1:A:998:TYR:CE2	1:A:1667:GLU:HB2	2.44	0.52
1:A:501:THR:N	1:A:886:GLU:OE1	2.30	0.52
1:B:341:GLN:O	1:B:345:VAL:HG12	2.10	0.52
2:G:1475:LYS:CB	2:G:1481:SER:HB2	2.39	0.52
2:G:1567:ARG:HG2	2:G:1567:ARG:HH11	1.72	0.52
2:G:1593:ILE:HD13	2:G:1626:ILE:HD13	1.92	0.52
2:G:1932:SER:O	2:G:1936:VAL:HG22	2.10	0.52
2:H:1359:MET:HE3	2:H:1404:MET:HB3	1.92	0.52
2:I:702:TYR:HB2	2:I:727:PRO:HB2	1.92	0.52
2:I:964:LEU:CD2	2:I:964:LEU:N	2.72	0.52
1:A:1305:CYS:SG	1:A:1583:HIS:NE2	2.83	0.52
1:A:430:ARG:NH1	1:A:493:VAL:O	2.40	0.52
1:A:59:ARG:HH11	2:G:1896:GLN:NE2	2.07	0.52
2:G:2026:PHE:CD2	2:G:2045:TRP:HZ3	2.27	0.52
1:A:2:LYS:CD	2:G:2050:GLN:HB3	2.38	0.52
2:G:955:GLU:HG2	2:G:987:TYR:CE2	2.45	0.52
2:H:615:TYR:CZ	2:H:1074:MET:HB3	2.43	0.52
2:H:1292:ILE:O	2:H:1368:VAL:O	2.27	0.52
2:H:1776:PHE:O	2:H:1779:PRO:HD2	2.09	0.52
2:H:747:HIS:O	2:H:751:LEU:HB2	2.10	0.52
2:I:1004:LEU:HD21	2:I:1020:VAL:HG23	1.91	0.52
2:I:1159:ILE:HG12	2:I:1169:PRO:CD	2.39	0.52
2:I:913:ASP:H	2:I:916:THR:CG2	2.23	0.52
1:B:529:MET:HG2	1:B:638:LEU:HG	1.92	0.52
1:B:893:VAL:HG11	1:B:930:LEU:CD2	2.36	0.52
1:C:1431:GLU:CD	1:C:1433:HIS:CE1	2.83	0.52
1:C:27:ARG:HB2	2:I:2016:ALA:HB2	1.91	0.52
1:C:607:LYS:HG2	1:C:608:ASP:N	2.24	0.52
2:G:1177:SER:O	2:G:1180:MET:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:926:LEU:HB3	2:G:947:THR:HG22	1.92	0.52
2:H:599:PRO:HD2	4:H:3051:FMN:H6	1.92	0.52
2:H:418:ASN:HD22	2:H:418:ASN:N	2.08	0.52
2:I:1282:ARG:HH21	2:I:1423:PHE:HB3	1.74	0.52
2:I:1597:ALA:HB1	2:I:1638:ILE:CD1	2.39	0.52
2:I:1918:LYS:HG2	2:I:1919:LEU:HD23	1.92	0.52
2:I:751:LEU:HD23	2:I:791:TYR:CZ	2.44	0.52
1:A:1475:GLU:HG3	1:A:1761:LYS:O	2.10	0.52
1:A:521:LYS:HE2	1:A:605:LEU:HD11	1.92	0.52
1:A:705:VAL:CG2	1:A:732:LEU:HD21	2.39	0.52
1:C:1577:GLN:HE22	1:C:1591:TRP:C	2.13	0.52
1:C:340:ARG:HH12	1:C:344:GLN:NE2	2.08	0.52
1:C:705:VAL:CG2	1:C:732:LEU:HD21	2.40	0.52
2:G:1093:ASP:HB3	2:G:1096:LYS:HG3	1.90	0.52
2:G:121:GLU:HA	2:G:124:LYS:HD2	1.91	0.52
2:G:1745:LYS:HD3	2:G:1747:LYS:HE2	1.91	0.52
2:G:176:LEU:HD22	2:G:247:ALA:HB1	1.90	0.52
2:G:1873:TYR:CE1	2:G:1877:ARG:NE	2.75	0.52
2:G:768:GLY:HA3	2:G:800:LEU:CD2	2.38	0.52
2:H:278:VAL:HG11	2:H:303:LEU:HD13	1.92	0.52
2:H:553:ASN:O	2:H:556:LYS:CE	2.58	0.52
2:I:1223:MET:CE	2:I:1238:LEU:HD12	2.40	0.52
2:I:273:HIS:CB	2:I:512:LEU:HD22	2.40	0.52
2:I:747:HIS:O	2:I:751:LEU:HB2	2.10	0.52
1:A:1183:ARG:NH1	1:A:1344:GLY:HA2	2.24	0.52
1:A:1577:GLN:HE22	1:A:1591:TRP:C	2.13	0.52
1:A:280:GLU:O	1:A:280:GLU:HG2	2.10	0.52
1:A:607:LYS:HG2	1:A:608:ASP:N	2.25	0.52
1:A:674:LYS:O	1:A:675:ASP:HB2	2.09	0.52
1:C:156:ALA:HA	1:C:166:ILE:CD1	2.40	0.52
2:G:278:VAL:HG11	2:G:303:LEU:HD13	1.92	0.52
2:H:281:VAL:HG12	2:H:282:ALA:N	2.24	0.52
2:H:577:ILE:HD13	2:H:1097:ILE:CD1	2.40	0.52
2:H:892:ILE:HG12	2:H:903:TRP:CG	2.45	0.52
2:I:1871:LEU:HD22	2:I:1888:ILE:HD11	1.92	0.52
2:I:2026:PHE:CD2	2:I:2045:TRP:HZ3	2.27	0.52
1:A:881:ASN:HA	1:A:944:ARG:NH2	2.25	0.51
1:B:1056:ILE:CD1	1:B:1193:TRP:HD1	2.22	0.51
1:B:1238:VAL:HG12	1:B:1239:HIS:N	2.25	0.51
1:B:1748:ASN:C	1:B:1750:ILE:H	2.13	0.51
1:C:1665:ILE:CG1	1:C:1669:ARG:HD3	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1774:THR:HA	2:G:1777:THR:HB	1.90	0.51
2:G:234:ILE:CG1	2:G:235:PRO:HD3	2.40	0.51
2:H:1673:GLU:N	2:H:1676:MET:HE3	2.25	0.51
2:H:654:VAL:HG23	2:H:683:ALA:HB1	1.92	0.51
1:B:985:ARG:HH12	2:H:953:ARG:NH2	2.07	0.51
2:I:1745:LYS:HD3	2:I:1747:LYS:HE2	1.93	0.51
1:A:1123:GLN:HG3	1:A:1124:GLU:N	2.24	0.51
1:A:1411:THR:HG22	1:A:1412:ASP:N	2.25	0.51
1:B:1104:ARG:O	1:B:1185:VAL:HG13	2.11	0.51
1:B:1665:ILE:HG12	1:B:1666:THR:N	2.25	0.51
1:C:1238:VAL:HG12	1:C:1239:HIS:N	2.25	0.51
1:C:1303:GLY:N	1:C:1307:THR:HG22	2.26	0.51
1:C:156:ALA:HA	1:C:166:ILE:HD12	1.92	0.51
1:C:1840:VAL:HG23	1:C:1848:ALA:HB3	1.92	0.51
2:G:376:ASN:C	2:G:376:ASN:HD22	2.13	0.51
2:H:131:ILE:CD1	2:H:182:VAL:CG1	2.88	0.51
2:I:1697:HIS:CE1	2:I:1829:GLU:HG2	2.45	0.51
2:I:1868:GLN:HG3	2:I:1898:TYR:CZ	2.45	0.51
2:I:715:GLN:O	2:I:719:ILE:HG12	2.10	0.51
1:A:1303:GLY:N	1:A:1307:THR:HG22	2.25	0.51
1:A:1411:THR:HG22	1:A:1412:ASP:H	1.76	0.51
1:A:1474:ALA:HA	1:A:1478:PRO:CD	2.41	0.51
1:C:46:GLU:OE1	1:C:53:LEU:HB2	2.11	0.51
1:C:674:LYS:O	1:C:675:ASP:HB2	2.11	0.51
2:G:1293:THR:HG22	2:G:1296:GLU:CG	2.40	0.51
2:G:1328:VAL:HG23	2:G:1557:SER:HA	1.92	0.51
2:G:1493:LEU:HD11	2:G:1499:VAL:CG2	2.40	0.51
2:G:124:LYS:HG2	2:G:179:THR:HA	1.90	0.51
2:G:213:LEU:HG	2:G:213:LEU:O	2.10	0.51
2:G:489:LYS:O	2:G:493:THR:HG22	2.10	0.51
2:G:702:TYR:HB2	2:G:727:PRO:HB2	1.93	0.51
2:H:1293:THR:HG22	2:H:1296:GLU:CG	2.41	0.51
2:H:1475:LYS:CB	2:H:1481:SER:HB2	2.40	0.51
2:H:545:GLN:NE2	2:H:545:GLN:H	2.07	0.51
2:H:758:ARG:NH2	2:H:797:ASP:OD1	2.35	0.51
1:B:985:ARG:NH1	2:H:953:ARG:CZ	2.73	0.51
1:B:1411:THR:HG22	1:B:1412:ASP:N	2.26	0.51
1:B:335:HIS:HD2	1:B:335:HIS:O	1.93	0.51
1:C:983:GLN:NE2	2:I:962:LYS:HD2	2.25	0.51
2:G:1081:HIS:O	2:G:1085:LEU:HB2	2.10	0.51
1:A:12:ILE:CD1	2:G:2041:ILE:CD1	2.83	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:654:VAL:HG12	2:G:654:VAL:O	2.09	0.51
2:H:1081:HIS:O	2:H:1085:LEU:HB2	2.10	0.51
2:H:582:LYS:HE2	2:H:1108:PRO:HB3	1.92	0.51
2:H:1475:LYS:HG3	2:H:1481:SER:HB2	1.93	0.51
2:H:1491:VAL:HB	2:H:1501:ILE:HD12	1.92	0.51
2:I:1475:LYS:CB	2:I:1481:SER:HB2	2.41	0.51
2:I:652:ILE:HD12	2:I:652:ILE:N	2.25	0.51
2:I:732:TRP:CD2	2:I:750:MET:HE3	2.45	0.51
2:I:732:TRP:CD2	2:I:750:MET:HE1	2.43	0.51
2:G:816:ASP:HB3	2:G:1048:VAL:CG2	2.41	0.51
2:H:1561:ASN:OD1	2:H:1563:ILE:HB	2.10	0.51
2:I:460:TYR:HA	2:I:466:SER:O	2.11	0.51
1:A:157:HIS:HE1	1:A:228:LEU:HD22	1.76	0.51
1:A:1840:VAL:HG23	1:A:1848:ALA:HB3	1.91	0.51
1:B:1194:ASN:HB3	1:B:1197:THR:HG22	1.91	0.51
1:B:1477:ILE:H	1:B:1478:PRO:CD	2.24	0.51
1:B:1840:VAL:HG23	1:B:1848:ALA:HB3	1.92	0.51
1:B:338:LEU:O	1:B:342:GLN:HG3	2.10	0.51
1:B:415:SER:O	1:B:419:GLU:HB2	2.10	0.51
1:C:328:LEU:HD22	1:C:328:LEU:C	2.30	0.51
1:C:644:THR:HG22	1:C:648:ASP:O	2.10	0.51
2:G:1417:THR:CG2	2:G:1419:PHE:CE2	2.93	0.51
2:G:1427:VAL:HG12	2:G:1427:VAL:O	2.09	0.51
2:G:145:LEU:O	2:G:149:VAL:HG12	2.10	0.51
2:H:1493:LEU:HD11	2:H:1499:VAL:HG21	1.93	0.51
2:H:432:LEU:HB3	2:H:484:ILE:HG23	1.92	0.51
2:H:55:THR:HB	2:H:59:GLU:OE2	2.10	0.51
2:I:1015:VAL:HG11	2:I:1017:PHE:CE1	2.45	0.51
1:A:1310:GLU:OE1	1:A:1649:LYS:CE	2.56	0.51
2:G:1431:TYR:CE1	2:G:1526:THR:HG23	2.45	0.51
2:G:1589:VAL:HG11	2:G:1640:PHE:CE1	2.45	0.51
2:G:1579:ILE:HD11	2:G:1615:MET:SD	2.51	0.51
2:G:1764:PHE:HB2	2:G:1770:LEU:HD21	1.93	0.51
2:H:1419:PHE:O	2:H:1420:GLU:C	2.49	0.51
2:H:1716:ASN:OD1	2:H:1765:ARG:HA	2.11	0.51
2:H:260:PRO:HD3	2:H:289:TRP:CZ2	2.46	0.51
2:H:1054:LEU:HB3	4:H:3051:FMN:HM82	1.93	0.51
2:H:732:TRP:CD1	2:H:750:MET:HE3	2.46	0.51
2:I:1428:GLU:HB2	2:I:1468:THR:HG22	1.93	0.51
2:I:1566:SER:HB3	2:I:1568:HIS:CE1	2.45	0.51
2:I:306:ILE:HA	2:I:439:ILE:CD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1498:GLU:HB2	1:A:1876:LEU:CD1	2.37	0.51
1:A:254:TRP:HZ3	1:A:292:GLN:HG3	1.75	0.51
1:A:465:ASN:O	1:A:469:VAL:HG23	2.11	0.51
1:B:864:VAL:CG2	1:B:921:PRO:HB3	2.40	0.51
1:C:1123:GLN:HB2	1:C:1177:LYS:HE2	1.93	0.51
1:C:1411:THR:HG22	1:C:1412:ASP:H	1.75	0.51
1:C:1009:LEU:HG	1:C:1664:ALA:HB2	1.93	0.51
1:C:513:GLU:OE2	1:C:873:ARG:NH1	2.44	0.51
2:G:1986:LYS:HA	2:G:1989:LYS:HB3	1.92	0.51
2:H:1236:LEU:HD11	2:H:1262:ILE:HG12	1.92	0.51
2:H:533:LEU:HD13	2:H:545:GLN:HG3	1.92	0.51
2:H:667:LYS:HD2	2:H:697:THR:CG2	2.35	0.51
2:I:157:VAL:HG11	2:I:496:PHE:CZ	2.46	0.51
2:I:346:GLN:HA	2:I:377:LEU:HD21	1.92	0.51
2:I:950:PHE:O	2:I:954:VAL:HG23	2.11	0.51
1:B:1705:PRO:HB2	1:B:1733:PHE:CE1	2.46	0.51
1:C:733:ILE:CD1	1:C:761:LEU:HD11	2.40	0.51
2:G:1422:THR:O	2:G:1422:THR:CG2	2.59	0.51
2:G:16:LEU:HG	2:G:48:PHE:CZ	2.45	0.51
2:G:443:LEU:HD22	2:G:448:VAL:CG1	2.41	0.51
2:G:566:HIS:O	2:G:568:LYS:HG3	2.10	0.51
2:G:786:SER:CB	2:G:794:MET:HE2	2.41	0.51
2:H:807:ILE:HG21	2:H:1066:ILE:HA	1.92	0.51
2:H:2046:GLU:C	2:H:2048:TYR:H	2.14	0.51
2:H:332:GLU:OE2	2:H:394:ARG:HD3	2.10	0.51
2:H:461:ASP:HB3	2:H:464:ASP:HB2	1.93	0.51
2:I:1313:SER:O	2:I:1314:ARG:HD3	2.11	0.51
2:I:1359:MET:HA	2:I:1359:MET:HE3	1.92	0.51
2:I:807:ILE:HG21	2:I:1066:ILE:HA	1.93	0.51
1:A:400:ARG:HH11	1:A:400:ARG:HG3	1.67	0.51
1:A:889:GLU:HG3	1:A:893:VAL:O	2.11	0.51
1:B:1455:ARG:NH2	1:B:1459:ILE:HG12	2.26	0.51
1:B:822:VAL:HG12	1:B:824:LEU:HD22	1.93	0.51
1:C:157:HIS:HE1	1:C:228:LEU:HD22	1.75	0.51
1:C:411:GLN:HE22	1:C:1628:SER:H	1.58	0.51
2:G:1135:GLU:OE2	2:G:1175:LYS:HE3	2.11	0.51
2:G:1452:LEU:HA	2:G:1502:GLY:HA3	1.92	0.51
2:G:418:ASN:N	2:G:418:ASN:HD22	2.09	0.51
2:G:751:LEU:HD23	2:G:791:TYR:CZ	2.46	0.51
2:G:868:PHE:HB3	2:G:873:PHE:CE2	2.46	0.51
2:H:1678:MET:CE	2:H:1707:LEU:HD22	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2026:PHE:HD2	2:H:2045:TRP:HZ3	1.59	0.51
2:H:233:SER:HA	2:H:424:ALA:CB	2.41	0.51
2:H:460:TYR:HA	2:H:466:SER:O	2.11	0.51
2:H:741:HIS:HB2	2:H:853:PRO:O	2.11	0.51
1:A:1105:LEU:HD23	1:A:1185:VAL:HG22	1.93	0.50
1:A:635:ILE:HG22	1:A:651:TYR:CD1	2.46	0.50
1:A:985:ARG:NH1	2:G:953:ARG:CZ	2.74	0.50
1:B:1524:GLY:HA2	1:B:1527:ALA:HB3	1.93	0.50
1:B:386:PHE:O	1:B:390:VAL:HB	2.11	0.50
1:B:50:SER:HB2	1:B:51:PRO:CD	2.40	0.50
2:G:1223:MET:CE	2:G:1238:LEU:HD12	2.40	0.50
2:G:1697:HIS:HE1	2:G:1829:GLU:HG2	1.74	0.50
2:G:194:THR:CG2	2:G:300:ILE:HD11	2.41	0.50
2:G:601:THR:HG22	2:G:620:ALA:H	1.75	0.50
2:H:1265:MET:HE1	2:H:1562:PRO:HG2	1.92	0.50
2:H:408:PRO:HG3	2:H:836:TYR:CD2	2.46	0.50
2:I:1493:LEU:HD11	2:I:1499:VAL:HG21	1.93	0.50
2:I:1776:PHE:O	2:I:1779:PRO:HD2	2.10	0.50
1:A:1533:ILE:HD11	1:A:1564:LEU:HD13	1.93	0.50
1:A:433:VAL:O	1:A:437:ILE:HG13	2.12	0.50
1:B:1158:PRO:HD2	1:B:1159:GLU:OE2	2.10	0.50
1:B:1196:LYS:HE3	1:B:1202:ASP:CG	2.31	0.50
1:B:1411:THR:HG22	1:B:1412:ASP:H	1.75	0.50
1:B:635:ILE:HG22	1:B:651:TYR:CD1	2.46	0.50
1:C:34:VAL:O	1:C:38:ASP:HB2	2.11	0.50
1:C:828:PRO:HG3	1:C:868:ILE:HG22	1.94	0.50
1:C:655:LEU:CD2	1:C:916:LEU:HD11	2.41	0.50
2:G:281:VAL:HG12	2:G:282:ALA:N	2.26	0.50
2:G:526:ARG:HH11	2:G:558:ASN:HD21	1.59	0.50
2:G:7:ARG:CZ	2:G:24:THR:HA	2.41	0.50
2:H:1597:ALA:HB1	2:H:1638:ILE:CD1	2.41	0.50
2:H:1861:ARG:HD2	2:H:1964:PHE:O	2.12	0.50
2:I:281:VAL:HG12	2:I:282:ALA:N	2.25	0.50
2:I:611:THR:HA	2:I:615:TYR:O	2.11	0.50
2:I:750:MET:CG	2:I:796:PHE:HZ	2.24	0.50
2:I:85:ASN:HD22	2:I:135:ARG:NH1	2.04	0.50
1:A:20:TYR:CE1	2:G:2033:THR:HG21	2.47	0.50
1:A:24:SER:O	2:G:1977:HIS:CD2	2.65	0.50
1:A:34:VAL:O	1:A:38:ASP:HB2	2.10	0.50
1:A:59:ARG:HH11	2:G:1896:GLN:HE22	1.58	0.50
2:G:1272:ASP:O	2:G:1273:GLU:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1918:LYS:HG2	2:G:1919:LEU:HD23	1.93	0.50
2:G:652:ILE:CD1	2:G:658:MET:HE3	2.42	0.50
2:H:1774:THR:HA	2:H:1777:THR:HB	1.93	0.50
2:H:1775:GLN:HG2	2:H:1836:MET:SD	2.51	0.50
2:H:344:LEU:HB3	2:H:349:VAL:HG23	1.94	0.50
2:H:491:GLU:HA	2:H:494:THR:HG22	1.93	0.50
2:I:1027:ILE:O	2:I:1031:LYS:HB2	2.11	0.50
2:I:1945:ASP:O	2:I:1949:LYS:HG3	2.10	0.50
2:I:173:LEU:HD13	2:I:219:LEU:HD21	1.94	0.50
2:I:376:ASN:C	2:I:376:ASN:HD22	2.14	0.50
1:A:286:PHE:O	1:A:290:MET:HG2	2.10	0.50
1:B:1303:GLY:N	1:B:1307:THR:HG22	2.25	0.50
1:B:421:ILE:HG12	1:B:469:VAL:HG21	1.93	0.50
1:C:1116:PRO:HB2	1:C:1184:LEU:HD12	1.93	0.50
1:C:280:GLU:O	1:C:280:GLU:HG2	2.11	0.50
1:C:415:SER:O	1:C:419:GLU:HB2	2.12	0.50
1:C:702:LYS:HE2	1:C:729:GLY:O	2.11	0.50
2:G:545:GLN:NE2	2:G:545:GLN:H	2.09	0.50
2:H:1148:ASN:ND2	2:H:1151:HIS:H	2.08	0.50
2:H:1102:TYR:CE2	2:H:1152:ALA:HB2	2.47	0.50
2:H:1389:ILE:HG13	2:H:1411:PHE:HD1	1.76	0.50
2:H:1435:ILE:HG22	2:H:1435:ILE:O	2.10	0.50
2:H:463:PHE:CE1	2:H:486:LEU:HD22	2.47	0.50
2:I:1491:VAL:HB	2:I:1501:ILE:HD12	1.93	0.50
1:A:1004:ILE:HG22	1:A:1660:TYR:CE2	2.46	0.50
1:B:156:ALA:HA	1:B:166:ILE:CD1	2.41	0.50
1:B:156:ALA:HA	1:B:166:ILE:HD12	1.93	0.50
1:C:1431:GLU:HB3	1:C:1520:ALA:HB2	1.92	0.50
2:G:1871:LEU:HD22	2:G:1888:ILE:HD11	1.93	0.50
2:G:611:THR:HA	2:G:615:TYR:O	2.11	0.50
2:G:663:ILE:HB	2:G:664:PRO:CD	2.40	0.50
2:G:676:ILE:HG12	2:G:676:ILE:O	2.11	0.50
2:G:732:TRP:CG	2:G:750:MET:HE3	2.46	0.50
2:G:784:GLU:O	2:G:787:THR:HB	2.11	0.50
2:H:1428:GLU:HB2	2:H:1468:THR:HG22	1.94	0.50
2:I:1135:GLU:OE2	2:I:1175:LYS:HE3	2.12	0.50
2:I:1716:ASN:OD1	2:I:1765:ARG:HA	2.11	0.50
2:I:2035:SER:HB3	2:I:2038:ILE:CD1	2.40	0.50
2:I:955:GLU:HG2	2:I:987:TYR:CE2	2.46	0.50
1:A:1523:ARG:NH2	1:A:1564:LEU:O	2.45	0.50
1:A:487:ASP:O	1:A:488:PRO:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1009:LEU:HA	1:B:1445:MET:HE2	1.93	0.50
1:C:1019:ILE:HG21	1:C:1316:VAL:HG22	1.94	0.50
1:C:1474:ALA:HA	1:C:1478:PRO:CD	2.42	0.50
1:C:985:ARG:HH12	2:I:953:ARG:NH2	2.09	0.50
2:G:1350:LEU:HD11	2:G:1410:PHE:HB3	1.94	0.50
2:G:1840:VAL:O	2:G:1840:VAL:HG12	2.11	0.50
2:G:774:ALA:HB1	2:G:1081:HIS:CD2	2.37	0.50
2:H:826:GLY:HA2	2:H:1060:ALA:HB3	1.94	0.50
2:H:2036:GLU:HG2	2:H:2039:LYS:NZ	2.27	0.50
2:I:1953:VAL:HG12	2:I:1953:VAL:O	2.11	0.50
2:I:712:ALA:O	2:I:715:GLN:HB3	2.12	0.50
2:I:866:LYS:O	2:I:870:GLU:HG3	2.12	0.50
1:A:1104:ARG:O	1:A:1185:VAL:HG13	2.12	0.50
1:A:12:ILE:CD1	2:G:2041:ILE:HD11	2.41	0.50
1:A:359:ARG:NH2	1:C:1153:ASP:OD2	2.43	0.50
1:B:1347:LYS:O	1:B:1347:LYS:HD3	2.11	0.50
1:B:825:PRO:HB2	1:B:843:LYS:NZ	2.27	0.50
2:G:440:ASN:ND2	2:G:477:GLU:HG2	2.26	0.50
2:G:894:ARG:NH1	2:G:898:ASP:OD2	2.43	0.50
2:G:949:ASP:CB	2:G:1006:MET:HE2	2.38	0.50
2:H:121:GLU:HA	2:H:124:LYS:HD2	1.93	0.50
1:B:20:TYR:OH	2:H:2035:SER:HB2	2.12	0.50
2:H:161:GLY:HA3	2:H:506:PRO:HD2	1.93	0.50
2:H:638:VAL:HG22	2:H:675:PRO:HG2	1.93	0.50
2:I:1986:LYS:HA	2:I:1989:LYS:HB3	1.93	0.50
1:C:13:LEU:HB2	2:I:2026:PHE:CE1	2.45	0.50
1:A:930:LEU:HD22	1:A:933:VAL:HG11	1.93	0.50
1:B:408:TRP:CZ3	1:B:1628:SER:HB3	2.47	0.50
1:C:157:HIS:CE1	1:C:228:LEU:HD22	2.47	0.50
1:C:328:LEU:HD13	1:C:329:GLU:N	2.27	0.50
1:C:702:LYS:HD3	1:C:731:THR:CG2	2.41	0.50
2:G:1776:PHE:O	2:G:1779:PRO:HD2	2.12	0.50
2:G:2035:SER:HB3	2:G:2038:ILE:CD1	2.42	0.50
2:G:24:THR:O	2:G:26:SER:N	2.44	0.50
2:G:306:ILE:HA	2:G:439:ILE:CD1	2.42	0.50
2:G:606:PHE:CE1	2:G:811:VAL:HG13	2.46	0.50
2:G:60:LEU:O	2:G:63:LYS:HB2	2.12	0.50
2:G:682:GLY:O	2:G:683:ALA:HB3	2.12	0.50
2:H:2035:SER:HB3	2:H:2038:ILE:CD1	2.42	0.50
2:H:747:HIS:HE1	2:H:780:TYR:OH	1.95	0.50
2:I:1417:THR:C	2:I:1419:PHE:H	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:344:LEU:HB3	2:I:349:VAL:HG23	1.93	0.50
1:A:1125:VAL:HG21	1:A:1175:ILE:CD1	2.42	0.50
1:A:1116:PRO:HB2	1:A:1184:LEU:HD12	1.94	0.50
1:A:1347:LYS:HD3	1:A:1347:LYS:O	2.11	0.50
1:A:1459:ILE:O	1:A:1463:VAL:HG23	2.12	0.50
1:A:156:ALA:HA	1:A:166:ILE:HD12	1.93	0.50
1:B:46:GLU:OE1	1:B:53:LEU:HB2	2.12	0.50
1:C:1460:LYS:CE	1:C:1774:GLU:OE1	2.59	0.50
1:C:1566:ARG:HB3	1:C:1623:TYR:CE1	2.46	0.50
1:C:1705:PRO:HB2	1:C:1733:PHE:CE1	2.46	0.50
1:C:385:PHE:HD2	1:C:787:LYS:HA	1.77	0.50
2:G:1552:PRO:O	2:G:1556:VAL:HG23	2.12	0.50
2:G:1716:ASN:OD1	2:G:1765:ARG:HA	2.12	0.50
2:G:1697:HIS:HE1	2:G:1829:GLU:CG	2.25	0.50
2:G:428:HIS:CD2	2:G:488:VAL:HG23	2.47	0.50
2:H:1004:LEU:HD21	2:H:1020:VAL:CG2	2.41	0.50
2:H:2030:TYR:CE1	2:H:2034:GLY:HA2	2.46	0.50
2:H:441:LYS:O	2:H:444:VAL:HG12	2.12	0.50
2:H:7:ARG:CZ	2:H:24:THR:HA	2.42	0.50
2:I:777:THR:HG23	2:I:1081:HIS:CE1	2.47	0.50
2:I:1673:GLU:N	2:I:1676:MET:HE3	2.25	0.50
2:I:455:ILE:HG12	2:I:469:ARG:HG2	1.93	0.50
1:A:142:ASP:CG	1:A:257:PRO:HB2	2.32	0.49
1:B:1451:GLN:OE1	1:B:1451:GLN:HA	2.12	0.49
1:B:1533:ILE:HG13	1:B:1564:LEU:HB3	1.94	0.49
1:B:413:LEU:HB2	1:B:439:ILE:HD13	1.94	0.49
1:C:1665:ILE:HG12	1:C:1666:THR:N	2.27	0.49
1:C:267:VAL:O	1:C:290:MET:HE1	2.12	0.49
2:G:131:ILE:CB	2:G:182:VAL:CG1	2.85	0.49
2:G:1441:ILE:HD11	2:G:1445:ARG:NH2	2.25	0.49
2:G:1868:GLN:HG3	2:G:1898:TYR:CZ	2.48	0.49
2:G:2029:VAL:O	2:G:2033:THR:HG22	2.12	0.49
2:H:1227:ARG:HG3	2:H:1227:ARG:NH1	2.01	0.49
2:H:777:THR:HG23	2:H:1081:HIS:CE1	2.47	0.49
2:I:1632:ILE:HG23	2:I:1632:ILE:O	2.12	0.49
2:I:72:VAL:HG12	2:I:73:GLU:N	2.27	0.49
2:I:7:ARG:HE	2:I:27:PHE:CB	2.24	0.49
1:A:1460:LYS:HE3	1:A:1774:GLU:HA	1.94	0.49
1:A:335:HIS:O	1:A:338:LEU:HB3	2.12	0.49
1:B:1125:VAL:HG21	1:B:1175:ILE:CD1	2.42	0.49
1:B:1474:ALA:HA	1:B:1478:PRO:CD	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:674:LYS:O	1:B:675:ASP:HB2	2.11	0.49
2:G:871:THR:HG21	2:G:887:LYS:HZ2	1.77	0.49
2:H:1148:ASN:HD22	2:H:1151:HIS:H	1.60	0.49
2:H:1162:ASP:O	2:H:1163:LYS:HB2	2.11	0.49
2:H:1745:LYS:HD3	2:H:1747:LYS:HE2	1.94	0.49
2:H:7:ARG:HE	2:H:27:PHE:CB	2.26	0.49
2:H:871:THR:HG21	2:H:887:LYS:NZ	2.26	0.49
2:I:24:THR:O	2:I:26:SER:N	2.45	0.49
2:I:259:THR:HG22	2:I:262:GLU:CB	2.41	0.49
2:H:28:PHE:CE1	2:I:27:PHE:CE2	3.00	0.49
2:I:274:SER:OG	2:I:428:HIS:HE1	1.95	0.49
2:I:60:LEU:O	2:I:63:LYS:HB2	2.11	0.49
1:A:1276:GLN:O	1:A:1282:THR:HG21	2.13	0.49
1:A:1501:LEU:CD1	1:A:1775:LEU:HG	2.43	0.49
1:C:1264:ARG:NH1	1:C:1270:VAL:HB	2.27	0.49
1:C:1455:ARG:O	1:C:1459:ILE:HG13	2.12	0.49
1:C:889:GLU:HG3	1:C:893:VAL:O	2.13	0.49
2:G:1493:LEU:HD11	2:G:1499:VAL:HG21	1.93	0.49
2:G:1486:PHE:HA	2:G:1504:VAL:O	2.12	0.49
2:G:463:PHE:CE1	2:G:486:LEU:HD22	2.47	0.49
2:G:463:PHE:O	2:G:463:PHE:HD2	1.95	0.49
2:H:894:ARG:NH1	2:H:898:ASP:OD2	2.41	0.49
2:I:1352:HIS:HE1	2:I:1583:MET:CE	2.25	0.49
2:I:324:LEU:HD12	2:I:324:LEU:O	2.12	0.49
2:I:751:LEU:HA	2:I:794:MET:HE3	1.94	0.49
1:A:1189:ILE:HG23	1:A:1190:PRO:HD2	1.95	0.49
1:A:1009:LEU:HD13	1:A:1445:MET:HE1	1.94	0.49
1:A:1460:LYS:CG	1:A:1773:VAL:O	2.60	0.49
1:C:1392:LEU:HD22	1:C:1396:MET:HG3	1.93	0.49
1:C:790:PHE:CE2	1:C:794:ILE:HD11	2.48	0.49
2:G:1427:VAL:HG22	2:G:1469:GLU:HG2	1.94	0.49
2:G:677:GLN:O	2:G:678:PHE:HB3	2.13	0.49
2:G:706:LYS:HE2	2:G:731:GLN:OE1	2.13	0.49
2:G:950:PHE:O	2:G:954:VAL:HG23	2.13	0.49
2:H:942:THR:HG21	2:H:1012:GLN:HA	1.95	0.49
2:H:1889:VAL:HG13	2:H:1977:HIS:HB3	1.93	0.49
2:H:273:HIS:CB	2:H:512:LEU:HD22	2.41	0.49
2:H:682:GLY:O	2:H:683:ALA:HB3	2.13	0.49
2:I:1293:THR:CG2	2:I:1296:GLU:H	2.20	0.49
2:I:1678:MET:CE	2:I:1707:LEU:HD22	2.41	0.49
2:I:238:CYS:CB	2:I:239:PRO:HD3	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1234:MET:HG2	1:A:1326:ILE:HD12	1.94	0.49
1:A:20:TYR:CD1	2:G:2033:THR:OG1	2.59	0.49
1:A:46:GLU:OE1	1:A:53:LEU:HB2	2.12	0.49
1:B:1305:CYS:SG	1:B:1583:HIS:NE2	2.85	0.49
1:B:1460:LYS:HE3	1:B:1774:GLU:CD	2.33	0.49
1:B:435:GLU:O	1:B:439:ILE:HG13	2.12	0.49
1:C:1050:CYS:HB3	1:C:1089:VAL:HG12	1.94	0.49
1:C:50:SER:HB2	1:C:51:PRO:CD	2.43	0.49
2:G:1738:PHE:HE1	2:G:1837:THR:HG23	1.76	0.49
2:H:1303:ALA:HB2	2:H:1556:VAL:HG21	1.93	0.49
2:H:1417:THR:O	2:H:1419:PHE:N	2.45	0.49
2:H:598:THR:O	2:H:602:VAL:HB	2.11	0.49
1:A:1451:GLN:OE1	1:A:1451:GLN:HA	2.12	0.49
1:A:157:HIS:CE1	1:A:228:LEU:HD22	2.48	0.49
1:A:489:VAL:HG22	1:A:671:VAL:N	2.28	0.49
1:B:1362:PRO:HA	1:B:1365:MET:HG3	1.94	0.49
1:B:1600:LEU:HD11	1:B:1655:VAL:HG12	1.94	0.49
1:B:170:LYS:HD3	1:B:175:LEU:HD23	1.93	0.49
1:B:764:ASP:OD2	1:B:818:ARG:HD3	2.11	0.49
2:G:465:GLY:HA2	2:G:493:THR:HA	1.95	0.49
2:H:138:ASP:O	2:H:139:LYS:HG3	2.12	0.49
2:H:1566:SER:HB3	2:H:1568:HIS:CE1	2.47	0.49
2:H:7:ARG:HH11	2:H:24:THR:HG23	1.75	0.49
2:H:22:VAL:HG11	2:H:27:PHE:HA	1.94	0.49
2:H:369:SER:O	2:H:370:LEU:HD23	2.13	0.49
2:H:715:GLN:O	2:H:719:ILE:HG12	2.13	0.49
2:H:949:ASP:CB	2:H:1006:MET:HE2	2.42	0.49
2:I:1015:VAL:HG13	2:I:1017:PHE:CE2	2.47	0.49
2:I:1265:MET:CE	2:I:1562:PRO:HG2	2.41	0.49
2:I:1435:ILE:O	2:I:1435:ILE:HG22	2.12	0.49
2:I:7:ARG:CZ	2:I:24:THR:HA	2.42	0.49
2:I:16:LEU:HG	2:I:48:PHE:CZ	2.48	0.49
2:I:161:GLY:HA3	2:I:506:PRO:HD2	1.93	0.49
2:I:55:THR:CG2	2:I:56:THR:HG22	2.33	0.49
1:A:1264:ARG:NH1	1:A:1270:VAL:HB	2.28	0.49
1:A:1705:PRO:HB2	1:A:1733:PHE:CE1	2.47	0.49
1:A:256:LEU:HD22	1:A:260:ARG:HB3	1.94	0.49
1:A:328:LEU:HD13	1:A:329:GLU:N	2.27	0.49
1:B:1105:LEU:HD23	1:B:1185:VAL:HG22	1.94	0.49
1:C:636:PRO:HB2	1:C:638:LEU:O	2.13	0.49
1:C:980:VAL:HG23	2:I:968:GLN:OE1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1266:TYR:HB2	2:G:1347:LEU:HD23	1.95	0.49
1:A:18:LEU:HD21	2:G:1815:LEU:HD12	1.95	0.49
2:G:618:GLU:HG2	2:G:678:PHE:CZ	2.48	0.49
2:H:161:GLY:N	2:H:505:GLY:HA3	2.25	0.49
2:H:1873:TYR:HE1	2:H:1877:ARG:HH21	1.59	0.49
2:H:463:PHE:O	2:H:463:PHE:HD2	1.96	0.49
2:H:455:ILE:HD11	2:H:469:ARG:NE	2.27	0.49
2:I:1169:PRO:O	2:I:1173:VAL:HG23	2.13	0.49
2:I:1873:TYR:CE2	2:I:1940:LEU:HD21	2.47	0.49
2:I:740:HIS:CE1	2:I:852:GLU:OE1	2.65	0.49
1:A:21:GLN:HG3	2:G:2013:ASN:HB2	1.93	0.49
1:B:1642:THR:HG22	1:B:1652:GLN:HG3	1.93	0.49
1:C:1114:TYR:CD1	1:C:1337:GLU:HG3	2.48	0.49
2:G:157:VAL:HG11	2:G:496:PHE:CZ	2.47	0.49
2:G:491:GLU:HA	2:G:494:THR:HG22	1.95	0.49
2:G:732:TRP:CD1	2:G:750:MET:HE3	2.47	0.49
2:H:569:LEU:HD12	2:H:1090:TYR:CD1	2.48	0.49
2:H:1593:ILE:O	2:H:1597:ALA:HB3	2.12	0.49
2:H:1634:GLY:HA3	2:H:1799:PRO:HA	1.94	0.49
2:H:1666:PHE:CD1	2:H:1814:ALA:HA	2.48	0.49
2:H:173:LEU:O	2:H:173:LEU:HD22	2.13	0.49
2:H:702:TYR:HB2	2:H:727:PRO:HB2	1.94	0.49
2:H:932:ILE:HD12	2:H:939:PHE:HD1	1.78	0.49
2:I:949:ASP:CB	2:I:1006:MET:HE2	2.43	0.49
2:I:573:LYS:HE3	2:I:1101:GLU:OE1	2.12	0.49
2:I:597:MET:H	2:I:601:THR:HB	1.78	0.49
2:I:11:LEU:HD11	2:I:64:PHE:CD2	2.48	0.49
1:C:982:ILE:HD11	2:I:965:SER:HB2	1.95	0.49
1:A:1362:PRO:HA	1:A:1365:MET:HG3	1.95	0.49
1:A:1219:VAL:CA	1:A:1384:ILE:HD11	2.31	0.49
1:B:186:ILE:O	1:B:190:LEU:HG	2.13	0.49
1:C:1020:VAL:CG1	1:C:1400:ILE:HG23	2.42	0.49
1:C:267:VAL:HG12	1:C:290:MET:CE	2.42	0.49
2:G:1130:THR:H	2:G:1133:THR:CG2	2.26	0.49
2:G:161:GLY:N	2:G:505:GLY:HA3	2.24	0.49
2:G:273:HIS:CB	2:G:512:LEU:HD22	2.42	0.49
2:H:1749:GLU:OE2	2:H:1840:VAL:HG13	2.12	0.49
2:H:428:HIS:HD2	2:H:486:LEU:O	1.96	0.49
2:I:1567:ARG:HH11	2:I:1567:ARG:HG2	1.70	0.49
2:I:173:LEU:O	2:I:173:LEU:HD22	2.13	0.49
1:C:18:LEU:HD21	2:I:1815:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:TYR:CD2	2:I:2033:THR:OG1	2.66	0.49
2:I:306:ILE:HA	2:I:439:ILE:HD13	1.94	0.49
1:A:1009:LEU:HG	1:A:1664:ALA:HB2	1.95	0.49
1:A:1022:THR:HG22	1:A:1226:SER:CB	2.43	0.49
1:A:1749:THR:CB	1:A:1874:ASP:N	2.75	0.49
1:B:1312:VAL:CG2	1:B:1329:VAL:HG11	2.39	0.49
1:C:335:HIS:O	1:C:335:HIS:CD2	2.65	0.49
1:C:32:GLN:NE2	1:C:57:ALA:HA	2.28	0.49
2:G:1666:PHE:CD1	2:G:1814:ALA:HA	2.48	0.49
2:G:173:LEU:HD22	2:G:173:LEU:O	2.13	0.49
2:G:1913:VAL:O	2:G:1917:ILE:HG13	2.12	0.49
2:G:2036:GLU:HG2	2:G:2039:LYS:NZ	2.28	0.49
2:G:259:THR:HG22	2:G:262:GLU:CB	2.43	0.49
2:G:560:ASN:OD1	2:G:560:ASN:O	2.30	0.49
2:G:653:TYR:HD1	2:G:659:LEU:HD21	1.78	0.49
2:G:715:GLN:O	2:G:719:ILE:HG12	2.13	0.49
2:G:807:ILE:HD12	2:G:1063:THR:HG23	1.95	0.49
2:H:1002:HIS:NE2	2:H:1006:MET:HE3	2.27	0.49
2:H:860:ARG:HB2	2:H:1049:GLN:HG3	1.94	0.49
2:I:1567:ARG:NH1	2:I:1568:HIS:HB3	2.28	0.49
2:I:428:HIS:HD2	2:I:486:LEU:O	1.95	0.49
2:I:881:VAL:N	2:I:882:PRO:CD	2.76	0.49
1:A:1021:VAL:HG22	1:A:1387:ILE:HG22	1.95	0.48
1:A:1312:VAL:CG2	1:A:1329:VAL:HG11	2.41	0.48
1:B:182:VAL:O	1:B:186:ILE:HG13	2.12	0.48
1:B:1753:ALA:HB2	1:B:1872:SER:OG	2.13	0.48
1:B:916:LEU:HD22	1:B:922:VAL:HG22	1.94	0.48
1:C:1105:LEU:HD23	1:C:1185:VAL:HG22	1.94	0.48
2:G:402:LEU:HD12	2:G:404:GLN:HG2	1.95	0.48
2:G:598:THR:O	2:G:602:VAL:HB	2.13	0.48
2:H:739:GLY:HA2	2:H:1054:LEU:HG	1.95	0.48
2:H:1931:LEU:HB3	2:H:1935:GLU:CG	2.36	0.48
2:H:465:GLY:HA2	2:H:493:THR:HA	1.95	0.48
2:I:1697:HIS:HE1	2:I:1829:GLU:CG	2.26	0.48
2:I:161:GLY:N	2:I:505:GLY:HA3	2.24	0.48
2:I:663:ILE:HB	2:I:664:PRO:CD	2.42	0.48
2:I:835:THR:HG22	2:I:844:VAL:HA	1.95	0.48
1:C:1693:ILE:CD1	2:I:998:GLN:HB2	2.40	0.48
1:B:187:LEU:HD22	1:B:201:PRO:HB2	1.94	0.48
1:B:465:ASN:O	1:B:469:VAL:HG23	2.12	0.48
2:G:1745:LYS:HE2	2:G:1747:LYS:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2046:GLU:C	2:G:2048:TYR:H	2.15	0.48
2:G:376:ASN:C	2:G:376:ASN:ND2	2.67	0.48
2:G:597:MET:H	2:G:601:THR:HB	1.77	0.48
2:G:11:LEU:HD11	2:G:64:PHE:CD2	2.48	0.48
2:H:901:LYS:NZ	2:H:1031:LYS:O	2.46	0.48
2:H:1272:ASP:O	2:H:1273:GLU:HG3	2.13	0.48
2:H:1868:GLN:HG3	2:H:1898:TYR:CZ	2.48	0.48
2:H:259:THR:HG22	2:H:262:GLU:CB	2.42	0.48
2:H:306:ILE:HA	2:H:439:ILE:CD1	2.42	0.48
2:H:786:SER:CB	2:H:794:MET:HE2	2.43	0.48
2:I:1674:GLN:OE1	2:I:1712:ASN:HA	2.13	0.48
2:I:629:GLY:O	2:I:632:ALA:HB3	2.13	0.48
2:I:682:GLY:O	2:I:683:ALA:HB3	2.13	0.48
2:I:970:TYR:O	2:I:973:LEU:HB2	2.14	0.48
1:A:1477:ILE:H	1:A:1478:PRO:HD3	1.78	0.48
1:B:157:HIS:HE1	1:B:228:LEU:HD22	1.77	0.48
1:B:413:LEU:C	1:B:415:SER:H	2.17	0.48
1:B:2:LYS:HE2	1:B:4:GLU:CD	2.34	0.48
1:C:1305:CYS:SG	3:C:2748:CER:C5	3.01	0.48
1:C:1523:ARG:NH2	1:C:1564:LEU:O	2.46	0.48
1:C:256:LEU:HD22	1:C:260:ARG:HB3	1.95	0.48
2:G:1330:GLY:HA2	2:G:1374:THR:HG21	1.94	0.48
2:G:1428:GLU:HG2	2:G:1470:THR:HG22	1.94	0.48
2:G:533:LEU:HD13	2:G:545:GLN:HG3	1.94	0.48
2:G:754:TYR:CE2	2:G:794:MET:HG3	2.48	0.48
2:G:7:ARG:HE	2:G:27:PHE:CB	2.25	0.48
2:H:33:LEU:HD21	2:H:80:PHE:CE2	2.49	0.48
2:H:40:ILE:O	2:H:42:PRO:HD3	2.13	0.48
2:H:463:PHE:CD1	2:H:486:LEU:HD22	2.48	0.48
2:H:955:GLU:HG2	2:H:987:TYR:HE2	1.78	0.48
2:I:1130:THR:H	2:I:1133:THR:CG2	2.25	0.48
2:I:1873:TYR:CE1	2:I:1877:ARG:NE	2.77	0.48
2:I:278:VAL:HG11	2:I:303:LEU:HD13	1.95	0.48
2:I:786:SER:CB	2:I:794:MET:HE2	2.42	0.48
1:A:340:ARG:HH12	1:A:344:GLN:HE21	1.60	0.48
1:B:328:LEU:HD13	1:B:329:GLU:N	2.29	0.48
1:B:335:HIS:O	1:B:338:LEU:HB3	2.14	0.48
1:B:702:LYS:HD3	1:B:731:THR:CG2	2.44	0.48
1:B:332:THR:HG22	1:C:331:ILE:CD1	2.44	0.48
1:C:331:ILE:HG23	1:C:332:THR:N	2.28	0.48
2:G:1980:TYR:HD1	2:G:1981:LEU:HD12	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:455:ILE:HG12	2:G:469:ARG:HG2	1.94	0.48
2:G:720:ALA:HA	2:G:728:ILE:CD1	2.43	0.48
2:H:1422:THR:HG23	2:H:1474:PHE:CD1	2.48	0.48
2:H:1624:THR:HB	2:H:1642:THR:OG1	2.14	0.48
2:H:428:HIS:CD2	2:H:488:VAL:HG23	2.49	0.48
2:H:995:LEU:HB3	2:H:1000:ILE:HD11	1.94	0.48
2:I:146:PHE:HA	2:I:149:VAL:HG12	1.92	0.48
2:I:1850:SER:HB2	2:I:1973:SER:HB2	1.95	0.48
2:I:249:TYR:CD2	2:I:283:ILE:HD11	2.48	0.48
2:I:402:LEU:HD12	2:I:404:GLN:HG2	1.94	0.48
2:I:455:ILE:O	2:I:455:ILE:HG13	2.13	0.48
2:I:551:THR:HG22	2:I:552:SER:N	2.29	0.48
2:I:593:LEU:HD21	2:I:800:LEU:HB3	1.95	0.48
2:I:995:LEU:HB3	2:I:1000:ILE:HD11	1.95	0.48
1:A:1714:VAL:HG22	1:A:1738:ILE:HD11	1.96	0.48
1:B:408:TRP:CH2	1:B:1628:SER:HB3	2.47	0.48
1:B:21:GLN:HG3	2:H:2013:ASN:HB2	1.95	0.48
1:B:998:TYR:CE2	1:B:1667:GLU:HB2	2.49	0.48
1:C:988:ILE:HD13	1:C:1048:GLU:CB	2.43	0.48
1:C:1477:ILE:H	1:C:1478:PRO:HD3	1.78	0.48
1:C:1642:THR:HG22	1:C:1652:GLN:HG3	1.96	0.48
2:G:1567:ARG:CG	2:G:1567:ARG:NH1	2.51	0.48
2:G:995:LEU:HB3	2:G:1000:ILE:HD11	1.96	0.48
2:H:1100:VAL:CG2	2:H:1147:ILE:HG21	2.43	0.48
2:H:145:LEU:HD21	2:H:156:LEU:HD21	1.95	0.48
2:H:1918:LYS:HG2	2:H:1919:LEU:HD23	1.96	0.48
2:H:1953:VAL:O	2:H:1953:VAL:HG12	2.14	0.48
2:H:1986:LYS:HA	2:H:1989:LYS:HB3	1.95	0.48
2:I:1081:HIS:O	2:I:1085:LEU:HB2	2.14	0.48
2:I:569:LEU:HD12	2:I:1090:TYR:CD1	2.48	0.48
2:I:1266:TYR:HB2	2:I:1347:LEU:HD23	1.95	0.48
2:I:1382:VAL:HA	2:I:1422:THR:OG1	2.12	0.48
1:A:1401:TYR:C	1:A:1658:PRO:HG3	2.33	0.48
1:A:19:ALA:O	1:A:22:PHE:HB2	2.14	0.48
1:A:444:ASN:HB2	1:A:447:LEU:N	2.14	0.48
1:B:503:ILE:HD12	1:B:950:THR:HG21	1.96	0.48
1:C:430:ARG:NH1	1:C:493:VAL:O	2.44	0.48
1:C:764:ASP:OD2	1:C:818:ARG:HD3	2.12	0.48
2:G:569:LEU:HD12	2:G:1090:TYR:CD1	2.48	0.48
2:G:1148:ASN:C	2:G:1148:ASN:HD22	2.17	0.48
2:G:1213:LEU:O	2:G:1214:LEU:HD23	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:TYR:CE1	2:G:2033:THR:CG2	2.97	0.48
2:G:593:LEU:HD21	2:G:800:LEU:HB3	1.96	0.48
2:G:72:VAL:HG12	2:G:73:GLU:N	2.28	0.48
2:H:1632:ILE:O	2:H:1632:ILE:HG23	2.13	0.48
2:H:397:LYS:HB3	2:H:416:PHE:CE2	2.48	0.48
2:H:99:ASN:HA	2:H:550:VAL:HG21	1.95	0.48
2:H:784:GLU:O	2:H:787:THR:HB	2.13	0.48
2:I:1159:ILE:CG1	2:I:1169:PRO:CD	2.90	0.48
2:I:121:GLU:HA	2:I:124:LYS:HD2	1.96	0.48
2:I:1738:PHE:CE1	2:I:1837:THR:HG23	2.48	0.48
2:I:7:ARG:HH11	2:I:24:THR:HG23	1.77	0.48
2:I:533:LEU:HG	2:I:533:LEU:O	2.13	0.48
2:I:586:LEU:HD12	2:I:764:MET:SD	2.54	0.48
1:A:988:ILE:HA	1:A:1048:GLU:CG	2.44	0.48
1:A:182:VAL:O	1:A:186:ILE:HG13	2.14	0.48
1:A:420:ILE:HG22	1:A:469:VAL:HG22	1.96	0.48
1:C:1276:GLN:O	1:C:1282:THR:HG21	2.13	0.48
1:C:1300:THR:HA	1:C:1301:PRO:HD3	1.67	0.48
1:C:1312:VAL:CG2	1:C:1329:VAL:HG11	2.44	0.48
1:C:1396:MET:O	1:C:1680:ARG:NH1	2.46	0.48
1:C:1451:GLN:OE1	1:C:1451:GLN:HA	2.13	0.48
1:C:1617:ILE:O	1:C:1620:GLN:HG2	2.13	0.48
1:C:852:ARG:CG	1:C:852:ARG:NH1	2.66	0.48
2:G:1590:ARG:HG3	2:G:1608:TYR:CD2	2.48	0.48
2:G:2026:PHE:HD2	2:G:2045:TRP:HZ3	1.59	0.48
2:G:240:LEU:O	2:G:244:ILE:HG13	2.13	0.48
2:H:1674:GLN:OE1	2:H:1712:ASN:HA	2.12	0.48
2:H:561:TRP:CZ3	2:H:792:PRO:HB2	2.49	0.48
2:H:751:LEU:HD23	2:H:791:TYR:CZ	2.49	0.48
2:I:1697:HIS:HE1	2:I:1829:GLU:HG2	1.77	0.48
2:I:667:LYS:HD2	2:I:697:THR:CG2	2.35	0.48
2:I:762:ASN:HD22	2:I:762:ASN:N	1.88	0.48
1:A:1037:TRP:HB2	1:A:1598:GLN:OE1	2.13	0.48
1:A:539:SER:O	1:A:540:GLN:C	2.52	0.48
1:B:1056:ILE:HD13	1:B:1193:TRP:CD1	2.45	0.48
1:B:1183:ARG:NH1	1:B:1344:GLY:HA2	2.29	0.48
1:B:625:THR:HG23	1:B:661:ASP:OD1	2.13	0.48
1:B:790:PHE:CE2	1:B:794:ILE:HD11	2.47	0.48
1:C:1738:ILE:O	1:C:1739:GLN:HB2	2.14	0.48
1:C:888:ILE:HD12	1:C:939:PHE:CE2	2.47	0.48
2:G:1180:MET:HB2	2:G:1197:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1040:LEU:O	2:H:1046:GLN:HG3	2.13	0.48
2:H:169:TYR:CG	2:H:170:PHE:N	2.81	0.48
2:H:214:ASN:ND2	2:H:217:GLU:HB2	2.27	0.48
2:H:317:THR:HG21	2:I:1309:GLU:CG	2.42	0.48
2:H:490:TRP:HA	2:H:493:THR:HG22	1.96	0.48
2:H:597:MET:H	2:H:601:THR:HB	1.78	0.48
2:I:1325:PHE:CE1	2:I:1328:VAL:HG11	2.49	0.48
2:I:1586:SER:O	2:I:1590:ARG:HB2	2.14	0.48
2:I:845:THR:HG22	2:I:855:HIS:CD2	2.49	0.48
1:A:427:ASN:HB2	1:A:468:LEU:HD21	1.95	0.48
1:A:695:GLY:HA3	1:A:906:LEU:HD11	1.94	0.48
1:B:243:ILE:O	1:B:247:ARG:HG3	2.13	0.48
2:G:306:ILE:HA	2:G:439:ILE:HD13	1.96	0.48
2:G:432:LEU:HB3	2:G:484:ILE:HG23	1.96	0.48
2:G:481:ASP:OD2	2:G:485:ARG:NH1	2.47	0.48
2:H:489:LYS:O	2:H:493:THR:HG22	2.13	0.48
2:H:868:PHE:HB3	2:H:873:PHE:CE2	2.48	0.48
2:I:1159:ILE:HG22	2:I:1160:THR:N	2.28	0.48
2:I:772:GLY:O	2:I:804:ARG:HD3	2.14	0.48
1:A:1639:VAL:HG12	1:A:1640:SER:N	2.28	0.48
1:A:328:LEU:N	1:A:330:GLU:H	2.12	0.48
1:A:927:ASN:O	1:A:929:GLY:N	2.41	0.48
1:B:1319:ILE:HA	1:B:1324:ALA:O	2.13	0.48
1:B:328:LEU:N	1:B:330:GLU:H	2.11	0.48
1:B:683:ALA:HA	1:B:689:GLY:HA3	1.95	0.48
1:B:930:LEU:HD23	1:B:930:LEU:HA	1.67	0.48
1:C:386:PHE:O	1:C:390:VAL:HB	2.14	0.48
1:C:751:PHE:CZ	1:C:761:LEU:HD13	2.49	0.48
2:G:1148:ASN:ND2	2:G:1151:HIS:H	2.12	0.48
2:G:1325:PHE:CE1	2:G:1328:VAL:HG11	2.48	0.48
2:G:173:LEU:HD13	2:G:219:LEU:HD21	1.94	0.48
2:G:461:ASP:HB3	2:G:464:ASP:HB2	1.95	0.48
2:H:157:VAL:HG11	2:H:496:PHE:CZ	2.49	0.48
2:H:232:LEU:HD21	2:H:423:VAL:HA	1.95	0.48
2:H:706:LYS:HE2	2:H:731:GLN:OE1	2.14	0.48
2:I:2026:PHE:HD2	2:I:2045:TRP:HZ3	1.60	0.48
2:I:214:ASN:ND2	2:I:217:GLU:HB2	2.28	0.48
2:I:489:LYS:O	2:I:493:THR:HG22	2.13	0.48
2:I:753:MET:O	2:I:757:ILE:HG13	2.14	0.48
1:A:187:LEU:HD22	1:A:201:PRO:HB2	1.96	0.47
1:B:1646:PHE:CE1	3:B:2748:CER:H31	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HE3	1:B:9:LEU:HD12	1.96	0.47
1:C:1392:LEU:CD2	1:C:1396:MET:HG3	2.44	0.47
1:C:440:MET:HE3	1:C:483:VAL:HG21	1.95	0.47
1:C:529:MET:HG2	1:C:638:LEU:HG	1.95	0.47
2:G:1027:ILE:O	2:G:1031:LYS:HB2	2.14	0.47
2:G:1566:SER:HB3	2:G:1568:HIS:CE1	2.49	0.47
2:G:22:VAL:HG11	2:G:27:PHE:HA	1.96	0.47
2:G:567:PRO:HG3	2:G:781:LEU:CD1	2.44	0.47
2:H:873:PHE:CD1	2:H:1026:GLU:HB2	2.49	0.47
2:H:1590:ARG:NH2	2:H:1594:GLU:OE2	2.47	0.47
2:H:943:TRP:CZ2	2:H:1016:PRO:HG3	2.49	0.47
2:I:1002:HIS:NE2	2:I:1006:MET:HE3	2.29	0.47
2:I:1015:VAL:HA	2:I:1016:PRO:HD3	1.74	0.47
2:I:176:LEU:HD22	2:I:247:ALA:HB1	1.96	0.47
2:I:1834:ARG:NH1	2:I:1834:ARG:CG	2.66	0.47
2:I:594:VAL:CG2	2:I:610:THR:HG21	2.44	0.47
2:I:900:GLN:NE2	2:I:1051:THR:HA	2.28	0.47
1:A:1501:LEU:O	1:A:1505:GLN:HG3	2.14	0.47
1:A:176:VAL:HG12	1:A:178:GLY:H	1.79	0.47
1:B:1367:ARG:HH12	1:B:1372:THR:CB	2.20	0.47
1:B:256:LEU:HD22	1:B:260:ARG:HB3	1.95	0.47
1:C:1021:VAL:HG11	1:C:1597:LEU:CD1	2.44	0.47
1:C:1125:VAL:HG21	1:C:1175:ILE:CD1	2.43	0.47
1:C:427:ASN:HB2	1:C:468:LEU:HD21	1.95	0.47
2:G:777:THR:HG23	2:G:1081:HIS:CE1	2.49	0.47
2:G:40:ILE:O	2:G:42:PRO:HD3	2.14	0.47
2:H:159:ILE:CG2	2:H:501:ILE:HG22	2.44	0.47
2:H:1749:GLU:OE2	2:H:1840:VAL:CG1	2.62	0.47
2:H:213:LEU:HG	2:H:213:LEU:O	2.14	0.47
2:H:732:TRP:CD2	2:H:750:MET:HE1	2.49	0.47
2:H:950:PHE:O	2:H:954:VAL:HG23	2.13	0.47
1:A:1238:VAL:CG1	1:A:1242:GLU:HB2	2.44	0.47
1:A:1303:GLY:C	1:A:1307:THR:HG22	2.35	0.47
1:A:683:ALA:HA	1:A:689:GLY:HA3	1.95	0.47
1:A:852:ARG:HB3	1:A:858:TRP:HZ2	1.80	0.47
1:B:1116:PRO:HB2	1:B:1184:LEU:HD12	1.95	0.47
1:B:1209:ASP:OD2	1:B:1253:GLY:HA2	2.14	0.47
1:B:530:ALA:HA	1:B:636:PRO:HB3	1.97	0.47
1:C:1516:ASP:HA	1:C:1517:PRO:HD3	1.66	0.47
1:C:1010:GLU:HA	1:C:1664:ALA:HA	1.95	0.47
2:G:1624:THR:HB	2:G:1642:THR:OG1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1666:PHE:CD1	2:G:1814:ALA:HB2	2.49	0.47
2:G:428:HIS:HD2	2:G:486:LEU:O	1.97	0.47
2:G:804:ARG:NH2	2:G:1068:GLU:OE1	2.48	0.47
2:H:1438:SER:O	2:H:1441:ILE:HG23	2.13	0.47
2:H:589:ARG:HB3	2:H:590:PRO:CD	2.43	0.47
2:I:1579:ILE:HD11	2:I:1615:MET:SD	2.53	0.47
2:I:1752:PHE:HZ	2:I:1836:MET:HE3	1.80	0.47
2:I:926:LEU:HB3	2:I:947:THR:CG2	2.43	0.47
1:C:1133:PRO:HG3	1:C:1166:LYS:HG3	1.96	0.47
1:C:1138:LYS:HG3	1:C:1163:TYR:CE1	2.48	0.47
1:C:998:TYR:CE2	1:C:1667:GLU:HB2	2.49	0.47
1:C:370:GLU:O	1:C:373:ALA:HB3	2.14	0.47
1:C:526:VAL:HG12	1:C:626:VAL:HG11	1.96	0.47
1:C:987:ASN:HD22	2:I:957:ARG:CD	2.26	0.47
2:G:169:TYR:CG	2:G:170:PHE:N	2.83	0.47
2:G:33:LEU:HD21	2:G:80:PHE:CE2	2.50	0.47
2:G:512:LEU:O	2:G:516:THR:HG23	2.15	0.47
2:H:1425:LYS:HG2	2:H:1471:GLU:HG3	1.95	0.47
2:H:1472:VAL:CG2	2:H:1483:VAL:HG22	2.44	0.47
2:H:1486:PHE:HA	2:H:1504:VAL:O	2.14	0.47
2:H:597:MET:HA	4:H:3051:FMN:N5	2.30	0.47
2:H:634:ILE:HD11	2:H:649:ILE:CD1	2.40	0.47
2:H:677:GLN:O	2:H:678:PHE:HB3	2.15	0.47
2:I:1804:PHE:CD2	2:I:1818:LEU:HD22	2.49	0.47
2:I:233:SER:HA	2:I:424:ALA:CB	2.44	0.47
2:I:562:LEU:HG	2:I:793:PRO:CB	2.44	0.47
1:A:1208:VAL:HG11	1:A:1212:THR:HB	1.96	0.47
1:A:1319:ILE:HA	1:A:1324:ALA:O	2.14	0.47
1:A:1012:LEU:HD23	1:A:1445:MET:CE	2.43	0.47
1:B:1477:ILE:H	1:B:1478:PRO:HD3	1.79	0.47
1:B:20:TYR:CG	2:H:2033:THR:OG1	2.67	0.47
1:B:331:ILE:HG23	1:B:332:THR:N	2.29	0.47
1:B:531:LEU:HD21	1:B:629:THR:HG22	1.97	0.47
1:C:1303:GLY:CA	1:C:1649:LYS:HE2	2.36	0.47
1:C:142:ASP:CG	1:C:257:PRO:HB2	2.34	0.47
1:C:328:LEU:N	1:C:330:GLU:H	2.12	0.47
2:G:1651:LEU:O	2:G:1652:THR:HG23	2.14	0.47
2:G:1949:LYS:O	2:G:1953:VAL:HG23	2.15	0.47
2:G:463:PHE:CD1	2:G:486:LEU:HD22	2.48	0.47
2:G:123:ILE:CD1	2:G:533:LEU:CD2	2.93	0.47
2:G:732:TRP:CD2	2:G:750:MET:HE3	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2037:PRO:O	2:H:2041:ILE:HG13	2.15	0.47
2:H:376:ASN:C	2:H:376:ASN:HD22	2.18	0.47
2:H:455:ILE:HG13	2:H:455:ILE:O	2.13	0.47
2:H:750:MET:CG	2:H:796:PHE:HZ	2.25	0.47
2:H:860:ARG:H	2:H:1049:GLN:HG3	1.79	0.47
2:I:873:PHE:CE1	2:I:1026:GLU:HB2	2.49	0.47
2:I:1378:ILE:O	2:I:1378:ILE:HG12	2.14	0.47
2:I:2037:PRO:O	2:I:2041:ILE:HG13	2.14	0.47
2:I:350:GLN:HA	2:I:353:VAL:HG13	1.96	0.47
2:I:55:THR:HB	2:I:59:GLU:OE2	2.13	0.47
1:A:983:GLN:HE22	2:G:962:LYS:HD2	1.77	0.47
1:B:157:HIS:CE1	1:B:228:LEU:HD22	2.49	0.47
1:B:1305:CYS:SG	3:B:2748:CER:C5	3.03	0.47
1:C:335:HIS:O	1:C:338:LEU:HB3	2.14	0.47
2:G:1422:THR:O	2:G:1422:THR:HG23	2.14	0.47
2:H:579:VAL:CG2	2:H:1078:HIS:CD2	2.95	0.47
2:H:1854:MET:CG	2:H:1901:ALA:HB2	2.45	0.47
2:H:355:LYS:HB3	2:H:355:LYS:HE2	1.65	0.47
2:H:652:ILE:N	2:H:652:ILE:HD12	2.30	0.47
2:H:751:LEU:HD23	2:H:791:TYR:CD2	2.49	0.47
2:I:1103:PHE:O	2:I:1247:GLY:HA3	2.14	0.47
2:I:1389:ILE:HG13	2:I:1411:PHE:HD1	1.80	0.47
2:I:1590:ARG:NH2	2:I:1594:GLU:OE2	2.48	0.47
2:I:455:ILE:HD11	2:I:469:ARG:NE	2.29	0.47
2:I:553:ASN:O	2:I:556:LYS:HE3	2.15	0.47
2:I:706:LYS:HE2	2:I:731:GLN:OE1	2.15	0.47
2:I:748:THR:CB	2:I:749:PRO:HD3	2.44	0.47
1:A:1061:SER:HB2	1:A:1078:SER:HB3	1.96	0.47
1:A:1010:GLU:HA	1:A:1664:ALA:HA	1.97	0.47
1:A:243:ILE:O	1:A:247:ARG:HG3	2.14	0.47
1:A:413:LEU:HD13	1:A:451:MET:HG2	1.97	0.47
1:B:34:VAL:O	1:B:38:ASP:HB2	2.14	0.47
1:B:776:GLU:OE1	1:B:795:MET:HE1	2.13	0.47
1:B:827:SER:HA	1:B:828:PRO:HD3	1.73	0.47
1:B:889:GLU:HG3	1:B:893:VAL:O	2.15	0.47
1:C:1183:ARG:NH1	1:C:1344:GLY:HA2	2.30	0.47
1:C:1305:CYS:SG	1:C:1585:LYS:HA	2.55	0.47
1:C:254:TRP:HZ3	1:C:292:GLN:HG3	1.77	0.47
2:G:1102:TYR:HB3	2:G:1244:PRO:CA	2.44	0.47
2:G:232:LEU:HD21	2:G:423:VAL:HA	1.97	0.47
2:G:732:TRP:CE2	2:G:750:MET:HE3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1130:THR:H	2:H:1133:THR:CG2	2.27	0.47
2:H:1378:ILE:HG12	2:H:1378:ILE:O	2.13	0.47
2:H:176:LEU:HD22	2:H:247:ALA:HB1	1.95	0.47
2:H:560:ASN:OD1	2:H:560:ASN:O	2.33	0.47
2:H:606:PHE:HZ	2:H:805:VAL:CG1	2.28	0.47
2:H:111:LEU:HD11	2:H:64:PHE:CD2	2.50	0.47
2:H:741:HIS:HE1	2:H:845:THR:HG21	1.61	0.47
2:I:1148:ASN:ND2	2:I:1151:HIS:H	2.13	0.47
2:I:22:VAL:HG11	2:I:27:PHE:HA	1.97	0.47
2:I:461:ASP:HB3	2:I:464:ASP:HB2	1.95	0.47
2:I:732:TRP:CE2	2:I:750:MET:HE3	2.50	0.47
1:A:1158:PRO:HD2	1:A:1159:GLU:OE2	2.14	0.47
1:A:406:TRP:CE3	1:A:1619:GLU:HG3	2.49	0.47
1:A:930:LEU:CD2	1:A:933:VAL:HG11	2.44	0.47
1:B:1276:GLN:O	1:B:1282:THR:HG21	2.14	0.47
1:B:705:VAL:CG2	1:B:732:LEU:HD21	2.43	0.47
1:B:968:VAL:O	2:H:1512:HIS:HB2	2.14	0.47
1:C:338:LEU:O	1:C:342:GLN:HG3	2.15	0.47
2:G:1567:ARG:NH1	2:G:1568:HIS:HB3	2.28	0.47
2:G:369:SER:O	2:G:370:LEU:HD23	2.14	0.47
2:G:629:GLY:O	2:G:632:ALA:HB3	2.15	0.47
2:H:1980:TYR:HD1	2:H:1981:LEU:HD12	1.79	0.47
2:H:1819:ALA:CA	2:H:2005:ARG:HH11	2.26	0.47
2:H:967:ILE:HD12	2:H:972:LEU:HD22	1.96	0.47
2:I:1004:LEU:CD2	2:I:1019:PRO:HB2	2.44	0.47
2:I:443:LEU:HD22	2:I:448:VAL:CG1	2.45	0.47
2:I:747:HIS:HE1	2:I:780:TYR:OH	1.97	0.47
2:I:768:GLY:HA3	2:I:800:LEU:CD2	2.41	0.47
2:I:955:GLU:HG2	2:I:987:TYR:HE2	1.79	0.47
1:A:529:MET:HE3	1:A:529:MET:CA	2.36	0.47
1:A:988:ILE:HD13	1:A:1048:GLU:HA	1.97	0.47
1:B:1523:ARG:NH2	1:B:1564:LEU:O	2.48	0.47
1:B:253:ARG:O	1:B:254:TRP:CD1	2.68	0.47
1:B:142:ASP:CG	1:B:257:PRO:HB2	2.35	0.47
1:C:1544:THR:O	1:C:1545:SER:HB3	2.15	0.47
2:G:1159:ILE:CG1	2:G:1169:PRO:CD	2.93	0.47
2:G:1666:PHE:CE1	2:G:1814:ALA:HA	2.50	0.47
2:G:1873:TYR:CE2	2:G:1940:LEU:HD21	2.49	0.47
2:G:55:THR:HB	2:G:59:GLU:OE2	2.14	0.47
2:H:1004:LEU:CD2	2:H:1019:PRO:HB2	2.44	0.47
2:H:586:LEU:HD12	2:H:764:MET:SD	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:826:GLY:HA3	2:H:1061:GLN:CB	2.44	0.47
2:I:1418:ASP:C	2:I:1420:GLU:H	2.18	0.47
2:I:194:THR:CG2	2:I:300:ILE:HD11	2.40	0.47
2:I:376:ASN:C	2:I:376:ASN:ND2	2.68	0.47
2:I:42:PRO:HG2	2:I:52:ASP:CG	2.35	0.47
1:B:1305:CYS:SG	3:B:2748:CER:H51	2.54	0.47
1:C:1012:LEU:HD23	1:C:1445:MET:HE3	1.97	0.47
1:C:237:MET:HG3	1:C:241:PHE:HB3	1.95	0.47
2:G:826:GLY:HA2	2:G:1060:ALA:HB3	1.97	0.47
2:G:1850:SER:HB2	2:G:1973:SER:HB2	1.96	0.47
2:G:730:LEU:C	2:G:730:LEU:HD12	2.35	0.47
2:G:772:GLY:O	2:G:804:ARG:HD3	2.15	0.47
2:H:127:ILE:HD12	2:H:180:TYR:HD2	1.80	0.47
2:H:131:ILE:CD1	2:H:182:VAL:CB	2.71	0.47
2:I:1553:TYR:OH	2:I:1583:MET:HB3	2.15	0.47
1:C:18:LEU:HD21	2:I:1815:LEU:CD1	2.45	0.47
2:I:606:PHE:HZ	2:I:805:VAL:CG1	2.28	0.47
1:A:1430:ARG:O	1:A:1430:ARG:HG2	2.15	0.47
1:A:1830:GLY:HA2	1:A:1831:GLY:HA2	1.57	0.47
1:A:36:LEU:CD2	1:A:61:LEU:HD21	2.37	0.47
1:B:1009:LEU:HD13	1:B:1445:MET:HE1	1.97	0.47
1:B:254:TRP:HZ3	1:B:292:GLN:HG3	1.76	0.47
1:B:32:GLN:NE2	1:B:57:ALA:HA	2.29	0.47
1:B:883:ILE:HD12	1:B:947:LEU:HD12	1.97	0.47
1:C:1189:ILE:HG23	1:C:1190:PRO:HD2	1.97	0.47
2:G:1273:GLU:HB3	2:G:1274:PRO:CD	2.45	0.47
2:G:1493:LEU:HB3	2:G:1494:PRO:HD2	1.96	0.47
2:G:1844:ARG:NH1	2:G:1844:ARG:HG2	2.09	0.47
1:A:29:ILE:HG13	2:G:1891:TYR:O	2.15	0.47
2:G:739:GLY:HA2	2:G:1054:LEU:HG	1.97	0.47
2:G:745:ASP:HA	2:G:832:TRP:CH2	2.48	0.47
2:G:881:VAL:N	2:G:882:PRO:CD	2.78	0.47
2:H:1015:VAL:HG11	2:H:1017:PHE:CE1	2.50	0.47
2:H:1054:LEU:HB2	4:H:3051:FMN:HM71	1.96	0.47
2:H:1273:GLU:HB3	2:H:1274:PRO:CD	2.45	0.47
2:H:1428:GLU:HG2	2:H:1470:THR:HG22	1.97	0.47
2:H:1473:THR:O	2:H:1481:SER:HB3	2.15	0.47
2:H:1764:PHE:HB2	2:H:1770:LEU:HD21	1.97	0.47
2:H:238:CYS:CB	2:H:239:PRO:HD3	2.43	0.47
2:H:720:ALA:HA	2:H:728:ILE:CD1	2.45	0.47
2:I:1148:ASN:HD22	2:I:1148:ASN:C	2.19	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:490:TRP:HA	2:I:493:THR:HG22	1.96	0.47
1:A:186:ILE:O	1:A:190:LEU:HG	2.14	0.46
1:A:702:LYS:HD3	1:A:731:THR:CG2	2.44	0.46
1:B:1544:THR:O	1:B:1545:SER:HB3	2.15	0.46
1:C:709:ARG:O	1:C:714:VAL:HG21	2.16	0.46
1:C:930:LEU:CD2	1:C:933:VAL:HG11	2.45	0.46
2:G:1015:VAL:HG11	2:G:1017:PHE:CE1	2.50	0.46
2:G:2035:SER:HB3	2:G:2038:ILE:CG1	2.41	0.46
2:G:249:TYR:CD2	2:G:283:ILE:HD11	2.50	0.46
2:H:7:ARG:NH2	2:H:24:THR:O	2.48	0.46
2:H:440:ASN:ND2	2:H:477:GLU:HG2	2.30	0.46
2:I:1913:VAL:O	2:I:1917:ILE:HG13	2.15	0.46
2:I:533:LEU:HD13	2:I:545:GLN:HG3	1.97	0.46
2:I:573:LYS:C	2:I:575:GLY:H	2.19	0.46
2:I:99:ASN:HA	2:I:550:VAL:HG23	1.97	0.46
1:A:1056:ILE:HG13	1:A:1057:MET:N	2.30	0.46
1:A:1238:VAL:CG1	1:A:1239:HIS:N	2.78	0.46
1:A:183:GLN:NE2	1:A:202:GLU:HG2	2.29	0.46
1:A:908:LEU:HA	1:A:913:VAL:HG21	1.96	0.46
1:B:1133:PRO:HG3	1:B:1166:LYS:HG3	1.97	0.46
1:C:1303:GLY:C	1:C:1307:THR:HG22	2.35	0.46
1:C:1646:PHE:CE1	3:C:2748:CER:H31	2.50	0.46
1:C:293:LYS:O	1:C:297:ILE:HG13	2.15	0.46
1:C:499:PRO:HD3	1:C:516:ARG:HH21	1.80	0.46
2:G:1293:THR:HG22	2:G:1296:GLU:CD	2.35	0.46
2:G:279:THR:O	2:G:283:ILE:HB	2.15	0.46
2:G:598:THR:CB	2:G:599:PRO:HD3	2.46	0.46
2:G:652:ILE:HD12	2:G:652:ILE:N	2.29	0.46
2:G:751:LEU:HA	2:G:794:MET:HE3	1.96	0.46
2:H:101:ILE:H	2:H:101:ILE:HG13	1.30	0.46
2:H:1258:ARG:O	2:H:1262:ILE:HG13	2.15	0.46
2:H:1269:LEU:O	2:H:1560:LEU:HD23	2.15	0.46
2:H:1804:PHE:CD2	2:H:1818:LEU:HD22	2.50	0.46
2:H:218:TRP:HB3	2:H:225:THR:OG1	2.15	0.46
2:H:736:ARG:H	2:H:736:ARG:HG3	1.55	0.46
2:H:926:LEU:HB3	2:H:947:THR:HG22	1.97	0.46
2:I:1080:GLY:O	2:I:1084:LYS:HG3	2.15	0.46
2:I:1148:ASN:HD22	2:I:1151:HIS:H	1.63	0.46
2:I:213:LEU:HG	2:I:213:LEU:O	2.16	0.46
2:I:345:THR:HG22	2:I:347:GLU:N	2.23	0.46
2:I:758:ARG:NH2	2:I:797:ASP:OD1	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:LEU:HD13	1:A:272:GLU:CB	2.44	0.46
1:A:702:LYS:HE2	1:A:729:GLY:O	2.15	0.46
1:B:1239:HIS:CD2	1:B:1241:SER:H	2.33	0.46
1:B:1303:GLY:C	1:B:1307:THR:HG22	2.35	0.46
1:B:1114:TYR:CD1	1:B:1337:GLU:HG3	2.50	0.46
1:B:1639:VAL:CG1	1:B:1640:SER:N	2.79	0.46
1:B:237:MET:HG3	1:B:241:PHE:HB3	1.97	0.46
1:C:1004:ILE:HG22	1:C:1660:TYR:CE2	2.49	0.46
1:C:186:ILE:O	1:C:190:LEU:HG	2.15	0.46
1:C:420:ILE:HG22	1:C:469:VAL:HG22	1.96	0.46
1:C:908:LEU:HA	1:C:913:VAL:HG21	1.96	0.46
2:G:1422:THR:HG23	2:G:1474:PHE:CD1	2.51	0.46
2:G:1579:ILE:HG22	2:G:1580:THR:O	2.15	0.46
2:G:9:LEU:HB2	2:G:27:PHE:HE1	1.81	0.46
2:G:7:ARG:NH2	2:G:24:THR:O	2.48	0.46
2:G:826:GLY:HA3	2:G:1061:GLN:CB	2.44	0.46
2:H:1079:ASP:O	2:H:1082:ILE:HG22	2.16	0.46
2:H:1359:MET:CE	2:H:1404:MET:HB3	2.44	0.46
2:H:1552:PRO:O	2:H:1556:VAL:HG23	2.15	0.46
1:B:14:LEU:HD11	2:H:1821:VAL:HG11	1.97	0.46
2:H:1945:ASP:O	2:H:1949:LYS:HG3	2.15	0.46
2:H:350:GLN:HA	2:H:353:VAL:HG13	1.97	0.46
2:H:598:THR:CB	2:H:599:PRO:HD3	2.44	0.46
2:H:72:VAL:HG12	2:H:73:GLU:N	2.30	0.46
2:H:879:LYS:HA	2:H:879:LYS:HD3	1.71	0.46
2:I:1593:ILE:HD13	2:I:1626:ILE:HD13	1.97	0.46
2:I:826:GLY:HA3	2:I:1061:GLN:CB	2.46	0.46
1:A:986:ALA:CB	1:A:1047:LEU:HD13	2.45	0.46
1:A:1544:THR:O	1:A:1545:SER:HB3	2.15	0.46
1:A:1639:VAL:CG1	1:A:1640:SER:N	2.78	0.46
1:A:1646:PHE:CE1	3:A:2748:CER:H31	2.50	0.46
1:A:338:LEU:O	1:A:342:GLN:HG3	2.16	0.46
1:B:1305:CYS:SG	1:B:1585:LYS:HA	2.56	0.46
1:B:741:SER:HB3	1:B:744:ASP:HB2	1.97	0.46
1:C:1238:VAL:CG1	1:C:1242:GLU:HB2	2.45	0.46
1:C:451:MET:HE2	1:C:451:MET:HB3	1.71	0.46
1:C:784:ILE:HG23	1:C:788:SER:HB2	1.98	0.46
2:G:1749:GLU:OE2	2:G:1840:VAL:HG13	2.16	0.46
2:G:355:LYS:HE2	2:G:355:LYS:HB3	1.64	0.46
2:H:807:ILE:HD12	2:H:1063:THR:HG23	1.96	0.46
2:H:1266:TYR:HB2	2:H:1347:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1666:PHE:CD1	2:H:1814:ALA:HB2	2.49	0.46
2:H:1908:ASP:HA	2:H:1911:THR:HG22	1.98	0.46
2:H:42:PRO:HG2	2:H:52:ASP:CG	2.36	0.46
2:H:573:LYS:HE3	2:H:1101:GLU:OE1	2.15	0.46
2:H:881:VAL:N	2:H:882:PRO:CD	2.79	0.46
2:I:1272:ASP:O	2:I:1273:GLU:HG3	2.15	0.46
2:I:131:ILE:HG21	2:I:182:VAL:HG12	1.97	0.46
2:I:1624:THR:HB	2:I:1642:THR:CG2	2.43	0.46
2:I:1764:PHE:HB2	2:I:1770:LEU:HD21	1.97	0.46
1:A:1050:CYS:HB3	1:A:1089:VAL:HG12	1.98	0.46
1:B:1618:LEU:HD23	1:B:1621:PHE:CE2	2.51	0.46
1:B:183:GLN:NE2	1:B:202:GLU:HG2	2.29	0.46
1:B:451:MET:HE2	1:B:451:MET:HB3	1.73	0.46
1:C:256:LEU:HA	1:C:257:PRO:HD3	1.72	0.46
1:C:2:LYS:HE2	1:C:4:GLU:CD	2.35	0.46
2:G:873:PHE:CD1	2:G:1026:GLU:HB2	2.50	0.46
2:G:109:LEU:HD11	2:G:116:LEU:CD2	2.41	0.46
2:G:1834:ARG:CG	2:G:1834:ARG:NH1	2.68	0.46
1:A:26:VAL:CG2	2:G:1890:ASN:ND2	2.78	0.46
2:G:455:ILE:O	2:G:455:ILE:HG13	2.14	0.46
2:G:702:TYR:HB3	2:G:727:PRO:HB2	1.97	0.46
2:H:1169:PRO:O	2:H:1173:VAL:HG23	2.15	0.46
2:H:1195:VAL:HG13	2:H:1211:LEU:CB	2.44	0.46
2:H:1441:ILE:HD11	2:H:1445:ARG:NH2	2.27	0.46
2:H:1567:ARG:NH1	2:H:1568:HIS:HB3	2.29	0.46
2:H:1638:ILE:HD12	2:H:1657:ILE:CG1	2.43	0.46
2:I:1666:PHE:CD1	2:I:1814:ALA:HA	2.50	0.46
2:I:584:SER:CB	2:I:591:PRO:HG3	2.41	0.46
1:A:170:LYS:HD3	1:A:175:LEU:HD23	1.97	0.46
1:A:2:LYS:HE2	1:A:4:GLU:CD	2.36	0.46
1:B:1303:GLY:CA	1:B:1649:LYS:HE2	2.40	0.46
1:B:702:LYS:HE2	1:B:729:GLY:O	2.15	0.46
1:C:1319:ILE:HA	1:C:1324:ALA:O	2.14	0.46
1:C:1362:PRO:HA	1:C:1365:MET:HG3	1.97	0.46
1:C:1367:ARG:HH12	1:C:1372:THR:CB	2.20	0.46
1:C:1533:ILE:HD11	1:C:1564:LEU:HD13	1.98	0.46
1:C:243:ILE:O	1:C:247:ARG:HG3	2.16	0.46
2:G:1886:VAL:HG22	2:G:1906:ALA:HB1	1.97	0.46
2:G:209:PHE:CE2	2:G:213:LEU:HD22	2.51	0.46
2:G:214:ASN:ND2	2:G:217:GLU:HB2	2.30	0.46
2:G:309:ARG:HA	2:G:309:ARG:HD3	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:441:LYS:O	2:G:444:VAL:HG12	2.15	0.46
2:G:669:LEU:HD12	2:G:669:LEU:HA	1.62	0.46
2:G:719:ILE:H	2:G:719:ILE:HG12	1.57	0.46
2:G:844:VAL:HG22	2:G:858:ALA:HB2	1.98	0.46
2:H:582:LYS:HE2	2:H:761:PRO:O	2.16	0.46
2:I:1071:LYS:HE3	2:I:1075:ASP:OD2	2.14	0.46
2:H:321:PRO:HD2	2:I:1599:ASP:OD1	2.16	0.46
2:I:1932:SER:O	2:I:1936:VAL:HG22	2.16	0.46
2:I:2026:PHE:HB3	2:I:2042:ILE:HD13	1.98	0.46
2:I:843:ILE:HD11	2:I:1055:HIS:HB3	1.98	0.46
1:A:1270:VAL:HG11	1:A:1274:ILE:HD13	1.97	0.46
1:A:1487:LEU:C	1:A:1487:LEU:HD23	2.35	0.46
1:A:1617:ILE:O	1:A:1620:GLN:HG2	2.16	0.46
1:A:709:ARG:O	1:A:714:VAL:HG21	2.16	0.46
1:B:11:HIS:C	1:B:11:HIS:CD2	2.89	0.46
1:B:792:HIS:CE1	1:B:796:LEU:HD23	2.51	0.46
1:C:1263:ASP:HB2	1:C:1270:VAL:HG21	1.98	0.46
1:C:1577:GLN:NE2	1:C:1591:TRP:HB3	2.30	0.46
1:C:1233:GLU:CD	1:C:1680:ARG:HH21	2.19	0.46
1:C:774:ILE:HA	1:C:775:PRO:HD3	1.74	0.46
2:G:1378:ILE:O	2:G:1378:ILE:HG12	2.13	0.46
2:G:1854:MET:CG	2:G:1901:ALA:HB2	2.46	0.46
2:G:553:ASN:O	2:G:556:LYS:HE3	2.16	0.46
2:H:1180:MET:HB2	2:H:1197:LEU:HD21	1.98	0.46
2:H:1624:THR:HB	2:H:1642:THR:CG2	2.45	0.46
2:H:1738:PHE:CE1	2:H:1837:THR:HG23	2.50	0.46
2:H:1850:SER:HB2	2:H:1973:SER:HB2	1.97	0.46
2:H:1858:ASN:HA	2:H:1896:GLN:O	2.16	0.46
2:H:306:ILE:HA	2:H:439:ILE:HD13	1.96	0.46
2:H:481:ASP:OD2	2:H:485:ARG:NH1	2.48	0.46
2:H:653:TYR:HD1	2:H:659:LEU:HD21	1.80	0.46
2:H:845:THR:HG22	2:H:855:HIS:CD2	2.51	0.46
2:I:860:ARG:HB2	2:I:1049:GLN:HG3	1.97	0.46
2:I:109:LEU:HD11	2:I:116:LEU:CD2	2.43	0.46
2:I:109:LEU:HD22	2:I:114:THR:HG23	1.96	0.46
2:I:1418:ASP:C	2:I:1420:GLU:N	2.68	0.46
2:I:589:ARG:HB3	2:I:590:PRO:CD	2.43	0.46
2:I:653:TYR:HD1	2:I:659:LEU:HD21	1.79	0.46
1:A:37:LYS:HB2	1:A:65:TYR:CE1	2.48	0.46
1:A:427:ASN:ND2	1:A:610:THR:H	2.08	0.46
1:A:49:PRO:O	1:A:82:SER:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1021:VAL:HG22	1:B:1387:ILE:HG22	1.98	0.46
1:B:1595:GLY:O	1:B:1599:ILE:HG13	2.15	0.46
1:C:182:VAL:O	1:C:186:ILE:HG13	2.16	0.46
2:G:1168:ASN:HA	2:G:1169:PRO:HD3	1.81	0.46
2:G:1303:ALA:HB2	2:G:1556:VAL:HG21	1.98	0.46
2:G:131:ILE:CG2	2:G:182:VAL:HG11	2.43	0.46
2:G:2037:PRO:O	2:G:2041:ILE:HG13	2.16	0.46
2:G:785:TRP:CG	2:G:786:SER:N	2.83	0.46
2:G:845:THR:HG22	2:G:855:HIS:CD2	2.50	0.46
2:G:955:GLU:HG2	2:G:987:TYR:HE2	1.80	0.46
2:H:1344:ASP:O	2:H:1416:TYR:HE2	1.99	0.46
2:H:1427:VAL:HG22	2:H:1469:GLU:HG2	1.96	0.46
2:H:1491:VAL:HB	2:H:1501:ILE:CD1	2.45	0.46
2:H:1651:LEU:O	2:H:1652:THR:HG23	2.16	0.46
2:H:1846:GLU:C	2:H:1848:GLY:H	2.19	0.46
2:H:1873:TYR:CE1	2:H:1877:ARG:NE	2.77	0.46
2:H:551:THR:HG22	2:H:552:SER:N	2.30	0.46
2:H:60:LEU:O	2:H:63:LYS:HB2	2.16	0.46
2:I:1180:MET:HB3	2:I:1199:GLU:HG2	1.98	0.46
2:I:1543:ASP:OD1	2:I:1623:LYS:HG2	2.15	0.46
2:I:490:TRP:CZ2	2:I:512:LEU:HD21	2.51	0.46
1:A:331:ILE:HG23	1:A:332:THR:N	2.31	0.46
1:A:35:PHE:HA	1:A:39:PHE:HD2	1.81	0.46
1:A:489:VAL:CG2	1:A:670:GLY:C	2.84	0.46
1:A:507:GLY:N	1:A:954:ARG:HG2	2.31	0.46
1:C:1196:LYS:HE3	1:C:1202:ASP:CG	2.37	0.46
1:C:11:His:C	1:C:11:His:CD2	2.89	0.46
1:C:1209:ASP:OD2	1:C:1253:GLY:HA2	2.16	0.46
2:G:123:ILE:HD11	2:G:533:LEU:HD22	1.98	0.46
2:G:1418:ASP:O	2:G:1421:ASN:N	2.43	0.46
2:G:970:TYR:O	2:G:973:LEU:HB2	2.16	0.46
2:H:1236:LEU:HA	2:H:1237:PRO:HD3	1.78	0.46
2:H:1374:THR:HG23	2:H:1396:LEU:CD1	2.46	0.46
2:H:1227:ARG:NE	2:H:1565:VAL:HG12	2.30	0.46
2:H:490:TRP:CZ2	2:H:512:LEU:HD21	2.51	0.46
2:H:702:TYR:HB3	2:H:727:PRO:HB2	1.97	0.46
2:I:1031:LYS:O	2:I:1032:ASP:C	2.54	0.46
2:I:1054:LEU:HB3	4:I:3051:FMN:HM82	1.98	0.46
2:I:1228:THR:HG21	2:I:1234:VAL:HG23	1.98	0.46
2:I:1418:ASP:O	2:I:1420:GLU:N	2.49	0.46
2:I:740:HIS:HE1	2:I:852:GLU:OE1	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:860:ARG:H	2:I:1049:GLN:HG3	1.80	0.46
1:A:1709:GLU:HG3	1:A:1709:GLU:H	1.46	0.46
1:A:386:PHE:O	1:A:390:VAL:HB	2.16	0.46
1:B:143:GLU:H	1:B:260:ARG:HG2	1.81	0.46
1:B:601:VAL:O	1:B:602:GLU:C	2.54	0.46
1:C:1459:ILE:O	1:C:1463:VAL:HG23	2.16	0.46
1:C:539:SER:O	1:C:540:GLN:C	2.52	0.46
2:G:1002:HIS:NE2	2:G:1006:MET:CE	2.79	0.46
2:G:1311:PHE:HD1	2:G:1320:LEU:O	1.99	0.46
2:G:1435:ILE:O	2:G:1435:ILE:HG22	2.15	0.46
2:G:233:SER:HA	2:G:424:ALA:CB	2.46	0.46
2:H:1021:LEU:HA	2:H:1021:LEU:HD22	1.58	0.46
2:H:913:ASP:H	2:H:916:THR:CG2	2.29	0.46
2:I:1222:GLU:HG3	2:I:1235:SER:OG	2.16	0.46
2:I:1282:ARG:NH2	2:I:1423:PHE:HB3	2.31	0.46
2:I:1561:ASN:OD1	2:I:1563:ILE:HB	2.15	0.46
2:I:232:LEU:HD21	2:I:423:VAL:HA	1.98	0.46
2:I:391:LEU:CD2	2:I:394:ARG:NH2	2.78	0.46
2:I:670:ARG:HD2	2:I:676:ILE:O	2.16	0.46
2:I:785:TRP:CG	2:I:786:SER:N	2.84	0.46
2:I:751:LEU:HD11	2:I:789:PHE:CD1	2.51	0.46
2:I:844:VAL:HG22	2:I:858:ALA:HB2	1.97	0.46
1:A:1533:ILE:HG13	1:A:1564:LEU:HB3	1.98	0.45
1:A:411:GLN:NE2	1:A:1628:SER:H	2.13	0.45
1:A:1557:ILE:HD11	1:A:1642:THR:HG21	1.97	0.45
1:A:792:HIS:CE1	1:A:796:LEU:HD23	2.51	0.45
1:B:1234:MET:HG2	1:B:1326:ILE:CD1	2.46	0.45
1:B:516:ARG:NH2	1:B:889:GLU:OE1	2.49	0.45
1:B:881:ASN:HA	1:B:944:ARG:HH22	1.78	0.45
1:C:1040:GLU:HB2	1:C:1580:LEU:HD12	1.98	0.45
1:C:1376:PHE:CB	1:C:1544:THR:HG22	2.45	0.45
1:C:1573:ILE:HG23	1:C:1627:PRO:HG3	1.98	0.45
1:C:400:ARG:HH11	1:C:400:ARG:HG3	1.72	0.45
2:G:1586:SER:O	2:G:1590:ARG:HB2	2.16	0.45
2:G:159:ILE:CG2	2:G:501:ILE:HG22	2.46	0.45
2:G:1738:PHE:CD1	2:G:1837:THR:HG23	2.51	0.45
2:H:1031:LYS:O	2:H:1032:ASP:C	2.54	0.45
2:H:1135:GLU:OE2	2:H:1175:LYS:HE3	2.15	0.45
2:H:1417:THR:C	2:H:1419:PHE:H	2.19	0.45
2:H:1388:LYS:HE3	2:H:1418:ASP:OD2	2.16	0.45
2:H:1593:ILE:HD13	2:H:1626:ILE:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1666:PHE:CE1	2:H:1814:ALA:HA	2.50	0.45
2:H:1873:TYR:CE1	2:H:1877:ARG:NH2	2.83	0.45
2:H:2026:PHE:HB3	2:H:2042:ILE:HD13	1.98	0.45
2:H:391:LEU:CD2	2:H:394:ARG:NH2	2.80	0.45
2:H:730:LEU:HD12	2:H:730:LEU:C	2.36	0.45
2:I:738:GLY:HA3	4:I:3051:FMN:HM81	1.98	0.45
2:I:807:ILE:HD12	2:I:1063:THR:HG23	1.98	0.45
1:A:1114:TYR:CE1	1:A:1337:GLU:HG3	2.50	0.45
1:A:408:TRP:CZ3	1:A:1628:SER:HB3	2.51	0.45
1:A:764:ASP:OD2	1:A:818:ARG:HD3	2.17	0.45
1:B:1431:GLU:OE2	1:B:1433:HIS:HE1	2.00	0.45
1:B:19:ALA:O	1:B:22:PHE:HB2	2.15	0.45
1:B:26:VAL:HG13	2:H:2013:ASN:ND2	2.31	0.45
1:B:2:LYS:HE2	1:B:4:GLU:OE1	2.15	0.45
1:B:719:GLN:HG3	1:B:720:SER:N	2.31	0.45
1:C:170:LYS:HD3	1:C:175:LEU:HD23	1.97	0.45
1:C:430:ARG:NH2	1:C:605:LEU:HD13	2.31	0.45
1:C:529:MET:CE	1:C:894:ARG:HD2	2.46	0.45
2:G:1219:ILE:HD11	2:G:1242:PHE:HB2	1.98	0.45
2:G:1222:GLU:HG3	2:G:1235:SER:OG	2.16	0.45
2:G:1472:VAL:CG2	2:G:1483:VAL:HG22	2.46	0.45
2:G:1673:GLU:N	2:G:1676:MET:HE3	2.25	0.45
2:G:191:SER:HA	2:G:194:THR:CG2	2.46	0.45
2:G:1976:PHE:HA	2:G:1981:LEU:CD2	2.46	0.45
2:G:161:GLY:HA3	2:G:506:PRO:HD2	1.98	0.45
2:H:1579:ILE:HG22	2:H:1580:THR:O	2.16	0.45
2:H:1768:LYS:HE2	2:H:1772:SER:HB3	1.98	0.45
2:H:246:LEU:HD12	2:H:246:LEU:HA	1.85	0.45
2:H:324:LEU:HD12	2:H:324:LEU:O	2.16	0.45
2:H:612:ASN:HD21	2:H:641:ILE:HA	1.81	0.45
2:I:1359:MET:HE3	2:I:1404:MET:HB3	1.98	0.45
2:I:369:SER:O	2:I:370:LEU:HD23	2.16	0.45
2:I:601:THR:HB	2:I:620:ALA:HB2	1.98	0.45
2:I:669:LEU:HD12	2:I:669:LEU:HA	1.65	0.45
1:A:1367:ARG:HH12	1:A:1372:THR:CB	2.18	0.45
1:A:1431:GLU:OE2	1:A:1523:ARG:NH1	2.48	0.45
1:A:751:PHE:CZ	1:A:761:LEU:HD13	2.51	0.45
1:B:1639:VAL:HG12	1:B:1640:SER:N	2.31	0.45
1:B:235:SER:HA	1:B:276:ARG:NH2	2.32	0.45
1:B:37:LYS:HB2	1:B:65:TYR:CE1	2.51	0.45
1:B:444:ASN:HB2	1:B:447:LEU:N	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:827:SER:HA	1:C:828:PRO:HD3	1.70	0.45
1:C:982:ILE:HD11	2:I:965:SER:CB	2.46	0.45
1:A:18:LEU:HD21	2:G:1815:LEU:CD1	2.46	0.45
2:G:1953:VAL:O	2:G:1953:VAL:HG12	2.16	0.45
2:G:247:ALA:O	2:G:251:VAL:HG13	2.15	0.45
2:G:460:TYR:HA	2:G:466:SER:O	2.17	0.45
2:G:562:LEU:HG	2:G:793:PRO:CG	2.43	0.45
2:G:860:ARG:HB2	2:G:1049:GLN:HG3	1.97	0.45
2:H:1590:ARG:HG3	2:H:1608:TYR:CD2	2.51	0.45
2:H:1776:PHE:C	2:H:1779:PRO:HD2	2.37	0.45
2:H:249:TYR:CD2	2:H:283:ILE:HD11	2.52	0.45
2:H:439:ILE:HD12	2:H:484:ILE:CD1	2.46	0.45
2:H:562:LEU:HG	2:H:793:PRO:CB	2.47	0.45
2:I:1180:MET:HB2	2:I:1197:LEU:HD21	1.97	0.45
2:I:1775:GLN:HG2	2:I:1836:MET:SD	2.57	0.45
2:I:1854:MET:CG	2:I:1901:ALA:HB2	2.47	0.45
2:I:618:GLU:HG2	2:I:678:PHE:CZ	2.51	0.45
2:I:739:GLY:HA2	2:I:1054:LEU:HG	1.97	0.45
1:A:168:MET:HA	1:A:206:LEU:HB2	1.98	0.45
1:A:413:LEU:C	1:A:415:SER:H	2.18	0.45
1:A:625:THR:HG23	1:A:627:SER:H	1.82	0.45
1:A:630:ILE:O	1:A:653:ARG:NH2	2.48	0.45
1:A:798:ASN:HA	1:A:801:ARG:HB2	1.98	0.45
1:B:1310:GLU:OE1	1:B:1649:LYS:CE	2.62	0.45
1:B:32:GLN:NE2	1:B:57:ALA:CA	2.80	0.45
1:B:988:ILE:HD13	1:B:1048:GLU:CB	2.47	0.45
1:C:1533:ILE:HG13	1:C:1564:LEU:HB3	1.98	0.45
2:G:1015:VAL:HG13	2:G:1017:PHE:CE2	2.52	0.45
2:G:1148:ASN:HD22	2:G:1151:HIS:H	1.63	0.45
2:G:1314:ARG:HA	2:G:1314:ARG:HD3	1.62	0.45
2:G:1844:ARG:HA	2:G:1849:ARG:O	2.16	0.45
2:G:582:LYS:HE2	2:G:1108:PRO:HB3	1.97	0.45
2:G:807:ILE:HA	2:G:818:LYS:HG2	1.97	0.45
2:H:1735:ALA:O	2:H:1737:ILE:HG13	2.16	0.45
2:H:463:PHE:CD2	2:H:463:PHE:C	2.90	0.45
2:H:601:THR:O	2:H:601:THR:CG2	2.65	0.45
2:H:835:THR:CB	2:H:845:THR:HG23	2.43	0.45
2:I:1199:GLU:OE2	2:I:1567:ARG:CZ	2.65	0.45
2:I:1327:ILE:HA	2:I:1327:ILE:HD12	1.80	0.45
2:I:1609:THR:O	2:I:1653:GLY:HA3	2.16	0.45
2:I:463:PHE:CE1	2:I:486:LEU:HD22	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1196:LYS:HE3	1:A:1202:ASP:CG	2.36	0.45
1:A:143:GLU:H	1:A:260:ARG:HG2	1.81	0.45
1:A:293:LYS:O	1:A:297:ILE:HG13	2.16	0.45
1:B:1020:VAL:CG1	1:B:1400:ILE:HG23	2.46	0.45
1:B:1061:SER:HB2	1:B:1078:SER:HB3	1.99	0.45
1:B:1019:ILE:HG21	1:B:1316:VAL:HG22	1.98	0.45
1:B:1464:GLU:HG3	1:B:1773:VAL:HG11	1.91	0.45
1:B:1376:PHE:CB	1:B:1544:THR:HG22	2.45	0.45
1:C:1104:ARG:O	1:C:1185:VAL:HG13	2.17	0.45
1:C:776:GLU:OE1	1:C:795:MET:HE1	2.17	0.45
2:G:357:ASN:OD1	2:G:365:GLN:HB3	2.16	0.45
2:H:1027:ILE:O	2:H:1031:LYS:HB2	2.16	0.45
2:H:1383:ASN:HD21	2:H:1418:ASP:CB	2.30	0.45
2:H:24:THR:O	2:H:26:SER:N	2.49	0.45
2:H:319:LEU:HA	2:H:319:LEU:HD22	1.68	0.45
2:H:611:THR:HA	2:H:615:TYR:O	2.16	0.45
2:H:659:LEU:HA	2:H:659:LEU:HD12	1.82	0.45
2:H:754:TYR:CE2	2:H:794:MET:HG3	2.52	0.45
2:I:1776:PHE:C	2:I:1779:PRO:HD2	2.37	0.45
2:I:1976:PHE:CB	2:I:1981:LEU:CD2	2.94	0.45
2:I:2036:GLU:HG2	2:I:2039:LYS:HZ3	1.82	0.45
2:I:894:ARG:NH1	2:I:898:ASP:OD2	2.42	0.45
2:I:938:TRP:CD1	2:I:944:ARG:HG3	2.52	0.45
1:C:1682:LYS:HB3	2:I:994:PHE:CD2	2.51	0.45
1:A:1120:GLU:O	1:A:1121:MET:HG3	2.16	0.45
1:A:776:GLU:OE1	1:A:795:MET:HE1	2.16	0.45
1:A:658:LEU:HD13	1:A:916:LEU:HD12	1.99	0.45
1:B:1533:ILE:HD11	1:B:1564:LEU:HD13	1.98	0.45
1:C:1491:ARG:NH1	1:C:1744:TYR:O	2.50	0.45
1:C:197:THR:HG22	1:C:198:PRO:O	2.15	0.45
1:C:225:SER:OG	1:C:266:LEU:HD21	2.16	0.45
1:C:143:GLU:H	1:C:260:ARG:HG2	1.81	0.45
1:B:332:THR:HG22	1:C:331:ILE:HD11	1.98	0.45
2:G:1080:GLY:O	2:G:1084:LYS:HG3	2.16	0.45
2:G:1241:ASN:N	2:G:1252:SER:O	2.49	0.45
2:G:142:ASN:HB2	2:G:550:VAL:HG13	1.99	0.45
2:G:1466:PHE:HE2	2:G:1489:ILE:HD13	1.81	0.45
2:G:1976:PHE:CB	2:G:1981:LEU:CD2	2.95	0.45
2:G:315:PRO:O	2:H:1314:ARG:NH2	2.50	0.45
2:G:712:ALA:O	2:G:715:GLN:HB3	2.16	0.45
2:H:1085:LEU:HD12	2:H:1085:LEU:HA	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1159:ILE:HG22	2:H:1160:THR:N	2.32	0.45
2:H:1325:PHE:O	2:H:1328:VAL:HG12	2.16	0.45
2:H:618:GLU:HG2	2:H:678:PHE:CZ	2.52	0.45
2:H:785:TRP:CG	2:H:786:SER:N	2.84	0.45
2:I:1195:VAL:HG13	2:I:1211:LEU:CB	2.46	0.45
2:I:1637:LEU:HD23	2:I:1637:LEU:HA	1.79	0.45
2:I:440:ASN:ND2	2:I:477:GLU:HG2	2.31	0.45
2:I:23:PRO:HG2	2:I:86:LEU:HD11	1.98	0.45
1:A:1300:THR:HA	1:A:1301:PRO:HD3	1.70	0.45
1:B:66:GLU:HA	1:B:66:GLU:OE1	2.15	0.45
1:C:1670:TYR:O	1:C:1674:VAL:HG23	2.17	0.45
1:C:1305:CYS:SG	3:C:2748:CER:H51	2.57	0.45
1:C:521:LYS:HB3	1:C:523:SER:HB3	1.98	0.45
2:G:1858:ASN:ND2	2:G:1861:ARG:HG3	2.32	0.45
2:G:1873:TYR:HE1	2:G:1877:ARG:HH21	1.59	0.45
2:G:665:LEU:O	2:G:665:LEU:HD22	2.17	0.45
2:G:754:TYR:CG	2:G:794:MET:HG2	2.51	0.45
2:H:1678:MET:HE3	2:H:1707:LEU:CD2	2.41	0.45
2:H:2035:SER:HB3	2:H:2038:ILE:CG1	2.44	0.45
2:H:594:VAL:CG2	2:H:610:THR:HG21	2.45	0.45
2:I:1162:ASP:O	2:I:1163:LYS:HB2	2.16	0.45
2:I:1949:LYS:O	2:I:1953:VAL:HG23	2.17	0.45
1:C:21:GLN:HG3	2:I:2013:ASN:HB2	1.98	0.45
2:I:478:ARG:O	2:I:482:CYS:HB2	2.17	0.45
2:I:784:GLU:O	2:I:787:THR:HB	2.17	0.45
1:A:1239:HIS:CD2	1:A:1241:SER:H	2.35	0.45
1:A:1443:LEU:HA	1:A:1443:LEU:HD23	1.75	0.45
1:B:1004:ILE:HG22	1:B:1660:TYR:CE2	2.52	0.45
1:B:1459:ILE:O	1:B:1463:VAL:HG23	2.17	0.45
1:B:1584:PRO:CG	1:B:1591:TRP:CZ3	3.00	0.45
1:B:1239:HIS:HE1	1:B:1714:VAL:O	2.00	0.45
2:G:101:ILE:HG13	2:G:101:ILE:H	1.31	0.45
2:G:1265:MET:HE1	2:G:1562:PRO:HG2	1.98	0.45
2:G:218:TRP:HB3	2:G:225:THR:OG1	2.16	0.45
2:G:350:GLN:HA	2:G:353:VAL:HG13	1.97	0.45
2:G:455:ILE:HD11	2:G:469:ARG:NE	2.32	0.45
2:G:879:LYS:HA	2:G:879:LYS:HD3	1.68	0.45
2:H:1100:VAL:HG23	2:H:1147:ILE:HB	1.99	0.45
2:H:1845:ASP:HB2	2:H:1849:ARG:N	2.15	0.45
2:H:751:LEU:HA	2:H:794:MET:HE3	1.98	0.45
2:I:1002:HIS:NE2	2:I:1006:MET:CE	2.80	0.45

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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	0.45
2:I:1258:ARG:O	2:I:1262:ILE:HG13	2.17	0.45
2:I:1308:CYS:HB3	2:I:1311:PHE:CE2	2.51	0.45
2:I:161:GLY:H	2:I:505:GLY:CA	2.28	0.45
2:I:355:LYS:HE2	2:I:355:LYS:HB3	1.70	0.45
2:I:654:VAL:O	2:I:654:VAL:HG12	2.17	0.45
2:I:677:GLN:O	2:I:678:PHE:HB3	2.17	0.45
1:A:483:VAL:O	1:A:484:LEU:C	2.56	0.45
1:A:929:GLY:C	1:A:931:GLN:H	2.19	0.45
1:B:1617:ILE:O	1:B:1620:GLN:HG2	2.17	0.45
1:B:340:ARG:HH12	1:B:344:GLN:HE21	1.64	0.45
1:B:420:ILE:HG22	1:B:469:VAL:HG22	1.99	0.45
1:C:378:LEU:HA	1:C:378:LEU:HD12	1.84	0.45
1:C:927:ASN:O	1:C:929:GLY:N	2.41	0.45
2:G:1491:VAL:HB	2:G:1501:ILE:HD12	1.99	0.45
2:G:1543:ASP:OD1	2:G:1623:LYS:HG2	2.16	0.45
2:G:1227:ARG:CZ	2:G:1565:VAL:HG12	2.47	0.45
2:G:624:TYR:HB2	2:G:630:MET:HE3	1.99	0.45
2:H:1327:ILE:HG12	2:H:1583:MET:HE3	1.99	0.45
2:H:512:LEU:O	2:H:516:THR:HG23	2.17	0.45
2:I:1491:VAL:HB	2:I:1501:ILE:CD1	2.47	0.45
2:I:653:TYR:OH	2:I:690:VAL:HG11	2.17	0.45
1:A:1516:ASP:HA	1:A:1517:PRO:HD3	1.61	0.45
1:A:204:THR:HA	1:A:205:PRO:HD3	1.85	0.45
1:A:335:HIS:CD2	1:A:335:HIS:O	2.69	0.45
1:B:1119:LYS:HE2	1:B:1341:PHE:CG	2.52	0.45
1:B:1300:THR:HA	1:B:1301:PRO:HD3	1.69	0.45
1:B:1592:MET:HE2	1:B:1641:ILE:HG23	1.98	0.45
1:B:196:THR:O	1:B:213:PHE:HE2	2.00	0.45
1:B:43:ARG:O	2:H:1662:THR:HA	2.16	0.45
1:B:32:GLN:HE21	1:B:57:ALA:HB2	1.82	0.45
1:B:67:SER:OG	2:G:359:HIS:HE1	1.99	0.45
1:B:44:VAL:HG13	1:B:78:ILE:HG12	1.98	0.45
1:C:1061:SER:HB2	1:C:1078:SER:HB3	1.99	0.45
1:C:478:GLU:OE1	1:C:478:GLU:HA	2.17	0.45
1:C:916:LEU:HD22	1:C:922:VAL:HG22	1.99	0.45
2:G:1002:HIS:NE2	2:G:1006:MET:HE3	2.32	0.45
2:G:109:LEU:HA	2:G:109:LEU:HD23	1.79	0.45
2:G:1325:PHE:O	2:G:1328:VAL:HG12	2.17	0.45
2:G:1389:ILE:HG13	2:G:1411:PHE:CD1	2.52	0.45
2:G:1417:THR:C	2:G:1419:PHE:N	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1418:ASP:C	2:G:1420:GLU:H	2.19	0.45
2:G:42:PRO:HG2	2:G:52:ASP:CG	2.38	0.45
2:H:641:ILE:HG12	2:H:645:SER:CB	2.46	0.45
2:I:1256:GLU:O	2:I:1257:ASP:HB2	2.17	0.45
2:I:231:LEU:HA	2:I:236:ILE:HD12	1.99	0.45
2:I:298:LYS:HG2	2:I:448:VAL:CG2	2.38	0.45
1:A:1283:MET:O	1:A:1287:VAL:HG23	2.18	0.44
1:A:242:THR:HG22	1:A:243:ILE:H	1.81	0.44
1:A:636:PRO:HB2	1:A:638:LEU:O	2.16	0.44
1:B:1029:PRO:HA	1:B:1188:GLN:O	2.17	0.44
1:B:1455:ARG:HD2	1:B:1455:ARG:HA	1.86	0.44
1:B:411:GLN:NE2	1:B:1628:SER:H	2.15	0.44
1:B:427:ASN:HB2	1:B:468:LEU:HD21	1.99	0.44
1:B:612:GLU:O	1:B:615:SER:HB3	2.17	0.44
1:B:626:VAL:HG23	1:B:664:GLU:OE2	2.17	0.44
1:B:733:ILE:CD1	1:B:761:LEU:HD11	2.46	0.44
1:C:1257:LEU:HA	1:C:1257:LEU:HD23	1.83	0.44
1:C:1494:HIS:CE1	1:C:1877:GLN:CG	2.99	0.44
1:C:253:ARG:O	1:C:254:TRP:CD1	2.70	0.44
1:C:641:ARG:HD3	1:C:649:TRP:O	2.17	0.44
2:G:1071:LYS:HE3	2:G:1075:ASP:OD2	2.16	0.44
2:G:1294:ALA:HA	2:G:1368:VAL:CG2	2.47	0.44
2:G:1855:ILE:HB	2:G:1907:LEU:HD12	2.00	0.44
2:G:607:VAL:O	2:G:611:THR:HB	2.17	0.44
2:G:717:ILE:O	2:G:720:ALA:HB3	2.18	0.44
2:G:741:HIS:HB3	2:G:853:PRO:HB2	1.98	0.44
2:G:741:HIS:HE1	2:G:855:HIS:NE2	2.13	0.44
2:G:926:LEU:HB3	2:G:947:THR:CG2	2.46	0.44
2:H:109:LEU:HD22	2:H:114:THR:HG23	1.99	0.44
2:H:1308:CYS:HB3	2:H:1311:PHE:CE2	2.52	0.44
2:H:1321:ALA:HA	2:H:1322:PRO:HD3	1.84	0.44
2:H:1529:GLN:O	2:H:1632:ILE:HG13	2.16	0.44
1:B:13:LEU:HB2	2:H:2026:PHE:CE1	2.52	0.44
2:H:443:LEU:HD22	2:H:448:VAL:CG1	2.46	0.44
2:I:1159:ILE:CG2	2:I:1160:THR:N	2.81	0.44
2:I:1589:VAL:HG21	2:I:1651:LEU:HD12	1.99	0.44
2:I:272:GLY:HA3	2:I:276:GLY:C	2.37	0.44
1:A:1012:LEU:HD23	1:A:1445:MET:HE2	1.99	0.44
1:A:1373:ARG:NE	1:A:1550:ASP:HB2	2.32	0.44
1:A:1666:THR:HG23	1:A:1669:ARG:CB	2.47	0.44
1:A:225:SER:OG	1:A:266:LEU:HD21	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:MET:HA	1:B:206:LEU:HB2	2.00	0.44
1:B:256:LEU:HA	1:B:257:PRO:HD3	1.73	0.44
1:B:330:GLU:O	1:B:330:GLU:HG2	2.16	0.44
1:C:1234:MET:HG2	1:C:1326:ILE:HD12	1.98	0.44
1:C:1238:VAL:CG1	1:C:1239:HIS:N	2.80	0.44
2:G:1609:THR:O	2:G:1653:GLY:HA3	2.16	0.44
2:G:7:ARG:HH11	2:G:24:THR:HG23	1.76	0.44
2:G:463:PHE:C	2:G:463:PHE:CD2	2.90	0.44
2:G:595:PRO:HD3	2:G:800:LEU:HB2	1.99	0.44
2:H:120:LYS:HB3	2:H:124:LYS:HE3	1.99	0.44
2:H:1330:GLY:HA2	2:H:1374:THR:HG21	1.98	0.44
2:H:1543:ASP:OD1	2:H:1623:LYS:HG2	2.17	0.44
2:H:560:ASN:H	2:H:564:GLU:HG2	1.82	0.44
2:H:786:SER:HB2	2:H:794:MET:HE2	1.99	0.44
2:H:854:ILE:HG22	2:H:856:LYS:HG3	1.99	0.44
2:I:1303:ALA:HB2	2:I:1556:VAL:HG21	1.98	0.44
2:I:1314:ARG:HD3	2:I:1314:ARG:HA	1.64	0.44
2:I:191:SER:HA	2:I:194:THR:CG2	2.43	0.44
2:I:441:LYS:O	2:I:444:VAL:HG12	2.17	0.44
2:I:659:LEU:HD12	2:I:659:LEU:HA	1.84	0.44
1:A:1431:GLU:HB3	1:A:1520:ALA:HB2	1.99	0.44
1:A:27:ARG:HH21	2:G:2015:THR:HA	1.82	0.44
1:A:267:VAL:HG12	1:A:290:MET:CE	2.48	0.44
1:B:183:GLN:O	1:B:187:LEU:HG	2.17	0.44
1:B:225:SER:OG	1:B:266:LEU:HD21	2.18	0.44
1:B:479:ASN:O	1:B:483:VAL:HG23	2.17	0.44
1:B:539:SER:O	1:B:540:GLN:C	2.54	0.44
1:B:655:LEU:HD23	1:B:655:LEU:HA	1.82	0.44
1:B:833:PHE:O	1:B:834:GLY:O	2.35	0.44
1:C:1487:LEU:C	1:C:1487:LEU:HD23	2.38	0.44
1:C:180:SER:O	1:C:183:GLN:N	2.50	0.44
2:G:1015:VAL:HA	2:G:1016:PRO:HD3	1.79	0.44
2:G:120:LYS:HB3	2:G:124:LYS:HE3	1.99	0.44
2:G:231:LEU:HA	2:G:236:ILE:HD12	2.00	0.44
2:G:566:HIS:O	2:G:567:PRO:O	2.34	0.44
2:H:161:GLY:H	2:H:505:GLY:CA	2.29	0.44
2:H:427:PHE:HB3	2:H:428:HIS:ND1	2.32	0.44
2:H:607:VAL:O	2:H:611:THR:HB	2.17	0.44
2:I:1735:ALA:O	2:I:1737:ILE:HG13	2.17	0.44
2:I:1757:GLU:H	2:I:1757:GLU:HG3	1.50	0.44
2:I:703:LEU:HD21	2:I:705:LEU:CD2	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:780:TYR:HB2	2:I:799:PHE:CE2	2.53	0.44
2:I:901:LYS:NZ	2:I:1031:LYS:O	2.51	0.44
1:A:1020:VAL:CG1	1:A:1400:ILE:HG23	2.47	0.44
1:A:1056:ILE:CD1	1:A:1193:TRP:CD1	3.00	0.44
1:A:66:GLU:HA	1:A:66:GLU:OE1	2.17	0.44
1:B:1040:GLU:OE2	1:B:1577:GLN:HB2	2.18	0.44
1:B:232:LEU:HD13	1:B:272:GLU:CB	2.47	0.44
1:B:32:GLN:HE22	1:B:57:ALA:N	2.16	0.44
1:C:1022:THR:HG22	1:C:1226:SER:CB	2.47	0.44
1:C:1657:HIS:CG	1:C:1658:PRO:HD2	2.53	0.44
1:C:625:THR:HG23	1:C:627:SER:H	1.83	0.44
1:C:930:LEU:HD23	1:C:930:LEU:HA	1.76	0.44
2:G:1590:ARG:NH2	2:G:1594:GLU:OE2	2.50	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:1908:ASP:HA	2:G:1911:THR:HG22	2.00	0.44
2:G:1945:ASP:O	2:G:1949:LYS:HG3	2.17	0.44
2:G:932:ILE:HD12	2:G:939:PHE:HD1	1.83	0.44
2:H:1311:PHE:HD1	2:H:1320:LEU:O	2.00	0.44
2:H:1697:HIS:CE1	2:H:1829:GLU:CG	3.00	0.44
2:H:209:PHE:CE2	2:H:213:LEU:HD22	2.52	0.44
2:H:663:ILE:HB	2:H:664:PRO:CD	2.44	0.44
2:H:778:TYR:N	2:H:779:PRO:CD	2.80	0.44
2:I:1330:GLY:HA2	2:I:1374:THR:HG21	1.99	0.44
2:I:1418:ASP:OD1	2:I:1420:GLU:HG3	2.17	0.44
2:I:1651:LEU:HA	2:I:1651:LEU:HD23	1.73	0.44
2:I:1054:LEU:CB	4:I:3051:FMN:HM71	2.46	0.44
2:I:665:LEU:HD22	2:I:665:LEU:O	2.18	0.44
1:B:496:PRO:HB2	1:B:519:VAL:HG12	1.99	0.44
1:C:503:ILE:HD12	1:C:950:THR:HG21	1.98	0.44
1:C:44:VAL:HG13	1:C:78:ILE:HG12	1.99	0.44
2:G:109:LEU:HD22	2:G:114:THR:HG23	2.00	0.44
2:G:1632:ILE:O	2:G:1632:ILE:HG23	2.16	0.44
2:G:297:ARG:O	2:G:301:THR:HG22	2.17	0.44
2:G:490:TRP:HA	2:G:493:THR:HG22	1.98	0.44
2:G:589:ARG:HB3	2:G:590:PRO:CD	2.48	0.44
2:H:109:LEU:HD11	2:H:116:LEU:CD2	2.43	0.44
2:H:641:ILE:CG1	2:H:645:SER:HB2	2.45	0.44
2:I:1590:ARG:HG3	2:I:1608:TYR:CD2	2.53	0.44
2:I:1846:GLU:C	2:I:1848:GLY:H	2.20	0.44
2:I:468:LEU:O	2:I:471:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:245:GLN:HG2	2:I:505:GLY:HA2	2.00	0.44
2:I:835:THR:HG22	2:I:844:VAL:CA	2.48	0.44
2:I:9:LEU:HB2	2:I:27:PHE:HE1	1.82	0.44
1:A:1022:THR:CG2	1:A:1226:SER:OG	2.66	0.44
1:A:1135:GLU:CD	1:B:242:THR:HG21	2.38	0.44
1:A:1305:CYS:SG	1:A:1585:LYS:HA	2.57	0.44
1:B:1238:VAL:CG1	1:B:1239:HIS:N	2.81	0.44
1:B:1516:ASP:HA	1:B:1517:PRO:HD3	1.65	0.44
1:B:267:VAL:HG12	1:B:290:MET:CE	2.48	0.44
1:C:1557:ILE:HD11	1:C:1642:THR:HG21	2.00	0.44
1:C:503:ILE:HD11	1:C:947:LEU:HD22	1.98	0.44
2:G:1784:MET:HE2	2:G:1784:MET:O	2.17	0.44
2:G:551:THR:C	2:G:553:ASN:H	2.20	0.44
2:G:551:THR:HG22	2:G:552:SER:N	2.31	0.44
2:G:751:LEU:HD11	2:G:789:PHE:CD1	2.53	0.44
2:G:751:LEU:HD23	2:G:791:TYR:CD2	2.53	0.44
2:H:1389:ILE:HG13	2:H:1411:PHE:CD1	2.52	0.44
2:H:305:PHE:CD1	2:H:442:ASP:HB3	2.53	0.44
2:H:807:ILE:HA	2:H:818:LYS:HG2	1.99	0.44
2:I:1257:ASP:O	2:I:1261:ARG:HG3	2.17	0.44
2:I:159:ILE:CG2	2:I:501:ILE:HG22	2.47	0.44
2:I:1896:GLN:HE21	2:I:1896:GLN:HB3	1.58	0.44
2:I:305:PHE:CD1	2:I:442:ASP:HB3	2.52	0.44
2:I:40:ILE:O	2:I:42:PRO:HD3	2.17	0.44
2:I:720:ALA:HA	2:I:728:ILE:CD1	2.47	0.44
1:A:1194:ASN:OD1	1:A:1196:LYS:HB2	2.18	0.44
1:A:1220:VAL:O	1:A:1224:ILE:HG12	2.18	0.44
1:A:1464:GLU:HG3	1:A:1773:VAL:HG11	1.77	0.44
1:A:458:THR:OG1	1:A:470:LYS:HD2	2.18	0.44
1:B:1012:LEU:HD23	1:B:1445:MET:CE	2.48	0.44
1:B:1195:ALA:HB1	1:B:1200:ILE:HD12	1.99	0.44
1:C:1673:TYR:CZ	1:C:1677:VAL:HG21	2.51	0.44
2:H:1148:ASN:HD22	2:H:1148:ASN:C	2.21	0.44
2:H:1579:ILE:HD11	2:H:1615:MET:SD	2.58	0.44
1:B:29:ILE:HG12	2:H:1892:ASN:C	2.37	0.44
2:H:272:GLY:HA3	2:H:276:GLY:C	2.38	0.44
2:H:376:ASN:C	2:H:376:ASN:ND2	2.70	0.44
2:H:455:ILE:C	2:H:455:ILE:HD12	2.38	0.44
2:I:1739:GLU:HB2	2:I:1987:PRO:CB	2.29	0.44
2:I:184:VAL:HG12	2:I:188:ILE:HG12	1.99	0.44
2:I:1976:PHE:HB3	2:I:1981:LEU:CD2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:297:ARG:O	2:I:301:THR:HG22	2.18	0.44
2:I:517:HIS:CE1	2:I:540:ASP:O	2.71	0.44
1:A:1133:PRO:HG3	1:A:1166:LYS:HG3	1.99	0.44
1:A:11:HIS:CD2	1:A:11:HIS:C	2.92	0.44
1:A:499:PRO:HD3	1:A:516:ARG:HH21	1.83	0.44
1:A:530:ALA:HA	1:A:636:PRO:HB3	1.99	0.44
1:B:1037:TRP:HB2	1:B:1598:GLN:OE1	2.18	0.44
1:B:1455:ARG:O	1:B:1459:ILE:HG13	2.18	0.44
1:B:1842:VAL:O	1:B:1843:ASN:C	2.57	0.44
1:B:42:GLU:O	1:B:77:GLU:N	2.47	0.44
1:C:1270:VAL:HG11	1:C:1274:ILE:HD13	1.99	0.44
1:C:1234:MET:CE	1:C:1326:ILE:HG21	2.48	0.44
1:C:187:LEU:HD22	1:C:201:PRO:HB2	1.99	0.44
1:C:601:VAL:O	1:C:602:GLU:C	2.56	0.44
1:C:706:THR:HB	1:C:737:PHE:HB3	2.00	0.44
1:C:852:ARG:HB3	1:C:858:TRP:HZ2	1.83	0.44
2:G:615:TYR:CE2	2:G:1074:MET:HB3	2.52	0.44
2:G:1257:ASP:O	2:G:1261:ARG:HG3	2.18	0.44
2:G:1551:GLU:HB2	2:G:1552:PRO:HD3	2.00	0.44
2:G:1589:VAL:HG21	2:G:1651:LEU:HD12	1.99	0.44
2:G:1776:PHE:C	2:G:1779:PRO:HD2	2.38	0.44
2:G:1662:THR:HB	2:G:1799:PRO:HG2	1.99	0.44
2:H:1228:THR:HG21	2:H:1234:VAL:HG23	2.00	0.44
2:H:184:VAL:HG12	2:H:188:ILE:HG12	2.00	0.44
1:B:20:TYR:CD2	2:H:2033:THR:OG1	2.71	0.44
2:H:732:TRP:CE2	2:H:750:MET:HE3	2.52	0.44
2:H:780:TYR:HB2	2:H:799:PHE:CE2	2.53	0.44
2:H:938:TRP:CE2	2:H:944:ARG:HG3	2.52	0.44
2:I:142:ASN:HB2	2:I:550:VAL:HG13	1.99	0.44
2:I:1579:ILE:HG22	2:I:1580:THR:O	2.18	0.44
2:I:1666:PHE:CE1	2:I:1814:ALA:HA	2.53	0.44
2:I:1886:VAL:HG22	2:I:1906:ALA:HB1	1.98	0.44
1:A:1501:LEU:HD11	1:A:1775:LEU:CG	2.47	0.44
1:A:1842:VAL:O	1:A:1843:ASN:C	2.57	0.44
1:B:1430:ARG:HG2	1:B:1430:ARG:O	2.18	0.44
1:B:267:VAL:O	1:B:290:MET:HE1	2.17	0.44
1:C:1181:PHE:CZ	1:C:1341:PHE:HA	2.53	0.44
1:C:1291:LEU:HD21	1:C:1698:PHE:CE1	2.53	0.44
1:C:295:ALA:HB1	1:C:300:VAL:O	2.18	0.44
1:C:833:PHE:O	1:C:834:GLY:O	2.36	0.44
2:G:1004:LEU:CD2	2:G:1019:PRO:HB2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1352:HIS:HE1	2:G:1583:MET:CE	2.27	0.44
2:G:159:ILE:HD11	2:G:512:LEU:CG	2.48	0.44
2:G:459:VAL:HG12	2:G:468:LEU:HD12	2.00	0.44
2:G:566:HIS:O	2:G:567:PRO:C	2.57	0.44
2:G:901:LYS:NZ	2:G:1031:LYS:O	2.50	0.44
2:H:102:HIS:HE1	2:H:180:TYR:OH	2.00	0.44
2:H:1496:LYS:HE2	2:H:1693:ARG:HH21	1.82	0.44
2:H:1739:GLU:HB2	2:H:1987:PRO:CB	2.30	0.44
2:I:914:LEU:HD21	2:I:1003:PHE:CD2	2.53	0.44
2:I:1493:LEU:HB3	2:I:1494:PRO:CD	2.48	0.44
2:I:1684:SER:O	2:I:1688:GLN:HG3	2.18	0.44
2:I:218:TRP:HB3	2:I:225:THR:OG1	2.18	0.44
2:I:246:LEU:O	2:I:250:VAL:HG23	2.18	0.44
1:A:181:THR:O	1:A:185:GLU:HG3	2.18	0.43
1:A:406:TRP:CE3	1:A:407:ASN:HB2	2.53	0.43
1:A:933:VAL:HG22	1:A:933:VAL:O	2.18	0.43
1:B:1460:LYS:CE	1:B:1774:GLU:CD	2.86	0.43
1:B:35:PHE:HA	1:B:39:PHE:HD2	1.83	0.43
1:B:888:ILE:HD12	1:B:939:PHE:CE2	2.43	0.43
1:C:1332:TYR:HB3	1:C:1382:ALA:CB	2.48	0.43
1:C:1373:ARG:NE	1:C:1550:ASP:HB2	2.33	0.43
1:B:1129:GLU:OE1	1:C:348:ARG:HD3	2.18	0.43
1:C:413:LEU:C	1:C:415:SER:H	2.21	0.43
2:G:1236:LEU:HD11	2:G:1262:ILE:HG12	1.99	0.43
2:G:245:GLN:HG2	2:G:505:GLY:HA2	1.99	0.43
2:G:543:PHE:CB	2:G:545:GLN:NE2	2.81	0.43
2:G:566:HIS:ND1	2:G:567:PRO:HD2	2.33	0.43
2:G:726:PHE:HA	2:G:727:PRO:HD3	1.89	0.43
2:G:753:MET:O	2:G:757:ILE:HG13	2.18	0.43
2:G:866:LYS:O	2:G:870:GLU:HG3	2.18	0.43
2:H:1222:GLU:HG3	2:H:1235:SER:OG	2.17	0.43
2:H:1586:SER:O	2:H:1590:ARG:HB2	2.17	0.43
2:H:1638:ILE:CD1	2:H:1657:ILE:HG13	2.41	0.43
2:H:9:LEU:HB2	2:H:27:PHE:HE1	1.83	0.43
2:H:123:ILE:HD11	2:H:533:LEU:CD2	2.48	0.43
2:H:670:ARG:HD2	2:H:676:ILE:O	2.18	0.43
2:H:567:PRO:CG	2:H:781:LEU:CD1	2.94	0.43
2:I:1427:VAL:HG22	2:I:1469:GLU:HG2	1.99	0.43
2:I:1551:GLU:HB2	2:I:1552:PRO:HD3	2.00	0.43
2:I:1782:THR:CG2	2:I:1827:LEU:HD21	2.45	0.43
2:I:427:PHE:HB3	2:I:428:HIS:ND1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:432:LEU:HB3	2:I:484:ILE:HG23	2.00	0.43
2:I:932:ILE:HD12	2:I:939:PHE:HD1	1.83	0.43
1:A:1584:PRO:CG	1:A:1591:TRP:CZ3	3.02	0.43
1:A:626:VAL:HG23	1:A:664:GLU:OE2	2.18	0.43
1:A:930:LEU:HD23	1:A:930:LEU:HA	1.75	0.43
1:B:1279:PHE:HB2	1:B:1282:THR:HG23	2.00	0.43
1:C:1279:PHE:HB2	1:C:1282:THR:HG23	2.00	0.43
1:C:1720:ALA:O	1:C:1721:ARG:HG2	2.17	0.43
1:C:196:THR:O	1:C:213:PHE:HE2	2.01	0.43
1:C:168:MET:HA	1:C:206:LEU:HB2	2.00	0.43
2:G:1195:VAL:HG13	2:G:1211:LEU:CB	2.48	0.43
2:G:1227:ARG:CD	2:G:1565:VAL:HG11	2.44	0.43
2:G:195:LEU:O	2:G:199:ILE:HG13	2.18	0.43
2:G:581:THR:O	2:G:585:LYS:HB2	2.18	0.43
2:G:754:TYR:CD2	2:G:794:MET:CG	3.01	0.43
2:G:900:GLN:NE2	2:G:1051:THR:HA	2.32	0.43
2:H:666:ILE:HG22	2:H:698:LEU:HD22	2.00	0.43
2:I:1778:GLN:HB2	2:I:1779:PRO:HD3	2.00	0.43
2:I:1976:PHE:HA	2:I:1981:LEU:CD2	2.48	0.43
2:I:428:HIS:CD2	2:I:488:VAL:HG23	2.53	0.43
2:I:751:LEU:HD23	2:I:791:TYR:CD2	2.53	0.43
2:I:938:TRP:CE2	2:I:944:ARG:HG3	2.53	0.43
1:A:1209:ASP:OD2	1:A:1253:GLY:HA2	2.19	0.43
1:A:237:MET:HG3	1:A:241:PHE:HB3	2.00	0.43
1:A:235:SER:HA	1:A:276:ARG:NH2	2.32	0.43
1:A:28:TRP:HB3	2:G:1892:ASN:HA	2.00	0.43
1:A:411:GLN:O	1:A:415:SER:HB2	2.18	0.43
1:B:1248:GLY:HA3	1:B:1301:PRO:HD2	1.99	0.43
1:B:1014:ASP:N	1:B:1510:ASN:HD21	2.06	0.43
1:B:807:LYS:HD3	1:B:807:LYS:C	2.39	0.43
1:C:988:ILE:HD13	1:C:1048:GLU:HB3	2.01	0.43
1:C:1056:ILE:CD1	1:C:1193:TRP:CD1	2.99	0.43
1:C:340:ARG:HH12	1:C:344:GLN:HE21	1.65	0.43
1:C:421:ILE:HG12	1:C:469:VAL:HG21	1.98	0.43
1:C:627:SER:HB3	1:C:661:ASP:OD1	2.18	0.43
1:C:639:HIS:HB2	1:C:656:SER:OG	2.18	0.43
2:G:1327:ILE:HD12	2:G:1327:ILE:HA	1.79	0.43
2:G:1473:THR:O	2:G:1481:SER:HB3	2.18	0.43
2:G:1768:LYS:HE2	2:G:1772:SER:HB3	2.00	0.43
2:H:856:LYS:CE	2:H:1052:CYS:SG	3.06	0.43
2:H:369:SER:C	2:H:370:LEU:HD23	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:439:ILE:HD12	2:H:484:ILE:HD11	1.99	0.43
2:H:732:TRP:CH2	2:H:749:PRO:HG2	2.53	0.43
2:H:772:GLY:O	2:H:804:ARG:HD3	2.18	0.43
2:H:970:TYR:O	2:H:973:LEU:HB2	2.18	0.43
2:I:1241:ASN:N	2:I:1252:SER:O	2.50	0.43
2:I:159:ILE:HG12	2:I:512:LEU:HD23	2.01	0.43
2:I:1624:THR:CB	2:I:1642:THR:HG23	2.47	0.43
2:I:551:THR:C	2:I:553:ASN:H	2.22	0.43
2:I:572:ASN:CB	2:I:576:LYS:H	2.27	0.43
2:I:754:TYR:CG	2:I:794:MET:HG2	2.53	0.43
2:I:843:ILE:HD13	2:I:1055:HIS:O	2.18	0.43
1:B:1244:GLY:C	1:B:1327:CYS:HB2	2.38	0.43
1:B:176:VAL:HG12	1:B:178:GLY:H	1.83	0.43
1:C:980:VAL:HG21	2:I:952:ARG:HH21	1.83	0.43
2:G:1016:PRO:HD2	2:G:1017:PHE:CE2	2.53	0.43
2:G:1040:LEU:O	2:G:1046:GLN:HG3	2.19	0.43
2:G:1162:ASP:O	2:G:1163:LYS:HB2	2.19	0.43
2:G:1223:MET:HE3	2:G:1238:LEU:CD1	2.49	0.43
2:G:1308:CYS:HB3	2:G:1311:PHE:CE2	2.53	0.43
2:G:1674:GLN:OE1	2:G:1712:ASN:HA	2.18	0.43
2:G:1678:MET:HE3	2:G:1707:LEU:CD2	2.43	0.43
2:G:1804:PHE:CD2	2:G:1818:LEU:HD22	2.53	0.43
2:G:1846:GLU:C	2:G:1848:GLY:H	2.20	0.43
2:G:455:ILE:C	2:G:455:ILE:HD12	2.39	0.43
2:G:967:ILE:HD12	2:G:972:LEU:HD22	2.00	0.43
2:H:309:ARG:HD3	2:H:309:ARG:HA	1.63	0.43
2:I:1210:ILE:O	2:I:1210:ILE:HG22	2.18	0.43
2:I:1325:PHE:O	2:I:1328:VAL:HG12	2.18	0.43
2:I:1428:GLU:HG2	2:I:1470:THR:HG22	1.99	0.43
2:I:430:HIS:CE1	2:I:431:LEU:HD13	2.53	0.43
2:I:439:ILE:HD12	2:I:484:ILE:CD1	2.48	0.43
2:I:835:THR:HG21	2:I:855:HIS:NE2	2.33	0.43
1:A:1291:LEU:HD21	1:A:1698:PHE:CE1	2.53	0.43
1:A:1375:GLY:HA2	1:A:1546:THR:HG22	2.01	0.43
1:A:1553:GLU:HA	1:A:1556:THR:HG23	2.01	0.43
1:A:1556:THR:O	1:A:1560:MET:HG2	2.18	0.43
1:A:1673:TYR:CZ	1:A:1677:VAL:HG21	2.53	0.43
1:A:254:TRP:CZ3	1:A:302:LEU:HD13	2.53	0.43
1:A:413:LEU:HG	1:A:413:LEU:O	2.17	0.43
1:A:496:PRO:HB2	1:A:519:VAL:HG12	2.01	0.43
1:A:893:VAL:HG11	1:A:930:LEU:CD2	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:THR:HB	1:B:244:THR:HB	2.01	0.43
1:C:1021:VAL:HG22	1:C:1387:ILE:HG22	2.01	0.43
1:C:1625:LEU:O	1:C:1627:PRO:HD3	2.18	0.43
1:C:221:LEU:HA	1:C:221:LEU:HD23	1.89	0.43
1:C:235:SER:HA	1:C:276:ARG:NH2	2.33	0.43
2:G:1458:ASP:O	2:G:1462:LYS:HE3	2.19	0.43
2:G:1493:LEU:HB3	2:G:1494:PRO:CD	2.48	0.43
2:G:272:GLY:HA3	2:G:276:GLY:C	2.38	0.43
2:G:397:LYS:HB3	2:G:416:PHE:CE2	2.53	0.43
2:G:156:LEU:HD23	2:G:500:HIS:HB2	1.99	0.43
2:G:653:TYR:OH	2:G:690:VAL:HG11	2.18	0.43
2:H:1015:VAL:HG13	2:H:1017:PHE:CE2	2.53	0.43
2:H:1422:THR:CG2	2:H:1422:THR:O	2.66	0.43
2:H:726:PHE:HA	2:H:727:PRO:HD3	1.88	0.43
2:H:745:ASP:HA	2:H:832:TRP:CH2	2.51	0.43
2:I:1651:LEU:O	2:I:1652:THR:HG23	2.17	0.43
2:I:1496:LYS:CE	2:I:1693:ARG:HH21	2.31	0.43
2:I:397:LYS:HB3	2:I:416:PHE:CE2	2.53	0.43
2:I:439:ILE:HD12	2:I:484:ILE:HD11	1.99	0.43
2:I:562:LEU:HD23	2:I:562:LEU:HA	1.79	0.43
2:I:852:GLU:HG3	2:I:852:GLU:H	1.39	0.43
2:I:972:LEU:HD23	2:I:979:ALA:HB2	2.00	0.43
1:A:242:THR:HB	1:A:244:THR:HB	2.00	0.43
1:A:641:ARG:HD3	1:A:649:TRP:O	2.18	0.43
1:A:627:SER:HB2	1:A:657:SER:CB	2.48	0.43
1:A:790:PHE:CE2	1:A:794:ILE:HD11	2.53	0.43
1:B:1208:VAL:HG11	1:B:1212:THR:HB	1.97	0.43
1:B:1270:VAL:HG11	1:B:1274:ILE:HD13	2.00	0.43
1:C:1234:MET:HE3	1:C:1326:ILE:HG21	2.01	0.43
1:C:1446:LYS:O	1:C:1450:ARG:HG3	2.18	0.43
1:C:232:LEU:HD13	1:C:272:GLU:CB	2.48	0.43
2:G:1889:VAL:HG13	2:G:1977:HIS:HB3	1.97	0.43
2:G:419:ARG:HG3	2:G:420:PHE:N	2.33	0.43
2:G:99:ASN:HA	2:G:550:VAL:CG2	2.49	0.43
2:H:1241:ASN:N	2:H:1252:SER:O	2.51	0.43
2:H:1419:PHE:C	2:H:1421:ASN:N	2.71	0.43
2:H:360:LEU:HA	2:H:361:PRO:HD3	1.90	0.43
2:H:160:PHE:CE2	2:H:504:PHE:HB2	2.54	0.43
2:H:73:GLU:OE2	2:H:76:LYS:HD2	2.18	0.43
2:I:1079:ASP:O	2:I:1082:ILE:HG22	2.19	0.43
2:I:1236:LEU:HD22	2:I:1238:LEU:HG	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1959:LYS:HG2	2:I:1959:LYS:O	2.19	0.43
2:I:279:THR:O	2:I:283:ILE:HB	2.19	0.43
2:I:871:THR:HG21	2:I:887:LYS:HZ1	1.83	0.43
1:A:1431:GLU:OE2	1:A:1433:HIS:HE1	2.02	0.43
1:A:267:VAL:O	1:A:290:MET:HE1	2.19	0.43
1:A:988:ILE:CD1	1:A:1048:GLU:HA	2.48	0.43
1:B:1219:VAL:CA	1:B:1384:ILE:HD11	2.32	0.43
1:B:1233:GLU:CD	1:B:1680:ARG:HH21	2.22	0.43
1:B:370:GLU:O	1:B:373:ALA:HB3	2.19	0.43
1:C:1248:GLY:HA3	1:C:1301:PRO:HD2	2.01	0.43
1:C:1375:GLY:HA2	1:C:1546:THR:HG22	1.99	0.43
1:C:1553:GLU:HA	1:C:1556:THR:HG23	2.01	0.43
1:C:1539:ALA:O	1:C:1574:GLY:HA2	2.18	0.43
1:C:1599:ILE:HD11	1:C:1606:PRO:HD2	2.01	0.43
1:C:49:PRO:O	1:C:82:SER:HB2	2.19	0.43
2:G:184:VAL:HG12	2:G:188:ILE:HG12	2.00	0.43
2:G:184:VAL:O	2:G:184:VAL:HG12	2.19	0.43
2:G:324:LEU:O	2:G:324:LEU:HD12	2.18	0.43
2:G:566:HIS:C	2:G:566:HIS:ND1	2.72	0.43
2:G:573:LYS:C	2:G:575:GLY:H	2.21	0.43
2:G:652:ILE:HD13	2:G:658:MET:HE3	1.99	0.43
2:G:854:ILE:HG22	2:G:856:LYS:HG3	2.01	0.43
2:H:1223:MET:HE3	2:H:1238:LEU:CD1	2.46	0.43
2:H:573:LYS:C	2:H:575:GLY:H	2.21	0.43
2:H:629:GLY:O	2:H:632:ALA:HB3	2.18	0.43
2:H:643:LYS:HA	2:H:1163:LYS:HG2	1.99	0.43
2:H:653:TYR:OH	2:H:690:VAL:HG11	2.18	0.43
2:I:607:VAL:O	2:I:611:THR:HB	2.18	0.43
2:I:7:ARG:NH2	2:I:24:THR:O	2.52	0.43
1:A:1009:LEU:CD1	1:A:1445:MET:HE1	2.48	0.43
1:A:644:THR:HG23	1:A:648:ASP:N	2.34	0.43
1:A:827:SER:HA	1:A:828:PRO:HD3	1.70	0.43
1:B:1375:GLY:HA2	1:B:1546:THR:HG22	2.01	0.43
1:B:1446:LYS:O	1:B:1450:ARG:HG3	2.19	0.43
1:B:1498:GLU:HG2	1:B:1876:LEU:HB3	1.89	0.43
1:B:681:THR:HA	1:B:706:THR:OG1	2.19	0.43
1:C:1158:PRO:HD2	1:C:1159:GLU:OE2	2.18	0.43
1:A:335:HIS:ND1	1:C:335:HIS:HE1	2.17	0.43
1:C:384:GLU:O	1:C:388:ASN:HB2	2.19	0.43
2:G:1004:LEU:HD21	2:G:1020:VAL:CG2	2.48	0.43
2:G:1175:LYS:HG3	2:G:1176:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:324:LEU:O	2:G:328:LEU:HG	2.18	0.43
2:G:601:THR:O	2:G:601:THR:CG2	2.67	0.43
2:G:786:SER:HB3	2:G:794:MET:HE2	2.01	0.43
2:G:860:ARG:H	2:G:1049:GLN:HG3	1.83	0.43
2:H:1567:ARG:HH11	2:H:1567:ARG:HG2	1.72	0.43
2:H:1940:LEU:HD12	2:H:1941:PHE:N	2.34	0.43
2:H:654:VAL:HG12	2:H:654:VAL:O	2.18	0.43
2:I:1168:ASN:HA	2:I:1169:PRO:HD3	1.84	0.43
2:I:1552:PRO:O	2:I:1556:VAL:HG23	2.19	0.43
2:I:169:TYR:CG	2:I:170:PHE:N	2.87	0.43
2:I:2030:TYR:CD1	2:I:2034:GLY:HA2	2.54	0.43
2:I:425:SER:HA	2:I:426:PRO:HD3	1.78	0.43
2:I:846:VAL:CG1	2:I:865:TRP:NE1	2.82	0.43
1:A:1431:GLU:CG	1:A:1433:HIS:CE1	3.00	0.43
1:A:1670:TYR:O	1:A:1674:VAL:HG23	2.18	0.43
1:A:833:PHE:HA	1:A:937:LYS:HD2	2.00	0.43
1:B:1431:GLU:CG	1:B:1433:HIS:CE1	3.02	0.43
1:B:1657:HIS:HA	1:B:1658:PRO:HD3	1.89	0.43
1:B:460:GLU:CG	1:B:470:LYS:HD3	2.48	0.43
1:C:1600:LEU:HD11	1:C:1655:VAL:HG12	2.00	0.43
2:G:884:LEU:HD22	2:G:1021:LEU:CD1	2.49	0.43
2:G:1219:ILE:HB	2:G:1240:TYR:HB2	2.01	0.43
2:G:1875:VAL:HG22	2:G:1910:VAL:HG11	2.01	0.43
2:G:2042:ILE:HG12	2:G:2042:ILE:H	1.39	0.43
2:G:28:PHE:CE2	2:H:7:ARG:CD	2.73	0.43
2:G:486:LEU:HA	2:G:487:PRO:HD3	1.90	0.43
2:G:15:SER:H	2:G:48:PHE:HE2	1.67	0.43
2:G:835:THR:HG22	2:G:844:VAL:HA	2.00	0.43
2:H:1862:VAL:HG22	2:H:1863:ALA:N	2.33	0.43
2:H:543:PHE:CB	2:H:545:GLN:NE2	2.81	0.43
2:H:717:ILE:HG23	2:H:760:HIS:CE1	2.54	0.43
2:I:615:TYR:CE2	2:I:1074:MET:HB3	2.53	0.43
2:I:1561:ASN:HA	2:I:1562:PRO:HD3	1.80	0.43
2:I:1662:THR:HB	2:I:1799:PRO:HG2	2.00	0.43
2:I:1873:TYR:CE1	2:I:1877:ARG:NH2	2.81	0.43
2:I:209:PHE:CE2	2:I:213:LEU:HD22	2.53	0.43
2:I:573:LYS:C	2:I:575:GLY:N	2.72	0.43
2:I:702:TYR:HB3	2:I:727:PRO:HB2	2.00	0.43
2:I:967:ILE:HD12	2:I:972:LEU:HD22	2.00	0.43
1:A:1107:GLU:HA	1:A:1108:PRO:HD3	1.90	0.43
1:A:1498:GLU:HG2	1:A:1876:LEU:HB3	1.68	0.43

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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	0.43
1:A:460:GLU:CG	1:A:470:LYS:HD3	2.49	0.43
1:A:32:GLN:HE22	1:A:57:ALA:N	2.16	0.43
1:A:44:VAL:HG11	1:A:78:ILE:HG12	1.96	0.43
1:B:1283:MET:O	1:B:1287:VAL:HG23	2.18	0.43
1:B:1553:GLU:HA	1:B:1556:THR:HG23	2.00	0.43
1:B:260:ARG:HH12	1:B:300:VAL:CG2	2.20	0.43
1:B:335:HIS:C	1:B:335:HIS:CD2	2.92	0.43
1:B:411:GLN:O	1:B:415:SER:HB2	2.18	0.43
1:C:1047:LEU:O	1:C:1051:VAL:HG23	2.19	0.43
1:C:1107:GLU:HA	1:C:1108:PRO:HD3	1.89	0.43
1:C:1208:VAL:HG11	1:C:1212:THR:HB	1.98	0.43
1:C:852:ARG:NH1	1:C:856:GLU:OE1	2.52	0.43
2:G:1339:PHE:N	2:G:1340:PRO:CD	2.82	0.43
2:G:1348:LEU:HD12	2:G:1348:LEU:HA	1.81	0.43
2:G:1327:ILE:HG12	2:G:1583:MET:HE3	2.01	0.43
2:G:1858:ASN:HA	2:G:1896:GLN:O	2.18	0.43
2:G:339:LEU:HD23	2:G:419:ARG:O	2.19	0.43
2:G:441:LYS:O	2:G:445:LYS:HG3	2.18	0.43
2:G:634:ILE:CD1	2:G:649:ILE:HD11	2.43	0.43
2:H:1293:THR:CG2	2:H:1296:GLU:H	2.24	0.43
2:H:595:PRO:HD3	2:H:800:LEU:HB2	2.01	0.43
2:I:652:ILE:CD1	2:I:658:MET:HE3	2.48	0.43
2:I:950:PHE:O	2:I:953:ARG:HB3	2.19	0.43
1:A:1396:MET:O	1:A:1680:ARG:NH1	2.52	0.42
1:A:1539:ALA:O	1:A:1574:GLY:HA2	2.18	0.42
1:A:155:VAL:O	1:A:159:LEU:HG	2.19	0.42
1:A:2:LYS:HE2	1:A:4:GLU:OE1	2.19	0.42
1:A:705:VAL:HG23	1:A:732:LEU:CD2	2.48	0.42
1:B:1050:CYS:HB3	1:B:1089:VAL:HG12	2.00	0.42
1:B:1263:ASP:HB2	1:B:1270:VAL:HG21	2.00	0.42
1:B:1406:MET:HE1	1:B:1428:THR:HB	2.01	0.42
1:B:335:HIS:CD2	1:B:335:HIS:O	2.70	0.42
1:B:350:LEU:HB2	1:B:352:MET:HG2	2.01	0.42
1:B:430:ARG:NH2	1:B:605:LEU:HD13	2.33	0.42
1:C:1175:ILE:HA	1:C:1176:PRO:HD3	1.89	0.42
1:C:1243:VAL:O	1:C:1296:GLY:HA3	2.18	0.42
2:G:561:TRP:O	2:G:563:GLU:N	2.51	0.42
2:G:23:PRO:HG2	2:G:86:LEU:HD11	2.00	0.42
2:H:1257:ASP:O	2:H:1261:ARG:HG3	2.19	0.42
2:H:1458:ASP:O	2:H:1462:LYS:HE3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1847:LEU:H	2:H:1847:LEU:CD1	2.12	0.42
2:H:551:THR:C	2:H:553:ASN:H	2.21	0.42
2:I:1311:PHE:HD1	2:I:1320:LEU:O	2.02	0.42
2:I:1868:GLN:HG3	2:I:1898:TYR:HH	1.83	0.42
2:I:1878:VAL:CG1	2:I:1910:VAL:HG22	2.36	0.42
2:I:7:ARG:CG	2:I:22:VAL:O	2.67	0.42
2:I:516:THR:O	2:I:519:ASN:HB2	2.19	0.42
2:I:736:ARG:HG3	2:I:736:ARG:H	1.57	0.42
2:I:835:THR:HB	2:I:845:THR:HG23	2.01	0.42
1:A:1195:ALA:HB1	1:A:1200:ILE:HD12	2.02	0.42
1:A:1495:ASN:HD22	1:A:1495:ASN:HA	1.67	0.42
1:A:32:GLN:NE2	1:A:57:ALA:HA	2.34	0.42
1:B:1119:LYS:HE2	1:B:1341:PHE:CD1	2.54	0.42
1:B:417:TYR:HH	1:B:458:THR:HG22	1.84	0.42
1:C:1308:SER:HB3	1:C:1589:GLY:HA3	2.01	0.42
1:C:1618:LEU:HD23	1:C:1621:PHE:CE2	2.55	0.42
1:C:1657:HIS:CE1	1:C:1658:PRO:HD2	2.54	0.42
1:C:1239:HIS:HE1	1:C:1714:VAL:O	2.02	0.42
1:C:949:GLU:O	1:C:953:VAL:CG1	2.67	0.42
2:G:1320:LEU:HD12	2:G:1320:LEU:HA	1.88	0.42
2:G:238:CYS:CB	2:G:239:PRO:HD3	2.45	0.42
2:G:612:ASN:HD21	2:G:641:ILE:HA	1.85	0.42
2:H:1070:ILE:CD1	2:H:1074:MET:HG2	2.49	0.42
2:H:1149:TRP:HA	2:H:1242:PHE:CD1	2.54	0.42
2:H:1335:ILE:O	2:H:1338:ILE:HG12	2.19	0.42
2:H:127:ILE:HD12	2:H:180:TYR:CD2	2.54	0.42
1:B:12:ILE:CD1	2:H:2041:ILE:HD11	2.49	0.42
2:H:245:GLN:HG2	2:H:505:GLY:HA2	2.00	0.42
2:H:274:SER:OG	2:H:428:HIS:HE1	2.02	0.42
2:H:279:THR:O	2:H:283:ILE:HB	2.20	0.42
2:H:665:LEU:HD22	2:H:665:LEU:O	2.19	0.42
2:H:866:LYS:O	2:H:870:GLU:HG3	2.19	0.42
2:H:938:TRP:CD1	2:H:944:ARG:HG3	2.53	0.42
2:I:896:ASN:O	2:I:1050:ARG:NH2	2.52	0.42
2:I:1321:ALA:HA	2:I:1322:PRO:HD3	1.83	0.42
2:I:1666:PHE:CD1	2:I:1814:ALA:HB2	2.54	0.42
2:I:503:ASP:O	2:I:530:ALA:HB3	2.19	0.42
2:I:538:ASP:HB2	2:I:540:ASP:HB2	2.01	0.42
2:I:810:GLU:OE2	2:I:1070:ILE:N	2.43	0.42
2:I:856:LYS:CE	2:I:1052:CYS:SG	3.07	0.42
1:A:1131:LEU:HD12	1:A:1131:LEU:HA	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1132:GLU:HA	1:A:1133:PRO:HD3	1.94	0.42
1:A:290:MET:HB3	1:A:290:MET:HE2	1.93	0.42
1:B:1145:LYS:HD3	1:B:1154:ILE:HG12	2.01	0.42
1:B:1420:ALA:HA	1:B:1421:PRO:HD3	1.74	0.42
1:B:155:VAL:HG22	1:B:186:ILE:CG2	2.50	0.42
1:B:280:GLU:O	1:B:284:LYS:HG3	2.20	0.42
1:B:828:PRO:HG3	1:B:868:ILE:HG22	2.00	0.42
1:B:908:LEU:HA	1:B:913:VAL:HG21	2.00	0.42
1:C:1114:TYR:CE1	1:C:1337:GLU:HG3	2.55	0.42
1:C:408:TRP:CH2	1:C:1628:SER:HB3	2.55	0.42
1:C:330:GLU:O	1:C:330:GLU:HG2	2.18	0.42
2:G:1031:LYS:O	2:G:1032:ASP:C	2.57	0.42
2:G:1986:LYS:N	2:G:1987:PRO:CD	2.82	0.42
2:G:2026:PHE:HB3	2:G:2042:ILE:HD13	2.00	0.42
2:G:421:LEU:HA	2:G:422:PRO:HD3	1.81	0.42
2:G:543:PHE:HB2	2:G:545:GLN:NE2	2.25	0.42
2:G:586:LEU:HD12	2:G:764:MET:SD	2.59	0.42
2:H:1080:GLY:O	2:H:1084:LYS:HG3	2.19	0.42
2:H:1159:ILE:CG2	2:H:1160:THR:N	2.82	0.42
2:H:1383:ASN:HD21	2:H:1418:ASP:HB3	1.84	0.42
2:H:1497:GLU:OE1	2:H:2002:LYS:CE	2.66	0.42
2:H:1551:GLU:HB2	2:H:1552:PRO:HD3	2.00	0.42
2:H:240:LEU:HA	2:H:240:LEU:HD12	1.78	0.42
2:H:258:PHE:N	2:H:258:PHE:CD1	2.87	0.42
2:H:38:ASN:HA	2:H:41:LEU:HD12	2.01	0.42
2:H:967:ILE:CD1	2:H:972:LEU:HD22	2.50	0.42
2:I:1085:LEU:HD12	2:I:1085:LEU:HA	1.82	0.42
2:I:190:PHE:O	2:I:194:THR:HG22	2.19	0.42
2:I:234:ILE:HG13	2:I:235:PRO:CD	2.46	0.42
2:I:309:ARG:HD3	2:I:309:ARG:HA	1.61	0.42
2:I:726:PHE:HA	2:I:727:PRO:HD3	1.86	0.42
2:I:778:TYR:N	2:I:779:PRO:CD	2.82	0.42
1:A:1002:LYS:HZ1	1:A:1782:GLU:HG2	1.83	0.42
1:A:460:GLU:H	1:A:460:GLU:HG3	1.34	0.42
1:B:874:GLY:O	1:B:875:THR:C	2.58	0.42
1:C:1219:VAL:CA	1:C:1384:ILE:CD1	2.94	0.42
1:C:21:GLN:HB3	1:C:21:GLN:HE21	1.69	0.42
1:C:406:TRP:CE3	1:C:407:ASN:HB2	2.53	0.42
1:C:798:ASN:HA	1:C:801:ARG:HB2	2.02	0.42
2:G:1878:VAL:CG1	2:G:1910:VAL:HG22	2.34	0.42
2:G:503:ASP:OD2	2:G:513:GLY:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1159:ILE:HG13	2:H:1169:PRO:CD	2.50	0.42
2:H:1427:VAL:HG22	2:H:1469:GLU:CG	2.50	0.42
2:H:176:LEU:CD2	2:H:184:VAL:HG21	2.50	0.42
2:H:1986:LYS:N	2:H:1987:PRO:CD	2.81	0.42
2:H:520:LYS:O	2:H:521:ASP:C	2.58	0.42
2:H:536:ASN:HD21	2:H:540:ASP:HB3	1.84	0.42
2:H:741:HIS:CE1	2:H:855:HIS:NE2	2.88	0.42
2:I:1102:TYR:HB3	2:I:1244:PRO:CA	2.49	0.42
2:I:1175:LYS:HG3	2:I:1176:PRO:HD2	2.00	0.42
2:I:120:LYS:HB3	2:I:124:LYS:HE3	2.01	0.42
2:I:1590:ARG:HG3	2:I:1608:TYR:CG	2.54	0.42
2:I:2042:ILE:HG12	2:I:2042:ILE:H	1.36	0.42
2:I:441:LYS:O	2:I:445:LYS:HG3	2.19	0.42
2:I:674:TYR:HA	2:I:675:PRO:HD3	1.69	0.42
1:A:1195:ALA:CB	1:A:1213:LEU:HD13	2.49	0.42
1:A:382:LEU:HA	1:A:382:LEU:HD23	1.79	0.42
1:B:1022:THR:HG22	1:B:1226:SER:CB	2.49	0.42
1:B:1234:MET:HE3	1:B:1326:ILE:HG21	2.01	0.42
1:B:1385:GLN:HE21	1:B:1385:GLN:HB3	1.66	0.42
1:B:1534:ASP:OD1	1:B:1566:ARG:HD3	2.19	0.42
1:B:157:HIS:CE1	1:B:269:LEU:HD11	2.55	0.42
1:B:272:GLU:HA	1:B:273:PRO:HD3	1.92	0.42
1:C:1455:ARG:HD2	1:C:1455:ARG:HA	1.82	0.42
1:C:1592:MET:HE2	1:C:1641:ILE:HG23	2.00	0.42
1:C:408:TRP:CZ3	1:C:1628:SER:HB3	2.54	0.42
1:C:413:LEU:O	1:C:413:LEU:HG	2.19	0.42
1:C:32:GLN:NE2	1:C:57:ALA:CA	2.82	0.42
2:G:1135:GLU:HG2	2:G:1176:PRO:HG2	2.02	0.42
2:G:517:HIS:CE1	2:G:540:ASP:O	2.73	0.42
2:G:638:VAL:HG22	2:G:675:PRO:HG2	2.01	0.42
2:H:1149:TRP:NE1	2:H:1213:LEU:HD12	2.34	0.42
2:H:1294:ALA:HA	2:H:1368:VAL:CG2	2.49	0.42
1:B:20:TYR:HE1	2:H:2035:SER:HB2	1.82	0.42
2:H:676:ILE:O	2:H:676:ILE:HG12	2.17	0.42
2:H:751:LEU:HD11	2:H:789:PHE:CD1	2.55	0.42
2:I:463:PHE:CD1	2:I:486:LEU:HD22	2.54	0.42
2:I:730:LEU:C	2:I:730:LEU:HD12	2.40	0.42
2:I:786:SER:HB3	2:I:794:MET:HE2	2.01	0.42
2:I:754:TYR:CE2	2:I:794:MET:HG3	2.53	0.42
2:I:835:THR:HG22	2:I:844:VAL:C	2.40	0.42
1:A:1420:ALA:HA	1:A:1421:PRO:HD3	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:MET:HG2	1:A:638:LEU:CG	2.50	0.42
1:B:1239:HIS:CD2	1:B:1241:SER:OG	2.59	0.42
1:B:1784:ASP:O	1:B:1788:GLU:HB2	2.20	0.42
1:B:706:THR:HB	1:B:737:PHE:HB3	2.01	0.42
1:B:982:ILE:HG23	2:H:956:GLU:HG2	2.01	0.42
1:C:1220:VAL:O	1:C:1224:ILE:HG12	2.19	0.42
1:C:406:TRP:CD2	1:C:1619:GLU:HG3	2.55	0.42
1:C:1639:VAL:CG1	1:C:1640:SER:N	2.82	0.42
1:C:475:GLN:CD	1:C:614:ALA:HB2	2.40	0.42
2:G:1180:MET:HB3	2:G:1199:GLU:HG2	2.00	0.42
2:G:1418:ASP:O	2:G:1419:PHE:C	2.58	0.42
2:G:786:SER:HB2	2:G:794:MET:HE2	2.00	0.42
2:H:345:THR:HG22	2:H:347:GLU:N	2.25	0.42
2:H:562:LEU:HG	2:H:793:PRO:HG2	2.02	0.42
2:H:60:LEU:O	2:H:60:LEU:HD23	2.20	0.42
2:H:900:GLN:NE2	2:H:1051:THR:HA	2.34	0.42
2:I:1217:ASN:HD22	2:I:1217:ASN:HA	1.60	0.42
2:I:1344:ASP:O	2:I:1416:TYR:HE2	2.02	0.42
2:I:1359:MET:CE	2:I:1404:MET:HB3	2.50	0.42
2:I:298:LYS:HA	2:I:448:VAL:CG2	2.49	0.42
2:I:33:LEU:HD21	2:I:80:PHE:CE2	2.54	0.42
1:A:1019:ILE:HG13	1:A:1316:VAL:HG13	2.01	0.42
1:A:1263:ASP:HB2	1:A:1270:VAL:HG21	2.01	0.42
1:A:181:THR:HG22	1:A:185:GLU:OE2	2.19	0.42
1:A:1:MET:HE3	1:A:9:LEU:HD12	2.01	0.42
1:A:489:VAL:CG2	1:A:671:VAL:N	2.83	0.42
1:B:1238:VAL:CG1	1:B:1242:GLU:HB2	2.49	0.42
1:B:1264:ARG:NH1	1:B:1270:VAL:HB	2.35	0.42
1:B:1244:GLY:O	1:B:1327:CYS:HB2	2.20	0.42
1:B:1682:LYS:HB3	2:H:994:PHE:CE2	2.54	0.42
1:B:242:THR:HG22	1:B:243:ILE:H	1.83	0.42
1:B:625:THR:HG23	1:B:627:SER:H	1.84	0.42
1:C:1067:LEU:HA	1:C:1067:LEU:HD23	1.76	0.42
1:C:438:ASN:HD21	1:C:698:GLN:HE21	1.66	0.42
2:G:1044:VAL:HG21	2:G:1050:ARG:NE	2.34	0.42
2:G:856:LYS:CE	2:G:1052:CYS:SG	3.08	0.42
2:G:1149:TRP:NE1	2:G:1213:LEU:HD12	2.35	0.42
2:G:507:GLY:O	2:G:508:GLY:C	2.58	0.42
2:G:810:GLU:OE2	2:G:1070:ILE:N	2.44	0.42
2:G:938:TRP:CE2	2:G:944:ARG:HG3	2.54	0.42
2:H:1002:HIS:NE2	2:H:1006:MET:CE	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:804:ARG:NH1	2:H:1062:PHE:O	2.52	0.42
2:H:1175:LYS:HG3	2:H:1176:PRO:HD2	2.02	0.42
2:H:1339:PHE:N	2:H:1340:PRO:CD	2.83	0.42
2:H:567:PRO:HG3	2:H:781:LEU:HD11	1.99	0.42
2:H:581:THR:O	2:H:585:LYS:HB2	2.20	0.42
2:H:712:ALA:O	2:H:716:VAL:HG23	2.20	0.42
2:H:754:TYR:CG	2:H:794:MET:HG2	2.55	0.42
2:H:949:ASP:HB3	2:H:1006:MET:CE	2.47	0.42
2:I:1129:ALA:HB2	2:I:1138:TRP:CH2	2.55	0.42
2:I:1273:GLU:HB3	2:I:1274:PRO:CD	2.50	0.42
2:I:1343:VAL:HG22	2:I:1343:VAL:O	2.20	0.42
2:I:1989:LYS:NZ	2:I:2037:PRO:HG2	2.35	0.42
2:I:2046:GLU:C	2:I:2048:TYR:N	2.73	0.42
2:I:44:PRO:HA	2:I:53:GLU:OE2	2.19	0.42
2:I:703:LEU:CD2	2:I:705:LEU:HG	2.50	0.42
2:I:73:GLU:OE2	2:I:76:LYS:HD2	2.18	0.42
2:I:740:HIS:HA	2:I:854:ILE:HD13	2.01	0.42
2:I:745:ASP:HA	2:I:832:TRP:CH2	2.49	0.42
1:A:1260:MET:HB2	1:A:1274:ILE:HD12	2.02	0.42
1:A:408:TRP:CH2	1:A:1628:SER:HB3	2.55	0.42
1:A:655:LEU:HA	1:A:655:LEU:HD23	1.81	0.42
1:A:800:LEU:HA	1:A:800:LEU:HD23	1.84	0.42
1:B:1012:LEU:HD23	1:B:1445:MET:HE3	2.00	0.42
1:B:1830:GLY:HA2	1:B:1831:GLY:HA2	1.57	0.42
1:B:458:THR:OG1	1:B:470:LYS:HD2	2.20	0.42
1:B:798:ASN:HA	1:B:801:ARG:HB2	2.02	0.42
1:C:1310:GLU:OE1	1:C:1649:LYS:CE	2.65	0.42
1:C:155:VAL:O	1:C:159:LEU:HG	2.19	0.42
1:C:1842:VAL:O	1:C:1843:ASN:C	2.57	0.42
1:C:2:LYS:HE2	1:C:4:GLU:OE1	2.19	0.42
1:C:37:LYS:HB2	1:C:65:TYR:CE1	2.52	0.42
2:G:1014:PRO:HG2	2:G:1032:ASP:HB2	2.01	0.42
2:G:1079:ASP:O	2:G:1082:ILE:HG22	2.19	0.42
2:G:1217:ASN:HA	2:G:1217:ASN:HD22	1.62	0.42
2:G:1383:ASN:OD1	2:G:1388:LYS:HG3	2.20	0.42
2:G:237:SER:O	2:G:241:ILE:HG13	2.20	0.42
2:G:258:PHE:HD1	2:G:258:PHE:N	2.18	0.42
2:G:732:TRP:CH2	2:G:749:PRO:HG2	2.55	0.42
2:G:7:ARG:NH1	2:G:24:THR:CG2	2.79	0.42
2:G:827:VAL:HG21	2:G:840:THR:CG2	2.49	0.42
1:A:987:ASN:HD22	2:G:957:ARG:CD	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1642:THR:HB	2:H:1651:LEU:HB2	2.01	0.42
2:H:33:LEU:HD13	2:H:68:VAL:HG22	2.02	0.42
2:H:624:TYR:HB2	2:H:630:MET:HE3	2.02	0.42
2:H:844:VAL:HG22	2:H:858:ALA:HB2	2.01	0.42
2:I:732:TRP:CH2	2:I:749:PRO:HG2	2.55	0.42
1:A:1332:TYR:HB3	1:A:1382:ALA:CB	2.50	0.42
1:A:1618:LEU:HD23	1:A:1621:PHE:CE2	2.54	0.42
1:A:155:VAL:HG22	1:A:186:ILE:CG2	2.50	0.42
1:A:335:HIS:CD2	1:A:335:HIS:C	2.92	0.42
1:A:444:ASN:CB	1:A:446:ALA:H	2.32	0.42
1:A:453:TYR:O	1:A:457:ASN:HB2	2.20	0.42
1:B:1189:ILE:HG23	1:B:1190:PRO:HD2	2.01	0.42
1:B:1539:ALA:O	1:B:1574:GLY:HA2	2.20	0.42
1:B:1705:PRO:HB2	1:B:1733:PHE:CD1	2.55	0.42
1:B:1:MET:HE3	1:B:6:GLU:HA	2.01	0.42
1:B:780:GLU:O	1:B:781:LEU:C	2.58	0.42
1:B:44:VAL:HG11	1:B:78:ILE:HG12	2.00	0.42
1:C:1012:LEU:HD23	1:C:1445:MET:HE2	2.02	0.42
1:C:1154:ILE:O	1:C:1154:ILE:HG13	2.20	0.42
1:C:1244:GLY:HA3	1:C:1297:PRO:HD2	2.02	0.42
2:G:1666:PHE:CD1	2:G:1814:ALA:CB	3.02	0.42
2:G:1840:VAL:O	2:G:1840:VAL:HG13	2.18	0.42
2:G:2036:GLU:HB2	2:G:2037:PRO:CD	2.48	0.42
2:G:892:ILE:HD11	2:G:903:TRP:CD2	2.51	0.42
2:H:1889:VAL:HG22	2:H:1977:HIS:O	2.19	0.42
1:B:31:THR:CG2	2:H:2011:ILE:HG21	2.40	0.42
1:B:20:TYR:CZ	2:H:2035:SER:HB2	2.53	0.42
2:H:433:VAL:N	2:H:434:PRO:CD	2.83	0.42
2:H:641:ILE:CD1	2:H:645:SER:HB2	2.50	0.42
2:H:995:LEU:HB3	2:H:1000:ILE:CD1	2.50	0.42
2:I:1135:GLU:HG2	2:I:1176:PRO:HG2	2.02	0.42
2:I:1223:MET:HE3	2:I:1238:LEU:CD1	2.49	0.42
2:I:1593:ILE:O	2:I:1597:ALA:HB3	2.20	0.42
2:I:360:LEU:HA	2:I:361:PRO:HD3	1.89	0.42
2:I:879:LYS:HA	2:I:879:LYS:HD3	1.73	0.42
1:A:1234:MET:HE3	1:A:1326:ILE:HG21	2.02	0.42
1:A:998:TYR:CD2	1:A:1667:GLU:HG3	2.55	0.42
1:A:350:LEU:HD23	1:A:350:LEU:HA	1.89	0.42
1:A:521:LYS:HB3	1:A:523:SER:HB3	2.01	0.42
1:A:32:GLN:HE21	1:A:57:ALA:HB2	1.85	0.42
1:A:780:GLU:O	1:A:781:LEU:C	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1175:ILE:HA	1:B:1176:PRO:HD3	1.89	0.42
1:B:140:ILE:CG2	1:B:141:ALA:N	2.83	0.42
1:B:438:ASN:ND2	1:B:698:GLN:HE21	2.14	0.42
1:C:1029:PRO:HA	1:C:1188:GLN:O	2.20	0.42
1:C:1370:THR:HG22	1:C:1371:THR:N	2.35	0.42
1:C:19:ALA:O	1:C:22:PHE:HB2	2.19	0.42
2:G:1236:LEU:HA	2:G:1237:PRO:HD3	1.76	0.42
2:G:1360:ILE:HA	2:G:1361:PRO:HD3	1.91	0.42
2:G:1782:THR:CG2	2:G:1827:LEU:HD21	2.48	0.42
2:G:298:LYS:HA	2:G:448:VAL:CG2	2.50	0.42
2:G:427:PHE:HB3	2:G:428:HIS:ND1	2.34	0.42
2:G:468:LEU:O	2:G:471:LEU:HB2	2.20	0.42
2:G:670:ARG:HD2	2:G:676:ILE:O	2.20	0.42
2:G:736:ARG:H	2:G:736:ARG:HG3	1.59	0.42
2:H:1180:MET:HB3	2:H:1199:GLU:HG2	2.02	0.42
2:H:1343:VAL:HG22	2:H:1343:VAL:O	2.20	0.42
2:H:1666:PHE:CD1	2:H:1814:ALA:CB	3.03	0.42
2:H:1855:ILE:HB	2:H:1907:LEU:HD12	2.01	0.42
2:H:2036:GLU:HB2	2:H:2037:PRO:CD	2.47	0.42
2:H:234:ILE:HG13	2:H:235:PRO:CD	2.47	0.42
2:H:23:PRO:HG2	2:H:86:LEU:HD11	2.01	0.42
2:H:421:LEU:HA	2:H:422:PRO:HD3	1.78	0.42
2:I:804:ARG:NH2	2:I:1068:GLU:OE1	2.53	0.42
2:I:1214:LEU:HD11	2:I:1220:GLN:NE2	2.35	0.42
2:I:1335:ILE:O	2:I:1338:ILE:HG12	2.20	0.42
2:I:1738:PHE:HE1	2:I:1837:THR:HG23	1.85	0.42
2:I:258:PHE:N	2:I:258:PHE:CD1	2.87	0.42
1:A:1279:PHE:HB2	1:A:1282:THR:HG23	2.01	0.41
1:A:1308:SER:HB3	1:A:1589:GLY:HA3	2.01	0.41
1:A:1019:ILE:HG21	1:A:1316:VAL:HG22	2.01	0.41
1:A:1657:HIS:CG	1:A:1658:PRO:HD2	2.55	0.41
1:A:32:GLN:NE2	1:A:57:ALA:CA	2.83	0.41
1:B:1019:ILE:HG13	1:B:1316:VAL:HG13	2.02	0.41
1:B:1673:TYR:CZ	1:B:1677:VAL:HG21	2.55	0.41
1:C:1215:VAL:O	1:C:1219:VAL:HG23	2.20	0.41
1:C:12:ILE:HD11	2:I:2041:ILE:HD11	2.01	0.41
1:C:616:LEU:HB2	1:C:617:PRO:HD3	2.01	0.41
1:C:635:ILE:CG2	1:C:651:TYR:CG	3.03	0.41
2:G:1128:LYS:HG2	2:G:1181:VAL:HG22	2.02	0.41
2:G:1579:ILE:CD1	2:G:1615:MET:SD	3.08	0.41
2:G:1496:LYS:CE	2:G:1693:ARG:HH21	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:439:ILE:HD12	2:G:484:ILE:HD11	2.01	0.41
2:G:638:VAL:HA	2:G:641:ILE:CG2	2.50	0.41
2:H:896:ASN:O	2:H:1050:ARG:NH2	2.53	0.41
2:H:2010:TYR:O	2:H:2012:PRO:HD3	2.20	0.41
2:H:240:LEU:O	2:H:244:ILE:HG13	2.19	0.41
2:H:258:PHE:N	2:H:258:PHE:HD1	2.18	0.41
2:I:1815:LEU:O	2:I:1821:VAL:HG23	2.20	0.41
2:I:1697:HIS:CE1	2:I:1829:GLU:CG	3.03	0.41
2:I:1980:TYR:HD1	2:I:1981:LEU:HD12	1.85	0.41
2:I:441:LYS:HG2	2:I:445:LYS:HE3	2.02	0.41
2:I:512:LEU:O	2:I:516:THR:HG23	2.20	0.41
2:I:659:LEU:O	2:I:663:ILE:HG12	2.20	0.41
1:A:1233:GLU:CD	1:A:1680:ARG:HH21	2.24	0.41
1:A:280:GLU:O	1:A:284:LYS:HG3	2.21	0.41
1:A:28:TRP:CE2	1:A:53:LEU:HD22	2.55	0.41
1:A:340:ARG:NH1	1:A:344:GLN:CG	2.70	0.41
1:A:50:SER:CB	1:A:51:PRO:CD	2.98	0.41
1:B:290:MET:HE2	1:B:290:MET:HB3	1.96	0.41
1:C:1584:PRO:CG	1:C:1591:TRP:CZ3	3.03	0.41
1:C:12:ILE:O	1:C:15:THR:HG23	2.20	0.41
1:C:889:GLU:C	1:C:891:MET:H	2.24	0.41
2:G:1553:TYR:OH	2:G:1583:MET:HB3	2.20	0.41
2:G:1755:ILE:HD11	2:G:1762:TYR:HB2	2.03	0.41
1:A:29:ILE:HD13	2:G:1894:GLU:HA	2.01	0.41
2:G:2035:SER:OG	2:G:2037:PRO:HD2	2.21	0.41
2:G:717:ILE:HG23	2:G:760:HIS:CE1	2.55	0.41
1:A:983:GLN:HE21	2:G:962:LYS:HD2	1.80	0.41
2:G:992:GLU:HA	2:G:992:GLU:OE1	2.20	0.41
2:H:142:ASN:HB2	2:H:550:VAL:HG13	2.01	0.41
2:H:1713:ASN:HA	2:H:1714:PRO:HD3	1.89	0.41
2:H:15:SER:H	2:H:48:PHE:HE2	1.66	0.41
2:H:584:SER:CB	2:H:591:PRO:HG3	2.46	0.41
2:I:1149:TRP:HA	2:I:1242:PHE:CD1	2.54	0.41
2:I:1495:THR:O	2:I:1496:LYS:HB2	2.20	0.41
2:I:524:GLY:HA2	2:I:558:ASN:O	2.20	0.41
2:I:592:LEU:O	2:I:616:THR:HG23	2.19	0.41
2:I:84:LEU:HA	2:I:84:LEU:HD23	1.89	0.41
1:A:1666:THR:HG23	1:A:1669:ARG:HB2	2.01	0.41
1:A:1784:ASP:O	1:A:1788:GLU:HB2	2.20	0.41
1:B:1047:LEU:O	1:B:1051:VAL:HG23	2.20	0.41
1:B:455:ILE:HD13	1:B:455:ILE:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:852:ARG:HB3	1:B:858:TRP:HZ2	1.83	0.41
1:C:1047:LEU:HD23	1:C:1047:LEU:HA	1.89	0.41
1:C:1208:VAL:HG13	1:C:1209:ASP:O	2.20	0.41
1:C:335:HIS:C	1:C:335:HIS:CD2	2.91	0.41
1:C:792:HIS:CE1	1:C:796:LEU:HD23	2.55	0.41
2:G:1258:ARG:O	2:G:1262:ILE:HG13	2.20	0.41
2:G:1380:SER:HB3	2:G:1424:GLN:HB2	2.02	0.41
2:G:1359:MET:HB3	2:G:1606:ARG:NH2	2.35	0.41
2:G:1624:THR:HB	2:G:1642:THR:CG2	2.50	0.41
2:G:520:LYS:O	2:G:521:ASP:C	2.58	0.41
2:G:667:LYS:HD2	2:G:697:THR:CG2	2.38	0.41
2:G:888:ARG:O	2:G:892:ILE:HB	2.21	0.41
2:H:1314:ARG:HD3	2:H:1314:ARG:HA	1.63	0.41
2:I:1493:LEU:HB3	2:I:1494:PRO:HD2	2.02	0.41
2:I:195:LEU:O	2:I:199:ILE:HG13	2.20	0.41
2:I:339:LEU:HD23	2:I:419:ARG:O	2.20	0.41
2:I:507:GLY:O	2:I:508:GLY:C	2.59	0.41
2:I:581:THR:O	2:I:585:LYS:HB2	2.20	0.41
2:I:807:ILE:HA	2:I:818:LYS:HG2	2.02	0.41
1:A:1154:ILE:O	1:A:1154:ILE:HG13	2.19	0.41
1:A:1305:CYS:SG	3:A:2748:CER:C5	3.08	0.41
1:A:12:ILE:O	1:A:15:THR:HG23	2.20	0.41
1:A:1720:ALA:O	1:A:1721:ARG:HG2	2.21	0.41
1:A:330:GLU:O	1:A:330:GLU:HG2	2.20	0.41
1:A:28:TRP:CZ2	1:A:53:LEU:HD22	2.56	0.41
1:A:807:LYS:C	1:A:807:LYS:HD3	2.40	0.41
1:B:1216:LEU:HA	1:B:1216:LEU:HD23	1.93	0.41
1:B:1448:ARG:HD2	1:B:1508:TRP:O	2.21	0.41
1:B:378:LEU:HA	1:B:378:LEU:HD12	1.75	0.41
1:B:992:PHE:CD2	1:B:1399:PRO:HG3	2.55	0.41
1:C:495:LYS:HA	1:C:496:PRO:HD3	1.86	0.41
1:C:496:PRO:HB2	1:C:519:VAL:HG12	2.02	0.41
1:C:521:LYS:HE2	1:C:605:LEU:HD11	2.02	0.41
1:C:719:GLN:HG3	1:C:720:SER:N	2.35	0.41
2:G:439:ILE:HD12	2:G:484:ILE:CD1	2.50	0.41
2:G:760:HIS:HA	2:G:761:PRO:HD3	1.85	0.41
2:G:846:VAL:HG13	2:G:865:TRP:CD1	2.55	0.41
2:G:950:PHE:O	2:G:953:ARG:HB3	2.20	0.41
2:H:1071:LYS:HE3	2:H:1075:ASP:OD2	2.20	0.41
2:H:1752:PHE:HZ	2:H:1836:MET:HE3	1.84	0.41
2:H:1886:VAL:HG22	2:H:1906:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:455:ILE:HG12	2:H:469:ARG:CG	2.49	0.41
2:H:601:THR:HB	2:H:620:ALA:HB2	2.01	0.41
2:H:561:TRP:CG	2:H:754:TYR:HE2	2.39	0.41
2:I:1021:LEU:HD22	2:I:1021:LEU:HA	1.61	0.41
2:I:1457:PHE:CD2	2:I:1459:LEU:HD23	2.55	0.41
2:I:1458:ASP:O	2:I:1462:LYS:HE3	2.21	0.41
2:I:156:LEU:HD23	2:I:500:HIS:HB2	2.02	0.41
2:I:258:PHE:HD1	2:I:258:PHE:N	2.18	0.41
2:I:654:VAL:CG2	2:I:683:ALA:HB1	2.50	0.41
2:I:949:ASP:HB3	2:I:1006:MET:CE	2.48	0.41
1:A:12:ILE:O	1:A:16:GLU:HG2	2.20	0.41
1:A:1477:ILE:N	1:A:1478:PRO:CD	2.83	0.41
1:A:601:VAL:O	1:A:602:GLU:C	2.59	0.41
1:A:82:SER:OG	1:A:83:LYS:HG3	2.20	0.41
1:B:1244:GLY:HA3	1:B:1297:PRO:HD2	2.03	0.41
1:B:1257:LEU:HD23	1:B:1257:LEU:HA	1.76	0.41
1:B:1303:GLY:H	1:B:1307:THR:CG2	2.31	0.41
1:B:1308:SER:HB3	1:B:1589:GLY:HA3	2.03	0.41
1:B:1232:TYR:CE2	1:B:1701:LYS:HD2	2.55	0.41
1:B:453:TYR:O	1:B:457:ASN:HB2	2.21	0.41
1:B:504:ASP:CB	1:B:508:ASN:HB2	2.49	0.41
1:B:949:GLU:O	1:B:953:VAL:HG12	2.21	0.41
1:C:1408:ALA:O	1:C:1651:GLY:HA2	2.21	0.41
1:C:1443:LEU:HA	1:C:1443:LEU:HD23	1.77	0.41
1:C:1830:GLY:HA2	1:C:1831:GLY:HA2	1.57	0.41
1:C:242:THR:HB	1:C:244:THR:HB	2.02	0.41
2:G:1676:MET:HE1	2:G:1781:LEU:CD2	2.47	0.41
2:G:1706:ILE:HD12	2:G:1706:ILE:HA	1.89	0.41
2:G:1862:VAL:HG22	2:G:1863:ALA:N	2.36	0.41
1:A:9:LEU:HD21	2:G:2047:LYS:HD2	2.02	0.41
1:B:2:LYS:CD	2:H:2050:GLN:HB3	2.44	0.41
2:H:231:LEU:HA	2:H:236:ILE:HD12	2.03	0.41
2:H:339:LEU:HD23	2:H:419:ARG:O	2.20	0.41
2:H:478:ARG:O	2:H:482:CYS:HB2	2.20	0.41
2:I:177:TYR:CD1	2:I:188:ILE:HG21	2.55	0.41
2:I:1940:LEU:HD12	2:I:1941:PHE:N	2.35	0.41
2:I:566:HIS:ND1	2:I:567:PRO:HD2	2.35	0.41
2:I:572:ASN:HA	2:I:572:ASN:HD22	1.70	0.41
2:I:712:ALA:O	2:I:716:VAL:HG23	2.21	0.41
2:I:780:TYR:HB2	2:I:799:PHE:HE2	1.85	0.41
2:I:786:SER:HB2	2:I:794:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:800:LEU:H	2:I:800:LEU:HD23	1.85	0.41
1:A:1842:VAL:O	1:A:1843:ASN:O	2.39	0.41
1:A:370:GLU:O	1:A:373:ALA:HB3	2.20	0.41
1:A:825:PRO:HB2	1:A:843:LYS:HZ2	1.86	0.41
1:A:529:MET:HE1	1:A:894:ARG:HD2	2.00	0.41
1:A:932:PHE:O	1:A:934:PRO:HD3	2.20	0.41
1:B:1066:ASN:HD22	1:B:1071:PRO:HA	1.86	0.41
1:B:238:PRO:CG	1:B:283:ALA:HB2	2.50	0.41
1:B:406:TRP:CD2	1:B:1619:GLU:HG3	2.55	0.41
1:B:495:LYS:HA	1:B:496:PRO:HD3	1.89	0.41
1:C:1709:GLU:H	1:C:1709:GLU:HG3	1.42	0.41
1:C:1784:ASP:O	1:C:1788:GLU:HB2	2.20	0.41
2:G:1169:PRO:O	2:G:1173:VAL:HG23	2.20	0.41
2:G:1352:HIS:HD2	2:G:1410:PHE:CD2	2.38	0.41
2:G:1495:THR:O	2:G:1496:LYS:HB2	2.20	0.41
2:G:1642:THR:HB	2:G:1651:LEU:HB2	2.01	0.41
2:G:1815:LEU:O	2:G:1821:VAL:HG23	2.20	0.41
2:G:1979:THR:O	2:G:1982:MET:HB2	2.21	0.41
2:G:597:MET:HA	4:G:3051:FMN:C5A	2.51	0.41
2:G:490:TRP:CZ2	2:G:512:LEU:HD21	2.55	0.41
2:G:754:TYR:CG	2:G:794:MET:CG	3.04	0.41
2:H:1236:LEU:HD22	2:H:1238:LEU:HG	2.03	0.41
2:H:1680:LEU:HD13	2:H:1687:ALA:CB	2.45	0.41
2:H:624:TYR:CD1	2:H:630:MET:HE2	2.56	0.41
2:H:712:ALA:O	2:H:715:GLN:HB3	2.20	0.41
2:H:717:ILE:CG2	2:H:760:HIS:CE1	3.04	0.41
2:H:722:ALA:CB	2:H:723:HIS:CE1	3.04	0.41
2:H:950:PHE:O	2:H:953:ARG:HB3	2.20	0.41
2:I:1417:THR:C	2:I:1419:PHE:N	2.74	0.41
2:I:1423:PHE:N	2:I:1423:PHE:CD1	2.71	0.41
2:I:1054:LEU:HD22	4:I:3051:FMN:HM72	2.03	0.41
2:I:663:ILE:HG13	2:I:694:TYR:CE1	2.51	0.41
2:I:638:VAL:HG22	2:I:675:PRO:HG2	2.03	0.41
1:A:32:GLN:O	1:A:36:LEU:HB2	2.21	0.41
1:A:774:ILE:HA	1:A:775:PRO:HD3	1.76	0.41
1:A:988:ILE:HD13	1:A:1048:GLU:CG	2.50	0.41
1:B:1105:LEU:HA	1:B:1105:LEU:HD23	1.89	0.41
1:B:1126:ILE:CD1	1:B:1172:THR:HG22	2.51	0.41
1:B:1666:THR:HG23	1:B:1669:ARG:CB	2.50	0.41
1:C:1119:LYS:HE2	1:C:1341:PHE:CG	2.55	0.41
1:C:1131:LEU:HA	1:C:1131:LEU:HD12	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1418:VAL:N	1:C:1419:PRO:CD	2.83	0.41
1:C:35:PHE:HA	1:C:39:PHE:HD2	1.86	0.41
2:G:843:ILE:CD1	2:G:1055:HIS:HB3	2.50	0.41
2:G:571:LYS:HB2	2:G:1099:ALA:HB2	2.02	0.41
2:G:1344:ASP:O	2:G:1416:TYR:HE2	2.03	0.41
2:G:1427:VAL:HG22	2:G:1469:GLU:CG	2.51	0.41
2:G:246:LEU:HD12	2:G:246:LEU:HA	1.82	0.41
2:G:425:SER:HA	2:G:426:PRO:HD3	1.79	0.41
2:G:587:ILE:HD11	2:G:589:ARG:HB2	2.03	0.41
2:G:835:THR:HG21	2:G:855:HIS:NE2	2.35	0.41
2:H:1128:LYS:HG2	2:H:1181:VAL:HG22	2.01	0.41
2:H:11:LEU:HD23	2:H:11:LEU:HA	1.93	0.41
2:H:1503:ILE:HG22	2:H:1504:VAL:C	2.41	0.41
2:H:236:ILE:HD13	2:H:236:ILE:C	2.40	0.41
2:H:821:ILE:HA	2:H:857:ILE:HD11	2.02	0.41
2:H:827:VAL:HG12	2:H:828:PRO:O	2.19	0.41
2:I:1357:TYR:HD1	2:I:1406:VAL:HG22	1.85	0.41
2:I:159:ILE:HD11	2:I:512:LEU:CG	2.49	0.41
2:I:1642:THR:HB	2:I:1651:LEU:HB2	2.03	0.41
2:I:1981:LEU:HD12	2:I:1981:LEU:N	2.36	0.41
2:I:463:PHE:O	2:I:463:PHE:HD2	2.04	0.41
2:I:634:ILE:CD1	2:I:649:ILE:HD11	2.44	0.41
2:I:595:PRO:HD3	2:I:800:LEU:HB2	2.01	0.41
1:A:16:GLU:HA	1:A:16:GLU:OE2	2.21	0.41
1:A:1239:HIS:HE1	1:A:1714:VAL:O	2.03	0.41
1:A:441:ASN:OD1	1:A:488:PRO:HA	2.21	0.41
1:A:91:THR:HA	1:A:92:PRO:HD3	1.81	0.41
1:B:521:LYS:HB3	1:B:523:SER:HB3	2.03	0.41
1:B:949:GLU:O	1:B:953:VAL:CG1	2.68	0.41
1:C:1420:ALA:HA	1:C:1421:PRO:HD3	1.78	0.41
1:C:658:LEU:HD13	1:C:916:LEU:HD12	2.02	0.41
2:G:1070:ILE:O	2:G:1070:ILE:HD13	2.21	0.41
2:G:131:ILE:HD12	2:G:182:VAL:CG1	2.49	0.41
2:G:1428:GLU:CG	2:G:1468:THR:HG22	2.51	0.41
2:G:236:ILE:HG12	2:G:240:LEU:HD22	2.02	0.41
2:G:270:ALA:O	2:G:459:VAL:HA	2.20	0.41
2:G:123:ILE:CD1	2:G:533:LEU:HD23	2.50	0.41
2:H:159:ILE:HG12	2:H:512:LEU:HD23	2.02	0.41
2:H:1662:THR:HB	2:H:1799:PRO:HG2	2.02	0.41
2:H:1959:LYS:HG2	2:H:1959:LYS:O	2.20	0.41
2:H:320:PRO:HA	2:H:321:PRO:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:674:TYR:HA	2:H:675:PRO:HD3	1.73	0.41
2:H:719:ILE:HG12	2:H:719:ILE:H	1.63	0.41
2:H:805:VAL:HG12	2:H:805:VAL:O	2.21	0.41
2:I:1374:THR:HG23	2:I:1396:LEU:CD1	2.49	0.41
2:I:2035:SER:OG	2:I:2037:PRO:HD2	2.21	0.41
2:I:705:LEU:HD23	2:I:705:LEU:HA	1.80	0.41
1:A:152:HIS:HD2	1:A:163:LEU:CB	2.32	0.41
1:A:612:GLU:O	1:A:615:SER:HB3	2.21	0.41
1:A:719:GLN:HG3	1:A:720:SER:N	2.36	0.41
1:B:1418:VAL:N	1:B:1419:PRO:CD	2.83	0.41
1:B:1618:LEU:HD23	1:B:1621:PHE:HE2	1.85	0.41
1:B:1709:GLU:HG3	1:B:1709:GLU:H	1.45	0.41
1:C:1239:HIS:CD2	1:C:1241:SER:H	2.38	0.41
1:C:1244:GLY:C	1:C:1327:CYS:HB2	2.41	0.41
1:C:1431:GLU:O	1:C:1431:GLU:HG3	2.19	0.41
1:C:1842:VAL:O	1:C:1843:ASN:O	2.39	0.41
1:C:453:TYR:O	1:C:457:ASN:HB2	2.19	0.41
1:C:32:GLN:HE22	1:C:57:ALA:N	2.19	0.41
1:C:683:ALA:HA	1:C:689:GLY:HA3	2.02	0.41
2:G:1210:ILE:O	2:G:1210:ILE:HG22	2.19	0.41
2:G:1884:TRP:HB3	2:G:1885:LEU:H	1.74	0.41
2:H:1300:PHE:CB	2:H:1556:VAL:HG11	2.50	0.41
2:H:1815:LEU:O	2:H:1821:VAL:HG23	2.21	0.41
2:H:1868:GLN:HG3	2:H:1898:TYR:HH	1.83	0.41
2:H:195:LEU:O	2:H:199:ILE:HG13	2.20	0.41
2:H:827:VAL:HG21	2:H:840:THR:CG2	2.51	0.41
2:I:1219:ILE:HB	2:I:1240:TYR:HB2	2.03	0.41
2:I:1503:ILE:HG22	2:I:1504:VAL:C	2.41	0.41
2:I:1514:ASN:HA	2:I:1515:PRO:HD3	1.86	0.41
2:I:1579:ILE:CD1	2:I:1615:MET:SD	3.09	0.41
2:I:827:VAL:HG12	2:I:828:PRO:O	2.20	0.41
1:A:1460:LYS:CE	1:A:1774:GLU:OE1	2.62	0.41
1:A:253:ARG:O	1:A:254:TRP:CD1	2.74	0.41
1:A:438:ASN:HD21	1:A:698:GLN:HE21	1.68	0.41
1:A:930:LEU:HD22	1:A:933:VAL:CG1	2.51	0.41
1:B:1657:HIS:CG	1:B:1658:PRO:HD2	2.55	0.41
1:B:444:ASN:CB	1:B:446:ALA:H	2.31	0.41
1:C:1076:VAL:CG1	1:C:1081:LYS:HA	2.50	0.41
1:C:1705:PRO:HB2	1:C:1733:PHE:CD1	2.56	0.41
1:C:1829:GLY:O	1:C:1830:GLY:O	2.39	0.41
1:C:739:GLN:HB3	1:C:794:ILE:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:949:GLU:O	1:C:953:VAL:HG12	2.21	0.41
2:G:1352:HIS:CD2	2:G:1410:PHE:CD2	3.09	0.41
2:G:1778:GLN:HB2	2:G:1779:PRO:HD3	2.02	0.41
2:G:1889:VAL:HG22	2:G:1977:HIS:O	2.20	0.41
2:G:1981:LEU:HD12	2:G:1981:LEU:N	2.36	0.41
2:G:1989:LYS:NZ	2:G:2037:PRO:HG2	2.35	0.41
2:G:258:PHE:N	2:G:258:PHE:CD1	2.87	0.41
2:G:260:PRO:HD3	2:G:289:TRP:CZ2	2.54	0.41
2:G:735:GLY:O	2:G:741:HIS:CD2	2.73	0.41
2:G:748:THR:CB	2:G:749:PRO:HD3	2.47	0.41
2:G:780:TYR:HB2	2:G:799:PHE:CE2	2.56	0.41
2:G:995:LEU:HB3	2:G:1000:ILE:CD1	2.50	0.41
2:H:615:TYR:CE2	2:H:1074:MET:HB3	2.56	0.41
2:H:1213:LEU:O	2:H:1214:LEU:HD23	2.19	0.41
2:H:1270:TRP:HZ3	2:H:1347:LEU:HD21	1.85	0.41
2:H:1589:VAL:HG21	2:H:1651:LEU:HD12	2.02	0.41
2:H:425:SER:HA	2:H:426:PRO:HD3	1.78	0.41
2:H:753:MET:O	2:H:757:ILE:HG13	2.21	0.41
2:H:804:ARG:NH2	2:H:1068:GLU:OE1	2.54	0.41
2:H:892:ILE:HD11	2:H:903:TRP:CD2	2.53	0.41
2:I:248:HIS:CE1	2:I:531:GLY:HA2	2.55	0.41
2:I:455:ILE:C	2:I:455:ILE:HD12	2.42	0.41
2:I:582:LYS:HE2	2:I:761:PRO:O	2.21	0.41
1:A:1705:PRO:HB2	1:A:1733:PHE:CD1	2.56	0.41
1:A:36:LEU:O	1:A:76:ARG:NH1	2.53	0.41
1:A:908:LEU:O	1:A:913:VAL:HG22	2.21	0.41
1:B:1029:PRO:HG2	1:B:1581:THR:O	2.21	0.41
1:B:197:THR:HG22	1:B:198:PRO:O	2.21	0.41
1:B:187:LEU:CD2	1:B:201:PRO:HB2	2.51	0.41
1:B:32:GLN:HE22	1:B:57:ALA:CA	2.34	0.41
1:B:489:VAL:HG22	1:B:670:GLY:HA3	2.02	0.41
1:B:427:ASN:ND2	1:B:610:THR:H	2.14	0.41
1:B:82:SER:OG	1:B:83:LYS:HG3	2.20	0.41
1:B:504:ASP:O	1:B:954:ARG:HD3	2.21	0.41
1:C:1019:ILE:HG13	1:C:1316:VAL:HG13	2.03	0.41
1:C:1666:THR:HG23	1:C:1669:ARG:CB	2.51	0.41
1:C:237:MET:HA	1:C:238:PRO:HD3	1.93	0.41
1:C:294:TYR:CZ	1:C:298:VAL:HG21	2.55	0.41
1:C:427:ASN:HB2	1:C:468:LEU:CD2	2.51	0.41
1:C:644:THR:HG23	1:C:648:ASP:N	2.34	0.41
2:G:2049:GLU:O	2:G:2050:GLN:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:339:LEU:HB2	2:G:386:LEU:HD22	2.03	0.41
2:G:44:PRO:HA	2:G:53:GLU:OE2	2.21	0.41
2:G:455:ILE:HD13	2:G:457:ILE:O	2.21	0.41
2:H:1063:THR:HG22	2:H:1063:THR:O	2.21	0.41
2:H:1387:GLY:HA2	2:H:1414:GLY:O	2.21	0.41
2:H:1949:LYS:O	2:H:1953:VAL:HG23	2.21	0.41
2:I:118:LYS:O	2:I:121:GLU:HB2	2.20	0.41
2:I:1327:ILE:O	2:I:1331:TRP:HB2	2.21	0.41
2:I:2020:GLN:NE2	2:I:2020:GLN:HA	2.36	0.41
2:I:319:LEU:HA	2:I:319:LEU:HD22	1.67	0.41
2:I:717:ILE:O	2:I:720:ALA:HB3	2.21	0.41
2:I:754:TYR:CG	2:I:794:MET:CG	3.04	0.41
2:I:827:VAL:HG21	2:I:840:THR:CG2	2.51	0.41
1:A:1418:VAL:N	1:A:1419:PRO:CD	2.84	0.40
1:A:197:THR:HG22	1:A:198:PRO:O	2.21	0.40
1:A:232:LEU:O	1:A:236:LYS:HB2	2.21	0.40
1:A:681:THR:HA	1:A:706:THR:OG1	2.21	0.40
1:B:1056:ILE:HG13	1:B:1057:MET:N	2.36	0.40
1:B:1557:ILE:HD11	1:B:1642:THR:HG21	2.03	0.40
1:B:483:VAL:O	1:B:483:VAL:HG12	2.21	0.40
1:B:91:THR:HA	1:B:92:PRO:HD3	1.81	0.40
1:B:933:VAL:HA	1:B:934:PRO:HD3	1.63	0.40
1:B:989:GLN:NE2	2:H:993:GLN:OE1	2.53	0.40
1:B:998:TYR:CD2	1:B:1667:GLU:HG3	2.56	0.40
1:C:1308:SER:OG	1:C:1590:ALA:N	2.54	0.40
1:C:187:LEU:CD2	1:C:201:PRO:HB2	2.51	0.40
2:G:1343:VAL:HG22	2:G:1343:VAL:O	2.20	0.40
2:G:1844:ARG:HD2	2:G:1848:GLY:O	2.21	0.40
1:A:29:ILE:HG21	2:G:1894:GLU:HB2	2.04	0.40
2:G:430:HIS:CE1	2:G:431:LEU:HD13	2.56	0.40
2:G:159:ILE:HG12	2:G:512:LEU:HD23	2.03	0.40
2:G:73:GLU:OE2	2:G:76:LYS:HD2	2.21	0.40
2:G:938:TRP:CD1	2:G:944:ARG:HG3	2.56	0.40
2:H:1227:ARG:CZ	2:H:1565:VAL:HG12	2.51	0.40
2:H:338:MET:HG3	2:H:423:VAL:HG21	2.02	0.40
2:H:566:HIS:O	2:H:567:PRO:C	2.59	0.40
2:H:888:ARG:O	2:H:892:ILE:HB	2.21	0.40
2:I:1676:MET:HE1	2:I:1781:LEU:CD2	2.50	0.40
2:I:1880:LYS:HB2	2:I:1880:LYS:HE3	1.90	0.40
2:I:1889:VAL:HG21	2:I:1901:ALA:HB3	2.03	0.40
2:I:2036:GLU:HB2	2:I:2037:PRO:CD	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2039:LYS:HA	2:I:2042:ILE:HG13	2.03	0.40
2:I:247:ALA:O	2:I:251:VAL:HG13	2.21	0.40
2:I:280:ALA:O	2:I:283:ILE:HG22	2.21	0.40
2:I:846:VAL:CG2	2:I:866:LYS:HB2	2.51	0.40
1:A:1021:VAL:HG11	1:A:1597:LEU:CD1	2.50	0.40
1:A:1146:HIS:O	1:A:1146:HIS:HD2	2.04	0.40
1:A:1665:ILE:HD11	1:A:1669:ARG:CG	2.51	0.40
1:A:44:VAL:HG13	1:A:78:ILE:HG12	1.99	0.40
1:A:833:PHE:O	1:A:834:GLY:O	2.39	0.40
1:B:1583:HIS:HA	1:B:1584:PRO:HD3	1.84	0.40
1:B:1829:GLY:O	1:B:1830:GLY:O	2.39	0.40
1:C:1105:LEU:HA	1:C:1105:LEU:HD23	1.84	0.40
1:C:148:SER:O	1:C:152:HIS:HB2	2.21	0.40
1:C:411:GLN:O	1:C:415:SER:HB2	2.21	0.40
2:G:1227:ARG:NE	2:G:1565:VAL:HG12	2.36	0.40
2:G:1678:MET:HG2	2:G:1711:ILE:HG12	2.03	0.40
2:G:1940:LEU:HD12	2:G:1941:PHE:N	2.37	0.40
1:A:23:ALA:O	2:G:1977:HIS:HA	2.20	0.40
2:G:562:LEU:HD23	2:G:562:LEU:HA	1.85	0.40
2:G:601:THR:HB	2:G:620:ALA:HB2	2.01	0.40
2:G:638:VAL:O	2:G:641:ILE:HG22	2.20	0.40
2:G:805:VAL:O	2:G:805:VAL:HG12	2.21	0.40
2:G:827:VAL:HG12	2:G:828:PRO:O	2.21	0.40
2:H:1214:LEU:HD11	2:H:1220:GLN:NE2	2.36	0.40
2:H:1506:TYR:CZ	2:H:1515:PRO:HG2	2.56	0.40
2:H:1609:THR:O	2:H:1653:GLY:HA3	2.21	0.40
2:H:203:LEU:HD12	2:H:203:LEU:HA	1.91	0.40
2:H:462:THR:HB	2:H:482:CYS:SG	2.61	0.40
2:H:573:LYS:C	2:H:575:GLY:N	2.75	0.40
2:H:590:PRO:HA	2:H:591:PRO:HD3	1.81	0.40
2:H:638:VAL:HA	2:H:641:ILE:CG2	2.52	0.40
2:H:723:HIS:ND1	2:H:723:HIS:N	2.70	0.40
2:H:960:LYS:CE	2:H:960:LYS:HA	2.44	0.40
2:I:1091:GLY:O	2:I:1093:ASP:N	2.55	0.40
2:I:1339:PHE:N	2:I:1340:PRO:CD	2.85	0.40
2:I:1359:MET:HB3	2:I:1606:ARG:NH2	2.36	0.40
2:I:1889:VAL:HG13	2:I:1977:HIS:HB3	2.00	0.40
2:I:246:LEU:HA	2:I:246:LEU:HD12	1.79	0.40
2:I:536:ASN:HD21	2:I:540:ASP:HB3	1.85	0.40
2:I:543:PHE:CB	2:I:545:GLN:NE2	2.82	0.40
2:I:703:LEU:HD23	2:I:705:LEU:HG	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:816:ASP:HB3	2:I:1048:VAL:HG21	2.03	0.40
1:A:238:PRO:CG	1:A:283:ALA:HB2	2.51	0.40
1:A:852:ARG:NH1	1:A:852:ARG:CG	2.73	0.40
1:B:1303:GLY:CA	1:B:1307:THR:HG22	2.52	0.40
1:B:221:LEU:HD23	1:B:221:LEU:HA	1.94	0.40
1:B:293:LYS:O	1:B:297:ILE:HG13	2.20	0.40
1:B:774:ILE:HA	1:B:775:PRO:HD3	1.74	0.40
1:C:1303:GLY:CA	1:C:1307:THR:HG22	2.52	0.40
1:C:43:ARG:O	2:I:1662:THR:HA	2.22	0.40
2:G:1637:LEU:HA	2:G:1637:LEU:HD23	1.77	0.40
2:G:1875:VAL:HA	2:G:1878:VAL:CG1	2.52	0.40
2:G:248:HIS:CE1	2:G:531:GLY:HA2	2.56	0.40
2:G:319:LEU:HA	2:G:319:LEU:HD22	1.62	0.40
2:G:391:LEU:CD2	2:G:394:ARG:NH2	2.85	0.40
2:G:441:LYS:HG2	2:G:445:LYS:HE3	2.02	0.40
2:G:573:LYS:C	2:G:575:GLY:N	2.75	0.40
2:G:582:LYS:HE2	2:G:761:PRO:O	2.22	0.40
2:G:852:GLU:H	2:G:852:GLU:HG3	1.40	0.40
2:H:1166:VAL:CG1	2:H:1167:SER:N	2.85	0.40
2:H:1528:GLU:C	2:H:1530:LYS:H	2.17	0.40
2:H:1597:ALA:HB1	2:H:1657:ILE:HD12	2.02	0.40
2:H:517:HIS:HB2	2:H:527:VAL:HG21	2.04	0.40
2:H:517:HIS:CE1	2:H:540:ASP:O	2.75	0.40
2:H:560:ASN:O	2:H:562:LEU:N	2.54	0.40
2:H:810:GLU:OE2	2:H:1070:ILE:N	2.45	0.40
2:H:912:ARG:HB2	2:H:916:THR:HG23	2.03	0.40
2:I:1213:LEU:O	2:I:1214:LEU:HD23	2.20	0.40
2:I:1271:ILE:HG22	2:I:1273:GLU:HB2	2.04	0.40
2:I:1855:ILE:HB	2:I:1907:LEU:HD12	2.02	0.40
2:I:612:ASN:HD21	2:I:641:ILE:HA	1.84	0.40
2:I:864:LEU:HD13	2:I:894:ARG:HB3	2.04	0.40
1:A:1209:ASP:OD1	1:A:1210:PRO:HD2	2.21	0.40
1:A:1406:MET:CE	1:A:1428:THR:HB	2.52	0.40
1:A:157:HIS:CE1	1:A:269:LEU:HD11	2.57	0.40
1:A:916:LEU:HD22	1:A:922:VAL:HG22	2.02	0.40
1:B:1370:THR:HG22	1:B:1371:THR:N	2.36	0.40
1:B:12:ILE:O	1:B:16:GLU:HG2	2.20	0.40
1:B:509:ILE:HG13	1:B:509:ILE:H	1.50	0.40
1:B:74:LEU:O	1:B:74:LEU:HD12	2.22	0.40
1:C:1063:HIS:CE1	1:C:1067:LEU:CD2	3.04	0.40
1:C:1195:ALA:HB1	1:C:1200:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1639:VAL:HG12	1:C:1640:SER:N	2.35	0.40
1:C:1749:THR:O	1:C:1874:ASP:HB3	2.21	0.40
1:C:406:TRP:CZ3	1:C:407:ASN:HB2	2.57	0.40
1:C:655:LEU:HD23	1:C:655:LEU:HA	1.79	0.40
2:G:260:PRO:HD3	2:G:289:TRP:CD2	2.56	0.40
2:G:612:ASN:C	2:G:614:GLY:H	2.24	0.40
2:H:1281:PRO:O	2:H:1378:ILE:HG23	2.22	0.40
2:H:1593:ILE:HD13	2:H:1626:ILE:CD1	2.51	0.40
2:H:1716:ASN:HA	2:H:1770:LEU:HD11	2.04	0.40
2:H:538:ASP:HB2	2:H:540:ASP:HB2	2.03	0.40
2:H:607:VAL:HG23	2:H:617:ILE:CG2	2.51	0.40
2:I:240:LEU:HA	2:I:240:LEU:HD12	1.81	0.40
2:I:717:ILE:CG2	2:I:760:HIS:CE1	3.05	0.40
2:I:812:LYS:HA	2:I:812:LYS:HD3	1.82	0.40
1:A:350:LEU:HB2	1:A:352:MET:HG2	2.03	0.40
1:A:427:ASN:HB2	1:A:468:LEU:CD2	2.51	0.40
1:B:1577:GLN:NE2	1:B:1591:TRP:HB3	2.36	0.40
1:B:709:ARG:O	1:B:714:VAL:HG21	2.21	0.40
1:C:187:LEU:HD11	1:C:202:GLU:HG3	2.03	0.40
1:C:413:LEU:HD13	1:C:451:MET:HG2	2.03	0.40
2:G:119:THR:HG22	2:G:120:LYS:N	2.36	0.40
2:G:1830:VAL:HA	2:G:1991:PHE:HE2	1.86	0.40
2:G:2039:LYS:HA	2:G:2042:ILE:HG13	2.03	0.40
2:G:533:LEU:HG	2:G:533:LEU:O	2.21	0.40
2:G:606:PHE:HZ	2:G:805:VAL:CG1	2.33	0.40
2:H:1172:LYS:HZ1	2:H:1574:ASN:HA	1.85	0.40
2:H:1327:ILE:HA	2:H:1327:ILE:HD12	1.77	0.40
2:H:283:ILE:HD12	2:H:283:ILE:HA	1.89	0.40
2:H:233:SER:HA	2:H:424:ALA:HB3	2.03	0.40
2:H:441:LYS:O	2:H:445:LYS:HG3	2.22	0.40
2:H:298:LYS:HA	2:H:448:VAL:CG2	2.52	0.40
2:H:156:LEU:HD23	2:H:500:HIS:HB2	2.04	0.40
2:H:816:ASP:HB3	2:H:1048:VAL:CG2	2.52	0.40
2:I:225:THR:HA	2:I:226:PRO:HD3	1.98	0.40
2:I:601:THR:O	2:I:601:THR:CG2	2.68	0.40
2:I:612:ASN:C	2:I:614:GLY:H	2.25	0.40

All (54) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1784:ASP:CA	2:G:1087:HIS:CE1[7_655]	0.16	2.04
1:A:1784:ASP:CG	2:I:1087:HIS:CE1[7_545]	0.52	1.68
1:C:1784:ASP:C	2:G:1087:HIS:NE2[7_655]	0.54	1.66
1:C:1784:ASP:CB	2:G:1087:HIS:ND1[7_655]	0.56	1.64
1:A:1784:ASP:OD2	2:I:1087:HIS:ND1[7_545]	0.58	1.62
1:B:1480:GLU:OE2	2:H:290:GLU:CB[6_555]	0.74	1.46
1:C:1784:ASP:CB	2:G:1087:HIS:CG[7_655]	0.83	1.37
1:A:1784:ASP:CG	2:I:1087:HIS:NE2[7_545]	0.91	1.29
1:A:1784:ASP:CB	2:I:1087:HIS:NE2[7_545]	0.97	1.23
1:A:1784:ASP:OD2	2:I:1087:HIS:CE1[7_545]	1.05	1.15
1:C:1784:ASP:CA	2:G:1087:HIS:ND1[7_655]	1.19	1.01
1:A:1784:ASP:OD2	2:I:1087:HIS:CG[7_545]	1.20	1.00
1:C:1784:ASP:O	2:G:1087:HIS:NE2[7_655]	1.22	0.98
1:B:1480:GLU:CD	2:H:290:GLU:CB[6_555]	1.29	0.91
2:G:77:VAL:CB	2:I:1929:LYS:CD[6_455]	1.31	0.89
1:C:1784:ASP:C	2:G:1087:HIS:CE1[7_655]	1.38	0.82
1:A:1784:ASP:OD1	2:I:1087:HIS:CE1[7_545]	1.38	0.82
1:C:1784:ASP:CA	2:G:1087:HIS:NE2[7_655]	1.42	0.78
1:B:1480:GLU:OE2	2:H:290:GLU:CG[6_555]	1.43	0.77
2:G:77:VAL:CG2	2:I:1929:LYS:NZ[6_455]	1.46	0.74
1:C:1784:ASP:N	2:G:1087:HIS:CE1[7_655]	1.46	0.74
1:C:1784:ASP:CG	2:G:1087:HIS:ND1[7_655]	1.47	0.73
2:G:77:VAL:CG2	2:I:1929:LYS:CE[6_455]	1.51	0.69
1:A:1784:ASP:OD2	2:I:1087:HIS:NE2[7_545]	1.60	0.60
1:A:1784:ASP:CG	2:I:1087:HIS:ND1[7_545]	1.64	0.56
2:G:79:GLN:OE1	2:I:1930:SER:O[6_455]	1.64	0.56
1:C:1784:ASP:CB	2:G:1087:HIS:CE1[7_655]	1.64	0.56
1:A:1784:ASP:OD2	2:I:1087:HIS:CD2[7_545]	1.68	0.52
1:C:1785:THR:N	2:G:1087:HIS:NE2[7_655]	1.70	0.50
2:G:77:VAL:CB	2:I:1929:LYS:CE[6_455]	1.71	0.49
1:C:1784:ASP:CB	2:G:1087:HIS:CD2[7_655]	1.81	0.39
1:B:1480:GLU:OE1	2:H:290:GLU:CB[6_555]	1.83	0.37
1:A:1784:ASP:CB	2:I:1087:HIS:CE1[7_545]	1.84	0.36
1:C:1784:ASP:C	2:G:1087:HIS:CD2[7_655]	1.86	0.34
2:G:77:VAL:O	2:I:1929:LYS:CB[6_455]	1.92	0.28
2:G:77:VAL:O	2:I:1929:LYS:CA[6_455]	1.93	0.27
1:A:1784:ASP:CG	2:I:1087:HIS:CD2[7_545]	1.94	0.26
2:G:77:VAL:CG1	2:I:1929:LYS:CD[6_455]	1.95	0.25
1:C:1784:ASP:CG	2:G:1087:HIS:CG[7_655]	1.97	0.23
2:G:77:VAL:O	2:I:1929:LYS:CG[6_455]	1.97	0.23
1:A:1784:ASP:OD1	2:I:1087:HIS:NE2[7_545]	1.98	0.22
1:C:1784:ASP:N	2:G:1087:HIS:ND1[7_655]	1.98	0.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1784:ASP:CB	2:G:1087:HIS:CB[7_655]	2.03	0.17
1:C:1784:ASP:OD2	2:G:1087:HIS:CB[7_655]	2.03	0.17
2:H:6:THR:CG2	2:I:1935:GLU:OE2[6_455]	2.05	0.15
2:H:6:THR:CG2	2:I:1935:GLU:CD[6_455]	2.06	0.14
1:C:1784:ASP:OD1	2:G:1087:HIS:ND1[7_655]	2.11	0.09
1:C:1784:ASP:CB	2:G:1087:HIS:NE2[7_655]	2.11	0.09
1:C:1784:ASP:O	2:G:1087:HIS:CD2[7_655]	2.12	0.08
1:C:1784:ASP:CA	2:G:1087:HIS:CG[7_655]	2.13	0.07
2:G:77:VAL:CB	2:I:1929:LYS:CG[6_455]	2.15	0.05
1:A:1784:ASP:CB	2:I:1087:HIS:CD2[7_545]	2.15	0.05
1:A:852:ARG:NH2	1:B:837:GLY:O[7_645]	2.19	0.01
1:B:1480:GLU:OE1	2:H:290:GLU:CA[6_555]	2.19	0.01

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	1736/1887 (92%)	1614 (93%)	100 (6%)	22 (1%)	12	48
1	B	1736/1887 (92%)	1619 (93%)	100 (6%)	17 (1%)	15	53
1	C	1736/1887 (92%)	1618 (93%)	96 (6%)	22 (1%)	12	48
2	G	2029/2051 (99%)	1825 (90%)	173 (8%)	31 (2%)	10	45
2	H	2029/2051 (99%)	1826 (90%)	173 (8%)	30 (2%)	10	45
2	I	2029/2051 (99%)	1829 (90%)	174 (9%)	26 (1%)	12	48
All	All	11295/11814 (96%)	10331 (92%)	816 (7%)	148 (1%)	12	48

All (148) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	488	PRO
1	A	504	ASP
1	A	538	GLU

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Mol	Chain	Res	Type
1	A	605	LEU
1	A	834	GLY
1	A	935	GLU
1	A	1763	LYS
1	A	1830	GLY
1	A	1843	ASN
1	B	504	ASP
1	B	538	GLU
1	B	605	LEU
1	B	834	GLY
1	B	1763	LYS
1	B	1830	GLY
1	B	1843	ASN
1	C	504	ASP
1	C	538	GLU
1	C	605	LEU
1	C	834	GLY
1	C	935	GLU
1	C	1763	LYS
1	C	1830	GLY
1	C	1843	ASN
2	G	521	ASP
2	G	561	TRP
2	G	1177	SER
2	G	1955	PRO
2	H	521	ASP
2	H	561	TRP
2	H	1418	ASP
2	H	1955	PRO
2	I	521	ASP
2	I	1955	PRO
1	A	1252	GLY
1	A	1585	LYS
1	A	1608	ASN
1	B	179	LYS
1	B	1252	GLY
1	B	1585	LYS
1	B	1608	ASN
1	C	1252	GLY
1	C	1585	LYS
1	C	1608	ASN
2	G	203	LEU

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Mol	Chain	Res	Type
2	G	562	LEU
2	G	1044	VAL
2	G	1418	ASP
2	G	1419	PHE
2	G	1722	GLY
2	H	203	LEU
2	H	1044	VAL
2	H	1177	SER
2	H	1420	GLU
2	H	1529	GLN
2	H	1722	GLY
2	I	203	LEU
2	I	1044	VAL
2	I	1177	SER
2	I	1418	ASP
2	I	1722	GLY
1	A	179	LYS
1	A	1749	THR
1	B	1749	THR
1	C	1749	THR
2	G	112	ASN
2	G	139	LYS
2	G	567	PRO
2	G	1101	GLU
2	G	2034	GLY
2	H	112	ASN
2	H	562	LEU
2	H	1101	GLU
2	I	374	ALA
2	I	1092	ASP
2	I	1101	GLU
2	I	2034	GLY
2	G	25	ALA
2	G	26	SER
2	G	374	ALA
2	G	742	SER
2	G	769	SER
2	G	1092	ASP
2	G	1510	ALA
2	H	26	SER
2	H	374	ALA
2	H	567	PRO

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Mol	Chain	Res	Type
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
2	I	1419	PHE
1	A	485	ASP
1	A	1130	ASP
1	A	1477	ILE
1	A	1536	LEU
1	B	970	GLY
1	B	1477	ILE
1	C	179	LYS
1	C	934	PRO
1	C	1477	ILE
2	H	769	SER
2	H	1092	ASP
2	H	1257	ASP
2	I	25	ALA
2	I	136	PRO
2	I	769	SER
2	I	823	ALA
2	I	1510	ALA
1	A	178	GLY
1	A	970	GLY
1	C	930	LEU
1	C	970	GLY
1	C	1536	LEU
2	G	574	SER
2	H	1419	PHE
2	I	139	LYS
2	I	574	SER
1	A	1543	GLY
1	B	1543	GLY
1	C	1543	GLY
2	G	136	PRO
2	G	335	PRO
2	H	136	PRO
2	H	335	PRO
2	H	1661	VAL

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Mol	Chain	Res	Type
1	B	178	GLY
2	G	1340	PRO
2	G	1956	ARG
2	H	772	GLY
1	A	934	PRO
1	C	178	GLY
1	C	1240	VAL
2	G	772	GLY
2	G	1176	PRO
2	G	1840	VAL
2	I	772	GLY
1	B	726	GLY
1	C	726	GLY
2	G	470	VAL
2	H	470	VAL
2	H	2012	PRO
2	I	335	PRO
2	I	1956	ARG
2	I	1340	PRO

### 5.3.2 Protein sidechains ⓘ

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	1460/1566 (93%)	1308 (90%)	152 (10%)	7	28
1	B	1460/1566 (93%)	1312 (90%)	148 (10%)	7	29
1	C	1460/1566 (93%)	1310 (90%)	150 (10%)	7	28
2	G	1772/1789 (99%)	1563 (88%)	209 (12%)	5	24
2	H	1772/1789 (99%)	1560 (88%)	212 (12%)	5	23
2	I	1772/1789 (99%)	1561 (88%)	211 (12%)	5	24
All	All	9696/10065 (96%)	8614 (89%)	1082 (11%)	6	25

All (1082) 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	487	ASP
1	A	490	TYR
1	A	493	VAL
1	A	506	ASN
1	A	509	ILE
1	A	527	GLN
1	A	529	MET
1	A	536	THR

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Mol	Chain	Res	Type
1	A	599	MET
1	A	600	ASP
1	A	603	ASP
1	A	606	ASP
1	A	607	LYS
1	A	615	SER
1	A	621	THR
1	A	622	ILE
1	A	625	THR
1	A	629	THR
1	A	635	ILE
1	A	644	THR
1	A	648	ASP
1	A	654	GLN
1	A	711	SER
1	A	719	GLN
1	A	728	LYS
1	A	731	THR
1	A	732	LEU
1	A	748	LEU
1	A	749	ILE
1	A	776	GLU
1	A	782	GLU
1	A	793	ARG
1	A	797	THR
1	A	806	VAL
1	A	817	THR
1	A	825	PRO
1	A	852	ARG
1	A	860	ASN
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	931	GLN
1	A	933	VAL
1	A	935	GLU
1	A	947	LEU
1	A	949	GLU
1	A	953	VAL

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Mol	Chain	Res	Type
1	A	964	GLU
1	A	980	VAL
1	A	1016	GLU
1	A	1020	VAL
1	A	1022	THR
1	A	1047	LEU
1	A	1056	ILE
1	A	1070	ARG
1	A	1087	LYS
1	A	1095	THR
1	A	1101	SER
1	A	1125	VAL
1	A	1127	VAL
1	A	1131	LEU
1	A	1172	THR
1	A	1173	LEU
1	A	1179	LEU
1	A	1184	LEU
1	A	1196	LYS
1	A	1197	THR
1	A	1208	VAL
1	A	1218	SER
1	A	1226	SER
1	A	1229	THR
1	A	1255	SER
1	A	1274	ILE
1	A	1283	MET
1	A	1307	THR
1	A	1327	CYS
1	A	1338	GLU
1	A	1367	ARG
1	A	1372	THR
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

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Mol	Chain	Res	Type
1	A	1515	ARG
1	A	1522	LEU
1	A	1523	ARG
1	A	1532	THR
1	A	1533	ILE
1	A	1549	ASN
1	A	1556	THR
1	A	1566	ARG
1	A	1580	LEU
1	A	1585	LYS
1	A	1612	ASP
1	A	1625	LEU
1	A	1665	ILE
1	A	1666	THR
1	A	1692	MET
1	A	1693	ILE
1	A	1707	THR
1	A	1709	GLU
1	A	1721	ARG
1	A	1775	LEU
1	A	1782	GLU
1	A	1788	GLU
1	A	1794	GLN
1	A	1841	ARG
1	A	1873	HIS
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

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Mol	Chain	Res	Type
1	B	375	LEU
1	B	385	PHE
1	B	390	VAL
1	B	392	THR
1	B	400	ARG
1	B	401	THR
1	B	412	SER
1	B	413	LEU
1	B	415	SER
1	B	416	LEU
1	B	428	VAL
1	B	432	VAL
1	B	435	GLU
1	B	447	LEU
1	B	457	ASN
1	B	460	GLU
1	B	461	THR
1	B	484	LEU
1	B	489	VAL
1	B	493	VAL
1	B	499	PRO
1	B	506	ASN
1	B	509	ILE
1	B	510	THR
1	B	527	GLN
1	B	529	MET
1	B	536	THR
1	B	599	MET
1	B	600	ASP
1	B	603	ASP
1	B	606	ASP
1	B	607	LYS
1	B	615	SER
1	B	621	THR
1	B	622	ILE
1	B	625	THR
1	B	629	THR
1	B	635	ILE
1	B	644	THR
1	B	648	ASP
1	B	711	SER
1	B	719	GLN

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Mol	Chain	Res	Type
1	B	728	LYS
1	B	731	THR
1	B	732	LEU
1	B	748	LEU
1	B	749	ILE
1	B	776	GLU
1	B	782	GLU
1	B	793	ARG
1	B	797	THR
1	B	806	VAL
1	B	852	ARG
1	B	860	ASN
1	B	864	VAL
1	B	873	ARG
1	B	881	ASN
1	B	891	MET
1	B	913	VAL
1	B	930	LEU
1	B	933	VAL
1	B	947	LEU
1	B	949	GLU
1	B	953	VAL
1	B	964	GLU
1	B	980	VAL
1	B	1016	GLU
1	B	1020	VAL
1	B	1047	LEU
1	B	1056	ILE
1	B	1070	ARG
1	B	1078	SER
1	B	1080	THR
1	B	1087	LYS
1	B	1095	THR
1	B	1101	SER
1	B	1125	VAL
1	B	1127	VAL
1	B	1131	LEU
1	B	1172	THR
1	B	1173	LEU
1	B	1179	LEU
1	B	1184	LEU
1	B	1196	LYS

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Mol	Chain	Res	Type
1	B	1197	THR
1	B	1208	VAL
1	B	1218	SER
1	B	1229	THR
1	B	1255	SER
1	B	1274	ILE
1	B	1283	MET
1	B	1307	THR
1	B	1327	CYS
1	B	1338	GLU
1	B	1367	ARG
1	B	1372	THR
1	B	1384	ILE
1	B	1385	GLN
1	B	1392	LEU
1	B	1414	ILE
1	B	1426	LEU
1	B	1442	ASN
1	B	1465	ASN
1	B	1479	SER
1	B	1502	ARG
1	B	1515	ARG
1	B	1522	LEU
1	B	1523	ARG
1	B	1532	THR
1	B	1533	ILE
1	B	1549	ASN
1	B	1556	THR
1	B	1566	ARG
1	B	1577	GLN
1	B	1580	LEU
1	B	1585	LYS
1	B	1612	ASP
1	B	1625	LEU
1	B	1665	ILE
1	B	1666	THR
1	B	1692	MET
1	B	1693	ILE
1	B	1707	THR
1	B	1709	GLU
1	B	1721	ARG
1	B	1775	LEU

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Mol	Chain	Res	Type
1	B	1782	GLU
1	B	1788	GLU
1	B	1794	GLN
1	B	1841	ARG
1	B	1873	HIS
1	C	14	LEU
1	C	15	THR
1	C	21	GLN
1	C	22	PHE
1	C	145	VAL
1	C	149	LEU
1	C	158	LYS
1	C	165	SER
1	C	171	THR
1	C	202	GLU
1	C	217	PHE
1	C	242	THR
1	C	253	ARG
1	C	328	LEU
1	C	331	ILE
1	C	332	THR
1	C	375	LEU
1	C	378	LEU
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

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Mol	Chain	Res	Type
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
1	C	621	THR
1	C	622	ILE
1	C	625	THR
1	C	629	THR
1	C	635	ILE
1	C	644	THR
1	C	648	ASP
1	C	711	SER
1	C	719	GLN
1	C	728	LYS
1	C	731	THR
1	C	732	LEU
1	C	748	LEU
1	C	749	ILE
1	C	776	GLU
1	C	782	GLU
1	C	797	THR
1	C	806	VAL
1	C	824	LEU
1	C	852	ARG
1	C	860	ASN
1	C	864	VAL
1	C	873	ARG
1	C	881	ASN
1	C	891	MET
1	C	913	VAL
1	C	930	LEU
1	C	931	GLN
1	C	933	VAL
1	C	935	GLU
1	C	947	LEU
1	C	949	GLU

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Mol	Chain	Res	Type
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
1	C	1127	VAL
1	C	1131	LEU
1	C	1172	THR
1	C	1173	LEU
1	C	1179	LEU
1	C	1184	LEU
1	C	1196	LYS
1	C	1197	THR
1	C	1208	VAL
1	C	1218	SER
1	C	1229	THR
1	C	1255	SER
1	C	1274	ILE
1	C	1283	MET
1	C	1307	THR
1	C	1327	CYS
1	C	1338	GLU
1	C	1367	ARG
1	C	1372	THR
1	C	1384	ILE
1	C	1385	GLN
1	C	1392	LEU
1	C	1414	ILE
1	C	1426	LEU
1	C	1430	ARG
1	C	1432	HIS
1	C	1442	ASN
1	C	1455	ARG
1	C	1465	ASN

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Mol	Chain	Res	Type
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
1	C	1585	LYS
1	C	1612	ASP
1	C	1625	LEU
1	C	1665	ILE
1	C	1666	THR
1	C	1692	MET
1	C	1693	ILE
1	C	1707	THR
1	C	1709	GLU
1	C	1721	ARG
1	C	1775	LEU
1	C	1782	GLU
1	C	1788	GLU
1	C	1794	GLN
1	C	1841	ARG
1	C	1873	HIS
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

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Mol	Chain	Res	Type
2	G	117	VAL
2	G	122	LEU
2	G	149	VAL
2	G	153	ASN
2	G	155	GLN
2	G	159	ILE
2	G	173	LEU
2	G	175	ASP
2	G	176	LEU
2	G	178	GLN
2	G	182	VAL
2	G	210	THR
2	G	227	ASP
2	G	236	ILE
2	G	240	LEU
2	G	246	LEU
2	G	281	VAL
2	G	286	THR
2	G	295	SER
2	G	297	ARG
2	G	300	ILE
2	G	303	LEU
2	G	319	LEU
2	G	339	LEU
2	G	340	SER
2	G	342	SER
2	G	344	LEU
2	G	353	VAL
2	G	371	VAL
2	G	376	ASN
2	G	389	LEU
2	G	392	THR
2	G	402	LEU
2	G	418	ASN
2	G	425	SER
2	G	431	LEU
2	G	448	VAL
2	G	455	ILE
2	G	462	THR
2	G	463	PHE
2	G	471	LEU
2	G	476	SER

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Mol	Chain	Res	Type
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	566	HIS
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
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

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Mol	Chain	Res	Type
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
2	G	1048	VAL
2	G	1066	ILE
2	G	1070	ILE
2	G	1082	ILE
2	G	1109	VAL
2	G	1123	ASP
2	G	1124	SER
2	G	1145	SER
2	G	1148	ASN
2	G	1160	THR
2	G	1171	ARG
2	G	1189	THR
2	G	1197	LEU
2	G	1211	LEU
2	G	1219	ILE
2	G	1227	ARG
2	G	1260	GLN
2	G	1265	MET
2	G	1284	VAL
2	G	1314	ARG
2	G	1318	THR
2	G	1328	VAL
2	G	1335	ILE
2	G	1348	LEU

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Mol	Chain	Res	Type
2	G	1359	MET
2	G	1360	ILE
2	G	1378	ILE
2	G	1397	SER
2	G	1407	THR
2	G	1408	SER
2	G	1417	THR
2	G	1418	ASP
2	G	1420	GLU
2	G	1424	GLN
2	G	1426	THR
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
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

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Mol	Chain	Res	Type
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	1844	ARG
2	G	1847	LEU
2	G	1857	ILE
2	G	1862	VAL
2	G	1886	VAL
2	G	1914	LEU
2	G	1936	VAL
2	G	1937	GLU
2	G	1941	PHE
2	G	1982	MET
2	G	2003	VAL
2	G	2042	ILE
2	G	2044	ASN
2	G	2047	LYS
2	G	2048	TYR
2	G	2050	GLN
2	H	6	THR
2	H	7	ARG
2	H	45	THR
2	H	46	GLU
2	H	48	PHE
2	H	56	THR
2	H	65	LEU
2	H	84	LEU
2	H	86	LEU
2	H	93	ASN
2	H	99	ASN
2	H	101	ILE
2	H	109	LEU
2	H	117	VAL

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Mol	Chain	Res	Type
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
2	H	297	ARG
2	H	300	ILE
2	H	317	THR
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

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Mol	Chain	Res	Type
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	566	HIS
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
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

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Mol	Chain	Res	Type
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
2	H	1066	ILE
2	H	1070	ILE
2	H	1082	ILE
2	H	1109	VAL
2	H	1123	ASP
2	H	1145	SER
2	H	1148	ASN
2	H	1160	THR
2	H	1171	ARG
2	H	1189	THR
2	H	1197	LEU
2	H	1211	LEU
2	H	1219	ILE
2	H	1227	ARG
2	H	1260	GLN
2	H	1265	MET
2	H	1284	VAL
2	H	1314	ARG
2	H	1318	THR
2	H	1328	VAL
2	H	1335	ILE
2	H	1348	LEU

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Mol	Chain	Res	Type
2	H	1359	MET
2	H	1360	ILE
2	H	1378	ILE
2	H	1397	SER
2	H	1407	THR
2	H	1408	SER
2	H	1420	GLU
2	H	1422	THR
2	H	1426	THR
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
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	1530	LYS
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	1657	ILE
2	H	1661	VAL

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Mol	Chain	Res	Type
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
2	H	1982	MET
2	H	2003	VAL
2	H	2038	ILE
2	H	2042	ILE
2	H	2044	ASN
2	H	2047	LYS
2	H	2048	TYR
2	H	2050	GLN
2	I	6	THR
2	I	7	ARG
2	I	45	THR
2	I	46	GLU
2	I	48	PHE
2	I	56	THR
2	I	65	LEU
2	I	84	LEU
2	I	86	LEU
2	I	93	ASN
2	I	99	ASN
2	I	101	ILE

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Mol	Chain	Res	Type
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
2	I	319	LEU
2	I	339	LEU
2	I	340	SER
2	I	342	SER
2	I	344	LEU
2	I	353	VAL
2	I	371	VAL
2	I	376	ASN
2	I	389	LEU
2	I	392	THR
2	I	402	LEU
2	I	418	ASN
2	I	425	SER
2	I	431	LEU
2	I	444	VAL
2	I	448	VAL
2	I	455	ILE
2	I	462	THR
2	I	463	PHE

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
2	I	810	GLU
2	I	825	THR
2	I	832	TRP
2	I	835	THR
2	I	844	VAL
2	I	846	VAL
2	I	852	GLU
2	I	855	HIS
2	I	857	ILE
2	I	865	TRP
2	I	869	ASP
2	I	880	LEU
2	I	881	VAL
2	I	892	ILE
2	I	907	VAL
2	I	929	LEU
2	I	945	THR
2	I	952	ARG
2	I	953	ARG
2	I	964	LEU
2	I	971	SER
2	I	993	GLN
2	I	1015	VAL
2	I	1021	LEU
2	I	1024	ARG
2	I	1048	VAL
2	I	1066	ILE
2	I	1070	ILE
2	I	1082	ILE
2	I	1109	VAL
2	I	1123	ASP
2	I	1124	SER
2	I	1145	SER
2	I	1148	ASN
2	I	1160	THR
2	I	1171	ARG
2	I	1189	THR
2	I	1197	LEU
2	I	1211	LEU
2	I	1219	ILE
2	I	1227	ARG
2	I	1260	GLN

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Mol	Chain	Res	Type
2	I	1265	MET
2	I	1284	VAL
2	I	1314	ARG
2	I	1318	THR
2	I	1328	VAL
2	I	1335	ILE
2	I	1348	LEU
2	I	1359	MET
2	I	1360	ILE
2	I	1378	ILE
2	I	1397	SER
2	I	1407	THR
2	I	1408	SER
2	I	1420	GLU
2	I	1421	ASN
2	I	1423	PHE
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
2	I	1470	THR
2	I	1472	VAL
2	I	1473	THR
2	I	1501	ILE
2	I	1511	SER
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

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (294) 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

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Mol	Chain	Res	Type
1	A	214	GLN
1	A	271	ASN
1	A	335	HIS
1	A	341	GLN
1	A	344	GLN
1	A	374	GLN
1	A	411	GLN
1	A	427	ASN
1	A	438	ASN
1	A	506	ASN
1	A	527	GLN
1	A	618	ASN
1	A	694	GLN
1	A	738	ASN
1	A	758	ASN
1	A	792	HIS
1	A	860	ASN
1	A	898	GLN
1	A	983	GLN
1	A	987	ASN
1	A	989	GLN
1	A	1000	GLN
1	A	1003	GLN
1	A	1063	HIS
1	A	1064	ASN
1	A	1066	ASN
1	A	1146	HIS
1	A	1239	HIS
1	A	1385	GLN
1	A	1432	HIS
1	A	1433	HIS
1	A	1442	ASN
1	A	1458	GLN
1	A	1482	GLN
1	A	1494	HIS
1	A	1495	ASN
1	A	1505	GLN
1	A	1510	ASN
1	A	1542	HIS
1	A	1549	ASN
1	A	1563	HIS
1	A	1577	GLN

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Mol	Chain	Res	Type
1	A	1610	ASN
1	A	1652	GLN
1	A	1690	ASN
1	A	1852	HIS
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
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

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Mol	Chain	Res	Type
1	B	1458	GLN
1	B	1482	GLN
1	B	1494	HIS
1	B	1495	ASN
1	B	1505	GLN
1	B	1510	ASN
1	B	1542	HIS
1	B	1549	ASN
1	B	1563	HIS
1	B	1577	GLN
1	B	1610	ASN
1	B	1652	GLN
1	B	1690	ASN
1	B	1794	GLN
1	B	1852	HIS
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	411	GLN
1	C	427	ASN
1	C	438	ASN
1	C	506	ASN
1	C	527	GLN
1	C	618	ASN
1	C	694	GLN
1	C	738	ASN
1	C	758	ASN
1	C	792	HIS
1	C	860	ASN
1	C	898	GLN
1	C	987	ASN
1	C	989	GLN

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Mol	Chain	Res	Type
1	C	1000	GLN
1	C	1003	GLN
1	C	1063	HIS
1	C	1064	ASN
1	C	1066	ASN
1	C	1146	HIS
1	C	1239	HIS
1	C	1385	GLN
1	C	1432	HIS
1	C	1433	HIS
1	C	1442	ASN
1	C	1458	GLN
1	C	1482	GLN
1	C	1495	ASN
1	C	1505	GLN
1	C	1510	ASN
1	C	1542	HIS
1	C	1549	ASN
1	C	1563	HIS
1	C	1577	GLN
1	C	1610	ASN
1	C	1652	GLN
1	C	1690	ASN
1	C	1852	HIS
2	G	34	GLN
2	G	36	GLN
2	G	85	ASN
2	G	102	HIS
2	G	178	GLN
2	G	359	HIS
2	G	376	ASN
2	G	418	ASN
2	G	428	HIS
2	G	440	ASN
2	G	447	ASN
2	G	500	HIS
2	G	517	HIS
2	G	545	GLN
2	G	558	ASN
2	G	572	ASN
2	G	612	ASN
2	G	650	ASN

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Mol	Chain	Res	Type
2	G	718	ASN
2	G	740	HIS
2	G	741	HIS
2	G	747	HIS
2	G	752	GLN
2	G	762	ASN
2	G	855	HIS
2	G	900	GLN
2	G	910	GLN
2	G	1046	GLN
2	G	1148	ASN
2	G	1217	ASN
2	G	1220	GLN
2	G	1260	GLN
2	G	1341	ASN
2	G	1352	HIS
2	G	1355	ASN
2	G	1367	GLN
2	G	1384	GLN
2	G	1595	ASN
2	G	1659	GLN
2	G	1669	GLN
2	G	1672	GLN
2	G	1697	HIS
2	G	1890	ASN
2	G	1896	GLN
2	G	1977	HIS
2	G	2013	ASN
2	G	2020	GLN
2	H	34	GLN
2	H	85	ASN
2	H	102	HIS
2	H	178	GLN
2	H	359	HIS
2	H	376	ASN
2	H	418	ASN
2	H	428	HIS
2	H	440	ASN
2	H	447	ASN
2	H	500	HIS
2	H	517	HIS
2	H	545	GLN

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Mol	Chain	Res	Type
2	H	558	ASN
2	H	572	ASN
2	H	612	ASN
2	H	650	ASN
2	H	718	ASN
2	H	740	HIS
2	H	741	HIS
2	H	747	HIS
2	H	752	GLN
2	H	762	ASN
2	H	900	GLN
2	H	910	GLN
2	H	1039	HIS
2	H	1046	GLN
2	H	1148	ASN
2	H	1217	ASN
2	H	1220	GLN
2	H	1260	GLN
2	H	1341	ASN
2	H	1352	HIS
2	H	1355	ASN
2	H	1367	GLN
2	H	1669	GLN
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	36	GLN
2	I	85	ASN
2	I	102	HIS
2	I	178	GLN
2	I	359	HIS
2	I	376	ASN
2	I	418	ASN
2	I	428	HIS
2	I	440	ASN
2	I	447	ASN
2	I	500	HIS

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Mol	Chain	Res	Type
2	I	517	HIS
2	I	545	GLN
2	I	558	ASN
2	I	572	ASN
2	I	612	ASN
2	I	718	ASN
2	I	740	HIS
2	I	741	HIS
2	I	747	HIS
2	I	752	GLN
2	I	762	ASN
2	I	855	HIS
2	I	900	GLN
2	I	910	GLN
2	I	1046	GLN
2	I	1055	HIS
2	I	1148	ASN
2	I	1217	ASN
2	I	1220	GLN
2	I	1260	GLN
2	I	1341	ASN
2	I	1352	HIS
2	I	1355	ASN
2	I	1367	GLN
2	I	1421	ASN
2	I	1595	ASN
2	I	1669	GLN
2	I	1672	GLN
2	I	1697	HIS
2	I	1868	GLN
2	I	1890	ASN
2	I	1896	GLN
2	I	1977	HIS
2	I	2013	ASN
2	I	2020	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

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

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

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

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	3051	FMN	C4A-C10	16.06	1.54	1.38
4	H	3051	FMN	C4A-C10	15.15	1.53	1.38
4	I	3051	FMN	C4A-C10	14.86	1.53	1.38
4	G	3051	FMN	C4A-N5	12.70	1.51	1.33
4	I	3051	FMN	C4A-N5	12.26	1.50	1.33
4	H	3051	FMN	C4A-N5	12.20	1.50	1.33
3	C	2748	CER	O1-C4	11.69	1.41	1.21
3	A	2748	CER	O1-C4	11.67	1.41	1.21
3	B	2748	CER	O1-C4	11.63	1.41	1.21
4	G	3051	FMN	C10-N1	11.49	1.48	1.33
4	H	3051	FMN	C10-N1	11.35	1.47	1.33
4	I	3051	FMN	C6-C5A	11.06	1.59	1.41
4	I	3051	FMN	C10-N1	10.87	1.47	1.33
4	G	3051	FMN	C6-C5A	10.78	1.58	1.41
4	H	3051	FMN	C6-C5A	10.58	1.58	1.41
4	H	3051	FMN	C4-N3	10.22	1.50	1.33
4	I	3051	FMN	C5A-N5	9.86	1.51	1.35
4	G	3051	FMN	C4-N3	9.85	1.50	1.33
4	I	3051	FMN	C4-N3	9.83	1.50	1.33
4	G	3051	FMN	C5A-N5	9.70	1.51	1.35
4	H	3051	FMN	C5A-N5	9.56	1.51	1.35
4	G	3051	FMN	C9-C9A	9.45	1.59	1.40
4	H	3051	FMN	C9-C9A	9.33	1.59	1.40
4	I	3051	FMN	C9-C9A	9.29	1.59	1.40
4	G	3051	FMN	C9A-N10	8.68	1.50	1.38
4	H	3051	FMN	C9A-N10	8.32	1.49	1.38
4	I	3051	FMN	C9A-N10	8.27	1.49	1.38
4	G	3051	FMN	C6-C7	7.90	1.57	1.37
4	I	3051	FMN	C6-C7	7.71	1.57	1.37
4	G	3051	FMN	C2-N1	7.69	1.53	1.38
4	H	3051	FMN	C2-N3	7.68	1.53	1.38
4	H	3051	FMN	C6-C7	7.55	1.57	1.37
4	H	3051	FMN	C2-N1	7.51	1.53	1.38
4	I	3051	FMN	C2-N1	7.45	1.52	1.38
4	I	3051	FMN	C9-C8	7.33	1.56	1.37
4	I	3051	FMN	C8-C7	7.29	1.59	1.40
4	G	3051	FMN	C2-N3	7.27	1.52	1.38
4	G	3051	FMN	O4-C4	7.17	1.42	1.24
4	I	3051	FMN	C2-N3	7.10	1.52	1.38
4	G	3051	FMN	C9-C8	7.10	1.55	1.37
4	G	3051	FMN	C4-C4A	7.09	1.53	1.41
4	H	3051	FMN	O4-C4	7.08	1.42	1.24

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

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2748	CER	O1-C4-C5	-7.72	107.97	121.70
3	A	2748	CER	O1-C4-C5	-7.67	108.06	121.70
4	H	3051	FMN	C4-N3-C2	7.46	121.44	115.14
3	B	2748	CER	O1-C4-C5	-7.34	108.64	121.70
4	G	3051	FMN	C4-N3-C2	7.33	121.33	115.14
4	I	3051	FMN	C4-N3-C2	7.00	121.05	115.14
4	G	3051	FMN	C1'-N10-C9A	4.68	121.97	118.29
4	H	3051	FMN	C1'-N10-C9A	4.30	121.68	118.29
4	H	3051	FMN	C4A-C4-N3	-3.94	118.04	123.43
4	G	3051	FMN	C4A-C4-N3	-3.90	118.10	123.43
4	I	3051	FMN	C1'-N10-C9A	3.89	121.35	118.29
3	A	2748	CER	C5-C4-C3	-3.86	110.87	117.94
3	B	2748	CER	C5-C4-C3	-3.77	111.03	117.94
3	C	2748	CER	C5-C4-C3	-3.76	111.05	117.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	3051	FMN	C4A-C4-N3	-3.67	118.41	123.43
3	A	2748	CER	C6-C5-C4	-3.35	108.47	113.88
3	C	2748	CER	C6-C5-C4	-3.30	108.56	113.88
4	G	3051	FMN	C4A-N5-C5A	3.29	120.06	116.77
4	H	3051	FMN	C4A-N5-C5A	3.17	119.94	116.77
4	G	3051	FMN	C10-C4A-N5	-3.15	119.08	121.26
3	B	2748	CER	C6-C5-C4	-3.05	108.95	113.88
4	H	3051	FMN	C10-C4A-N5	-2.98	119.20	121.26
4	I	3051	FMN	C4A-N5-C5A	2.97	119.74	116.77
4	G	3051	FMN	C5A-C9A-N10	2.97	119.86	117.72
4	I	3051	FMN	C4'-C3'-C2'	-2.76	107.62	113.36
4	H	3051	FMN	C4'-C3'-C2'	-2.72	107.71	113.36
4	G	3051	FMN	C4'-C3'-C2'	-2.70	107.74	113.36
4	I	3051	FMN	C5A-C9A-N10	2.59	119.59	117.72
4	H	3051	FMN	C5A-C9A-N10	2.51	119.53	117.72
4	I	3051	FMN	C10-C4A-N5	-2.41	119.59	121.26
4	H	3051	FMN	O5'-C5'-C4'	-2.03	103.94	109.36

There are no chirality outliers.

All (30) torsion outliers are listed below:

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

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

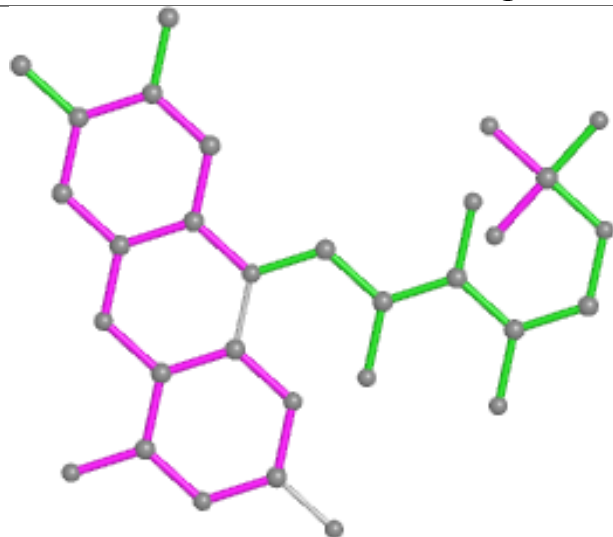
There are no ring outliers.

6 monomers are involved in 32 short contacts:

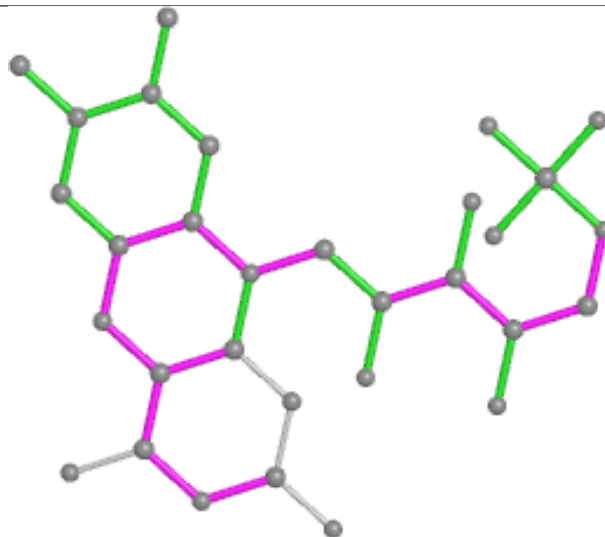
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	3051	FMN	6	0
4	G	3051	FMN	7	0
3	A	2748	CER	3	0
3	C	2748	CER	4	0
4	I	3051	FMN	8	0
3	B	2748	CER	4	0

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

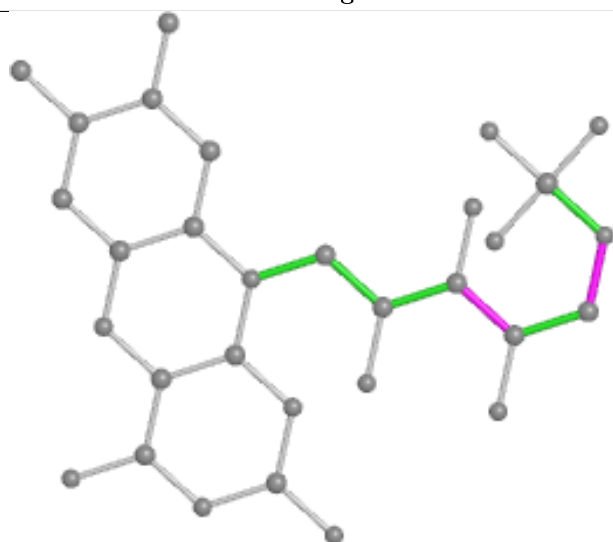
## Ligand FMN H 3051



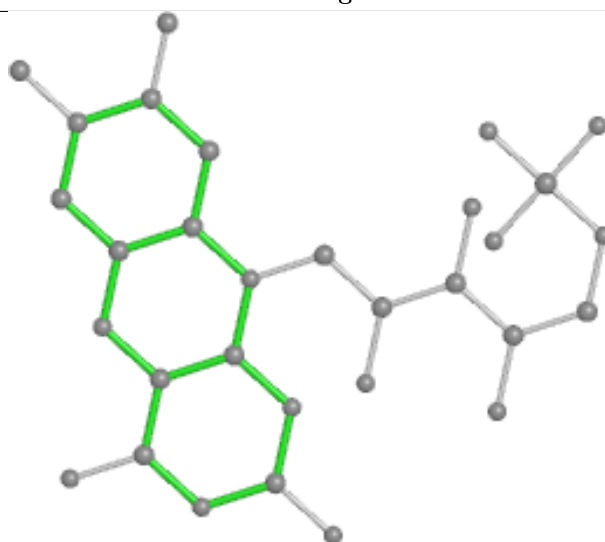
Bond lengths



Bond angles

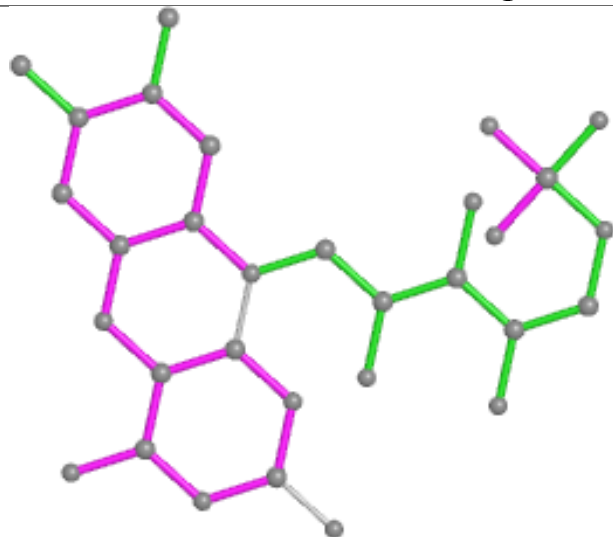


Torsions

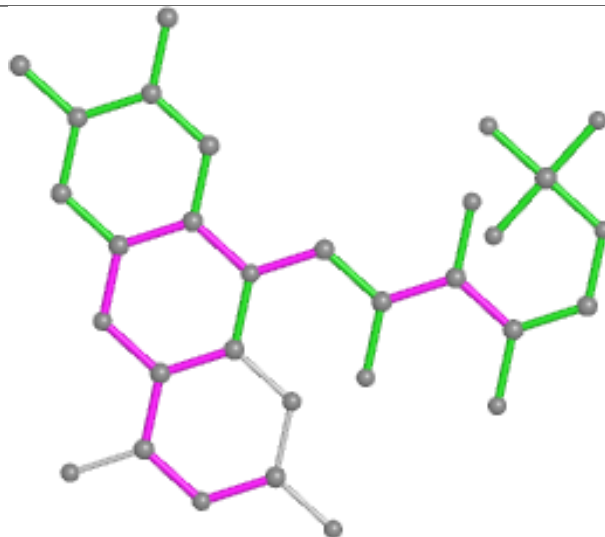


Rings

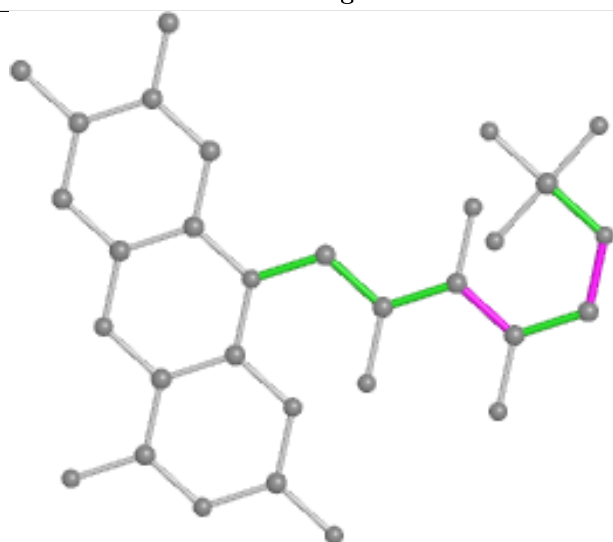
## Ligand FMN G 3051



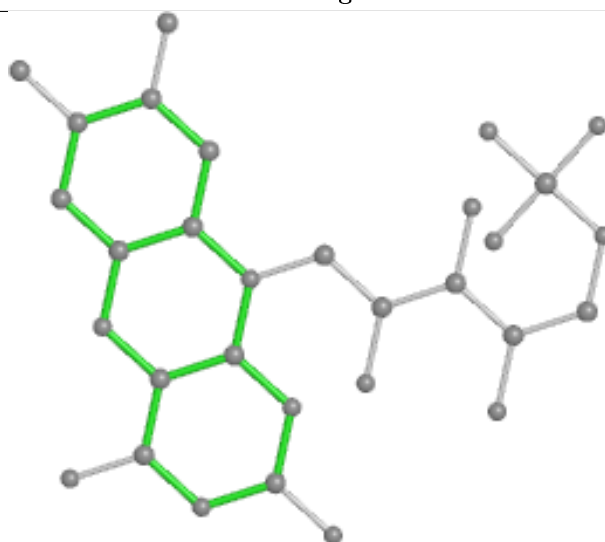
Bond lengths



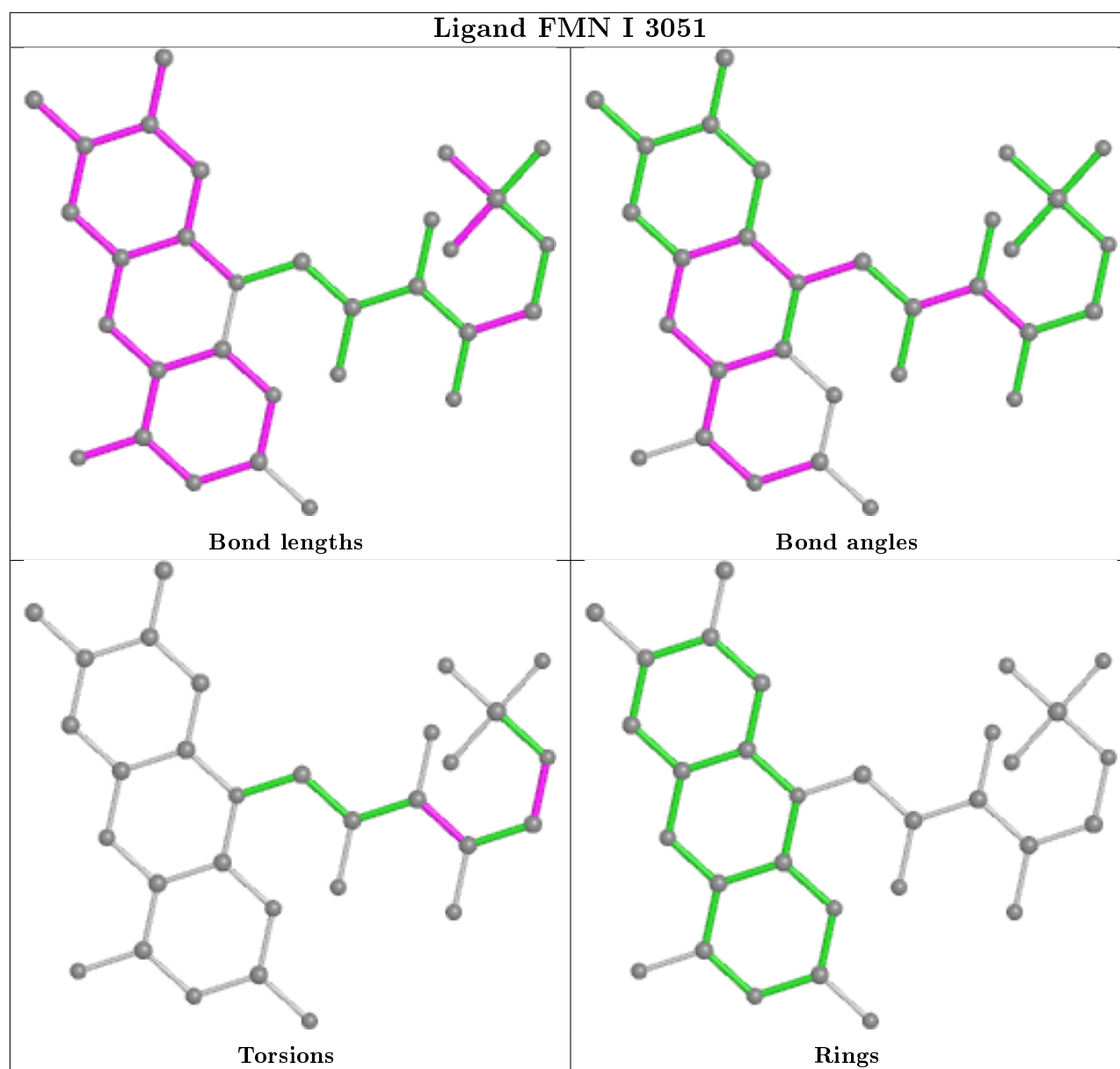
Bond angles



Torsions



Rings



## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1750/1887 (92%)	-0.30	46 (2%) 56 46	95, 134, 347, 457	0
1	B	1750/1887 (92%)	-0.34	32 (1%) 68 59	96, 133, 302, 419	0
1	C	1750/1887 (92%)	-0.26	62 (3%) 44 35	98, 135, 423, 568	0
2	G	2033/2051 (99%)	-0.45	1 (0%) 100 100	131, 169, 218, 267	0
2	H	2033/2051 (99%)	-0.36	10 (0%) 91 85	130, 170, 215, 265	0
2	I	2033/2051 (99%)	-0.43	6 (0%) 94 90	131, 171, 215, 261	0
All	All	11349/11814 (96%)	-0.36	157 (1%) 75 65	95, 162, 239, 568	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1882	ALA	10.4
1	C	1831	GLY	9.1
1	A	1829	GLY	8.0
1	C	1830	GLY	7.7
1	C	1870	SER	7.6
1	C	1850	GLU	7.3
1	C	1884	SER	7.3
1	C	1838	GLU	7.2
1	C	1832	ALA	6.8
1	C	1883	VAL	6.1
1	A	1827	SER	5.7
1	A	1763	LYS	5.3
1	A	1882	ALA	5.2
1	C	1872	SER	5.2
1	C	875	THR	5.1
1	C	1869	VAL	5.0
1	C	1794	GLN	4.8
1	A	1881	VAL	4.8
1	B	875	THR	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	1830	GLY	4.5
1	C	1797	GLU	4.5
1	B	539	SER	4.5
1	C	1766	ASN	4.4
1	C	1833	ALA	4.4
1	C	1857	LYS	4.3
1	A	974	ASP	4.2
1	C	1803	PRO	4.2
1	A	539	SER	4.2
1	C	1874	ASP	4.1
1	B	141	ALA	4.1
1	A	875	THR	4.0
1	C	1804	SER	4.0
1	C	1873	HIS	4.0
1	A	1762	GLU	3.9
1	C	1868	LYS	3.9
1	A	975	ALA	3.9
1	A	1843	ASN	3.8
1	A	1875	ASP	3.8
1	C	1880	ALA	3.8
1	B	1833	ALA	3.7
2	G	1956	ARG	3.7
1	B	599	MET	3.6
2	H	1929	LYS	3.6
1	A	1853	GLY	3.6
1	B	1762	GLU	3.6
1	C	540	GLN	3.5
1	A	208	GLU	3.5
1	B	1830	GLY	3.5
1	A	1880	ALA	3.5
1	C	1837	ILE	3.5
1	C	1783	ASN	3.5
1	B	140	ILE	3.5
1	A	1866	ASP	3.4
1	C	200	LYS	3.4
1	C	1842	VAL	3.4
1	B	1854	ASN	3.4
1	A	1826	LYS	3.4
1	A	1850	GLU	3.4
1	B	1874	ASP	3.4
2	H	1953	VAL	3.3
1	C	1765	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	1793	PRO	3.3
2	I	1928	GLN	3.3
2	H	1671	SER	3.3
1	A	1770	GLY	3.3
1	B	540	GLN	3.2
1	A	1870	SER	3.2
1	B	976	ALA	3.1
1	A	1831	GLY	3.1
2	H	1959	LYS	3.0
1	B	1875	ASP	3.0
1	B	1837	ILE	3.0
1	C	1816	LYS	3.0
1	A	1884	SER	3.0
1	B	1868	LYS	2.9
1	A	1873	HIS	2.9
1	C	1875	ASP	2.9
2	H	1964	PHE	2.9
1	C	1793	PRO	2.9
1	B	1829	GLY	2.9
1	C	141	ALA	2.9
1	C	1843	ASN	2.9
1	A	540	GLN	2.8
1	A	1883	VAL	2.8
1	C	1771	VAL	2.8
1	B	1836	ASP	2.8
1	B	1883	VAL	2.8
1	B	219	GLY	2.8
1	C	204	THR	2.7
1	B	1802	GLN	2.7
1	B	1850	GLU	2.7
1	B	1826	LYS	2.7
2	H	1956	ARG	2.7
1	B	1784	ASP	2.6
1	C	202	GLU	2.6
1	C	1820	PHE	2.6
1	C	1841	ARG	2.6
2	I	401	GLY	2.6
1	B	1804	SER	2.6
1	A	1476	GLU	2.6
1	B	600	ASP	2.6
1	C	1770	GLY	2.6
1	A	1780	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	215	ASP	2.6
1	A	1860	GLU	2.5
1	C	1840	VAL	2.5
1	C	539	SER	2.5
1	C	164	ASP	2.4
1	C	1768	GLY	2.4
1	C	1800	SER	2.4
2	I	43	GLU	2.4
1	A	1748	ASN	2.4
1	A	1868	LYS	2.4
1	C	1829	GLY	2.4
1	C	1812	THR	2.4
1	B	195	GLY	2.4
1	C	1789	ARG	2.3
1	C	203	GLU	2.3
1	C	301	ASP	2.3
1	A	1792	THR	2.3
1	C	223	LYS	2.3
2	H	2033	THR	2.3
1	C	1828	LEU	2.3
2	H	1853	GLY	2.3
2	I	1880	LYS	2.3
1	C	1822	SER	2.3
1	A	1842	VAL	2.2
1	A	1844	LYS	2.2
1	A	1885	THR	2.2
1	C	1845	ASN	2.2
1	A	1874	ASP	2.2
1	B	1801	ALA	2.2
1	A	1838	GLU	2.2
1	A	1872	SER	2.2
1	B	1831	GLY	2.2
1	A	293	LYS	2.2
1	C	1867	VAL	2.2
1	A	1782	GLU	2.2
1	A	1828	LEU	2.2
1	B	1803	PRO	2.2
1	A	1836	ASP	2.2
1	C	1805	VAL	2.2
2	I	75	SER	2.2
1	C	1782	GLU	2.2
1	C	971	ASN	2.1

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	A	973	ALA	2.1
1	A	981	GLU	2.1
1	C	1811	GLY	2.1
2	I	74	PRO	2.1
1	B	1886	LYS	2.1
2	H	1739	GLU	2.1
1	B	1812	THR	2.0
1	C	1772	ASP	2.0
1	B	1810	ALA	2.0
1	A	199	GLU	2.0
2	H	1740	THR	2.0
1	C	1802	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

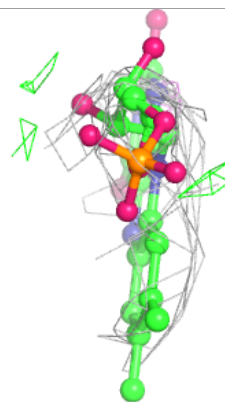
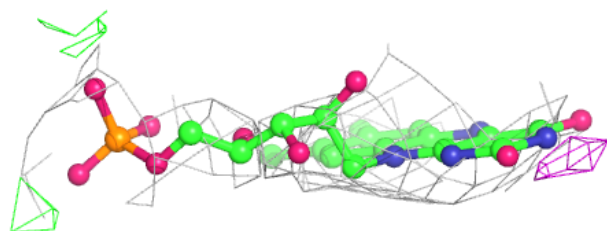
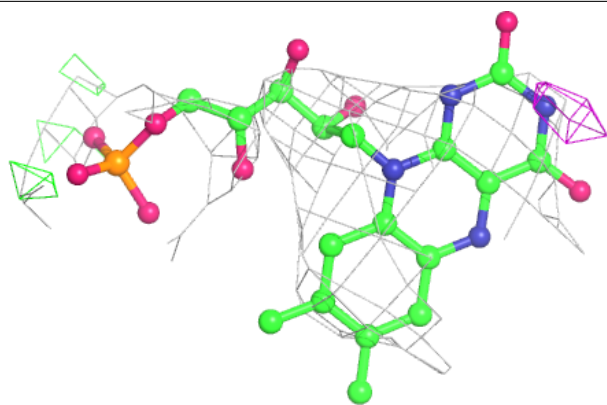
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	FMN	H	3051	31/31	0.80	0.32	131,157,181,186	0
4	FMN	G	3051	31/31	0.82	0.27	135,158,184,203	0
4	FMN	I	3051	31/31	0.82	0.26	129,161,178,201	0
3	CER	A	2748	12/16	0.84	0.30	67,131,240,249	0
3	CER	C	2748	12/16	0.90	0.34	67,131,249,250	0
3	CER	B	2748	12/16	0.91	0.20	67,131,249,250	0

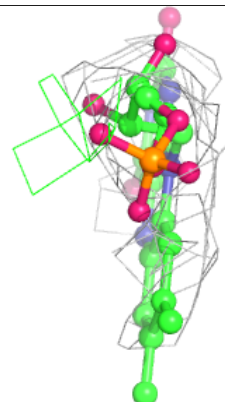
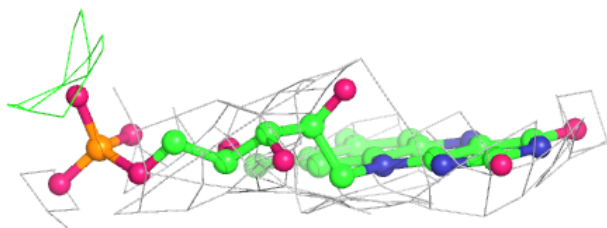
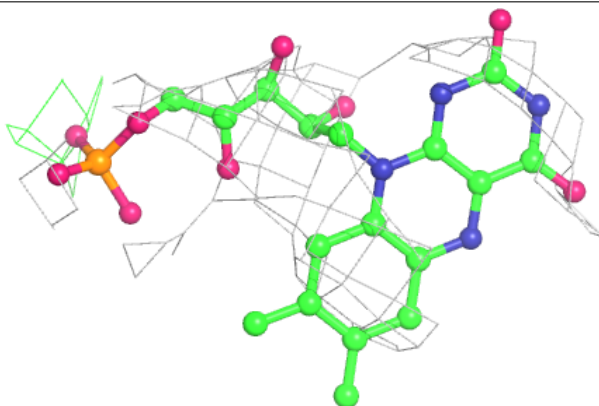
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

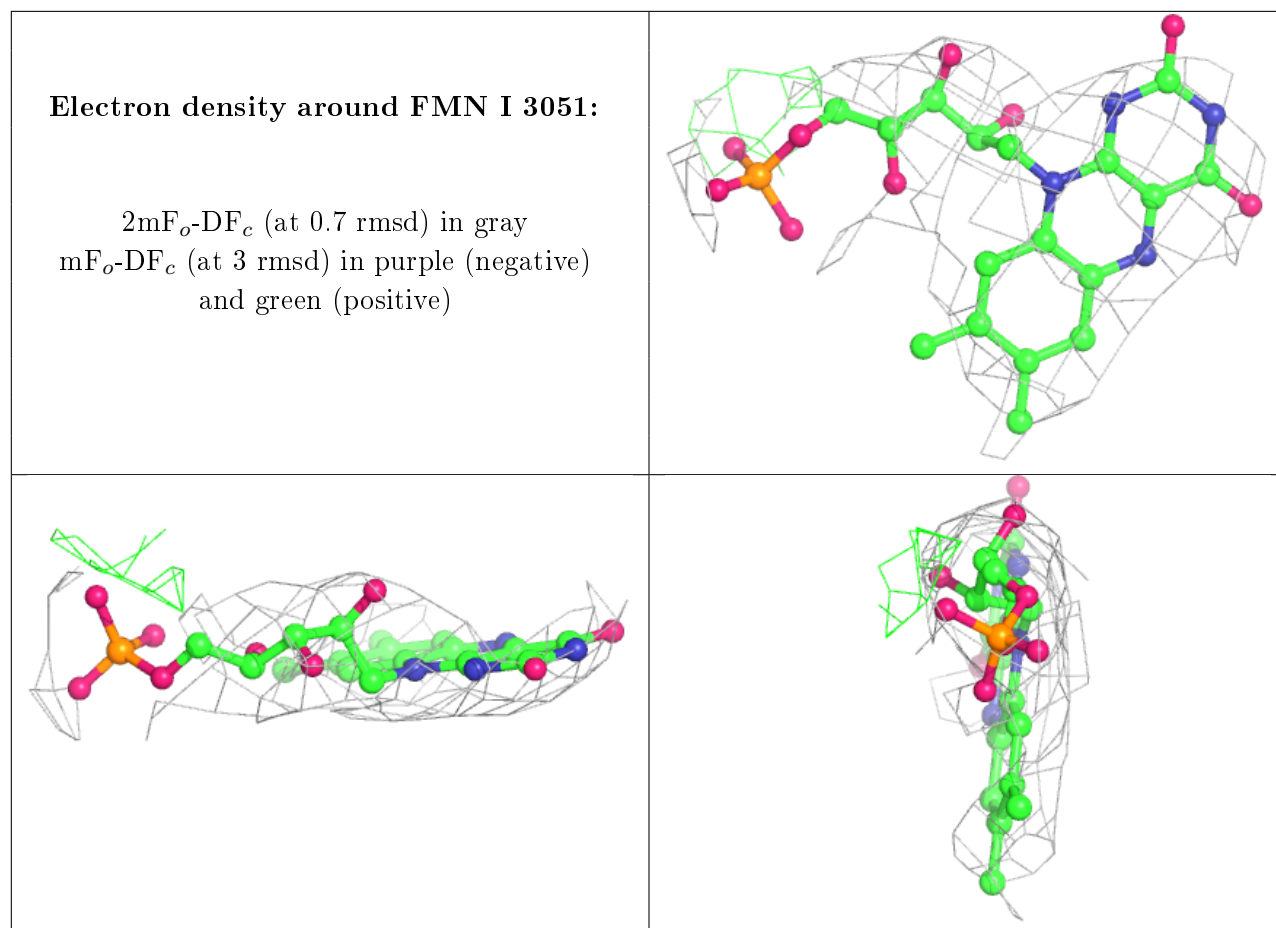
**Electron density around FMN H 3051:**

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

**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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.