



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 25, 2017 – 11:04 am GMT

PDB ID : 5LUQ
Title : Crystal Structure of Human DNA-dependent Protein Kinase Catalytic Subunit (DNA-PKcs)
Authors : Sibanda, B.L.; Chirgadze, D.Y.; Ascher, D.B.; Blundell, T.L.
Deposited on : 2016-09-09
Resolution : 4.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : recalc29047
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

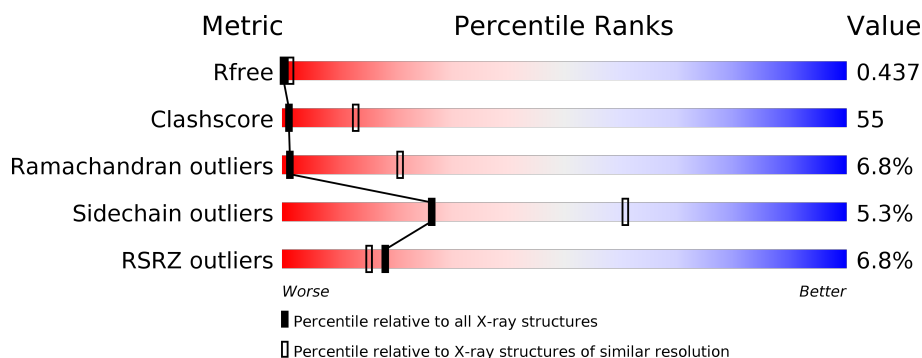
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1002 (4.92-3.62)
Clashscore	112137	1001 (4.92-3.68)
Ramachandran outliers	110173	1012 (4.92-3.64)
Sidechain outliers	110143	1021 (4.92-3.62)
RSRZ outliers	101464	1009 (4.92-3.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	4128	<div> <div>6%</div> <div>29%</div> <div>53%</div> <div>8%</div> <div>10%</div> </div>
1	B	4128	<div> <div>6%</div> <div>28%</div> <div>53%</div> <div>8%</div> <div>10%</div> </div>
2	K	194	<div> <div>23%</div> <div>5%</div> <div>72%</div> </div>
2	S	194	<div> <div>23%</div> <div>5%</div> <div>72%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 59694 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 DNA-dependent protein kinase catalytic subunit,DNA-dependent Protein Kinase Catalytic Subunit,DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	3725	Total	C	N	O	S	Se	0	0	0
			29574	18907	5016	5460	81	110			
1	B	3725	Total	C	N	O	S	Se	0	0	0
			29574	18907	5016	5460	81	110			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP P78527
A	4128	MSE	-	expression tag	UNP P78527
B	1	MSE	-	expression tag	UNP P78527
B	4128	MSE	-	expression tag	UNP P78527

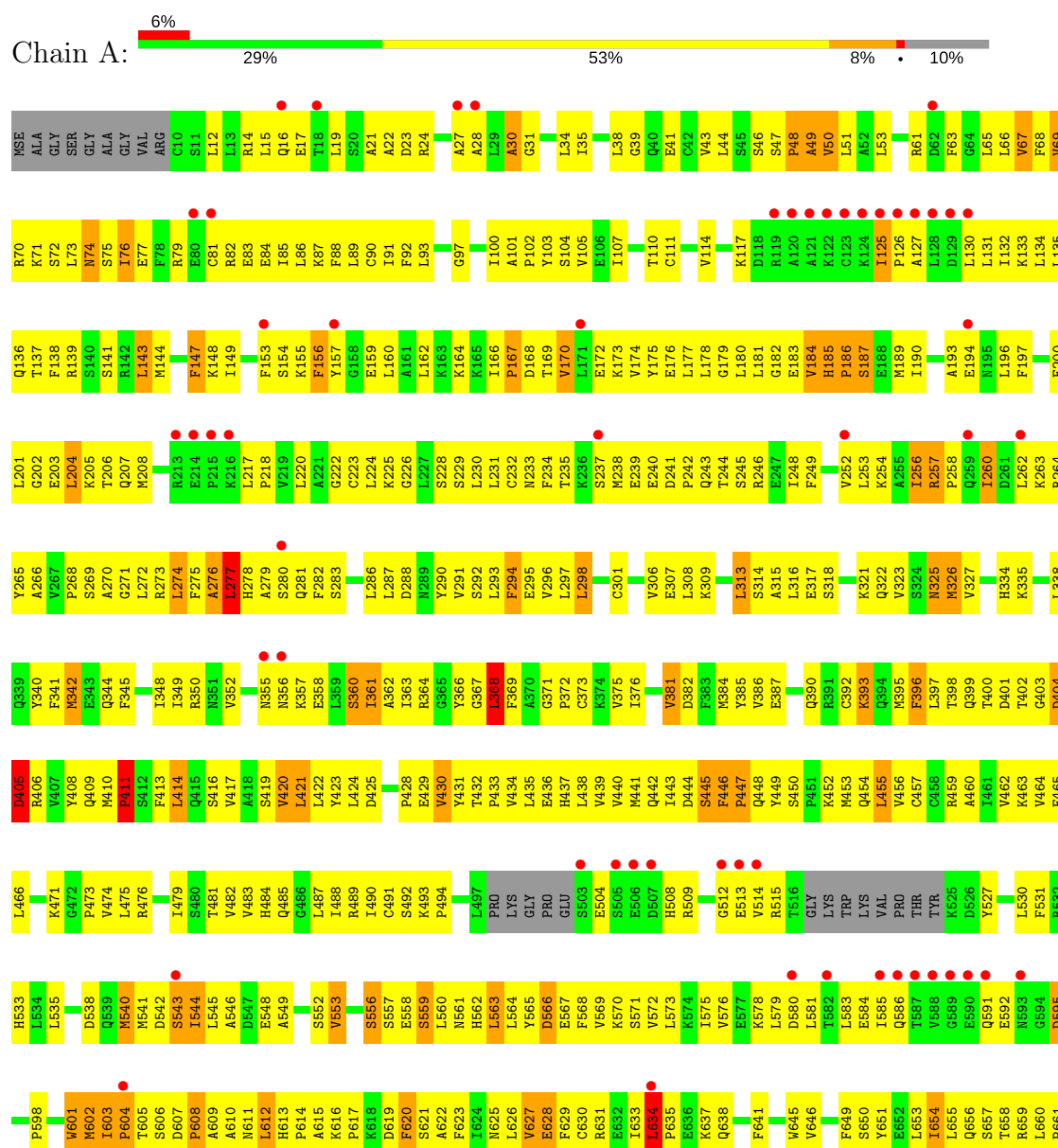
- Molecule 2 is a protein called C-terminal fragment of KU80 (KU80ct194).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	54	Total	C	N	O	Se	0	0	0
			273	164	54	54	1			
2	S	54	Total	C	N	O	Se	0	0	0
			273	164	54	54	1			

3 Residue-property plots [i](#)

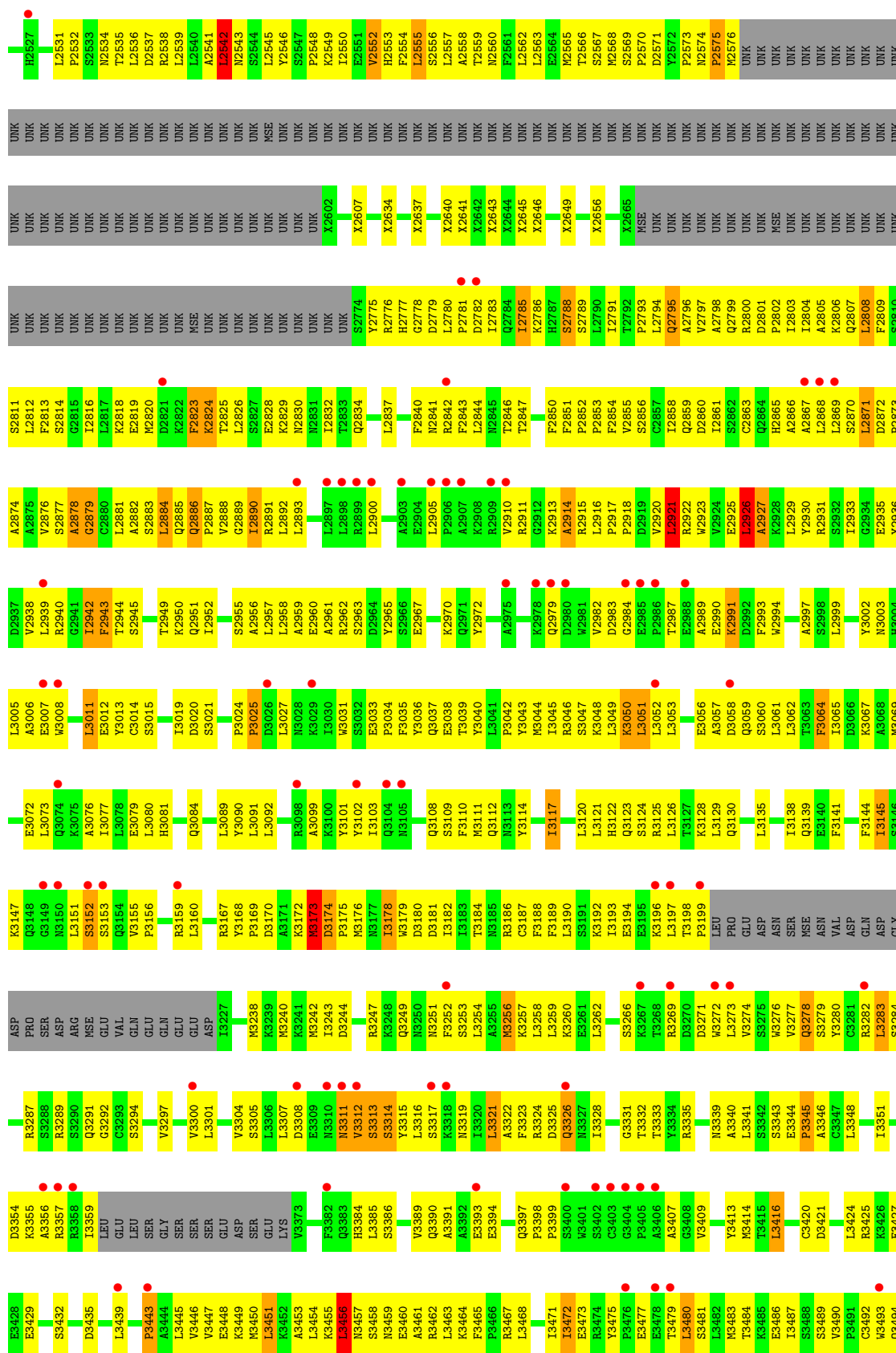
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

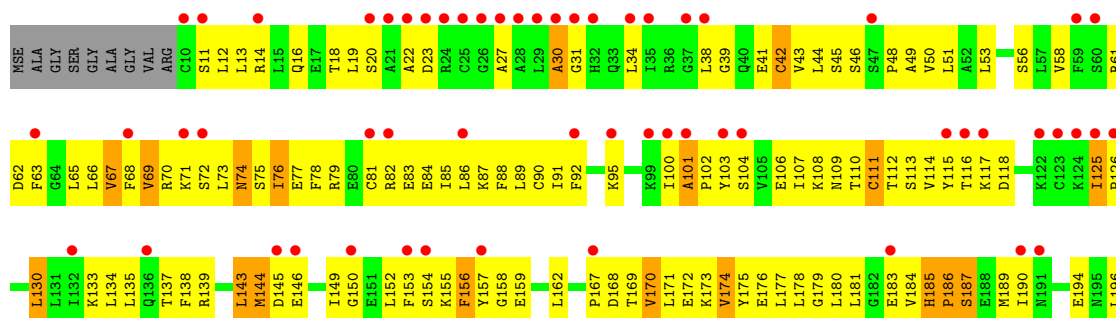
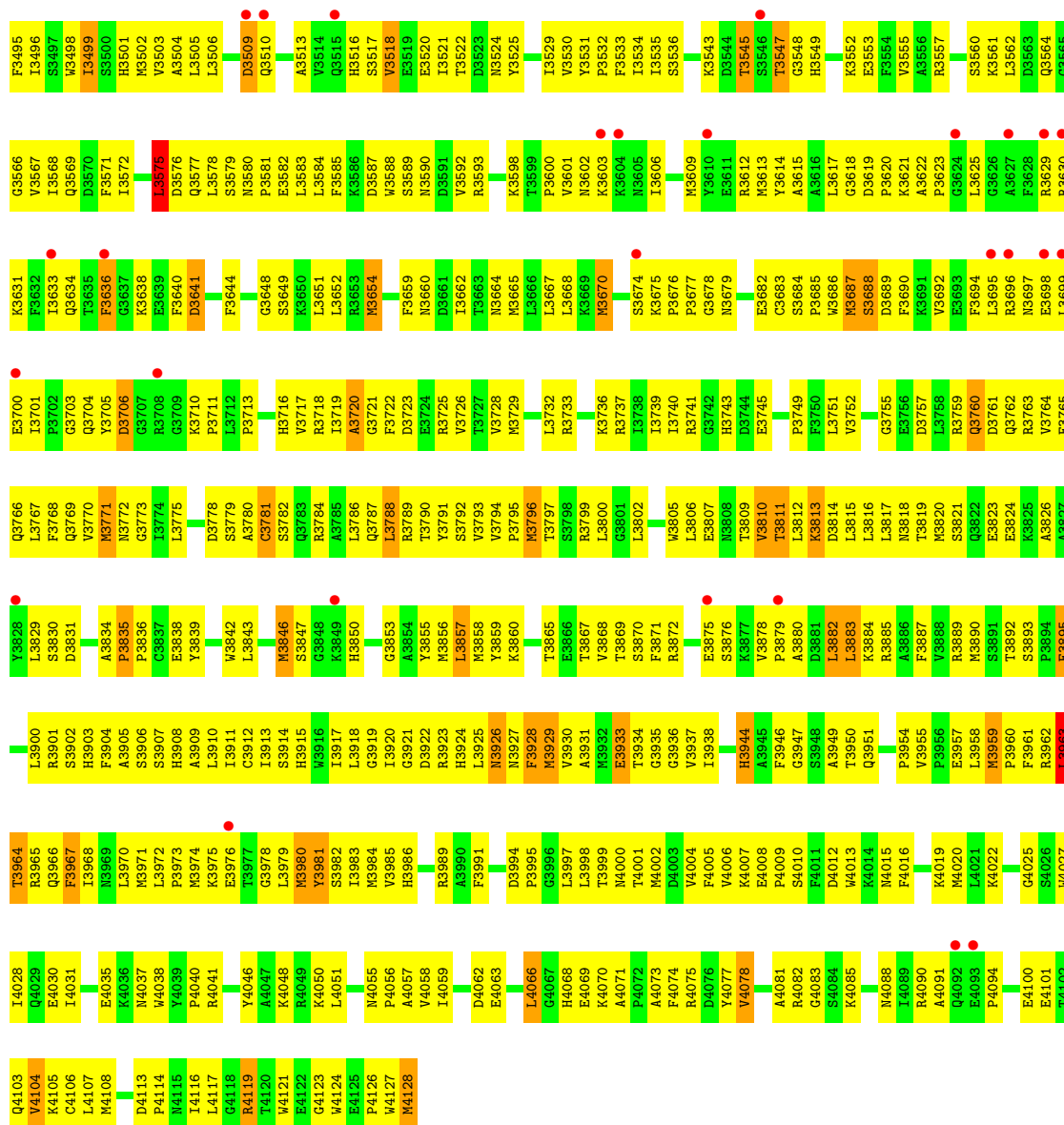
- Molecule 1: DNA-dependent protein kinase catalytic subunit,DNA-dependent Protein Kinase Catalytic Subunit,DNA-dependent protein kinase catalytic subunit





WORLDWIDE
PDB
PROTEIN DATA BANK



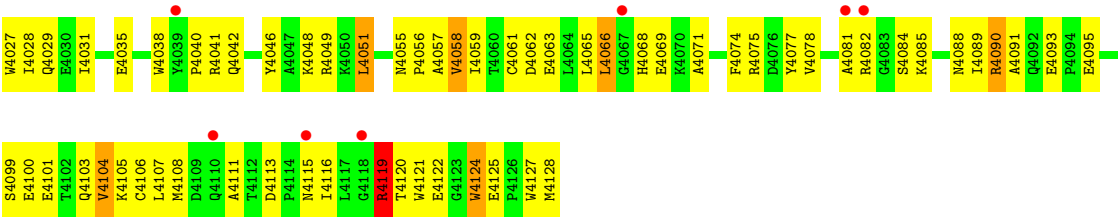


A1103	W1039	V979	T915	L848	P787	A727	P661	P598	L530	L468	Y408	L338	Y283	F197
L1104	K1042	T980	E916	E849	Y788	S728	L662	W601	F531	L468	Q409	L338	R264	F200
V1105	Q1043	R981	L917	E850	Y789	C729	L663	M602	R532	K471	Q410	F341	Y285	F200
Y1106	T1044	Q982	L917	T851		L730			H533	Q472	M410		A266	L201
Y1107	T1045	L983	S922	R852	Y792	T731	F666	I603	L534	P473	F412	F345	V267	L204
E1108	T1046	E985	R924	R854	Y794	T732	Y667	T605	L535	V474	F413	Y346	P268	K205
S1110	Q1049	P986	Q925	W855	C795	L733	K668	S606	S536	L475	L414	G347	S269	L206
L1111	E1050	L987	T926	W856	T796	L734	L669	S606	S537	R476	Q415	I348	A270	T207
A1112	E1051	V988	K927	Q857	D797	L736	S671	P608	D538		S416	I349	G271	M208
L1113	L1107	V989	V928	W858	G798	P737	L672	A609	Q539	S480	V417	R350	L272	T209
A1114	S1052	Q990	A929	L859	Y799	H738	T673	A610	M540	T481	A418	R351	R273	
H1115	P1053	L991	A930	G860	L800	H739		M611	M541	S419	L274	V352	L274	
	V1054	I992	C931	S861	K901	I740		M612	D542	V482	Y420	V353	F275	V212
E1118	M1055	H993	E932	L862	T902	I741		H613	S543	V483	L421	A276	A276	R213
A1119	W994	L933	E932		S903	E742	W680	H614	I544	H484	L422	L277	E214	E214
S1120	L1059	F995	L934	Q865	A904	L743	K681	P614	L545	Q485	Y423	H278	P215	P215
L1121	F1060	T996	H935	T866	L805	D744	V682	K616	A546	Q486	L424	A279	K216	K216
G1122	K1061	N997	S936	K867	S906	V745	PHE	P617	F550	T488	D425	S280	S280	
T1123	R1062	H998	S937	K868	D907	R746	GLU	K618	F551	T489	V426	S360	D281	P218
	L1063	K999	V938	N869	E908	A747	GLY	D619	F552	K489	V427	I361	F282	P219
C1127	Y1064	F1000	M939	L870	T809	Y748	VAL	F620	V553	Q491	A228	A362	L286	L286
D1129	S1065	E1002	F940	L871	LYS	V749	SER	S821	M554	S492	V430	I363	G222	G222
A1130	L1066	S1003	L942	T872	ASN	P750	PRO	A622	S555	K493	T432	G365	C223	C223
T1131	A1067	Q1004	C943	W873	TRP	A751	LYS	F623	S556	P494	T432	G367	L224	L224
	L1068	D1005	R944		GLU	L752	SER	I624	S557	V495	P433		K225	K225
H1132	P1069	T1006	A945	D877	LEU	Q753	LEU	N625	S558	V496	V434	L227	G226	G226
L1133	F1070	L1008	A945	E878	LYS	M754	LYS	N625	S559	L497	L435	L227	L227	L227
L1134	N1071	V1007	T946	W884	ALA	A755	HIS	V627	M560	PRO	A436	A370	S228	S228
C1135	A1072	A1008	Q947	V886	ALA	F756	SER	E628	N561	LYS	H437	G371	E295	E295
R1136	F1073	L1009	M948	N886	LEU	K757	PRO	F629	H562	GLY	L438	P372	V296	V296
I1137	K1074	L1010	P949	W886	SER	L758	GLU	C630	L563	PRO	V439		L297	L297
I1138	R1075	E1011		N887	ASP	G759	ASP	R631	L564	GLY	V440	I376	L298	L298
L1139	L1076	A1012	G951	R888	ALA	L760	PRO	E632	F565	SS03	Q442	V381	V306	V306
K1140	G1077	I1013	G952	R889	ALA	S761	GLU	I633	D666	E504	Q442	V381	E307	E307
L1141	A1078	L1014	Q953	K890	GLN	Y762	GLY	L634	E567	S505	I443	M364	L308	L308
H1142	S1079	D1015	G954	R891	LYS	T763	Y701	P635	F568	E506	I444	Y385	L313	L313
V1143	L1080	G1016	A955	L892	GLY	P764		E636	V569	D507	S445	Y385	S314	S314
S1144	A1081	I1017	P956	S893	PHE	L765	F704	K637	K570	H508	F446	V387	L241	L241
F1082	F1082	V1018	P957	F894	ASN	A766	A705	Q638	S571	R509	P447	L388	A315	A315
N1083	N1083	D1019	M958	A895	LYS	E767	L706		V572	A510	Q448	L388	L316	L316
K1146	E1088	P1020	Y959	V896	VAL	V768	F707	F641	L573	SS11	Y449	I389	Q243	Q243
N1084	I1085	V1021	Q960	R897	VAL	G769	V708	F642	K574	G512	S450	Q390	T244	T244
I1086	T1086	D1022	L961	F898	LEU	L770	K709		I575	E513	P451	R391	S245	S245
K1149	R1087	S1023	Y962	R899	LYS	M771	F710	W845	V576	V514	K452	C392	F319	F319
L1150	E1087	T1024	K963	E900	HIS	A772	G711	V846	E577	R515	M453	K393	L320	L320
R1151	F1089	L1025	R964	M901	LEU	L773	K712	Y647	K578	T516	Q454	Q394	K321	K321
L1152	R1026	R1026	T965	K902	LYS	E774	E713	S648	L579	GLY	L455	R395	Q322	Q322
P1154	E1091	D1027	F966	P903	LYS	E775	V714	F649	D580	LYS	V456	F396	V251	V251
R1155	E1092	F1028	P967	V904	THR	V776	A715	S650	L581	TRP	C457	L397	V252	V252
G1156	E1093	C1029	V968	I905	LYS	S777	V716	S651	T582	LYS	C458	T398	L253	L253
F1157	S1094	G1030	P906	F906	ASN	T778	K717	E652	L583	VAL	R459	K326	K254	K254
P1158	L1095	L970	L907	N907	LEU	V779	M718	L653	E584	PRO	A460	T400	V327	V327
P1159	V1096	C1032	R971	L908	SER	V779	M719	I654	I585	THR	I461	D401	I256	I256
R1159	E1097	L1033	L972	V909	SER	D781	Q720	L655	Q586	TVR	V462	T403	R257	R257
S1160	G1098	H1034	L973	F910	ASN	R782	W721	D656			K525	G403	P258	P258
A1161	E1098	E1035	C974	L911	GLU	H783	K722	S657	Q591		V464	D404	Q259	Q259
S1162	F1099	F1036	L912	P912	ALA	V784	K722	T658	E592		F465	D405	L260	L260
L1163	V1100	L1037	R913	W885		V784	L725	R659	M593		V466	R406	D261	D261
C1164	F1101					Q786	L726					K337	L262	L262
L1165	E1102	K1038	Q978	V914	S847			L660			A467			

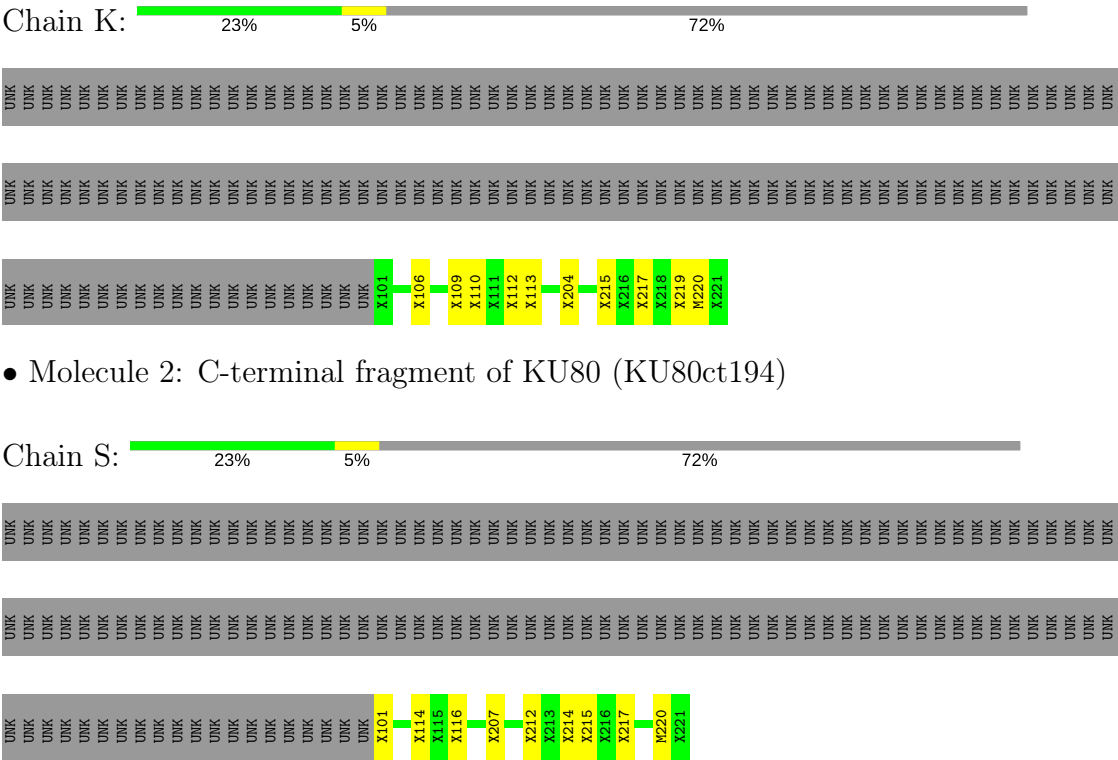
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C1229	G1230	Q1231	P1232	A1237	Q1238	P1239	T1240	L1241	L1244	P1247	F1248	L1249	L1250	Q1251	H1252	L1253	L1254	W1256	L1257	D1258	L1259	L1260	A1263	L1264	E1265	C1266	Y1267	T1268	C1269	I1270	I1271	C1272	E1273	L1274	T1275	V1276	L1279	Q1280	V1281	L1282	G1283	T1284	E1285	Q1286	Q1287	S1288	S1289	L1290	L1291	K1292	A1293	V1294	A1295										
F1296	F1297	L1298	E1299	S1300	L1301	A1302	M1303	H1304	D1305	L1306	I1307	A1308	ALA	GLU	LYS	PHE	THR	GLY	ALA	GLY	ALA	GLY	ASN	ARG	THR	S1323	P1324	Y1330	S1333	K1334	L1335	T1336	V1337	V1338	V1339	R1340	T1341	M1342	E1343	F1344	T1345	T1346	T1347	L1348	L1349	M1350	T1351	S1352	Q1353	E1354	G1355	W1356	K1357	L1358	L1359	K1360							
K1361	D1362	C1363	E1364	L1365	T1366	H1367	L1368	M1369	R1370	L1371	L1372	V1373	Q1374	T1375	L1376	C1377	E1378	G1379	I1382	N1385	L1386	G1387	D1388	V1389	Q1390	M1392	A1393	D1397	L1463	L1464	C1399	V1400	N1401	L1402	M1403	L1404	A1405	L1406	K1407	M1408	S1409	Y1411	Y1412	D1413	I1414	L1415	E1416	T1417	H1418	L1419	G1420	E1421	I1422	L1423	T1424								
A1425	Q1426	E1430	L1431	P1432	S1433	M1434	D1435	Y1436	L1437	S1438	P1439	D1440	A1441	Q1442	R1443	S1444	R1445	L1446	L1447	L1448	A1449	L1450	V1451	S1452	S1453	A1454	C1455	L1456	L1457	L1458	H1459	R1460	L1463	L1464	H1465	N1466	L1467	L1468	P1469	S1470	Q1471	S1472	T1473	D1474	L1475	SER	H1476	V1479	L1483	L1484	I1485	H1486	Y1488	H1489	G1490	I1491	A1492	P1493	G1494				
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S1561	L1562	F1563	L1564	T1565	N1566	M1567	L1568	E1569	L1570	L1571	K1572	N1573	N1574	D1575	L1576	L1577	A1578	G1579	L1580	E1581	M1582	M1583	Q1584	S1585	S1586	L1587	D1588	G1589	L1590	K1591	M1592	L1593	ASN	S1594	PRO	A1595	V1596	L1597	N1598	G1599	M1600	L1601	D1602	Q1603	S1604	F1605	E1606	R1608	A1609	ASN	GLN	LYS	GLN	S1677	L1678	L1679	A1680	L1681	T1682	K1683	L1684	LEU	THR
THR	ILE	LEU	GLN	HIS	TRP	LYS	LYS	CYS	D1630	S1631	V1632	M1633	A1634	K1635	D1636	S1637	P1638	L1639	E1640	M1643	A1644	V1645	L1646	A1647	L1648	L1649	A1650	K1651	L1652	L1653	Q1654	L1655	S1658	VAL	SER	PHE	ASN	THR	THR	SER	HIS	GLY	SER	PRO	GLU	V1671	F1672	S1677	L1678	L1679	A1680	L1681	T1682	K1683	L1684	LEU	THR						
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E1751	L1752	Q1753	Q1754	P1755	M1756	L1757	L1758	L1759	E1760	L1761	M1762	T1763	GLU	VAL	LEU	CYS	ARG	GLU	GLN	HIS	VAL	MSE	VAL	VAL	GLU	GLU	LEU	PHE	GLN	ASP	VAL	LEU	LYS	SER	ARG	ILE	ALA	R1787	L1797	L1798	E1799	S1800	V1801	Y1802	F1805	R1806	K1807	D1808	L1809	P1810	R1811	L1812	S1813	L1814	T1815	R1816	Q1817	V1818	F1819				
R1822	SER	LEU	LEU	THR	LEU	LEU	TRP	HIS	CYS	SER	LEU	ASP	ALA	LEU	ARG	GLU	PHE	PHE	SER	THR	ILE	VAL	VAL	VAL	ASP	ALA	ILE	ASP	ARG	ARG	PHE	LYS	SER	ARG	ARG	PHE	T1856	K1857	L1858	M1859	E1860	S1861	T1862	F1863	D1864	T1865	Q1866	I1867	T1868	K1869	K1870	M1871	G1872	Y1873	Y1874	K1875	L1876	L1877	D1878	V1879	M1880		
Y1881	S1882	R1883	L1884	P1885	K1886	D1887	L1888	V1889	H1890	L1891	S1894	K1895	L1896	F1897	N1898	Q1899	F1900	S1903	C1904	T1905	T1906	E1907	G1908	M1909	L1910	L1911	T1912	K1913	T1914	L1915	F1916	L1917	L1918	C1919	Y1920	F1923	T1924	E1925	N1926	M1927	A1928	G1929	E1930	N1931	Q1932	L1933	L1934	R1937	M1938	E1939	R2000	K2001	H1941	C1942	A1943	Y1944	E2006						
N1946	C1947	A1948	L1949	S1950	P1951	I1952	C1953	L1954	F1955	V1956	N1957	E1958	L1959	F1960	Q1961	Y1962	Q1963	G1964	F1965	L1966	S1967	S1968	E1969	K1970	P1971	E1972	K1973	L1974	L1975	L1976	L1977	F1978	E1979	N1980	L1981	L1984	K1985	R1986	R1987	Y1988	N1989	F1990	P1991	V1992	V1993	V1994	E1995	V1996	P1997	M1998	E1999	R2000	K2001	K2002	K2003	Y2004	E2006						
L2007	R2008	K2009	E2010	A2011	R2012	E2013	A2014	A2015	N2016	G2017	D2018	S2019	P2022	S2023	S2026	S2027	L2028	S2029	L2030	L2031	A2032	D2033	L2036	S2037	E2038	E2039	M2040	S2041	Q2042	F2043	D2044	F2045	S2046	T2047	G2048	V2049	Q2050	S2051	Y2052	S2053	Y2054	D2058	P2059	R2060	P2061	A2062	T2063	G2064	R2065	R2066	R2067	R2068	E2069	E2070	Q2071								

N3093	E2960	L2893	K2820	UNK	UNK	UNK	L2536	P2465	V2401	K3334	V2272	L2144	R2072
P3024	A2961	E2894	D2821	UNK	UNK	UNK	D2537	S2496	L2402	N3335	G2273	F2145	D2073
P3025	P2962	E2895	F2822	UNK	UNK	UNK	R2538	T2467	C2403	L2336	L2274	L2146	P2074
D3026	S2963	A2896	F2823	UNK	UNK	UNK	L2539	K2404	R2403	Q2275	Q2276	A2147	L2075
L3027	L2897	MSE	K2824	UNK	UNK	UNK	L2540	R2470	E2406	V2405	L2276	K2148	V2076
N3028	L2898	UNK	T2825	UNK	UNK	UNK	L2541	Q2471	G2407	L2338	L2277	L2149	H2077
K3029	Y2965	UNK	L2826	UNK	UNK	UNK	L2542	Q2472	M2408	L2341	G2278	V2150	D2078
K3030	S2966	UNK	L2826	UNK	UNK	UNK	L2543	M2473	M2408	L2344	L2279	L2151	D2079
I3030	E2967	UNK	UNK	UNK	UNK	UNK	L2544	Q2474	T2409	V2345	L2280	L2152	V2080
W3031	A2968	UNK	UNK	UNK	UNK	UNK	L2545	M2475	L2410	M2281	M2220	T2153	L2081
S3032	K2970	UNK	UNK	UNK	UNK	UNK	L2546	L2476	E2411	A2282	K2221	E2154	E2082
E3033	Q2971	UNK	UNK	UNK	UNK	UNK	S2547	L2477	Y2412	N2283	V2222	S2155	L2083
P3034	Q2972	UNK	UNK	UNK	UNK	UNK	S2548	M2478	Y2413	L2349	V2223	V2156	E2084
Y3035	K2973	UNK	X2802	UNK	UNK	UNK	K2549	S2479	K2416	K2350	L2285	F2157	M2085
Q3037	E2974	UNK	X2803	UNK	UNK	UNK	K2550	D2480	K2481	Q2351	L2286	R2158	M2086
E3038	A2975	UNK	X2834	UNK	UNK	UNK	H2551	H2481	D2482	H2352	P2287	E2159	E2087
L3039	L2910	UNK	X2835	UNK	UNK	UNK	H2552	D2482	D2419	Q2353	P2226	V2160	L2088
Y3040	Q2912	UNK	H2553	UNK	UNK	UNK	H2554	R2485	F2420	D2288	V2288	A2161	N2089
L3041	K2978	UNK	L2554	UNK	UNK	UNK	L2555	R2486	Y2421	T2355	D2289	K2162	K2090
P3042	Q2979	UNK	L2556	UNK	UNK	UNK	L2556	D2487	Q2422	M2356	Q2291	H2163	H2091
Y3043	R2915	UNK	L2557	UNK	UNK	UNK	L2557	E2488	M2424	E2357	C2292	W2164	C2093
M3044	L2916	UNK	L2558	UNK	UNK	UNK	L2558	E2488	R2425	D2358	G2293	L2165	M2094
I3045	V2982	UNK	L2559	UNK	UNK	UNK	L2559	T2491	H2426	K2359	L2294	S2166	C2094
S3046	D2983	UNK	T2559	UNK	UNK	UNK	K2560	K2491	H2426	F2360	Q2295	L2167	A2095
R3047	G2984	UNK	K2560	UNK	UNK	UNK	K2561	S2495	D2427	I2361	E2298	L2168	P2096
K3048	E2985	UNK	F2561	UNK	UNK	UNK	L2562	S2495	E2430	V2382	E2299	L2169	L2097
L3049	P2986	UNK	L2562	UNK	UNK	UNK	L2563	T2498	E2430	C2363	Y2299	L2170	T2098
K3050	T2921	UNK	L2563	UNK	UNK	UNK	L2564	K2498	D2433	L2364	F2300	L2171	A2099
L3051	Q2987	UNK	L2564	UNK	UNK	UNK	L2565	L2501	K2433	N2365	Q2301	L2100	L2100
L3052	E2988	UNK	L2566	UNK	UNK	UNK	L2566	L2501	V2434	K2366	K2369	S2174	V2101
L3053	A2989	UNK	L2567	UNK	UNK	UNK	L2567	A2502	C2435	V2367	V2304	R2175	K2102
E3056	L2992	UNK	L2568	UNK	UNK	UNK	L2568	V2505	D2437	K2369	M2307	R2176	H2103
A3057	K2928	UNK	L2569	UNK	UNK	UNK	L2569	L2506	L2438	S2370	C2244	N2177	M2104
D3058	L2930	UNK	L2570	UNK	UNK	UNK	L2570	L2507	I2439	F2371	M2245	L2182	P2110
Q3059	E2994	UNK	L2571	UNK	UNK	UNK	L2571	Q2508	Y2440	P2372	K2246	H2183	P2111
S3060	E2995	UNK	L2572	UNK	UNK	UNK	L2572	G2509	K2441	P2373	V2310	Y2184	Q2112
L3061	S2998	UNK	L2573	UNK	UNK	UNK	L2573	L2510	M2442	L2374	R2311	M2185	D2116
F3064	L2999	UNK	L2574	UNK	UNK	UNK	L2574	UNK	M2443	D2376	Y2253	V2186	L2122
I3065	D3000	UNK	L2575	UNK	UNK	UNK	L2575	P2515	P2444	A2377	E2314	E2188	P2119
M3069	Y3002	UNK	UNK	UNK	UNK	UNK	UNK	Q2516	L2446	F2378	V2315	L2189	R2120
H3070	H3003	UNK	UNK	UNK	UNK	UNK	UNK	L2517	K2447	M2379	Y2316	D2121	D2121
G3071	L3004	UNK	UNK	UNK	UNK	UNK	UNK	Q2518	P2448	A2317	L2355	L2193	L2122
L3072	L3005	UNK	UNK	UNK	UNK	UNK	UNK	L2519	V2449	V2382	A2318	L2194	W2125
L3073	A3006	UNK	UNK	UNK	UNK	UNK	UNK	L2520	E2450	F2383	A2319	S2195	M2126
Q3074	E3007	UNK	UNK	UNK	UNK	UNK	UNK	L2521	L2451	F2384	E2258	K2196	K2127
K3075	W3008	UNK	UNK	UNK	UNK	UNK	UNK	R2522	R2452	L2385	E2321	K2259	F2128
A3076	K3009	UNK	UNK	UNK	UNK	UNK	UNK	R2523	E2453	L2386	K2322	K2260	L2129
L3080	S3010	UNK	UNK	UNK	UNK	UNK	UNK	R2524	L2454	P2387	S2261	V2205	P2139
Y3081	E3012	UNK	UNK	UNK	UNK	UNK	UNK	R2525	L2455	K2388	G2262	P2206	L2140
Q3084	L3011	UNK	UNK	UNK	UNK	UNK	UNK	S2526	N2456	F2389	L2325	T2201	M2135
E3085	Y3013	UNK	UNK	UNK	UNK	UNK	UNK	H2527	P2457	H2390	I2326	P2202	P2136
L3086	C3014	UNK	UNK	UNK	UNK	UNK	UNK	G2391	V2458	G2391	L2327	T2203	L2137
L3089	S3015	UNK	UNK	UNK	UNK	UNK	UNK	R2530	V2459	L2386	P2266	G2204	V2138
Y3090	Q2951	UNK	UNK	UNK	UNK	UNK	UNK	L2531	E2460	C2397	S2267	V2205	P2139
L3091	Q2954	UNK	UNK	UNK	UNK	UNK	UNK	P2532	F2461	V2330	K2268	P2206	L2140
L3092	D3020	UNK	UNK	UNK	UNK	UNK	UNK	S2533	V2462	E2331	D2269	D2207	M2141
E3022	L2957	UNK	UNK	UNK	UNK	UNK	UNK	N2534	S2463	L2398	E2332	R2270	L2142
		UNK	UNK	UNK	UNK	UNK	UNK	T2535	H2464	V2400	R2333	E2209	R2143





● Molecule 2: C-terminal fragment of KU80 (KU80ct194)



● Molecule 2: C-terminal fragment of KU80 (KU80ct194)

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	169.12Å 132.64Å 296.59Å 90.00° 105.53° 90.00°	Depositor
Resolution (Å)	49.92 – 4.30 49.92 – 4.30	Depositor EDS
% Data completeness (in resolution range)	97.8 (49.92-4.30) 97.6 (49.92-4.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 4.29Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.386 , 0.437 0.385 , 0.437	Depositor DCC
R_{free} test set	1977 reflections (2.34%)	DCC
Wilson B-factor (Å ²)	184.6	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 188.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	59694	wwPDB-VP
Average B, all atoms (Å ²)	253.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.45	3/29743 (0.0%)	0.77	47/40014 (0.1%)
1	B	0.46	6/29743 (0.0%)	0.77	49/40014 (0.1%)
2	K	0.22	0/7	0.50	0/7
2	S	0.45	0/7	0.34	0/7
All	All	0.46	9/59500 (0.0%)	0.77	96/80042 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	6
All	All	0	14

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1069	HIS	C-N	-9.65	1.16	1.34
1	B	3794	VAL	C-N	-8.26	1.18	1.34
1	B	1069	HIS	C-N	7.70	1.48	1.34
1	B	4124	TRP	CB-CG	-6.16	1.39	1.50
1	A	601	TRP	CB-CG	-5.75	1.40	1.50
1	B	3981	TYR	CD1-CE1	-5.53	1.31	1.39
1	B	2546	TYR	CB-CG	-5.38	1.43	1.51
1	B	2546	TYR	CD2-CE2	-5.37	1.31	1.39
1	A	2362	VAL	CB-CG1	-5.04	1.42	1.52

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	726	LEU	CA-CB-CG	-10.22	91.80	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3456	LEU	CA-CB-CG	9.67	137.54	115.30
1	B	1009	LEU	CB-CG-CD1	-9.35	95.11	111.00
1	A	3456	LEU	CA-CB-CG	9.33	136.75	115.30
1	B	726	LEU	CA-CB-CG	-9.12	94.32	115.30
1	B	1010	LEU	CA-CB-CG	9.01	136.02	115.30
1	A	2926	LEU	CA-CB-CG	8.88	135.71	115.30
1	A	1010	LEU	CA-CB-CG	8.37	134.55	115.30
1	A	3882	LEU	CA-CB-CG	-8.14	96.57	115.30
1	B	2542	LEU	CA-CB-CG	7.94	133.56	115.30
1	A	3575	LEU	CA-CB-CG	7.75	133.12	115.30
1	A	1165	LEU	CA-CB-CG	7.67	132.95	115.30
1	A	2542	LEU	CA-CB-CG	7.53	132.63	115.30
1	B	1165	LEU	CA-CB-CG	7.50	132.54	115.30
1	A	1976	LEU	CB-CG-CD1	-7.38	98.45	111.00
1	B	1695	LEU	CA-CB-CG	7.22	131.91	115.30
1	B	4051	LEU	CA-CB-CG	6.89	131.15	115.30
1	A	3321	LEU	CB-CG-CD2	-6.88	99.31	111.00
1	A	3788	LEU	CA-CB-CG	-6.87	99.49	115.30
1	B	1717	LEU	CA-CB-CG	-6.85	99.53	115.30
1	A	1025	LEU	CA-CB-CG	-6.81	99.63	115.30
1	B	3397	GLN	CA-CB-CG	6.52	127.75	113.40
1	B	220	LEU	CA-CB-CG	6.52	130.29	115.30
1	B	515	ARG	NE-CZ-NH1	-6.47	117.07	120.30
1	A	3480	LEU	CA-CB-CG	6.27	129.73	115.30
1	A	455	LEU	CA-CB-CG	6.26	129.70	115.30
1	B	862	LEU	CB-CG-CD2	-6.26	100.36	111.00
1	A	3665	MSE	CB-CG-SE	6.25	131.43	112.70
1	B	1580	LEU	CA-CB-CG	6.24	129.65	115.30
1	A	1111	LEU	CA-CB-CG	-6.24	100.95	115.30
1	A	2241	LEU	CA-CB-CG	-6.19	101.07	115.30
1	B	1984	LEU	CA-CB-CG	6.17	129.49	115.30
1	B	2892	LEU	CA-CB-CG	6.14	129.43	115.30
1	B	1812	LEU	CA-CB-CG	6.14	129.43	115.30
1	A	1524	LEU	CA-CB-CG	6.13	129.41	115.30
1	A	1145	LEU	CA-CB-CG	6.13	129.40	115.30
1	B	2921	LEU	CA-CB-CG	6.09	129.30	115.30
1	B	3667	LEU	CA-CB-CG	6.07	129.26	115.30
1	B	3416	LEU	CA-CB-CG	6.03	129.16	115.30
1	A	718	MSE	CB-CG-SE	-6.02	94.64	112.70
1	B	942	LEU	CB-CG-CD1	-6.02	100.77	111.00
1	A	1648	LEU	CA-CB-CG	5.95	128.99	115.30
1	A	901	MSE	CA-CB-CG	-5.94	103.20	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1025	LEU	CA-CB-CG	-5.93	101.66	115.30
1	B	3988	LEU	CA-CB-CG	-5.87	101.80	115.30
1	A	204	LEU	CA-CB-CG	-5.84	101.87	115.30
1	B	913	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	3230	LEU	CA-CB-CG	5.79	128.61	115.30
1	A	1984	LEU	CA-CB-CG	5.75	128.52	115.30
1	A	3963	LEU	CA-CB-CG	5.75	128.52	115.30
1	B	942	LEU	CA-CB-CG	5.73	128.47	115.30
1	B	734	LEU	CA-CB-CG	-5.71	102.17	115.30
1	B	130	LEU	CB-CG-CD1	-5.69	101.33	111.00
1	B	545	LEU	CA-CB-CG	5.68	128.37	115.30
1	B	1686	LEU	CA-CB-CG	-5.66	102.29	115.30
1	B	3734	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	2097	LEU	CB-CG-CD2	-5.62	101.44	111.00
1	A	1752	LEU	CA-CB-CG	-5.56	102.50	115.30
1	B	612	LEU	CA-CB-CG	5.56	128.08	115.30
1	A	1812	LEU	CA-CB-CG	5.54	128.05	115.30
1	B	1643	MSE	CB-CG-SE	-5.52	96.14	112.70
1	B	583	LEU	CA-CB-CG	5.51	127.97	115.30
1	B	2539	LEU	CA-CB-CG	5.50	127.95	115.30
1	A	2921	LEU	CA-CB-CG	5.49	127.92	115.30
1	A	414	LEU	CA-CB-CG	-5.43	102.81	115.30
1	B	3788	LEU	CA-CB-CG	-5.38	102.94	115.30
1	A	2235	LEU	CA-CB-CG	5.37	127.65	115.30
1	A	1415	LEU	CA-CB-CG	-5.37	102.96	115.30
1	A	1976	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	1915	LEU	CA-CB-CG	5.33	127.55	115.30
1	A	3667	LEU	CA-CB-CG	5.33	127.56	115.30
1	B	1572	LEU	CA-CB-CG	5.28	127.44	115.30
1	B	359	LEU	CA-CB-CG	5.25	127.39	115.30
1	A	313	LEU	CA-CB-CG	5.25	127.37	115.30
1	A	421	LEU	CA-CB-CG	5.24	127.35	115.30
1	B	1930	GLU	CA-CB-CG	5.22	124.89	113.40
1	B	421	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	933	LEU	CA-CB-CG	-5.21	103.32	115.30
1	A	2808	LEU	CB-CG-CD1	-5.20	102.16	111.00
1	A	563	LEU	CB-CG-CD1	-5.17	102.20	111.00
1	A	3152	SER	C-N-CA	5.17	134.63	121.70
1	A	1095	LEU	CA-CB-CG	5.16	127.17	115.30
1	B	2926	LEU	CB-CG-CD2	-5.16	102.23	111.00
1	B	3575	LEU	CA-CB-CG	5.14	127.13	115.30
1	A	892	LEU	CA-CB-CG	-5.13	103.51	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2398	LEU	CA-CB-CG	5.12	127.09	115.30
1	A	1762	MSE	CB-CG-SE	5.12	128.06	112.70
1	B	2122	LEU	CA-CB-CG	5.12	127.07	115.30
1	A	2396	LEU	CB-CG-CD2	-5.11	102.31	111.00
1	A	758	LEU	CA-CB-CG	-5.07	103.65	115.30
1	B	564	LEU	CA-CB-CG	5.05	126.91	115.30
1	B	475	LEU	CA-CB-CG	5.04	126.89	115.30
1	B	871	LEU	CA-CB-CG	5.03	126.86	115.30
1	A	1582	LEU	CA-CB-CG	-5.01	103.77	115.30
1	B	670	LEU	CA-CB-CG	5.01	126.83	115.30
1	B	3159	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1323	SER	Peptide
1	A	2283	ASN	Peptide
1	A	2372	PRO	Peptide
1	A	3547	THR	Peptide
1	A	3980	MSE	Peptide
1	A	411	PRO	Peptide
1	A	4119	ARG	Peptide
1	A	634	LEU	Peptide
1	B	1323	SER	Peptide
1	B	2372	PRO	Peptide
1	B	3547	THR	Peptide
1	B	411	PRO	Peptide
1	B	4119	ARG	Peptide
1	B	634	LEU	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	29574	0	29642	3223	0
1	B	29574	0	29642	3283	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	273	0	70	9	0
2	S	273	0	73	8	0
All	All	59694	0	59427	6514	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 55.

All (6514) 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:B:2183:HIS:O	1:B:2187:VAL:HB	1.30	1.31
1:B:662:LEU:O	1:B:666:PHE:HB2	1.28	1.30
1:A:3521:ILE:O	1:A:3525:TYR:HB2	1.32	1.28
1:B:3683:CYS:SG	1:B:3736:LYS:NZ	2.12	1.23
1:B:2167:PRO:O	1:B:2171:LEU:HB2	1.39	1.18
1:B:1344:PHE:O	1:B:1348:LEU:HB2	1.41	1.18
1:A:3923:ARG:HG2	1:A:3962:ARG:HH22	1.07	1.17
1:B:1407:LYS:NZ	1:B:1460:ARG:O	1.77	1.16
1:B:3521:ILE:O	1:B:3525:TYR:HB2	1.43	1.16
1:A:2183:HIS:O	1:A:2187:VAL:HB	1.39	1.16
1:A:368:LEU:HD21	1:A:384:MSE:HB2	1.25	1.15
1:B:3868:VAL:O	1:B:3872:ARG:HB3	1.44	1.15
1:B:2872:ASP:O	1:B:2913:LYS:NZ	1.80	1.15
1:B:2477:LEU:O	1:B:2481:HIS:HB3	1.44	1.14
1:B:3467:ARG:O	1:B:3471:ILE:HB	1.46	1.14
1:B:1931:ASN:O	1:B:1938:ARG:NH2	1.80	1.13
1:B:974:CYS:HA	1:B:981:ARG:HD2	1.17	1.13
1:A:3167:ARG:HD3	1:A:3186:ARG:HG2	1.29	1.12
1:B:67:VAL:O	1:B:71:LYS:HB2	1.50	1.12
1:B:2100:LEU:HD21	1:B:2104:MSE:HE3	1.31	1.11
1:B:3099:ALA:O	1:B:3103:ILE:HB	1.47	1.11
1:A:3812:LEU:O	1:A:3816:LEU:HB2	1.49	1.11
1:A:560:LEU:HB3	1:A:616:LYS:HZ3	1.12	1.11
1:B:2960:GLU:OE2	1:B:3289:ARG:NH1	1.83	1.10
1:B:19:LEU:O	1:B:23:ASP:HB2	1.51	1.10
1:B:2891:ARG:HH22	1:B:3884:LYS:HD3	0.97	1.10
1:B:3581:PRO:HG2	1:B:3674:SER:HB2	1.34	1.09
1:A:3467:ARG:O	1:A:3471:ILE:HB	1.49	1.09
1:B:909:VAL:HG13	1:B:913:ARG:HH11	1.16	1.08
1:B:899:ARG:HH12	1:B:2570:PRO:HB2	1.17	1.08
1:B:3772:ASN:HB2	1:B:3787:GLN:HG3	1.36	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3868:VAL:O	1:A:3872:ARG:HB3	1.54	1.07
1:B:3117:ILE:HD12	1:B:3125:ARG:HH11	1.15	1.07
1:A:887:ASP:HB3	1:A:3889:ARG:HB3	1.35	1.04
1:B:2304:VAL:HG11	1:B:2344:LEU:HB3	1.40	1.04
1:B:3534:ILE:HG12	1:B:3704:GLN:HE22	1.22	1.03
1:B:2991:LYS:NZ	1:B:2995:GLU:OE2	1.91	1.03
1:A:2227:LYS:HD2	1:A:2235:LEU:HG	1.37	1.03
1:A:4082:ARG:HG3	1:A:4091:ALA:HB2	1.40	1.03
1:A:963:LYS:NZ	1:A:1006:THR:OG1	1.92	1.02
1:B:90:CYS:HB3	1:B:137:THR:HG22	1.40	1.02
1:A:327:VAL:HG22	1:A:338:LEU:HD13	1.38	1.02
1:B:2887:PRO:HB3	1:B:2922:ARG:HH11	1.24	1.02
1:B:4071:ALA:O	1:B:4075:ARG:HB3	1.58	1.01
1:B:3917:ILE:O	1:B:4048:LYS:NZ	1.92	1.01
1:A:1491:ILE:O	1:A:1497:ARG:NH1	1.93	1.00
1:B:3284:SER:HB2	1:B:3287:ARG:HH21	1.23	1.00
1:A:974:CYS:HA	1:A:981:ARG:HD2	1.41	1.00
1:A:1808:ASP:HB2	1:A:1814:PHE:HB3	1.41	0.99
1:B:2216:LEU:HD22	1:B:2249:LEU:HD11	1.43	0.99
1:B:2166:SER:O	1:B:2170:GLN:HB3	1.60	0.99
1:A:1471:GLN:O	1:A:1475:LEU:HB3	1.63	0.98
1:B:985:GLU:HG3	1:B:1031:ARG:HH22	1.25	0.98
1:B:2879:GLY:HA2	1:B:2886:GLN:HG2	1.42	0.98
1:B:3284:SER:HA	1:B:3287:ARG:HE	1.24	0.98
1:B:3699:LEU:O	1:B:3718:ARG:NH1	1.97	0.98
1:A:4103:GLN:O	1:A:4107:LEU:HB2	1.64	0.98
1:B:963:LYS:NZ	1:B:1006:THR:OG1	1.96	0.98
1:A:3819:THR:OG1	1:A:3889:ARG:NH1	1.96	0.97
1:B:1959:LEU:HD13	1:B:1998:MSE:HE3	1.44	0.97
1:A:357:LYS:HB3	1:A:360:SER:HB2	1.46	0.97
1:B:366:TYR:O	1:B:369:PHE:HB3	1.62	0.97
1:A:366:TYR:O	1:A:369:PHE:HB3	1.63	0.97
1:B:357:LYS:HB3	1:B:360:SER:HB2	1.44	0.97
1:B:2424:MSE:HG2	1:B:2433:LYS:HD2	1.47	0.96
1:B:3923:ARG:HG2	1:B:3962:ARG:HH22	1.30	0.96
1:A:2943:PHE:HD1	1:A:2944:THR:H	1.13	0.96
1:B:1093:GLU:N	1:B:1097:GLU:OE2	1.98	0.96
1:A:2070:GLU:HG3	1:A:2072:ARG:HG3	1.47	0.96
1:B:2243:GLU:HA	1:B:2246:LYS:HD2	1.46	0.96
1:A:2375:ALA:O	1:A:2379:MSE:HB3	1.66	0.96
1:B:1249:SER:O	1:B:1253:THR:HB	1.64	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1435:ASN:OD1	1:B:1489:LYS:NZ	1.99	0.96
1:B:3931:ALA:O	1:B:3935:GLY:HA2	1.63	0.96
1:A:3182:ILE:HB	1:A:3186:ARG:NH1	1.80	0.95
1:A:3923:ARG:O	1:A:3962:ARG:NH1	1.98	0.95
1:A:385:TYR:HD1	1:A:420:VAL:HG13	1.30	0.95
1:B:3819:THR:OG1	1:B:3889:ARG:NH1	2.00	0.95
1:B:2228:ARG:NH1	1:B:2269:ASP:OD1	1.98	0.95
1:A:560:LEU:HB3	1:A:616:LYS:NZ	1.81	0.95
1:A:2962:ARG:HB2	1:A:3253:SER:HB3	1.47	0.95
1:B:440:VAL:HB	1:B:483:VAL:HG12	1.46	0.95
1:B:2308:SER:HB3	1:B:2348:GLN:HG2	1.49	0.95
1:B:2538:ARG:HH11	1:B:2565:MSE:HB3	1.32	0.95
1:B:801:LYS:NZ	1:B:877:ASP:OD2	2.00	0.95
1:A:1685:ASP:HB2	1:A:1727:ARG:HH22	1.28	0.94
1:B:3887:PHE:HB3	1:B:3897:PHE:HE1	1.31	0.94
1:A:1010:LEU:HB2	1:A:1028:PHE:CD1	2.02	0.94
1:A:1733:THR:HG21	1:A:1877:LEU:HB3	1.47	0.94
1:A:3885:ARG:HE	1:A:3889:ARG:HD2	1.32	0.94
1:A:1883:ARG:HB2	1:A:1927:MSE:HE1	1.48	0.94
1:B:3923:ARG:HG2	1:B:3962:ARG:NH2	1.82	0.94
1:B:2416:LYS:O	1:B:2420:PHE:HB3	1.68	0.94
1:B:3772:ASN:HD22	1:B:3788:LEU:H	1.16	0.94
1:B:3722:PHE:HE1	1:B:3740:ILE:HG12	1.31	0.93
1:B:753:GLN:O	1:B:757:LYS:HB2	1.68	0.93
1:A:3923:ARG:HG2	1:A:3962:ARG:NH2	1.83	0.93
1:B:3920:ILE:HG13	1:B:3923:ARG:HD2	1.50	0.93
1:B:977:ASP:HB2	1:B:981:ARG:HB3	1.50	0.93
1:B:2891:ARG:NH2	1:B:3884:LYS:HD3	1.81	0.93
1:B:61:ARG:O	1:B:65:LEU:HB2	1.68	0.93
1:A:2443:MSE:HE3	1:A:2476:ILE:HB	1.48	0.93
1:A:3789:ARG:NH2	1:A:3806:LEU:HD22	1.83	0.93
1:B:1966:LEU:HD22	1:B:1991:PRO:HB3	1.50	0.93
1:A:964:ARG:HB2	1:A:1009:LEU:HD22	1.49	0.93
1:A:3521:ILE:O	1:A:3525:TYR:CB	2.16	0.93
1:A:473:PRO:HA	1:A:476:ARG:HH22	1.33	0.93
1:B:760:LEU:HD11	1:B:799:TYR:HB2	1.48	0.93
1:A:2549:LYS:HZ1	1:A:2557:LEU:HD22	1.30	0.92
1:B:659:ARG:HH22	1:B:662:LEU:HG	1.33	0.92
1:B:3462:ARG:HB2	1:B:3498:TRP:HB3	1.47	0.92
1:A:2330:VAL:HG21	1:A:2338:GLU:HB3	1.52	0.92
1:A:2457:PRO:HA	1:A:2460:GLU:HB2	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3872:ARG:HH11	1:A:3965:ARG:NH1	1.67	0.92
1:B:1949:ILE:HD12	1:B:1952:ILE:HG21	1.51	0.92
1:B:2330:VAL:HG22	1:B:2335:ASN:HA	1.51	0.92
1:B:756:PHE:HA	1:B:773:LEU:HD13	1.50	0.92
1:B:1343:GLU:O	1:B:1347:THR:OG1	1.88	0.92
1:B:1729:PHE:HE2	1:B:1870:LYS:HA	1.32	0.91
1:B:2390:HIS:HA	1:B:2397:CYS:HB2	1.52	0.91
1:A:3462:ARG:HB2	1:A:3498:TRP:HB3	1.49	0.91
1:B:970:LEU:HD22	1:B:1031:ARG:HH21	1.34	0.91
1:B:2330:VAL:HG21	1:B:2338:GLU:HB3	1.52	0.91
1:B:2011:ALA:HB3	1:B:2014:ALA:HB2	1.50	0.91
1:A:363:ILE:O	1:A:367:GLY:N	2.03	0.91
1:A:2375:ALA:O	1:A:2379:MSE:CB	2.19	0.91
1:A:616:LYS:O	1:A:620:PHE:HB2	1.71	0.91
1:B:808:GLU:HG2	1:B:852:ARG:HH21	1.31	0.91
1:B:1107:TYR:O	1:B:1110:SER:HB2	1.71	0.91
1:B:2361:ILE:HD12	1:B:2364:LEU:HD12	1.49	0.91
1:B:2559:THR:HG21	1:B:2808:LEU:HD13	1.53	0.91
1:B:1743:MSE:SE	1:B:1880:MSE:SE	2.90	0.90
1:A:3498:TRP:CD1	1:A:3502:MSE:HB2	2.05	0.90
1:B:1010:LEU:HD13	1:B:1028:PHE:HE1	1.36	0.90
1:B:3839:TYR:HE1	1:B:3867:THR:HB	1.36	0.90
1:B:429:GLU:O	1:B:431:TYR:N	2.04	0.90
1:A:1905:ILE:HG12	1:A:1951:VAL:HG11	1.51	0.90
1:A:1987:ARG:O	1:A:1991:PRO:HD3	1.71	0.90
1:A:2837:LEU:HD22	1:A:2868:LEU:HG	1.51	0.90
1:A:1106:ILE:O	1:A:1110:SER:N	2.05	0.89
1:A:1155:ARG:NH1	1:A:1155:ARG:O	2.04	0.89
1:B:4082:ARG:HG3	1:B:4091:ALA:HB2	1.54	0.89
1:B:2562:LEU:HD12	1:B:2812:LEU:HD21	1.53	0.89
1:A:1090:ARG:HH21	1:A:1100:VAL:HG11	1.35	0.89
1:A:2467:THR:HB	1:A:2518:GLN:HE22	1.35	0.89
1:A:2552:VAL:HG23	1:A:2852:PRO:HG2	1.54	0.89
1:B:1552:HIS:O	1:B:1555:HIS:ND1	2.05	0.89
1:B:2142:ILE:HA	1:B:2145:PHE:CD2	2.07	0.89
1:A:429:GLU:O	1:A:431:TYR:N	2.06	0.89
1:B:2352:HIS:HB3	1:B:2360:PHE:HB3	1.54	0.89
1:B:1651:LYS:HB2	1:B:1684:LEU:HD11	1.53	0.89
1:B:3887:PHE:HB3	1:B:3897:PHE:CE1	2.08	0.89
1:A:1931:ASN:O	1:A:1938:ARG:NH2	2.06	0.89
1:A:3816:LEU:HD13	1:A:3966:GLN:HE22	1.36	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3696:ARG:NH1	1:A:3720:ALA:O	2.05	0.88
1:B:3259:LEU:O	1:B:3263:HIS:HB2	1.73	0.88
1:B:2891:ARG:HD3	1:B:3972:LEU:HD22	1.55	0.88
1:A:1729:PHE:HE2	1:A:1870:LYS:HA	1.39	0.88
1:A:2957:LEU:HB3	1:A:3989:ARG:NH1	1.87	0.88
1:B:993:HIS:HB2	1:B:1038:LYS:HG2	1.55	0.88
1:B:3048:LYS:HD3	1:B:3061:LEU:HD23	1.55	0.88
1:B:3762:GLN:HA	1:B:3793:VAL:HG21	1.54	0.88
1:B:473:PRO:HA	1:B:476:ARG:HH22	1.36	0.88
1:A:2390:HIS:HA	1:A:2397:CYS:HB2	1.54	0.88
1:B:1241:LEU:HD11	1:B:1253:THR:HG21	1.54	0.88
1:B:2326:ILE:O	1:B:2330:VAL:HB	1.74	0.88
1:A:1010:LEU:HB2	1:A:1028:PHE:HD1	1.36	0.88
1:B:3923:ARG:O	1:B:3962:ARG:NH1	2.07	0.88
1:A:3589:SER:O	1:A:3593:ARG:HB2	1.74	0.88
1:A:3772:ASN:HB2	1:A:3787:GLN:HG3	1.55	0.88
1:A:801:LYS:HB2	1:A:805:LEU:HD12	1.56	0.88
1:B:1582:LEU:HD22	1:B:1600:MSE:HE1	1.52	0.88
1:A:90:CYS:HB3	1:A:137:THR:HG22	1.56	0.88
1:A:3772:ASN:ND2	1:A:3788:LEU:O	2.06	0.88
1:A:185:HIS:H	1:A:186:PRO:HD2	1.38	0.88
1:A:2022:PRO:HB2	1:A:2072:ARG:HH21	1.36	0.88
1:A:658:THR:HA	1:A:733:LEU:HD22	1.55	0.88
1:B:1018:VAL:HB	1:B:1074:LYS:HB2	1.54	0.88
1:B:741:ILE:O	1:B:744:ASP:N	2.05	0.88
1:B:662:LEU:O	1:B:666:PHE:CB	2.20	0.87
1:B:658:THR:HA	1:B:733:LEU:HD22	1.55	0.87
1:A:473:PRO:HA	1:A:476:ARG:NH2	1.88	0.87
1:A:535:LEU:HD21	1:A:623:PHE:HA	1.55	0.87
1:B:1808:ASP:HB2	1:B:1814:PHE:HB3	1.54	0.87
1:B:2546:TYR:CE1	1:B:2558:ALA:HB2	2.09	0.87
1:A:105:VAL:HG21	1:A:149:ILE:HD13	1.53	0.87
1:B:252:VAL:HG11	1:B:265:TYR:HB2	1.56	0.87
1:A:3003:ASN:ND2	1:A:3014:CYS:SG	2.47	0.87
1:A:2378:PHE:HE1	1:A:2408:MSE:HE1	1.40	0.87
1:B:2307:MSE:HB3	1:B:2348:GLN:HE22	1.39	0.87
1:A:2477:LEU:O	1:A:2481:HIS:HB3	1.74	0.87
1:B:591:GLN:OE1	1:B:1026:ARG:NH1	2.08	0.87
1:B:2253:TYR:HD1	1:B:2256:ILE:HD12	1.37	0.86
1:A:866:ILE:HD13	1:A:3129:LEU:HB3	1.57	0.86
1:B:3530:VAL:HG11	1:B:3702:PRO:HD3	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1107:TYR:O	1:A:1110:SER:HB2	1.74	0.86
1:A:3492:CYS:O	1:A:3495:PHE:HB3	1.74	0.86
1:B:2286:PRO:HB2	1:B:2289:ASP:HA	1.57	0.86
1:A:1407:LYS:O	1:A:1409:SER:N	2.08	0.86
1:A:1919:CYS:O	1:A:1923:PHE:HB2	1.76	0.86
1:A:793:LEU:HA	1:A:796:LEU:HG	1.58	0.86
1:A:2563:LEU:O	1:A:2567:SER:OG	1.93	0.86
1:B:2837:LEU:HA	1:B:2840:PHE:HD2	1.40	0.86
1:A:1603:GLN:OE1	1:A:1606:ARG:NH2	2.08	0.86
1:A:4071:ALA:O	1:A:4075:ARG:HB3	1.76	0.86
1:B:2253:TYR:HB2	1:B:2291:GLN:HG2	1.56	0.86
1:B:2443:MSE:SE	1:B:2476:ILE:HB	2.25	0.86
1:A:1749:ALA:HA	1:A:1752:LEU:HD12	1.55	0.86
1:B:3167:ARG:HH11	1:B:3167:ARG:HG3	1.40	0.86
1:B:658:THR:HG22	1:B:659:ARG:NH1	1.89	0.86
1:A:3326:GLN:HB2	1:A:3393:GLU:HG2	1.56	0.86
1:A:659:ARG:HH22	1:A:662:LEU:HG	1.41	0.86
1:A:1762:MSE:SE	1:A:1896:ILE:HG23	2.26	0.85
1:A:3581:PRO:HG2	1:A:3674:SER:HB2	1.58	0.85
1:B:1733:THR:HG21	1:B:1877:LEU:HB3	1.55	0.85
1:A:2142:ILE:HA	1:A:2145:PHE:CD2	2.11	0.85
1:B:745:VAL:HG11	1:B:776:TRP:HZ2	1.39	0.85
1:A:527:TYR:OH	1:A:615:ALA:O	1.93	0.85
1:A:1010:LEU:HA	1:A:1013:ILE:HG12	1.56	0.85
1:B:2358:ASP:HB2	1:B:2396:LEU:HD21	1.57	0.85
1:B:3326:GLN:HB2	1:B:3393:GLU:HG2	1.57	0.85
1:B:3868:VAL:O	1:B:3872:ARG:CB	2.24	0.85
1:A:3613:MSE:HE1	1:A:3617:LEU:HD12	1.56	0.85
1:A:4007:LYS:HG3	1:A:4041:ARG:HD2	1.55	0.85
1:B:3632:PHE:O	1:B:3637:GLY:N	2.08	0.85
1:A:2330:VAL:HG22	1:A:2335:ASN:HA	1.57	0.85
1:B:3487:ILE:HG21	1:B:3495:PHE:HB2	1.58	0.85
1:B:725:LEU:O	1:B:728:SER:OG	1.94	0.85
1:A:2043:PHE:O	1:A:2047:THR:OG1	1.93	0.85
1:B:2227:LYS:HD2	1:B:2235:LEU:HG	1.58	0.85
1:B:2375:ALA:O	1:B:2379:MSE:HB3	1.76	0.85
1:B:2478:MSE:O	1:B:2482:ASP:HB3	1.76	0.85
1:A:971:ARG:HG3	1:A:972:LEU:N	1.90	0.85
1:A:2007:ILE:HG22	1:A:2009:LYS:HB2	1.57	0.85
1:B:2070:GLU:HG3	1:B:2072:ARG:HG3	1.57	0.85
1:B:3589:SER:O	1:B:3593:ARG:HB2	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:974:CYS:HA	1:A:981:ARG:CD	2.07	0.84
1:B:1010:LEU:HB2	1:B:1028:PHE:HD1	1.40	0.84
1:B:2481:HIS:HE1	1:B:2485:ARG:NH1	1.75	0.84
1:B:3583:LEU:HD11	1:B:3733:ARG:HB3	1.57	0.84
1:A:2161:ALA:HA	1:A:2164:TRP:HD1	1.42	0.84
1:B:2300:PHE:CZ	1:B:2341:LEU:HB2	2.12	0.84
1:B:3811:THR:OG1	1:B:3813:LYS:NZ	2.09	0.84
1:A:2292:CYS:HB3	1:A:2300:PHE:HB2	1.57	0.84
1:A:2837:LEU:HA	1:A:2840:PHE:HD2	1.41	0.84
1:B:2196:TRP:CD2	1:B:2199:LEU:HD11	2.12	0.84
1:B:3182:ILE:HB	1:B:3186:ARG:NH1	1.91	0.84
1:A:286:LEU:HB2	1:A:290:TYR:HB2	1.59	0.84
1:B:978:GLN:HA	1:B:981:ARG:HE	1.42	0.84
1:B:3243:ILE:HG12	1:B:3258:LEU:HD11	1.58	0.84
1:B:3725:ARG:HH12	1:B:3737:ARG:NH2	1.74	0.84
1:B:3879:PRO:HA	1:B:3882:LEU:HB2	1.58	0.84
1:A:3174:ASP:H	1:A:3175:PRO:HD2	1.42	0.84
1:A:3868:VAL:HG11	1:A:4114:PRO:HB3	1.60	0.84
1:B:3117:ILE:HD12	1:B:3125:ARG:NH1	1.91	0.84
1:A:3092:LEU:HA	1:A:3192:LYS:HE3	1.58	0.84
1:A:361:ILE:HB	1:A:364:ARG:NH2	1.92	0.84
1:B:1162:SER:H	1:B:1165:LEU:HD12	1.42	0.84
1:B:2552:VAL:HG23	1:B:2852:PRO:HG2	1.57	0.84
1:B:3486:GLU:HG3	1:B:3487:ILE:H	1.43	0.84
1:B:3858:MSE:HE3	1:B:4119:ARG:HA	1.60	0.84
1:B:2161:ALA:HA	1:B:2164:TRP:HD1	1.43	0.84
1:B:2329:TYR:O	1:B:2333:ARG:N	2.11	0.84
1:A:1410:PRO:HB2	1:A:1414:ILE:HD12	1.58	0.84
1:A:1743:MSE:O	1:A:1747:LEU:HB2	1.78	0.83
1:A:1992:VAL:O	1:A:1996:VAL:HG22	1.78	0.83
1:A:2542:LEU:HB2	1:A:2546:TYR:HE2	1.42	0.83
1:B:3687:MSE:O	1:B:3689:ASP:N	2.11	0.83
1:B:2152:ASN:HB3	1:B:2153:THR:HA	1.60	0.83
1:B:3900:LEU:HD21	1:B:3935:GLY:HA3	1.59	0.83
1:B:4103:GLN:O	1:B:4107:LEU:HB2	1.77	0.83
1:A:2415:LEU:O	1:A:2419:ASP:HB2	1.78	0.83
1:A:968:VAL:HG23	1:A:971:ARG:HD3	1.60	0.83
1:B:2813:PHE:HD2	1:B:2859:GLN:HG3	1.43	0.83
1:B:3499:ILE:HG23	1:B:3535:ILE:HD13	1.60	0.83
1:B:971:ARG:HG3	1:B:972:LEU:N	1.93	0.83
1:A:352:VAL:HG23	1:A:357:LYS:H	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3521:ILE:O	1:B:3525:TYR:CB	2.27	0.83
1:B:2274:ILE:HD13	1:B:2318:ALA:HB2	1.60	0.83
1:A:4090:ARG:HH11	1:A:4106:CYS:HA	1.41	0.83
1:A:61:ARG:O	1:A:65:LEU:HB2	1.77	0.83
1:B:1073:PHE:HD1	1:B:1074:LYS:H	1.27	0.83
1:B:609:ALA:H	1:B:1798:LEU:HD12	1.43	0.83
1:B:3725:ARG:NH1	1:B:3737:ARG:HH22	1.76	0.83
2:K:106:UNK:O	2:K:110:UNK:N	2.11	0.83
1:A:2361:ILE:HD12	1:A:2364:LEU:HD12	1.61	0.83
1:A:2478:MSE:O	1:A:2482:ASP:HB3	1.78	0.83
1:B:658:THR:HG22	1:B:659:ARG:HH11	1.41	0.83
1:A:1886:LYS:HZ2	1:A:1924:THR:HB	1.44	0.83
1:B:215:PRO:HG3	1:B:251:PHE:HB3	1.59	0.83
1:B:2435:CYS:O	1:B:2439:ILE:HB	1.77	0.83
1:B:245:SER:HA	1:B:248:ILE:HD12	1.58	0.83
1:B:1087:ARG:HD3	1:B:1134:LEU:HB3	1.60	0.83
1:B:3012:GLU:HB2	1:B:3050:LYS:NZ	1.94	0.83
1:A:575:ILE:HA	1:A:578:LYS:HB2	1.61	0.83
1:B:3034:PRO:HG2	1:B:3037:GLN:HB2	1.61	0.83
1:A:1138:ILE:HD13	1:A:1150:LYS:HE2	1.60	0.82
1:A:3961:PHE:CE1	1:A:3963:LEU:HB2	2.14	0.82
1:A:3972:LEU:O	1:A:3974:MSE:N	2.10	0.82
1:B:2957:LEU:HD22	1:B:4100:GLU:HG3	1.61	0.82
1:B:598:PRO:HB3	1:B:1022:ASP:HB2	1.59	0.82
1:B:1010:LEU:HB2	1:B:1028:PHE:CD1	2.14	0.82
1:A:1751:GLU:O	1:A:1755:SER:N	2.11	0.82
1:B:3737:ARG:HH11	1:B:3739:ILE:HD11	1.43	0.82
1:B:3816:LEU:HD21	1:B:3883:LEU:HD13	1.59	0.82
1:A:1651:LYS:HB3	1:A:1680:ALA:HB1	1.59	0.82
1:A:2196:TRP:CD2	1:A:2199:LEU:HD11	2.14	0.82
1:A:1007:VAL:O	1:A:1011:GLU:HB2	1.79	0.82
1:A:2002:LYS:O	1:A:2004:TYR:N	2.12	0.82
1:A:1070:PRO:HB2	1:A:1073:PHE:CZ	2.14	0.82
1:A:2049:VAL:HA	1:A:2052:TYR:HD2	1.42	0.82
1:A:203:GLU:O	1:A:207:GLN:HB2	1.78	0.82
1:A:3722:PHE:HE1	1:A:3740:ILE:HG12	1.44	0.82
1:A:4057:ALA:HB3	1:A:4059:ILE:HB	1.60	0.82
1:B:3751:LEU:O	1:B:3802:LEU:HG	1.80	0.82
1:A:3789:ARG:HH22	1:A:3806:LEU:HD22	1.42	0.82
1:A:70:ARG:HD3	1:A:82:ARG:HD3	1.59	0.82
1:A:959:TYR:O	1:A:963:LYS:HB2	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2375:ALA:O	1:B:2379:MSE:CB	2.28	0.82
1:B:488:ILE:HG21	1:B:616:LYS:HD2	1.60	0.82
1:A:3152:SER:HB3	1:A:3153:SER:HB3	1.61	0.82
1:B:1346:THR:HG21	1:B:1401:ASN:HB3	1.62	0.82
1:B:1729:PHE:CE2	1:B:1870:LYS:HA	2.15	0.82
1:A:3820:MSE:HA	1:A:3882:LEU:HD22	1.62	0.81
1:A:978:GLN:HA	1:A:981:ARG:HE	1.44	0.81
1:B:2126:MSE:HG3	1:B:2129:LEU:HD12	1.61	0.81
1:B:2531:LEU:HG	1:B:2538:ARG:HB2	1.62	0.81
1:B:974:CYS:HA	1:B:981:ARG:CD	2.07	0.81
1:A:3872:ARG:O	1:A:3876:SER:OG	1.98	0.81
1:B:3449:LYS:HA	1:B:3452:LYS:HD2	1.62	0.81
1:B:956:PRO:HB2	1:B:957:PRO:HD3	1.62	0.81
1:A:1155:ARG:HH12	1:A:1159:PRO:HD3	1.45	0.81
1:A:1696:LEU:HA	1:A:1700:THR:HG21	1.61	0.81
1:A:3762:GLN:HA	1:A:3793:VAL:HG21	1.62	0.81
1:B:1729:PHE:CZ	1:B:1870:LYS:HG3	2.15	0.81
1:B:1744:LYS:HG3	1:B:1880:MSE:HE3	1.60	0.81
1:B:1930:GLU:N	1:B:1930:GLU:OE2	2.13	0.81
1:B:3044:MSE:O	1:B:3047:SER:OG	1.96	0.81
1:A:2167:PRO:O	1:A:2171:LEU:CB	2.28	0.81
1:B:1987:ARG:O	1:B:1991:PRO:HD3	1.80	0.81
1:A:2167:PRO:O	1:A:2171:LEU:HB2	1.79	0.81
1:B:3498:TRP:CD1	1:B:3502:MSE:HB2	2.14	0.81
1:B:3572:ILE:HA	1:B:3575:LEU:HD22	1.62	0.81
1:A:2538:ARG:NH1	1:A:2562:LEU:O	2.13	0.81
1:A:3269:ARG:NH1	1:A:3312:VAL:HA	1.96	0.81
1:B:1877:LEU:O	1:B:1920:TYR:OH	1.98	0.81
1:B:3238:MSE:SE	1:B:3242:MSE:SE	2.99	0.81
1:B:431:TYR:HA	1:B:434:VAL:HG12	1.63	0.81
1:A:1080:LEU:HD12	1:A:1081:ALA:H	1.46	0.81
1:B:2260:PHE:HD1	1:B:2274:ILE:HG22	1.46	0.81
1:B:916:GLU:HB3	1:B:930:ALA:HB1	1.63	0.81
1:A:741:ILE:O	1:A:744:ASP:N	2.09	0.81
1:B:2031:LEU:HB2	1:B:2033:ASP:HB2	1.61	0.81
1:A:1729:PHE:CZ	1:A:1870:LYS:HG3	2.16	0.81
1:A:2239:LYS:HG3	1:A:2279:ILE:HG23	1.62	0.81
1:A:3319:ASN:HD22	1:A:3407:ALA:HB1	1.45	0.81
1:A:382:ASP:O	1:A:386:VAL:HB	1.79	0.81
1:B:1017:ILE:HG21	1:B:1025:LEU:HD22	1.63	0.81
1:A:1594:SER:O	1:A:1598:ASN:HB2	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1090:ARG:HH21	1:B:1100:VAL:HG11	1.45	0.81
1:A:977:ASP:HB3	1:A:981:ARG:H	1.46	0.81
1:B:2379:MSE:HE1	1:B:2404:ARG:HD3	1.61	0.81
1:B:2446:LEU:O	1:B:2451:LEU:HB2	1.81	0.81
1:B:891:ARG:HE	1:B:894:PHE:HB3	1.46	0.81
1:A:1552:HIS:O	1:A:1555:HIS:ND1	2.14	0.80
1:A:970:LEU:CD2	1:A:1031:ARG:HH21	1.94	0.80
1:B:959:TYR:O	1:B:963:LYS:HB2	1.81	0.80
1:A:3872:ARG:HH11	1:A:3965:ARG:HH12	1.27	0.80
1:A:459:ARG:HG2	1:A:540:MSE:HE1	1.60	0.80
1:B:1729:PHE:HZ	1:B:1870:LYS:HG3	1.45	0.80
1:B:3530:VAL:HG21	1:B:3701:ILE:HA	1.63	0.80
1:A:2559:THR:HG21	1:A:2808:LEU:HD13	1.61	0.80
1:A:805:LEU:HD22	1:A:3125:ARG:HH11	1.45	0.80
1:B:1090:ARG:HH12	1:B:1096:VAL:HG13	1.45	0.80
1:B:893:SER:HB3	1:B:906:PHE:HB2	1.63	0.80
1:B:931:CYS:SG	1:B:984:TYR:OH	2.39	0.80
1:A:2243:GLU:HA	1:A:2246:LYS:HD2	1.63	0.80
1:B:266:ALA:HB2	1:B:308:LEU:HG	1.63	0.80
1:A:3638:LYS:HA	1:A:3641:ASP:HB2	1.63	0.80
1:A:369:PHE:CD1	1:A:416:SER:HA	2.17	0.80
1:A:619:ASP:O	1:A:622:ALA:N	2.14	0.80
1:B:2253:TYR:CD1	1:B:2256:ILE:HD12	2.16	0.80
1:A:725:LEU:O	1:A:728:SER:OG	1.99	0.80
1:B:1996:VAL:HG11	1:B:2048:GLY:HA2	1.63	0.80
1:A:939:MSE:SE	1:A:2783:ILE:HG12	2.30	0.80
1:A:3046:ARG:NH2	1:A:3181:ASP:OD2	2.14	0.80
1:A:627:VAL:HG12	1:A:628:GLU:H	1.46	0.80
1:B:295:GLU:HA	1:B:298:LEU:HD22	1.63	0.80
1:A:1429:GLU:O	1:A:1433:ALA:HB2	1.81	0.79
1:A:705:ALA:HB1	1:A:1385:ASN:HD21	1.46	0.79
1:B:16:GLN:O	1:B:20:SER:HB3	1.81	0.79
1:B:3255:ALA:O	1:B:3282:ARG:NH2	2.15	0.79
1:B:1112:ALA:HA	1:B:1115:HIS:CE1	2.17	0.79
1:B:2546:TYR:HE1	1:B:2558:ALA:HB2	1.43	0.79
1:A:2861:ILE:HG21	1:A:2889:GLY:HA2	1.61	0.79
1:B:286:LEU:HB2	1:B:290:TYR:HB2	1.65	0.79
1:B:3252:PHE:HA	1:B:3282:ARG:HD2	1.65	0.79
1:B:1918:LEU:HD11	1:B:1957:ASN:HB3	1.63	0.79
1:B:2423:VAL:O	1:B:2425:ARG:N	2.15	0.79
1:B:2837:LEU:HD22	1:B:2868:LEU:HG	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2987:THR:HB	1:B:2991:LYS:H	1.46	0.79
1:B:726:LEU:HA	1:B:729:CYS:SG	2.22	0.79
1:A:1886:LYS:HG3	1:A:1890:HIS:HE1	1.46	0.79
1:A:770:LEU:HD12	1:A:851:ILE:HD13	1.61	0.79
1:B:1410:PRO:HB2	1:B:1414:ILE:HD12	1.64	0.79
1:A:2474:TYR:HB3	1:A:2478:MSE:HE3	1.64	0.79
1:A:3989:ARG:HH21	1:A:4100:GLU:CB	1.95	0.79
1:B:12:LEU:HD22	1:B:38:LEU:HA	1.65	0.79
1:A:3450:MSE:SE	1:A:3464:LYS:HG2	2.33	0.79
1:B:637:LYS:O	1:B:641:PHE:HB3	1.81	0.79
1:A:2351:GLN:O	1:A:2355:THR:OG1	2.00	0.79
1:B:1718:ILE:HG23	1:B:1750:LEU:HD11	1.62	0.79
1:B:298:LEU:HD23	1:B:316:LEU:HD13	1.62	0.79
1:A:1000:LYS:O	1:A:1002:GLU:N	2.15	0.79
1:A:796:LEU:HA	1:A:799:TYR:CE2	2.18	0.79
1:A:767:GLU:HG3	1:A:851:ILE:HD11	1.65	0.79
1:B:1655:ILE:HG23	1:B:1677:SER:HB3	1.65	0.79
1:B:2121:ASP:HA	1:B:2126:MSE:HB3	1.63	0.79
1:B:2443:MSE:HB3	1:B:2480:ILE:HG12	1.65	0.79
1:A:162:LEU:HD21	1:A:196:LEU:HD13	1.65	0.79
1:A:3955:VAL:HG12	1:A:4027:TRP:HE1	1.47	0.79
1:B:527:TYR:OH	1:B:619:ASP:N	2.16	0.79
1:B:627:VAL:HG12	1:B:628:GLU:H	1.46	0.79
1:A:3314:SER:HA	1:A:3315:TYR:HB3	1.64	0.78
1:A:3397:GLN:HE22	1:A:3449:LYS:HD3	1.49	0.78
1:A:714:VAL:HG13	1:A:734:LEU:HD13	1.65	0.78
1:B:1011:GLU:OE2	1:B:1062:ARG:NE	2.17	0.78
1:B:1029:CYS:HB3	1:B:1085:ILE:HG13	1.63	0.78
1:A:2890:ILE:HG21	1:A:2922:ARG:HH12	1.49	0.78
1:B:1762:MSE:SE	1:B:1896:ILE:HG23	2.33	0.78
1:B:2100:LEU:O	1:B:2104:MSE:HB2	1.82	0.78
1:B:2153:THR:OG1	1:B:2154:GLU:N	2.14	0.78
1:A:3736:LYS:HB3	1:A:3752:VAL:HB	1.64	0.78
1:A:3868:VAL:O	1:A:3872:ARG:CB	2.29	0.78
1:B:1986:ARG:HH12	1:B:2036:LEU:HD22	1.46	0.78
1:A:15:LEU:HD23	1:A:2359:LYS:HZ3	1.48	0.78
1:A:2379:MSE:HE1	1:A:2404:ARG:HH11	1.49	0.78
1:A:903:PRO:HB2	1:A:2811:SER:HB2	1.65	0.78
1:B:1802:TYR:HA	1:B:1805:PHE:HD2	1.47	0.78
1:B:2911:ARG:HG2	1:B:2914:ALA:HB3	1.66	0.78
1:B:538:ASP:HB3	1:B:627:VAL:HG13	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3499:ILE:HG23	1:A:3535:ILE:HD13	1.63	0.78
1:A:3904:PHE:O	1:A:3907:SER:OG	2.01	0.78
1:B:3529:ILE:HG23	1:B:3532:PRO:HD2	1.63	0.78
1:B:439:VAL:HG11	1:B:479:ILE:HD13	1.65	0.78
1:A:2467:THR:HA	1:A:2470:ARG:HG3	1.64	0.78
1:A:376:ILE:HG13	1:A:381:VAL:HG21	1.65	0.78
1:B:808:GLU:CG	1:B:852:ARG:HH21	1.96	0.78
1:A:960:GLN:HG3	1:A:1009:LEU:HD21	1.65	0.78
1:B:3575:LEU:HG	1:B:3687:MSE:HG2	1.65	0.78
1:B:3923:ARG:NH2	1:B:3941:ASP:O	2.17	0.78
1:A:980:THR:HG23	1:A:984:TYR:HE1	1.49	0.78
1:B:281:GLN:HA	1:B:326:MSE:SE	2.34	0.78
1:A:1582:LEU:HD22	1:A:1600:MSE:HE1	1.66	0.77
1:A:3922:ASP:O	1:A:3927:ASN:ND2	2.17	0.77
1:B:2538:ARG:NH1	1:B:2565:MSE:HB3	1.98	0.77
1:B:3421:ASP:OD2	1:B:3464:LYS:NZ	2.16	0.77
1:A:87:LYS:HG2	1:A:133:LYS:HG3	1.66	0.77
1:A:1886:LYS:HG3	1:A:1890:HIS:CE1	2.19	0.77
1:A:2190:VAL:HG21	1:A:2241:LEU:HD13	1.66	0.77
1:A:3479:THR:O	1:A:3483:MSE:HB2	1.83	0.77
1:B:1407:LYS:O	1:B:1409:SER:N	2.14	0.77
1:B:2193:ILE:HA	1:B:2196:TRP:CZ2	2.20	0.77
1:B:909:VAL:HG13	1:B:913:ARG:NH1	1.96	0.77
1:A:1640:GLU:O	1:A:1644:ALA:HB2	1.85	0.77
1:A:1890:HIS:HB3	1:A:1937:ARG:HA	1.65	0.77
1:A:2253:TYR:CD1	1:A:2256:ILE:HD12	2.18	0.77
1:A:2879:GLY:HA2	1:A:2886:GLN:HG2	1.65	0.77
1:B:3684:SER:O	1:B:3688:SER:OG	2.01	0.77
1:B:3732:LEU:HD21	1:B:3926:ASN:HD21	1.48	0.77
1:A:1073:PHE:HD1	1:A:1074:LYS:H	1.30	0.77
1:A:1374:GLN:HB3	1:A:1377:CYS:HB3	1.64	0.77
1:A:1590:THR:O	1:A:1592:MSE:N	2.16	0.77
1:A:1718:ILE:HA	1:A:1725:GLN:HE21	1.50	0.77
1:A:1946:ASN:ND2	1:A:1993:GLU:OE2	2.17	0.77
1:B:2235:LEU:O	1:B:2239:LYS:N	2.16	0.77
1:B:2457:PRO:HA	1:B:2460:GLU:HB2	1.66	0.77
1:B:979:VAL:HG21	1:B:2656:UNK:HA	1.66	0.77
1:B:3137:GLU:OE1	1:B:3167:ARG:NH1	2.18	0.77
1:B:805:LEU:HD22	1:B:3125:ARG:NH1	2.00	0.77
1:A:2412:TYR:HE1	1:A:2415:LEU:HD23	1.48	0.77
1:A:2467:THR:HG22	1:A:2470:ARG:NH1	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:SER:O	1:A:556:SER:OG	2.02	0.77
1:A:977:ASP:HB2	1:A:981:ARG:HB3	1.64	0.77
1:B:1080:LEU:HD13	1:B:1127:CYS:HB3	1.66	0.77
1:A:2083:LEU:O	1:A:2087:GLU:N	2.17	0.77
1:A:2161:ALA:HA	1:A:2164:TRP:CD1	2.19	0.77
1:A:2847:THR:HB	1:A:2850:PHE:CD2	2.20	0.77
1:A:2891:ARG:NH2	1:A:3884:LYS:HD3	2.00	0.77
1:B:2300:PHE:HZ	1:B:2341:LEU:HB2	1.46	0.77
1:B:3148:GLN:HB2	1:B:3156:PRO:HB3	1.67	0.77
1:B:852:ARG:NH1	1:B:3111:MSE:SE	2.68	0.77
1:A:2049:VAL:HG11	1:A:2100:LEU:HD12	1.66	0.77
1:A:2890:ILE:HG21	1:A:2922:ARG:NH1	2.00	0.77
1:B:2459:VAL:HG21	1:B:2501:LEU:HD21	1.67	0.77
1:B:4057:ALA:HB3	1:B:4059:ILE:HB	1.65	0.77
1:A:2462:VAL:HB	1:A:2473:MSE:SE	2.35	0.77
1:A:3704:GLN:HB2	1:A:3796:MSE:HE2	1.66	0.77
1:A:3813:LYS:HE2	1:A:3926:ASN:HB2	1.67	0.77
1:A:67:VAL:O	1:A:71:LYS:HB2	1.83	0.77
1:B:2236:GLU:HA	1:B:2239:LYS:HB3	1.67	0.77
1:B:3152:SER:HB3	1:B:3153:SER:HB3	1.65	0.77
1:B:3923:ARG:CG	1:B:3962:ARG:HH22	1.97	0.77
1:B:385:TYR:HD1	1:B:420:VAL:HG13	1.49	0.77
1:B:446:PHE:HA	1:B:449:TYR:CE2	2.20	0.77
1:B:936:SER:HB3	1:B:2791:ILE:HG12	1.66	0.77
1:A:1343:GLU:O	1:A:1347:THR:HB	1.85	0.77
1:A:753:GLN:O	1:A:757:LYS:HB2	1.84	0.77
1:B:1350:ASN:HD21	1:B:1404:LYS:HG2	1.47	0.77
1:B:1919:CYS:O	1:B:1923:PHE:HB2	1.85	0.77
1:B:323:VAL:O	1:B:327:VAL:HB	1.84	0.77
1:B:1469:PRO:HA	1:B:1472:SER:HB3	1.67	0.77
1:A:1356:TRP:CZ2	1:A:1409:SER:HB3	2.20	0.76
1:A:2239:LYS:O	1:A:2242:VAL:HB	1.85	0.76
1:A:2220:MSE:SE	1:A:2256:ILE:HD11	2.34	0.76
1:A:2560:ASN:HB2	1:A:2800:ARG:HD3	1.66	0.76
1:B:2382:VAL:HG21	1:B:2404:ARG:HG3	1.64	0.76
1:B:3590:ASN:OD1	1:B:3593:ARG:NH2	2.18	0.76
1:A:1086:TYR:HE2	1:A:1090:ARG:HE	1.33	0.76
1:A:1930:GLU:OE1	1:A:1987:ARG:NH1	2.18	0.76
1:A:2809:PHE:HB3	1:A:2859:GLN:NE2	1.99	0.76
1:A:46:SER:H	1:A:51:LEU:HD13	1.49	0.76
1:B:16:GLN:O	1:B:20:SER:CB	2.32	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:942:LEU:HD22	1:B:2783:ILE:HG21	1.67	0.76
1:A:1081:ALA:O	1:A:1085:ILE:HG12	1.86	0.76
1:A:3057:ALA:HB1	1:A:3062:LEU:HD11	1.67	0.76
1:A:805:LEU:CD2	1:A:3125:ARG:HH11	1.99	0.76
1:B:1987:ARG:O	1:B:1990:PHE:N	2.18	0.76
1:A:2253:TYR:CE2	1:A:2287:PRO:HB3	2.19	0.76
1:A:890:LYS:HG3	1:A:891:ARG:HD3	1.66	0.76
1:B:2473:MSE:O	1:B:2476:ILE:HG12	1.85	0.76
1:B:3019:ILE:HG23	1:B:3021:SER:H	1.51	0.76
1:A:1966:LEU:HD22	1:A:1991:PRO:HB3	1.66	0.76
1:B:1594:SER:O	1:B:1598:ASN:HB2	1.85	0.76
1:B:2147:ALA:HB1	1:B:2151:ILE:HD12	1.67	0.76
1:B:2281:MSE:HE2	1:B:2322:VAL:HA	1.66	0.76
1:B:2883:SER:O	1:B:2886:GLN:HG3	1.84	0.76
1:A:2397:CYS:O	1:A:2401:VAL:HB	1.86	0.76
1:A:971:ARG:HG3	1:A:972:LEU:H	1.50	0.76
1:B:3479:THR:O	1:B:3483:MSE:HB2	1.86	0.76
1:B:891:ARG:HE	1:B:894:PHE:CB	1.99	0.76
1:A:3243:ILE:HD13	1:A:3262:LEU:HD22	1.65	0.76
1:A:385:TYR:CD1	1:A:420:VAL:HG13	2.18	0.76
1:A:638:GLN:HE22	1:A:669:LEU:HB2	1.51	0.76
1:B:1178:ARG:HB3	1:B:1179:PRO:HD3	1.68	0.76
1:B:185:HIS:H	1:B:186:PRO:HD2	1.49	0.76
1:B:2453:GLU:O	1:B:2457:PRO:HD3	1.85	0.76
1:A:1655:ILE:HD13	1:A:1681:ASP:HB3	1.68	0.76
1:A:2364:LEU:O	1:A:2368:THR:OG1	2.03	0.76
1:B:1138:ILE:HG21	1:B:1150:LYS:HE2	1.68	0.76
1:B:2891:ARG:HH22	1:B:3884:LYS:CD	1.88	0.76
1:B:3629:ARG:HH22	1:B:3638:LYS:NZ	1.84	0.76
1:B:576:VAL:HG13	1:B:601:TRP:HE3	1.51	0.76
1:A:3019:ILE:HG23	1:A:3021:SER:H	1.49	0.76
1:B:1091:GLU:HG2	1:B:1137:ILE:HG21	1.68	0.76
1:B:138:PHE:HD2	1:B:173:LYS:HE3	1.51	0.76
1:B:904:VAL:O	1:B:906:PHE:N	2.18	0.76
1:A:1700:THR:HA	1:A:1703:THR:HB	1.67	0.76
1:A:2313:LYS:HA	1:A:2316:TYR:CE2	2.21	0.76
1:B:1036:PHE:HA	1:B:1055:ASN:HD21	1.50	0.76
1:B:1070:PRO:HD3	1:B:1075:ARG:HD2	1.67	0.76
1:B:3534:ILE:HG12	1:B:3704:GLN:NE2	1.99	0.76
1:A:1007:VAL:O	1:A:1011:GLU:CB	2.33	0.75
1:A:1060:PHE:HA	1:A:1063:LEU:HD12	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LEU:H	1:A:143:LEU:HD12	1.51	0.75
1:A:3176:MSE:HE2	1:A:3251:ASN:ND2	2.01	0.75
1:A:891:ARG:HG3	1:A:894:PHE:HB2	1.68	0.75
1:A:926:THR:O	1:A:930:ALA:HB3	1.85	0.75
1:A:3487:ILE:HG21	1:A:3495:PHE:HB2	1.67	0.75
1:A:661:PRO:HG2	1:A:733:LEU:HA	1.67	0.75
1:B:2062:ALA:HB1	1:B:2066:PHE:HE2	1.52	0.75
1:B:2542:LEU:HB2	1:B:2546:TYR:HE2	1.51	0.75
1:B:3520:GLU:OE1	1:B:3524:ASN:ND2	2.19	0.75
1:B:3872:ARG:O	1:B:3876:SER:OG	2.00	0.75
1:B:3989:ARG:HH21	1:B:4100:GLU:CG	1.99	0.75
1:A:2183:HIS:CE1	1:A:2237:ILE:HG21	2.21	0.75
1:A:3487:ILE:HD11	1:A:3498:TRP:HH2	1.51	0.75
1:B:608:PRO:HG2	1:B:1798:LEU:HG	1.68	0.75
1:B:19:LEU:O	1:B:23:ASP:CB	2.33	0.75
1:B:3284:SER:CB	1:B:3287:ARG:HH21	1.99	0.75
1:A:1637:SER:O	1:A:1640:GLU:N	2.19	0.75
1:A:1751:GLU:HG2	1:A:1870:LYS:HE2	1.68	0.75
1:A:3305:SER:HA	1:A:3308:ASP:HB3	1.68	0.75
1:A:1118:GLU:HG3	1:A:3743:HIS:HE1	1.51	0.75
1:A:1587:VAL:HB	1:A:1643:MSE:HE2	1.68	0.75
1:A:2449:VAL:HA	1:A:2452:ARG:HD2	1.67	0.75
1:A:3979:LEU:HA	1:A:3981:TYR:HB3	1.67	0.75
1:B:1039:TRP:HZ2	1:B:1049:GLN:HA	1.52	0.75
1:B:1356:TRP:CZ2	1:B:1409:SER:HB3	2.22	0.75
1:B:153:PHE:HB2	1:B:157:TYR:HE2	1.52	0.75
1:B:1992:VAL:O	1:B:1996:VAL:HG22	1.85	0.75
1:B:3414:MSE:SE	1:B:3450:MSE:SE	3.04	0.75
1:A:3269:ARG:NH1	1:A:3312:VAL:HG12	2.02	0.75
1:B:2458:VAL:HA	1:B:2461:PHE:CE2	2.22	0.75
1:B:2887:PRO:HG3	1:B:2921:LEU:HD13	1.68	0.75
1:B:3243:ILE:HG21	1:B:3262:LEU:HD22	1.68	0.75
1:A:2363:CYS:O	1:A:2367:VAL:HG12	1.87	0.75
1:B:1086:TYR:CD2	1:B:1090:ARG:HG2	2.22	0.75
1:B:3144:PHE:CD1	1:B:3160:LEU:HD11	2.21	0.75
1:B:3491:PRO:HB3	1:B:3711:PRO:HB3	1.69	0.75
1:A:2300:PHE:CZ	1:A:2341:LEU:HB2	2.22	0.74
1:A:2372:PRO:HB2	1:A:2374:LEU:HD13	1.68	0.74
1:B:353:ASP:O	1:B:1859:ASN:ND2	2.19	0.74
1:B:2806:LYS:HD3	1:B:2855:VAL:HG13	1.67	0.74
1:B:253:LEU:HD21	1:B:297:LEU:HA	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3583:LEU:HD11	1:A:3733:ARG:HB3	1.66	0.74
1:B:3012:GLU:HB2	1:B:3050:LYS:HZ1	1.51	0.74
1:B:385:TYR:HE1	1:B:421:LEU:HD23	1.52	0.74
1:B:1217:VAL:HG13	1:B:1274:ARG:HH12	1.50	0.74
1:B:1977:ILE:O	1:B:1979:GLU:N	2.17	0.74
1:B:2253:TYR:CZ	1:B:2287:PRO:HB3	2.22	0.74
1:B:2311:ARG:HG3	1:B:2363:CYS:HB2	1.70	0.74
1:B:971:ARG:HG3	1:B:972:LEU:H	1.52	0.74
1:A:1010:LEU:HD13	1:A:1028:PHE:HE1	1.51	0.74
1:A:3974:MSE:HB3	1:A:3976:GLU:H	1.52	0.74
1:A:766:ALA:O	1:A:768:VAL:N	2.17	0.74
1:B:4021:LEU:HD22	1:B:4028:ILE:HD12	1.68	0.74
1:B:714:VAL:HG12	1:B:734:LEU:HD11	1.69	0.74
1:B:978:GLN:O	1:B:981:ARG:HG2	1.88	0.74
1:A:2960:GLU:OE2	1:A:3289:ARG:NH1	2.19	0.74
1:B:1221:ILE:HG13	1:B:1274:ARG:HH11	1.53	0.74
1:B:3314:SER:HA	1:B:3315:TYR:HB3	1.68	0.74
1:B:3447:VAL:HG12	1:B:3468:LEU:HD22	1.69	0.74
1:B:616:LYS:HB3	1:B:617:PRO:HD2	1.68	0.74
1:A:1976:LEU:HD11	1:A:2031:LEU:HB3	1.69	0.74
1:B:2810:SER:HA	1:B:2813:PHE:CE2	2.23	0.74
1:B:3503:VAL:HG11	1:B:3535:ILE:HB	1.70	0.74
1:A:242:PRO:HB3	1:A:282:PHE:CD1	2.22	0.74
1:A:3323:PHE:O	1:A:3326:GLN:N	2.19	0.74
1:A:2549:LYS:NZ	1:A:2554:PHE:HA	2.02	0.74
1:B:1012:ALA:O	1:B:1015:ASP:HB3	1.87	0.74
1:B:3397:GLN:N	1:B:3397:GLN:OE1	2.19	0.74
1:B:3459:ASN:O	1:B:3462:ARG:HG2	1.87	0.74
1:B:4071:ALA:O	1:B:4075:ARG:CB	2.35	0.74
1:B:4084:SER:O	1:B:4088:ASN:N	2.21	0.74
1:B:793:LEU:HG	1:B:796:LEU:HD12	1.68	0.74
1:A:3575:LEU:O	1:A:3577:GLN:N	2.21	0.74
1:A:3762:GLN:NE2	1:A:3763:ARG:HH11	1.85	0.74
1:B:2260:PHE:CD1	1:B:2274:ILE:HG22	2.23	0.74
1:B:4089:ILE:HB	1:B:4090:ARG:NH2	2.02	0.74
1:A:2274:ILE:O	1:A:2277:LEU:N	2.21	0.74
1:A:2404:ARG:HG2	1:A:2408:MSE:HE3	1.68	0.74
1:A:940:PHE:CE2	1:A:2576:MSE:SE	2.91	0.74
1:A:2877:SER:O	1:A:2879:GLY:N	2.21	0.74
1:A:273:ARG:HD2	1:A:314:SER:HB3	1.69	0.74
1:A:726:LEU:HA	1:A:729:CYS:SG	2.28	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1871:MSE:HA	1:B:1874:TYR:HB2	1.70	0.74
1:B:2379:MSE:HE1	1:B:2404:ARG:NH1	2.03	0.74
1:B:3110:PHE:O	1:B:3114:TYR:HD1	1.69	0.74
1:B:968:VAL:HG23	1:B:971:ARG:HD3	1.70	0.74
1:A:3034:PRO:HG2	1:A:3037:GLN:HB2	1.69	0.73
1:A:432:THR:HG23	1:A:475:LEU:HD13	1.70	0.73
1:B:2068:ARG:O	1:B:2070:GLU:N	2.20	0.73
1:B:2253:TYR:CE2	1:B:2287:PRO:HB3	2.23	0.73
1:B:2379:MSE:SE	1:B:2404:ARG:HD3	2.38	0.73
1:B:3928:PHE:HD2	1:B:3962:ARG:HH21	1.35	0.73
1:A:1132:ASP:HA	1:A:1135:CYS:SG	2.28	0.73
1:A:3176:MSE:HE1	1:A:3179:TRP:HE3	1.54	0.73
1:B:1073:PHE:CE2	1:B:3745:GLU:HA	2.23	0.73
1:B:1985:LYS:HD2	1:B:2037:SER:HB3	1.69	0.73
1:B:2507:ILE:HA	1:B:2510:LEU:HD12	1.69	0.73
1:A:2142:ILE:HA	1:A:2145:PHE:HD2	1.51	0.73
1:A:2222:HIS:O	1:A:2225:HIS:N	2.16	0.73
1:A:760:LEU:HD13	1:A:802:THR:OG1	1.88	0.73
1:B:1342:MSE:HE2	1:B:1398:VAL:HG12	1.70	0.73
1:B:3493:TRP:HE3	1:B:3713:PRO:HB3	1.53	0.73
1:B:886:TRP:HD1	1:B:889:GLU:H	1.35	0.73
1:B:363:ILE:O	1:B:367:GLY:N	2.18	0.73
1:A:2872:ASP:O	1:A:2913:LYS:NZ	2.21	0.73
1:B:2404:ARG:NH1	1:B:2412:TYR:CZ	2.56	0.73
1:B:2917:PRO:HA	1:B:2920:VAL:HG12	1.70	0.73
1:B:3432:SER:HB2	1:B:3435:ASP:HB2	1.69	0.73
1:A:2253:TYR:HB2	1:A:2291:GLN:HG2	1.70	0.73
1:A:4066:LEU:HG	1:A:4075:ARG:HA	1.71	0.73
1:B:1142:HIS:O	1:B:1144:SER:N	2.20	0.73
1:B:174:VAL:O	1:B:178:LEU:HG	1.88	0.73
1:B:2851:PHE:HA	1:B:2854:PHE:CD2	2.24	0.73
1:B:3323:PHE:O	1:B:3326:GLN:HG2	1.88	0.73
1:A:1115:HIS:O	1:A:1119:LYS:N	2.22	0.73
1:A:170:VAL:HG23	1:A:173:LYS:HD3	1.71	0.73
1:A:2883:SER:O	1:A:2886:GLN:HG3	1.87	0.73
1:B:989:MSE:HE2	1:B:1031:ARG:HH12	1.54	0.73
1:B:2004:TYR:CD1	1:B:2054:TYR:HB3	2.23	0.73
1:B:3167:ARG:NH1	1:B:3167:ARG:HG3	2.02	0.73
1:B:4010:SER:O	1:B:4015:ASN:N	2.21	0.73
1:B:629:PHE:CZ	1:B:666:PHE:HD1	2.07	0.73
1:A:70:ARG:HH22	1:A:117:LYS:HE3	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4010:SER:O	1:A:4015:ASN:N	2.22	0.73
1:A:567:GLU:OE2	1:A:1798:LEU:HB3	1.89	0.73
1:B:1070:PRO:HB2	1:B:1073:PHE:CZ	2.24	0.73
1:B:153:PHE:HB2	1:B:157:TYR:CE2	2.24	0.73
1:B:2027:SER:HB2	1:B:2030:TYR:OH	1.87	0.73
1:B:2321:GLU:OE2	1:B:2325:LEU:HD22	1.89	0.73
1:B:3944:HIS:HA	1:B:4016:PHE:HZ	1.53	0.73
1:A:1984:LEU:O	1:A:1988:TYR:HB3	1.89	0.73
1:A:2571:ASP:O	1:A:2789:SER:OG	2.06	0.73
1:A:3167:ARG:O	1:A:3186:ARG:NH2	2.22	0.73
1:B:1014:LEU:HB2	1:B:1078:ALA:HB1	1.71	0.73
1:B:1890:HIS:HB3	1:B:1937:ARG:HA	1.69	0.73
1:A:1009:LEU:O	1:A:1012:ALA:N	2.22	0.73
1:A:1890:HIS:HB2	1:A:1937:ARG:HD2	1.71	0.73
1:A:19:LEU:O	1:A:23:ASP:HB2	1.89	0.73
1:A:2157:PHE:CE1	1:A:2203:THR:HB	2.23	0.73
1:A:2925:GLU:HB3	1:A:3121:LEU:HD11	1.70	0.73
1:B:730:LEU:HA	1:B:733:LEU:HD12	1.71	0.73
1:A:3048:LYS:HD3	1:A:3061:LEU:HD23	1.71	0.72
1:A:609:ALA:O	1:A:613:HIS:ND1	2.20	0.72
1:B:1651:LYS:O	1:B:1655:ILE:HD12	1.89	0.72
1:B:2918:PRO:HA	1:B:2921:LEU:HG	1.70	0.72
1:A:1087:ARG:HD3	1:A:1134:LEU:HD22	1.71	0.72
1:A:1374:GLN:O	1:A:1378:GLU:N	2.21	0.72
1:A:253:LEU:HD11	1:A:297:LEU:HB3	1.71	0.72
1:A:3276:TRP:HB3	1:A:3280:TYR:CZ	2.24	0.72
1:B:398:THR:HG22	1:B:1865:THR:HG21	1.70	0.72
1:B:2896:ALA:HA	1:B:2899:ARG:NH2	2.04	0.72
1:B:3876:SER:HB3	1:B:4127:TRP:O	1.87	0.72
1:B:535:LEU:HD22	1:B:626:LEU:HG	1.72	0.72
1:B:990:GLN:HA	1:B:993:HIS:CD2	2.24	0.72
1:A:1070:PRO:HG3	1:A:1075:ARG:HB2	1.70	0.72
1:A:1743:MSE:SE	1:A:1880:MSE:SE	3.07	0.72
1:B:1349:LEU:HD21	1:B:1359:LEU:HB2	1.70	0.72
1:B:471:LYS:HA	1:B:1553:PHE:HE2	1.53	0.72
1:B:1886:LYS:NZ	1:B:1948:ALA:HB2	2.05	0.72
1:B:2222:HIS:O	1:B:2225:HIS:N	2.19	0.72
1:A:2311:ARG:HG3	1:A:2363:CYS:HB2	1.69	0.72
1:A:3284:SER:HA	1:A:3287:ARG:HE	1.55	0.72
1:A:978:GLN:O	1:A:981:ARG:HG2	1.89	0.72
1:B:1014:LEU:HA	1:B:1025:LEU:HD13	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1115:HIS:O	1:B:1119:LYS:N	2.22	0.72
1:B:526:ASP:HB2	1:B:529:ASP:OD2	1.89	0.72
1:B:967:PRO:HA	1:B:970:LEU:HD23	1.69	0.72
1:A:1456:LYS:HA	1:A:1459:HIS:HD2	1.53	0.72
1:A:4082:ARG:HG3	1:A:4091:ALA:CB	2.19	0.72
1:A:1456:LYS:HA	1:A:1459:HIS:CD2	2.23	0.72
1:A:2260:PHE:O	1:A:2262:GLY:N	2.22	0.72
1:A:2542:LEU:HB2	1:A:2546:TYR:CE2	2.25	0.72
1:A:3045:ILE:O	1:A:3048:LYS:HB3	1.89	0.72
1:A:3130:GLN:HG3	1:A:3178:ILE:HG12	1.72	0.72
1:B:2860:ASP:HB3	1:B:2868:LEU:HD22	1.72	0.72
1:A:1871:MSE:HA	1:A:1874:TYR:HB2	1.71	0.72
1:A:2193:ILE:HA	1:A:2196:TRP:CZ2	2.24	0.72
1:A:737:PRO:HA	1:A:740:ILE:HD12	1.70	0.72
1:B:3583:LEU:O	1:B:3587:ASP:HB2	1.88	0.72
1:A:3015:SER:O	1:A:3019:ILE:N	2.21	0.72
1:A:349:ILE:HG12	1:A:364:ARG:HD2	1.72	0.72
1:A:434:VAL:HA	1:A:437:HIS:CE1	2.24	0.72
1:B:1802:TYR:O	1:B:1805:PHE:N	2.22	0.72
1:B:2177:ASN:HD22	1:B:2182:ILE:HG22	1.54	0.72
1:B:2563:LEU:O	1:B:2567:SER:OG	2.06	0.72
1:A:2300:PHE:HZ	1:A:2341:LEU:HB2	1.54	0.72
1:A:3592:VAL:HG22	1:A:3609:MSE:SE	2.40	0.72
1:B:2837:LEU:HA	1:B:2840:PHE:CD2	2.25	0.72
1:B:3579:SER:OG	1:B:3580:ASN:N	2.22	0.72
1:B:868:LYS:HA	1:B:871:LEU:HD12	1.71	0.72
1:A:3256:MSE:HE2	1:A:3282:ARG:NH1	2.03	0.72
1:A:3432:SER:HB2	1:A:3435:ASP:HB2	1.72	0.72
1:A:358:GLU:HA	1:A:1858:LEU:HD22	1.71	0.72
1:A:871:LEU:HD11	1:A:3122:HIS:HE1	1.55	0.72
1:B:1090:ARG:HA	1:B:1090:ARG:NE	2.05	0.72
1:B:2313:LYS:HG3	1:B:2314:GLU:OE2	1.90	0.72
1:B:2961:ALA:HB1	1:B:3002:TYR:HD1	1.54	0.72
1:B:649:PHE:CE1	1:B:657:SER:HB2	2.25	0.72
1:B:721:TYR:CE1	1:B:1121:LEU:HD21	2.24	0.72
1:A:1870:LYS:HG2	1:A:1871:MSE:HE2	1.71	0.71
1:B:2239:LYS:HG3	1:B:2279:ILE:HG23	1.72	0.71
1:B:3326:GLN:OE1	1:B:3393:GLU:HA	1.90	0.71
1:A:1306:ILE:HG12	1:A:1334:LYS:HB3	1.72	0.71
1:A:2323:LEU:HD21	1:A:2345:VAL:HG21	1.72	0.71
1:A:2423:VAL:HG13	1:A:2424:MSE:H	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2433:LYS:HG3	1:A:2436:LEU:HD12	1.70	0.71
1:B:1032:CYS:HB3	1:B:1036:PHE:CZ	2.25	0.71
1:B:932:GLU:HG3	1:B:2636:UNK:HA	1.72	0.71
1:B:3593:ARG:HA	1:B:3596:LEU:HD12	1.72	0.71
1:A:2312:TYR:HE2	1:A:2314:GLU:HG2	1.55	0.71
1:A:2453:GLU:O	1:A:2457:PRO:HD3	1.90	0.71
1:A:3503:VAL:HG11	1:A:3535:ILE:HB	1.72	0.71
1:A:3982:SER:O	1:A:3986:HIS:ND1	2.22	0.71
1:B:1349:LEU:HA	1:B:1353:PRO:HD2	1.71	0.71
1:B:1761:LEU:HD22	1:B:1860:GLU:HB3	1.73	0.71
1:B:2806:LYS:NZ	1:B:2858:ILE:HG21	2.06	0.71
1:B:602:MSE:SE	1:B:726:LEU:HD13	2.40	0.71
1:A:1977:ILE:O	1:A:1979:GLU:N	2.18	0.71
1:A:2070:GLU:HA	1:A:2071:GLN:HB2	1.72	0.71
1:A:922:SER:HB3	1:A:926:THR:HG23	1.72	0.71
1:A:967:PRO:HA	1:A:970:LEU:HD23	1.70	0.71
1:A:2281:MSE:HE2	1:A:2322:VAL:HA	1.73	0.71
1:A:2435:CYS:O	1:A:2439:ILE:HB	1.89	0.71
1:A:3677:PRO:O	1:A:3679:ASN:N	2.22	0.71
1:A:616:LYS:HB3	1:A:617:PRO:HD2	1.72	0.71
1:B:1762:MSE:HB2	1:B:1896:ILE:HG12	1.72	0.71
1:B:2883:SER:O	1:B:2885:GLN:N	2.22	0.71
1:B:2884:LEU:HB3	1:B:3895:GLU:HG3	1.73	0.71
1:B:2970:LYS:NZ	1:B:2974:GLU:OE2	2.22	0.71
1:B:3130:GLN:HG3	1:B:3178:ILE:HG12	1.73	0.71
1:B:491:CYS:SG	1:B:492:SER:N	2.62	0.71
1:B:560:LEU:HB3	1:B:616:LYS:HE2	1.73	0.71
1:A:2535:THR:O	1:A:2538:ARG:HG2	1.89	0.71
1:B:204:LEU:HD22	1:B:219:VAL:HG12	1.71	0.71
1:B:3471:ILE:HG23	1:B:3472:ILE:HG13	1.73	0.71
1:B:553:VAL:HB	1:B:637:LYS:HZ2	1.56	0.71
1:B:808:GLU:HG2	1:B:852:ARG:NH2	2.06	0.71
1:A:1256:TRP:O	1:A:1260:LEU:N	2.17	0.71
1:A:3257:LYS:HA	1:A:3260:LYS:HD2	1.73	0.71
1:A:3427:GLU:HB3	1:A:3439:LEU:HD22	1.71	0.71
1:A:3835:PRO:HA	1:A:3871:PHE:HE1	1.54	0.71
1:A:3875:GLU:HG2	1:A:4127:TRP:HB3	1.72	0.71
1:B:1702:LEU:O	1:B:1706:SER:HB3	1.91	0.71
1:B:3587:ASP:HB3	1:B:4022:LYS:HZ2	1.55	0.71
1:A:1609:ALA:HB3	1:A:1806:ARG:NH2	2.06	0.71
1:A:1745:LYS:O	1:A:1747:LEU:N	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2538:ARG:HH12	1:A:2566:THR:H	1.36	0.71
1:A:396:PHE:CZ	1:A:397:LEU:HG	2.25	0.71
1:A:705:ALA:HB1	1:A:1385:ASN:ND2	2.05	0.71
1:A:756:PHE:HA	1:A:773:LEU:HD13	1.73	0.71
1:B:2043:PHE:O	1:B:2047:THR:OG1	2.09	0.71
1:B:2200:ALA:HA	1:B:2203:THR:HG22	1.73	0.71
1:A:2152:ASN:HB3	1:A:2153:THR:HA	1.72	0.71
1:A:446:PHE:O	1:A:533:HIS:NE2	2.24	0.71
1:A:621:SER:HB3	1:A:659:ARG:NH2	2.06	0.71
1:B:1798:LEU:O	1:B:1802:TYR:HB2	1.90	0.71
1:B:3464:LYS:HG3	1:B:3468:LEU:HD11	1.72	0.71
1:B:454:GLN:HG3	1:B:533:HIS:HE1	1.54	0.71
1:A:1681:ASP:OD1	1:A:1682:THR:N	2.23	0.71
1:A:2478:MSE:O	1:A:2482:ASP:CB	2.37	0.71
1:A:3813:LYS:HG2	1:A:3926:ASN:HA	1.73	0.71
1:B:1267:TYR:O	1:B:1271:ILE:HG13	1.90	0.71
1:B:1464:LEU:HB2	1:B:1468:LEU:HD12	1.73	0.71
1:B:3155:VAL:HG21	1:B:3159:ARG:NH2	2.06	0.71
1:B:3875:GLU:O	1:B:3879:PRO:HD3	1.91	0.71
1:B:560:LEU:HD11	1:B:645:TRP:CZ2	2.26	0.71
1:A:1880:MSE:SE	1:A:1881:TYR:HD1	2.23	0.70
1:A:2260:PHE:CZ	1:A:2303:LEU:HA	2.25	0.70
1:A:2312:TYR:CE2	1:A:2314:GLU:HG2	2.25	0.70
1:A:660:LEU:O	1:A:664:SER:OG	2.08	0.70
1:A:941:MSE:HB2	1:A:958:MSE:HE3	1.73	0.70
1:B:1060:PHE:HA	1:B:1063:LEU:HD12	1.72	0.70
1:B:1138:ILE:HD13	1:B:1150:LYS:HE2	1.73	0.70
1:B:2161:ALA:HA	1:B:2164:TRP:CD1	2.25	0.70
1:B:2227:LYS:HG3	1:B:2232:ARG:HA	1.73	0.70
1:B:3772:ASN:ND2	1:B:3788:LEU:H	1.89	0.70
1:B:4048:LYS:O	1:B:4051:LEU:HB3	1.91	0.70
1:B:514:VAL:HG12	1:B:604:PRO:HG3	1.73	0.70
1:B:982:GLN:O	1:B:986:PRO:HD3	1.91	0.70
1:A:1655:ILE:HG23	1:A:1677:SER:HB3	1.73	0.70
1:A:3498:TRP:HD1	1:A:3502:MSE:HB2	1.56	0.70
1:B:3340:ALA:O	1:B:3343:SER:N	2.24	0.70
1:B:575:ILE:HD11	1:B:579:LEU:HD22	1.70	0.70
1:B:913:ARG:NE	1:B:916:GLU:OE2	2.24	0.70
1:A:1403:MSE:HE1	1:A:1419:LEU:HD21	1.73	0.70
1:A:2137:ILE:HB	1:A:2170:GLN:HE22	1.55	0.70
1:A:3989:ARG:HH21	1:A:4100:GLU:HB3	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2086:ASP:HB3	1:B:2090:ARG:HH21	1.55	0.70
1:B:2896:ALA:HA	1:B:2899:ARG:HH21	1.57	0.70
1:B:1472:SER:HA	1:B:1476:HIS:CD2	2.26	0.70
1:B:2161:ALA:HB1	1:B:2211:LEU:HD13	1.71	0.70
1:B:2260:PHE:O	1:B:2262:GLY:N	2.24	0.70
1:A:1593:VAL:O	1:A:1597:LEU:HB2	1.91	0.70
1:A:3044:MSE:O	1:A:3047:SER:OG	2.04	0.70
1:A:527:TYR:OH	1:A:619:ASP:N	2.22	0.70
1:B:989:MSE:HE2	1:B:1031:ARG:NH1	2.07	0.70
1:B:1155:ARG:NH2	1:B:1230:GLY:O	2.24	0.70
1:B:2379:MSE:CE	1:B:2404:ARG:HD3	2.20	0.70
1:A:446:PHE:H	1:A:446:PHE:HD1	1.36	0.70
1:B:1017:ILE:HB	1:B:1025:LEU:HB2	1.74	0.70
1:B:2412:TYR:HD2	1:B:2416:LYS:HE3	1.57	0.70
1:B:2936:TYR:HD2	1:B:3979:LEU:HD21	1.56	0.70
1:A:2030:TYR:HD1	1:A:2031:LEU:HG	1.57	0.70
1:A:3917:ILE:HG22	1:A:3918:LEU:HD22	1.72	0.70
1:B:1416:GLU:O	1:B:1420:ARG:HB2	1.91	0.70
1:B:2535:THR:O	1:B:2538:ARG:HG2	1.92	0.70
1:B:2945:SER:O	1:B:2949:THR:HG23	1.90	0.70
1:A:3592:VAL:HA	1:A:3609:MSE:SE	2.41	0.70
1:B:2112:GLN:OE1	1:B:2120:ARG:NH2	2.24	0.70
1:B:848:LEU:HA	1:B:851:ILE:HD12	1.74	0.70
1:A:1592:MSE:O	1:A:1594:SER:N	2.24	0.70
1:B:1445:ARG:HA	1:B:1448:LEU:HD12	1.74	0.70
1:B:2260:PHE:CE2	1:B:2303:LEU:HA	2.27	0.70
1:B:3498:TRP:HE1	1:B:3502:MSE:SE	2.25	0.70
1:B:3638:LYS:HA	1:B:3641:ASP:OD2	1.91	0.70
1:B:3772:ASN:HB2	1:B:3787:GLN:CG	2.19	0.70
1:B:932:GLU:HB3	1:B:2794:LEU:HD13	1.73	0.70
1:A:1014:LEU:HD13	1:A:1078:ALA:HB1	1.72	0.70
1:A:1918:LEU:HD22	1:A:1958:GLU:HB3	1.72	0.70
1:A:2239:LYS:HE2	1:A:2240:THR:HG22	1.73	0.70
1:A:527:TYR:CE1	1:A:615:ALA:HB1	2.26	0.70
1:B:177:LEU:O	1:B:180:LEU:N	2.25	0.70
1:B:19:LEU:HD22	1:B:30:ALA:HB1	1.72	0.70
1:B:970:LEU:CD2	1:B:1031:ARG:HH21	2.05	0.70
1:A:1249:SER:O	1:A:1253:THR:HB	1.92	0.69
1:A:114:VAL:HG11	1:A:130:LEU:HD11	1.72	0.69
1:A:1877:LEU:O	1:A:1920:TYR:OH	2.09	0.69
1:A:2781:PRO:HB2	1:A:2786:LYS:HD3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3687:MSE:O	1:A:3689:ASP:N	2.25	0.69
1:A:990:GLN:HA	1:A:993:HIS:HD2	1.57	0.69
1:B:1985:LYS:O	1:B:1989:ASN:ND2	2.22	0.69
1:B:2253:TYR:HB2	1:B:2291:GLN:CG	2.22	0.69
1:B:2452:ARG:HA	1:B:2455:LEU:HD12	1.73	0.69
1:B:3284:SER:HB2	1:B:3287:ARG:NH2	2.04	0.69
1:B:3119:VAL:HG21	1:B:3899:ALA:HB1	1.74	0.69
1:B:3910:LEU:O	1:B:3914:SER:OG	2.07	0.69
1:B:629:PHE:HZ	1:B:666:PHE:HD1	1.40	0.69
1:A:1378:GLU:OE2	1:A:1382:ILE:HG23	1.92	0.69
1:A:1469:PRO:HA	1:A:1472:SER:HB3	1.74	0.69
1:B:436:GLU:OE2	1:B:475:LEU:HD12	1.93	0.69
1:B:743:LEU:O	1:B:746:ARG:NH1	2.25	0.69
1:A:1996:VAL:HG23	1:A:1997:PRO:CD	2.22	0.69
1:A:2071:GLN:HA	1:A:2074:PRO:HG2	1.73	0.69
1:A:2958:LEU:O	1:A:3289:ARG:NH2	2.25	0.69
1:A:718:MSE:HE3	1:A:731:THR:HG22	1.74	0.69
1:A:718:MSE:HE2	1:A:754:MSE:HG3	1.75	0.69
1:B:660:LEU:O	1:B:663:ILE:HG13	1.91	0.69
1:A:1583:MSE:SE	1:A:1643:MSE:SE	3.09	0.69
1:A:1651:LYS:O	1:A:1655:ILE:HD12	1.92	0.69
1:A:2038:GLU:OE1	1:A:2076:VAL:HG22	1.93	0.69
1:A:2153:THR:OG1	1:A:2154:GLU:N	2.18	0.69
1:B:1087:ARG:HD2	1:B:1137:ILE:HD11	1.74	0.69
1:B:1412:LYS:HA	1:B:1415:LEU:HD12	1.72	0.69
1:B:3979:LEU:HA	1:B:3981:TYR:HB3	1.74	0.69
1:B:512:GLY:HA2	1:B:602:MSE:HG3	1.73	0.69
1:B:629:PHE:CE2	1:B:668:LYS:HB2	2.28	0.69
1:A:334:HIS:CE1	1:A:338:LEU:HD21	2.28	0.69
1:B:2813:PHE:CD2	1:B:2859:GLN:HG3	2.25	0.69
1:B:272:LEU:HB3	1:B:319:PHE:CZ	2.27	0.69
1:B:722:LYS:HB3	1:B:727:ALA:HA	1.74	0.69
1:B:86:LEU:HD23	1:B:89:LEU:HD12	1.72	0.69
1:A:2216:LEU:HD22	1:A:2249:LEU:HD11	1.73	0.69
1:A:2452:ARG:HE	1:A:2498:ILE:HD11	1.57	0.69
1:A:3810:VAL:HG23	1:A:3815:LEU:HD11	1.74	0.69
1:B:170:VAL:HG23	1:B:173:LYS:HZ1	1.57	0.69
1:B:2413:PHE:CE1	1:B:2442:MSE:HB3	2.27	0.69
1:B:2430:GLU:HG3	1:B:2465:PRO:HB3	1.74	0.69
1:B:2884:LEU:C	1:B:2887:PRO:HD2	2.13	0.69
1:B:3574:ALA:HA	1:B:3577:GLN:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1445:ARG:HA	1:A:1448:LEU:HD12	1.74	0.69
1:A:2304:VAL:HG13	1:A:2348:GLN:HE21	1.57	0.69
1:A:2329:TYR:O	1:A:2333:ARG:N	2.25	0.69
1:A:2464:HIS:H	1:A:2465:PRO:HD3	1.56	0.69
1:A:723:ASP:HB2	1:A:726:LEU:HD12	1.74	0.69
1:B:2196:TRP:HE1	1:B:2200:ALA:HB2	1.58	0.69
1:B:3654:MSE:SE	1:B:3659:PHE:HB3	2.42	0.69
1:B:65:LEU:O	1:B:69:VAL:HB	1.93	0.69
1:A:1018:VAL:HB	1:A:1074:LYS:HA	1.75	0.69
1:A:1059:LEU:HD22	1:A:1063:LEU:HD11	1.75	0.69
1:A:1507:CYS:SG	1:A:1508:LYS:N	2.65	0.69
1:A:1685:ASP:HB2	1:A:1727:ARG:NH2	2.06	0.69
1:A:2125:TRP:O	1:A:2127:LYS:N	2.25	0.69
1:A:19:LEU:HB2	1:A:34:LEU:HD13	1.75	0.69
1:A:368:LEU:HD23	1:A:372:PRO:HG2	1.74	0.69
1:A:3974:MSE:HB3	1:A:3976:GLU:HB3	1.74	0.69
1:A:462:VAL:HG11	1:A:540:MSE:SE	2.42	0.69
1:B:135:LEU:HD13	1:B:170:VAL:HB	1.75	0.69
1:B:2351:GLN:O	1:B:2355:THR:OG1	2.07	0.69
1:B:2555:LEU:O	1:B:2558:ALA:HB3	1.92	0.69
1:A:602:MSE:SE	1:A:726:LEU:HD13	2.42	0.69
1:B:414:LEU:HD23	1:B:460:ALA:HB1	1.74	0.69
1:B:434:VAL:HA	1:B:437:HIS:CE1	2.28	0.69
1:A:2187:VAL:O	1:A:2190:VAL:HG22	1.93	0.69
1:A:4121:TRP:HD1	1:A:4123:GLY:H	1.40	0.69
1:A:870:LEU:HA	1:A:873:VAL:HB	1.75	0.69
1:B:1086:TYR:HD2	1:B:1090:ARG:HG2	1.58	0.69
1:B:1955:VAL:HG12	1:B:1957:ASN:HB2	1.75	0.69
1:A:1569:THR:O	1:A:1573:LYS:HB2	1.93	0.69
1:A:3048:LYS:NZ	1:A:3089:LEU:HB3	2.08	0.69
1:A:934:LEU:HD21	1:A:962:TYR:CE1	2.28	0.69
1:B:1799:GLU:HA	1:B:1802:TYR:HB2	1.74	0.69
1:B:3587:ASP:HB3	1:B:4022:LYS:NZ	2.08	0.69
1:B:3772:ASN:ND2	1:B:3788:LEU:O	2.26	0.69
1:B:917:LEU:HD21	1:B:934:LEU:HD13	1.74	0.69
1:B:935:HIS:NE2	1:B:987:LEU:HG	2.09	0.69
1:A:1763:THR:OG1	1:A:1864:ASP:OD2	2.09	0.68
1:A:3114:TYR:CE1	1:A:3128:LYS:HD3	2.28	0.68
1:A:970:LEU:HD22	1:A:1031:ARG:HH21	1.58	0.68
1:A:977:ASP:HB3	1:A:981:ARG:N	2.08	0.68
1:B:999:LYS:HD3	1:B:1000:LYS:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1080:LEU:CD1	1:B:1127:CYS:HB3	2.23	0.68
1:B:2074:PRO:O	1:B:2077:HIS:N	2.26	0.68
1:B:2283:ASN:O	1:B:2287:PRO:HD3	1.92	0.68
1:B:2365:ASN:HD21	1:B:2382:VAL:HG11	1.58	0.68
1:B:2951:GLN:OE1	1:B:2972:TYR:OH	2.10	0.68
1:A:3312:VAL:O	1:A:3314:SER:N	2.26	0.68
1:B:3631:LYS:HB3	1:B:3682:GLU:HA	1.76	0.68
1:B:745:VAL:HG11	1:B:776:TRP:CZ2	2.27	0.68
1:A:1722:PHE:CD2	1:A:1754:GLN:HG2	2.29	0.68
1:B:3435:ASP:O	1:B:3439:LEU:CB	2.41	0.68
1:B:345:PHE:HD2	1:B:367:GLY:HA3	1.59	0.68
1:B:398:THR:O	1:B:401:ASP:N	2.24	0.68
1:A:2177:ASN:HD22	1:A:2182:ILE:HG22	1.57	0.68
1:A:2283:ASN:ND2	1:A:2284:ASP:OD2	2.26	0.68
1:B:1165:LEU:HA	1:B:1168:LEU:HD12	1.76	0.68
1:B:2242:VAL:HG12	1:B:2246:LYS:HE3	1.75	0.68
1:A:1937:ARG:O	1:A:1941:HIS:HB2	1.92	0.68
1:A:1917:LYS:HE2	1:A:1955:VAL:HB	1.74	0.68
1:A:2271:SER:HB2	1:A:2314:GLU:HG3	1.75	0.68
1:A:2900:LEU:HB2	1:A:2910:VAL:HA	1.75	0.68
1:A:3955:VAL:HG23	1:A:4121:TRP:CE3	2.28	0.68
1:B:1989:ASN:HB3	1:B:2040:MSE:HB3	1.75	0.68
1:B:2274:ILE:O	1:B:2277:LEU:N	2.27	0.68
1:B:4113:ASP:HB3	1:B:4116:ILE:HG13	1.75	0.68
1:B:721:TYR:HE1	1:B:1121:LEU:HD21	1.58	0.68
1:A:1382:ILE:HB	1:A:1386:ILE:HD11	1.75	0.68
1:A:793:LEU:HG	1:A:796:LEU:HD12	1.75	0.68
1:A:940:PHE:CZ	1:A:2791:ILE:HG21	2.28	0.68
1:B:1682:THR:OG1	1:B:1727:ARG:NH2	2.27	0.68
1:B:1981:LEU:O	1:B:1984:LEU:HG	1.93	0.68
1:B:2423:VAL:HG23	1:B:2426:HIS:HB3	1.76	0.68
1:A:3583:LEU:O	1:A:3587:ASP:HB2	1.92	0.68
1:A:3816:LEU:HD11	1:A:3883:LEU:HG	1.74	0.68
1:A:4066:LEU:HD23	1:A:4075:ARG:HG3	1.76	0.68
1:A:543:SER:C	1:A:545:LEU:H	1.95	0.68
1:B:1403:MSE:HE1	1:B:1419:LEU:HD21	1.75	0.68
1:B:1643:MSE:HA	1:B:1646:LEU:HG	1.74	0.68
1:B:3084:GLN:OE1	1:B:3084:GLN:N	2.21	0.68
1:B:3339:ASN:O	1:B:3341:LEU:N	2.26	0.68
1:B:3737:ARG:NH1	1:B:3739:ILE:HD11	2.07	0.68
1:B:3840:LYS:HE2	1:B:4122:GLU:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:669:LEU:HD22	1:B:672:ILE:HG13	1.75	0.68
1:B:926:THR:O	1:B:930:ALA:HB3	1.92	0.68
1:A:2094:MSE:HE1	1:A:2143:ARG:HA	1.75	0.68
1:A:2936:TYR:HB3	1:A:3979:LEU:HD11	1.75	0.68
1:A:484:HIS:CD2	1:A:616:LYS:HE3	2.29	0.68
1:A:580:ASP:OD1	1:A:581:LEU:N	2.26	0.68
1:B:2477:LEU:HB3	1:B:2506:LEU:HD21	1.76	0.68
1:B:3031:TRP:CE3	1:B:3034:PRO:HD3	2.29	0.68
1:B:3981:TYR:OH	1:B:4101:GLU:HB3	1.93	0.68
1:A:1437:TYR:CD2	1:A:1444:ASP:OD2	2.47	0.68
1:A:3830:SER:HB2	1:A:3835:PRO:HG3	1.76	0.68
1:B:2260:PHE:CZ	1:B:2303:LEU:HA	2.29	0.68
1:B:574:LYS:O	1:B:577:GLU:HG2	1.94	0.68
1:A:1802:TYR:O	1:A:1805:PHE:N	2.27	0.68
1:A:265:TYR:O	1:A:268:PRO:HD2	1.94	0.68
1:A:3049:LEU:HD13	1:A:3184:THR:HB	1.76	0.68
1:A:3790:THR:HG22	1:A:3791:TYR:H	1.58	0.68
1:A:882:SER:HB2	1:A:3892:THR:H	1.59	0.68
1:A:3883:LEU:HD13	1:A:3970:LEU:HD13	1.74	0.68
1:B:1886:LYS:HZ3	1:B:1948:ALA:HB2	1.59	0.68
1:B:2316:TYR:CG	1:B:2317:ALA:N	2.62	0.68
1:B:655:LEU:O	1:B:659:ARG:HG2	1.93	0.68
1:A:1080:LEU:HD12	1:A:1081:ALA:N	2.08	0.67
1:A:260:ILE:HG22	1:A:264:ARG:HH12	1.59	0.67
1:B:2258:GLU:OE2	1:B:2295:GLN:NE2	2.22	0.67
1:B:2542:LEU:HB2	1:B:2546:TYR:CE2	2.29	0.67
1:B:3620:PRO:HA	1:B:3625:LEU:HD12	1.76	0.67
1:B:411:PRO:HA	1:B:414:LEU:HB3	1.75	0.67
1:B:968:VAL:HA	1:B:971:ARG:HG2	1.76	0.67
1:A:1403:MSE:HA	1:A:1406:LEU:HB2	1.76	0.67
1:A:172:GLU:O	1:A:176:GLU:HG3	1.94	0.67
1:A:990:GLN:HA	1:A:993:HIS:CD2	2.29	0.67
1:B:2390:HIS:HD1	1:B:2397:CYS:HG	1.41	0.67
1:B:2440:TYR:HD2	1:B:2476:ILE:HD12	1.58	0.67
1:B:899:ARG:NH1	1:B:2570:PRO:HB2	2.00	0.67
1:B:4063:GLU:HA	1:B:4066:LEU:HD22	1.75	0.67
1:A:323:VAL:O	1:A:327:VAL:HB	1.94	0.67
1:A:367:GLY:C	1:A:369:PHE:H	1.98	0.67
1:B:2776:ARG:HA	1:B:2776:ARG:NH1	2.08	0.67
1:B:797:ASP:HA	1:B:800:LEU:HD12	1.77	0.67
1:A:3788:LEU:HG	1:A:3789:ARG:H	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ILE:HG13	1:A:381:VAL:CG2	2.24	0.67
1:A:848:LEU:HA	1:A:851:ILE:HD12	1.76	0.67
1:A:909:VAL:HG13	1:A:913:ARG:NH1	2.09	0.67
1:B:3797:THR:HG22	1:B:3800:LEU:HG	1.77	0.67
1:B:3761:ASP:HB3	1:B:3942:PHE:HB2	1.76	0.67
1:B:429:GLU:N	1:B:429:GLU:OE1	2.27	0.67
1:B:554:ASN:CG	1:B:637:LYS:HZ3	1.98	0.67
1:A:1163:LEU:HD13	1:A:1256:TRP:CD1	2.29	0.67
1:A:1723:PRO:C	1:A:1725:GLN:H	1.97	0.67
1:A:2239:LYS:HG3	1:A:2279:ILE:CG2	2.23	0.67
1:A:3174:ASP:OD2	1:A:3782:SER:HB3	1.94	0.67
1:A:3964:THR:O	1:A:3967:PHE:HD1	1.78	0.67
1:A:3858:MSE:HB3	1:A:4119:ARG:NH2	2.10	0.67
1:A:411:PRO:HA	1:A:414:LEU:HB3	1.76	0.67
1:A:571:SER:HB2	1:A:606:SER:H	1.59	0.67
1:B:446:PHE:HD1	1:B:446:PHE:H	1.42	0.67
1:B:969:LEU:O	1:B:973:ALA:CB	2.42	0.67
1:A:2538:ARG:HH11	1:A:2565:MSE:HB3	1.59	0.67
1:A:3959:MSE:HE1	1:A:4124:TRP:CD2	2.30	0.67
1:A:756:PHE:O	1:A:760:LEU:HG	1.95	0.67
1:B:1504:ASP:HA	1:B:1507:CYS:HB3	1.76	0.67
1:B:550:PHE:HZ	1:B:632:GLU:HG2	1.57	0.67
1:A:144:MSE:HE2	1:A:184:VAL:HG11	1.76	0.67
1:A:2477:LEU:HD13	1:A:2505:VAL:HG11	1.76	0.67
1:A:3974:MSE:HA	1:A:3975:LYS:HB3	1.75	0.67
1:A:767:GLU:HG2	1:A:846:ILE:O	1.94	0.67
1:B:1643:MSE:O	1:B:1646:LEU:N	2.27	0.67
1:A:1017:ILE:HD12	1:A:1025:LEU:HD22	1.77	0.67
1:A:1744:LYS:HA	1:A:1880:MSE:HE3	1.75	0.67
1:A:2223:VAL:HB	1:A:2238:ILE:HD12	1.76	0.67
1:A:2851:PHE:HA	1:A:2854:PHE:CD2	2.29	0.67
1:A:3344:GLU:O	1:A:3348:LEU:HG	1.94	0.67
1:A:3505:LEU:HD12	1:A:3509:ASP:HB3	1.76	0.67
1:A:3583:LEU:HD11	1:A:3733:ARG:HD3	1.77	0.67
1:A:4066:LEU:HD11	1:A:4078:VAL:HG11	1.77	0.67
1:B:2140:LEU:HA	1:B:2143:ARG:HD2	1.75	0.67
1:B:2420:PHE:HE1	1:B:2436:LEU:HD22	1.59	0.67
1:B:3812:LEU:HG	1:B:3813:LYS:N	2.08	0.67
1:B:406:ARG:O	1:B:409:GLN:N	2.26	0.67
1:B:463:LYS:O	1:B:466:LEU:HB3	1.94	0.67
1:B:865:GLN:N	1:B:865:GLN:OE1	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:LYS:NZ	1:A:1328:GLU:OE2	2.24	0.67
1:A:173:LYS:O	1:A:177:LEU:HG	1.94	0.67
1:A:2253:TYR:CZ	1:A:2287:PRO:HB3	2.30	0.67
1:B:1145:LEU:HB2	1:B:1149:LYS:NZ	2.10	0.67
1:B:1344:PHE:O	1:B:1348:LEU:CB	2.33	0.67
1:B:1483:LEU:HA	1:B:1500:LEU:HD21	1.75	0.67
1:B:1963:GLN:HE21	1:B:1995:GLU:HG2	1.60	0.67
1:B:2001:LYS:HA	1:B:2054:TYR:CE2	2.29	0.67
1:B:2440:TYR:CD2	1:B:2476:ILE:HD12	2.29	0.67
1:B:2854:PHE:CG	1:B:2882:ALA:HB2	2.30	0.67
1:B:327:VAL:HG22	1:B:338:LEU:HD22	1.77	0.67
1:B:985:GLU:HG3	1:B:1031:ARG:NH2	2.03	0.67
1:A:2033:ASP:O	1:A:2037:SER:OG	2.13	0.67
1:A:2224:PHE:CZ	1:A:2276:LEU:HD22	2.30	0.67
1:A:2806:LYS:HA	1:A:2809:PHE:CD2	2.30	0.67
1:A:3879:PRO:HB2	1:A:3966:GLN:OE1	1.94	0.67
1:B:1491:ILE:O	1:B:1497:ARG:NH1	2.27	0.67
1:B:1751:GLU:OE2	1:B:1884:LEU:HD13	1.95	0.67
1:B:1894:SER:O	1:B:1897:ASN:N	2.21	0.67
1:B:2507:ILE:HG12	1:B:2548:PRO:HB2	1.77	0.67
1:B:794:PRO:HA	1:B:869:ASN:HB3	1.77	0.67
1:A:1292:LYS:NZ	1:A:1361:LYS:NZ	2.44	0.66
1:A:1464:LEU:HB2	1:A:1468:LEU:HD12	1.75	0.66
1:A:1880:MSE:SE	1:A:1881:TYR:CD1	2.98	0.66
1:A:2066:PHE:HB3	1:A:2067:ARG:HG2	1.76	0.66
1:A:2913:LYS:O	1:A:2916:LEU:N	2.22	0.66
1:A:646:VAL:HG22	1:A:660:LEU:HD23	1.76	0.66
1:A:76:ILE:HG13	1:A:77:GLU:H	1.59	0.66
1:B:3007:GLU:O	1:B:3010:SER:OG	2.13	0.66
1:A:1036:PHE:CD1	1:A:1059:LEU:HD11	2.30	0.66
1:A:1214:GLU:HG2	1:A:1218:SER:HB3	1.77	0.66
1:A:2256:ILE:HD13	1:A:2276:LEU:HD11	1.77	0.66
1:A:3072:GLU:O	1:A:3076:ALA:HB2	1.96	0.66
1:A:3471:ILE:HG23	1:A:3472:ILE:HG13	1.75	0.66
1:A:610:ALA:HA	1:A:613:HIS:CE1	2.29	0.66
1:B:2323:LEU:HG	1:B:2341:LEU:HD21	1.77	0.66
1:B:3414:MSE:HE1	1:B:3450:MSE:HA	1.76	0.66
1:B:980:THR:CG2	1:B:984:TYR:HE2	2.09	0.66
1:A:3019:ILE:HG13	1:A:3020:ASP:H	1.60	0.66
1:A:3467:ARG:HG3	1:A:3471:ILE:HD12	1.77	0.66
1:A:931:CYS:SG	1:A:932:GLU:N	2.68	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1103:ALA:O	1:B:1106:ILE:HG12	1.95	0.66
1:B:2009:LYS:HG2	1:B:2011:ALA:H	1.58	0.66
1:B:3042:PRO:HA	1:B:3045:ILE:HG12	1.76	0.66
1:B:266:ALA:CB	1:B:308:LEU:HG	2.25	0.66
1:B:659:ARG:HH22	1:B:662:LEU:CG	2.05	0.66
1:A:1548:GLY:O	1:A:1552:HIS:ND1	2.28	0.66
1:A:2121:ASP:HA	1:A:2126:MSE:HB3	1.77	0.66
1:A:3040:TYR:HA	1:A:3043:TYR:CD2	2.31	0.66
1:A:3061:LEU:HD21	1:A:3089:LEU:HD13	1.76	0.66
1:A:3182:ILE:HB	1:A:3186:ARG:HH11	1.58	0.66
1:A:3579:SER:OG	1:A:3580:ASN:N	2.25	0.66
1:A:3725:ARG:HH12	1:A:3737:ARG:HH22	1.43	0.66
1:A:3875:GLU:O	1:A:3879:PRO:HD3	1.95	0.66
1:B:1113:LEU:HD13	1:B:1162:SER:HB3	1.76	0.66
1:B:1266:CYS:O	1:B:1269:THR:OG1	2.12	0.66
1:B:1364:CYS:HB3	1:B:1367:HIS:ND1	2.10	0.66
1:B:1952:ILE:HG23	1:B:1953:CYS:O	1.96	0.66
1:B:3606:ILE:HD13	1:B:3609:MSE:HE3	1.76	0.66
1:B:3820:MSE:HA	1:B:3882:LEU:HD22	1.77	0.66
1:B:776:TRP:CZ2	1:B:780:ILE:HD12	2.30	0.66
1:A:1702:LEU:O	1:A:1706:SER:HB3	1.95	0.66
1:A:2891:ARG:HD3	1:A:3972:LEU:HD22	1.77	0.66
1:A:3008:TRP:O	1:A:3011:LEU:N	2.22	0.66
1:A:3582:GLU:HB2	1:A:3674:SER:OG	1.95	0.66
1:A:886:TRP:HZ3	1:A:954:GLY:O	1.78	0.66
1:B:3160:LEU:O	1:B:3163:THR:HG22	1.96	0.66
1:B:638:GLN:OE1	1:B:638:GLN:N	2.25	0.66
1:A:657:SER:O	1:A:661:PRO:HD3	1.95	0.66
1:B:2137:ILE:O	1:B:2141:ASN:N	2.27	0.66
1:B:2167:PRO:HB2	1:B:2171:LEU:HD22	1.77	0.66
1:B:3721:GLY:O	1:B:3741:ARG:HB2	1.95	0.66
1:B:3842:TRP:CH2	1:B:3846:MSE:HE2	2.30	0.66
1:B:362:ALA:HB2	1:B:409:GLN:HE21	1.61	0.66
1:B:69:VAL:O	1:B:73:LEU:HG	1.96	0.66
1:A:1170:LYS:HA	1:A:1173:LEU:HD12	1.77	0.66
1:A:2886:GLN:HG3	1:A:2887:PRO:HD3	1.77	0.66
1:A:3493:TRP:CE3	1:A:3496:ILE:HG13	2.30	0.66
1:A:514:VAL:HA	1:A:604:PRO:HG3	1.78	0.66
1:B:4002:MSE:SE	1:B:4048:LYS:HE3	2.46	0.66
1:B:793:LEU:HA	1:B:796:LEU:HG	1.78	0.66
1:A:1306:ILE:CG1	1:A:1334:LYS:HB3	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1649:LEU:HA	1:A:1652:ILE:HD12	1.76	0.66
1:A:175:TYR:HE1	1:A:200:PHE:HB3	1.59	0.66
1:A:2254:ARG:HG3	1:A:2255:LEU:H	1.61	0.66
1:A:2549:LYS:HZ2	1:A:2554:PHE:HA	1.59	0.66
1:A:260:ILE:HG23	1:A:263:LYS:HD2	1.75	0.66
1:A:3323:PHE:O	1:A:3326:GLN:HG3	1.96	0.66
1:A:3703:GLY:O	1:A:3706:ASP:HB2	1.95	0.66
1:A:612:LEU:O	1:A:615:ALA:HB3	1.96	0.66
1:B:178:LEU:HB3	1:B:197:PHE:CZ	2.30	0.66
1:B:2462:VAL:HG21	1:B:2473:MSE:SE	2.46	0.66
1:B:3446:VAL:HA	1:B:3449:LYS:HD2	1.78	0.66
1:B:3486:GLU:HG3	1:B:3487:ILE:N	2.09	0.66
1:B:3725:ARG:HH12	1:B:3737:ARG:HH22	1.31	0.66
1:B:649:PHE:CZ	1:B:657:SER:HB2	2.31	0.66
1:A:3125:ARG:O	1:A:3128:LYS:N	2.29	0.66
1:A:3414:MSE:HG3	1:A:3456:LEU:HD21	1.76	0.66
1:A:3460:GLU:HA	1:A:3463:LEU:HD12	1.78	0.66
1:A:3619:ASP:HA	1:A:3622:ALA:HB3	1.76	0.66
1:A:680:ILE:HG12	1:A:701:TYR:CD1	2.30	0.66
1:B:186:PRO:HB2	1:B:189:MSE:HB3	1.78	0.66
1:B:1993:GLU:O	1:B:1997:PRO:HD2	1.96	0.66
1:B:2155:GLU:O	1:B:2157:PHE:N	2.29	0.66
1:B:2190:VAL:HG21	1:B:2241:LEU:HD13	1.76	0.66
1:B:2408:MSE:HE2	1:B:2408:MSE:HA	1.78	0.66
1:B:294:PHE:HZ	1:B:319:PHE:CD2	2.14	0.66
1:B:3887:PHE:HE2	1:B:3904:PHE:HD2	1.43	0.66
1:B:3944:HIS:CE1	1:B:4020:MSE:HE2	2.30	0.66
1:B:617:PRO:O	1:B:620:PHE:N	2.29	0.66
1:A:2382:VAL:HG21	1:A:2404:ARG:HG3	1.79	0.65
1:A:971:ARG:HB3	1:A:1027:ASP:OD2	1.96	0.65
1:B:1081:ALA:O	1:B:1085:ILE:HG12	1.95	0.65
1:B:3262:LEU:HD21	1:B:3274:VAL:HG12	1.78	0.65
1:B:403:GLY:C	1:B:405:ASP:H	1.98	0.65
1:A:2011:ALA:O	1:A:2013:GLU:N	2.28	0.65
1:A:2023:SER:HA	1:A:2070:GLU:OE2	1.96	0.65
1:A:2183:HIS:O	1:A:2187:VAL:CB	2.30	0.65
1:A:2962:ARG:HE	1:A:3254:LEU:HA	1.60	0.65
1:A:3042:PRO:HA	1:A:3045:ILE:HG12	1.77	0.65
1:A:3287:ARG:HH11	1:A:3331:GLY:HA3	1.61	0.65
1:A:446:PHE:CD1	1:A:447:PRO:HD3	2.30	0.65
1:B:1681:ASP:OD1	1:B:1682:THR:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2478:MSE:O	1:B:2482:ASP:CB	2.44	0.65
1:B:3589:SER:O	1:B:3593:ARG:CB	2.44	0.65
1:B:717:LYS:NZ	1:B:1121:LEU:HD11	2.10	0.65
1:A:135:LEU:HD13	1:A:173:LYS:HB3	1.78	0.65
1:A:1802:TYR:HA	1:A:1805:PHE:HD2	1.61	0.65
1:A:2794:LEU:HA	1:A:2797:VAL:HG22	1.78	0.65
1:A:3847:SER:HA	1:A:3857:LEU:HD13	1.77	0.65
1:B:2224:PHE:CZ	1:B:2276:LEU:HD22	2.32	0.65
1:B:253:LEU:HD11	1:B:297:LEU:HB3	1.78	0.65
1:B:2571:ASP:O	1:B:2789:SER:OG	2.14	0.65
1:B:2935:GLU:HG3	1:B:2936:TYR:H	1.62	0.65
1:B:3630:ARG:HG2	1:B:3686:TRP:NE1	2.11	0.65
1:B:393:LYS:HA	1:B:396:PHE:CD1	2.31	0.65
1:B:3998:LEU:O	1:B:4001:THR:OG1	2.13	0.65
1:B:649:PHE:O	1:B:652:GLU:N	2.15	0.65
1:A:1101:PHE:O	1:A:1104:LEU:HB2	1.97	0.65
1:A:1934:LEU:CD1	1:A:1937:ARG:H	2.09	0.65
1:A:3429:GLU:OE1	1:A:4046:TYR:OH	2.13	0.65
1:A:3946:PHE:CE2	1:A:4048:LYS:HD2	2.31	0.65
1:A:939:MSE:HE2	1:A:942:LEU:HD13	1.79	0.65
1:B:1349:LEU:HD23	1:B:1353:PRO:HG2	1.78	0.65
1:B:1816:ARG:HB3	1:B:1819:PHE:HE1	1.60	0.65
1:A:1121:LEU:HG	1:A:1122:GLY:N	2.11	0.65
1:A:1292:LYS:NZ	1:A:1361:LYS:HZ1	1.95	0.65
1:A:1423:ILE:HG13	1:A:1424:THR:H	1.60	0.65
1:A:1718:ILE:HG23	1:A:1750:LEU:HD21	1.78	0.65
1:A:2034:SER:O	1:A:2036:LEU:N	2.29	0.65
1:A:2182:ILE:O	1:A:2186:VAL:HG12	1.97	0.65
1:A:2253:TYR:HD1	1:A:2256:ILE:HD12	1.59	0.65
1:A:3480:LEU:O	1:A:3484:THR:OG1	2.14	0.65
1:B:1101:PHE:CG	1:B:1138:ILE:HG12	2.32	0.65
1:B:385:TYR:O	1:B:389:ILE:HB	1.95	0.65
1:B:753:GLN:O	1:B:757:LYS:CB	2.43	0.65
1:A:1737:ASN:C	1:A:1739:TYR:H	2.00	0.65
1:A:2049:VAL:O	1:A:2052:TYR:N	2.28	0.65
1:A:2507:ILE:HA	1:A:2510:LEU:HD12	1.78	0.65
1:A:2886:GLN:OE1	1:A:2921:LEU:HB2	1.97	0.65
1:B:471:LYS:HA	1:B:1553:PHE:CE2	2.31	0.65
1:B:173:LYS:O	1:B:177:LEU:HG	1.97	0.65
1:B:3677:PRO:O	1:B:3679:ASN:N	2.28	0.65
1:B:736:LEU:O	1:B:740:ILE:HG13	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:938:VAL:HG21	1:B:962:TYR:CZ	2.32	0.65
1:A:1346:THR:HG21	1:A:1401:ASN:HB3	1.79	0.65
1:A:2049:VAL:HA	1:A:2052:TYR:CD2	2.30	0.65
1:A:2058:ASP:HB3	1:A:2059:PRO:HD3	1.78	0.65
1:A:2274:ILE:HA	1:A:2277:LEU:HG	1.76	0.65
1:A:2304:VAL:HG13	1:A:2348:GLN:NE2	2.10	0.65
1:A:3630:ARG:HA	1:A:3686:TRP:CD1	2.32	0.65
1:A:393:LYS:HA	1:A:396:PHE:CD1	2.32	0.65
1:A:4004:VAL:O	1:A:4008:GLU:HB2	1.97	0.65
1:A:759:GLY:HA2	1:A:763:THR:OG1	1.95	0.65
1:A:895:ALA:HB3	1:A:904:VAL:HG21	1.78	0.65
1:B:1651:LYS:O	1:B:1654:GLN:HB2	1.97	0.65
1:B:2062:ALA:HB1	1:B:2066:PHE:CE2	2.30	0.65
1:B:2937:ASP:OD1	1:B:3979:LEU:HD12	1.96	0.65
1:A:2240:THR:HG21	2:K:113:UNK:N	2.12	0.65
1:A:1039:TRP:HZ2	1:A:1049:GLN:HA	1.62	0.65
1:A:1107:TYR:O	1:A:1111:LEU:N	2.29	0.65
1:A:1138:ILE:HG21	1:A:1150:LYS:HE2	1.78	0.65
1:A:1373:VAL:HB	1:A:1418:HIS:CE1	2.31	0.65
1:A:1437:TYR:CE2	1:A:1444:ASP:OD2	2.48	0.65
1:A:2854:PHE:CG	1:A:2882:ALA:HB2	2.32	0.65
1:A:660:LEU:O	1:A:663:ILE:HG13	1.96	0.65
1:A:757:LYS:HA	1:A:760:LEU:HD12	1.78	0.65
1:B:1249:SER:O	1:B:1253:THR:CB	2.44	0.65
1:B:220:LEU:O	1:B:224:LEU:HG	1.97	0.65
1:B:3141:PHE:HE1	1:B:3193:ILE:HG13	1.62	0.65
1:B:3705:TYR:HE2	1:B:3708:ARG:NH1	1.95	0.65
1:B:4099:SER:O	1:B:4103:GLN:NE2	2.27	0.65
1:A:1949:ILE:HD12	1:A:1952:ILE:HG21	1.79	0.65
1:A:2375:ALA:O	1:A:2379:MSE:HB2	1.96	0.65
1:A:940:PHE:HE2	1:A:2576:MSE:SE	2.29	0.65
1:A:3416:LEU:HD13	1:A:3446:VAL:HG12	1.78	0.65
1:A:909:VAL:HG13	1:A:913:ARG:HH11	1.62	0.65
1:B:2070:GLU:HB2	1:B:2072:ARG:N	2.12	0.65
1:B:2270:ASN:O	1:B:2274:ILE:HG23	1.95	0.65
1:B:2412:TYR:CD2	1:B:2416:LYS:HE3	2.31	0.65
1:B:3152:SER:HB2	1:B:3155:VAL:HB	1.77	0.65
1:B:3257:LYS:HA	1:B:3260:LYS:HD2	1.77	0.65
1:B:3722:PHE:CD1	1:B:3740:ILE:HA	2.32	0.65
1:B:3704:GLN:HE21	1:B:3796:MSE:SE	2.30	0.65
1:A:3176:MSE:HE1	1:A:3179:TRP:CE3	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3843:LEU:HD22	1:A:3858:MSE:HE1	1.79	0.65
1:B:2196:TRP:CG	1:B:2199:LEU:HD11	2.31	0.65
1:B:2413:PHE:CD2	1:B:2445:LYS:HG3	2.32	0.65
1:B:2883:SER:HA	1:B:2886:GLN:HE21	1.62	0.65
1:B:2936:TYR:CE1	1:B:2949:THR:HG21	2.32	0.65
1:B:3499:ILE:HG13	1:B:3531:TYR:CZ	2.32	0.65
1:B:3594:ALA:HB1	1:B:4028:ILE:HG21	1.79	0.65
1:B:4062:ASP:O	1:B:4066:LEU:HD13	1.97	0.65
1:B:416:SER:O	1:B:420:VAL:HB	1.97	0.65
1:A:3141:PHE:HE1	1:A:3193:ILE:HG13	1.62	0.64
1:A:757:LYS:HA	1:A:760:LEU:CD1	2.27	0.64
1:B:1094:SER:N	1:B:1097:GLU:OE2	2.28	0.64
1:B:1163:LEU:HD22	1:B:1260:LEU:HD11	1.79	0.64
1:B:217:LEU:HD22	1:B:264:ARG:HG3	1.79	0.64
1:B:446:PHE:CZ	1:B:530:LEU:HB3	2.32	0.64
1:A:1145:LEU:HD13	1:A:1149:LYS:HD3	1.80	0.64
1:A:1915:LEU:HD12	1:A:1916:ILE:HG13	1.78	0.64
1:A:3011:LEU:HD12	1:A:3047:SER:HB3	1.79	0.64
1:A:3421:ASP:OD2	1:A:3467:ARG:HD3	1.97	0.64
1:A:404:ASP:O	1:A:406:ARG:N	2.29	0.64
1:B:1655:ILE:HG13	1:B:1677:SER:HA	1.79	0.64
1:B:172:GLU:O	1:B:176:GLU:HG3	1.97	0.64
1:B:2538:ARG:NH1	1:B:2562:LEU:O	2.30	0.64
1:B:2539:LEU:HA	1:B:2542:LEU:HD23	1.79	0.64
1:B:3015:SER:O	1:B:3019:ILE:N	2.28	0.64
1:B:3931:ALA:O	1:B:3935:GLY:CA	2.43	0.64
1:A:1889:VAL:HG22	1:A:1900:PHE:CD2	2.33	0.64
1:A:2412:TYR:CE1	1:A:2415:LEU:HD23	2.32	0.64
1:B:171:LEU:HD13	1:B:219:VAL:HG13	1.80	0.64
1:B:1909:ASN:O	1:B:1912:THR:HG23	1.98	0.64
1:B:385:TYR:CE1	1:B:421:LEU:HD23	2.31	0.64
1:A:2094:MSE:HE2	1:A:2142:ILE:HG22	1.79	0.64
1:A:183:GLU:HA	1:A:233:ASN:HD21	1.62	0.64
1:A:2452:ARG:HG2	1:A:2498:ILE:HD11	1.79	0.64
1:A:3048:LYS:HZ2	1:A:3089:LEU:HB3	1.63	0.64
1:A:866:ILE:HB	1:A:3129:LEU:HD13	1.78	0.64
1:A:3503:VAL:HG21	1:A:3535:ILE:O	1.97	0.64
1:B:1649:LEU:HA	1:B:1652:ILE:HD12	1.78	0.64
1:B:2999:LEU:HD12	1:B:3002:TYR:HE2	1.63	0.64
1:B:3496:ILE:O	1:B:3498:TRP:N	2.31	0.64
1:B:4020:MSE:HE3	1:B:4027:TRP:NE1	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:710:PHE:O	1:B:714:VAL:HG23	1.96	0.64
1:A:1107:TYR:CE1	1:A:1111:LEU:HD13	2.33	0.64
1:A:1349:LEU:HD21	1:A:1359:LEU:HD13	1.78	0.64
1:A:2782:ASP:HA	1:A:2786:LYS:HB2	1.80	0.64
1:A:3046:ARG:HH22	1:A:3181:ASP:CG	1.99	0.64
1:A:3721:GLY:O	1:A:3741:ARG:HB2	1.97	0.64
1:B:111:CYS:HA	1:B:134:LEU:HD22	1.80	0.64
1:B:1279:LEU:HG	1:B:1292:LYS:NZ	2.13	0.64
1:B:3864:ARG:NH1	1:B:4115:ASN:OD1	2.30	0.64
1:A:1269:THR:HG22	1:A:1275:THR:HG21	1.78	0.64
1:A:1649:LEU:HD12	1:A:1652:ILE:HD12	1.78	0.64
1:A:3998:LEU:O	1:A:4002:MSE:HG3	1.97	0.64
1:A:512:GLY:HA3	1:A:726:LEU:HD22	1.79	0.64
1:A:743:LEU:HG	1:A:783:HIS:HE1	1.62	0.64
1:A:854:ARG:O	1:A:858:MSE:HB2	1.98	0.64
1:B:1039:TRP:CZ2	1:B:1049:GLN:HA	2.32	0.64
1:B:177:LEU:HA	1:B:180:LEU:HB2	1.79	0.64
1:B:2467:THR:HB	1:B:2518:GLN:HE22	1.62	0.64
1:B:2850:PHE:HB2	1:B:2853:PRO:HG2	1.80	0.64
1:B:2870:SER:O	1:B:2872:ASP:N	2.30	0.64
1:B:3974:MSE:SE	1:B:3976:GLU:HB3	2.47	0.64
1:B:85:ILE:O	1:B:89:LEU:HG	1.97	0.64
1:A:1165:LEU:HB3	1:A:1169:VAL:HG23	1.79	0.64
1:A:1345:THR:HG21	1:A:1368:LEU:HD13	1.78	0.64
1:A:1609:ALA:HB3	1:A:1806:ARG:HH22	1.61	0.64
1:A:1890:HIS:CE1	1:A:1941:HIS:HA	2.33	0.64
1:A:2307:MSE:HG2	1:A:2348:GLN:NE2	2.12	0.64
1:A:3589:SER:O	1:A:3593:ARG:CB	2.45	0.64
1:A:3676:PRO:O	1:A:3679:ASN:ND2	2.30	0.64
1:A:3425:ARG:NH2	1:A:4000:ASN:OD1	2.31	0.64
1:B:2276:LEU:HA	1:B:2279:ILE:HG12	1.80	0.64
1:B:2939:LEU:HD21	1:B:2994:TRP:CD2	2.33	0.64
1:A:1084:ASN:HD21	1:A:1131:ILE:HG22	1.63	0.64
1:A:720:GLN:HB3	1:A:1123:THR:HG21	1.78	0.64
1:A:2413:PHE:CE1	1:A:2442:MSE:HG2	2.33	0.64
1:A:2555:LEU:HD11	1:A:2803:ILE:HD11	1.79	0.64
1:A:3498:TRP:NE1	1:A:3502:MSE:SE	2.81	0.64
1:B:1973:LYS:O	1:B:1974:ASN:HB2	1.98	0.64
1:B:2423:VAL:HG13	1:B:2424:MSE:H	1.63	0.64
1:B:2433:LYS:NZ	1:B:2461:PHE:CZ	2.65	0.64
1:B:2555:LEU:HD12	1:B:2556:SER:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:LEU:HB3	1:B:319:PHE:HZ	1.63	0.64
1:B:3705:TYR:CE2	1:B:3708:ARG:NH1	2.66	0.64
1:B:393:LYS:HA	1:B:396:PHE:HD1	1.62	0.64
1:B:66:LEU:HD21	1:B:89:LEU:HD11	1.78	0.64
1:A:1700:THR:O	1:A:1702:LEU:N	2.30	0.64
1:A:884:VAL:HB	1:A:3892:THR:OG1	1.98	0.64
1:A:995:PHE:CD1	1:A:1003:SER:HA	2.33	0.64
1:B:101:ALA:HB3	1:B:102:PRO:HD3	1.80	0.64
1:B:1069:HIS:HB3	1:B:3741:ARG:CZ	2.28	0.64
1:B:1598:ASN:CG	1:B:1811:ARG:HG2	2.19	0.64
1:B:1696:LEU:HA	1:B:1700:THR:HG21	1.79	0.64
1:B:3282:ARG:HB2	1:B:3282:ARG:NH1	2.13	0.64
1:B:345:PHE:CD2	1:B:367:GLY:HA3	2.32	0.64
1:B:3816:LEU:O	1:B:3820:MSE:HB3	1.97	0.64
1:B:411:PRO:HG2	1:B:457:CYS:SG	2.37	0.64
1:A:2253:TYR:HA	1:A:2256:ILE:HB	1.80	0.64
1:A:14:ARG:HB3	1:A:2359:LYS:HE2	1.79	0.64
1:A:3855:TYR:HB3	1:A:4074:PHE:CZ	2.32	0.64
1:A:771:ASN:O	1:A:773:LEU:N	2.30	0.64
1:B:1471:GLN:O	1:B:1475:LEU:HB3	1.98	0.64
1:B:207:GLN:O	1:B:212:VAL:HG12	1.98	0.64
1:B:2379:MSE:HE1	1:B:2404:ARG:HH11	1.60	0.64
1:B:909:VAL:O	1:B:913:ARG:HG2	1.98	0.64
1:A:1039:TRP:CZ2	1:A:1049:GLN:HA	2.33	0.63
1:A:1939:LEU:HD13	1:A:1986:ARG:HH21	1.62	0.63
1:A:2194:LEU:HD13	1:A:2244:CYS:HB3	1.79	0.63
1:A:3110:PHE:O	1:A:3114:TYR:HD1	1.81	0.63
1:A:2929:LEU:HG	1:A:3784:ARG:HG2	1.79	0.63
1:A:3788:LEU:HG	1:A:3789:ARG:N	2.13	0.63
1:A:66:LEU:HD21	1:A:89:LEU:HD11	1.80	0.63
1:B:2912:GLY:HA2	1:B:2915:ARG:HH21	1.64	0.63
1:B:3725:ARG:NH1	1:B:3737:ARG:NH2	2.38	0.63
1:A:1640:GLU:O	1:A:1644:ALA:CB	2.46	0.63
1:A:2866:ALA:O	1:A:2869:LEU:N	2.31	0.63
1:A:3781:CYS:HA	1:A:3786:LEU:HD12	1.78	0.63
1:A:3985:VAL:HG11	1:A:4101:GLU:HG2	1.79	0.63
1:A:493:LYS:HB3	1:A:494:PRO:HD2	1.80	0.63
1:B:139:ARG:HA	1:B:173:LYS:HD3	1.80	0.63
1:B:1970:LYS:HE2	1:B:2017:GLY:HA3	1.80	0.63
1:B:4038:TRP:CH2	1:B:4040:PRO:HB3	2.32	0.63
1:A:1259:LEU:HD11	1:A:1337:VAL:HA	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2352:HIS:HB3	1:A:2360:PHE:HB3	1.78	0.63
1:B:2171:LEU:HG	1:B:2177:ASN:HD21	1.63	0.63
1:B:3687:MSE:C	1:B:3689:ASP:H	1.99	0.63
1:B:617:PRO:HB3	1:B:659:ARG:HG3	1.80	0.63
1:A:132:ILE:HA	1:A:135:LEU:HD12	1.80	0.63
1:A:1981:LEU:HD21	1:A:2031:LEU:O	1.98	0.63
1:A:1982:ILE:HA	1:A:1985:LYS:HE2	1.80	0.63
1:A:2281:MSE:SE	1:A:2286:PRO:HB3	2.48	0.63
1:A:2404:ARG:NH1	1:A:2412:TYR:CZ	2.67	0.63
1:A:3192:LYS:N	1:A:3192:LYS:HD2	2.13	0.63
1:B:995:PHE:CD1	1:B:1003:SER:HA	2.33	0.63
1:B:1296:PHE:O	1:B:1299:GLU:N	2.28	0.63
1:B:2145:PHE:HD1	1:B:2188:GLU:HG2	1.62	0.63
1:B:2433:LYS:HG3	1:B:2436:LEU:HD12	1.79	0.63
1:B:3974:MSE:HA	1:B:3975:LYS:HB3	1.80	0.63
1:B:2933:ILE:HG23	1:B:3979:LEU:HB2	1.80	0.63
1:B:744:ASP:C	1:B:746:ARG:H	2.01	0.63
1:B:984:TYR:O	1:B:988:VAL:HG13	1.99	0.63
1:A:1093:GLU:N	1:A:1097:GLU:OE2	2.22	0.63
1:A:720:GLN:HG3	1:A:1121:LEU:HD22	1.81	0.63
1:A:1424:THR:O	1:A:1427:SER:N	2.28	0.63
1:A:1685:ASP:CB	1:A:1727:ARG:HH22	2.06	0.63
1:A:278:HIS:O	1:A:281:GLN:HB3	1.98	0.63
1:A:2936:TYR:CD1	1:A:2949:THR:HG21	2.33	0.63
1:A:904:VAL:O	1:A:906:PHE:N	2.32	0.63
1:B:1006:THR:HG22	1:B:1010:LEU:HG	1.81	0.63
1:B:2022:PRO:HB2	1:B:2072:ARG:HH21	1.62	0.63
1:B:2144:LEU:HB3	1:B:2148:LYS:HE3	1.80	0.63
1:B:2449:VAL:HA	1:B:2452:ARG:HD2	1.80	0.63
1:B:3155:VAL:HG23	1:B:3158:LYS:HD2	1.80	0.63
1:B:3630:ARG:HG2	1:B:3686:TRP:HE1	1.63	0.63
1:B:473:PRO:HA	1:B:476:ARG:NH2	2.11	0.63
1:B:726:LEU:HD23	1:B:729:CYS:SG	2.38	0.63
1:A:1070:PRO:HB2	1:A:1073:PHE:CE1	2.34	0.63
1:A:1729:PHE:CE2	1:A:1870:LYS:HG3	2.33	0.63
1:A:345:PHE:HD2	1:A:367:GLY:HA3	1.64	0.63
1:B:1251:GLN:O	1:B:1255:CYS:HB2	1.98	0.63
1:B:2788:SER:O	1:B:2791:ILE:HB	1.98	0.63
1:B:3763:ARG:NH2	1:B:4009:PRO:HG3	2.13	0.63
1:B:3834:ALA:HB1	1:B:3838:GLU:OE1	1.98	0.63
1:B:766:ALA:O	1:B:768:VAL:N	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ILE:HG22	1:A:257:ARG:HG3	1.80	0.63
1:A:3684:SER:OG	1:A:3685:PRO:HD3	1.98	0.63
1:A:414:LEU:HD23	1:A:460:ALA:HB1	1.80	0.63
1:A:988:VAL:O	1:A:992:ILE:HG23	1.99	0.63
1:B:1583:MSE:HE1	1:B:1640:GLU:OE2	1.98	0.63
1:B:1711:ARG:HG3	1:B:1712:ARG:N	2.13	0.63
1:B:3919:GLY:H	1:B:3946:PHE:H	1.47	0.63
1:B:942:LEU:HD11	1:B:991:LEU:HD11	1.80	0.63
1:A:1419:LEU:O	1:A:1421:GLU:N	2.31	0.63
1:A:1575:LEU:HD13	1:A:1604:SER:HB3	1.80	0.63
1:A:1952:ILE:HG12	1:A:1953:CYS:H	1.63	0.63
1:A:3816:LEU:HD13	1:A:3966:GLN:NE2	2.12	0.63
1:A:4050:LYS:HB3	1:A:4055:ASN:HD21	1.63	0.63
1:B:1100:VAL:O	1:B:1104:LEU:N	2.29	0.63
1:B:1279:LEU:HG	1:B:1292:LYS:HZ1	1.62	0.63
1:B:1306:ILE:HG12	1:B:1334:LYS:HB3	1.81	0.63
1:B:3167:ARG:HG2	1:B:3186:ARG:NE	2.14	0.63
1:B:3982:SER:O	1:B:3986:HIS:ND1	2.32	0.63
1:B:4088:ASN:OD1	1:B:4091:ALA:HB3	1.99	0.63
1:B:988:VAL:O	1:B:992:ILE:HG23	1.99	0.63
1:A:1887:ASP:OD1	1:A:1937:ARG:NH2	2.31	0.63
1:A:2256:ILE:HG21	1:A:2280:VAL:HG21	1.81	0.63
1:A:2327:LEU:O	1:A:2331:MSE:HG2	1.99	0.63
1:B:114:VAL:CG1	1:B:130:LEU:HD11	2.29	0.63
1:B:2226:PRO:O	1:B:2230:VAL:N	2.27	0.63
1:B:2799:GLN:HG3	1:B:2808:LEU:HD11	1.81	0.63
1:B:2936:TYR:HE1	1:B:2949:THR:HG21	1.64	0.63
1:B:3045:ILE:O	1:B:3048:LYS:HB2	1.99	0.63
1:B:4035:GLU:HG2	1:B:4038:TRP:CE3	2.34	0.63
1:B:559:SER:O	1:B:563:LEU:HG	1.98	0.63
1:A:999:LYS:HD3	1:A:1000:LYS:H	1.64	0.62
1:A:1029:CYS:HB3	1:A:1085:ILE:HG13	1.81	0.62
1:A:2379:MSE:SE	1:A:2408:MSE:SE	3.17	0.62
1:A:31:GLY:O	1:A:34:LEU:HB3	1.98	0.62
1:A:4048:LYS:O	1:A:4051:LEU:HB3	1.99	0.62
1:A:649:PHE:O	1:A:651:TYR:N	2.32	0.62
1:A:802:THR:O	1:A:806:SER:OG	2.15	0.62
1:A:935:HIS:O	1:A:938:VAL:HB	1.99	0.62
1:B:3250:ASN:OD1	1:B:3285:HIS:HB3	1.98	0.62
1:A:1745:LYS:C	1:A:1747:LEU:H	2.02	0.62
1:A:4056:PRO:HG2	1:A:4094:PRO:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1459:HIS:CE1	1:B:1510:LEU:HG	2.35	0.62
1:B:1604:SER:HB2	1:B:1632:TRP:HB3	1.80	0.62
1:B:2146:LEU:HA	1:B:2149:LEU:HG	1.80	0.62
1:B:3107:ILE:HA	1:B:3110:PHE:CE2	2.34	0.62
1:B:3778:ASP:OD2	1:B:3781:CYS:N	2.32	0.62
1:B:452:LYS:O	1:B:455:LEU:HG	1.99	0.62
1:B:585:ILE:HG22	1:B:586:GLN:H	1.64	0.62
1:A:101:ALA:HB3	1:A:102:PRO:HD3	1.81	0.62
1:A:2147:ALA:HB1	1:A:2151:ILE:HD12	1.82	0.62
1:A:2378:PHE:CE1	1:A:2408:MSE:HE1	2.29	0.62
1:A:956:PRO:HB2	1:A:957:PRO:HD3	1.79	0.62
1:B:3592:VAL:HG13	1:B:3609:MSE:SE	2.50	0.62
1:B:4046:TYR:CZ	1:B:4049:ARG:NH2	2.68	0.62
1:A:2074:PRO:O	1:A:2077:HIS:N	2.32	0.62
1:A:252:VAL:HG11	1:A:265:TYR:HB2	1.81	0.62
1:A:2900:LEU:HD12	1:A:2905:LEU:HD21	1.80	0.62
1:A:3176:MSE:HE2	1:A:3251:ASN:HD22	1.64	0.62
1:A:3256:MSE:HE2	1:A:3282:ARG:HH12	1.62	0.62
1:A:3762:GLN:NE2	1:A:3763:ARG:NH1	2.46	0.62
1:A:3812:LEU:O	1:A:3816:LEU:CB	2.38	0.62
1:B:1637:SER:O	1:B:1640:GLU:N	2.32	0.62
1:B:154:SER:OG	1:B:189:MSE:HG2	1.99	0.62
1:B:200:PHE:O	1:B:204:LEU:HG	1.98	0.62
1:B:2936:TYR:CD2	1:B:3979:LEU:HD21	2.33	0.62
1:B:2943:PHE:CD2	1:B:2944:THR:HG23	2.34	0.62
1:B:508:HIS:HD2	1:B:725:LEU:HD13	1.65	0.62
1:B:891:ARG:CD	1:B:905:ILE:HG12	2.30	0.62
1:A:2239:LYS:HD3	2:K:110:UNK:CB	2.30	0.62
1:A:2260:PHE:CD1	1:A:2274:ILE:HG22	2.35	0.62
1:A:2900:LEU:HB3	1:A:2905:LEU:HD11	1.80	0.62
1:A:3486:GLU:HG3	1:A:3487:ILE:H	1.65	0.62
1:A:870:LEU:HD11	1:A:3125:ARG:HG3	1.80	0.62
1:B:1080:LEU:HD12	1:B:1081:ALA:N	2.14	0.62
1:B:1708:GLU:HB2	1:B:1709:GLU:OE2	2.00	0.62
1:B:2386:LEU:O	1:B:2390:HIS:HB2	2.00	0.62
1:B:3824:GLU:HB3	1:B:3829:LEU:HD11	1.81	0.62
1:A:971:ARG:HD2	1:A:1024:THR:HG23	1.80	0.62
1:A:1033:ILE:HB	1:A:1085:ILE:HG22	1.81	0.62
1:A:1292:LYS:HZ2	1:A:1361:LYS:NZ	1.96	0.62
1:A:2239:LYS:HD2	1:A:2279:ILE:HD12	1.81	0.62
1:A:245:SER:HA	1:A:248:ILE:HD12	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2555:LEU:O	1:A:2558:ALA:HB3	1.99	0.62
1:A:2837:LEU:HA	1:A:2840:PHE:CD2	2.30	0.62
1:A:2869:LEU:HG	1:A:2893:LEU:HD12	1.80	0.62
1:B:1265:GLU:O	1:B:1269:THR:HG23	2.00	0.62
1:B:1293:ALA:HA	1:B:1296:PHE:HD2	1.65	0.62
1:B:3174:ASP:OD2	1:B:3779:SER:HA	2.00	0.62
1:B:3582:GLU:O	1:B:3586:LYS:HB3	2.00	0.62
1:B:3630:ARG:HG2	1:B:3686:TRP:CD1	2.35	0.62
1:B:3812:LEU:HA	1:B:3815:LEU:HD12	1.81	0.62
1:B:414:LEU:HA	1:B:417:VAL:HB	1.80	0.62
1:B:508:HIS:CD2	1:B:725:LEU:HD13	2.35	0.62
1:A:2847:THR:HB	1:A:2850:PHE:HD2	1.65	0.62
1:A:345:PHE:CD2	1:A:367:GLY:HA3	2.34	0.62
1:A:3810:VAL:CG2	1:A:3815:LEU:HD11	2.29	0.62
1:A:3931:ALA:O	1:A:3935:GLY:HA2	2.00	0.62
1:A:509:ARG:HB3	1:A:729:CYS:SG	2.40	0.62
1:B:1574:ASN:HB3	1:B:1582:LEU:HD21	1.82	0.62
1:B:2925:GLU:HA	1:B:3121:LEU:HD11	1.80	0.62
1:B:3393:GLU:OE1	1:B:3416:LEU:HD13	1.99	0.62
1:B:3872:ARG:HH11	1:B:3965:ARG:NH1	1.97	0.62
1:B:796:LEU:HA	1:B:799:TYR:CE2	2.34	0.62
1:B:870:LEU:HA	1:B:873:VAL:HB	1.81	0.62
1:A:1119:LYS:HZ1	1:A:1256:TRP:HZ2	1.47	0.62
1:A:1220:LEU:HD13	1:A:1274:ARG:HG3	1.82	0.62
1:A:1216:GLY:HA3	1:A:1271:ILE:HG22	1.80	0.62
1:A:1342:MSE:SE	1:A:1372:LEU:HB2	2.50	0.62
1:A:1429:GLU:O	1:A:1433:ALA:CB	2.46	0.62
1:A:1880:MSE:HE2	1:A:1884:LEU:HD11	1.81	0.62
1:A:2002:LYS:C	1:A:2004:TYR:H	2.03	0.62
1:A:2227:LYS:HA	1:A:2234:ASN:HD22	1.64	0.62
1:A:2416:LYS:HB3	1:A:2442:MSE:SE	2.49	0.62
1:A:3930:VAL:HG12	1:A:3937:VAL:HG22	1.81	0.62
1:A:398:THR:O	1:A:401:ASP:N	2.33	0.62
1:A:794:PRO:HA	1:A:869:ASN:HB3	1.81	0.62
1:A:801:LYS:NZ	1:A:877:ASP:OD2	2.29	0.62
1:B:1090:ARG:HA	1:B:1090:ARG:HE	1.64	0.62
1:B:1221:ILE:HG13	1:B:1274:ARG:NH1	2.14	0.62
1:B:2157:PHE:HE2	1:B:2199:LEU:CD1	2.12	0.62
1:B:2310:VAL:HG23	1:B:2315:VAL:HG21	1.81	0.62
1:B:2416:LYS:O	1:B:2420:PHE:CB	2.47	0.62
1:B:2776:ARG:HA	1:B:2776:ARG:HH11	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3019:ILE:HG13	1:B:3020:ASP:H	1.65	0.62
1:B:446:PHE:HA	1:B:449:TYR:HE2	1.62	0.62
1:A:1449:ALA:HA	1:A:1452:VAL:HB	1.80	0.62
1:A:2283:ASN:O	1:A:2287:PRO:HD3	2.00	0.62
1:A:3465:PHE:HA	1:A:3468:LEU:HD12	1.81	0.62
1:A:572:VAL:HG13	1:A:573:LEU:H	1.64	0.62
1:B:1269:THR:HG22	1:B:1275:THR:HG21	1.82	0.62
1:B:18:THR:O	1:B:22:ALA:HB3	1.99	0.62
1:B:232:CYS:SG	1:B:274:LEU:HD13	2.40	0.62
1:B:3228:SER:HA	1:B:3231:ILE:HD12	1.80	0.62
1:B:3513:ALA:O	1:B:3516:HIS:N	2.33	0.62
1:B:634:LEU:HB3	1:B:638:GLN:HE22	1.65	0.62
1:A:2874:ALA:HB1	1:A:2878:ALA:HB3	1.81	0.62
1:A:2913:LYS:O	1:A:2915:ARG:N	2.32	0.62
1:A:538:ASP:O	1:A:545:LEU:HD13	1.99	0.62
1:A:789:TYR:HA	1:A:793:LEU:HD12	1.82	0.62
1:B:3243:ILE:HD13	1:B:3262:LEU:HD22	1.82	0.62
1:B:358:GLU:HG3	1:B:359:LEU:H	1.64	0.62
1:A:1928:ALA:HB2	1:A:1941:HIS:CE1	2.35	0.61
1:A:242:PRO:O	1:A:246:ARG:HB3	2.00	0.61
1:A:753:GLN:O	1:A:757:LYS:CB	2.48	0.61
1:A:935:HIS:HB2	1:A:984:TYR:HE2	1.65	0.61
1:B:1073:PHE:CZ	1:B:3745:GLU:HA	2.35	0.61
1:B:1280:GLN:HA	1:B:1361:LYS:NZ	2.15	0.61
1:B:1298:LEU:HA	1:B:1301:ILE:HB	1.82	0.61
1:B:732:PHE:HB2	1:B:733:LEU:HD23	1.82	0.61
1:A:1604:SER:HB2	1:A:1632:TRP:HB3	1.82	0.61
1:A:202:GLY:O	1:A:206:THR:OG1	2.10	0.61
1:A:2399:GLU:O	1:A:2402:LEU:HG	2.00	0.61
1:A:2549:LYS:HZ1	1:A:2557:LEU:CD2	2.10	0.61
1:A:3008:TRP:HA	1:A:3050:LYS:HG2	1.82	0.61
1:A:3684:SER:O	1:A:3688:SER:OG	2.14	0.61
1:A:3809:THR:HA	1:A:3931:ALA:HA	1.82	0.61
1:A:713:GLU:O	1:A:717:LYS:HG2	2.00	0.61
1:B:1214:GLU:HB2	1:B:1218:SER:HB3	1.82	0.61
1:B:1374:GLN:O	1:B:1378:GLU:HB2	2.00	0.61
1:B:2142:ILE:HA	1:B:2145:PHE:HD2	1.62	0.61
1:B:592:GLU:HB3	1:B:601:TRP:HZ2	1.65	0.61
1:B:913:ARG:HG3	1:B:937:MSE:SE	2.50	0.61
1:A:1108:MSE:O	1:A:1112:ALA:N	2.32	0.61
1:A:83:GLU:HG3	1:A:130:LEU:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1996:VAL:HG23	1:A:1997:PRO:HD2	1.82	0.61
1:A:2274:ILE:HD13	1:A:2318:ALA:HB2	1.81	0.61
1:A:287:LEU:C	1:A:291:VAL:HB	2.21	0.61
1:A:3037:GLN:HG3	1:A:3040:TYR:HE2	1.65	0.61
1:A:3578:LEU:HD13	1:A:3683:CYS:SG	2.40	0.61
1:A:3924:HIS:H	1:A:3927:ASN:HD22	1.46	0.61
1:B:1403:MSE:HA	1:B:1406:LEU:HB2	1.81	0.61
1:B:2177:ASN:HD22	1:B:2182:ILE:CG2	2.12	0.61
1:B:2399:GLU:O	1:B:2402:LEU:HG	2.00	0.61
1:B:2957:LEU:HB3	1:B:3989:ARG:HH22	1.63	0.61
1:B:980:THR:HG22	1:B:984:TYR:HE2	1.66	0.61
1:A:2167:PRO:O	1:A:2171:LEU:HB3	2.01	0.61
1:A:2925:GLU:O	1:A:2927:ALA:N	2.30	0.61
1:A:440:VAL:HG21	1:A:1814:PHE:CZ	2.36	0.61
1:A:913:ARG:NE	1:A:916:GLU:OE2	2.32	0.61
1:B:1431:LEU:HD11	1:B:1479:VAL:HG22	1.81	0.61
1:B:2538:ARG:HH11	1:B:2565:MSE:CB	2.08	0.61
1:B:2961:ALA:HB1	1:B:3002:TYR:CD1	2.33	0.61
1:A:1086:TYR:CD2	1:A:1090:ARG:HG2	2.36	0.61
1:A:1574:ASN:HB3	1:A:1582:LEU:HD21	1.81	0.61
1:A:2936:TYR:O	1:A:2940:ARG:HB2	2.00	0.61
1:A:3630:ARG:HD2	1:A:3633:ILE:HG12	1.83	0.61
1:A:3962:ARG:CZ	1:A:3962:ARG:HB2	2.30	0.61
1:A:508:HIS:HD2	1:A:725:LEU:HD22	1.65	0.61
1:B:2220:MSE:SE	1:B:2256:ILE:HD11	2.51	0.61
1:B:2849:SER:HB3	1:B:2881:LEU:HD12	1.82	0.61
1:B:3152:SER:HB3	1:B:3153:SER:CB	2.31	0.61
1:B:3167:ARG:HD3	1:B:3186:ARG:HG2	1.82	0.61
1:A:1076:LEU:HD22	1:A:1111:LEU:HG	1.83	0.61
1:A:2517:LEU:HA	1:A:2520:ILE:HG22	1.82	0.61
1:A:3765:GLU:O	1:A:3768:PHE:HB2	2.00	0.61
1:A:3962:ARG:NH1	1:A:4124:TRP:CZ3	2.66	0.61
1:A:575:ILE:HG12	1:A:579:LEU:HB2	1.81	0.61
1:B:1378:GLU:O	1:B:1382:ILE:HG12	2.01	0.61
1:B:2011:ALA:O	1:B:2013:GLU:N	2.33	0.61
1:B:3435:ASP:O	1:B:3439:LEU:HB3	2.01	0.61
1:B:4082:ARG:CG	1:B:4091:ALA:HB2	2.30	0.61
1:B:612:LEU:O	1:B:616:LYS:N	2.31	0.61
1:A:1178:ARG:HB3	1:A:1179:PRO:HD3	1.82	0.61
1:A:2396:LEU:HA	1:A:2400:VAL:HG23	1.82	0.61
1:A:3885:ARG:O	1:A:3889:ARG:HB2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:PHE:CE2	1:A:530:LEU:HB3	2.34	0.61
1:B:1108:MSE:O	1:B:1112:ALA:N	2.33	0.61
1:B:146:GLU:HB2	1:B:149:ILE:HB	1.83	0.61
1:B:3314:SER:HB3	1:B:3318:LYS:HE3	1.82	0.61
1:B:3493:TRP:HB3	1:B:3711:PRO:HA	1.81	0.61
1:B:3491:PRO:CB	1:B:3711:PRO:HB3	2.30	0.61
1:A:1352:SER:HB3	1:A:1353:PRO:HD3	1.83	0.61
1:A:3435:ASP:O	1:A:3439:LEU:CB	2.49	0.61
1:A:3414:MSE:HE1	1:A:3450:MSE:HA	1.82	0.61
1:A:3797:THR:HG22	1:A:3800:LEU:HG	1.82	0.61
1:A:934:LEU:HA	1:A:937:MSE:HE3	1.83	0.61
1:A:970:LEU:HD21	1:A:1031:ARG:HH21	1.65	0.61
1:B:1270:PHE:HZ	1:B:1347:THR:HB	1.66	0.61
1:B:2847:THR:HB	1:B:2850:PHE:HD2	1.65	0.61
1:B:3047:SER:O	1:B:3050:LYS:HG3	2.01	0.61
1:B:367:GLY:C	1:B:369:PHE:H	2.03	0.61
1:B:3729:MSE:HE2	1:B:3737:ARG:HB2	1.82	0.61
1:B:3835:PRO:HA	1:B:3871:PHE:HE1	1.65	0.61
1:B:3923:ARG:CD	1:B:3962:ARG:HH22	2.14	0.61
1:B:938:VAL:O	1:B:942:LEU:HB2	2.00	0.61
1:A:1142:HIS:O	1:A:1144:SER:N	2.30	0.61
1:A:1270:PHE:CZ	1:A:1347:THR:HG23	2.35	0.61
1:A:2204:GLY:HA2	1:A:2208:ASP:OD2	2.00	0.61
1:A:2479:TRP:CZ3	1:A:2480:ILE:HD13	2.36	0.61
1:A:349:ILE:CD1	1:A:368:LEU:HD12	2.31	0.61
1:A:3517:SER:HA	1:A:3520:GLU:HB2	1.81	0.61
1:A:3543:LYS:HE2	1:A:3545:THR:HG22	1.82	0.61
1:A:1248:PHE:HB3	1:A:3695:LEU:HD23	1.83	0.61
1:A:935:HIS:HB2	1:A:984:TYR:CE2	2.34	0.61
1:B:1352:SER:O	1:B:1354:GLU:N	2.33	0.61
1:B:1587:VAL:HG23	1:B:1647:ALA:HB2	1.82	0.61
1:B:206:THR:HA	1:B:209:THR:OG1	2.01	0.61
1:B:2814:SER:O	1:B:2818:LYS:HB2	2.00	0.61
1:A:114:VAL:HG12	1:A:130:LEU:HD21	1.81	0.61
1:A:1740:VAL:O	1:A:1743:MSE:HG3	1.99	0.61
1:A:239:GLU:HG3	1:A:240:GLU:HG3	1.83	0.61
1:A:273:ARG:HG3	1:A:274:LEU:N	2.15	0.61
1:A:2960:GLU:HG2	1:A:3252:PHE:CD2	2.36	0.61
1:A:2933:ILE:HD13	1:A:3976:GLU:HG3	1.83	0.61
1:A:437:HIS:O	1:A:440:VAL:HG22	2.00	0.61
1:A:484:HIS:CD2	1:A:556:SER:HB3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:SER:HB3	1:A:659:ARG:CZ	2.31	0.61
1:A:645:TRP:CE3	1:A:660:LEU:HD11	2.35	0.61
1:B:2157:PHE:HE2	1:B:2199:LEU:HD13	1.66	0.61
1:B:2345:VAL:O	1:B:2349:LEU:HG	2.01	0.61
1:B:2943:PHE:C	1:B:2945:SER:H	2.04	0.61
1:B:3247:ARG:NE	1:B:3278:GLN:OE1	2.30	0.61
1:B:3614:TYR:O	1:B:3618:GLY:N	2.29	0.61
1:B:3631:LYS:HA	1:B:3634:GLN:HB3	1.83	0.61
1:A:177:LEU:O	1:A:180:LEU:N	2.34	0.60
1:A:2183:HIS:CE1	1:A:2237:ILE:HD13	2.36	0.60
1:A:2260:PHE:HD1	1:A:2274:ILE:HG22	1.65	0.60
1:A:3915:HIS:O	1:A:3918:LEU:N	2.33	0.60
1:A:446:PHE:HD1	1:A:447:PRO:HD3	1.65	0.60
1:A:637:LYS:O	1:A:641:PHE:HB3	2.01	0.60
1:B:1886:LYS:HE3	1:B:1924:THR:HG21	1.82	0.60
1:B:2274:ILE:HA	1:B:2277:LEU:HG	1.83	0.60
1:B:2481:HIS:HE1	1:B:2485:ARG:HH11	1.49	0.60
1:B:2575:PRO:HD2	1:B:2785:ILE:HD11	1.81	0.60
1:B:2806:LYS:HZ1	1:B:2858:ILE:HG21	1.64	0.60
1:B:3498:TRP:O	1:B:3498:TRP:CD1	2.54	0.60
1:B:659:ARG:NH2	1:B:662:LEU:HG	2.10	0.60
1:A:1087:ARG:HD2	1:A:1137:ILE:HD11	1.83	0.60
1:A:1118:GLU:HG3	1:A:3743:HIS:CE1	2.35	0.60
1:A:1155:ARG:O	1:A:1158:PRO:HD2	2.01	0.60
1:A:135:LEU:HD21	1:A:173:LYS:HD2	1.83	0.60
1:A:1885:PRO:O	1:A:1889:VAL:HG23	2.00	0.60
1:A:3117:ILE:HG13	1:A:3120:LEU:HB3	1.82	0.60
1:A:3283:LEU:HD11	1:A:3297:VAL:HG13	1.82	0.60
1:A:3788:LEU:HD13	1:A:3910:LEU:HD23	1.82	0.60
1:A:3947:GLY:O	1:A:3950:THR:N	2.34	0.60
1:B:1419:LEU:O	1:B:1421:GLU:N	2.34	0.60
1:B:1711:ARG:HG3	1:B:1712:ARG:H	1.65	0.60
1:B:175:TYR:HA	1:B:178:LEU:HD12	1.82	0.60
1:B:1903:SER:O	1:B:1906:THR:OG1	2.18	0.60
1:B:2316:TYR:CZ	1:B:2317:ALA:HB2	2.36	0.60
1:B:2989:ALA:O	1:B:2993:PHE:N	2.32	0.60
1:B:3595:GLU:HA	1:B:3598:LYS:HD2	1.81	0.60
1:B:627:VAL:HG12	1:B:628:GLU:N	2.15	0.60
1:B:775:GLU:O	1:B:779:TYR:HD2	1.84	0.60
1:A:1424:THR:OG1	1:A:1425:ALA:N	2.34	0.60
1:A:1452:VAL:HG11	1:A:1502:SER:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1805:PHE:HA	1:A:1808:ASP:OD2	2.00	0.60
1:A:2167:PRO:HB2	1:A:2171:LEU:HD22	1.83	0.60
1:A:246:ARG:HA	1:A:249:PHE:HD2	1.66	0.60
1:A:2813:PHE:HA	1:A:2816:ILE:HG22	1.82	0.60
1:A:607:ASP:HA	1:A:610:ALA:HB3	1.81	0.60
1:B:1762:MSE:HE2	1:B:1899:VAL:HG11	1.83	0.60
1:B:2353:GLN:HG2	1:B:2361:ILE:HD13	1.83	0.60
1:B:2775:TYR:HB3	1:B:2776:ARG:NH2	2.16	0.60
1:B:242:PRO:HB3	1:B:282:PHE:CD1	2.35	0.60
1:B:3048:LYS:O	1:B:3052:LEU:N	2.31	0.60
1:B:3265:GLU:HA	1:B:3267:LYS:HE3	1.84	0.60
1:B:404:ASP:O	1:B:406:ARG:N	2.33	0.60
1:A:1761:LEU:HD22	1:A:1860:GLU:HB3	1.83	0.60
1:A:1981:LEU:O	1:A:1985:LYS:HG2	2.02	0.60
1:A:2088:LEU:O	1:A:2092:GLU:N	2.34	0.60
1:A:3876:SER:O	1:A:3879:PRO:HD2	2.00	0.60
1:A:390:GLN:O	1:A:393:LYS:HG2	2.01	0.60
1:B:108:LYS:HG2	1:B:138:PHE:HA	1.81	0.60
1:B:3065:ILE:HD13	1:B:3089:LEU:HD21	1.83	0.60
1:B:3594:ALA:HB1	1:B:4028:ILE:HD13	1.83	0.60
1:B:3954:PRO:HB3	1:B:4027:TRP:HA	1.82	0.60
1:A:1131:ILE:HA	1:A:1134:LEU:HG	1.84	0.60
1:A:1978:PHE:O	1:A:1981:LEU:HB3	2.01	0.60
1:A:1983:ASP:O	1:A:1987:ARG:HB2	2.02	0.60
1:A:2430:GLU:OE2	1:A:2461:PHE:HD1	1.83	0.60
1:A:2413:PHE:CD1	1:A:2442:MSE:HG2	2.36	0.60
1:A:908:ASP:HB3	1:A:2807:GLN:OE1	2.01	0.60
1:A:3181:ASP:O	1:A:3184:THR:OG1	2.13	0.60
1:A:4004:VAL:O	1:A:4008:GLU:CB	2.50	0.60
1:A:617:PRO:HB3	1:A:659:ARG:HG2	1.82	0.60
1:B:1259:LEU:HG	1:B:1337:VAL:HG22	1.83	0.60
1:B:1743:MSE:HG2	1:B:1747:LEU:HD12	1.83	0.60
1:B:224:LEU:HD22	1:B:248:ILE:HD11	1.83	0.60
1:B:3389:VAL:HG11	1:B:3419:PHE:CZ	2.35	0.60
1:B:327:VAL:HG22	1:B:338:LEU:HD13	1.83	0.60
1:B:3965:ARG:HE	1:B:3969:ASN:HD21	1.49	0.60
1:B:730:LEU:HD23	1:B:733:LEU:HD12	1.83	0.60
1:A:1100:VAL:O	1:A:1104:LEU:N	2.33	0.60
1:A:1935:GLU:HB2	1:A:1986:ARG:CZ	2.31	0.60
1:A:3155:VAL:N	1:A:3156:PRO:HD2	2.17	0.60
1:A:3725:ARG:NH1	1:A:3737:ARG:HH22	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:GLY:C	1:A:405:ASP:H	2.04	0.60
1:A:966:PHE:O	1:A:969:LEU:HB3	2.02	0.60
1:B:1742:CYS:HA	1:B:1745:LYS:HD2	1.83	0.60
1:B:2472:GLN:O	1:B:2476:ILE:HG23	2.02	0.60
1:B:3483:MSE:O	1:B:3516:HIS:NE2	2.35	0.60
1:B:3670:MSE:O	1:B:3674:SER:HB3	2.00	0.60
1:B:613:HIS:ND1	1:B:614:PRO:HD3	2.16	0.60
1:A:249:PHE:O	1:A:253:LEU:HG	2.01	0.60
1:A:3503:VAL:HG23	1:A:3536:SER:HA	1.83	0.60
1:A:3760:GLN:OE1	1:A:3760:GLN:N	2.34	0.60
1:A:566:ASP:OD2	1:A:1800:SER:HA	2.02	0.60
1:B:1066:LEU:HA	1:B:1069:HIS:CD2	2.36	0.60
1:B:1220:LEU:HD13	1:B:1274:ARG:HG3	1.81	0.60
1:B:1700:THR:OG1	1:B:1701:SER:N	2.33	0.60
1:B:1946:ASN:O	1:B:1949:ILE:HG22	2.02	0.60
1:B:2326:ILE:HG21	1:B:2341:LEU:HD23	1.82	0.60
1:B:3723:ASP:HB2	1:B:3741:ARG:HE	1.66	0.60
1:A:3152:SER:HB3	1:A:3153:SER:CB	2.32	0.60
1:A:3487:ILE:CG2	1:A:3495:PHE:HB2	2.31	0.60
1:A:752:LEU:HB2	1:A:756:PHE:CE1	2.37	0.60
1:A:936:SER:O	1:A:939:MSE:N	2.35	0.60
1:B:1130:ALA:O	1:B:1134:LEU:HG	2.01	0.60
1:B:1146:ASN:O	1:B:1150:LYS:HB3	2.02	0.60
1:B:2975:ALA:C	1:B:2977:ASN:H	2.05	0.60
1:B:3344:GLU:O	1:B:3348:LEU:HG	2.02	0.60
1:B:3928:PHE:HE2	1:B:3962:ARG:HE	1.47	0.60
1:B:3962:ARG:NH1	1:B:4124:TRP:CH2	2.70	0.60
1:B:649:PHE:HE1	1:B:653:LEU:H	1.49	0.60
1:A:1063:LEU:HD13	1:A:1082:PHE:CZ	2.37	0.60
1:A:1583:MSE:HE2	1:A:1639:LEU:HB2	1.83	0.60
1:A:2083:LEU:H	1:A:2086:ASP:HB2	1.67	0.60
1:A:2274:ILE:CG1	1:A:2314:GLU:HB3	2.32	0.60
1:A:2554:PHE:O	1:A:2557:LEU:N	2.35	0.60
1:A:3351:ILE:O	1:A:3355:LYS:HG2	2.02	0.60
1:A:416:SER:O	1:A:420:VAL:HB	2.01	0.60
1:A:999:LYS:HB3	1:A:1001:PHE:CE2	2.37	0.60
1:B:1520:ALA:O	1:B:1524:LEU:HD13	2.01	0.60
1:B:3916:TRP:CE3	1:B:3917:ILE:HD12	2.36	0.60
1:B:3950:THR:OG1	1:B:3957:GLU:O	2.09	0.60
1:A:2157:PHE:HE1	1:A:2203:THR:HB	1.66	0.60
1:A:2389:PHE:CD2	1:A:2396:LEU:HD22	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:PHE:CD1	1:A:297:LEU:HD13	2.37	0.60
1:A:3971:MSE:HE1	1:A:3980:MSE:SE	2.52	0.60
1:B:1762:MSE:HG2	1:B:1896:ILE:HA	1.83	0.60
1:B:2145:PHE:HZ	1:B:2185:MSE:HA	1.66	0.60
1:B:2981:TRP:O	1:B:2985:GLU:HB2	2.02	0.60
1:B:3444:ALA:HA	1:B:3475:TYR:OH	2.02	0.60
1:B:3571:PHE:O	1:B:3575:LEU:CB	2.49	0.60
1:A:2183:HIS:HE1	1:A:2237:ILE:HG21	1.67	0.59
1:A:2436:LEU:O	1:A:2439:ILE:HG22	2.02	0.59
1:A:3498:TRP:HE1	1:A:3502:MSE:SE	2.35	0.59
1:A:3572:ILE:O	1:A:3575:LEU:HB2	2.01	0.59
1:A:3584:LEU:O	1:A:3588:TRP:HB3	2.02	0.59
1:A:396:PHE:CD2	1:A:441:MSE:HG3	2.37	0.59
1:A:414:LEU:HA	1:A:417:VAL:HB	1.84	0.59
1:A:722:LYS:HB3	1:A:727:ALA:HA	1.84	0.59
1:A:933:LEU:HD11	1:A:2795:GLN:OE1	2.02	0.59
1:B:1166:LEU:HB3	1:B:1170:LYS:NZ	2.17	0.59
1:B:1569:THR:O	1:B:1573:LYS:HB2	2.02	0.59
1:B:1750:LEU:O	1:B:1754:GLN:HG3	2.02	0.59
1:B:18:THR:O	1:B:22:ALA:CB	2.49	0.59
1:B:3722:PHE:CE1	1:B:3740:ILE:HG12	2.23	0.59
1:B:913:ARG:HA	1:B:916:GLU:CD	2.23	0.59
1:A:1344:PHE:HA	1:A:1347:THR:HB	1.84	0.59
1:A:1438:GLY:O	1:A:1441:ALA:HB2	2.01	0.59
1:A:1916:ILE:HG23	1:A:1920:TYR:CE1	2.36	0.59
1:A:2139:PRO:O	1:A:2143:ARG:HD2	2.01	0.59
1:A:2352:HIS:HB2	1:A:2364:LEU:HD11	1.83	0.59
1:A:2549:LYS:NZ	1:A:2557:LEU:HD22	2.11	0.59
1:A:3047:SER:HB2	1:A:3050:LYS:HE2	1.84	0.59
1:A:3435:ASP:O	1:A:3439:LEU:HB3	2.02	0.59
1:A:3572:ILE:HA	1:A:3575:LEU:HG	1.82	0.59
1:A:3723:ASP:HB2	1:A:3741:ARG:HE	1.67	0.59
1:B:2430:GLU:HG3	1:B:2465:PRO:CB	2.32	0.59
1:B:850:GLU:OE2	1:B:854:ARG:NH2	2.34	0.59
1:B:977:ASP:HB3	1:B:981:ARG:H	1.67	0.59
1:A:1651:LYS:O	1:A:1654:GLN:HB2	2.02	0.59
1:A:2325:LEU:HG	1:A:2329:TYR:CE2	2.37	0.59
1:A:393:LYS:HA	1:A:396:PHE:HD1	1.67	0.59
1:A:3913:ILE:HD11	1:A:3984:MSE:HB3	1.83	0.59
1:A:3946:PHE:HE2	1:A:4048:LYS:HD2	1.68	0.59
1:A:913:ARG:CB	1:A:934:LEU:HD12	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:980:THR:O	1:A:984:TYR:HD1	1.85	0.59
1:B:1175:HIS:O	1:B:1179:PRO:HD3	2.01	0.59
1:B:610:ALA:HA	1:B:613:HIS:CE1	2.37	0.59
1:A:1029:CYS:SG	1:A:1085:ILE:HG13	2.42	0.59
1:A:1142:HIS:C	1:A:1144:SER:H	2.05	0.59
1:A:1894:SER:HB2	1:A:1896:ILE:HG13	1.83	0.59
1:A:1996:VAL:HG21	1:A:2047:THR:OG1	2.02	0.59
1:A:2510:LEU:HG	1:A:2522:ARG:HE	1.68	0.59
1:A:3080:LEU:HB3	1:A:3102:TYR:CE1	2.37	0.59
1:A:3090:TYR:HB2	1:A:3099:ALA:HB2	1.84	0.59
1:A:3439:LEU:O	1:A:3443:PRO:HD3	2.02	0.59
1:A:3583:LEU:HD13	1:A:3755:GLY:HA3	1.85	0.59
1:A:966:PHE:HB3	1:A:967:PRO:HD3	1.83	0.59
1:B:1005:ASP:OD1	1:B:1005:ASP:N	2.34	0.59
1:B:108:LYS:HB3	1:B:138:PHE:CD1	2.37	0.59
1:B:2129:LEU:HD22	1:B:2144:LEU:HD11	1.83	0.59
1:B:2330:VAL:CG2	1:B:2335:ASN:HA	2.28	0.59
1:B:2420:PHE:CZ	1:B:2436:LEU:HB3	2.37	0.59
1:B:2542:LEU:CB	1:B:2546:TYR:HE2	2.14	0.59
1:B:2886:GLN:CD	1:B:2887:PRO:HD3	2.23	0.59
1:B:3333:THR:OG1	1:B:3385:LEU:HB3	2.01	0.59
1:B:3887:PHE:HE1	1:B:3900:LEU:HB3	1.67	0.59
2:S:217:UNK:HA	2:S:220:MSE:SE	2.52	0.59
1:A:136:GLN:HA	1:A:139:ARG:HD3	1.84	0.59
1:A:2274:ILE:HG12	1:A:2314:GLU:HB3	1.83	0.59
1:A:2420:PHE:CZ	1:A:2436:LEU:HB3	2.37	0.59
1:A:3811:THR:HG22	1:A:3929:MSE:SE	2.53	0.59
1:A:4081:ALA:HA	1:A:4113:ASP:OD2	2.02	0.59
1:B:1908:GLY:HA3	1:B:1952:ILE:HG13	1.84	0.59
1:B:232:CYS:HG	1:B:275:PHE:HE1	1.50	0.59
1:B:3069:MSE:HA	1:B:3072:GLU:HB3	1.84	0.59
1:B:3389:VAL:O	1:B:3393:GLU:HG3	2.02	0.59
1:B:633:ILE:HG22	1:B:634:LEU:HD23	1.84	0.59
1:A:1416:GLU:O	1:A:1420:ARG:HB2	2.03	0.59
1:A:1711:ARG:HB3	1:A:1739:TYR:HE1	1.68	0.59
1:A:1925:GLU:O	1:A:1928:ALA:N	2.32	0.59
1:A:2326:ILE:O	1:A:2330:VAL:HB	2.03	0.59
1:A:3156:PRO:HB2	1:A:3197:LEU:HD12	1.84	0.59
1:A:3581:PRO:O	1:A:3585:PHE:HD1	1.85	0.59
1:B:1142:HIS:C	1:B:1144:SER:H	2.05	0.59
1:B:1368:LEU:HA	1:B:1371:VAL:HG12	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:GLU:OE2	1:B:264:ARG:NH2	2.36	0.59
1:B:2239:LYS:O	1:B:2242:VAL:HB	2.02	0.59
1:B:2281:MSE:SE	1:B:2286:PRO:HB3	2.52	0.59
1:B:2501:LEU:O	1:B:2505:VAL:HG23	2.02	0.59
1:B:2921:LEU:HD12	1:B:2922:ARG:N	2.17	0.59
1:B:3592:VAL:HA	1:B:3609:MSE:SE	2.53	0.59
1:A:1267:TYR:O	1:A:1271:ILE:HG13	2.03	0.59
1:A:1467:ILE:HG13	1:A:1468:LEU:HG	1.84	0.59
1:A:1962:TYR:O	1:A:1965:PHE:N	2.35	0.59
1:A:2299:TYR:O	1:A:2302:ALA:N	2.35	0.59
1:A:2319:ALA:O	1:A:2323:LEU:HD12	2.03	0.59
1:A:2851:PHE:HA	1:A:2854:PHE:CE2	2.38	0.59
1:A:2957:LEU:HB3	1:A:3989:ARG:HH12	1.63	0.59
1:A:253:LEU:HD21	1:A:297:LEU:HA	1.84	0.59
1:A:3031:TRP:CE3	1:A:3034:PRO:HD3	2.37	0.59
1:A:3492:CYS:O	1:A:3495:PHE:CB	2.50	0.59
1:A:3612:ARG:HD3	1:A:3799:ARG:NH2	2.17	0.59
1:A:3963:LEU:HD12	1:A:3967:PHE:HZ	1.66	0.59
1:A:940:PHE:CE1	1:A:2791:ILE:HG21	2.37	0.59
1:B:1594:SER:OG	1:B:1683:LYS:HD3	2.02	0.59
1:B:2040:MSE:HA	1:B:2043:PHE:HD1	1.68	0.59
1:B:2136:PRO:C	1:B:2139:PRO:HD2	2.22	0.59
1:B:2144:LEU:HB3	1:B:2148:LYS:CE	2.33	0.59
1:B:2291:GLN:O	1:B:2293:GLY:N	2.35	0.59
1:B:2638:UNK:O	1:B:2790:LEU:HD13	2.02	0.59
1:B:3000:ASP:O	1:B:3004:HIS:N	2.35	0.59
1:B:327:VAL:HG13	1:B:338:LEU:HD13	1.84	0.59
1:A:2270:ASN:O	1:A:2274:ILE:HG23	2.03	0.59
1:A:2543:ASN:HA	1:A:2546:TYR:HD2	1.67	0.59
1:A:2960:GLU:CD	1:A:3289:ARG:HH12	2.05	0.59
1:B:1655:ILE:HG12	1:B:1681:ASP:HB3	1.83	0.59
1:B:179:GLY:HA3	1:B:229:SER:HB3	1.84	0.59
1:B:2419:ASP:O	1:B:2422:GLN:HB3	2.02	0.59
1:B:2645:UNK:HA	1:B:2649:UNK:C	2.33	0.59
1:B:270:ALA:O	1:B:274:LEU:HG	2.03	0.59
1:B:3273:LEU:O	1:B:3277:VAL:HG12	2.03	0.59
1:B:4062:ASP:O	1:B:4065:LEU:HG	2.03	0.59
1:B:886:TRP:CH2	1:B:892:LEU:HD13	2.37	0.59
1:A:1060:PHE:O	1:A:1064:TYR:HD2	1.85	0.59
1:A:1437:TYR:O	1:A:1439:PRO:HD2	2.02	0.59
1:A:1571:LEU:HD13	1:A:1599:GLY:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1647:ALA:O	1:A:1651:LYS:HE3	2.02	0.59
1:A:194:GLU:HA	1:A:197:PHE:HD2	1.68	0.59
1:A:242:PRO:O	1:A:246:ARG:CB	2.50	0.59
1:A:2546:TYR:CE1	1:A:2558:ALA:HB2	2.38	0.59
1:A:2868:LEU:O	1:A:2872:ASP:HB2	2.03	0.59
1:A:3269:ARG:HH11	1:A:3312:VAL:HA	1.66	0.59
1:A:3638:LYS:O	1:A:3641:ASP:N	2.36	0.59
1:A:3811:THR:OG1	1:A:3811:THR:O	2.19	0.59
1:A:4006:VAL:HA	1:A:4012:ASP:OD2	2.03	0.59
1:A:980:THR:HG23	1:A:984:TYR:CE1	2.34	0.59
1:B:1018:VAL:HB	1:B:1074:LYS:CB	2.28	0.59
1:B:437:HIS:HA	1:B:1814:PHE:CZ	2.38	0.59
1:B:2185:MSE:O	1:B:2189:ILE:HG13	2.02	0.59
1:B:197:PHE:CZ	1:B:230:LEU:HD22	2.37	0.59
1:B:3753:LYS:HD3	1:B:3758:LEU:HD21	1.85	0.59
1:B:3909:ALA:HB2	1:B:3980:MSE:HE2	1.83	0.59
1:B:390:GLN:NE2	1:B:1723:PRO:HG2	2.18	0.59
1:B:392:CYS:HA	1:B:395:MSE:HB2	1.83	0.59
1:B:767:GLU:HG2	1:B:846:ILE:O	2.03	0.59
1:A:1866:GLN:O	1:A:1870:LYS:HB2	2.03	0.59
1:A:1992:VAL:HG21	1:A:2044:ASP:OD1	2.03	0.59
1:A:2330:VAL:CG2	1:A:2335:ASN:HA	2.31	0.59
1:A:3076:ALA:HB1	1:A:3080:LEU:HD11	1.85	0.59
1:A:3324:ARG:O	1:A:3328:ILE:HG13	2.02	0.59
1:A:3505:LEU:HB3	1:A:3510:GLN:OE1	2.03	0.59
1:B:1016:GLY:O	1:B:1019:ASP:HB2	2.03	0.59
1:B:1084:ASN:CG	1:B:1134:LEU:HD11	2.22	0.59
1:B:3908:HIS:O	1:B:3911:ILE:HG12	2.03	0.59
1:A:1736:PHE:O	1:A:1740:VAL:HG23	2.02	0.58
1:A:2462:VAL:CB	1:A:2473:MSE:SE	3.00	0.58
1:A:3585:PHE:HE2	1:A:3617:LEU:HD11	1.68	0.58
1:A:535:LEU:HD13	1:A:626:LEU:HD21	1.84	0.58
1:A:982:GLN:O	1:A:986:PRO:HD3	2.03	0.58
1:B:3149:GLY:HA3	1:B:3196:LYS:HE3	1.84	0.58
1:B:3351:ILE:HG23	1:B:3355:LYS:HE2	1.84	0.58
1:B:3503:VAL:HG22	1:B:3539:SER:HB2	1.84	0.58
1:B:3516:HIS:CG	1:B:3517:SER:N	2.70	0.58
1:B:673:THR:HG22	1:B:704:PHE:HE1	1.68	0.58
1:B:806:SER:O	1:B:809:THR:N	2.36	0.58
1:A:1102:GLU:HA	1:A:1150:LYS:NZ	2.18	0.58
1:A:1330:TYR:O	1:A:1334:LYS:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2058:ASP:H	1:A:2061:PRO:HG2	1.68	0.58
1:A:2221:LYS:O	1:A:2225:HIS:ND1	2.36	0.58
1:A:2560:ASN:OD1	1:A:2800:ARG:NH1	2.36	0.58
1:A:3274:VAL:O	1:A:3277:VAL:HG22	2.04	0.58
1:A:3769:GLN:HA	1:A:3772:ASN:OD1	2.03	0.58
1:A:3813:LYS:CE	1:A:3926:ASN:HB2	2.31	0.58
1:A:3872:ARG:NH1	1:A:3965:ARG:HH12	1.98	0.58
1:A:2936:TYR:CD2	1:A:3979:LEU:HD21	2.38	0.58
1:A:437:HIS:CD2	1:A:438:LEU:N	2.70	0.58
1:B:1036:PHE:CD1	1:B:1059:LEU:HD11	2.38	0.58
1:B:111:CYS:HB2	1:B:134:LEU:HB3	1.86	0.58
1:B:1648:LEU:HD13	1:B:1688:LEU:HD21	1.85	0.58
1:B:1737:ASN:C	1:B:1739:TYR:H	2.06	0.58
1:B:176:GLU:HG2	1:B:225:LYS:HD3	1.83	0.58
1:B:2145:PHE:CZ	1:B:2185:MSE:HA	2.39	0.58
1:B:3190:LEU:HD21	1:B:3235:LYS:HG2	1.85	0.58
1:B:3583:LEU:HD21	1:B:3733:ARG:HD3	1.84	0.58
1:B:3637:GLY:O	1:B:3641:ASP:HB3	2.03	0.58
1:B:738:HIS:ND1	1:B:745:VAL:HG13	2.18	0.58
1:A:1386:ILE:HA	1:A:1389:VAL:HB	1.85	0.58
1:A:1454:ALA:O	1:A:1457:GLN:HB2	2.03	0.58
1:A:2378:PHE:O	1:A:2382:VAL:HG22	2.02	0.58
1:A:2942:ILE:HD12	1:A:2987:THR:HG22	1.85	0.58
1:A:3505:LEU:HA	1:A:3509:ASP:HB2	1.84	0.58
1:A:368:LEU:CD2	1:A:384:MSE:HB2	2.18	0.58
1:B:143:LEU:O	1:B:144:MSE:HB2	2.03	0.58
1:B:1918:LEU:HD13	1:B:1958:GLU:HB3	1.85	0.58
1:B:2003:LYS:O	1:B:2007:ILE:HG13	2.03	0.58
1:B:2157:PHE:HA	1:B:2160:TYR:CD2	2.38	0.58
1:B:2182:ILE:O	1:B:2186:VAL:HG12	2.03	0.58
1:B:2775:TYR:HB3	1:B:2776:ARG:CZ	2.33	0.58
1:B:2936:TYR:HA	1:B:2939:LEU:HB2	1.85	0.58
1:B:321:LYS:O	1:B:325:ASN:ND2	2.26	0.58
1:B:3427:GLU:HB3	1:B:3439:LEU:HD22	1.85	0.58
1:B:435:LEU:O	1:B:439:VAL:HG23	2.03	0.58
1:B:535:LEU:HD21	1:B:622:ALA:O	2.03	0.58
1:B:752:LEU:HA	1:B:755:ALA:HB3	1.84	0.58
1:A:1296:PHE:HD1	1:A:1299:GLU:OE2	1.86	0.58
1:A:1711:ARG:HB3	1:A:1739:TYR:CE1	2.37	0.58
1:A:1919:CYS:O	1:A:1923:PHE:CB	2.50	0.58
1:A:2884:LEU:HD22	1:A:3895:GLU:OE2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3099:ALA:O	1:A:3103:ILE:HB	2.02	0.58
1:A:3454:LEU:HA	1:A:3456:LEU:HD12	1.85	0.58
1:A:446:PHE:HA	1:A:449:TYR:CE2	2.39	0.58
1:A:613:HIS:ND1	1:A:614:PRO:HD3	2.18	0.58
1:A:633:ILE:HG22	1:A:637:LYS:HG2	1.86	0.58
1:A:727:ALA:O	1:A:731:THR:HG23	2.03	0.58
1:A:985:GLU:HB3	1:A:986:PRO:HD3	1.84	0.58
1:B:1963:GLN:NE2	1:B:1995:GLU:HG2	2.18	0.58
1:B:2070:GLU:HA	1:B:2071:GLN:HB2	1.85	0.58
1:B:2913:LYS:HG3	1:B:2914:ALA:N	2.18	0.58
1:B:571:SER:O	1:B:605:THR:OG1	2.19	0.58
1:A:1386:ILE:HB	1:A:1391:VAL:HG21	1.84	0.58
1:A:1959:LEU:HD13	1:A:1998:MSE:HE3	1.84	0.58
1:A:2420:PHE:CE1	1:A:2436:LEU:HB3	2.38	0.58
1:A:3092:LEU:HD22	1:A:3192:LYS:HE2	1.86	0.58
1:A:3587:ASP:HB3	1:A:4022:LYS:NZ	2.19	0.58
1:B:971:ARG:HD2	1:B:1024:THR:OG1	2.04	0.58
1:B:1583:MSE:HE3	1:B:1643:MSE:CB	2.33	0.58
1:B:503:SER:O	1:B:507:ASP:HB2	2.02	0.58
1:B:713:GLU:O	1:B:717:LYS:HG2	2.04	0.58
1:B:722:LYS:HD2	1:B:730:LEU:HB2	1.85	0.58
1:A:1648:LEU:HD22	1:A:1684:LEU:HD22	1.86	0.58
1:A:2275:GLN:O	1:A:2279:ILE:HG12	2.03	0.58
1:A:2962:ARG:NH2	1:A:3006:ALA:HB1	2.18	0.58
1:A:3092:LEU:HD22	1:A:3192:LYS:CE	2.33	0.58
1:A:3339:ASN:O	1:A:3341:LEU:N	2.36	0.58
1:A:450:SER:O	1:A:454:GLN:HB2	2.04	0.58
1:A:566:ASP:O	1:A:570:LYS:NZ	2.36	0.58
1:A:491:CYS:SG	1:A:615:ALA:HB2	2.43	0.58
1:B:1651:LYS:HB2	1:B:1684:LEU:CD1	2.29	0.58
1:B:2011:ALA:HB3	1:B:2014:ALA:CB	2.29	0.58
1:B:2126:MSE:HE2	1:B:2156:VAL:HG22	1.86	0.58
1:B:2167:PRO:O	1:B:2171:LEU:CB	2.33	0.58
1:B:2900:LEU:HD12	1:B:2905:LEU:HD11	1.84	0.58
1:B:572:VAL:HG13	1:B:573:LEU:H	1.67	0.58
1:A:1059:LEU:O	1:A:1063:LEU:HG	2.03	0.58
1:A:1101:PHE:CD2	1:A:1138:ILE:HG12	2.38	0.58
1:A:1327:GLY:O	1:A:1330:TYR:HB3	2.04	0.58
1:A:1594:SER:HA	1:A:1687:HIS:HE1	1.69	0.58
1:A:205:LYS:HA	1:A:208:MSE:HG2	1.84	0.58
1:A:2085:MSE:SE	1:A:2088:LEU:HD22	2.54	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2140:LEU:HA	1:A:2143:ARG:HD3	1.86	0.58
1:A:2454:LEU:O	1:A:2457:PRO:HD2	2.03	0.58
1:A:3910:LEU:O	1:A:3914:SER:OG	2.15	0.58
1:A:509:ARG:HD2	1:A:655:LEU:HD13	1.84	0.58
1:B:1063:LEU:HD13	1:B:1082:PHE:CE1	2.38	0.58
1:B:1086:TYR:HE2	1:B:1090:ARG:HE	1.51	0.58
1:B:1644:ALA:HA	1:B:1648:LEU:HD12	1.83	0.58
1:B:1925:GLU:OE2	1:B:1959:LEU:HG	2.03	0.58
1:B:204:LEU:HD13	1:B:223:CYS:HB2	1.84	0.58
1:B:2358:ASP:HB2	1:B:2396:LEU:CD2	2.30	0.58
1:B:3463:LEU:HD13	1:B:4000:ASN:HB2	1.86	0.58
1:B:410:MSE:HE1	1:B:445:SER:HB3	1.85	0.58
1:B:446:PHE:CD1	1:B:447:PRO:HD3	2.38	0.58
1:B:903:PRO:HG2	1:B:2811:SER:HB2	1.85	0.58
1:A:1074:LYS:O	1:A:1075:ARG:HG2	2.04	0.58
1:A:252:VAL:HG21	1:A:265:TYR:HB2	1.85	0.58
1:A:2920:VAL:HB	1:A:3036:TYR:OH	2.04	0.58
1:A:3454:LEU:O	1:A:3494:GLN:NE2	2.34	0.58
1:A:3464:LYS:O	1:A:3468:LEU:HG	2.03	0.58
1:A:3525:TYR:O	1:A:3529:ILE:HB	2.03	0.58
1:A:3631:LYS:HE2	1:A:3634:GLN:HG2	1.86	0.58
1:A:3879:PRO:HA	1:A:3882:LEU:HB2	1.86	0.58
1:A:617:PRO:O	1:A:620:PHE:N	2.36	0.58
1:B:1163:LEU:HA	1:B:1260:LEU:HD21	1.84	0.58
1:B:1606:ARG:HH11	1:B:1806:ARG:HB3	1.69	0.58
1:B:175:TYR:HE1	1:B:200:PHE:HB3	1.68	0.58
1:B:2167:PRO:HA	1:B:2171:LEU:HD13	1.86	0.58
1:B:419:SER:O	1:B:422:LEU:HB2	2.04	0.58
1:A:2338:GLU:O	1:A:2338:GLU:HG2	2.03	0.58
1:A:3047:SER:O	1:A:3050:LYS:HG3	2.04	0.58
1:A:3322:ALA:O	1:A:3325:ASP:HB3	2.04	0.58
1:A:352:VAL:HA	1:A:355:ASN:O	2.03	0.58
1:A:3772:ASN:O	1:A:3787:GLN:NE2	2.24	0.58
1:A:549:ALA:O	1:A:553:VAL:HG23	2.03	0.58
1:A:870:LEU:HD21	1:A:3129:LEU:HD11	1.86	0.58
1:B:2040:MSE:HA	1:B:2043:PHE:CD1	2.38	0.58
1:B:2481:HIS:O	1:B:2485:ARG:N	2.37	0.58
1:B:2477:LEU:CB	1:B:2506:LEU:HD21	2.34	0.58
1:B:3571:PHE:O	1:B:3575:LEU:HB2	2.03	0.58
1:B:3974:MSE:HB3	1:B:3976:GLU:HB3	1.86	0.58
1:B:510:ALA:O	1:B:513:GLU:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1010:LEU:HA	1:A:1013:ILE:CG1	2.30	0.58
1:A:1521:PHE:HB2	1:A:1589:ASN:OD1	2.04	0.58
1:A:2440:TYR:O	1:A:2443:MSE:HE2	2.04	0.58
1:A:2430:GLU:HG3	1:A:2465:PRO:HB3	1.86	0.58
1:A:435:LEU:HD11	1:A:475:LEU:HD21	1.85	0.58
1:A:627:VAL:HG12	1:A:628:GLU:N	2.17	0.58
1:A:806:SER:O	1:A:809:THR:N	2.26	0.58
1:B:1145:LEU:HB2	1:B:1149:LYS:HZ3	1.66	0.58
1:B:1883:ARG:HE	1:B:1923:PHE:HZ	1.50	0.58
1:B:3699:LEU:HB3	1:B:3718:ARG:HH12	1.69	0.58
1:B:669:LEU:O	1:B:671:SER:N	2.36	0.58
1:B:852:ARG:O	1:B:855:VAL:HB	2.04	0.58
1:A:2349:LEU:O	1:A:2353:GLN:HG3	2.02	0.57
1:A:2440:TYR:OH	1:A:2455:LEU:HG	2.04	0.57
1:A:2474:TYR:HE2	1:A:2518:GLN:HB3	1.69	0.57
1:A:2993:PHE:O	1:A:2997:ALA:N	2.25	0.57
1:A:3451:LEU:HG	1:A:3486:GLU:OE1	2.04	0.57
1:A:3649:SER:HA	1:A:3652:LEU:HG	1.86	0.57
1:A:3855:TYR:HB3	1:A:4074:PHE:HZ	1.66	0.57
1:A:3944:HIS:CG	1:A:3949:ALA:HA	2.39	0.57
1:A:488:ILE:O	1:A:612:LEU:HB2	2.04	0.57
1:A:852:ARG:O	1:A:855:VAL:HB	2.04	0.57
1:B:647:TYR:HE1	1:B:1389:VAL:HA	1.68	0.57
1:B:1810:PRO:O	1:B:1812:LEU:HG	2.03	0.57
1:B:2568:MSE:HG3	1:B:2569:SER:H	1.69	0.57
1:B:3104:GLN:HA	1:B:3107:ILE:HD12	1.86	0.57
1:B:3464:LYS:HE3	1:B:3468:LEU:HD21	1.86	0.57
1:B:3501:HIS:HA	1:B:4008:GLU:OE2	2.04	0.57
1:B:3981:TYR:CE1	1:B:4104:VAL:HB	2.39	0.57
1:A:1139:GLU:HG3	1:A:1175:HIS:NE2	2.18	0.57
1:A:1400:VAL:O	1:A:1404:LYS:HB2	2.04	0.57
1:A:1679:LEU:O	1:A:1683:LYS:HG3	2.04	0.57
1:A:2065:ARG:HD3	1:A:2100:LEU:HD11	1.86	0.57
1:A:2495:SER:O	1:A:2498:ILE:HB	2.04	0.57
1:A:2538:ARG:HH11	1:A:2565:MSE:CB	2.17	0.57
1:A:2782:ASP:HA	1:A:2786:LYS:CB	2.34	0.57
1:A:2950:LYS:HE2	1:A:4105:LYS:NZ	2.18	0.57
1:B:1761:LEU:O	1:B:1895:LYS:HB2	2.04	0.57
1:B:205:LYS:HA	1:B:208:MSE:HE3	1.86	0.57
1:B:2323:LEU:HD21	1:B:2345:VAL:HG21	1.86	0.57
1:B:2374:LEU:CD1	1:B:2377:ARG:HB2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ASP:HB3	1:B:282:PHE:CE2	2.39	0.57
1:B:2837:LEU:HD12	1:B:2867:ALA:HB3	1.86	0.57
1:B:571:SER:HB2	1:B:606:SER:H	1.68	0.57
1:B:781:ASP:OD2	1:B:862:LEU:HD21	2.03	0.57
1:B:966:PHE:O	1:B:969:LEU:HB3	2.03	0.57
1:B:986:PRO:O	1:B:989:MSE:N	2.37	0.57
1:B:997:ASN:HA	1:B:1042:LYS:HD3	1.86	0.57
1:A:1952:ILE:HG23	1:A:1953:CYS:O	2.04	0.57
1:A:2286:PRO:HD3	1:A:2325:LEU:HD23	1.85	0.57
1:A:2809:PHE:HB3	1:A:2859:GLN:CD	2.24	0.57
1:A:3287:ARG:NH1	1:A:3331:GLY:HA3	2.19	0.57
1:A:3496:ILE:O	1:A:3498:TRP:N	2.37	0.57
1:A:3686:TRP:CZ3	1:A:3687:MSE:HG3	2.39	0.57
1:A:75:SER:O	1:A:77:GLU:N	2.36	0.57
1:B:2094:MSE:HE1	1:B:2143:ARG:HA	1.85	0.57
1:B:2927:ALA:HB2	1:B:2930:TYR:HD2	1.68	0.57
1:B:3181:ASP:HA	1:B:3184:THR:HG23	1.86	0.57
1:B:3496:ILE:HG23	1:B:3499:ILE:HD11	1.86	0.57
1:B:3871:PHE:HB3	1:B:4127:TRP:CD1	2.39	0.57
1:B:450:SER:O	1:B:454:GLN:HB2	2.03	0.57
1:B:2366:LYS:NZ	2:S:101:UNK:HA	2.19	0.57
1:A:1063:LEU:HD13	1:A:1082:PHE:CE1	2.39	0.57
1:A:1655:ILE:HG12	1:A:1677:SER:O	2.05	0.57
1:A:1606:ARG:HA	1:A:1806:ARG:HD3	1.87	0.57
1:A:205:LYS:NZ	1:A:243:GLN:OE1	2.25	0.57
1:A:2562:LEU:O	1:A:2566:THR:HG22	2.04	0.57
1:A:2960:GLU:HG2	1:A:3252:PHE:CG	2.39	0.57
1:A:3034:PRO:O	1:A:3038:GLU:HB3	2.05	0.57
1:A:368:LEU:HA	1:A:372:PRO:HG2	1.86	0.57
1:A:756:PHE:O	1:A:759:GLY:N	2.36	0.57
1:A:871:LEU:HD21	1:A:3122:HIS:CE1	2.39	0.57
1:A:987:LEU:O	1:A:991:LEU:HD13	2.05	0.57
1:B:1000:LYS:O	1:B:1003:SER:N	2.30	0.57
1:B:1090:ARG:HH22	1:B:1096:VAL:C	2.07	0.57
1:B:1270:PHE:CZ	1:B:1347:THR:HB	2.38	0.57
1:B:1923:PHE:CE2	1:B:1927:MSE:HE1	2.40	0.57
1:B:1976:LEU:HD13	1:B:2031:LEU:CD2	2.34	0.57
1:B:2085:MSE:O	1:B:2089:ASN:ND2	2.37	0.57
1:B:16:GLN:O	1:B:20:SER:OG	2.21	0.57
1:B:2886:GLN:OE1	1:B:2921:LEU:HB2	2.03	0.57
1:B:3174:ASP:H	1:B:3175:PRO:HD2	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3568:ILE:O	1:B:3571:PHE:N	2.38	0.57
1:B:358:GLU:HA	1:B:1858:LEU:HD22	1.85	0.57
1:B:473:PRO:CA	1:B:476:ARG:HH22	2.12	0.57
1:B:886:TRP:HD1	1:B:889:GLU:N	2.02	0.57
1:A:131:LEU:O	1:A:135:LEU:HG	2.05	0.57
1:A:2227:LYS:HZ1	1:A:2232:ARG:HB3	1.69	0.57
1:A:2503:LYS:O	1:A:2507:ILE:HB	2.04	0.57
1:A:805:LEU:CD2	1:A:3125:ARG:NH1	2.68	0.57
1:A:373:CYS:O	1:A:423:TYR:OH	2.20	0.57
1:A:4057:ALA:HB2	1:A:4090:ARG:O	2.04	0.57
1:B:1238:GLN:HE22	1:B:1297:PHE:HD1	1.51	0.57
1:B:1632:TRP:HA	1:B:1635:LYS:HD2	1.85	0.57
1:B:2190:VAL:O	1:B:2193:ILE:HG22	2.04	0.57
1:B:2210:VAL:HG13	1:B:2211:LEU:H	1.70	0.57
1:B:2321:GLU:O	1:B:2324:GLY:N	2.36	0.57
1:B:2555:LEU:HB2	1:B:2809:PHE:CE1	2.40	0.57
1:B:3767:LEU:O	1:B:3771:MSE:HG3	2.04	0.57
1:B:3765:GLU:O	1:B:3768:PHE:HB2	2.05	0.57
1:B:575:ILE:HD13	1:B:603:ILE:HB	1.86	0.57
1:B:923:ASP:O	1:B:927:LYS:HE2	2.03	0.57
1:A:2913:LYS:HG3	1:A:2914:ALA:N	2.19	0.57
1:A:4027:TRP:HB3	1:A:4031:ILE:HD11	1.85	0.57
1:A:409:GLN:HG3	1:A:413:PHE:CZ	2.39	0.57
1:A:414:LEU:HD22	1:A:442:GLN:HG2	1.85	0.57
1:A:704:PHE:HA	1:A:707:PHE:CD1	2.39	0.57
1:A:797:ASP:HA	1:A:800:LEU:HD12	1.86	0.57
1:B:1715:GLU:HA	1:B:1718:ILE:HB	1.85	0.57
1:B:2562:LEU:O	1:B:2566:THR:HG22	2.04	0.57
1:B:3817:LEU:HA	1:B:3820:MSE:HE3	1.87	0.57
1:B:610:ALA:HA	1:B:613:HIS:ND1	2.19	0.57
1:A:2157:PHE:CZ	1:A:2203:THR:HB	2.40	0.57
1:A:2196:TRP:CG	1:A:2199:LEU:HD11	2.39	0.57
1:A:2349:LEU:HD23	1:A:2364:LEU:HD22	1.86	0.57
1:A:737:PRO:O	1:A:741:ILE:HG12	2.04	0.57
1:A:968:VAL:CG2	1:A:971:ARG:HD3	2.33	0.57
1:B:1681:ASP:HB2	1:B:1717:LEU:HD22	1.86	0.57
1:B:361:ILE:HD13	1:B:1858:LEU:HD23	1.86	0.57
1:B:2216:LEU:HD13	1:B:2249:LEU:HD21	1.85	0.57
1:B:2289:ASP:O	1:B:2292:CYS:N	2.24	0.57
1:B:262:LEU:HD22	1:B:306:VAL:HG12	1.86	0.57
1:B:680:ILE:HG12	1:B:701:TYR:HD2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:798:GLY:HA2	1:B:873:VAL:HG11	1.87	0.57
1:B:969:LEU:O	1:B:973:ALA:HB3	2.05	0.57
1:A:1982:ILE:O	1:A:1986:ARG:HB2	2.04	0.57
1:A:182:GLY:O	1:A:233:ASN:ND2	2.36	0.57
1:A:257:ARG:H	1:A:258:PRO:CD	2.17	0.57
1:A:3907:SER:CB	1:A:3937:VAL:H	2.17	0.57
1:A:567:GLU:HB3	1:A:606:SER:HB3	1.87	0.57
1:A:585:ILE:HG22	1:A:586:GLN:H	1.68	0.57
1:B:1216:GLY:HA3	1:B:1271:ILE:CG2	2.35	0.57
1:B:2319:ALA:O	1:B:2323:LEU:HD12	2.04	0.57
1:B:2801:ASP:HB2	1:B:2802:PRO:CD	2.35	0.57
1:B:3267:LYS:N	1:B:3271:ASP:OD2	2.37	0.57
1:B:3771:MSE:HE1	1:B:3917:ILE:HG21	1.85	0.57
1:B:990:GLN:HG3	1:B:2776:ARG:NH1	2.19	0.57
1:A:1635:LYS:O	1:A:1639:LEU:HG	2.05	0.57
1:A:1809:ASP:O	1:A:1815:THR:HG22	2.05	0.57
1:A:1989:ASN:HB3	1:A:2040:MSE:HB3	1.86	0.57
1:A:2555:LEU:HD13	1:A:2809:PHE:CZ	2.39	0.57
1:A:2883:SER:O	1:A:2885:GLN:N	2.38	0.57
1:A:3498:TRP:HB2	1:A:3501:HIS:HB2	1.86	0.57
1:A:3631:LYS:O	1:A:3631:LYS:HD3	2.05	0.57
1:A:3687:MSE:C	1:A:3689:ASP:H	2.06	0.57
1:A:3839:TYR:HE1	1:A:3867:THR:HB	1.70	0.57
1:A:576:VAL:HG13	1:A:601:TRP:CE3	2.40	0.57
1:B:1274:ARG:O	1:B:1279:LEU:N	2.28	0.57
1:B:1350:ASN:ND2	1:B:1404:LYS:HG2	2.18	0.57
1:B:1494:GLY:HA2	1:B:1497:ARG:HG3	1.87	0.57
1:B:2194:LEU:HD13	1:B:2244:CYS:SG	2.45	0.57
1:B:2267:SER:HB2	1:B:2269:ASP:OD2	2.05	0.57
1:B:2927:ALA:CB	1:B:2930:TYR:HD2	2.18	0.57
1:B:3903:HIS:O	1:B:3907:SER:OG	2.15	0.57
1:B:527:TYR:CE1	1:B:531:PHE:HZ	2.21	0.57
1:B:752:LEU:HD13	1:B:776:TRP:CZ3	2.40	0.57
1:A:1006:THR:O	1:A:1010:LEU:HG	2.05	0.57
1:A:1146:ASN:O	1:A:1150:LYS:HB3	2.05	0.57
1:A:283:SER:HA	1:A:286:LEU:HG	1.85	0.57
1:A:3167:ARG:HG2	1:A:3186:ARG:CZ	2.35	0.57
1:A:3529:ILE:HG23	1:A:3532:PRO:HD2	1.86	0.57
1:A:3980:MSE:HB2	1:A:3983:ILE:HD12	1.86	0.57
1:A:575:ILE:HD11	1:A:579:LEU:HD13	1.87	0.57
1:A:891:ARG:HB2	1:A:905:ILE:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:SER:HA	1:B:181:LEU:HD22	1.87	0.57
1:B:2019:SER:O	1:B:2023:SER:OG	2.10	0.57
1:B:385:TYR:HD1	1:B:420:VAL:CG1	2.18	0.57
1:B:460:ALA:O	1:B:464:VAL:HG12	2.05	0.57
1:B:566:ASP:O	1:B:570:LYS:NZ	2.38	0.57
1:B:70:ARG:HD3	1:B:82:ARG:HD3	1.87	0.57
1:A:175:TYR:CE1	1:A:200:PHE:HB3	2.39	0.56
1:A:2324:GLY:HA2	1:A:2371:PHE:HB3	1.87	0.56
1:A:2911:ARG:HG2	1:A:2914:ALA:HB3	1.87	0.56
1:A:3459:ASN:O	1:A:3462:ARG:HG2	2.05	0.56
1:A:3483:MSE:C	1:A:3516:HIS:HE2	2.08	0.56
1:A:2930:TYR:HH	1:A:3902:SER:HG	1.48	0.56
1:B:1007:VAL:O	1:B:1011:GLU:HB3	2.04	0.56
1:B:1293:ALA:HA	1:B:1296:PHE:CD2	2.40	0.56
1:B:144:MSE:HE2	1:B:144:MSE:HA	1.86	0.56
1:B:2359:LYS:HA	1:B:2362:VAL:HG13	1.87	0.56
1:B:2481:HIS:CE1	1:B:2485:ARG:NH1	2.65	0.56
1:B:3167:ARG:HG2	1:B:3186:ARG:CZ	2.35	0.56
1:B:3238:MSE:O	1:B:3242:MSE:HG3	2.05	0.56
1:B:3629:ARG:HH22	1:B:3638:LYS:CE	2.18	0.56
1:B:647:TYR:O	1:B:650:SER:OG	2.12	0.56
1:B:909:VAL:CG1	1:B:913:ARG:HH11	2.05	0.56
1:A:1042:LYS:NZ	1:A:1044:ILE:HD12	2.20	0.56
1:A:1343:GLU:O	1:A:1347:THR:CB	2.52	0.56
1:A:2193:ILE:HA	1:A:2196:TRP:CE2	2.39	0.56
1:A:3493:TRP:CZ2	1:A:3496:ILE:HG21	2.40	0.56
1:A:4005:PHE:O	1:A:4009:PRO:HD3	2.05	0.56
1:A:488:ILE:HG13	1:A:612:LEU:HD12	1.86	0.56
1:B:1475:LEU:O	1:B:1479:VAL:HG23	2.04	0.56
1:B:2452:ARG:HE	1:B:2498:ILE:HD11	1.71	0.56
1:B:2877:SER:C	1:B:2879:GLY:H	2.08	0.56
1:B:2967:GLU:O	1:B:2971:GLN:NE2	2.38	0.56
1:B:3345:PRO:O	1:B:3347:CYS:N	2.34	0.56
1:B:3448:GLU:HG3	1:B:3449:LYS:HG3	1.87	0.56
1:B:3530:VAL:CG1	1:B:3702:PRO:HD3	2.31	0.56
1:A:1491:ILE:HG22	1:A:1497:ARG:HH22	1.70	0.56
1:A:1722:PHE:CE2	1:A:1754:GLN:HG2	2.39	0.56
1:A:205:LYS:HA	1:A:208:MSE:HE3	1.86	0.56
1:A:2086:ASP:HB3	1:A:2090:ARG:NH2	2.20	0.56
1:A:3425:ARG:HH12	1:A:3999:THR:HG22	1.70	0.56
1:A:4063:GLU:HA	1:A:4066:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:LYS:HD2	1:A:730:LEU:HB2	1.88	0.56
1:B:1046:PRO:O	1:B:1049:GLN:HB3	2.05	0.56
1:B:1080:LEU:HB3	1:B:1111:LEU:CD2	2.36	0.56
1:B:1115:HIS:O	1:B:1118:GLU:C	2.44	0.56
1:B:1582:LEU:HD13	1:B:1600:MSE:SE	2.55	0.56
1:B:1987:ARG:O	1:B:1989:ASN:N	2.38	0.56
1:B:2364:LEU:O	1:B:2368:THR:OG1	2.11	0.56
1:B:2420:PHE:CE1	1:B:2439:ILE:HG21	2.40	0.56
1:B:2485:ARG:NH1	1:B:2530:ARG:CZ	2.68	0.56
1:B:265:TYR:O	1:B:268:PRO:HD2	2.05	0.56
1:B:2945:SER:O	1:B:2949:THR:N	2.36	0.56
1:B:3791:TYR:OH	1:B:3942:PHE:HE2	1.88	0.56
1:B:4046:TYR:CE2	1:B:4049:ARG:NH2	2.74	0.56
1:B:642:PHE:CE2	1:B:710:PHE:HE2	2.23	0.56
1:B:657:SER:O	1:B:661:PRO:HD3	2.04	0.56
1:A:1698:PHE:HD1	1:A:1699:PHE:N	2.03	0.56
1:A:2808:LEU:O	1:A:2812:LEU:HB2	2.06	0.56
1:A:3179:TRP:CH2	1:A:3258:LEU:HG	2.39	0.56
1:A:369:PHE:CE1	1:A:419:SER:HB2	2.40	0.56
1:A:3907:SER:O	1:A:3911:ILE:HG23	2.05	0.56
1:A:993:HIS:HB2	1:A:1038:LYS:HG2	1.86	0.56
1:B:2157:PHE:CE2	1:B:2199:LEU:HD13	2.40	0.56
1:B:242:PRO:HD3	1:B:282:PHE:CE2	2.41	0.56
1:B:3420:CYS:O	1:B:3423:GLN:HB3	2.05	0.56
1:B:368:LEU:HD22	1:B:420:VAL:HG22	1.87	0.56
1:B:53:LEU:O	1:B:56:SER:OG	2.22	0.56
1:B:634:LEU:HD22	1:B:667:TYR:CD1	2.40	0.56
1:B:66:LEU:CD2	1:B:89:LEU:HD11	2.34	0.56
1:B:893:SER:OG	1:B:906:PHE:HD2	1.88	0.56
1:A:852:ARG:NH1	1:A:3111:MSE:HE2	2.21	0.56
1:A:3762:GLN:HE22	1:A:3763:ARG:HH11	1.53	0.56
1:B:1000:LYS:O	1:B:1002:GLU:N	2.39	0.56
1:B:3279:SER:O	1:B:3283:LEU:HB2	2.05	0.56
1:B:3397:GLN:OE1	1:B:3398:PRO:HD2	2.06	0.56
1:B:737:PRO:O	1:B:741:ILE:HG13	2.06	0.56
1:B:778:ILE:HG13	1:B:858:MSE:SE	2.56	0.56
1:A:1516:GLU:O	1:A:1519:PHE:N	2.38	0.56
1:A:164:LYS:HB3	1:A:166:ILE:HG13	1.88	0.56
1:A:2080:VAL:HG12	1:A:2081:LEU:H	1.70	0.56
1:A:2236:GLU:HA	1:A:2239:LYS:HB3	1.88	0.56
1:A:2538:ARG:NH1	1:A:2565:MSE:HB3	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3448:GLU:OE2	1:A:3449:LYS:HE3	2.04	0.56
1:A:3751:LEU:O	1:A:3802:LEU:HG	2.05	0.56
1:A:381:VAL:HB	1:A:384:MSE:HG2	1.88	0.56
1:A:484:HIS:NE2	1:A:616:LYS:HE3	2.20	0.56
1:B:1017:ILE:HG23	1:B:1018:VAL:HG13	1.87	0.56
1:B:1374:GLN:O	1:B:1378:GLU:N	2.39	0.56
1:B:2265:PRO:HD3	1:B:2309:PHE:CZ	2.41	0.56
1:B:3277:VAL:HB	1:B:3321:LEU:HD21	1.88	0.56
1:B:797:ASP:HB3	1:B:870:LEU:HB3	1.88	0.56
1:B:909:VAL:HG22	1:B:2807:GLN:HG3	1.88	0.56
1:B:926:THR:O	1:B:930:ALA:CB	2.54	0.56
1:B:931:CYS:SG	1:B:932:GLU:N	2.78	0.56
1:B:964:ARG:HH12	1:B:968:VAL:HB	1.70	0.56
1:A:1032:CYS:O	1:A:1035:GLU:N	2.37	0.56
1:A:1148:ALA:O	1:A:1152:ARG:HG3	2.06	0.56
1:A:1598:ASN:O	1:A:1602:ASP:HB3	2.05	0.56
1:A:168:ASP:O	1:A:170:VAL:N	2.36	0.56
1:A:1861:SER:O	1:A:1864:ASP:HB3	2.06	0.56
1:A:1934:LEU:HD12	1:A:1937:ARG:H	1.70	0.56
1:A:2799:GLN:HB3	1:A:2808:LEU:HD11	1.86	0.56
1:A:2879:GLY:HA2	1:A:2886:GLN:CG	2.35	0.56
1:A:361:ILE:HG12	1:A:1858:LEU:CD2	2.36	0.56
1:A:3960:PRO:HG2	1:A:3961:PHE:CD2	2.41	0.56
1:A:654:ILE:HG13	1:A:655:LEU:H	1.70	0.56
1:B:1090:ARG:NH2	1:B:1097:GLU:HA	2.21	0.56
1:B:1431:LEU:O	1:B:1434:VAL:HG12	2.05	0.56
1:B:2116:ASP:HB3	1:B:2119:PRO:HD2	1.88	0.56
1:B:313:LEU:HD11	1:B:359:LEU:HD21	1.88	0.56
1:A:3575:LEU:C	1:A:3686:TRP:HH2	2.09	0.56
1:A:3590:ASN:OD1	1:A:3593:ARG:NH2	2.36	0.56
1:A:381:VAL:HB	1:A:384:MSE:CG	2.36	0.56
1:A:395:MSE:SE	1:A:413:PHE:CE2	3.09	0.56
1:B:1128:CYS:HA	1:B:1131:ILE:HG23	1.88	0.56
1:B:1587:VAL:HB	1:B:1643:MSE:HE2	1.86	0.56
1:B:2330:VAL:HG21	1:B:2338:GLU:CB	2.29	0.56
1:B:2450:GLU:O	1:B:2454:LEU:HG	2.06	0.56
1:B:2843:PHE:CE2	1:B:2853:PRO:HG3	2.41	0.56
1:B:3141:PHE:HZ	1:B:3192:LYS:HB2	1.71	0.56
1:B:3331:GLY:O	1:B:3335:ARG:HD2	2.05	0.56
1:B:3821:SER:OG	1:B:3826:ALA:O	2.22	0.56
1:B:993:HIS:CD2	1:B:2776:ARG:HD3	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1077:GLY:HA2	1:A:1080:LEU:HD21	1.86	0.56
1:A:155:LYS:O	1:A:159:GLU:HG3	2.05	0.56
1:A:2073:ASP:HB3	1:A:2091:HIS:CE1	2.41	0.56
1:A:2093:CYS:HB3	1:A:2143:ARG:HH21	1.71	0.56
1:A:2552:VAL:CG2	1:A:2852:PRO:HG2	2.31	0.56
1:A:294:PHE:O	1:A:298:LEU:HG	2.05	0.56
1:A:3705:TYR:OH	1:A:3765:GLU:OE1	2.20	0.56
1:B:1069:HIS:O	1:B:3741:ARG:HD3	2.05	0.56
1:B:2810:SER:HA	1:B:2813:PHE:CD2	2.41	0.56
1:B:2858:ILE:HD12	1:B:3894:PRO:HG2	1.86	0.56
1:B:3090:TYR:HB3	1:B:3095:ASP:OD2	2.05	0.56
1:B:3103:ILE:HD13	1:B:3139:GLN:OE1	2.06	0.56
1:B:3593:ARG:HD2	1:B:3660:ASN:O	2.04	0.56
1:B:3847:SER:HA	1:B:3857:LEU:HD13	1.86	0.56
1:B:3908:HIS:CD2	1:B:3912:CYS:SG	2.99	0.56
1:B:3875:GLU:HG2	1:B:4127:TRP:HB3	1.88	0.56
1:B:886:TRP:CZ2	1:B:892:LEU:HD13	2.41	0.56
1:B:892:LEU:HB2	1:B:907:LEU:HD22	1.87	0.56
1:A:179:GLY:HA3	1:A:229:SER:HB3	1.86	0.56
1:A:2171:LEU:HG	1:A:2177:ASN:ND2	2.21	0.56
1:A:2382:VAL:CG2	1:A:2404:ARG:HG3	2.36	0.56
1:A:3954:PRO:HG2	1:A:4027:TRP:HA	1.88	0.56
1:A:855:VAL:O	1:A:859:LEU:HG	2.05	0.56
1:B:1348:LEU:HD23	1:B:1352:SER:HB3	1.87	0.56
1:B:1799:GLU:HA	1:B:1802:TYR:CB	2.36	0.56
1:B:4125:GLU:HA	1:B:4127:TRP:HE3	1.70	0.56
1:A:131:LEU:HD21	1:A:170:VAL:HG23	1.86	0.56
1:A:2430:GLU:HG3	1:A:2465:PRO:CB	2.36	0.56
1:A:2869:LEU:HB3	1:A:2893:LEU:HG	1.88	0.56
1:B:1090:ARG:NH2	1:B:1096:VAL:O	2.38	0.56
1:B:1131:ILE:HG12	1:B:1132:ASP:N	2.19	0.56
1:B:1909:ASN:ND2	1:B:1951:VAL:O	2.38	0.56
1:B:2886:GLN:CG	1:B:2887:PRO:HD3	2.36	0.56
1:B:756:PHE:O	1:B:760:LEU:HG	2.06	0.56
1:B:759:GLY:HA3	1:B:773:LEU:CD1	2.36	0.56
1:B:964:ARG:NH1	1:B:968:VAL:HB	2.21	0.56
1:B:978:GLN:H	1:B:981:ARG:HD3	1.70	0.56
1:A:2842:ARG:O	1:A:2846:THR:HG23	2.06	0.55
1:A:759:GLY:HA3	1:A:773:LEU:HD11	1.88	0.55
1:B:1805:PHE:HA	1:B:1808:ASP:OD2	2.06	0.55
1:B:1977:ILE:C	1:B:1979:GLU:H	2.02	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2065:ARG:NH1	1:B:2097:LEU:HD21	2.21	0.55
1:B:176:GLU:HG2	1:B:225:LYS:CD	2.36	0.55
1:B:2936:TYR:CE1	1:B:2940:ARG:HB2	2.40	0.55
1:B:3781:CYS:HA	1:B:3786:LEU:HD12	1.87	0.55
1:B:3900:LEU:HD11	1:B:3934:THR:O	2.05	0.55
1:B:3962:ARG:HB2	1:B:3962:ARG:CZ	2.35	0.55
1:A:2186:VAL:O	1:A:2190:VAL:HG13	2.06	0.55
1:A:2447:LYS:HA	1:A:2451:LEU:HD12	1.89	0.55
1:A:2918:PRO:HA	1:A:2921:LEU:HG	1.88	0.55
1:A:3584:LEU:O	1:A:3588:TRP:CB	2.55	0.55
1:A:714:VAL:HG12	1:A:715:ALA:N	2.21	0.55
1:B:2869:LEU:HG	1:B:2893:LEU:HD12	1.88	0.55
1:B:392:CYS:SG	1:B:438:LEU:HD21	2.46	0.55
1:B:3989:ARG:HH21	1:B:4100:GLU:CD	2.09	0.55
1:B:411:PRO:HG3	1:B:442:GLN:HE22	1.71	0.55
1:A:1231:GLN:H	1:A:1232:PRO:CD	2.20	0.55
1:A:1952:ILE:HG12	1:A:1953:CYS:N	2.21	0.55
1:A:2837:LEU:HD12	1:A:2867:ALA:HB3	1.89	0.55
1:A:3495:PHE:HZ	1:A:3521:ILE:HG13	1.71	0.55
1:A:3499:ILE:O	1:A:3503:VAL:HG12	2.07	0.55
1:A:4031:ILE:O	1:A:4035:GLU:N	2.37	0.55
1:A:4100:GLU:HG2	1:A:4101:GLU:H	1.71	0.55
1:A:805:LEU:HD22	1:A:3125:ARG:NH1	2.20	0.55
1:A:913:ARG:HA	1:A:916:GLU:CD	2.27	0.55
1:A:989:MSE:O	1:A:992:ILE:HG13	2.06	0.55
1:B:1292:LYS:O	1:B:1295:ALA:HB3	2.05	0.55
1:B:1583:MSE:HE3	1:B:1643:MSE:HB2	1.87	0.55
1:B:1726:SER:HB2	1:B:1866:GLN:HE22	1.71	0.55
1:B:1733:THR:OG1	1:B:1877:LEU:HD13	2.06	0.55
1:B:2026:SER:HB3	2:S:207:UNK:CB	2.37	0.55
1:B:2285:LEU:O	1:B:2288:TYR:N	2.39	0.55
1:B:2378:PHE:O	1:B:2382:VAL:HG22	2.06	0.55
1:B:658:THR:HA	1:B:733:LEU:CD2	2.32	0.55
1:B:968:VAL:HG22	1:B:972:LEU:HD23	1.87	0.55
1:A:204:LEU:HD13	1:A:223:CYS:HB2	1.87	0.55
1:A:2222:HIS:O	1:A:2226:PRO:HD2	2.07	0.55
1:A:3144:PHE:CD1	1:A:3160:LEU:HD11	2.42	0.55
1:A:960:GLN:HG2	1:A:961:LEU:HD22	1.89	0.55
1:B:1442:GLN:HE22	1:B:1495:ASP:HB3	1.70	0.55
1:B:3106:GLY:HA2	1:B:3109:SER:HB2	1.88	0.55
1:B:3283:LEU:HG	1:B:3300:VAL:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3966:GLN:H	1:B:4128:MSE:C	2.10	0.55
1:B:4125:GLU:HA	1:B:4127:TRP:CE3	2.41	0.55
1:B:760:LEU:HD13	1:B:802:THR:OG1	2.06	0.55
1:B:985:GLU:O	1:B:988:VAL:HG22	2.06	0.55
1:A:1636:ASP:O	1:A:1640:GLU:HB2	2.06	0.55
1:A:1641:THR:O	1:A:1645:VAL:HG23	2.07	0.55
1:A:1897:ASN:HB3	1:A:1901:HIS:HE1	1.71	0.55
1:A:2210:VAL:HG13	1:A:2211:LEU:H	1.71	0.55
1:A:2575:PRO:HD2	1:A:2785:ILE:HD11	1.87	0.55
1:A:2890:ILE:HD12	1:A:2918:PRO:HB3	1.87	0.55
1:A:3994:ASP:OD2	1:A:3997:LEU:HD13	2.06	0.55
1:B:2031:LEU:C	1:B:2033:ASP:H	2.07	0.55
1:B:2375:ALA:O	1:B:2379:MSE:HB2	2.04	0.55
1:B:2542:LEU:O	1:B:2545:LEU:N	2.38	0.55
1:B:2957:LEU:HB3	1:B:3989:ARG:NH2	2.22	0.55
1:B:3282:ARG:HB2	1:B:3282:ARG:HH11	1.70	0.55
1:B:4066:LEU:HD11	1:B:4078:VAL:HG11	1.88	0.55
1:B:922:SER:C	1:B:924:ARG:H	2.09	0.55
1:A:2236:GLU:HG2	2:K:110:UNK:CB	2.36	0.55
1:A:1567:ILE:HG12	1:A:1571:LEU:HD11	1.87	0.55
1:A:2145:PHE:HD1	1:A:2188:GLU:HG2	1.71	0.55
1:A:2556:SER:O	1:A:2559:THR:OG1	2.25	0.55
1:A:3722:PHE:CD1	1:A:3740:ILE:HA	2.41	0.55
1:A:3981:TYR:OH	1:A:4101:GLU:HB3	2.07	0.55
1:A:543:SER:O	1:A:545:LEU:N	2.34	0.55
1:A:793:LEU:HA	1:A:796:LEU:CG	2.33	0.55
1:B:1678:LEU:O	1:B:1682:THR:HG22	2.07	0.55
1:B:1976:LEU:HD13	1:B:2031:LEU:HD23	1.89	0.55
1:B:2099:ALA:O	1:B:2102:LYS:HB2	2.06	0.55
1:B:2239:LYS:HG3	1:B:2279:ILE:HD12	1.89	0.55
1:B:2289:ASP:O	1:B:2291:GLN:N	2.39	0.55
1:B:2806:LYS:HZ2	1:B:2858:ILE:HG13	1.71	0.55
1:A:1392:MSE:HA	1:A:1395:LEU:HB3	1.89	0.55
1:A:1431:LEU:O	1:A:1434:VAL:HG12	2.07	0.55
1:A:1946:ASN:HA	1:A:1949:ILE:HG22	1.89	0.55
1:A:1982:ILE:HG23	1:A:1986:ARG:HE	1.71	0.55
1:A:2271:SER:OG	1:A:2272:VAL:N	2.40	0.55
1:A:3499:ILE:CG2	1:A:3535:ILE:HG21	2.36	0.55
1:A:1069:HIS:O	1:A:3741:ARG:HD3	2.07	0.55
1:B:1011:GLU:OE2	1:B:1062:ARG:CZ	2.55	0.55
1:B:1102:GLU:HA	1:B:1150:LYS:NZ	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2254:ARG:HB2	1:B:2295:GLN:OE1	2.06	0.55
1:B:279:ALA:HA	1:B:282:PHE:CE2	2.41	0.55
1:B:2895:GLU:O	1:B:2899:ARG:NH2	2.40	0.55
1:B:3578:LEU:HB3	1:B:3579:SER:HA	1.89	0.55
1:B:629:PHE:CZ	1:B:666:PHE:CD1	2.92	0.55
1:B:706:LEU:HB3	1:B:710:PHE:CZ	2.42	0.55
1:B:776:TRP:CE2	1:B:780:ILE:HD12	2.41	0.55
1:A:1016:GLY:O	1:A:1019:ASP:HB2	2.05	0.55
1:A:1083:ASN:HD21	1:A:1104:LEU:HD21	1.71	0.55
1:A:1400:VAL:O	1:A:1404:LYS:CB	2.55	0.55
1:A:1606:ARG:O	1:A:1806:ARG:NH1	2.39	0.55
1:A:1880:MSE:O	1:A:1883:ARG:N	2.39	0.55
1:A:1918:LEU:HD11	1:A:1957:ASN:HB3	1.89	0.55
1:A:2098:THR:HG22	1:A:2146:LEU:HD13	1.89	0.55
1:A:2410:GLU:HA	1:A:2413:PHE:CZ	2.41	0.55
1:A:3424:LEU:HD13	1:A:3472:ILE:HD11	1.87	0.55
1:A:3472:ILE:HG22	1:A:3473:GLU:H	1.71	0.55
1:A:3676:PRO:HG2	1:A:3677:PRO:HD3	1.89	0.55
1:A:3722:PHE:CE1	1:A:3740:ILE:HG12	2.34	0.55
1:A:2957:LEU:HD11	1:A:3985:VAL:HG11	1.87	0.55
1:A:446:PHE:N	1:A:446:PHE:HD1	2.03	0.55
1:A:446:PHE:CZ	1:A:530:LEU:HB3	2.41	0.55
1:A:743:LEU:HD21	1:A:784:VAL:HG21	1.89	0.55
1:B:1424:THR:OG1	1:B:1425:ALA:N	2.40	0.55
1:B:1867:ILE:HG23	1:B:1871:MSE:HE3	1.89	0.55
1:B:2157:PHE:CE1	1:B:2203:THR:HB	2.42	0.55
1:B:3592:VAL:HG22	1:B:3609:MSE:SE	2.57	0.55
1:B:3791:TYR:HH	1:B:3942:PHE:HE2	1.54	0.55
1:B:2929:LEU:HD22	1:B:3983:ILE:HG12	1.89	0.55
1:B:3964:THR:HB	1:B:4128:MSE:O	2.06	0.55
1:B:568:PHE:O	1:B:571:SER:N	2.39	0.55
1:B:612:LEU:CD2	1:B:1800:SER:HB3	2.36	0.55
1:B:612:LEU:HD12	1:B:613:HIS:N	2.22	0.55
1:A:1335:CYS:HA	1:A:1338:VAL:HG12	1.89	0.55
1:A:1423:ILE:O	1:A:1427:SER:OG	2.20	0.55
1:A:1573:LYS:O	1:A:1576:ASP:HB3	2.07	0.55
1:A:1909:ASN:O	1:A:1912:THR:HG23	2.07	0.55
1:A:2789:SER:O	1:A:2793:PRO:HD3	2.07	0.55
1:A:2878:ALA:O	1:A:2886:GLN:HB3	2.07	0.55
1:A:3487:ILE:HA	1:A:3490:VAL:HG22	1.89	0.55
1:A:3901:ARG:HG2	1:A:3901:ARG:HH11	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3981:TYR:HE1	1:A:4105:LYS:N	2.05	0.55
1:A:892:LEU:HD11	1:A:958:MSE:HB2	1.87	0.55
1:B:1087:ARG:HD3	1:B:1134:LEU:HD22	1.89	0.55
1:B:1167:ASP:O	1:B:1171:TRP:HB2	2.06	0.55
1:B:1561:SER:HA	1:B:1564:SER:HB2	1.89	0.55
1:B:2088:LEU:HD21	1:B:2095:ALA:HB2	1.89	0.55
1:B:2190:VAL:HA	1:B:2193:ILE:HG22	1.88	0.55
1:B:3435:ASP:O	1:B:3439:LEU:HB2	2.06	0.55
1:A:1217:VAL:O	1:A:1221:ILE:HG13	2.07	0.55
1:A:1344:PHE:CE1	1:A:1348:LEU:HG	2.42	0.55
1:A:1729:PHE:HZ	1:A:1870:LYS:HG3	1.67	0.55
1:A:2046:SER:HB2	1:A:2096:PRO:HG2	1.89	0.55
1:A:2074:PRO:O	1:A:2076:VAL:N	2.40	0.55
1:A:2167:PRO:CA	1:A:2171:LEU:HB2	2.36	0.55
1:A:2951:GLN:OE1	1:A:2972:TYR:OH	2.18	0.55
1:A:3614:TYR:O	1:A:3618:GLY:N	2.29	0.55
1:A:3778:ASP:OD2	1:A:3781:CYS:N	2.40	0.55
1:A:3816:LEU:O	1:A:3820:MSE:HB3	2.07	0.55
1:A:4070:LYS:H	1:A:4074:PHE:HD2	1.55	0.55
1:A:385:TYR:OH	1:A:424:LEU:HD21	2.07	0.55
1:A:508:HIS:CD2	1:A:725:LEU:HD22	2.42	0.55
1:B:1346:THR:HG21	1:B:1401:ASN:CB	2.35	0.55
1:B:174:VAL:HG12	1:B:178:LEU:HD11	1.87	0.55
1:B:2387:PRO:HA	1:B:2390:HIS:HB3	1.88	0.55
1:B:3631:LYS:HA	1:B:3634:GLN:CB	2.37	0.55
1:B:3806:LEU:O	1:B:3809:THR:HG22	2.07	0.55
1:B:3915:HIS:O	1:B:3918:LEU:N	2.40	0.55
1:B:2957:LEU:HD21	1:B:4101:GLU:CD	2.27	0.55
1:B:431:TYR:HA	1:B:434:VAL:CG1	2.36	0.55
1:B:756:PHE:O	1:B:759:GLY:N	2.40	0.55
1:A:1007:VAL:O	1:A:1011:GLU:HB3	2.07	0.54
1:A:1080:LEU:HD22	1:A:1127:CYS:HB2	1.87	0.54
1:A:1253:THR:HA	1:A:1257:LEU:HD12	1.89	0.54
1:A:86:LEU:HD13	1:A:134:LEU:HD21	1.88	0.54
1:A:2145:PHE:CD1	1:A:2188:GLU:HG2	2.41	0.54
1:A:220:LEU:O	1:A:224:LEU:HG	2.06	0.54
1:A:3699:LEU:HG	1:A:3701:ILE:HG12	1.88	0.54
1:A:752:LEU:HA	1:A:755:ALA:HB3	1.88	0.54
1:B:114:VAL:HG11	1:B:130:LEU:HD11	1.90	0.54
1:B:170:VAL:HG23	1:B:173:LYS:NZ	2.21	0.54
1:B:1927:MSE:HG2	1:B:1941:HIS:CD2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2213:ASN:HB2	1:B:2250:SER:HB2	1.90	0.54
1:B:2793:PRO:O	1:B:2797:VAL:HG22	2.05	0.54
1:B:2944:THR:HG21	1:B:2983:ASP:OD2	2.07	0.54
1:B:358:GLU:N	1:B:361:ILE:HG23	2.22	0.54
1:B:3872:ARG:NH1	1:B:3965:ARG:NH1	2.54	0.54
1:B:454:GLN:HG3	1:B:533:HIS:CE1	2.40	0.54
1:B:784:VAL:O	1:B:787:PRO:HD2	2.07	0.54
1:A:1008:ALA:HA	1:A:1011:GLU:OE1	2.07	0.54
1:A:1240:THR:HA	1:A:1243:TYR:HD2	1.72	0.54
1:A:3122:HIS:O	1:A:3125:ARG:N	2.40	0.54
1:B:1276:VAL:HG13	1:B:1358:LEU:HD12	1.88	0.54
1:B:1378:GLU:HB3	1:B:1379:PRO:HD3	1.89	0.54
1:B:1636:ASP:O	1:B:1640:GLU:HB2	2.07	0.54
1:B:1682:THR:HB	1:B:1724:MSE:SE	2.57	0.54
1:B:1797:LEU:HD13	1:B:1805:PHE:CE2	2.41	0.54
1:B:356:ASN:OD1	1:B:1859:ASN:HB2	2.06	0.54
1:B:197:PHE:CE2	1:B:230:LEU:HD22	2.42	0.54
1:B:2224:PHE:HB3	1:B:2272:VAL:CG1	2.38	0.54
1:B:2304:VAL:O	1:B:2348:GLN:NE2	2.40	0.54
1:B:2352:HIS:CG	1:B:2364:LEU:HD21	2.42	0.54
1:B:3704:GLN:NE2	1:B:3796:MSE:SE	2.90	0.54
1:B:3493:TRP:CE3	1:B:3713:PRO:HB3	2.39	0.54
1:B:3876:SER:O	1:B:3879:PRO:HD2	2.07	0.54
1:A:1279:LEU:HG	1:A:1292:LYS:HZ3	1.72	0.54
1:A:1259:LEU:HG	1:A:1337:VAL:HG22	1.90	0.54
1:A:1363:LEU:C	1:A:1365:ASN:H	2.11	0.54
1:A:1675:TYR:CZ	1:A:1679:LEU:HD11	2.42	0.54
1:A:2040:MSE:HA	1:A:2043:PHE:HD1	1.73	0.54
1:A:2056:SER:HA	1:A:2061:PRO:HG3	1.88	0.54
1:A:2065:ARG:HB3	1:A:2125:TRP:CD1	2.42	0.54
1:A:245:SER:HB2	1:A:272:LEU:HD11	1.89	0.54
1:A:2796:ALA:O	1:A:2800:ARG:HG3	2.06	0.54
1:A:2870:SER:O	1:A:2872:ASP:N	2.41	0.54
1:A:3273:LEU:HB3	1:A:3321:LEU:CD2	2.37	0.54
1:A:3413:TYR:HD2	1:A:3453:ALA:HB2	1.72	0.54
1:A:887:ASP:O	1:A:3889:ARG:HG2	2.07	0.54
1:A:3967:PHE:CD1	1:A:3968:ILE:N	2.75	0.54
1:B:2636:UNK:O	1:B:2640:UNK:CB	2.55	0.54
1:B:2801:ASP:HB2	1:B:2802:PRO:HD3	1.88	0.54
1:B:2894:GLU:HA	1:B:2898:LEU:HB2	1.88	0.54
1:B:3464:LYS:O	1:B:3468:LEU:HG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3864:ARG:HD2	1:B:4115:ASN:OD1	2.08	0.54
1:A:1018:VAL:HB	1:A:1074:LYS:CA	2.37	0.54
1:A:1064:TYR:CD1	1:A:1106:ILE:HD11	2.42	0.54
1:A:1296:PHE:O	1:A:1299:GLU:N	2.39	0.54
1:A:1462:GLY:C	1:A:1464:LEU:H	2.11	0.54
1:A:1551:ILE:HA	1:A:1554:SER:HB3	1.89	0.54
1:A:15:LEU:HD23	1:A:2359:LYS:NZ	2.22	0.54
1:A:2164:TRP:HH2	1:A:2190:VAL:HG12	1.70	0.54
1:A:2923:TRP:CD1	1:A:2931:ARG:HD3	2.42	0.54
1:A:3294:SER:HB3	1:A:3341:LEU:HD22	1.90	0.54
1:B:1216:GLY:HA3	1:B:1271:ILE:HG22	1.88	0.54
1:B:2462:VAL:HG11	1:B:2473:MSE:SE	2.58	0.54
1:B:2474:TYR:CE1	1:B:2509:GLY:HA3	2.42	0.54
1:B:3472:ILE:HG22	1:B:3473:GLU:H	1.73	0.54
1:B:409:GLN:HG3	1:B:413:PHE:CZ	2.41	0.54
1:B:514:VAL:HA	1:B:604:PRO:HG3	1.90	0.54
1:B:575:ILE:N	1:B:605:THR:OG1	2.40	0.54
1:B:963:LYS:HB3	1:B:1009:LEU:HD11	1.88	0.54
1:A:1111:LEU:HA	1:A:1114:ALA:HB3	1.90	0.54
1:A:401:ASP:HB2	1:A:1763:THR:OG1	2.07	0.54
1:A:2461:PHE:HE1	1:A:2469:CYS:HG	1.55	0.54
1:A:2538:ARG:HH11	1:A:2565:MSE:CG	2.21	0.54
1:A:3008:TRP:H	1:A:3050:LYS:HG2	1.73	0.54
1:A:3114:TYR:OH	1:A:3128:LYS:HB3	2.07	0.54
1:A:759:GLY:HA3	1:A:773:LEU:CD1	2.38	0.54
1:B:1019:ASP:HB3	1:B:1020:PRO:HD2	1.89	0.54
1:B:1639:LEU:HD12	1:B:1640:GLU:N	2.23	0.54
1:B:3121:LEU:HB2	1:B:3124:SER:OG	2.08	0.54
1:B:4027:TRP:HB3	1:B:4031:ILE:HD11	1.90	0.54
1:B:3864:ARG:NH2	1:B:4119:ARG:HH21	2.05	0.54
1:B:649:PHE:C	1:B:651:TYR:N	2.61	0.54
1:B:659:ARG:HH22	1:B:662:LEU:CB	2.20	0.54
1:B:65:LEU:HD23	1:B:68:PHE:CE1	2.43	0.54
1:B:936:SER:HB3	1:B:2791:ILE:CG1	2.35	0.54
1:A:138:PHE:CD2	1:A:177:LEU:HD22	2.42	0.54
1:A:1424:THR:O	1:A:1426:GLN:N	2.41	0.54
1:A:1810:PRO:O	1:A:1811:ARG:HG2	2.08	0.54
1:A:269:SER:HB2	1:A:315:ALA:HB2	1.90	0.54
1:B:1693:VAL:O	1:B:1697:PRO:HD3	2.07	0.54
1:B:2039:GLU:HG2	1:B:2077:HIS:NE2	2.22	0.54
1:B:2220:MSE:SE	1:B:2276:LEU:HD11	2.58	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2363:CYS:O	1:B:2367:VAL:HG12	2.07	0.54
1:B:3907:SER:O	1:B:3911:ILE:HG23	2.08	0.54
1:B:633:ILE:O	1:B:637:LYS:HG2	2.08	0.54
1:B:897:PRO:HG2	1:B:898:PHE:CE1	2.43	0.54
1:A:1103:ALA:O	1:A:1106:ILE:HG12	2.07	0.54
1:A:2030:TYR:CD1	1:A:2031:LEU:HG	2.40	0.54
1:A:270:ALA:O	1:A:274:LEU:HG	2.08	0.54
1:A:2837:LEU:HD13	1:A:2868:LEU:N	2.23	0.54
1:A:3390:GLN:O	1:A:3394:GLU:HB2	2.08	0.54
1:A:3464:LYS:HE3	1:A:3468:LEU:HD21	1.88	0.54
1:A:3486:GLU:HG3	1:A:3487:ILE:N	2.22	0.54
1:A:3701:ILE:O	1:A:3701:ILE:HG13	2.08	0.54
1:A:3812:LEU:HG	1:A:3813:LYS:N	2.22	0.54
1:A:3963:LEU:HG	1:A:3967:PHE:HE1	1.71	0.54
1:A:69:VAL:HG12	1:A:70:ARG:N	2.22	0.54
1:B:2097:LEU:HA	1:B:2100:LEU:HB3	1.89	0.54
1:B:2224:PHE:HZ	1:B:2276:LEU:HD22	1.70	0.54
1:B:2386:LEU:HD11	1:B:2400:VAL:HG12	1.88	0.54
1:B:2543:ASN:HA	1:B:2546:TYR:HD2	1.72	0.54
1:B:3840:LYS:CE	1:B:4122:GLU:HB3	2.36	0.54
1:B:3858:MSE:HG2	1:B:4119:ARG:HD3	1.89	0.54
1:B:916:GLU:CB	1:B:930:ALA:HB1	2.36	0.54
1:A:1087:ARG:CD	1:A:1134:LEU:HD22	2.36	0.54
1:A:1406:LEU:HB3	1:A:1415:LEU:HD21	1.90	0.54
1:A:1609:ALA:HB2	1:A:1633:TRP:CZ2	2.42	0.54
1:A:2085:MSE:O	1:A:2088:LEU:HB3	2.08	0.54
1:A:2416:LYS:HD3	1:A:2442:MSE:SE	2.58	0.54
1:A:2935:GLU:HG3	1:A:2936:TYR:H	1.73	0.54
1:A:83:GLU:O	1:A:87:LYS:HG3	2.08	0.54
1:A:966:PHE:CZ	1:A:988:VAL:HG12	2.43	0.54
1:A:971:ARG:NE	1:A:1024:THR:OG1	2.40	0.54
1:B:2163:HIS:O	1:B:2167:PRO:HD3	2.07	0.54
1:B:2312:TYR:CE2	1:B:2313:LYS:HG2	2.43	0.54
1:B:2352:HIS:HB2	1:B:2364:LEU:HD11	1.89	0.54
1:B:2820:MSE:SE	1:B:2833:THR:HG21	2.58	0.54
1:B:3568:ILE:HD11	1:B:3691:LYS:HD2	1.90	0.54
1:B:649:PHE:C	1:B:651:TYR:H	2.10	0.54
1:B:855:VAL:O	1:B:859:LEU:HG	2.07	0.54
1:B:789:TYR:HD2	1:B:865:GLN:HG3	1.71	0.54
1:A:114:VAL:CG1	1:A:130:LEU:HD11	2.38	0.54
1:A:1886:LYS:HZ2	1:A:1924:THR:CB	2.17	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1907:GLU:OE2	1:A:1911:LEU:HD11	2.08	0.54
1:A:2177:ASN:HD22	1:A:2182:ILE:CG2	2.21	0.54
1:A:2304:VAL:HG11	1:A:2344:LEU:HB3	1.90	0.54
1:A:2412:TYR:CE1	1:A:2415:LEU:HB3	2.43	0.54
1:A:262:LEU:HD13	1:A:306:VAL:HG12	1.88	0.54
1:A:3039:THR:O	1:A:3042:PRO:HD2	2.08	0.54
1:A:3728:VAL:HG22	1:A:3736:LYS:HG3	1.89	0.54
1:A:3762:GLN:HE22	1:A:3763:ARG:NH1	2.05	0.54
1:B:87:LYS:HG2	1:B:133:LYS:HG3	1.89	0.54
1:B:1862:THR:O	1:B:1865:THR:HG22	2.07	0.54
1:B:2049:VAL:HG11	1:B:2100:LEU:HD12	1.90	0.54
1:B:2238:ILE:O	1:B:2242:VAL:HG23	2.08	0.54
1:B:276:ALA:HA	1:B:280:SER:OG	2.08	0.54
1:B:2806:LYS:HA	1:B:2809:PHE:CD2	2.43	0.54
1:B:278:HIS:O	1:B:281:GLN:HB3	2.08	0.54
1:B:2990:GLU:O	1:B:2994:TRP:HB2	2.07	0.54
1:B:3048:LYS:NZ	1:B:3064:PHE:CE2	2.74	0.54
1:B:3240:MSE:O	1:B:3242:MSE:N	2.41	0.54
1:B:39:GLY:HA2	1:B:92:PHE:HZ	1.71	0.54
1:B:620:PHE:CE1	1:B:623:PHE:HD2	2.26	0.54
1:B:718:MSE:SE	1:B:731:THR:HG22	2.58	0.54
1:B:981:ARG:HA	1:B:984:TYR:HD2	1.71	0.54
1:B:2366:LYS:HZ2	2:S:101:UNK:HA	1.73	0.54
1:A:1080:LEU:HD13	1:A:1127:CYS:CB	2.38	0.54
1:A:1087:ARG:HD3	1:A:1134:LEU:HB3	1.89	0.54
1:A:1166:LEU:HB3	1:A:1170:LYS:NZ	2.23	0.54
1:A:1582:LEU:O	1:A:1585:SER:HB3	2.08	0.54
1:A:1718:ILE:HG23	1:A:1750:LEU:HD11	1.89	0.54
1:A:2039:GLU:HG2	1:A:2077:HIS:NE2	2.23	0.54
1:A:2200:ALA:HA	1:A:2203:THR:HG22	1.89	0.54
1:A:2855:VAL:O	1:A:2859:GLN:HB2	2.08	0.54
1:A:3518:VAL:HA	1:A:3521:ILE:HG22	1.90	0.54
1:A:3857:LEU:HA	1:A:3859:TYR:CE2	2.43	0.54
1:A:2891:ARG:HH22	1:A:3884:LYS:HE2	1.73	0.54
1:A:508:HIS:HB3	1:A:725:LEU:HB3	1.90	0.54
1:B:2798:ALA:HB3	1:B:2799:GLN:NE2	2.23	0.54
1:B:3578:LEU:HD22	1:B:3683:CYS:SG	2.47	0.54
1:B:629:PHE:CZ	1:B:666:PHE:O	2.60	0.54
1:A:1008:ALA:O	1:A:1011:GLU:HB3	2.08	0.53
1:A:1175:HIS:O	1:A:1179:PRO:HD3	2.08	0.53
1:A:1804:MSE:O	1:A:1808:ASP:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1939:LEU:CD1	1:A:1986:ARG:HG2	2.38	0.53
1:A:2148:LYS:HD2	1:A:2188:GLU:OE2	2.08	0.53
1:A:3122:HIS:HB3	1:A:3126:LEU:HD13	1.89	0.53
1:A:3502:MSE:HE3	1:A:3517:SER:HB3	1.89	0.53
1:A:3525:TYR:CE1	1:A:3561:LYS:HD2	2.43	0.53
1:A:3974:MSE:HA	1:A:3975:LYS:CB	2.38	0.53
1:A:414:LEU:HG	1:A:414:LEU:O	2.01	0.53
1:A:548:GLU:O	1:A:552:SER:OG	2.21	0.53
1:B:1348:LEU:HD23	1:B:1353:PRO:HD3	1.90	0.53
1:B:1733:THR:HB	1:B:1877:LEU:HD22	1.90	0.53
1:B:2813:PHE:HA	1:B:2816:ILE:HG22	1.89	0.53
1:B:3047:SER:HB2	1:B:3050:LYS:HE2	1.90	0.53
1:B:3690:PHE:CZ	1:B:3722:PHE:HD2	2.26	0.53
1:B:3917:ILE:O	1:B:4048:LYS:CE	2.56	0.53
1:B:3965:ARG:HG3	1:B:3969:ASN:OD1	2.09	0.53
2:S:217:UNK:O	2:S:220:MSE:HG2	2.08	0.53
1:A:1817:GLN:HA	1:A:1820:VAL:HG22	1.90	0.53
1:A:3789:ARG:HD3	1:A:3938:ILE:HG21	1.89	0.53
1:A:3794:VAL:HG11	1:A:3796:MSE:HE3	1.90	0.53
1:A:3819:THR:HG1	1:A:3889:ARG:HH12	1.46	0.53
1:B:1575:LEU:HD13	1:B:1604:SER:HB3	1.90	0.53
1:B:1648:LEU:HD22	1:B:1684:LEU:HD22	1.89	0.53
1:B:356:ASN:ND2	1:B:1859:ASN:H	2.07	0.53
1:B:2049:VAL:HA	1:B:2052:TYR:HD2	1.71	0.53
1:B:2870:SER:HA	1:B:2897:LEU:HD22	1.89	0.53
1:B:294:PHE:O	1:B:297:LEU:HG	2.09	0.53
1:B:3469:LEU:O	1:B:3474:ARG:HG2	2.08	0.53
1:B:3636:PHE:C	1:B:3638:LYS:H	2.12	0.53
1:B:3927:ASN:O	1:B:3940:ILE:HG22	2.08	0.53
1:B:629:PHE:HZ	1:B:666:PHE:O	1.91	0.53
1:B:762:TYR:C	1:B:764:PRO:HD3	2.29	0.53
1:A:1046:PRO:O	1:A:1049:GLN:HB3	2.08	0.53
1:A:2078:ASP:HB3	1:A:2135:ASN:ND2	2.23	0.53
1:A:2168:LEU:HD13	1:A:2214:ARG:CZ	2.37	0.53
1:A:368:LEU:HD23	1:A:372:PRO:CG	2.37	0.53
1:A:489:ARG:HH22	1:A:492:SER:HB3	1.72	0.53
1:A:661:PRO:HG2	1:A:733:LEU:CA	2.38	0.53
1:A:926:THR:O	1:A:930:ALA:CB	2.56	0.53
1:B:1590:THR:O	1:B:1592:MSE:N	2.41	0.53
1:B:1723:PRO:C	1:B:1725:GLN:H	2.12	0.53
1:B:2009:LYS:NZ	1:B:2011:ALA:HA	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2196:TRP:CE2	1:B:2199:LEU:HD11	2.44	0.53
1:B:3585:PHE:HD1	1:B:3613:MSE:HE1	1.73	0.53
1:B:3790:THR:HG22	1:B:3791:TYR:H	1.73	0.53
1:B:641:PHE:CE1	1:B:663:ILE:HG21	2.42	0.53
1:B:757:LYS:HA	1:B:760:LEU:HD12	1.90	0.53
1:A:1032:CYS:HB3	1:A:1036:PHE:CZ	2.44	0.53
1:A:1083:ASN:HB2	1:A:1107:TYR:HE2	1.74	0.53
1:A:1111:LEU:HD23	1:A:1128:CYS:SG	2.48	0.53
1:A:306:VAL:O	1:A:309:LYS:HG3	2.08	0.53
1:A:3141:PHE:HZ	1:A:3192:LYS:HB2	1.73	0.53
1:A:3300:VAL:HG23	1:A:3328:ILE:HD13	1.89	0.53
1:A:3462:ARG:HE	1:A:3501:HIS:CD2	2.27	0.53
1:A:361:ILE:HG13	1:A:362:ALA:N	2.23	0.53
1:A:3944:HIS:NE2	1:A:4020:MSE:HE3	2.23	0.53
1:A:47:SER:H	1:A:51:LEU:HD12	1.74	0.53
1:A:535:LEU:HB3	1:A:626:LEU:HD11	1.91	0.53
1:A:756:PHE:O	1:A:759:GLY:C	2.47	0.53
1:B:1275:THR:HA	1:B:1279:LEU:HB2	1.90	0.53
1:B:1267:TYR:OH	1:B:1340:ARG:NH2	2.41	0.53
1:B:1941:HIS:ND1	1:B:1941:HIS:O	2.40	0.53
1:B:2300:PHE:CE2	1:B:2341:LEU:HB2	2.44	0.53
1:B:3311:ASN:O	1:B:3313:SER:N	2.39	0.53
1:B:3458:SER:OG	1:B:3494:GLN:NE2	2.42	0.53
1:B:3530:VAL:HA	1:B:3533:PHE:CD2	2.43	0.53
1:B:3629:ARG:NH2	1:B:3638:LYS:NZ	2.53	0.53
1:B:3699:LEU:HG	1:B:3701:ILE:HG23	1.90	0.53
1:B:969:LEU:O	1:B:973:ALA:HB2	2.07	0.53
1:B:977:ASP:O	1:B:980:THR:HB	2.09	0.53
1:A:1221:ILE:HG12	1:A:1274:ARG:NH1	2.24	0.53
1:A:1288:SER:O	1:A:1290:LEU:N	2.42	0.53
1:A:1306:ILE:HG22	1:A:1381:SER:HB3	1.90	0.53
1:A:1758:LEU:HD13	1:A:1860:GLU:HG2	1.89	0.53
1:A:2094:MSE:HE1	1:A:2143:ARG:CA	2.38	0.53
1:A:2352:HIS:CG	1:A:2364:LEU:HD21	2.44	0.53
1:A:276:ALA:HA	1:A:280:SER:OG	2.09	0.53
1:A:3529:ILE:HG13	1:A:3532:PRO:HG2	1.89	0.53
1:A:567:GLU:HB3	1:A:606:SER:CB	2.39	0.53
1:B:1015:ASP:HA	1:B:1018:VAL:HG22	1.90	0.53
1:B:1044:ILE:O	1:B:1045:THR:OG1	2.25	0.53
1:B:430:VAL:HG21	1:B:1682:THR:HG23	1.90	0.53
1:B:397:LEU:HD21	1:B:1813:SER:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3259:LEU:O	1:B:3263:HIS:CB	2.53	0.53
1:B:3605:ASN:O	1:B:3609:MSE:HG3	2.07	0.53
1:A:1348:LEU:O	1:A:1352:SER:N	2.35	0.53
1:A:2129:LEU:HB3	1:A:2156:VAL:HG13	1.90	0.53
1:A:3266:SER:HB2	1:A:3271:ASP:CG	2.29	0.53
1:A:3486:GLU:O	1:A:3489:SER:N	2.41	0.53
1:A:3617:LEU:HD13	1:A:3644:PHE:HD2	1.74	0.53
1:A:364:ARG:O	1:A:368:LEU:N	2.24	0.53
1:A:965:THR:HA	1:A:968:VAL:HG12	1.90	0.53
1:B:110:THR:O	1:B:114:VAL:HG23	2.07	0.53
1:B:1756:PRO:C	1:B:1758:LEU:H	2.11	0.53
1:B:2280:VAL:HG13	1:B:2287:PRO:HB2	1.91	0.53
1:B:3530:VAL:HG11	1:B:3700:GLU:O	2.09	0.53
1:B:4017:GLU:N	1:B:4017:GLU:OE1	2.39	0.53
1:B:69:VAL:HG12	1:B:70:ARG:N	2.24	0.53
1:B:884:VAL:HG11	1:B:3889:ARG:O	2.08	0.53
1:A:1004:GLN:O	1:A:1008:ALA:CB	2.56	0.53
1:A:1513:GLY:O	1:A:1517:LEU:HG	2.07	0.53
1:A:1567:ILE:O	1:A:1571:LEU:HG	2.09	0.53
1:A:1976:LEU:HD22	1:A:1981:LEU:HD22	1.91	0.53
1:A:2870:SER:C	1:A:2872:ASP:H	2.11	0.53
1:A:3464:LYS:HG3	1:A:3468:LEU:HD11	1.91	0.53
1:A:3493:TRP:HB2	1:A:3713:PRO:HG3	1.91	0.53
1:A:3818:ASN:O	1:A:3821:SER:HB3	2.08	0.53
1:A:361:ILE:HD11	1:A:413:PHE:CZ	2.44	0.53
1:A:947:GLN:HB2	1:A:949:PRO:HD3	1.89	0.53
1:B:1256:TRP:O	1:B:1260:LEU:HG	2.08	0.53
1:B:150:GLY:HA2	1:B:153:PHE:CE2	2.43	0.53
1:B:1914:THR:HG22	1:B:1955:VAL:HG21	1.89	0.53
1:B:1988:TYR:OH	1:B:2044:ASP:OD2	2.24	0.53
1:B:2349:LEU:HD23	1:B:2364:LEU:HD22	1.90	0.53
1:B:2798:ALA:O	1:B:2802:PRO:HD2	2.09	0.53
1:B:2890:ILE:HD12	1:B:2918:PRO:HB3	1.90	0.53
1:B:3588:TRP:O	1:B:3592:VAL:HG23	2.09	0.53
1:B:3459:ASN:ND2	1:B:3710:LYS:NZ	2.57	0.53
1:B:75:SER:O	1:B:77:GLU:N	2.41	0.53
1:A:995:PHE:CE1	1:A:1003:SER:HA	2.43	0.53
1:A:995:PHE:HZ	1:A:1006:THR:HB	1.74	0.53
1:A:1067:ALA:HB1	1:A:1111:LEU:CD1	2.38	0.53
1:A:361:ILE:HG12	1:A:1858:LEU:HD23	1.91	0.53
1:A:2094:MSE:HA	1:A:2094:MSE:HE3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:LEU:O	1:A:316:LEU:N	2.42	0.53
1:A:321:LYS:O	1:A:325:ASN:ND2	2.33	0.53
1:A:3280:TYR:O	1:A:3283:LEU:HB3	2.09	0.53
1:A:3620:PRO:HG2	1:A:3641:ASP:OD2	2.08	0.53
1:A:4002:MSE:SE	1:A:4048:LYS:HE3	2.58	0.53
1:A:771:ASN:C	1:A:773:LEU:H	2.12	0.53
1:B:1158:PRO:HB2	1:B:1159:PRO:HD3	1.91	0.53
1:B:1685:ASP:OD1	1:B:1717:LEU:HD13	2.09	0.53
1:B:179:GLY:O	1:B:183:GLU:HG3	2.08	0.53
1:B:2502:ALA:O	1:B:2506:LEU:HG	2.08	0.53
1:B:3133:GLN:O	1:B:3137:GLU:HG2	2.09	0.53
1:B:3487:ILE:HD11	1:B:3498:TRP:HH2	1.74	0.53
1:B:3908:HIS:CG	1:B:3967:PHE:CZ	2.97	0.53
1:B:3997:LEU:H	1:B:3997:LEU:HD12	1.73	0.53
1:B:808:GLU:OE1	1:B:3114:TYR:HB3	2.08	0.53
1:A:2186:VAL:HG21	1:A:2219:LEU:HD21	1.91	0.53
1:A:3024:PRO:HB2	1:A:3067:LYS:NZ	2.23	0.53
1:A:3251:ASN:ND2	1:A:3254:LEU:HB2	2.24	0.53
1:A:3578:LEU:HD11	1:A:3686:TRP:CZ3	2.43	0.53
1:A:3457:ASN:CG	1:A:3710:LYS:HZ2	2.12	0.53
1:B:1802:TYR:HA	1:B:1805:PHE:CD2	2.37	0.53
1:B:1916:ILE:O	1:B:1920:TYR:HD1	1.92	0.53
1:B:2009:LYS:HG2	1:B:2011:ALA:N	2.24	0.53
1:B:2379:MSE:SE	1:B:2408:MSE:SE	3.27	0.53
1:B:2532:PRO:HG2	1:B:2538:ARG:N	2.23	0.53
1:B:2870:SER:C	1:B:2872:ASP:H	2.04	0.53
1:B:2877:SER:O	1:B:2879:GLY:N	2.28	0.53
1:B:3080:LEU:HA	1:B:3086:LEU:HD22	1.91	0.53
1:B:3719:ILE:HG23	1:B:3720:ALA:H	1.73	0.53
1:B:3879:PRO:HG2	1:B:4128:MSE:HE3	1.91	0.53
1:B:3946:PHE:CE2	1:B:4048:LYS:HD2	2.44	0.53
1:B:3972:LEU:HB2	1:B:3974:MSE:HE2	1.91	0.53
1:B:531:PHE:CZ	1:B:619:ASP:HB2	2.43	0.53
1:B:550:PHE:CZ	1:B:632:GLU:HG2	2.42	0.53
1:A:1382:ILE:HD12	1:A:1386:ILE:HD11	1.91	0.53
1:A:139:ARG:O	1:A:141:SER:N	2.39	0.53
1:A:1982:ILE:HG23	1:A:1986:ARG:NE	2.24	0.53
1:A:2083:LEU:N	1:A:2086:ASP:HB2	2.24	0.53
1:A:2412:TYR:HD2	1:A:2416:LYS:HZ2	1.57	0.53
1:A:3238:MSE:O	1:A:3242:MSE:HG3	2.08	0.53
1:A:3498:TRP:NE1	1:A:3502:MSE:HB2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3696:ARG:O	1:A:3699:LEU:HB2	2.09	0.53
1:A:558:GLU:HA	1:A:561:ASN:ND2	2.24	0.53
1:A:562:HIS:HA	1:A:565:TYR:HB3	1.91	0.53
1:B:1349:LEU:CD2	1:B:1359:LEU:HB2	2.38	0.53
1:B:1652:ILE:HG13	1:B:1684:LEU:HD12	1.90	0.53
1:B:244:THR:O	1:B:248:ILE:HG13	2.09	0.53
1:B:2517:LEU:H	1:B:2517:LEU:HD23	1.73	0.53
1:B:3012:GLU:HB2	1:B:3050:LYS:HZ3	1.69	0.53
1:B:3425:ARG:NH1	1:B:4003:ASP:OD2	2.42	0.53
1:B:658:THR:N	1:B:733:LEU:HD13	2.24	0.53
1:A:1550:VAL:HG23	1:A:1551:ILE:H	1.74	0.52
1:A:1560:TYR:O	1:A:1563:PHE:N	2.30	0.52
1:A:1729:PHE:H	1:A:1730:PRO:HD2	1.74	0.52
1:A:3145:ILE:HG23	1:A:3196:LYS:HG2	1.91	0.52
1:A:3640:PHE:HB3	1:A:3644:PHE:CE2	2.44	0.52
1:A:659:ARG:NH2	1:A:662:LEU:HG	2.18	0.52
1:B:1733:THR:N	1:B:1734:PRO:HD3	2.24	0.52
1:B:1933:LEU:HD22	1:B:1937:ARG:HG2	1.90	0.52
1:B:2273:GLY:O	1:B:2276:LEU:HB3	2.09	0.52
1:B:2420:PHE:CE2	1:B:2424:MSE:HE3	2.44	0.52
1:B:3175:PRO:HB2	1:B:3178:ILE:HG13	1.90	0.52
1:B:357:LYS:HB2	1:B:361:ILE:HG22	1.89	0.52
1:B:385:TYR:CE2	1:B:424:LEU:HD21	2.44	0.52
1:B:986:PRO:O	1:B:990:GLN:HG2	2.10	0.52
1:A:1111:LEU:O	1:A:1114:ALA:HB3	2.09	0.52
1:A:2462:VAL:HG11	1:A:2473:MSE:HE1	1.91	0.52
1:A:3007:GLU:HA	1:A:3011:LEU:HB2	1.90	0.52
1:A:3051:LEU:HD22	1:A:3058:ASP:HB2	1.91	0.52
1:A:3170:ASP:O	1:A:3172:LYS:NZ	2.39	0.52
1:A:3397:GLN:NE2	1:A:3449:LYS:HD3	2.21	0.52
1:A:3498:TRP:O	1:A:3498:TRP:CD1	2.61	0.52
1:A:4081:ALA:HB2	1:A:4116:ILE:HD11	1.90	0.52
1:B:1096:VAL:HG23	1:B:1099:PHE:HE2	1.73	0.52
1:B:1356:TRP:HZ2	1:B:1409:SER:HB3	1.72	0.52
1:B:138:PHE:CD2	1:B:173:LYS:HE3	2.38	0.52
1:B:2223:VAL:HB	1:B:2238:ILE:HD12	1.92	0.52
1:B:245:SER:O	1:B:248:ILE:N	2.42	0.52
1:B:2461:PHE:O	1:B:2465:PRO:HD3	2.09	0.52
1:B:2999:LEU:HA	1:B:3002:TYR:CE2	2.44	0.52
1:B:3461:ALA:O	1:B:3464:LYS:N	2.41	0.52
1:B:396:PHE:CZ	1:B:397:LEU:HG	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:730:LEU:HA	1:B:733:LEU:CD1	2.39	0.52
1:B:933:LEU:O	1:B:936:SER:N	2.41	0.52
1:A:104:SER:HA	1:A:107:ILE:HD12	1.92	0.52
1:A:103:TYR:O	1:A:107:ILE:HG13	2.09	0.52
1:A:1520:ALA:O	1:A:1524:LEU:HD13	2.09	0.52
1:A:1725:GLN:OE1	1:A:1754:GLN:NE2	2.43	0.52
1:A:175:TYR:HE1	1:A:200:PHE:CB	2.23	0.52
1:A:1760:GLU:CB	1:A:1894:SER:HA	2.40	0.52
1:A:2281:MSE:SE	1:A:2286:PRO:CB	3.07	0.52
1:A:2395:THR:O	1:A:2399:GLU:HB2	2.09	0.52
1:A:2420:PHE:HE1	1:A:2436:LEU:HD22	1.75	0.52
1:A:231:LEU:HB2	1:A:275:PHE:CZ	2.44	0.52
1:A:3117:ILE:HD12	1:A:3125:ARG:NH1	2.23	0.52
1:A:4071:ALA:O	1:A:4075:ARG:CB	2.55	0.52
1:A:535:LEU:HD22	1:A:626:LEU:HG	1.91	0.52
1:B:1073:PHE:CD1	1:B:1074:LYS:N	2.74	0.52
1:B:1880:MSE:HE2	1:B:1884:LEU:HD21	1.92	0.52
1:B:217:LEU:N	1:B:218:PRO:HD2	2.23	0.52
1:B:249:PHE:HD1	1:B:265:TYR:CE1	2.27	0.52
1:B:3684:SER:OG	1:B:3685:PRO:HD3	2.10	0.52
1:B:580:ASP:OD1	1:B:581:LEU:N	2.42	0.52
1:B:70:ARG:HG3	1:B:78:PHE:HB3	1.90	0.52
1:B:922:SER:O	1:B:924:ARG:N	2.42	0.52
1:A:1369:MSE:HE1	1:A:1414:ILE:O	2.10	0.52
1:A:178:LEU:HB3	1:A:197:PHE:CZ	2.45	0.52
1:A:2542:LEU:CB	1:A:2546:TYR:HE2	2.18	0.52
1:A:3033:GLU:OE2	1:A:3079:GLU:OE2	2.27	0.52
1:A:307:GLU:H	1:A:307:GLU:CD	2.12	0.52
1:A:3416:LEU:CD1	1:A:3446:VAL:HG12	2.40	0.52
1:A:654:ILE:O	1:A:657:SER:N	2.42	0.52
1:A:703:CYS:O	1:A:707:PHE:HD1	1.92	0.52
1:A:947:GLN:C	1:A:949:PRO:HD3	2.30	0.52
1:B:1104:LEU:HD22	1:B:1135:CYS:SG	2.49	0.52
1:B:1698:PHE:HD1	1:B:1699:PHE:N	2.07	0.52
1:B:2464:HIS:H	1:B:2465:PRO:HD3	1.74	0.52
1:B:2824:LYS:O	1:B:2826:LEU:HG	2.09	0.52
1:B:937:MSE:O	1:B:941:MSE:HG3	2.08	0.52
1:A:1090:ARG:HH22	1:A:1096:VAL:HG22	1.74	0.52
1:A:608:PRO:HB2	1:A:1800:SER:HB2	1.91	0.52
1:A:2799:GLN:CB	1:A:2808:LEU:HD11	2.40	0.52
1:A:3331:GLY:O	1:A:3335:ARG:HD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3503:VAL:CG2	1:A:3536:SER:HA	2.39	0.52
1:A:3588:TRP:O	1:A:3592:VAL:HG23	2.08	0.52
1:A:3620:PRO:CB	1:A:3633:ILE:HG23	2.39	0.52
1:A:368:LEU:C	1:A:372:PRO:HG2	2.30	0.52
1:A:3769:GLN:O	1:A:3773:GLY:HA3	2.10	0.52
1:A:385:TYR:CE1	1:A:421:LEU:HD23	2.45	0.52
1:A:730:LEU:HA	1:A:733:LEU:HD12	1.90	0.52
1:B:1883:ARG:HB2	1:B:1923:PHE:CZ	2.44	0.52
1:B:1911:LEU:O	1:B:1913:LYS:N	2.37	0.52
1:B:1913:LYS:HG3	1:B:1916:ILE:HD12	1.91	0.52
1:B:194:GLU:HA	1:B:197:PHE:HD2	1.74	0.52
1:B:2002:LYS:O	1:B:2004:TYR:N	2.43	0.52
1:B:2308:SER:H	1:B:2348:GLN:NE2	2.08	0.52
1:B:2854:PHE:CZ	1:B:2881:LEU:HB2	2.45	0.52
1:B:2987:THR:HB	1:B:2991:LYS:N	2.20	0.52
1:B:3005:LEU:C	1:B:3254:LEU:HD21	2.28	0.52
1:B:3625:LEU:HD13	1:B:3633:ILE:HG13	1.91	0.52
1:B:1244:LEU:HD13	1:B:3698:GLU:OE2	2.10	0.52
1:B:88:PHE:O	1:B:91:ILE:HG13	2.09	0.52
1:B:981:ARG:CG	1:B:982:GLN:N	2.72	0.52
1:A:985:GLU:HG3	1:A:1031:ARG:NH2	2.25	0.52
1:A:1076:LEU:C	1:A:1078:ALA:H	2.12	0.52
1:A:1675:TYR:OH	1:A:1679:LEU:HD11	2.10	0.52
1:A:2405:VAL:O	1:A:2408:MSE:HB2	2.08	0.52
1:A:2854:PHE:CZ	1:A:2881:LEU:HB2	2.44	0.52
1:A:3251:ASN:HD21	1:A:3254:LEU:HD13	1.75	0.52
1:A:3464:LYS:HD2	1:A:3467:ARG:HD2	1.91	0.52
1:A:3602:ASN:HA	1:A:3606:ILE:HG12	1.92	0.52
1:A:3775:LEU:HB2	1:A:3787:GLN:NE2	2.24	0.52
1:A:476:ARG:O	1:A:479:ILE:HB	2.10	0.52
1:A:446:PHE:HB2	1:A:533:HIS:CD2	2.44	0.52
1:A:612:LEU:HD23	1:A:613:HIS:N	2.24	0.52
1:A:913:ARG:HB3	1:A:934:LEU:HD12	1.90	0.52
1:B:2002:LYS:C	1:B:2004:TYR:H	2.12	0.52
1:B:1993:GLU:HG2	1:B:2043:PHE:CD2	2.44	0.52
1:B:2210:VAL:HG13	1:B:2211:LEU:HG	1.90	0.52
1:B:2546:TYR:CE1	1:B:2558:ALA:CB	2.90	0.52
1:B:2546:TYR:HE1	1:B:2558:ALA:CB	2.20	0.52
1:B:2573:PRO:C	1:B:2575:PRO:HD3	2.30	0.52
1:B:3064:PHE:CG	1:B:3065:ILE:N	2.74	0.52
1:B:4077:TYR:CZ	1:B:4119:ARG:HG2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:GLU:O	1:B:571:SER:N	2.42	0.52
1:B:580:ASP:O	1:B:584:GLU:N	2.43	0.52
1:B:631:ARG:HG2	1:B:669:LEU:HD11	1.91	0.52
1:B:658:THR:CG2	1:B:659:ARG:HH11	2.17	0.52
1:A:1067:ALA:HB1	1:A:1111:LEU:HD11	1.91	0.52
1:A:3280:TYR:CD1	1:A:3328:ILE:HD11	2.44	0.52
1:A:408:TYR:HB2	1:A:453:MSE:HG2	1.91	0.52
1:A:736:LEU:O	1:A:740:ILE:HG13	2.10	0.52
1:A:967:PRO:O	1:A:970:LEU:N	2.42	0.52
1:B:1352:SER:HB3	1:B:1353:PRO:HD3	1.92	0.52
1:B:1399:CYS:O	1:B:1403:MSE:HG3	2.10	0.52
1:B:1885:PRO:O	1:B:1888:ASP:N	2.42	0.52
1:B:2031:LEU:CB	1:B:2033:ASP:HB2	2.37	0.52
1:B:2365:ASN:ND2	1:B:2382:VAL:HG11	2.24	0.52
1:B:2803:ILE:O	1:B:2805:ALA:N	2.43	0.52
1:B:2942:ILE:HG22	1:B:2943:PHE:CD1	2.45	0.52
1:B:3280:TYR:O	1:B:3283:LEU:HB3	2.09	0.52
1:B:3575:LEU:HG	1:B:3687:MSE:CG	2.36	0.52
1:B:3649:SER:HA	1:B:3652:LEU:HG	1.92	0.52
1:B:552:SER:O	1:B:556:SER:HB2	2.09	0.52
1:A:1733:THR:OG1	1:A:1877:LEU:HD13	2.09	0.52
1:A:2125:TRP:CZ2	1:A:2128:PHE:HB2	2.45	0.52
1:A:2427:ARG:HD3	1:A:2436:LEU:HD11	1.91	0.52
1:A:2538:ARG:HH11	1:A:2565:MSE:HG3	1.74	0.52
1:A:3461:ALA:O	1:A:3464:LYS:N	2.43	0.52
1:A:3496:ILE:HG23	1:A:3499:ILE:HD11	1.91	0.52
1:A:3964:THR:O	1:A:3967:PHE:CD1	2.59	0.52
1:A:433:PRO:HB2	1:A:1812:LEU:HA	1.91	0.52
1:A:653:LEU:HD12	1:A:656:GLN:HG3	1.92	0.52
1:B:1412:LYS:O	1:B:1415:LEU:HB2	2.10	0.52
1:A:14:ARG:HE	1:A:2396:LEU:CD1	2.23	0.52
1:A:2289:ASP:O	1:A:2291:GLN:N	2.43	0.52
1:A:2886:GLN:CG	1:A:2887:PRO:HD3	2.39	0.52
1:A:3109:SER:O	1:A:3112:GLN:HB3	2.10	0.52
1:A:3398:PRO:HG2	1:A:3399:PRO:HD3	1.92	0.52
1:A:872:THR:O	1:A:876:SER:HB2	2.09	0.52
1:B:1006:THR:HA	1:B:1009:LEU:HD12	1.91	0.52
1:B:2361:ILE:HA	1:B:2364:LEU:HG	1.92	0.52
1:B:3475:TYR:O	1:B:3479:THR:HG22	2.09	0.52
1:B:358:GLU:O	1:B:361:ILE:HG12	2.10	0.52
1:B:3840:LYS:O	1:B:3844:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:627:VAL:CG1	1:B:628:GLU:H	2.17	0.52
1:B:865:GLN:HB2	1:B:869:ASN:OD1	2.10	0.52
1:A:1070:PRO:O	1:A:1072:ALA:N	2.43	0.52
1:A:1574:ASN:CG	1:A:1582:LEU:HD21	2.30	0.52
1:A:1711:ARG:O	1:A:1715:GLU:HG3	2.10	0.52
1:A:181:LEU:CD1	1:A:189:MSE:HE2	2.39	0.52
1:A:3856:MSE:O	1:A:3859:TYR:OH	2.10	0.52
1:A:493:LYS:HB3	1:A:494:PRO:CD	2.39	0.52
1:A:611:ASN:C	1:A:614:PRO:HD2	2.30	0.52
1:B:2058:ASP:C	1:B:2061:PRO:HD2	2.30	0.52
1:B:2097:LEU:HD23	1:B:2100:LEU:HD22	1.90	0.52
1:B:2154:GLU:O	1:B:2157:PHE:HB2	2.10	0.52
1:B:2183:HIS:O	1:B:2187:VAL:CB	2.26	0.52
1:B:2199:LEU:HA	1:B:2202:PRO:HD2	1.92	0.52
1:B:2440:TYR:O	1:B:2443:MSE:HE2	2.10	0.52
1:B:3058:ASP:OD1	1:B:3060:SER:N	2.43	0.52
1:B:3277:VAL:HG23	1:B:3324:ARG:CD	2.40	0.52
1:B:3487:ILE:HA	1:B:3490:VAL:HG22	1.92	0.52
1:B:359:LEU:O	1:B:362:ALA:HB3	2.10	0.52
1:B:413:PHE:O	1:B:417:VAL:HG23	2.10	0.52
1:B:658:THR:O	1:B:661:PRO:HD2	2.09	0.52
1:B:805:LEU:HA	1:B:808:GLU:OE1	2.10	0.52
1:A:1010:LEU:HB2	1:A:1028:PHE:CE1	2.44	0.51
1:A:1014:LEU:HA	1:A:1025:LEU:HD13	1.91	0.51
1:A:111:CYS:HA	1:A:134:LEU:HD22	1.91	0.51
1:A:1632:TRP:HA	1:A:1635:LYS:HD2	1.91	0.51
1:A:3311:ASN:O	1:A:3313:SER:N	2.43	0.51
1:A:3333:THR:OG1	1:A:3385:LEU:HB3	2.10	0.51
1:A:3912:CYS:HB2	1:A:3984:MSE:HE2	1.91	0.51
1:A:655:LEU:HD12	1:A:658:THR:HB	1.91	0.51
1:B:1106:ILE:O	1:B:1109:GLU:HB3	2.11	0.51
1:B:1132:ASP:HA	1:B:1135:CYS:SG	2.50	0.51
1:B:1524:LEU:HD11	1:B:1592:MSE:HE3	1.92	0.51
1:B:1640:GLU:HG2	1:B:1691:GLN:HG2	1.92	0.51
1:B:1747:LEU:HD23	1:B:1750:LEU:HD12	1.92	0.51
1:B:1758:LEU:HD22	1:B:1759:LEU:HD22	1.92	0.51
1:B:1957:ASN:O	1:B:1961:PHE:N	2.43	0.51
1:B:2454:LEU:O	1:B:2457:PRO:HD2	2.10	0.51
1:B:2575:PRO:C	1:B:2576:MSE:HG3	2.31	0.51
1:B:2884:LEU:O	1:B:2887:PRO:HD2	2.10	0.51
1:B:2933:ILE:HG12	1:B:3979:LEU:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3781:CYS:SG	1:B:3786:LEU:HB2	2.50	0.51
1:A:1101:PHE:CG	1:A:1138:ILE:HG12	2.45	0.51
1:A:1330:TYR:O	1:A:1333:SER:OG	2.28	0.51
1:A:1590:THR:HG23	1:A:1591:LYS:N	2.25	0.51
1:A:2003:LYS:O	1:A:2007:ILE:HG13	2.11	0.51
1:A:2185:MSE:O	1:A:2189:ILE:HG12	2.11	0.51
1:A:2298:GLU:HB3	1:A:2301:GLN:HB3	1.92	0.51
1:A:2379:MSE:HE3	1:A:2383:PHE:HD1	1.75	0.51
1:A:3462:ARG:HH21	1:A:3501:HIS:CD2	2.28	0.51
1:A:3505:LEU:O	1:A:3510:GLN:HB2	2.11	0.51
1:A:3516:HIS:CG	1:A:3517:SER:N	2.77	0.51
1:A:3585:PHE:CE2	1:A:3613:MSE:SE	3.13	0.51
1:A:3631:LYS:HD2	1:A:3682:GLU:HG2	1.91	0.51
1:A:3659:PHE:CD1	1:A:3662:ILE:HD12	2.45	0.51
1:A:3705:TYR:HD2	1:A:3792:SER:HB2	1.74	0.51
1:A:4088:ASN:OD1	1:A:4091:ALA:HB3	2.09	0.51
1:A:557:SER:O	1:A:560:LEU:N	2.42	0.51
1:A:760:LEU:HD11	1:A:799:TYR:HB2	1.92	0.51
1:A:939:MSE:CE	1:A:942:LEU:HD13	2.40	0.51
1:B:1213:LYS:O	1:B:1215:GLU:N	2.43	0.51
1:B:1263:ALA:O	1:B:1267:TYR:HD1	1.94	0.51
1:B:1905:ILE:HG12	1:B:1951:VAL:HG11	1.92	0.51
1:B:2177:ASN:HB3	1:B:2182:ILE:N	2.24	0.51
1:B:2307:MSE:HB3	1:B:2348:GLN:NE2	2.17	0.51
1:B:2374:LEU:HD13	1:B:2377:ARG:HB2	1.91	0.51
1:B:276:ALA:HB2	1:B:318:SER:OG	2.10	0.51
1:B:2796:ALA:O	1:B:2800:ARG:HG3	2.10	0.51
1:B:3343:SER:O	1:B:3345:PRO:HD3	2.10	0.51
1:B:613:HIS:CE1	1:B:614:PRO:HD3	2.45	0.51
1:B:886:TRP:HZ3	1:B:954:GLY:O	1.93	0.51
1:A:127:ALA:O	1:A:131:LEU:HB2	2.11	0.51
1:A:135:LEU:CD2	1:A:173:LYS:HD2	2.40	0.51
1:A:1376:LEU:HD23	1:A:1376:LEU:H	1.75	0.51
1:A:17:GLU:OE2	1:A:61:ARG:NH1	2.43	0.51
1:A:1970:LYS:NZ	1:A:2017:GLY:HA3	2.24	0.51
1:A:21:ALA:O	1:A:24:ARG:HB2	2.11	0.51
1:A:352:VAL:HB	1:A:357:LYS:HG2	1.92	0.51
1:A:3909:ALA:HB2	1:A:3980:MSE:HE3	1.92	0.51
1:A:576:VAL:HG13	1:A:601:TRP:HE3	1.76	0.51
1:A:649:PHE:HE1	1:A:653:LEU:H	1.57	0.51
1:A:659:ARG:HH22	1:A:662:LEU:CG	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:LYS:HD2	1:A:746:ARG:HE	1.75	0.51
1:B:1029:CYS:CB	1:B:1085:ILE:HG13	2.36	0.51
1:B:1275:THR:HA	1:B:1279:LEU:CB	2.41	0.51
1:B:1579:VAL:HG12	1:B:1635:LYS:HG2	1.91	0.51
1:B:208:MSE:SE	1:B:220:LEU:HD21	2.61	0.51
1:B:2874:ALA:O	1:B:2877:SER:N	2.44	0.51
1:B:3107:ILE:HG23	1:B:3110:PHE:CZ	2.45	0.51
1:B:384:MSE:O	1:B:385:TYR:HB3	2.11	0.51
1:B:649:PHE:O	1:B:651:TYR:N	2.43	0.51
1:A:1072:ALA:HB1	1:A:1076:LEU:HD11	1.92	0.51
1:A:1266:CYS:O	1:A:1269:THR:OG1	2.25	0.51
1:A:1750:LEU:O	1:A:1754:GLN:HG3	2.10	0.51
1:A:2203:THR:O	1:A:2208:ASP:N	2.43	0.51
1:A:2450:GLU:O	1:A:2454:LEU:HG	2.11	0.51
1:A:2452:ARG:HG2	1:A:2498:ILE:CD1	2.40	0.51
1:A:266:ALA:CB	1:A:308:LEU:HG	2.41	0.51
1:A:3283:LEU:HD21	1:A:3297:VAL:HG22	1.92	0.51
1:A:3772:ASN:HB3	1:A:3788:LEU:H	1.74	0.51
1:A:906:PHE:O	1:A:909:VAL:N	2.35	0.51
1:B:1298:LEU:O	1:B:1302:ALA:HB2	2.10	0.51
1:B:111:CYS:O	1:B:134:LEU:HD13	2.10	0.51
1:B:2436:LEU:O	1:B:2439:ILE:HG22	2.10	0.51
1:B:3493:TRP:NE1	1:B:3708:ARG:O	2.40	0.51
1:B:3794:VAL:HB	1:B:3802:LEU:H	1.76	0.51
1:B:3967:PHE:O	1:B:3970:LEU:HD23	2.10	0.51
1:B:2957:LEU:CB	1:B:3989:ARG:HH22	2.22	0.51
1:B:4013:TRP:CZ3	1:B:4014:LYS:HB2	2.45	0.51
1:A:1503:LEU:O	1:A:1507:CYS:HB3	2.11	0.51
1:A:3588:TRP:HD1	1:A:3612:ARG:HD2	1.75	0.51
1:A:4019:LYS:HA	1:A:4019:LYS:HE2	1.93	0.51
1:A:413:PHE:O	1:A:417:VAL:HG23	2.11	0.51
1:A:863:GLY:HA2	1:A:866:ILE:HD11	1.91	0.51
1:B:1405:ALA:O	1:B:1410:PRO:HD3	2.10	0.51
1:B:1970:LYS:CE	1:B:2017:GLY:HA3	2.40	0.51
1:B:2094:MSE:SE	1:B:2143:ARG:HG3	2.60	0.51
1:B:2355:THR:O	1:B:2356:MSE:HG3	2.11	0.51
1:B:407:VAL:O	1:B:411:PRO:HD3	2.10	0.51
1:B:941:MSE:HE3	1:B:958:MSE:CG	2.40	0.51
1:A:1465:HIS:HA	1:A:1469:PRO:CD	2.41	0.51
1:A:2037:SER:O	1:A:2041:SER:HB3	2.10	0.51
1:A:2114:GLU:HG3	1:A:2116:ASP:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2224:PHE:HZ	1:A:2276:LEU:HD22	1.73	0.51
1:A:3147:LYS:O	1:A:3151:LEU:HG	2.10	0.51
1:A:3189:PHE:O	1:A:3193:ILE:HB	2.10	0.51
1:A:3813:LYS:HB3	1:A:3925:LEU:HG	1.93	0.51
1:A:4062:ASP:HB3	1:A:4078:VAL:HG21	1.93	0.51
1:A:543:SER:C	1:A:545:LEU:N	2.63	0.51
1:A:609:ALA:HB2	1:A:1800:SER:OG	2.11	0.51
1:A:619:ASP:O	1:A:621:SER:N	2.44	0.51
1:B:1266:CYS:HA	1:B:1344:PHE:CE1	2.46	0.51
1:B:1879:VAL:C	1:B:1882:SER:H	2.14	0.51
1:B:3134:ALA:O	1:B:3138:ILE:HG12	2.11	0.51
1:B:3298:LEU:HD11	1:B:3351:ILE:HD13	1.93	0.51
1:B:3525:TYR:CZ	1:B:3533:PHE:HE1	2.29	0.51
1:B:3954:PRO:HB2	1:B:4027:TRP:CD1	2.45	0.51
1:B:511:SER:HB2	1:B:515:ARG:HG2	1.93	0.51
1:A:1378:GLU:O	1:A:1382:ILE:HG12	2.11	0.51
1:A:1865:THR:HA	1:A:1868:THR:OG1	2.10	0.51
1:A:1876:ILE:O	1:A:1876:ILE:HG12	2.11	0.51
1:A:1993:GLU:O	1:A:1997:PRO:HD2	2.10	0.51
1:A:19:LEU:HD22	1:A:30:ALA:HB1	1.93	0.51
1:A:3173:MSE:HB3	1:A:3175:PRO:HD2	1.93	0.51
1:A:3173:MSE:HG2	1:A:3174:ASP:OD1	2.11	0.51
1:A:3518:VAL:O	1:A:3522:THR:OG1	2.10	0.51
1:A:514:VAL:HG11	1:A:610:ALA:O	2.10	0.51
1:A:917:LEU:HD22	1:A:969:LEU:HG	1.93	0.51
1:A:969:LEU:O	1:A:973:ALA:HB2	2.10	0.51
1:B:153:PHE:O	1:B:157:TYR:HD2	1.94	0.51
1:B:1975:LEU:HA	1:B:1976:LEU:HB3	1.91	0.51
1:B:3142:ILE:O	1:B:3145:ILE:HG22	2.11	0.51
1:B:3451:LEU:HD21	1:B:3483:MSE:HG2	1.93	0.51
1:B:3583:LEU:O	1:B:3587:ASP:CB	2.58	0.51
1:B:887:ASP:O	1:B:3889:ARG:HB3	2.11	0.51
1:B:798:GLY:HA2	1:B:873:VAL:CG1	2.41	0.51
1:A:1073:PHE:CD1	1:A:1074:LYS:N	2.76	0.51
1:A:1894:SER:C	1:A:1896:ILE:N	2.64	0.51
1:A:901:MSE:HG2	1:A:2819:GLU:HG2	1.92	0.51
1:A:2952:ILE:O	1:A:2955:SER:OG	2.18	0.51
1:A:3044:MSE:HE3	1:A:3060:SER:OG	2.11	0.51
1:A:3354:ASP:O	1:A:3357:ARG:HB2	2.11	0.51
1:A:371:GLY:O	1:A:375:VAL:N	2.44	0.51
1:A:3780:ALA:HB1	1:A:3784:ARG:NH1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3954:PRO:CG	1:A:4027:TRP:HA	2.41	0.51
1:A:421:LEU:C	1:A:423:TYR:H	2.13	0.51
1:A:968:VAL:HA	1:A:971:ARG:HG2	1.93	0.51
1:B:1729:PHE:H	1:B:1730:PRO:HD2	1.75	0.51
1:B:2038:GLU:HB3	1:B:2076:VAL:HG21	1.93	0.51
1:B:2365:ASN:HB2	1:B:2400:VAL:HG13	1.93	0.51
1:B:2470:ARG:HB3	1:B:2474:TYR:CE2	2.45	0.51
1:B:273:ARG:HE	1:B:314:SER:HB3	1.76	0.51
1:B:2923:TRP:HD1	1:B:2926:LEU:HD21	1.76	0.51
1:B:3450:MSE:HG2	1:B:3464:LYS:HG2	1.93	0.51
1:B:3448:GLU:HA	1:B:3451:LEU:HD22	1.91	0.51
1:B:19:LEU:HB2	1:B:34:LEU:HD22	1.92	0.51
1:B:3723:ASP:HB2	1:B:3741:ARG:NE	2.26	0.51
1:B:981:ARG:HG2	1:B:982:GLN:N	2.26	0.51
1:A:963:LYS:HB3	1:A:1009:LEU:HD11	1.93	0.51
1:A:2274:ILE:HD11	1:A:2314:GLU:HB3	1.92	0.51
1:A:2375:ALA:HB1	1:A:2411:LEU:HD22	1.93	0.51
1:A:2936:TYR:O	1:A:2940:ARG:CB	2.58	0.51
1:A:3705:TYR:CD2	1:A:3792:SER:HB2	2.46	0.51
1:A:3905:ALA:O	1:A:3908:HIS:N	2.44	0.51
1:A:479:ILE:O	1:A:483:VAL:HG13	2.11	0.51
1:B:1132:ASP:O	1:B:1135:CYS:N	2.44	0.51
1:B:125:ILE:H	1:B:126:PRO:CD	2.24	0.51
1:B:83:GLU:HG3	1:B:130:LEU:HD13	1.91	0.51
1:B:1700:THR:O	1:B:1702:LEU:N	2.44	0.51
1:B:178:LEU:HB3	1:B:197:PHE:HZ	1.75	0.51
1:B:287:LEU:C	1:B:291:VAL:HB	2.30	0.51
1:B:306:VAL:HG23	1:B:308:LEU:H	1.75	0.51
1:B:3696:ARG:O	1:B:3699:LEU:HB2	2.11	0.51
1:B:3751:LEU:HD13	1:B:3805:TRP:HB2	1.92	0.51
1:B:2928:LYS:HD2	1:B:3783:GLN:HB3	1.93	0.51
1:B:3883:LEU:HG	1:B:3970:LEU:HD13	1.93	0.51
1:B:3989:ARG:HH21	1:B:4100:GLU:CB	2.24	0.51
1:B:714:VAL:CG1	1:B:734:LEU:HD21	2.41	0.51
1:B:913:ARG:HE	1:B:916:GLU:CD	2.14	0.51
1:A:1004:GLN:O	1:A:1008:ALA:HB2	2.11	0.51
1:A:100:ILE:O	1:A:104:SER:N	2.44	0.51
1:A:2205:VAL:HB	1:A:2206:PRO:HD3	1.92	0.51
1:A:2356:MSE:SE	1:A:2360:PHE:CZ	3.14	0.51
1:A:273:ARG:HG3	1:A:274:LEU:H	1.76	0.51
1:A:3614:TYR:CE1	1:A:3618:GLY:HA3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:MSE:HG2	1:A:541:MSE:H	1.76	0.51
1:A:743:LEU:HD22	1:A:746:ARG:HH12	1.76	0.51
1:A:877:ASP:O	1:A:879:MSE:N	2.44	0.51
1:B:716:VAL:HG11	1:B:1121:LEU:HD13	1.93	0.51
1:B:1122:GLY:O	1:B:1123:THR:OG1	2.23	0.51
1:B:2495:SER:O	1:B:2498:ILE:HB	2.10	0.51
1:B:2890:ILE:HG21	1:B:2922:ARG:HH12	1.76	0.51
1:B:2943:PHE:O	1:B:2945:SER:N	2.41	0.51
1:B:3518:VAL:HG13	1:B:3554:PHE:CZ	2.46	0.51
1:B:3568:ILE:HD11	1:B:3691:LYS:CD	2.41	0.51
1:B:3572:ILE:HA	1:B:3575:LEU:HB3	1.93	0.51
1:B:3901:ARG:HG2	1:B:3901:ARG:HH11	1.75	0.51
1:B:4077:TYR:OH	1:B:4119:ARG:HG2	2.11	0.51
1:B:538:ASP:CB	1:B:627:VAL:HG13	2.39	0.51
1:B:63:PHE:CD1	1:B:89:LEU:HD13	2.46	0.51
1:B:947:GLN:C	1:B:949:PRO:HD3	2.32	0.51
1:A:1347:THR:O	1:A:1351:THR:OG1	2.27	0.50
1:A:1342:MSE:HE2	1:A:1398:VAL:HG12	1.93	0.50
1:A:1472:SER:HA	1:A:1476:HIS:CD2	2.46	0.50
1:A:1521:PHE:O	1:A:1524:LEU:HB2	2.11	0.50
1:A:2323:LEU:HD11	1:A:2345:VAL:HG21	1.93	0.50
1:A:2443:MSE:SE	1:A:2480:ILE:HG21	2.61	0.50
1:A:2464:HIS:H	1:A:2465:PRO:CD	2.24	0.50
1:A:2501:LEU:O	1:A:2505:VAL:HG23	2.10	0.50
1:A:2884:LEU:C	1:A:2887:PRO:HD2	2.32	0.50
1:A:3167:ARG:HG2	1:A:3186:ARG:NE	2.26	0.50
1:A:3280:TYR:CZ	1:A:3304:VAL:HG23	2.46	0.50
1:A:3979:LEU:CA	1:A:3981:TYR:HB3	2.39	0.50
1:A:4038:TRP:CH2	1:A:4040:PRO:HB3	2.46	0.50
1:A:406:ARG:O	1:A:409:GLN:N	2.27	0.50
1:A:575:ILE:HD11	1:A:579:LEU:HD22	1.93	0.50
1:A:87:LYS:HG2	1:A:133:LYS:CG	2.38	0.50
1:A:84:GLU:O	1:A:88:PHE:HD1	1.94	0.50
1:B:2152:ASN:CB	1:B:2153:THR:HA	2.36	0.50
1:B:2204:GLY:HA2	1:B:2208:ASP:OD2	2.12	0.50
1:B:217:LEU:O	1:B:221:ALA:HB2	2.10	0.50
1:B:3487:ILE:CG2	1:B:3495:PHE:HB2	2.37	0.50
1:B:3505:LEU:HD12	1:B:3509:ASP:HB3	1.91	0.50
1:B:2928:LYS:HG3	1:B:3783:GLN:O	2.11	0.50
1:B:3820:MSE:HB2	1:B:3882:LEU:HD13	1.94	0.50
1:B:3915:HIS:ND1	1:B:3920:ILE:HD12	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:886:TRP:CD1	1:B:889:GLU:N	2.69	0.50
1:B:929:ALA:O	1:B:933:LEU:HB2	2.11	0.50
1:B:928:VAL:O	1:B:932:GLU:HB2	2.11	0.50
1:A:1017:ILE:HG23	1:A:1018:VAL:HG13	1.92	0.50
1:A:1063:LEU:O	1:A:1066:LEU:HB3	2.11	0.50
1:A:1584:GLN:O	1:A:1588:ASP:OD1	2.29	0.50
1:A:1789:GLY:O	1:A:1793:THR:HG23	2.12	0.50
1:A:3011:LEU:HB3	1:A:3047:SER:HB3	1.94	0.50
1:A:3768:PHE:O	1:A:3771:MSE:N	2.44	0.50
1:A:3981:TYR:CE1	1:A:4104:VAL:HB	2.46	0.50
1:A:489:ARG:O	1:A:489:ARG:CZ	2.59	0.50
1:B:1376:LEU:HG	1:B:1377:CYS:N	2.26	0.50
1:B:1596:VAL:O	1:B:1600:MSE:HG3	2.11	0.50
1:B:2031:LEU:C	1:B:2033:ASP:N	2.64	0.50
1:B:2390:HIS:ND1	1:B:2397:CYS:SG	2.74	0.50
1:B:2462:VAL:CB	1:B:2473:MSE:SE	3.09	0.50
1:B:2935:GLU:O	1:B:2939:LEU:HG	2.10	0.50
1:B:348:ILE:HG23	1:B:357:LYS:HG3	1.93	0.50
1:B:3705:TYR:HE2	1:B:3708:ARG:HH12	1.60	0.50
1:B:3762:GLN:OE1	1:B:3795:PRO:HG3	2.11	0.50
1:B:390:GLN:O	1:B:393:LYS:HG2	2.11	0.50
1:B:411:PRO:O	1:B:415:GLN:HB2	2.12	0.50
1:B:419:SER:HA	1:B:422:LEU:HG	1.94	0.50
1:B:743:LEU:O	1:B:746:ARG:HG2	2.11	0.50
1:B:796:LEU:HD22	1:B:799:TYR:HE2	1.76	0.50
1:A:1042:LYS:HZ1	1:A:1044:ILE:HD12	1.76	0.50
1:A:1350:ASN:ND2	1:A:1404:LYS:HG2	2.27	0.50
1:A:1698:PHE:CD1	1:A:1699:PHE:N	2.79	0.50
1:A:173:LYS:HA	1:A:176:GLU:OE1	2.11	0.50
1:A:1815:THR:C	1:A:1816:ARG:HE	2.14	0.50
1:A:2095:ALA:HB3	1:A:2096:PRO:HD3	1.92	0.50
1:A:2190:VAL:HA	1:A:2193:ILE:HG22	1.93	0.50
1:A:2216:LEU:O	1:A:2220:MSE:HG3	2.11	0.50
1:A:2254:ARG:HG3	1:A:2255:LEU:N	2.27	0.50
1:A:2339:GLU:O	1:A:2343:GLU:HG3	2.10	0.50
1:A:237:SER:O	1:A:278:HIS:HB3	2.10	0.50
1:A:3007:GLU:OE2	1:A:3046:ARG:HD3	2.10	0.50
1:A:3108:GLN:HA	1:A:3111:MSE:HG3	1.94	0.50
1:A:3780:ALA:HB1	1:A:3784:ARG:HH12	1.77	0.50
1:A:703:CYS:O	1:A:706:LEU:HB2	2.11	0.50
1:B:1036:PHE:CZ	1:B:1082:PHE:HE2	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1076:LEU:HD11	1:B:1114:ALA:HB1	1.93	0.50
1:B:1238:GLN:HB2	1:B:1239:PRO:HD3	1.94	0.50
1:B:1469:PRO:HA	1:B:1472:SER:CB	2.38	0.50
1:B:2088:LEU:O	1:B:2092:GLU:N	2.43	0.50
1:B:2145:PHE:CE1	1:B:2188:GLU:HB3	2.47	0.50
1:B:3072:GLU:HG3	1:B:3080:LEU:HD11	1.94	0.50
1:B:3789:ARG:NH2	1:B:3806:LEU:HD22	2.26	0.50
1:B:410:MSE:HE1	1:B:445:SER:CB	2.42	0.50
1:A:964:ARG:N	1:A:1009:LEU:HD13	2.26	0.50
1:A:1265:GLU:O	1:A:1269:THR:HG23	2.10	0.50
1:A:1751:GLU:HG2	1:A:1870:LYS:CE	2.39	0.50
1:A:1856:THR:O	1:A:1860:GLU:HB2	2.12	0.50
1:A:1882:SER:C	1:A:1885:PRO:HD2	2.32	0.50
1:A:2000:ARG:HG2	1:A:2001:LYS:HG3	1.92	0.50
1:A:2097:LEU:HD13	1:A:2143:ARG:HG2	1.93	0.50
1:A:232:CYS:SG	1:A:274:LEU:HD13	2.51	0.50
1:A:2379:MSE:O	1:A:2383:PHE:HB2	2.11	0.50
1:A:2386:LEU:HD11	1:A:2400:VAL:HG12	1.94	0.50
1:A:2956:ALA:HA	1:A:2965:TYR:OH	2.11	0.50
1:A:367:GLY:C	1:A:369:PHE:N	2.64	0.50
1:A:568:PHE:CZ	1:A:653:LEU:HG	2.47	0.50
1:A:767:GLU:O	1:A:771:ASN:HB2	2.10	0.50
1:B:1162:SER:N	1:B:1165:LEU:HD12	2.20	0.50
1:B:1220:LEU:HD13	1:B:1274:ARG:CG	2.41	0.50
1:B:1503:LEU:O	1:B:1507:CYS:HB3	2.11	0.50
1:B:1956:PHE:HB3	1:B:1998:MSE:HE1	1.93	0.50
1:B:2129:LEU:HD13	1:B:2156:VAL:HG13	1.93	0.50
1:B:2220:MSE:SE	1:B:2256:ILE:CD1	3.10	0.50
1:B:3962:ARG:HD3	1:B:4124:TRP:CE3	2.46	0.50
1:B:554:ASN:O	1:B:557:SER:HB2	2.11	0.50
1:B:852:ARG:CZ	1:B:3111:MSE:SE	3.09	0.50
1:A:1102:GLU:O	1:A:1105:VAL:HG22	2.12	0.50
1:A:1107:TYR:HE1	1:A:1111:LEU:HD13	1.75	0.50
1:A:1678:LEU:O	1:A:1682:THR:HG22	2.12	0.50
1:A:1922:ALA:HA	1:A:1925:GLU:OE2	2.11	0.50
1:A:1886:LYS:NZ	1:A:1924:THR:HB	2.23	0.50
1:A:3593:ARG:HD2	1:A:3660:ASN:O	2.12	0.50
1:A:3763:ARG:O	1:A:3767:LEU:HB2	2.12	0.50
1:A:3901:ARG:HG2	1:A:3901:ARG:NH1	2.26	0.50
1:A:3981:TYR:O	1:A:3985:VAL:HG23	2.11	0.50
1:A:3962:ARG:HD3	1:A:4124:TRP:CE3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:LEU:O	1:A:490:ILE:HG22	2.11	0.50
1:B:1039:TRP:HH2	1:B:1052:SER:HB3	1.76	0.50
1:B:1101:PHE:O	1:B:1104:LEU:HB2	2.12	0.50
1:B:3151:LEU:O	1:B:3156:PRO:HD3	2.11	0.50
1:B:3810:VAL:HG23	1:B:3815:LEU:HD11	1.93	0.50
1:B:385:TYR:CD1	1:B:420:VAL:HG13	2.40	0.50
1:B:527:TYR:CE1	1:B:615:ALA:HA	2.46	0.50
1:B:67:VAL:O	1:B:71:LYS:CB	2.41	0.50
1:A:1502:SER:O	1:A:1505:LEU:N	2.43	0.50
1:A:175:TYR:OH	1:A:204:LEU:HD11	2.10	0.50
1:A:2166:SER:O	1:A:2170:GLN:HB3	2.12	0.50
1:A:288:ASP:N	1:A:288:ASP:OD1	2.43	0.50
1:A:3674:SER:O	1:A:3677:PRO:HD2	2.12	0.50
1:A:4007:LYS:CG	1:A:4041:ARG:HD2	2.35	0.50
1:A:801:LYS:O	1:A:805:LEU:HB2	2.11	0.50
1:A:85:ILE:O	1:A:89:LEU:HG	2.10	0.50
1:A:913:ARG:HB2	1:A:934:LEU:HD12	1.93	0.50
1:A:954:GLY:O	1:A:957:PRO:HD2	2.12	0.50
1:B:1406:LEU:HA	1:B:1410:PRO:HG3	1.94	0.50
1:B:1406:LEU:O	1:B:1415:LEU:HD21	2.12	0.50
1:B:2352:HIS:CD2	1:B:2364:LEU:HD21	2.47	0.50
1:B:2430:GLU:OE1	1:B:2433:LYS:HE3	2.11	0.50
1:B:2936:TYR:CZ	1:B:2940:ARG:HD2	2.47	0.50
1:B:3648:GLY:O	1:B:3651:LEU:HB2	2.11	0.50
1:B:3766:GLN:O	1:B:3770:VAL:HG23	2.11	0.50
1:B:512:GLY:CA	1:B:602:MSE:HG3	2.40	0.50
1:B:68:PHE:O	1:B:72:SER:OG	2.10	0.50
1:B:722:LYS:HB3	1:B:727:ALA:CA	2.42	0.50
1:B:734:LEU:C	1:B:737:PRO:HD2	2.32	0.50
1:A:1036:PHE:CZ	1:A:1082:PHE:HE2	2.30	0.50
1:A:1741:ASP:O	1:A:1745:LYS:HG3	2.11	0.50
1:A:2318:ALA:O	1:A:2322:VAL:HB	2.12	0.50
1:A:3049:LEU:HA	1:A:3188:PHE:CZ	2.46	0.50
1:A:334:HIS:O	1:A:338:LEU:HD11	2.12	0.50
1:A:3525:TYR:CZ	1:A:3533:PHE:HE1	2.30	0.50
1:A:3998:LEU:O	1:A:4001:THR:OG1	2.28	0.50
1:A:676:ASN:O	1:A:680:ILE:HG13	2.11	0.50
1:A:743:LEU:HG	1:A:783:HIS:CE1	2.44	0.50
1:A:66:LEU:CD2	1:A:89:LEU:HD11	2.42	0.50
1:B:1357:LYS:HG3	1:B:1360:LYS:NZ	2.26	0.50
1:B:152:LEU:O	1:B:156:PHE:HD1	1.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1696:LEU:HD23	1:B:1700:THR:HG21	1.92	0.50
1:B:1756:PRO:O	1:B:1758:LEU:N	2.34	0.50
1:B:1894:SER:O	1:B:1896:ILE:N	2.44	0.50
1:B:1972:GLU:CD	1:B:1987:ARG:HH12	2.14	0.50
1:B:2320:ALA:HB1	1:B:2370:SER:OG	2.10	0.50
1:B:2389:PHE:CD2	1:B:2396:LEU:HD22	2.46	0.50
1:B:2536:LEU:O	1:B:2539:LEU:HB2	2.11	0.50
1:B:368:LEU:HA	1:B:372:PRO:HG2	1.94	0.50
1:B:3726:VAL:HG21	1:B:3736:LYS:HD3	1.93	0.50
1:B:4066:LEU:HD23	1:B:4075:ARG:HG3	1.94	0.50
1:B:888:ARG:HA	1:B:907:LEU:HD21	1.94	0.50
1:A:1086:TYR:HD2	1:A:1090:ARG:HG2	1.76	0.50
1:A:1106:ILE:O	1:A:1109:GLU:HB3	2.12	0.50
1:A:1298:LEU:HA	1:A:1301:ILE:HB	1.94	0.50
1:A:1433:ALA:O	1:A:1437:TYR:CD2	2.65	0.50
1:A:1604:SER:HA	1:A:1632:TRP:CE3	2.47	0.50
1:A:1956:PHE:HB3	1:A:1998:MSE:CE	2.41	0.50
1:A:2512:ASP:H	1:A:2519:LEU:HD12	1.76	0.50
1:A:2814:SER:O	1:A:2818:LYS:HB2	2.11	0.50
1:A:293:LEU:O	1:A:296:VAL:HG12	2.12	0.50
1:A:3464:LYS:O	1:A:3467:ARG:HB3	2.12	0.50
1:A:3498:TRP:HD1	1:A:3498:TRP:O	1.95	0.50
1:A:3789:ARG:CZ	1:A:3806:LEU:HD22	2.40	0.50
1:A:4066:LEU:HD21	1:A:4078:VAL:HG21	1.94	0.50
1:A:741:ILE:O	1:A:743:LEU:N	2.45	0.50
1:A:969:LEU:O	1:A:973:ALA:CB	2.60	0.50
1:B:1074:LYS:O	1:B:1075:ARG:HG3	2.12	0.50
1:B:1586:SER:HB3	1:B:1643:MSE:HE1	1.94	0.50
1:B:1736:PHE:O	1:B:1740:VAL:HG23	2.11	0.50
1:B:175:TYR:HD2	1:B:222:GLY:HA3	1.76	0.50
1:B:1816:ARG:HB3	1:B:1819:PHE:CE1	2.45	0.50
1:B:2080:VAL:HG12	1:B:2081:LEU:H	1.75	0.50
1:B:2212:ALA:O	1:B:2215:LEU:N	2.44	0.50
1:B:2879:GLY:HA2	1:B:2886:GLN:CG	2.29	0.50
1:B:2964:ASP:O	1:B:2968:ALA:HB2	2.12	0.50
1:B:2960:GLU:O	1:B:2965:TYR:CD1	2.65	0.50
1:B:3179:TRP:CZ2	1:B:3258:LEU:HG	2.47	0.50
1:B:3383:GLN:HG3	1:B:3438:GLU:OE2	2.12	0.50
1:B:3510:GLN:O	1:B:3512:VAL:N	2.34	0.50
1:B:3572:ILE:HD13	1:B:3575:LEU:HD22	1.94	0.50
1:B:898:PHE:CE2	1:B:2566:THR:HG21	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:966:PHE:CE2	1:B:988:VAL:HG12	2.47	0.50
1:A:1655:ILE:CD1	1:A:1681:ASP:HB3	2.40	0.50
1:A:1747:LEU:O	1:A:1750:LEU:N	2.41	0.50
1:A:1935:GLU:HB2	1:A:1986:ARG:NH2	2.27	0.50
1:A:2171:LEU:CG	1:A:2177:ASN:HD21	2.25	0.50
1:A:2416:LYS:O	1:A:2420:PHE:HB3	2.12	0.50
1:A:2538:ARG:HH22	1:A:2566:THR:CG2	2.25	0.50
1:A:3495:PHE:CZ	1:A:3521:ILE:HG13	2.47	0.50
1:A:3865:THR:O	1:A:3869:THR:OG1	2.14	0.50
1:A:629:PHE:HA	1:A:634:LEU:HD21	1.91	0.50
1:B:1299:GLU:OE2	1:B:1367:HIS:HB2	2.12	0.50
1:B:1348:LEU:O	1:B:1352:SER:N	2.34	0.50
1:B:1455:CYS:O	1:B:1458:LEU:HB2	2.11	0.50
1:B:1882:SER:C	1:B:1885:PRO:HD2	2.33	0.50
1:B:2922:ARG:HD3	1:B:2930:TYR:HD1	1.77	0.50
1:B:3141:PHE:CZ	1:B:3192:LYS:HB2	2.47	0.50
1:B:3277:VAL:HG23	1:B:3324:ARG:HD2	1.94	0.50
1:B:3507:ASP:CG	1:B:3540:TYR:HA	2.32	0.50
1:B:3503:VAL:HG21	1:B:3535:ILE:O	2.12	0.50
1:B:12:LEU:HD13	1:B:42:CYS:SG	2.52	0.50
1:A:1014:LEU:HB2	1:A:1078:ALA:CB	2.41	0.49
1:A:2135:ASN:N	1:A:2136:PRO:CD	2.75	0.49
1:A:2196:TRP:HE1	1:A:2200:ALA:HB2	1.77	0.49
1:A:2373:PRO:HA	1:A:2378:PHE:HZ	1.77	0.49
1:A:242:PRO:HD3	1:A:282:PHE:CD2	2.47	0.49
1:A:232:CYS:HG	1:A:275:PHE:HE1	1.60	0.49
1:A:3397:GLN:HB3	1:A:3398:PRO:CD	2.42	0.49
1:A:3989:ARG:HH21	1:A:4100:GLU:HB2	1.77	0.49
1:A:4090:ARG:NH1	1:A:4106:CYS:HA	2.20	0.49
1:A:569:VAL:HG13	1:A:570:LYS:H	1.77	0.49
1:B:1553:PHE:O	1:B:1557:GLU:HB2	2.12	0.49
1:B:428:PRO:HB3	1:B:1679:LEU:HD13	1.94	0.49
1:B:2157:PHE:O	1:B:2160:TYR:N	2.45	0.49
1:B:2373:PRO:HB3	1:B:2407:GLY:O	2.11	0.49
1:B:2485:ARG:HH11	1:B:2530:ARG:CZ	2.25	0.49
1:B:294:PHE:CZ	1:B:319:PHE:CD2	2.96	0.49
1:B:2957:LEU:CA	1:B:3989:ARG:HH22	2.24	0.49
1:B:2939:LEU:HD21	1:B:2994:TRP:CE2	2.47	0.49
1:B:3484:THR:HA	1:B:3516:HIS:HE2	1.77	0.49
1:B:3858:MSE:HG3	1:B:4119:ARG:NE	2.27	0.49
1:B:661:PRO:HG2	1:B:733:LEU:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1905:ILE:HG23	1:A:1951:VAL:HG21	1.94	0.49
1:A:2066:PHE:HB3	1:A:2067:ARG:CG	2.41	0.49
1:A:2177:ASN:ND2	1:A:2182:ILE:HA	2.28	0.49
1:A:2168:LEU:HD13	1:A:2214:ARG:NE	2.27	0.49
1:A:2255:LEU:HA	1:A:2258:GLU:HB2	1.94	0.49
1:A:3531:TYR:HB3	1:A:3532:PRO:HD3	1.93	0.49
1:A:3578:LEU:HD11	1:A:3686:TRP:HZ3	1.77	0.49
1:A:2936:TYR:HB3	1:A:3979:LEU:CD1	2.41	0.49
1:A:455:LEU:HD13	1:A:459:ARG:CZ	2.42	0.49
1:A:476:ARG:HA	1:A:479:ILE:HD12	1.93	0.49
1:A:617:PRO:HB3	1:A:659:ARG:CG	2.41	0.49
1:A:63:PHE:O	1:A:66:LEU:HG	2.13	0.49
1:A:730:LEU:O	1:A:734:LEU:HG	2.12	0.49
1:B:114:VAL:HG12	1:B:130:LEU:HD21	1.94	0.49
1:B:1927:MSE:C	1:B:1929:GLY:H	2.15	0.49
1:B:1965:PHE:O	1:B:1968:SER:OG	2.18	0.49
1:B:2220:MSE:HB3	1:B:2224:PHE:CZ	2.47	0.49
1:B:2447:LYS:N	1:B:2448:PRO:HD2	2.28	0.49
1:B:2458:VAL:HA	1:B:2461:PHE:CD2	2.45	0.49
1:B:2961:ALA:HB1	1:B:3002:TYR:HB2	1.94	0.49
1:B:3272:TRP:CE3	1:B:3307:LEU:HD21	2.46	0.49
1:B:3280:TYR:CZ	1:B:3304:VAL:HG23	2.47	0.49
1:B:3774:ILE:HG22	1:B:3775:LEU:HD23	1.94	0.49
1:B:805:LEU:HD23	1:B:808:GLU:OE2	2.13	0.49
1:A:1119:LYS:NZ	1:A:1256:TRP:HZ2	2.10	0.49
1:A:1389:VAL:HG12	1:A:1389:VAL:O	2.12	0.49
1:A:1469:PRO:HA	1:A:1472:SER:CB	2.42	0.49
1:A:1574:ASN:CB	1:A:1582:LEU:HD21	2.40	0.49
1:A:2393:LEU:HD13	1:A:2426:HIS:CD2	2.46	0.49
1:A:282:PHE:CD1	1:A:283:SER:N	2.80	0.49
1:A:3005:LEU:O	1:A:3180:ASP:OD2	2.30	0.49
1:A:3012:GLU:HB2	1:A:3050:LYS:NZ	2.27	0.49
1:A:39:GLY:O	1:A:43:VAL:HG23	2.12	0.49
1:A:47:SER:N	1:A:51:LEU:HD12	2.27	0.49
1:A:884:VAL:HG22	1:A:888:ARG:HG2	1.93	0.49
1:A:965:THR:HA	1:A:968:VAL:CG1	2.42	0.49
1:A:986:PRO:O	1:A:990:GLN:HG2	2.12	0.49
1:B:1010:LEU:HD13	1:B:1028:PHE:CE1	2.28	0.49
1:B:1907:GLU:O	1:B:1911:LEU:HG	2.11	0.49
1:B:2328:ARG:O	1:B:2332:GLU:HG2	2.13	0.49
1:B:319:PHE:O	1:B:323:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3326:GLN:CB	1:B:3393:GLU:HG2	2.38	0.49
1:B:3493:TRP:CD1	1:B:3710:LYS:O	2.65	0.49
1:B:3923:ARG:HB3	1:B:3962:ARG:HH12	1.78	0.49
1:B:533:HIS:O	1:B:537:SER:HB3	2.13	0.49
1:B:941:MSE:HE3	1:B:958:MSE:HG3	1.95	0.49
1:A:1121:LEU:HG	1:A:1122:GLY:H	1.75	0.49
1:A:86:LEU:HD13	1:A:134:LEU:CD2	2.42	0.49
1:A:1491:ILE:N	1:A:1497:ARG:HH12	2.10	0.49
1:A:390:GLN:NE2	1:A:1723:PRO:HG2	2.28	0.49
1:A:1751:GLU:OE2	1:A:1884:LEU:HD13	2.11	0.49
1:A:1811:ARG:O	1:A:1815:THR:HG23	2.12	0.49
1:A:2280:VAL:HG13	1:A:2287:PRO:HB2	1.93	0.49
1:A:2420:PHE:CE1	1:A:2439:ILE:HG21	2.46	0.49
1:A:2927:ALA:HB2	1:A:3121:LEU:HD22	1.93	0.49
1:A:3174:ASP:N	1:A:3175:PRO:HD2	2.17	0.49
1:A:318:SER:O	1:A:321:LYS:HB2	2.12	0.49
1:A:3620:PRO:HB3	1:A:3633:ILE:HD12	1.94	0.49
1:A:481:THR:HG23	1:A:559:SER:OG	2.13	0.49
1:A:680:ILE:HG12	1:A:701:TYR:CE1	2.48	0.49
1:B:103:TYR:O	1:B:107:ILE:HG13	2.13	0.49
1:B:1086:TYR:CE2	1:B:1090:ARG:HG2	2.48	0.49
1:B:1139:GLU:HG3	1:B:1175:HIS:CD2	2.47	0.49
1:B:1702:LEU:O	1:B:1706:SER:CB	2.61	0.49
1:B:2193:ILE:HA	1:B:2196:TRP:CE2	2.48	0.49
1:B:2847:THR:HB	1:B:2850:PHE:CD2	2.47	0.49
1:B:3163:THR:OG1	1:B:3167:ARG:NH2	2.43	0.49
1:B:3323:PHE:CE1	1:B:3324:ARG:HG3	2.48	0.49
1:B:334:HIS:O	1:B:338:LEU:HD11	2.12	0.49
1:B:560:LEU:HD11	1:B:645:TRP:HZ2	1.74	0.49
1:B:954:GLY:O	1:B:957:PRO:HD2	2.11	0.49
1:A:1145:LEU:HD22	1:A:1149:LYS:HZ3	1.78	0.49
1:A:1155:ARG:HH12	1:A:1159:PRO:CD	2.21	0.49
1:A:1158:PRO:HB2	1:A:1159:PRO:HD3	1.95	0.49
1:A:1475:LEU:O	1:A:1478:SER:HB3	2.13	0.49
1:A:1808:ASP:OD1	1:A:1809:ASP:N	2.45	0.49
1:A:2027:SER:HB2	1:A:2030:TYR:OH	2.12	0.49
1:A:2144:LEU:C	1:A:2148:LYS:HE3	2.33	0.49
1:A:2944:THR:HG21	1:A:2983:ASP:OD2	2.12	0.49
1:A:2970:LYS:NZ	1:A:3013:TYR:OH	2.44	0.49
1:A:396:PHE:CG	1:A:397:LEU:N	2.80	0.49
1:A:4012:ASP:C	1:A:4016:PHE:HB2	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:VAL:HG11	1:A:776:TRP:HZ2	1.78	0.49
1:A:808:GLU:OE1	1:A:3114:TYR:HB3	2.13	0.49
1:A:767:GLU:CG	1:A:851:ILE:HD11	2.40	0.49
1:B:1645:VAL:HG22	1:B:1709:GLU:OE1	2.13	0.49
1:B:1945:TYR:CD1	1:B:1948:ALA:HB3	2.47	0.49
1:B:2094:MSE:O	1:B:2098:THR:HG23	2.13	0.49
1:B:2358:ASP:O	1:B:2361:ILE:HG22	2.12	0.49
1:B:2423:VAL:HG22	1:B:2424:MSE:N	2.27	0.49
1:B:2806:LYS:NZ	1:B:2858:ILE:HG13	2.26	0.49
1:B:2913:LYS:O	1:B:2915:ARG:N	2.45	0.49
1:B:3259:LEU:HD21	1:B:3279:SER:HB2	1.94	0.49
1:B:3696:ARG:HB2	1:B:3699:LEU:HB2	1.95	0.49
1:B:3825:LYS:HB2	1:B:3829:LEU:HD13	1.93	0.49
1:B:437:HIS:CD2	1:B:438:LEU:N	2.80	0.49
1:B:407:VAL:O	1:B:449:TYR:HE1	1.95	0.49
1:B:604:PRO:HG2	1:B:607:ASP:OD1	2.13	0.49
1:B:638:GLN:HG3	1:B:667:TYR:CD2	2.48	0.49
1:B:708:VAL:HG22	1:B:744:ASP:OD2	2.12	0.49
1:B:855:VAL:HG12	1:B:859:LEU:HD11	1.93	0.49
1:B:964:ARG:O	1:B:967:PRO:HD2	2.11	0.49
1:B:978:GLN:HA	1:B:981:ARG:NE	2.21	0.49
1:B:977:ASP:HB3	1:B:981:ARG:N	2.26	0.49
1:A:1060:PHE:HB3	1:A:1064:TYR:HE2	1.78	0.49
1:A:203:GLU:O	1:A:207:GLN:CB	2.55	0.49
1:A:2352:HIS:CD2	1:A:2364:LEU:HD21	2.48	0.49
1:A:2320:ALA:CA	1:A:2367:VAL:HG23	2.42	0.49
1:A:2960:GLU:HG3	1:A:3289:ARG:HH22	1.77	0.49
1:A:3356:ALA:CB	1:A:3384:HIS:HB3	2.43	0.49
1:A:704:PHE:O	1:A:707:PHE:HB2	2.11	0.49
1:A:871:LEU:HD11	1:A:3122:HIS:CE1	2.42	0.49
1:B:992:ILE:HD13	1:B:1031:ARG:HB3	1.95	0.49
1:B:1107:TYR:O	1:B:1111:LEU:N	2.40	0.49
1:B:2452:ARG:HG2	1:B:2498:ILE:HD11	1.94	0.49
1:B:3266:SER:HB2	1:B:3271:ASP:OD1	2.12	0.49
1:B:352:VAL:HG23	1:B:357:LYS:H	1.77	0.49
1:B:3793:VAL:O	1:B:3795:PRO:HD3	2.12	0.49
1:B:63:PHE:CE1	1:B:89:LEU:HD22	2.47	0.49
1:B:903:PRO:O	1:B:905:ILE:HG13	2.12	0.49
1:A:1102:GLU:O	1:A:1105:VAL:HG13	2.13	0.49
1:A:1643:MSE:O	1:A:1646:LEU:N	2.46	0.49
1:A:1723:PRO:C	1:A:1725:GLN:N	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2097:LEU:HA	1:A:2100:LEU:HB3	1.94	0.49
1:A:2148:LYS:NZ	1:A:2188:GLU:HG2	2.27	0.49
1:A:21:ALA:HA	1:A:24:ARG:HG3	1.94	0.49
1:A:2511:ILE:HA	1:A:2519:LEU:HD12	1.94	0.49
1:A:2542:LEU:HD12	1:A:2543:ASN:N	2.28	0.49
1:A:2567:SER:O	1:A:2571:ASP:HB2	2.11	0.49
1:A:933:LEU:HD22	1:A:2795:GLN:HA	1.93	0.49
1:A:3152:SER:HB2	1:A:3155:VAL:HB	1.94	0.49
1:A:899:ARG:HH22	1:A:2570:PRO:CB	2.25	0.49
1:A:892:LEU:H	1:A:907:LEU:HD22	1.78	0.49
1:B:1033:ILE:HA	1:B:1036:PHE:CD2	2.48	0.49
1:B:1960:LYS:HA	1:B:1963:GLN:OE1	2.13	0.49
1:B:2222:HIS:O	1:B:2226:PRO:HD2	2.12	0.49
1:B:2854:PHE:CE1	1:B:2878:ALA:HA	2.48	0.49
1:B:2999:LEU:HD12	1:B:3002:TYR:CE2	2.46	0.49
1:B:3003:ASN:O	1:B:3006:ALA:N	2.46	0.49
1:B:3163:THR:O	1:B:3167:ARG:HB2	2.13	0.49
1:B:3501:HIS:O	1:B:3505:LEU:HD13	2.12	0.49
1:B:3576:ASP:C	1:B:3578:LEU:HG	2.33	0.49
1:B:3667:LEU:HA	1:B:3670:MSE:HG2	1.92	0.49
1:B:3906:SER:O	1:B:3910:LEU:HD13	2.12	0.49
1:B:388:LEU:HG	1:B:420:VAL:HG21	1.94	0.49
1:B:479:ILE:O	1:B:483:VAL:HG13	2.12	0.49
1:B:789:TYR:CD2	1:B:865:GLN:HG3	2.47	0.49
1:A:1044:ILE:O	1:A:1045:THR:OG1	2.28	0.49
1:A:134:LEU:O	1:A:137:THR:OG1	2.25	0.49
1:A:1407:LYS:HG2	1:A:1462:GLY:N	2.28	0.49
1:A:2245:TRP:CE3	1:A:2245:TRP:HA	2.48	0.49
1:A:2365:ASN:HA	1:A:2368:THR:HB	1.94	0.49
1:A:2412:TYR:CD2	1:A:2416:LYS:HG3	2.47	0.49
1:A:270:ALA:HA	1:A:273:ARG:HG2	1.95	0.49
1:A:3052:LEU:HD13	1:A:3061:LEU:HG	1.94	0.49
1:A:3179:TRP:CZ2	1:A:3258:LEU:HG	2.46	0.49
1:A:3510:GLN:OE1	1:A:3513:ALA:HB2	2.13	0.49
1:A:3525:TYR:OH	1:A:3561:LYS:HB2	2.13	0.49
1:A:3885:ARG:HG3	1:A:3889:ARG:HD3	1.95	0.49
1:A:3929:MSE:O	1:A:3938:ILE:HG13	2.12	0.49
1:A:729:CYS:HA	1:A:732:PHE:CE2	2.48	0.49
1:B:1007:VAL:HA	1:B:1010:LEU:CD1	2.43	0.49
1:B:1220:LEU:O	1:B:1223:THR:OG1	2.26	0.49
1:B:1280:GLN:HA	1:B:1361:LYS:HZ2	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1459:HIS:NE2	1:B:1509:GLN:O	2.46	0.49
1:B:1751:GLU:O	1:B:1755:SER:N	2.42	0.49
1:B:1726:SER:HB2	1:B:1869:LYS:HD2	1.94	0.49
1:B:3117:ILE:CD1	1:B:3125:ARG:HH11	2.06	0.49
1:B:3293:CYS:O	1:B:3297:VAL:HB	2.13	0.49
1:B:3570:ASP:O	1:B:3573:ASN:HB3	2.13	0.49
1:B:3657:SER:O	1:B:3660:ASN:HB2	2.13	0.49
1:B:3971:MSE:HE2	1:B:3976:GLU:OE2	2.13	0.49
1:B:712:LYS:O	1:B:716:VAL:HG23	2.13	0.49
1:B:63:PHE:HD1	1:B:89:LEU:HD13	1.78	0.49
1:A:1139:GLU:HG3	1:A:1175:HIS:CD2	2.48	0.49
1:A:1684:LEU:HA	1:A:1687:HIS:HD2	1.77	0.49
1:A:175:TYR:HB2	1:A:222:GLY:C	2.33	0.49
1:A:2274:ILE:CD1	1:A:2314:GLU:HB3	2.43	0.49
1:A:3103:ILE:HD13	1:A:3139:GLN:OE1	2.13	0.49
1:A:3984:MSE:SE	1:A:4108:MSE:HE2	2.63	0.49
1:A:442:GLN:HA	1:A:445:SER:OG	2.12	0.49
1:B:1493:PRO:HG2	1:B:1495:ASP:HB2	1.94	0.49
1:B:2161:ALA:CB	1:B:2211:LEU:HD13	2.39	0.49
1:B:2357:GLU:OE1	1:B:2388:LYS:NZ	2.42	0.49
1:B:2778:GLY:O	1:B:2781:PRO:HD2	2.13	0.49
1:B:249:PHE:HB3	1:B:297:LEU:HD13	1.93	0.49
1:B:3522:THR:O	1:B:3526:PRO:HD3	2.13	0.49
1:B:3974:MSE:CG	1:B:3976:GLU:HB3	2.43	0.49
1:B:4041:ARG:HB2	1:B:4042:GLN:OE1	2.12	0.49
1:B:793:LEU:HA	1:B:796:LEU:HB2	1.94	0.49
1:B:891:ARG:HD2	1:B:905:ILE:HG12	1.94	0.49
1:A:1113:LEU:HA	1:A:1116:ALA:HB3	1.94	0.49
1:A:1695:LEU:HA	1:A:1698:PHE:CE2	2.48	0.49
1:A:1762:MSE:HE3	1:A:1864:ASP:OD1	2.13	0.49
1:A:3045:ILE:O	1:A:3048:LYS:HE2	2.13	0.49
1:A:3186:ARG:HD3	1:A:3242:MSE:SE	2.63	0.49
1:A:3247:ARG:HH21	1:A:3277:VAL:HG23	1.78	0.49
1:A:3651:LEU:HA	1:A:3654:MSE:HB2	1.95	0.49
1:A:3962:ARG:NH1	1:A:4124:TRP:CH2	2.81	0.49
1:A:903:PRO:HD2	1:A:904:VAL:HG23	1.95	0.49
1:A:927:LYS:HD3	1:A:976:VAL:HG12	1.94	0.49
1:B:1219:PHE:O	1:B:1223:THR:HG23	2.13	0.49
1:B:2467:THR:HA	1:B:2470:ARG:HG3	1.93	0.49
1:B:2842:ARG:O	1:B:2846:THR:HG23	2.11	0.49
1:B:2887:PRO:CB	1:B:2922:ARG:HH11	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3034:PRO:CG	1:B:3037:GLN:HB2	2.39	0.49
1:B:485:GLN:HA	1:B:488:ILE:HG12	1.94	0.49
1:B:567:GLU:HB3	1:B:606:SER:CB	2.43	0.49
1:B:990:GLN:HA	1:B:993:HIS:HD2	1.77	0.49
1:A:174:VAL:O	1:A:178:LEU:HG	2.13	0.48
1:A:181:LEU:HD13	1:A:189:MSE:HE2	1.95	0.48
1:A:2990:GLU:O	1:A:2994:TRP:HD1	1.96	0.48
1:A:3468:LEU:HD13	1:A:3483:MSE:HE1	1.93	0.48
1:A:3547:THR:HG21	1:A:3552:LYS:HB2	1.94	0.48
1:A:3648:GLY:O	1:A:3651:LEU:HB2	2.13	0.48
1:A:760:LEU:HD23	1:A:803:SER:HB3	1.95	0.48
1:A:901:MSE:HE1	1:A:2539:LEU:CD2	2.43	0.48
1:A:925:GLN:OE1	1:A:925:GLN:N	2.39	0.48
1:B:1059:LEU:O	1:B:1063:LEU:HG	2.13	0.48
1:B:13:LEU:O	1:B:16:GLN:HG2	2.13	0.48
1:B:1976:LEU:HG	1:B:1978:PHE:H	1.77	0.48
1:B:1959:LEU:CD1	1:B:1998:MSE:HE3	2.32	0.48
1:B:20:SER:HB2	1:B:65:LEU:HD22	1.95	0.48
1:B:2602:UNK:CB	1:B:2793:PRO:HG3	2.43	0.48
1:B:3061:LEU:HD21	1:B:3089:LEU:HD13	1.95	0.48
1:B:3155:VAL:N	1:B:3156:PRO:HD2	2.28	0.48
1:B:3972:LEU:O	1:B:3974:MSE:HG2	2.13	0.48
1:B:4085:LYS:HA	1:B:4088:ASN:CB	2.43	0.48
1:B:613:HIS:O	1:B:617:PRO:HG2	2.13	0.48
1:A:1122:GLY:O	1:A:1123:THR:OG1	2.29	0.48
1:A:1170:LYS:HD3	1:A:1267:TYR:CG	2.48	0.48
1:A:1722:PHE:H	1:A:1723:PRO:CD	2.26	0.48
1:A:398:THR:HG22	1:A:1865:THR:HG21	1.94	0.48
1:A:1869:LYS:O	1:A:1873:TYR:HD1	1.96	0.48
1:A:2110:PRO:HB2	1:A:2111:PRO:HD3	1.95	0.48
1:A:2171:LEU:HG	1:A:2177:ASN:HD21	1.78	0.48
1:A:2193:ILE:HD11	1:A:2245:TRP:CZ2	2.48	0.48
1:A:14:ARG:HD2	1:A:2358:ASP:OD2	2.13	0.48
1:A:3247:ARG:NH2	1:A:3277:VAL:HG23	2.27	0.48
1:A:3684:SER:HB3	1:A:3726:VAL:CG1	2.42	0.48
1:A:3950:THR:OG1	1:A:3957:GLU:O	2.22	0.48
1:A:3963:LEU:HG	1:A:3967:PHE:CE1	2.47	0.48
1:A:3974:MSE:HB3	1:A:3976:GLU:N	2.23	0.48
1:A:4103:GLN:H	1:A:4103:GLN:CD	2.17	0.48
1:A:531:PHE:CE2	1:A:619:ASP:HB2	2.47	0.48
1:B:1076:LEU:C	1:B:1078:ALA:H	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1238:GLN:NE2	1:B:1298:LEU:HG	2.28	0.48
1:B:1365:ASN:HA	1:B:1368:LEU:HD21	1.94	0.48
1:B:1708:GLU:HB2	1:B:1709:GLU:CD	2.33	0.48
1:B:1996:VAL:CG1	1:B:2048:GLY:HA2	2.37	0.48
1:B:2322:VAL:O	1:B:2326:ILE:HG12	2.13	0.48
1:B:3228:SER:O	1:B:3231:ILE:HB	2.13	0.48
1:B:280:SER:HB3	1:B:322:GLN:HB2	1.95	0.48
1:B:3284:SER:HA	1:B:3287:ARG:NE	2.09	0.48
1:B:3788:LEU:HD13	1:B:3907:SER:HA	1.96	0.48
1:B:3901:ARG:NH1	1:B:3901:ARG:HG2	2.27	0.48
1:B:4066:LEU:HG	1:B:4075:ARG:HA	1.95	0.48
1:B:575:ILE:HG12	1:B:579:LEU:HB2	1.95	0.48
1:B:669:LEU:HD13	1:B:672:ILE:HD12	1.95	0.48
1:A:2213:ASN:HB2	1:A:2250:SER:HB2	1.95	0.48
1:A:940:PHE:HZ	1:A:2791:ILE:HG21	1.73	0.48
1:A:583:LEU:HD23	1:A:592:GLU:OE2	2.13	0.48
1:A:848:LEU:HA	1:A:851:ILE:CD1	2.44	0.48
1:B:1299:GLU:HA	1:B:1302:ALA:CB	2.44	0.48
1:B:1330:TYR:O	1:B:1333:SER:OG	2.27	0.48
1:B:1889:VAL:HG13	1:B:1900:PHE:CD2	2.48	0.48
1:B:2031:LEU:HB2	1:B:2033:ASP:CB	2.40	0.48
1:B:2059:PRO:O	1:B:2062:ALA:HB3	2.13	0.48
1:B:2291:GLN:NE2	1:B:2294:ILE:HG13	2.28	0.48
1:B:2299:TYR:O	1:B:2302:ALA:N	2.46	0.48
1:B:2387:PRO:O	1:B:2390:HIS:HB3	2.12	0.48
1:B:249:PHE:O	1:B:253:LEU:HG	2.13	0.48
1:B:2459:VAL:HG11	1:B:2505:VAL:HG22	1.95	0.48
1:B:2549:LYS:HD2	1:B:2554:PHE:HB3	1.95	0.48
1:B:2851:PHE:O	1:B:2855:VAL:HG23	2.13	0.48
1:B:293:LEU:O	1:B:296:VAL:HG12	2.12	0.48
1:B:856:VAL:HG21	1:B:3110:PHE:CE1	2.48	0.48
1:B:3398:PRO:HG2	1:B:3399:PRO:HD3	1.94	0.48
1:B:358:GLU:HG3	1:B:359:LEU:N	2.27	0.48
1:B:3989:ARG:HE	1:B:4100:GLU:CB	2.26	0.48
1:B:611:ASN:C	1:B:614:PRO:HD2	2.33	0.48
1:B:758:LEU:O	1:B:762:TYR:HB3	2.13	0.48
1:B:884:VAL:HG22	1:B:888:ARG:HG2	1.95	0.48
1:B:892:LEU:HD12	1:B:892:LEU:O	2.13	0.48
1:B:996:THR:O	1:B:1042:LYS:HG2	2.12	0.48
1:A:1001:PHE:CD1	1:A:1002:GLU:N	2.82	0.48
1:A:1075:ARG:O	1:A:1078:ALA:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1029:CYS:CB	1:A:1085:ILE:HG13	2.43	0.48
1:A:1231:GLN:H	1:A:1232:PRO:HD3	1.78	0.48
1:A:1387:GLY:HA2	1:A:1392:MSE:SE	2.63	0.48
1:A:1889:VAL:HG22	1:A:1900:PHE:CE2	2.49	0.48
1:A:2122:LEU:HA	1:A:2127:LYS:HE2	1.96	0.48
1:A:2161:ALA:HB1	1:A:2211:LEU:HD13	1.95	0.48
1:A:2166:SER:N	1:A:2167:PRO:HD2	2.28	0.48
1:A:2573:PRO:C	1:A:2575:PRO:HD3	2.32	0.48
1:A:2778:GLY:O	1:A:2781:PRO:HD2	2.14	0.48
1:A:3020:ASP:HB3	1:A:3027:LEU:HD12	1.95	0.48
1:A:3612:ARG:O	1:A:3615:ALA:HB3	2.14	0.48
1:A:4117:LEU:HB3	1:A:4126:PRO:HB2	1.96	0.48
1:B:1741:ASP:O	1:B:1745:LYS:HG3	2.14	0.48
1:B:1884:LEU:HB2	1:B:1885:PRO:HD3	1.95	0.48
1:B:2086:ASP:CB	1:B:2090:ARG:HH21	2.24	0.48
1:B:2148:LYS:HD3	1:B:2160:TYR:HE1	1.78	0.48
1:B:2227:LYS:HD2	1:B:2235:LEU:CG	2.35	0.48
1:B:3076:ALA:O	1:B:3080:LEU:HG	2.14	0.48
1:B:3498:TRP:NE1	1:B:3502:MSE:HB2	2.28	0.48
1:B:3764:VAL:O	1:B:3768:PHE:HD1	1.96	0.48
1:B:3972:LEU:O	1:B:3974:MSE:N	2.46	0.48
1:B:706:LEU:HA	1:B:709:LYS:HB2	1.94	0.48
1:B:793:LEU:HA	1:B:796:LEU:CG	2.43	0.48
1:A:1389:VAL:O	1:A:1390:GLN:HB2	2.13	0.48
1:A:19:LEU:HA	1:A:22:ALA:HB3	1.95	0.48
1:A:2196:TRP:CE2	1:A:2199:LEU:HD11	2.47	0.48
1:A:2241:LEU:HA	1:A:2244:CYS:SG	2.53	0.48
1:A:2386:LEU:HD13	1:A:2401:VAL:HA	1.95	0.48
1:A:2437:ASP:HB3	1:A:2472:GLN:HG2	1.95	0.48
1:A:2532:PRO:O	1:A:2565:MSE:HE2	2.14	0.48
1:A:322:GLN:HA	1:A:325:ASN:HB2	1.95	0.48
1:A:3409:VAL:HB	1:A:3413:TYR:CE2	2.48	0.48
1:A:49:ALA:O	1:A:53:LEU:HB2	2.12	0.48
1:A:88:PHE:O	1:A:91:ILE:HG13	2.13	0.48
1:A:979:VAL:O	1:A:982:GLN:HB3	2.12	0.48
1:B:1228:GLY:O	1:B:1282:LEU:HD11	2.14	0.48
1:B:1698:PHE:CD1	1:B:1699:PHE:N	2.82	0.48
1:B:2063:THR:HA	1:B:2066:PHE:HB2	1.95	0.48
1:B:2085:MSE:O	1:B:2088:LEU:HB3	2.13	0.48
1:B:2837:LEU:HD22	1:B:2868:LEU:CG	2.41	0.48
1:B:3045:ILE:HB	1:B:3048:LYS:HZ1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3420:CYS:SG	1:B:3421:ASP:N	2.86	0.48
1:B:3629:ARG:HH22	1:B:3638:LYS:HE3	1.78	0.48
1:B:3771:MSE:O	1:B:3775:LEU:HG	2.14	0.48
1:B:3881:ASP:HA	1:B:3884:LYS:HD2	1.96	0.48
1:B:417:VAL:O	1:B:421:LEU:HG	2.14	0.48
1:B:629:PHE:CD2	1:B:668:LYS:HE2	2.48	0.48
1:B:741:ILE:O	1:B:743:LEU:N	2.46	0.48
1:A:1136:ARG:HG2	1:A:1171:TRP:CH2	2.48	0.48
1:A:1385:ASN:O	1:A:1389:VAL:HG23	2.13	0.48
1:A:1430:GLU:HA	1:A:1433:ALA:HB3	1.95	0.48
1:A:3464:LYS:CD	1:A:3467:ARG:HD2	2.43	0.48
1:A:3617:LEU:HD13	1:A:3644:PHE:CD2	2.49	0.48
1:A:3762:GLN:OE1	1:A:3795:PRO:HG3	2.13	0.48
1:A:4085:LYS:HA	1:A:4088:ASN:CB	2.43	0.48
1:A:65:LEU:HD23	1:A:68:PHE:CE1	2.48	0.48
1:A:934:LEU:C	1:A:934:LEU:HD23	2.33	0.48
1:A:978:GLN:HA	1:A:981:ARG:NE	2.23	0.48
1:B:1390:GLN:O	1:B:1393:ALA:HB3	2.14	0.48
1:B:1414:ILE:O	1:B:1418:HIS:HB2	2.13	0.48
1:B:1571:LEU:HD22	1:B:1600:MSE:HA	1.96	0.48
1:B:1894:SER:C	1:B:1896:ILE:N	2.66	0.48
1:B:1890:HIS:NE2	1:B:1941:HIS:HA	2.29	0.48
1:B:2231:PHE:CE1	1:B:2233:HIS:HB2	2.49	0.48
1:B:2782:ASP:HA	1:B:2786:LYS:HB3	1.96	0.48
1:B:3319:ASN:O	1:B:3323:PHE:HD2	1.95	0.48
1:B:3427:GLU:OE1	1:B:3435:ASP:HB3	2.14	0.48
1:B:3495:PHE:CZ	1:B:3521:ILE:HG13	2.49	0.48
1:B:3538:GLU:HG2	1:B:3759:ARG:NH1	2.29	0.48
1:B:3629:ARG:NH2	1:B:3634:GLN:HA	2.28	0.48
1:B:361:ILE:HA	1:B:364:ARG:HG2	1.94	0.48
1:B:3575:LEU:HD21	1:B:3687:MSE:SE	2.63	0.48
1:B:3981:TYR:O	1:B:3985:VAL:HG23	2.14	0.48
1:B:46:SER:H	1:B:51:LEU:HD13	1.78	0.48
1:B:749:VAL:N	1:B:750:PRO:CD	2.77	0.48
1:B:757:LYS:HA	1:B:760:LEU:CD1	2.44	0.48
1:B:938:VAL:HG21	1:B:962:TYR:OH	2.13	0.48
1:A:1340:ARG:NH1	1:A:1343:GLU:HG2	2.29	0.48
1:A:1465:HIS:HA	1:A:1469:PRO:HD2	1.95	0.48
1:A:2230:VAL:HB	1:A:2234:ASN:HD21	1.79	0.48
1:A:2467:THR:HB	1:A:2518:GLN:NE2	2.16	0.48
1:A:2890:ILE:CG2	1:A:2922:ARG:HH12	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:GLU:HA	1:A:298:LEU:HD12	1.96	0.48
1:A:3454:LEU:HD12	1:A:3490:VAL:HG11	1.95	0.48
1:A:358:GLU:N	1:A:361:ILE:HG23	2.29	0.48
1:A:449:TYR:CZ	1:A:457:CYS:SG	3.05	0.48
1:B:1007:VAL:O	1:B:1011:GLU:CB	2.61	0.48
1:B:1055:ASN:HA	1:B:1059:LEU:HG	1.94	0.48
1:B:1080:LEU:HB2	1:B:1131:ILE:HG22	1.94	0.48
1:B:1165:LEU:HB3	1:B:1169:VAL:HG23	1.96	0.48
1:B:86:LEU:HD13	1:B:134:LEU:HD21	1.95	0.48
1:B:1387:GLY:HA2	1:B:1392:MSE:HB2	1.94	0.48
1:B:1692:ALA:O	1:B:1695:LEU:HB2	2.14	0.48
1:B:1711:ARG:O	1:B:1715:GLU:HG3	2.12	0.48
1:B:1946:ASN:O	1:B:1949:ILE:N	2.35	0.48
1:B:1970:LYS:HB3	1:B:1971:PRO:HD3	1.95	0.48
1:B:1978:PHE:O	1:B:1981:LEU:HB3	2.13	0.48
1:B:2462:VAL:HB	1:B:2473:MSE:SE	2.63	0.48
1:B:901:MSE:HE1	1:B:2535:THR:HG21	1.96	0.48
1:B:3463:LEU:HD21	1:B:4001:THR:HA	1.96	0.48
1:B:3582:GLU:HB2	1:B:3674:SER:OG	2.14	0.48
1:B:3675:LYS:N	1:B:3676:PRO:HD2	2.29	0.48
1:B:3916:TRP:HE3	1:B:3917:ILE:HD12	1.77	0.48
1:B:4103:GLN:H	1:B:4103:GLN:CD	2.16	0.48
1:A:1066:LEU:HA	1:A:1069:HIS:CD2	2.49	0.48
1:A:1086:TYR:HE2	1:A:1090:ARG:NE	2.08	0.48
1:A:1105:VAL:HB	1:A:1153:LEU:HD22	1.95	0.48
1:A:1080:LEU:HD13	1:A:1127:CYS:HB3	1.96	0.48
1:A:1651:LYS:HD2	1:A:1684:LEU:CG	2.44	0.48
1:A:1737:ASN:O	1:A:1739:TYR:N	2.44	0.48
1:A:2224:PHE:CE2	1:A:2259:LYS:HD3	2.48	0.48
1:A:2467:THR:CB	1:A:2518:GLN:HE22	2.17	0.48
1:A:2911:ARG:CG	1:A:2914:ALA:HB3	2.43	0.48
1:A:2890:ILE:HD13	1:A:2922:ARG:HH12	1.78	0.48
1:A:3806:LEU:O	1:A:3809:THR:HG22	2.14	0.48
1:A:3917:ILE:O	1:A:4048:LYS:NZ	2.46	0.48
1:A:440:VAL:HG12	1:A:483:VAL:HG12	1.94	0.48
1:A:634:LEU:HD22	1:A:667:TYR:HD1	1.79	0.48
1:A:722:LYS:HB3	1:A:727:ALA:CA	2.44	0.48
1:A:883:TYR:CE2	1:A:961:LEU:HD12	2.49	0.48
1:B:1306:ILE:CG1	1:B:1334:LYS:HB3	2.42	0.48
1:B:429:GLU:OE2	1:B:1595:ALA:HB2	2.13	0.48
1:B:1916:ILE:HG23	1:B:1920:TYR:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2073:ASP:N	1:B:2074:PRO:CD	2.77	0.48
1:B:2142:ILE:HG12	1:B:2145:PHE:CE2	2.49	0.48
1:B:2164:TRP:HH2	1:B:2190:VAL:HG12	1.79	0.48
1:B:2304:VAL:HG13	1:B:2348:GLN:NE2	2.28	0.48
1:B:2877:SER:C	1:B:2879:GLY:N	2.67	0.48
1:B:2915:ARG:HG3	1:B:2915:ARG:HH11	1.78	0.48
1:B:3145:ILE:HG12	1:B:3196:LYS:HG2	1.95	0.48
1:B:3175:PRO:HG2	1:B:3178:ILE:HD11	1.95	0.48
1:B:345:PHE:O	1:B:349:ILE:HG13	2.13	0.48
1:B:3825:LYS:HD2	1:B:3829:LEU:HA	1.95	0.48
1:B:3835:PRO:HA	1:B:3871:PHE:CE1	2.47	0.48
1:B:3913:ILE:O	1:B:3917:ILE:HD13	2.14	0.48
1:B:645:TRP:CZ3	1:B:659:ARG:CB	2.97	0.48
1:B:994:TRP:HA	1:B:994:TRP:CE3	2.48	0.48
1:A:1042:LYS:HE3	1:A:1044:ILE:HG21	1.95	0.48
1:A:1072:ALA:CB	1:A:1114:ALA:HB1	2.44	0.48
1:A:1165:LEU:O	1:A:1168:LEU:N	2.46	0.48
1:A:1175:HIS:O	1:A:1178:ARG:HB3	2.13	0.48
1:A:1434:VAL:HB	1:A:1448:LEU:HD11	1.94	0.48
1:A:2193:ILE:CD1	1:A:2245:TRP:CZ2	2.97	0.48
1:A:2232:ARG:NH2	1:A:2313:LYS:NZ	2.62	0.48
1:A:2256:ILE:HG12	1:A:2276:LEU:HD21	1.96	0.48
1:A:2820:MSE:HE3	1:A:2829:LYS:HB3	1.96	0.48
1:A:280:SER:O	1:A:322:GLN:HG2	2.14	0.48
1:A:3638:LYS:C	1:A:3641:ASP:H	2.16	0.48
1:A:542:ASP:HA	1:A:545:LEU:CD1	2.44	0.48
1:A:611:ASN:O	1:A:614:PRO:HD2	2.13	0.48
1:A:509:ARG:CB	1:A:729:CYS:SG	3.02	0.48
1:A:889:GLU:OE2	1:A:950:GLU:HG2	2.13	0.48
1:B:1109:GLU:O	1:B:1113:LEU:HB3	2.14	0.48
1:B:1303:MSE:O	1:B:1307:ILE:HG13	2.13	0.48
1:B:1476:HIS:CE1	1:B:1507:CYS:HA	2.49	0.48
1:B:1574:ASN:CB	1:B:1582:LEU:HD21	2.42	0.48
1:B:1923:PHE:HE2	1:B:1927:MSE:HE1	1.79	0.48
1:B:19:LEU:HA	1:B:22:ALA:HB3	1.96	0.48
1:B:2146:LEU:HD22	1:B:2149:LEU:HD11	1.95	0.48
1:B:231:LEU:HD23	1:B:234:PHE:HB3	1.94	0.48
1:B:3460:GLU:HA	1:B:3463:LEU:HD12	1.96	0.48
1:B:39:GLY:O	1:B:43:VAL:HG23	2.13	0.48
1:B:446:PHE:HD2	1:B:533:HIS:CB	2.25	0.48
1:B:641:PHE:CZ	1:B:645:TRP:NE1	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:929:ALA:O	1:B:933:LEU:CB	2.62	0.48
1:A:1373:VAL:C	1:A:1375:THR:H	2.16	0.48
1:A:1723:PRO:O	1:A:1725:GLN:N	2.47	0.48
1:A:1984:LEU:HD12	1:A:1985:LYS:N	2.29	0.48
1:A:2004:TYR:CE1	1:A:2054:TYR:O	2.67	0.48
1:A:2328:ARG:O	1:A:2332:GLU:HG3	2.13	0.48
1:A:2854:PHE:HZ	1:A:2881:LEU:HB2	1.77	0.48
1:A:290:TYR:CD1	1:A:293:LEU:HD13	2.48	0.48
1:A:2979:GLN:O	1:A:2982:VAL:HG22	2.14	0.48
1:A:3008:TRP:CG	1:A:3257:LYS:NZ	2.81	0.48
1:A:3326:GLN:CB	1:A:3393:GLU:HG2	2.37	0.48
1:A:3806:LEU:HG	1:A:3807:GLU:O	2.13	0.48
1:A:3900:LEU:HD11	1:A:3934:THR:O	2.13	0.48
1:A:3980:MSE:HA	1:A:3983:ILE:HG13	1.94	0.48
1:B:1025:LEU:HA	1:B:1025:LEU:HD12	1.60	0.48
1:B:1087:ARG:CD	1:B:1134:LEU:HD22	2.44	0.48
1:B:1253:THR:HA	1:B:1257:LEU:HD12	1.95	0.48
1:B:2222:HIS:O	1:B:2224:PHE:N	2.47	0.48
1:B:2912:GLY:HA2	1:B:2915:ARG:NH2	2.28	0.48
1:B:2913:LYS:HG3	1:B:2914:ALA:H	1.76	0.48
1:B:3571:PHE:O	1:B:3575:LEU:HB3	2.13	0.48
1:B:3758:LEU:HD22	1:B:3761:ASP:OD2	2.13	0.48
1:B:3862:ALA:O	1:B:3865:THR:OG1	2.27	0.48
1:B:3816:LEU:HD11	1:B:3883:LEU:HD22	1.96	0.48
1:A:157:TYR:HA	1:A:160:LEU:HG	1.96	0.47
1:A:1762:MSE:SE	1:A:1867:ILE:HG21	2.64	0.47
1:A:1918:LEU:HD11	1:A:1957:ASN:ND2	2.29	0.47
1:A:1977:ILE:C	1:A:1979:GLU:H	2.13	0.47
1:A:2074:PRO:CB	1:A:2136:PRO:HB3	2.43	0.47
1:A:2358:ASP:N	1:A:2358:ASP:OD1	2.46	0.47
1:A:2390:HIS:ND1	1:A:2397:CYS:SG	2.64	0.47
1:A:2538:ARG:HG3	1:A:2539:LEU:N	2.28	0.47
1:A:3128:LYS:C	1:A:3130:GLN:H	2.15	0.47
1:A:3425:ARG:NH1	1:A:3999:THR:HG22	2.29	0.47
1:A:3725:ARG:HH12	1:A:3737:ARG:NH2	2.11	0.47
1:A:3870:SER:OG	1:A:3871:PHE:N	2.46	0.47
1:A:65:LEU:O	1:A:69:VAL:HB	2.14	0.47
1:B:1018:VAL:HB	1:B:1074:LYS:CA	2.44	0.47
1:B:1036:PHE:CZ	1:B:1082:PHE:CE2	3.02	0.47
1:B:1268:ASN:HA	1:B:1271:ILE:HD12	1.95	0.47
1:B:1299:GLU:C	1:B:1302:ALA:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1946:ASN:HA	1:B:1949:ILE:HG22	1.96	0.47
1:B:2193:ILE:HG13	1:B:2196:TRP:CZ2	2.49	0.47
1:B:2382:VAL:CG2	1:B:2404:ARG:HG3	2.40	0.47
1:B:2538:ARG:HG3	1:B:2539:LEU:N	2.28	0.47
1:B:2782:ASP:HA	1:B:2786:LYS:CB	2.44	0.47
1:B:3003:ASN:ND2	1:B:3010:SER:HB2	2.28	0.47
1:B:3110:PHE:HB2	1:B:3114:TYR:HE1	1.78	0.47
1:B:3136:THR:O	1:B:3140:GLU:HB2	2.14	0.47
1:B:3268:THR:H	1:B:3271:ASP:HB3	1.79	0.47
1:B:3525:TYR:HA	1:B:3529:ILE:HG21	1.96	0.47
1:B:3531:TYR:HB3	1:B:3532:PRO:HD3	1.95	0.47
1:B:3789:ARG:CZ	1:B:3806:LEU:HD22	2.44	0.47
1:B:3896:ALA:O	1:B:3899:ALA:HB3	2.14	0.47
1:B:4062:ASP:HA	1:B:4065:LEU:CD2	2.44	0.47
1:B:645:TRP:CZ3	1:B:659:ARG:HB3	2.49	0.47
1:B:76:ILE:HG13	1:B:77:GLU:H	1.79	0.47
1:B:989:MSE:HB2	1:B:990:GLN:NE2	2.29	0.47
1:B:942:LEU:HD11	1:B:991:LEU:CD1	2.44	0.47
1:A:1716:GLN:O	1:A:1719:VAL:N	2.40	0.47
1:A:1733:THR:N	1:A:1734:PRO:CD	2.77	0.47
1:A:2291:GLN:NE2	1:A:2294:ILE:HG21	2.29	0.47
1:A:290:TYR:O	1:A:294:PHE:HD1	1.97	0.47
1:A:335:LYS:HA	1:A:338:LEU:HD12	1.94	0.47
1:A:3493:TRP:CZ3	1:A:3496:ILE:HG13	2.49	0.47
1:A:1073:PHE:CZ	1:A:3745:GLU:HA	2.49	0.47
1:A:3954:PRO:HG3	1:A:4030:GLU:HB2	1.95	0.47
1:A:419:SER:O	1:A:422:LEU:HB2	2.15	0.47
1:A:31:GLY:HA3	1:A:81:CYS:SG	2.54	0.47
1:A:935:HIS:NE2	1:A:987:LEU:HG	2.29	0.47
1:B:1438:GLY:O	1:B:1441:ALA:HB2	2.14	0.47
1:B:1869:LYS:O	1:B:1873:TYR:HD1	1.96	0.47
1:B:2420:PHE:HZ	1:B:2436:LEU:HB3	1.76	0.47
1:B:2482:ASP:HA	1:B:2485:ARG:HB3	1.95	0.47
1:B:2911:ARG:O	1:B:2915:ARG:NE	2.47	0.47
1:B:3522:THR:HA	1:B:3525:TYR:HB3	1.96	0.47
1:B:3842:TRP:HH2	1:B:3846:MSE:HE2	1.73	0.47
1:B:58:VAL:O	1:B:62:ASP:HB2	2.14	0.47
1:B:650:SER:HA	1:B:652:GLU:OE2	2.13	0.47
1:B:659:ARG:HH12	1:B:662:LEU:CD2	2.28	0.47
1:B:922:SER:O	1:B:926:THR:OG1	2.28	0.47
1:A:292:SER:O	1:A:296:VAL:HB	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2960:GLU:HA	1:A:3251:ASN:O	2.14	0.47
1:A:3301:LEU:HB2	1:A:3328:ILE:CG2	2.44	0.47
1:A:3493:TRP:CE3	1:A:3713:PRO:HB3	2.49	0.47
1:A:3606:ILE:HD13	1:A:3609:MSE:HE3	1.96	0.47
1:B:1111:LEU:HD22	1:B:1131:ILE:HD13	1.96	0.47
1:B:1397:ASP:O	1:B:1400:VAL:HB	2.13	0.47
1:B:1501:PRO:O	1:B:1505:LEU:HB2	2.14	0.47
1:B:187:SER:O	1:B:190:ILE:HG22	2.13	0.47
1:B:2440:TYR:O	1:B:2440:TYR:CG	2.67	0.47
1:B:3334:TYR:CE1	1:B:3426:LYS:HD3	2.49	0.47
1:B:3797:THR:CG2	1:B:3800:LEU:HG	2.43	0.47
1:B:634:LEU:O	1:B:669:LEU:HD12	2.14	0.47
1:B:714:VAL:HG11	1:B:734:LEU:HD21	1.96	0.47
1:A:14:ARG:HH12	1:A:2392:VAL:HG21	1.79	0.47
1:A:2003:LYS:HG2	1:A:2006:GLU:OE1	2.14	0.47
1:A:2776:ARG:CZ	1:A:2776:ARG:HA	2.44	0.47
1:A:2841:ASN:OD1	1:A:2844:LEU:HD12	2.15	0.47
1:A:2917:PRO:HB2	1:A:2918:PRO:HD3	1.95	0.47
1:A:2940:ARG:HD3	1:A:3975:LYS:CD	2.44	0.47
1:A:3487:ILE:HG21	1:A:3524:ASN:HD21	1.78	0.47
1:A:368:LEU:CA	1:A:372:PRO:HG2	2.44	0.47
1:A:3878:VAL:HB	1:A:3879:PRO:HD3	1.96	0.47
1:A:403:GLY:O	1:A:405:ASP:N	2.44	0.47
1:A:455:LEU:O	1:A:459:ARG:HG3	2.15	0.47
1:A:69:VAL:O	1:A:73:LEU:HG	2.13	0.47
1:A:718:MSE:O	1:A:722:LYS:HB2	2.15	0.47
1:A:892:LEU:HD21	1:A:958:MSE:HG3	1.96	0.47
1:B:1080:LEU:HB2	1:B:1131:ILE:CG2	2.45	0.47
1:B:1472:SER:OG	1:B:1473:THR:N	2.48	0.47
1:B:2155:GLU:HB3	1:B:2156:VAL:H	1.40	0.47
1:B:2186:VAL:O	1:B:2190:VAL:HG13	2.13	0.47
1:B:2193:ILE:HG12	1:B:2193:ILE:O	2.14	0.47
1:B:2200:ALA:CA	1:B:2203:THR:HG22	2.41	0.47
1:B:2212:ALA:O	1:B:2215:LEU:HB3	2.15	0.47
1:B:2257:PHE:CE1	1:B:2299:TYR:HB3	2.49	0.47
1:B:3498:TRP:HD1	1:B:3502:MSE:HB2	1.77	0.47
1:B:3514:VAL:HG21	1:B:3551:ASN:HB3	1.95	0.47
1:B:3839:TYR:HB2	1:B:3871:PHE:CE1	2.49	0.47
1:B:411:PRO:O	1:B:415:GLN:CB	2.62	0.47
1:B:612:LEU:HD21	1:B:1800:SER:HB3	1.96	0.47
1:B:887:ASP:O	1:B:3889:ARG:NE	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:927:LYS:O	1:B:931:CYS:SG	2.73	0.47
1:A:1216:GLY:HA3	1:A:1271:ILE:CG2	2.45	0.47
1:A:1292:LYS:H	1:A:1292:LYS:HG3	1.52	0.47
1:A:1508:LYS:C	1:A:1510:LEU:H	2.18	0.47
1:A:1809:ASP:HA	1:A:1815:THR:HA	1.96	0.47
1:A:2549:LYS:HZ3	1:A:2554:PHE:HA	1.75	0.47
1:A:3008:TRP:CE3	1:A:3050:LYS:HB2	2.50	0.47
1:A:3114:TYR:CE2	1:A:3125:ARG:NH2	2.83	0.47
1:A:3775:LEU:HB3	1:A:3781:CYS:SG	2.53	0.47
1:A:3834:ALA:HB1	1:A:3838:GLU:OE1	2.14	0.47
1:A:749:VAL:N	1:A:750:PRO:HD3	2.30	0.47
1:B:1001:PHE:CD1	1:B:1002:GLU:N	2.81	0.47
1:B:1090:ARG:HH12	1:B:1096:VAL:CG1	2.22	0.47
1:B:205:LYS:HE3	1:B:243:GLN:HB3	1.96	0.47
1:B:2508:GLN:HG2	1:B:2508:GLN:O	2.14	0.47
1:B:2539:LEU:HG	1:B:2816:ILE:HG13	1.95	0.47
1:B:2603:UNK:CB	1:B:2793:PRO:HB2	2.44	0.47
1:B:3128:LYS:O	1:B:3132:VAL:HG13	2.14	0.47
1:B:3160:LEU:HA	1:B:3160:LEU:HD12	1.75	0.47
1:B:3330:LEU:C	1:B:3332:THR:H	2.17	0.47
1:B:3820:MSE:O	1:B:3824:GLU:N	2.41	0.47
1:B:428:PRO:O	1:B:430:VAL:HG23	2.14	0.47
1:B:539:GLN:HG3	1:B:626:LEU:O	2.14	0.47
1:B:756:PHE:O	1:B:759:GLY:C	2.52	0.47
1:B:801:LYS:HB2	1:B:805:LEU:HD12	1.96	0.47
1:B:927:LYS:HE3	1:B:928:VAL:HG13	1.96	0.47
1:A:1213:LYS:O	1:A:1215:GLU:N	2.48	0.47
1:A:82:ARG:NH2	1:A:130:LEU:HD22	2.30	0.47
1:A:1372:LEU:HG	1:A:1373:VAL:N	2.29	0.47
1:A:1396:PRO:O	1:A:1400:VAL:HG23	2.14	0.47
1:A:2164:TRP:CH2	1:A:2190:VAL:HG12	2.49	0.47
1:A:2325:LEU:HG	1:A:2329:TYR:CD2	2.49	0.47
1:A:238:MSE:HG3	1:A:239:GLU:HG2	1.96	0.47
1:A:3524:ASN:O	1:A:3529:ILE:HD13	2.14	0.47
1:A:3719:ILE:HG23	1:A:3720:ALA:H	1.79	0.47
1:A:3846:MSE:O	1:A:3857:LEU:HD22	2.14	0.47
1:A:4077:TYR:CG	1:A:4119:ARG:NH1	2.82	0.47
1:A:410:MSE:HE2	1:A:441:MSE:CE	2.44	0.47
1:A:977:ASP:O	1:A:980:THR:HB	2.14	0.47
1:B:1290:LEU:HD12	1:B:1294:VAL:HG21	1.97	0.47
1:B:1570:GLU:HA	1:B:1573:LYS:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1726:SER:CB	1:B:1866:GLN:HE22	2.27	0.47
1:B:2420:PHE:CZ	1:B:2424:MSE:HE3	2.49	0.47
1:B:2803:ILE:O	1:B:2803:ILE:HG12	2.14	0.47
1:B:2884:LEU:O	1:B:2888:VAL:HG23	2.15	0.47
1:B:2989:ALA:HB1	1:B:2993:PHE:CD2	2.49	0.47
1:B:3128:LYS:C	1:B:3130:GLN:H	2.17	0.47
1:B:324:SER:HB3	1:B:370:ALA:O	2.15	0.47
1:B:3762:GLN:HA	1:B:3793:VAL:CG2	2.36	0.47
1:B:458:CYS:SG	1:B:540:MSE:SE	3.23	0.47
1:B:749:VAL:N	1:B:750:PRO:HD3	2.30	0.47
2:K:215:UNK:O	2:K:219:UNK:N	2.48	0.47
1:A:1013:ILE:O	1:A:1016:GLY:N	2.48	0.47
1:A:1033:ILE:CG1	1:A:1089:PHE:HE2	2.27	0.47
1:A:1715:GLU:HA	1:A:1718:ILE:HB	1.95	0.47
1:A:1816:ARG:HD3	1:A:1819:PHE:CE1	2.49	0.47
1:A:2224:PHE:HB3	1:A:2272:VAL:HG13	1.96	0.47
1:A:2257:PHE:CD1	1:A:2299:TYR:HB3	2.49	0.47
1:A:2313:LYS:HA	1:A:2316:TYR:CD2	2.50	0.47
1:A:2390:HIS:CE1	1:A:2397:CYS:HG	2.33	0.47
1:A:2538:ARG:HD2	1:A:2562:LEU:HD22	1.96	0.47
1:A:282:PHE:CD1	1:A:282:PHE:C	2.88	0.47
1:A:2861:ILE:HD13	1:A:2889:GLY:HA2	1.96	0.47
1:A:2936:TYR:HD1	1:A:2949:THR:HG21	1.80	0.47
1:A:2939:LEU:HD21	1:A:2994:TRP:CD1	2.49	0.47
1:A:3090:TYR:O	1:A:3092:LEU:N	2.48	0.47
1:A:3284:SER:HB2	1:A:3287:ARG:HH21	1.79	0.47
1:A:3757:ASP:OD2	1:A:3759:ARG:HD3	2.14	0.47
1:A:4083:GLY:O	1:A:4088:ASN:ND2	2.44	0.47
1:A:4085:LYS:HA	1:A:4088:ASN:HB2	1.97	0.47
1:A:527:TYR:O	1:A:531:PHE:CE2	2.67	0.47
1:A:729:CYS:HA	1:A:732:PHE:CD2	2.50	0.47
1:B:1492:ALA:HB1	1:B:1493:PRO:CD	2.45	0.47
1:B:2549:LYS:HD2	1:B:2554:PHE:CB	2.44	0.47
1:B:3187:CYS:O	1:B:3190:LEU:N	2.48	0.47
1:B:3503:VAL:HG23	1:B:3536:SER:HA	1.96	0.47
1:B:3834:ALA:H	1:B:3835:PRO:HD3	1.79	0.47
1:B:3887:PHE:CE1	1:B:3900:LEU:HB3	2.47	0.47
1:B:3919:GLY:N	1:B:3946:PHE:H	2.09	0.47
1:A:1116:ALA:O	1:A:1119:LYS:HG2	2.14	0.47
1:A:1162:SER:H	1:A:1165:LEU:HD12	1.80	0.47
1:A:1689:LYS:O	1:A:1693:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1879:VAL:O	1:A:1882:SER:HB3	2.15	0.47
1:A:2023:SER:HB2	1:A:2024:TYR:CD1	2.49	0.47
1:A:2216:LEU:HD13	1:A:2249:LEU:HD21	1.97	0.47
1:A:2462:VAL:HG11	1:A:2473:MSE:CE	2.44	0.47
1:A:3447:VAL:HG11	1:A:3475:TYR:OH	2.15	0.47
1:A:3741:ARG:HG2	1:A:3741:ARG:NH1	2.29	0.47
1:A:3820:MSE:CB	1:A:3882:LEU:HD13	2.44	0.47
1:A:2936:TYR:HD2	1:A:3979:LEU:HD11	1.78	0.47
1:A:557:SER:O	1:A:560:LEU:HG	2.14	0.47
1:A:63:PHE:O	1:A:67:VAL:HG23	2.14	0.47
1:B:1076:LEU:HD11	1:B:1114:ALA:CB	2.45	0.47
1:B:1705:GLY:HA2	1:B:1739:TYR:OH	2.15	0.47
1:B:170:VAL:HG23	1:B:173:LYS:CE	2.44	0.47
1:B:1718:ILE:HA	1:B:1725:GLN:OE1	2.14	0.47
1:B:1737:ASN:O	1:B:1739:TYR:N	2.46	0.47
1:B:1760:GLU:HB2	1:B:1894:SER:HA	1.97	0.47
1:B:1945:TYR:OH	1:B:1959:LEU:HD12	2.15	0.47
1:B:2187:VAL:O	1:B:2190:VAL:HG22	2.14	0.47
1:B:2320:ALA:HA	1:B:2367:VAL:HG23	1.96	0.47
1:B:2809:PHE:HB3	1:B:2859:GLN:OE1	2.14	0.47
1:B:3011:LEU:O	1:B:3014:CYS:HB2	2.14	0.47
1:B:3196:LYS:C	1:B:3199:PRO:HD2	2.35	0.47
1:B:3499:ILE:HG13	1:B:3531:TYR:OH	2.15	0.47
1:B:3792:SER:OG	1:B:3804:GLU:HB2	2.14	0.47
1:B:2933:ILE:HG21	1:B:3976:GLU:HG3	1.96	0.47
1:B:895:ALA:HB2	1:B:904:VAL:HG21	1.96	0.47
1:B:966:PHE:CD1	1:B:969:LEU:HD13	2.50	0.47
1:B:986:PRO:C	1:B:990:GLN:HE21	2.18	0.47
2:K:217:UNK:O	2:K:220:MSE:HG2	2.15	0.47
1:A:1575:LEU:O	1:A:1635:LYS:NZ	2.39	0.47
1:A:1729:PHE:CE2	1:A:1873:TYR:CE1	3.03	0.47
1:A:174:VAL:HG12	1:A:178:LEU:HD11	1.96	0.47
1:A:2134:GLY:H	1:A:2137:ILE:HD11	1.80	0.47
1:A:2404:ARG:NH1	1:A:2412:TYR:CE1	2.82	0.47
1:A:2430:GLU:OE2	1:A:2461:PHE:CD1	2.65	0.47
1:A:3420:CYS:HB2	1:A:3446:VAL:HG11	1.96	0.47
1:A:3467:ARG:CG	1:A:3471:ILE:HD12	2.45	0.47
1:A:3920:ILE:HG13	1:A:3923:ARG:CD	2.45	0.47
1:A:3944:HIS:CD2	1:A:4020:MSE:HE3	2.49	0.47
1:A:3985:VAL:HG22	1:A:4104:VAL:HG21	1.95	0.47
1:A:4069:GLU:OE2	1:A:4070:LYS:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:PHE:O	1:A:72:SER:OG	2.23	0.47
1:A:798:GLY:HA2	1:A:873:VAL:HG11	1.96	0.47
1:B:1118:GLU:O	1:B:1120:SER:N	2.47	0.47
1:B:2385:LEU:HG	1:B:2389:PHE:CE2	2.49	0.47
1:B:3040:TYR:HA	1:B:3043:TYR:CD2	2.50	0.47
1:B:3122:HIS:O	1:B:3125:ARG:N	2.47	0.47
1:B:3251:ASN:HD21	1:B:3254:LEU:HD13	1.80	0.47
1:B:3247:ARG:HD3	1:B:3281:CYS:SG	2.55	0.47
1:B:3459:ASN:ND2	1:B:3710:LYS:HZ3	2.12	0.47
1:B:3659:PHE:CD1	1:B:3662:ILE:HD12	2.50	0.47
1:B:704:PHE:HA	1:B:707:PHE:CD1	2.50	0.47
1:B:858:MSE:O	1:B:861:SER:N	2.48	0.47
1:A:1036:PHE:CZ	1:A:1082:PHE:CE2	3.03	0.47
1:A:1131:ILE:HG12	1:A:1132:ASP:N	2.29	0.47
1:A:1701:SER:OG	1:A:1702:LEU:N	2.48	0.47
1:A:1970:LYS:HZ1	1:A:2018:ASP:N	2.13	0.47
1:A:205:LYS:O	1:A:208:MSE:HG2	2.15	0.47
1:A:257:ARG:H	1:A:258:PRO:HD2	1.78	0.47
1:A:241:ASP:HB2	1:A:282:PHE:HE2	1.80	0.47
1:A:3080:LEU:HD13	1:A:3102:TYR:OH	2.15	0.47
1:A:3386:SER:HA	1:A:3389:VAL:HG12	1.97	0.47
1:A:3393:GLU:OE1	1:A:3416:LEU:HD23	2.15	0.47
1:A:3510:GLN:CD	1:A:3513:ALA:HB2	2.35	0.47
1:A:3583:LEU:HD11	1:A:3733:ARG:CB	2.42	0.47
1:A:384:MSE:O	1:A:385:TYR:HB3	2.15	0.47
1:A:2891:ARG:HH21	1:A:3884:LYS:HD3	1.76	0.47
1:A:667:TYR:O	1:A:669:LEU:N	2.47	0.47
1:A:776:TRP:CZ2	1:A:780:ILE:HD12	2.50	0.47
1:A:928:VAL:HG23	1:A:929:ALA:N	2.29	0.47
1:B:963:LYS:HG3	1:B:1009:LEU:CD1	2.45	0.47
1:B:1036:PHE:HD1	1:B:1059:LEU:HD11	1.79	0.47
1:B:1068:LEU:HD11	1:B:1110:SER:OG	2.15	0.47
1:B:1302:ALA:O	1:B:1306:ILE:HB	2.15	0.47
1:B:2239:LYS:CG	1:B:2279:ILE:HD12	2.45	0.47
1:B:2254:ARG:HB2	1:B:2295:GLN:HB2	1.97	0.47
1:B:2379:MSE:HG2	1:B:2408:MSE:SE	2.65	0.47
1:B:2407:GLY:O	1:B:2409:THR:HG23	2.15	0.47
1:B:2987:THR:O	1:B:2990:GLU:HB2	2.14	0.47
1:B:3160:LEU:HB3	1:B:3164:TRP:CZ3	2.50	0.47
1:B:3243:ILE:HG23	1:B:3258:LEU:HD12	1.96	0.47
1:B:3244:ASP:O	1:B:3247:ARG:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3503:VAL:CG2	1:B:3536:SER:HA	2.45	0.47
1:B:3720:ALA:HB2	1:B:3743:HIS:HB2	1.96	0.47
1:B:3944:HIS:ND1	1:B:3949:ALA:HA	2.29	0.47
1:B:777:SER:HB2	1:B:858:MSE:HE1	1.97	0.47
1:B:943:GLY:O	1:B:945:ALA:N	2.45	0.47
1:B:987:LEU:O	1:B:991:LEU:HD13	2.15	0.47
1:A:1251:GLN:HE21	1:A:1329:ARG:NH1	2.13	0.47
1:A:125:ILE:H	1:A:126:PRO:CD	2.28	0.47
1:A:1292:LYS:O	1:A:1295:ALA:HB3	2.15	0.47
1:A:1335:CYS:SG	1:A:1382:ILE:HG21	2.55	0.47
1:A:474:VAL:HG11	1:A:1564:SER:HB2	1.97	0.47
1:A:1685:ASP:CB	1:A:1727:ARG:NH2	2.74	0.47
1:A:1745:LYS:C	1:A:1747:LEU:N	2.68	0.47
1:A:1598:ASN:ND2	1:A:1811:ARG:HB3	2.30	0.47
1:A:2260:PHE:HA	1:A:2273:GLY:HA3	1.96	0.47
1:A:234:PHE:O	1:A:235:THR:OG1	2.22	0.47
1:A:2637:UNK:O	1:A:2641:UNK:CB	2.63	0.47
1:A:2856:SER:O	1:A:2859:GLN:HB3	2.15	0.47
1:A:3011:LEU:HD11	1:A:3043:TYR:O	2.15	0.47
1:A:3053:LEU:HD11	1:A:3187:CYS:HB3	1.96	0.47
1:A:3147:LYS:O	1:A:3151:LEU:N	2.48	0.47
1:A:3533:PHE:CD1	1:A:3562:LEU:HB3	2.50	0.47
1:A:544:ILE:O	1:A:548:GLU:HB2	2.14	0.47
1:A:927:LYS:O	1:A:931:CYS:SG	2.73	0.47
1:B:1350:ASN:HD22	1:B:1404:LYS:HE3	1.79	0.47
1:B:1349:LEU:CA	1:B:1353:PRO:HD2	2.44	0.47
1:B:133:LYS:O	1:B:137:THR:HG23	2.15	0.47
1:B:1583:MSE:SE	1:B:1643:MSE:SE	3.32	0.47
1:B:1952:ILE:HG12	1:B:1953:CYS:H	1.79	0.47
1:B:2097:LEU:CD2	1:B:2100:LEU:HD22	2.45	0.47
1:B:257:ARG:N	1:B:258:PRO:CD	2.77	0.47
1:B:260:ILE:O	1:B:264:ARG:HG2	2.15	0.47
1:B:2970:LYS:O	1:B:2974:GLU:HG2	2.14	0.47
1:B:3059:GLN:CD	1:B:3059:GLN:H	2.17	0.47
1:B:3284:SER:CA	1:B:3287:ARG:HE	2.12	0.47
1:B:3298:LEU:HD11	1:B:3351:ILE:CD1	2.45	0.47
1:B:3585:PHE:HE1	1:B:3617:LEU:HD11	1.79	0.47
1:B:3904:PHE:CE1	1:B:3967:PHE:HE1	2.32	0.47
1:B:3965:ARG:HE	1:B:3969:ASN:ND2	2.14	0.47
1:B:3981:TYR:HA	1:B:4108:MSE:HE1	1.96	0.47
1:B:912:PRO:HB2	1:B:913:ARG:CZ	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1059:LEU:O	1:A:1062:ARG:N	2.48	0.46
1:A:1601:LEU:O	1:A:1605:PHE:HB2	2.14	0.46
1:A:1583:MSE:HE2	1:A:1639:LEU:HD13	1.97	0.46
1:A:1687:HIS:HB3	1:A:1691:GLN:NE2	2.30	0.46
1:A:2323:LEU:HD13	1:A:2371:PHE:CZ	2.50	0.46
1:A:2473:MSE:O	1:A:2476:ILE:HG12	2.14	0.46
1:A:2514:ASN:H	1:A:2515:PRO:CD	2.29	0.46
1:A:242:PRO:HD3	1:A:282:PHE:CE2	2.50	0.46
1:A:358:GLU:OE1	1:A:1858:LEU:HD13	2.15	0.46
1:A:3620:PRO:HB2	1:A:3633:ILE:HG23	1.95	0.46
1:A:3699:LEU:O	1:A:3718:ARG:NH1	2.47	0.46
1:A:3887:PHE:HZ	1:A:3904:PHE:CD2	2.33	0.46
1:A:3928:PHE:C	1:A:3928:PHE:CD1	2.88	0.46
1:A:443:ILE:HD11	1:A:465:PHE:HE2	1.80	0.46
1:A:797:ASP:HA	1:A:800:LEU:HB2	1.96	0.46
1:A:934:LEU:HD21	1:A:962:TYR:CZ	2.49	0.46
1:B:1563:PHE:CD1	1:B:1567:ILE:HG13	2.50	0.46
1:B:2404:ARG:NH1	1:B:2412:TYR:CE2	2.83	0.46
1:B:2439:ILE:HG21	1:B:2439:ILE:HD13	1.64	0.46
1:B:2554:PHE:O	1:B:2557:LEU:N	2.48	0.46
1:B:277:LEU:HD22	1:B:278:HIS:CD2	2.51	0.46
1:B:361:ILE:HB	1:B:364:ARG:NH2	2.30	0.46
1:B:3457:ASN:O	1:B:3710:LYS:NZ	2.47	0.46
1:B:3722:PHE:HD1	1:B:3740:ILE:HA	1.80	0.46
1:B:4081:ALA:HA	1:B:4113:ASP:OD2	2.13	0.46
1:B:670:LEU:HG	1:B:740:ILE:HG23	1.97	0.46
1:B:732:PHE:CE1	1:B:768:VAL:HG12	2.50	0.46
1:B:965:THR:HA	1:B:968:VAL:HG12	1.95	0.46
1:A:1010:LEU:O	1:A:1013:ILE:N	2.39	0.46
1:A:1373:VAL:O	1:A:1375:THR:N	2.41	0.46
1:A:186:PRO:O	1:A:189:MSE:HB3	2.16	0.46
1:A:1976:LEU:HD11	1:A:2031:LEU:CB	2.44	0.46
1:A:2186:VAL:O	1:A:2189:ILE:HG13	2.15	0.46
1:A:2199:LEU:HA	1:A:2202:PRO:HD2	1.97	0.46
1:A:2418:LYS:O	1:A:2421:VAL:HG12	2.15	0.46
1:A:2554:PHE:O	1:A:2557:LEU:HB2	2.16	0.46
1:A:2900:LEU:HD23	1:A:2910:VAL:HA	1.97	0.46
1:A:3008:TRP:CA	1:A:3050:LYS:HG2	2.44	0.46
1:A:348:ILE:O	1:A:364:ARG:HD3	2.16	0.46
1:A:3674:SER:C	1:A:3677:PRO:HD2	2.35	0.46
1:A:3931:ALA:HB3	1:A:3936:GLY:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4069:GLU:HA	1:A:4070:LYS:HA	1.64	0.46
1:B:1231:GLN:H	1:B:1232:PRO:CD	2.28	0.46
1:B:1259:LEU:HD11	1:B:1337:VAL:HA	1.97	0.46
1:B:135:LEU:O	1:B:139:ARG:HG3	2.15	0.46
1:B:401:ASP:HB2	1:B:1763:THR:HB	1.98	0.46
1:B:1874:TYR:OH	1:B:1884:LEU:HD12	2.15	0.46
1:B:2289:ASP:O	1:B:2290:PRO:C	2.53	0.46
1:B:381:VAL:O	1:B:384:MSE:HG2	2.14	0.46
1:B:763:THR:HG21	1:B:769:GLY:HA3	1.97	0.46
1:A:135:LEU:HD22	1:A:173:LYS:HB2	1.97	0.46
1:A:1376:LEU:HG	1:A:1377:CYS:N	2.30	0.46
1:A:1495:ASP:O	1:A:1498:GLN:HB2	2.15	0.46
1:A:1696:LEU:HD23	1:A:1700:THR:HG21	1.97	0.46
1:A:1985:LYS:HD2	1:A:2037:SER:HB3	1.98	0.46
1:A:2233:HIS:O	1:A:2237:ILE:HG13	2.15	0.46
1:A:2823:PHE:CG	1:A:2824:LYS:N	2.83	0.46
1:A:2949:THR:O	1:A:2952:ILE:N	2.46	0.46
1:A:3141:PHE:CE1	1:A:3189:PHE:HA	2.51	0.46
1:A:3762:GLN:HA	1:A:3793:VAL:CG2	2.41	0.46
1:A:399:GLN:OE1	1:A:405:ASP:HB2	2.16	0.46
1:A:385:TYR:HE1	1:A:421:LEU:HD23	1.79	0.46
1:A:436:GLU:OE2	1:A:475:LEU:CD1	2.63	0.46
1:A:777:SER:O	1:A:781:ASP:N	2.48	0.46
1:B:1455:CYS:O	1:B:1458:LEU:N	2.49	0.46
1:B:1602:ASP:HB2	1:B:1810:PRO:HB3	1.98	0.46
1:B:2009:LYS:HG3	1:B:2012:ARG:NH1	2.30	0.46
1:B:2067:ARG:O	1:B:2068:ARG:HB2	2.14	0.46
1:B:222:GLY:O	1:B:225:LYS:N	2.49	0.46
1:B:3616:ALA:O	1:B:3617:LEU:HD23	2.16	0.46
1:B:4002:MSE:SE	1:B:4048:LYS:CE	3.12	0.46
1:B:3855:TYR:HB3	1:B:4074:PHE:HZ	1.80	0.46
1:B:431:TYR:N	1:B:431:TYR:CD1	2.79	0.46
1:B:487:LEU:HD21	1:B:530:LEU:HB2	1.97	0.46
1:B:543:SER:O	1:B:545:LEU:N	2.37	0.46
1:B:789:TYR:HB2	1:B:865:GLN:HE21	1.81	0.46
1:A:1395:LEU:N	1:A:1396:PRO:HD2	2.30	0.46
1:A:1476:HIS:CE1	1:A:1507:CYS:HA	2.50	0.46
1:A:1589:ASN:O	1:A:1590:THR:HG22	2.16	0.46
1:A:1602:ASP:HB2	1:A:1810:PRO:HB3	1.96	0.46
1:A:1604:SER:CB	1:A:1632:TRP:HE3	2.28	0.46
1:A:1874:TYR:HD2	1:A:1885:PRO:HG3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2177:ASN:HB3	1:A:2182:ILE:N	2.30	0.46
1:A:2310:VAL:HG23	1:A:2315:VAL:HG21	1.98	0.46
1:A:2834:GLN:O	1:A:2837:LEU:HG	2.15	0.46
1:A:350:ARG:NH1	1:A:387:GLU:OE1	2.49	0.46
1:A:730:LEU:HA	1:A:730:LEU:HD23	1.82	0.46
1:A:764:PRO:HB3	1:A:770:LEU:HD11	1.97	0.46
1:A:849:GLU:H	1:A:849:GLU:CD	2.18	0.46
1:B:158:GLY:O	1:B:162:LEU:HD13	2.15	0.46
1:B:1809:ASP:O	1:B:1815:THR:HG22	2.14	0.46
1:B:1917:LYS:HE2	1:B:1953:CYS:O	2.14	0.46
1:B:2312:TYR:CZ	1:B:2313:LYS:HG2	2.50	0.46
1:B:241:ASP:HB3	1:B:282:PHE:HE2	1.78	0.46
1:B:3160:LEU:HD23	1:B:3164:TRP:CH2	2.51	0.46
1:B:3283:LEU:O	1:B:3283:LEU:HD22	2.16	0.46
1:B:3740:ILE:HD12	1:B:3750:PHE:CE1	2.51	0.46
1:B:3816:LEU:O	1:B:3820:MSE:CB	2.64	0.46
1:B:3463:LEU:HD13	1:B:4000:ASN:CB	2.45	0.46
1:B:70:ARG:HH12	1:B:117:LYS:HD2	1.80	0.46
1:B:852:ARG:HH12	1:B:3111:MSE:HG2	1.79	0.46
1:B:892:LEU:HD11	1:B:958:MSE:HG3	1.98	0.46
1:B:898:PHE:CD2	1:B:2566:THR:HG21	2.50	0.46
1:A:2240:THR:HG21	2:K:112:UNK:HA	1.98	0.46
1:A:964:ARG:CB	1:A:1009:LEU:HD22	2.35	0.46
1:A:1012:ALA:O	1:A:1015:ASP:HB3	2.15	0.46
1:A:993:HIS:HB2	1:A:1038:LYS:CG	2.45	0.46
1:A:1072:ALA:HB1	1:A:1076:LEU:CD1	2.46	0.46
1:A:1494:GLY:O	1:A:1498:GLN:HG3	2.15	0.46
1:A:1593:VAL:O	1:A:1597:LEU:CB	2.62	0.46
1:A:429:GLU:HG2	1:A:1594:SER:HB2	1.97	0.46
1:A:1636:ASP:HA	1:A:1639:LEU:HD11	1.98	0.46
1:A:1651:LYS:HD2	1:A:1684:LEU:HG	1.98	0.46
1:A:1897:ASN:HB3	1:A:1901:HIS:CE1	2.50	0.46
1:A:1933:LEU:H	1:A:1938:ARG:NH2	2.13	0.46
1:A:1934:LEU:HD11	1:A:1937:ARG:H	1.80	0.46
1:A:2923:TRP:CD1	1:A:2926:LEU:HD23	2.50	0.46
1:A:3121:LEU:O	1:A:3124:SER:HB2	2.14	0.46
1:A:3297:VAL:HG11	1:A:3332:THR:HG23	1.97	0.46
1:B:1423:ILE:HG13	1:B:1424:THR:H	1.81	0.46
1:B:1447:ARG:O	1:B:1451:VAL:HG23	2.15	0.46
1:B:1592:MSE:O	1:B:1596:VAL:HG12	2.16	0.46
1:B:1865:THR:O	1:B:1869:LYS:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:LEU:HB3	1:B:197:PHE:CE1	2.49	0.46
1:B:2383:PHE:CE1	1:B:2412:TYR:HD1	2.34	0.46
1:B:2413:PHE:HD2	1:B:2445:LYS:HG3	1.76	0.46
1:B:3334:TYR:HE1	1:B:3426:LYS:HD3	1.81	0.46
1:B:3813:LYS:HE3	1:B:3926:ASN:HB2	1.98	0.46
1:B:368:LEU:HD21	1:B:384:MSE:SE	2.66	0.46
1:B:4057:ALA:C	1:B:4059:ILE:N	2.69	0.46
1:B:4085:LYS:HA	1:B:4088:ASN:HB3	1.98	0.46
1:B:648:SER:O	1:B:651:TYR:HB2	2.15	0.46
1:A:1917:LYS:HD2	1:A:1953:CYS:HB3	1.98	0.46
1:A:2177:ASN:HB2	1:A:2182:ILE:HG23	1.97	0.46
1:A:2232:ARG:O	1:A:2234:ASN:N	2.49	0.46
1:A:2260:PHE:CZ	1:A:2306:ASN:HB2	2.51	0.46
1:A:2371:PHE:CG	1:A:2372:PRO:HD3	2.51	0.46
1:A:2555:LEU:HD12	1:A:2556:SER:H	1.79	0.46
1:A:2776:ARG:O	1:A:2780:LEU:HD23	2.15	0.46
1:A:2575:PRO:HB3	1:A:2789:SER:N	2.31	0.46
1:A:3463:LEU:HD13	1:A:4000:ASN:HB2	1.97	0.46
1:A:3549:HIS:NE2	1:A:3553:GLU:HG3	2.30	0.46
1:A:3578:LEU:HB3	1:A:3579:SER:HA	1.97	0.46
1:A:3722:PHE:CE1	1:A:3740:ILE:HA	2.51	0.46
1:A:3817:LEU:HD23	1:A:3820:MSE:CE	2.45	0.46
1:A:3966:GLN:HG2	1:A:4128:MSE:O	2.15	0.46
1:A:3944:HIS:HA	1:A:4016:PHE:HZ	1.81	0.46
1:A:434:VAL:HG23	1:A:437:HIS:CE1	2.51	0.46
1:A:471:LYS:HG3	1:A:1553:PHE:HZ	1.81	0.46
1:A:512:GLY:HA2	1:A:602:MSE:CE	2.45	0.46
1:A:649:PHE:C	1:A:651:TYR:H	2.18	0.46
1:A:749:VAL:N	1:A:750:PRO:CD	2.79	0.46
1:A:89:LEU:HA	1:A:92:PHE:CD2	2.50	0.46
1:B:1565:GLU:HG2	1:B:1566:THR:HG23	1.97	0.46
1:B:2142:ILE:O	1:B:2145:PHE:HB2	2.16	0.46
1:B:2159:PRO:HA	1:B:2162:LYS:HB2	1.98	0.46
1:B:2539:LEU:HB3	1:B:2816:ILE:CD1	2.46	0.46
1:B:3092:LEU:O	1:B:3192:LYS:NZ	2.42	0.46
1:B:3167:ARG:CD	1:B:3186:ARG:HG2	2.45	0.46
1:B:3578:LEU:HD13	1:B:3683:CYS:SG	2.56	0.46
1:B:3701:ILE:HG13	1:B:3701:ILE:O	2.15	0.46
1:B:12:LEU:HD12	1:B:58:VAL:HG21	1.97	0.46
1:B:617:PRO:CB	1:B:659:ARG:HD2	2.45	0.46
1:A:1138:ILE:HD13	1:A:1150:LYS:CE	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1382:ILE:HB	1:A:1386:ILE:CD1	2.44	0.46
1:A:1633:TRP:HA	1:A:1636:ASP:OD2	2.15	0.46
1:A:2004:TYR:C	1:A:2004:TYR:CD1	2.88	0.46
1:A:2097:LEU:HA	1:A:2097:LEU:HD23	1.77	0.46
1:A:2190:VAL:O	1:A:2193:ILE:HG22	2.16	0.46
1:A:2220:MSE:O	1:A:2223:VAL:HG12	2.16	0.46
1:A:2252:PRO:HA	1:A:2254:ARG:NH1	2.31	0.46
1:A:231:LEU:HD23	1:A:234:PHE:HB3	1.98	0.46
1:A:2433:LYS:HG3	1:A:2436:LEU:CD1	2.42	0.46
1:A:2861:ILE:HD12	1:A:2892:LEU:HD23	1.97	0.46
1:A:852:ARG:HH12	1:A:3110:PHE:HE1	1.61	0.46
1:A:3971:MSE:HE1	1:A:3980:MSE:HE1	1.97	0.46
1:A:4066:LEU:HD21	1:A:4078:VAL:CG2	2.46	0.46
1:A:608:PRO:HG2	1:A:1798:LEU:HD12	1.97	0.46
1:B:598:PRO:HG3	1:B:1022:ASP:O	2.16	0.46
1:B:1119:LYS:NZ	1:B:1256:TRP:HE1	2.13	0.46
1:B:1449:ALA:HA	1:B:1452:VAL:HB	1.96	0.46
1:B:2002:LYS:C	1:B:2004:TYR:N	2.68	0.46
1:B:2374:LEU:N	1:B:2378:PHE:HE1	2.14	0.46
1:B:2926:LEU:HD22	1:B:2931:ARG:NE	2.31	0.46
1:B:2962:ARG:HG3	1:B:3253:SER:OG	2.16	0.46
1:B:3173:MSE:HG2	1:B:3174:ASP:OD1	2.15	0.46
1:B:3323:PHE:O	1:B:3326:GLN:N	2.48	0.46
1:B:3630:ARG:HD2	1:B:3633:ILE:HG12	1.98	0.46
1:B:3878:VAL:HB	1:B:3879:PRO:HD3	1.98	0.46
1:B:655:LEU:HA	1:B:655:LEU:HD12	1.60	0.46
1:A:1132:ASP:O	1:A:1135:CYS:N	2.49	0.46
1:A:1378:GLU:O	1:A:1381:SER:N	2.49	0.46
1:A:1521:PHE:HA	1:A:1524:LEU:HD22	1.98	0.46
1:A:1652:ILE:HA	1:A:1655:ILE:HD12	1.97	0.46
1:A:2011:ALA:HB3	1:A:2014:ALA:HB2	1.98	0.46
1:A:2221:LYS:O	1:A:2225:HIS:CE1	2.69	0.46
1:A:2385:LEU:HG	1:A:2389:PHE:CZ	2.51	0.46
1:A:2828:GLU:O	1:A:2832:ILE:HG13	2.15	0.46
1:A:3024:PRO:N	1:A:3025:PRO:HD3	2.31	0.46
1:A:3059:GLN:H	1:A:3059:GLN:CD	2.19	0.46
1:A:3292:GLY:O	1:A:3297:VAL:HG23	2.15	0.46
1:A:3593:ARG:HH11	1:A:3593:ARG:HG2	1.81	0.46
1:A:3771:MSE:SE	1:A:3991:PHE:HE1	2.49	0.46
1:A:4077:TYR:CZ	1:A:4119:ARG:HD2	2.51	0.46
1:A:513:GLU:OE1	1:A:655:LEU:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1690:GLY:O	1:B:1694:THR:HG22	2.16	0.46
1:B:2000:ARG:HG2	1:B:2001:LYS:HG3	1.97	0.46
1:B:2369:LYS:HE3	1:B:2406:GLU:OE1	2.16	0.46
1:B:239:GLU:C	1:B:242:PRO:HD2	2.36	0.46
1:B:2869:LEU:HB3	1:B:2893:LEU:HG	1.96	0.46
1:B:3052:LEU:HD11	1:B:3092:LEU:HG	1.97	0.46
1:B:3241:LYS:C	1:B:3243:ILE:H	2.18	0.46
1:B:3272:TRP:CZ3	1:B:3307:LEU:HD21	2.51	0.46
1:B:3439:LEU:O	1:B:3443:PRO:HD3	2.16	0.46
1:B:3499:ILE:CG2	1:B:3535:ILE:HD13	2.41	0.46
1:B:3868:VAL:HG13	1:B:3872:ARG:HB2	1.98	0.46
1:B:575:ILE:HB	1:B:605:THR:CA	2.46	0.46
1:A:67:VAL:HG22	1:A:110:THR:HG21	1.97	0.46
1:A:1455:CYS:O	1:A:1458:LEU:HB2	2.16	0.46
1:A:1563:PHE:CE1	1:A:1567:ILE:HG13	2.51	0.46
1:A:1652:ILE:HG21	1:A:1716:GLN:OE1	2.15	0.46
1:A:1760:GLU:HB2	1:A:1894:SER:HA	1.97	0.46
1:A:2100:LEU:O	1:A:2104:MSE:HB2	2.16	0.46
1:A:2183:HIS:C	1:A:2187:VAL:HB	2.26	0.46
1:A:2164:TRP:HH2	1:A:2190:VAL:CG1	2.29	0.46
1:A:2232:ARG:HH22	1:A:2313:LYS:NZ	2.13	0.46
1:A:2255:LEU:HD12	1:A:2258:GLU:HB2	1.98	0.46
1:A:2517:LEU:HD23	1:A:2517:LEU:H	1.80	0.46
1:A:2801:ASP:HB2	1:A:2802:PRO:HD3	1.98	0.46
1:A:3092:LEU:O	1:A:3192:LYS:NZ	2.45	0.46
1:A:295:GLU:CD	1:A:341:PHE:HE1	2.19	0.46
1:A:3694:PHE:CD2	1:A:3697:ASN:HA	2.51	0.46
1:A:431:TYR:CD1	1:A:431:TYR:N	2.84	0.46
1:A:805:LEU:HD13	1:A:3117:ILE:HD13	1.98	0.46
1:A:878:GLU:C	1:A:880:MSE:H	2.19	0.46
1:A:971:ARG:CG	1:A:972:LEU:N	2.69	0.46
1:A:973:ALA:HB1	1:A:977:ASP:OD2	2.16	0.46
1:B:172:GLU:HG2	1:B:221:ALA:HB3	1.98	0.46
1:B:1747:LEU:HA	1:B:1747:LEU:HD23	1.77	0.46
1:B:2312:TYR:CG	1:B:2313:LYS:N	2.83	0.46
1:B:2900:LEU:HD23	1:B:2910:VAL:HA	1.98	0.46
1:B:3091:LEU:O	1:B:3192:LYS:HE2	2.15	0.46
1:B:3141:PHE:HA	1:B:3144:PHE:CE2	2.51	0.46
1:B:3408:GLY:O	1:B:3411:ASP:HB2	2.16	0.46
1:B:3534:ILE:H	1:B:3534:ILE:HD12	1.79	0.46
1:B:3829:LEU:HA	1:B:3829:LEU:HD12	1.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:THR:C	1:B:400:THR:N	2.68	0.46
1:B:403:GLY:C	1:B:405:ASP:N	2.67	0.46
1:B:560:LEU:CB	1:B:616:LYS:HG2	2.46	0.46
1:A:2069:ARG:HG2	2:K:204:UNK:CB	2.46	0.46
1:A:1133:HIS:CG	1:A:1133:HIS:O	2.68	0.46
1:A:1856:THR:HB	1:A:1860:GLU:OE1	2.16	0.46
1:A:1927:MSE:HE3	1:A:1927:MSE:HB2	1.62	0.46
1:A:2129:LEU:HD22	1:A:2144:LEU:HD11	1.96	0.46
1:A:2313:LYS:HA	1:A:2316:TYR:HE2	1.79	0.46
1:A:3583:LEU:HD21	1:A:3733:ARG:NH1	2.31	0.46
1:A:3780:ALA:CB	1:A:3784:ARG:HH12	2.29	0.46
1:A:3819:THR:O	1:A:3823:GLU:HG2	2.16	0.46
1:A:3900:LEU:HA	1:A:3900:LEU:HD12	1.80	0.46
1:A:4062:ASP:O	1:A:4066:LEU:HD13	2.16	0.46
1:A:982:GLN:O	1:A:986:PRO:CD	2.63	0.46
1:B:1430:GLU:OE1	1:B:1448:LEU:HA	2.16	0.46
1:B:1810:PRO:O	1:B:1811:ARG:HD2	2.16	0.46
1:B:1889:VAL:HG22	1:B:1900:PHE:CD2	2.51	0.46
1:B:1911:LEU:HD13	1:B:1916:ILE:HG22	1.97	0.46
1:B:2135:ASN:N	1:B:2136:PRO:CD	2.79	0.46
1:B:2161:ALA:O	1:B:2164:TRP:HB2	2.16	0.46
1:B:2241:LEU:H	1:B:2241:LEU:HG	1.53	0.46
1:B:2352:HIS:O	1:B:2360:PHE:HD2	1.99	0.46
1:B:2373:PRO:HA	1:B:2378:PHE:HZ	1.80	0.46
1:B:2386:LEU:O	1:B:2390:HIS:CB	2.64	0.46
1:B:257:ARG:H	1:B:258:PRO:CD	2.29	0.46
1:B:3483:MSE:O	1:B:3516:HIS:CE1	2.69	0.46
1:B:3872:ARG:O	1:B:3876:SER:CB	2.64	0.46
1:B:408:TYR:C	1:B:408:TYR:CD1	2.90	0.46
1:B:2957:LEU:HB3	1:B:4100:GLU:OE2	2.16	0.46
1:B:504:GLU:O	1:B:508:HIS:CG	2.69	0.46
1:B:578:LYS:O	1:B:581:LEU:HB2	2.16	0.46
1:B:620:PHE:HE1	1:B:623:PHE:HD2	1.64	0.46
1:B:752:LEU:HB2	1:B:756:PHE:CE1	2.51	0.46
1:A:1426:GLN:O	1:A:1430:GLU:HG3	2.16	0.45
1:A:1802:TYR:HA	1:A:1805:PHE:CD2	2.48	0.45
1:A:2035:THR:O	1:A:2039:GLU:HG3	2.16	0.45
1:A:2147:ALA:O	1:A:2151:ILE:N	2.49	0.45
1:A:2223:VAL:HG21	1:A:2238:ILE:HB	1.98	0.45
1:A:2356:MSE:HE2	1:A:2359:LYS:HD2	1.97	0.45
1:A:252:VAL:HB	1:A:265:TYR:HD1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2874:ALA:O	1:A:2878:ALA:N	2.50	0.45
1:A:2921:LEU:HD12	1:A:2922:ARG:N	2.31	0.45
1:A:3326:GLN:OE1	1:A:3393:GLU:OE2	2.34	0.45
1:A:3413:TYR:CD1	1:A:3449:LYS:HB3	2.51	0.45
1:A:3564:GLN:C	1:A:3566:GLY:H	2.19	0.45
1:A:382:ASP:O	1:A:386:VAL:CB	2.58	0.45
1:A:3997:LEU:O	1:A:4001:THR:HG23	2.17	0.45
1:A:752:LEU:HB2	1:A:756:PHE:HE1	1.79	0.45
1:A:93:LEU:HD23	1:A:93:LEU:HA	1.78	0.45
1:B:1014:LEU:HB2	1:B:1078:ALA:CB	2.43	0.45
1:B:1630:ASP:HA	1:B:1633:TRP:HE3	1.81	0.45
1:B:1879:VAL:HG23	1:B:1920:TYR:CD2	2.51	0.45
1:B:1989:ASN:HB3	1:B:2040:MSE:SE	2.66	0.45
1:B:2373:PRO:HA	1:B:2378:PHE:CZ	2.51	0.45
1:B:2389:PHE:CG	1:B:2396:LEU:HD22	2.51	0.45
1:B:2405:VAL:O	1:B:2408:MSE:HB2	2.16	0.45
1:B:2538:ARG:NH1	1:B:2562:LEU:HA	2.31	0.45
1:B:2908:LYS:HA	1:B:2908:LYS:HD3	1.72	0.45
1:B:3582:GLU:OE2	1:B:3675:LYS:HG3	2.16	0.45
1:B:3703:GLY:H	1:B:3717:VAL:HG13	1.80	0.45
1:B:3866:GLU:HA	1:B:3869:THR:OG1	2.16	0.45
1:B:3954:PRO:CB	1:B:4027:TRP:HA	2.46	0.45
1:B:406:ARG:HB3	1:B:408:TYR:CD2	2.51	0.45
1:B:528:VAL:HA	1:B:531:PHE:CE2	2.51	0.45
1:B:634:LEU:O	1:B:638:GLN:NE2	2.49	0.45
1:B:756:PHE:CD2	1:B:773:LEU:HB3	2.51	0.45
1:A:992:ILE:HD13	1:A:1035:GLU:HB2	1.98	0.45
1:A:1076:LEU:HD21	1:A:1114:ALA:HB1	1.99	0.45
1:A:1334:LYS:HA	1:A:1334:LYS:HD3	1.82	0.45
1:A:1386:ILE:HB	1:A:1391:VAL:CG2	2.45	0.45
1:A:1460:ARG:HD2	1:A:1460:ARG:H	1.81	0.45
1:A:1894:SER:O	1:A:1897:ASN:N	2.33	0.45
1:A:1966:LEU:HD22	1:A:1991:PRO:CB	2.42	0.45
1:A:2423:VAL:O	1:A:2425:ARG:N	2.50	0.45
1:A:264:ARG:O	1:A:268:PRO:HD3	2.15	0.45
1:A:2785:ILE:O	1:A:2785:ILE:HG12	2.16	0.45
1:A:2806:LYS:O	1:A:2806:LYS:HG2	2.15	0.45
1:A:3141:PHE:HA	1:A:3144:PHE:CE2	2.51	0.45
1:A:3530:VAL:HA	1:A:3533:PHE:CD2	2.51	0.45
1:A:356:ASN:OD1	1:A:1859:ASN:HB2	2.16	0.45
1:A:44:LEU:HG	1:A:44:LEU:H	1.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:760:LEU:O	1:A:764:PRO:HG3	2.16	0.45
1:A:968:VAL:O	1:A:971:ARG:HG2	2.16	0.45
1:B:1559:PHE:CE1	1:B:1592:MSE:HE2	2.52	0.45
1:B:1875:LYS:HG3	1:B:1876:ILE:HB	1.99	0.45
1:B:2157:PHE:CD1	1:B:2157:PHE:C	2.90	0.45
1:B:2316:TYR:O	1:B:2319:ALA:HB3	2.17	0.45
1:B:2893:LEU:O	1:B:2897:LEU:N	2.47	0.45
1:B:2957:LEU:HD21	1:B:4101:GLU:HG3	1.97	0.45
1:B:3243:ILE:HG12	1:B:3258:LEU:CD1	2.40	0.45
1:B:3393:GLU:O	1:B:3397:GLN:OE1	2.34	0.45
1:B:3920:ILE:HD13	1:B:3961:PHE:HA	1.98	0.45
1:B:3808:ASN:HB3	1:B:3933:GLU:HG2	1.98	0.45
1:B:4090:ARG:HD3	1:B:4090:ARG:HA	1.71	0.45
1:B:392:CYS:SG	1:B:438:LEU:HD11	2.57	0.45
1:B:637:LYS:O	1:B:641:PHE:CB	2.58	0.45
1:B:657:SER:O	1:B:660:LEU:HB2	2.16	0.45
1:B:910:PHE:HE2	1:B:941:MSE:SE	2.49	0.45
1:A:1099:PHE:CG	1:A:1100:VAL:N	2.84	0.45
1:A:1416:GLU:HB3	1:A:1420:ARG:HD2	1.97	0.45
1:A:1604:SER:HA	1:A:1632:TRP:HE3	1.80	0.45
1:A:1939:LEU:HD13	1:A:1986:ARG:NH2	2.30	0.45
1:A:19:LEU:O	1:A:23:ASP:CB	2.62	0.45
1:A:2074:PRO:HB3	1:A:2136:PRO:HB3	1.98	0.45
1:A:2126:MSE:HE2	1:A:2126:MSE:HB2	1.79	0.45
1:A:2260:PHE:HZ	1:A:2306:ASN:HB2	1.82	0.45
1:A:252:VAL:C	1:A:254:LYS:H	2.20	0.45
1:A:2940:ARG:HD3	1:A:3975:LYS:HD2	1.97	0.45
1:A:313:LEU:HD22	1:A:317:GLU:OE2	2.16	0.45
1:A:3291:GLN:NE2	1:A:3294:SER:OG	2.50	0.45
1:A:3477:GLU:HA	1:A:3480:LEU:HG	1.98	0.45
1:A:3513:ALA:O	1:A:3516:HIS:N	2.49	0.45
1:A:3771:MSE:HE1	1:A:3917:ILE:HG21	1.97	0.45
1:A:3612:ARG:HD3	1:A:3799:ARG:HH21	1.82	0.45
1:A:3853:GLY:C	1:A:3855:TYR:H	2.18	0.45
1:A:3981:TYR:CE1	1:A:4105:LYS:HA	2.51	0.45
1:B:1014:LEU:HD23	1:B:1028:PHE:CE2	2.51	0.45
1:B:1651:LYS:CE	1:B:1684:LEU:HD21	2.46	0.45
1:B:1801:VAL:HG12	1:B:1805:PHE:CE2	2.52	0.45
1:B:226:GLY:O	1:B:230:LEU:HD23	2.16	0.45
1:B:264:ARG:HA	1:B:264:ARG:HD3	1.75	0.45
1:B:2912:GLY:O	1:B:2915:ARG:CZ	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3459:ASN:CG	1:B:3710:LYS:HZ3	2.19	0.45
1:B:11:SER:OG	1:B:41:GLU:OE1	2.34	0.45
1:B:488:ILE:HG21	1:B:616:LYS:CD	2.38	0.45
1:B:617:PRO:HB3	1:B:659:ARG:CG	2.46	0.45
1:B:706:LEU:CD2	1:B:1385:ASN:HD22	2.29	0.45
1:B:789:TYR:HD2	1:B:865:GLN:CG	2.29	0.45
1:A:1685:ASP:HA	1:A:1728:GLU:OE2	2.16	0.45
1:A:1727:ARG:NH1	1:A:1728:GLU:OE1	2.50	0.45
1:A:185:HIS:N	1:A:186:PRO:HD2	2.18	0.45
1:A:2286:PRO:HD2	1:A:2329:TYR:CE2	2.50	0.45
1:A:244:THR:O	1:A:248:ILE:HG13	2.16	0.45
1:A:249:PHE:CG	1:A:297:LEU:HD13	2.52	0.45
1:A:2539:LEU:HA	1:A:2542:LEU:HD23	1.98	0.45
1:A:2563:LEU:O	1:A:2567:SER:CB	2.65	0.45
1:A:2553:HIS:ND1	1:A:2803:ILE:HD12	2.32	0.45
1:A:3141:PHE:HZ	1:A:3192:LYS:CB	2.30	0.45
1:A:3868:VAL:HG12	1:A:3872:ARG:HE	1.81	0.45
1:A:4059:ILE:HD11	1:A:4082:ARG:HD2	1.99	0.45
1:A:443:ILE:HD11	1:A:465:PHE:CE2	2.52	0.45
1:A:48:PRO:O	1:A:50:VAL:N	2.50	0.45
1:B:1093:GLU:O	1:B:1096:VAL:HG12	2.17	0.45
1:B:1577:LEU:HD12	1:B:1578:ALA:HB2	1.99	0.45
1:B:1879:VAL:O	1:B:1882:SER:N	2.48	0.45
1:B:2038:GLU:OE1	1:B:2076:VAL:HG22	2.17	0.45
1:B:2271:SER:OG	1:B:2272:VAL:N	2.50	0.45
1:B:396:PHE:CG	1:B:397:LEU:N	2.83	0.45
1:B:4108:MSE:O	1:B:4111:ALA:N	2.44	0.45
1:B:433:PRO:CB	1:B:1812:LEU:HB3	2.47	0.45
1:B:764:PRO:CB	1:B:848:LEU:HD11	2.46	0.45
1:A:1090:ARG:NH2	1:A:1100:VAL:HG11	2.17	0.45
1:A:1363:LEU:HA	1:A:1363:LEU:HD23	1.70	0.45
1:A:1479:VAL:O	1:A:1482:GLU:HB2	2.15	0.45
1:A:1894:SER:O	1:A:1896:ILE:N	2.49	0.45
1:A:2137:ILE:HG22	1:A:2141:ASN:HD21	1.82	0.45
1:A:2164:TRP:HZ3	1:A:2186:VAL:HG23	1.81	0.45
1:A:2196:TRP:NE1	1:A:2200:ALA:HB2	2.31	0.45
1:A:2538:ARG:NH1	1:A:2566:THR:N	2.64	0.45
1:A:933:LEU:HD21	1:A:2795:GLN:NE2	2.31	0.45
1:A:2808:LEU:O	1:A:2811:SER:OG	2.31	0.45
1:A:3764:VAL:O	1:A:3768:PHE:HD1	2.00	0.45
1:A:910:PHE:H	1:A:912:PRO:HD2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1468:LEU:O	1:B:1472:SER:N	2.50	0.45
1:B:1686:LEU:HA	1:B:1686:LEU:HD23	1.56	0.45
1:B:1971:PRO:O	1:B:1972:GLU:HG2	2.16	0.45
1:B:2028:LEU:HB2	1:B:2030:TYR:CE2	2.52	0.45
1:B:2193:ILE:CD1	1:B:2245:TRP:CZ2	2.99	0.45
1:B:2524:PHE:HA	1:B:2527:HIS:HB3	1.98	0.45
1:B:2937:ASP:OD2	1:B:3976:GLU:HB2	2.16	0.45
1:B:3005:LEU:HG	1:B:3005:LEU:H	1.60	0.45
1:B:3048:LYS:HB2	1:B:3048:LYS:HE3	1.77	0.45
1:B:3160:LEU:HB3	1:B:3164:TRP:CH2	2.52	0.45
1:B:3454:LEU:HA	1:B:3454:LEU:HD23	1.59	0.45
1:B:3881:ASP:OD1	1:B:3884:LYS:NZ	2.47	0.45
1:B:4066:LEU:CD2	1:B:4075:ARG:HG3	2.46	0.45
1:B:437:HIS:HA	1:B:1814:PHE:CE2	2.52	0.45
1:B:733:LEU:HD23	1:B:733:LEU:N	2.31	0.45
1:B:906:PHE:HA	1:B:909:VAL:HB	1.98	0.45
1:A:1147:LYS:O	1:A:1151:ARG:NE	2.50	0.45
1:A:1161:ALA:O	1:A:1260:LEU:HD13	2.17	0.45
1:A:706:LEU:HD21	1:A:1388:ASP:OD2	2.15	0.45
1:A:1917:LYS:HD2	1:A:1953:CYS:SG	2.57	0.45
1:A:2327:LEU:HA	1:A:2330:VAL:HG12	1.98	0.45
1:A:2379:MSE:HE1	1:A:2404:ARG:NH1	2.26	0.45
1:A:2427:ARG:HB3	1:A:2433:LYS:HB2	1.98	0.45
1:A:260:ILE:HG22	1:A:264:ARG:NH1	2.27	0.45
1:A:2806:LYS:HA	1:A:2809:PHE:CE2	2.50	0.45
1:A:2950:LYS:HE2	1:A:4105:LYS:HZ1	1.80	0.45
1:A:3944:HIS:CE1	1:A:4020:MSE:HE3	2.52	0.45
1:A:4013:TRP:HB2	1:A:4040:PRO:HG2	1.98	0.45
1:A:763:THR:HG21	1:A:769:GLY:HA3	1.99	0.45
1:A:971:ARG:HD2	1:A:1024:THR:CG2	2.44	0.45
1:A:977:ASP:CB	1:A:981:ARG:H	2.24	0.45
1:B:1299:GLU:HA	1:B:1302:ALA:HB3	1.99	0.45
1:B:1652:ILE:HG12	1:B:1717:LEU:HD11	1.99	0.45
1:B:279:ALA:HA	1:B:282:PHE:CD2	2.52	0.45
1:B:2913:LYS:O	1:B:2916:LEU:N	2.25	0.45
1:B:3268:THR:O	1:B:3271:ASP:HB3	2.17	0.45
1:B:3518:VAL:HA	1:B:3521:ILE:HG22	1.98	0.45
1:B:3890:MSE:O	1:B:3891:SER:OG	2.33	0.45
1:B:3916:TRP:CZ3	1:B:3917:ILE:HD12	2.52	0.45
1:B:3880:ALA:HB1	1:B:3969:ASN:HB3	1.99	0.45
1:B:542:ASP:HA	1:B:545:LEU:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:560:LEU:HA	1:B:563:LEU:HB2	1.99	0.45
1:B:586:GLN:OE1	1:B:1088:GLU:HG2	2.17	0.45
1:B:763:THR:N	1:B:764:PRO:HD3	2.31	0.45
1:B:982:GLN:O	1:B:986:PRO:CD	2.64	0.45
1:A:1147:LYS:HG2	1:A:1180:GLN:HG2	1.97	0.45
1:A:1996:VAL:HG23	1:A:1997:PRO:HD3	1.98	0.45
1:A:2004:TYR:OH	1:A:2055:SER:HB3	2.16	0.45
1:A:2077:HIS:HB3	1:A:2081:LEU:HG	1.99	0.45
1:A:2236:GLU:HG3	1:A:2236:GLU:H	1.46	0.45
1:A:2485:ARG:HA	1:A:2499:PHE:HE2	1.82	0.45
1:A:3077:ILE:O	1:A:3081:HIS:CG	2.70	0.45
1:A:313:LEU:HD13	1:A:317:GLU:OE2	2.16	0.45
1:A:3244:ASP:O	1:A:3247:ARG:HB3	2.16	0.45
1:A:3458:SER:OG	1:A:3494:GLN:NE2	2.49	0.45
1:A:3572:ILE:HD13	1:A:3575:LEU:HD12	1.97	0.45
1:A:3575:LEU:C	1:A:3577:GLN:H	2.18	0.45
1:A:3619:ASP:N	1:A:3620:PRO:CD	2.80	0.45
1:A:3670:MSE:HE3	1:A:3670:MSE:HB2	1.78	0.45
1:A:3834:ALA:H	1:A:3835:PRO:HD3	1.81	0.45
1:A:3955:VAL:HG12	1:A:4027:TRP:NE1	2.24	0.45
1:A:3958:LEU:O	1:A:3958:LEU:HD12	2.17	0.45
1:A:4077:TYR:OH	1:A:4116:ILE:HA	2.17	0.45
1:A:575:ILE:N	1:A:605:THR:OG1	2.50	0.45
1:A:65:LEU:HD23	1:A:68:PHE:CZ	2.52	0.45
1:A:799:TYR:O	1:A:801:LYS:N	2.50	0.45
1:A:916:GLU:HA	1:A:919:LEU:HG	1.99	0.45
1:B:1039:TRP:CH2	1:B:1052:SER:HB3	2.51	0.45
1:B:1269:THR:CG2	1:B:1275:THR:HG21	2.46	0.45
1:B:1378:GLU:HB3	1:B:1379:PRO:CD	2.46	0.45
1:B:1517:LEU:HD13	1:B:1585:SER:HB2	1.99	0.45
1:B:1876:ILE:O	1:B:1877:LEU:HG	2.16	0.45
1:B:2265:PRO:HD3	1:B:2309:PHE:HZ	1.79	0.45
1:B:2459:VAL:HG13	1:B:2505:VAL:HG13	1.98	0.45
1:B:2462:VAL:CG2	1:B:2473:MSE:SE	3.13	0.45
1:B:215:PRO:HB3	1:B:251:PHE:CD2	2.51	0.45
1:B:901:MSE:HG3	1:B:2819:GLU:HB2	1.98	0.45
1:B:3312:VAL:O	1:B:3314:SER:N	2.50	0.45
1:B:3315:TYR:CG	1:B:3316:LEU:N	2.84	0.45
1:B:348:ILE:HG23	1:B:357:LYS:HE3	1.98	0.45
1:B:3813:LYS:CE	1:B:3926:ASN:HB2	2.46	0.45
1:B:3812:LEU:O	1:B:3816:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:743:LEU:HD23	1:B:783:HIS:HE1	1.82	0.45
1:B:980:THR:HG23	1:B:984:TYR:HE2	1.80	0.45
1:A:1027:ASP:O	1:A:1031:ARG:HG2	2.17	0.45
1:A:1033:ILE:HG13	1:A:1089:PHE:HE2	1.82	0.45
1:A:1737:ASN:C	1:A:1739:TYR:N	2.69	0.45
1:A:2222:HIS:O	1:A:2224:PHE:N	2.49	0.45
1:A:2327:LEU:HD12	1:A:2371:PHE:HB2	1.98	0.45
1:A:3273:LEU:HD13	1:A:3321:LEU:HD13	1.99	0.45
1:A:3516:HIS:CE1	1:A:3517:SER:HG	2.34	0.45
1:A:3784:ARG:HB2	1:A:3786:LEU:HG	1.99	0.45
1:A:3820:MSE:HB2	1:A:3882:LEU:HD13	1.98	0.45
1:A:3967:PHE:CG	1:A:3968:ILE:N	2.84	0.45
1:A:436:GLU:O	1:A:440:VAL:HG13	2.17	0.45
1:A:460:ALA:O	1:A:464:VAL:HG12	2.17	0.45
1:A:557:SER:HA	1:A:560:LEU:CD2	2.47	0.45
1:A:933:LEU:HD12	1:A:933:LEU:HA	1.56	0.45
1:B:2196:TRP:NE1	1:B:2200:ALA:HB2	2.30	0.45
1:B:2402:LEU:HA	1:B:2405:VAL:HG22	1.97	0.45
1:B:252:VAL:C	1:B:254:LYS:H	2.20	0.45
1:B:3168:TYR:HB3	1:B:3169:PRO:HD3	1.99	0.45
1:B:3181:ASP:HA	1:B:3184:THR:CG2	2.45	0.45
1:B:3438:GLU:HB3	1:B:3442:TYR:HE2	1.82	0.45
1:B:3525:TYR:OH	1:B:3561:LYS:HB2	2.17	0.45
1:B:3594:ALA:CB	1:B:4028:ILE:HD13	2.45	0.45
1:B:3961:PHE:CE1	1:B:3963:LEU:HB2	2.51	0.45
1:B:4077:TYR:HB2	1:B:4119:ARG:NH2	2.32	0.45
1:B:63:PHE:O	1:B:66:LEU:HG	2.17	0.45
1:B:759:GLY:HA3	1:B:773:LEU:HD11	1.98	0.45
1:A:1402:LEU:O	1:A:1406:LEU:HD23	2.17	0.45
1:A:1685:ASP:HB3	1:A:1728:GLU:OE1	2.16	0.45
1:A:1762:MSE:HG2	1:A:1864:ASP:OD1	2.17	0.45
1:A:1858:LEU:O	1:A:1861:SER:HB2	2.16	0.45
1:A:1911:LEU:HD13	1:A:1916:ILE:CG2	2.45	0.45
1:A:1975:LEU:HA	1:A:1976:LEU:HD23	1.98	0.45
1:A:2226:PRO:O	1:A:2230:VAL:N	2.43	0.45
1:A:2253:TYR:HE1	1:A:2280:VAL:HG22	1.82	0.45
1:A:2439:ILE:C	1:A:2441:LYS:H	2.20	0.45
1:A:2777:HIS:O	1:A:2781:PRO:HD3	2.17	0.45
1:A:3930:VAL:HA	1:A:3937:VAL:HG13	1.98	0.45
1:A:16:GLN:OE1	1:A:61:ARG:HB2	2.17	0.45
1:A:513:GLU:HG2	1:A:653:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:VAL:HG12	1:B:130:LEU:HD11	1.98	0.45
1:B:1598:ASN:ND2	1:B:1811:ARG:HG2	2.32	0.45
1:B:1886:LYS:NZ	1:B:1944:ALA:O	2.47	0.45
1:B:2039:GLU:HG2	1:B:2077:HIS:CE1	2.52	0.45
1:B:2087:GLU:OE2	1:B:2138:VAL:HG12	2.17	0.45
1:B:262:LEU:H	1:B:262:LEU:HG	1.60	0.45
1:B:3110:PHE:C	1:B:3114:TYR:HD1	2.20	0.45
1:B:321:LYS:O	1:B:325:ASN:HB2	2.17	0.45
1:B:3498:TRP:HB2	1:B:3501:HIS:HB2	1.99	0.45
1:B:3550:LYS:HZ3	1:B:3554:PHE:HD2	1.58	0.45
1:B:3863:ASN:O	1:B:3867:THR:HG23	2.16	0.45
1:B:396:PHE:CZ	1:B:437:HIS:CD2	3.05	0.45
1:B:4056:PRO:HD2	1:B:4059:ILE:HG22	1.99	0.45
1:B:468:LEU:HD22	1:B:475:LEU:CD2	2.46	0.45
1:B:633:ILE:HG22	1:B:634:LEU:CD2	2.46	0.45
1:B:912:PRO:O	1:B:916:GLU:HG3	2.16	0.45
1:B:927:LYS:HE2	1:B:927:LYS:HB3	1.80	0.45
1:A:111:CYS:HB3	1:A:134:LEU:HB3	1.98	0.45
1:A:1300:SER:O	1:A:1304:HIS:ND1	2.36	0.45
1:A:1305:ASP:OD1	1:A:1306:ILE:N	2.50	0.45
1:A:1357:LYS:HG2	1:A:1357:LYS:O	2.17	0.45
1:A:1464:LEU:O	1:A:1468:LEU:N	2.43	0.45
1:A:1645:VAL:HG22	1:A:1709:GLU:OE1	2.17	0.45
1:A:1806:ARG:O	1:A:1810:PRO:HD3	2.17	0.45
1:A:1915:LEU:CD1	1:A:1916:ILE:HG13	2.46	0.45
1:A:1991:PRO:HD2	1:A:1992:VAL:H	1.81	0.45
1:A:2356:MSE:SE	1:A:2360:PHE:CE1	3.20	0.45
1:A:275:PHE:O	1:A:277:LEU:N	2.50	0.45
1:A:2959:ALA:O	1:A:3251:ASN:HA	2.17	0.45
1:A:2972:TYR:CE2	1:A:2991:LYS:NZ	2.84	0.45
1:A:3425:ARG:NH2	1:A:3467:ARG:NH1	2.65	0.45
1:A:763:THR:OG1	1:A:770:LEU:HD23	2.17	0.45
1:B:1032:CYS:HB3	1:B:1036:PHE:HZ	1.77	0.45
1:B:1301:ILE:HA	1:B:1304:HIS:HB2	1.99	0.45
1:B:1583:MSE:HE3	1:B:1643:MSE:HB3	1.98	0.45
1:B:1655:ILE:CG1	1:B:1681:ASP:HB3	2.47	0.45
1:B:2070:GLU:HG3	1:B:2072:ARG:CG	2.38	0.45
1:B:2164:TRP:HH2	1:B:2190:VAL:CG1	2.30	0.45
1:B:2219:LEU:HA	1:B:2219:LEU:HD23	1.76	0.45
1:B:2220:MSE:HE1	1:B:2256:ILE:HD11	1.98	0.45
1:B:2313:LYS:O	1:B:2316:TYR:HE1	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2555:LEU:HD22	1:B:2809:PHE:CE2	2.52	0.45
1:B:2883:SER:HA	1:B:2886:GLN:NE2	2.30	0.45
1:B:3493:TRP:CZ2	1:B:3496:ILE:HG21	2.52	0.45
1:B:362:ALA:HB2	1:B:409:GLN:NE2	2.29	0.45
1:A:1249:SER:O	1:A:1253:THR:CB	2.63	0.44
1:A:437:HIS:CE1	1:A:1813:SER:HG	2.35	0.44
1:A:2145:PHE:CE2	1:A:2185:MSE:SE	3.20	0.44
1:A:2203:THR:HG23	1:A:2245:TRP:HH2	1.82	0.44
1:A:2634:UNK:O	1:A:2637:UNK:N	2.50	0.44
1:A:3186:ARG:O	1:A:3189:PHE:HB2	2.17	0.44
1:A:1249:SER:HA	1:A:3698:GLU:OE2	2.17	0.44
1:A:3751:LEU:HD13	1:A:3805:TRP:HB2	1.98	0.44
1:A:3872:ARG:O	1:A:3876:SER:CB	2.65	0.44
1:A:3961:PHE:HE1	1:A:3963:LEU:HB2	1.76	0.44
1:A:4025:GLY:O	1:A:4028:ILE:HG22	2.17	0.44
1:A:4090:ARG:HD3	1:A:4090:ARG:HA	1.83	0.44
1:A:601:TRP:HE3	1:A:601:TRP:H	1.65	0.44
1:A:865:GLN:OE1	1:A:865:GLN:N	2.49	0.44
1:A:868:LYS:HA	1:A:871:LEU:HD12	1.99	0.44
1:A:909:VAL:HG12	1:A:937:MSE:SE	2.67	0.44
1:B:109:ASN:HA	1:B:112:THR:HG22	1.99	0.44
1:B:1137:ILE:O	1:B:1140:LYS:HD2	2.18	0.44
1:B:82:ARG:NH1	1:B:114:VAL:HG13	2.32	0.44
1:B:1438:GLY:HA2	1:B:1491:ILE:HD11	1.99	0.44
1:B:2147:ALA:O	1:B:2151:ILE:HG13	2.17	0.44
1:B:2960:GLU:O	1:B:2965:TYR:HD1	2.00	0.44
1:B:2970:LYS:CE	1:B:2974:GLU:OE2	2.65	0.44
1:B:3479:THR:OG1	1:B:3483:MSE:SE	2.85	0.44
1:B:3862:ALA:O	1:B:3866:GLU:HG3	2.17	0.44
1:B:4121:TRP:CG	1:B:4122:GLU:N	2.85	0.44
1:B:550:PHE:CE1	1:B:633:ILE:HA	2.52	0.44
1:B:805:LEU:HD13	1:B:3117:ILE:CD1	2.46	0.44
1:B:989:MSE:HG2	1:B:1031:ARG:NH1	2.32	0.44
1:A:1358:LEU:HD23	1:A:1358:LEU:O	2.17	0.44
1:A:1684:LEU:HD23	1:A:1687:HIS:HD2	1.83	0.44
1:A:187:SER:O	1:A:190:ILE:HG22	2.16	0.44
1:A:1918:LEU:HD11	1:A:1957:ASN:HD22	1.81	0.44
1:A:2227:LYS:C	1:A:2229:ALA:H	2.21	0.44
1:A:2866:ALA:O	1:A:2869:LEU:HB2	2.17	0.44
1:A:3172:LYS:HG3	1:A:3178:ILE:HG21	1.99	0.44
1:A:3427:GLU:HG3	1:A:3439:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:GLU:OE1	1:A:1798:LEU:HD13	2.18	0.44
1:A:74:ASN:HB3	1:A:75:SER:H	1.44	0.44
1:B:1701:SER:OG	1:B:1702:LEU:N	2.51	0.44
1:B:2007:ILE:HG22	1:B:2009:LYS:CB	2.47	0.44
1:B:2004:TYR:CG	1:B:2054:TYR:HB3	2.52	0.44
1:B:2093:CYS:C	1:B:2096:PRO:HD2	2.37	0.44
1:B:2442:MSE:H	1:B:2442:MSE:HG2	1.62	0.44
1:B:3619:ASP:N	1:B:3620:PRO:CD	2.80	0.44
1:B:3912:CYS:HB3	1:B:3961:PHE:CG	2.52	0.44
1:B:3764:VAL:HG13	1:B:3918:LEU:HD21	1.99	0.44
1:B:3974:MSE:HB3	1:B:3976:GLU:N	2.32	0.44
1:B:414:LEU:O	1:B:414:LEU:HG	2.14	0.44
1:B:732:PHE:HB2	1:B:733:LEU:CD2	2.47	0.44
1:B:84:GLU:O	1:B:88:PHE:HD2	2.01	0.44
1:B:89:LEU:HA	1:B:92:PHE:CD2	2.52	0.44
1:B:934:LEU:O	1:B:938:VAL:HG23	2.17	0.44
1:B:955:ALA:O	1:B:959:TYR:CB	2.66	0.44
1:B:91:ILE:O	1:B:95:LYS:HG3	2.17	0.44
1:A:1282:LEU:HD12	1:A:1282:LEU:HA	1.69	0.44
1:A:1476:HIS:HB2	1:A:1511:ALA:HB2	2.00	0.44
1:A:1583:MSE:HE1	1:A:1640:GLU:CD	2.37	0.44
1:A:1752:LEU:HD23	1:A:1752:LEU:HA	1.74	0.44
1:A:433:PRO:CB	1:A:1812:LEU:HA	2.48	0.44
1:A:185:HIS:H	1:A:186:PRO:CD	2.19	0.44
1:A:172:GLU:HA	1:A:222:GLY:HA3	1.99	0.44
1:A:2277:LEU:O	1:A:2280:VAL:HB	2.17	0.44
1:A:2310:VAL:O	1:A:2315:VAL:HG21	2.18	0.44
1:A:2320:ALA:HB2	1:A:2367:VAL:HA	1.99	0.44
1:A:3501:HIS:O	1:A:3505:LEU:HD13	2.18	0.44
1:A:3578:LEU:HD22	1:A:3683:CYS:SG	2.57	0.44
1:A:3739:ILE:CD1	1:A:3749:PRO:HB3	2.48	0.44
1:A:409:GLN:HG3	1:A:413:PHE:CE2	2.53	0.44
1:A:385:TYR:OH	1:A:421:LEU:HD23	2.18	0.44
1:A:456:VAL:O	1:A:459:ARG:HB2	2.18	0.44
1:B:1005:ASP:HB2	1:B:1006:THR:H	1.51	0.44
1:B:1119:LYS:HZ3	1:B:1256:TRP:HE1	1.64	0.44
1:B:1342:MSE:HG2	1:B:1402:LEU:HD23	1.99	0.44
1:B:1651:LYS:HD2	1:B:1684:LEU:HD21	2.00	0.44
1:B:2416:LYS:HE2	1:B:2439:ILE:HG12	1.99	0.44
1:B:307:GLU:O	1:B:308:LEU:HD13	2.17	0.44
1:B:3156:PRO:HB2	1:B:3197:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3477:GLU:O	1:B:3481:SER:HB2	2.17	0.44
1:B:3972:LEU:C	1:B:3974:MSE:HG2	2.38	0.44
1:B:4056:PRO:O	1:B:4058:VAL:N	2.51	0.44
1:B:487:LEU:HD23	1:B:530:LEU:HD12	1.99	0.44
1:B:527:TYR:HH	1:B:619:ASP:N	2.12	0.44
1:B:654:ILE:HG21	1:B:726:LEU:HB3	1.99	0.44
1:B:734:LEU:HD23	1:B:734:LEU:HA	1.52	0.44
1:A:1147:LYS:CG	1:A:1180:GLN:HG2	2.47	0.44
1:A:1583:MSE:SE	1:A:1643:MSE:HE3	2.67	0.44
1:A:1802:TYR:O	1:A:1805:PHE:HB2	2.17	0.44
1:A:1908:GLY:CA	1:A:1952:ILE:HG13	2.47	0.44
1:A:2506:LEU:H	1:A:2506:LEU:HG	1.56	0.44
1:A:939:MSE:SE	1:A:2783:ILE:HG23	2.67	0.44
1:A:334:HIS:ND1	1:A:338:LEU:HD21	2.31	0.44
1:A:3443:PRO:C	1:A:3445:LEU:H	2.20	0.44
1:A:352:VAL:HG23	1:A:357:LYS:N	2.23	0.44
1:A:368:LEU:O	1:A:420:VAL:HG23	2.17	0.44
1:A:3717:VAL:HG22	1:A:3718:ARG:H	1.83	0.44
1:A:3583:LEU:CD1	1:A:3733:ARG:HB3	2.43	0.44
1:A:3903:HIS:ND1	1:A:3934:THR:OG1	2.51	0.44
1:A:3966:GLN:HG2	1:A:4128:MSE:C	2.38	0.44
1:A:487:LEU:HG	1:A:530:LEU:HD13	2.00	0.44
1:A:658:THR:N	1:A:733:LEU:HD13	2.33	0.44
1:B:1101:PHE:HA	1:B:1104:LEU:HD12	1.98	0.44
1:B:1272:GLY:C	1:B:1274:ARG:H	2.21	0.44
1:B:1373:VAL:HG13	1:B:1374:GLN:HG2	2.00	0.44
1:B:1692:ALA:HA	1:B:1695:LEU:HD12	1.98	0.44
1:B:1949:ILE:HD12	1:B:1952:ILE:CG2	2.35	0.44
1:B:1958:GLU:HA	1:B:1961:PHE:HB3	2.00	0.44
1:B:2307:MSE:HE1	1:B:2367:VAL:HG11	1.98	0.44
1:B:2359:LYS:H	1:B:2359:LYS:HG3	1.62	0.44
1:B:2917:PRO:HB2	1:B:2918:PRO:HD3	1.99	0.44
1:B:481:THR:O	1:B:485:GLN:HG2	2.17	0.44
1:B:65:LEU:O	1:B:69:VAL:CB	2.64	0.44
1:B:669:LEU:C	1:B:671:SER:N	2.70	0.44
1:B:771:ASN:O	1:B:773:LEU:N	2.51	0.44
1:B:797:ASP:OD2	1:B:869:ASN:HB2	2.18	0.44
1:A:1076:LEU:O	1:A:1078:ALA:N	2.51	0.44
1:A:1086:TYR:CE1	1:A:1089:PHE:HB2	2.53	0.44
1:A:1115:HIS:O	1:A:1118:GLU:C	2.56	0.44
1:A:1151:ARG:O	1:A:1154:PRO:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:PHE:HB2	1:A:157:TYR:HE2	1.82	0.44
1:A:189:MSE:HE3	1:A:193:ALA:HB2	1.99	0.44
1:A:2145:PHE:CE1	1:A:2188:GLU:HB3	2.53	0.44
1:A:224:LEU:HD22	1:A:248:ILE:HD11	2.00	0.44
1:A:2379:MSE:HE1	1:A:2404:ARG:HD3	1.99	0.44
1:A:3125:ARG:HH21	1:A:3128:LYS:HD2	1.82	0.44
1:A:3835:PRO:HA	1:A:3871:PHE:CE1	2.43	0.44
1:A:432:THR:HB	1:A:433:PRO:CD	2.48	0.44
1:A:863:GLY:CA	1:A:866:ILE:HD11	2.47	0.44
1:B:1025:LEU:CD1	1:B:1028:PHE:HD2	2.30	0.44
1:B:1108:MSE:HB2	1:B:1132:ASP:OD1	2.17	0.44
1:B:2058:ASP:HB3	1:B:2059:PRO:HD3	1.98	0.44
1:B:2205:VAL:HB	1:B:2206:PRO:HD3	1.99	0.44
1:B:2539:LEU:O	1:B:2542:LEU:HG	2.18	0.44
1:B:602:MSE:SE	1:B:726:LEU:CD1	3.14	0.44
1:B:63:PHE:O	1:B:67:VAL:HG23	2.18	0.44
1:B:729:CYS:O	1:B:733:LEU:HG	2.17	0.44
1:B:954:GLY:O	1:B:958:MSE:HB3	2.17	0.44
1:B:971:ARG:CG	1:B:972:LEU:N	2.71	0.44
1:A:1340:ARG:O	1:A:1343:GLU:HB3	2.18	0.44
1:A:1433:ALA:O	1:A:1437:TYR:CG	2.71	0.44
1:A:1455:CYS:O	1:A:1458:LEU:N	2.50	0.44
1:A:1504:ASP:HA	1:A:1507:CYS:SG	2.57	0.44
1:A:2147:ALA:CB	1:A:2151:ILE:HD12	2.47	0.44
1:A:2164:TRP:CE3	1:A:2189:ILE:HD12	2.52	0.44
1:A:2167:PRO:C	1:A:2171:LEU:HB2	2.37	0.44
1:A:2253:TYR:CE1	1:A:2280:VAL:HG22	2.53	0.44
1:A:2320:ALA:HA	1:A:2367:VAL:HG23	1.99	0.44
1:A:249:PHE:HD1	1:A:265:TYR:CE1	2.36	0.44
1:A:268:PRO:O	1:A:271:GLY:N	2.51	0.44
1:A:3045:ILE:HG21	1:A:3064:PHE:CZ	2.52	0.44
1:A:3073:LEU:H	1:A:3073:LEU:HG	1.63	0.44
1:A:3155:VAL:HG11	1:A:3159:ARG:CZ	2.47	0.44
1:A:3168:TYR:HB3	1:A:3169:PRO:HD3	2.00	0.44
1:A:3283:LEU:HD22	1:A:3283:LEU:O	2.17	0.44
1:A:3305:SER:HA	1:A:3308:ASP:CB	2.45	0.44
1:A:3345:PRO:HB2	1:A:3346:ALA:H	1.58	0.44
1:A:3534:ILE:HG13	1:A:3569:GLN:OE1	2.17	0.44
1:A:430:VAL:HG11	1:A:1682:THR:HG21	2.00	0.44
1:A:530:LEU:HG	1:A:530:LEU:H	1.44	0.44
1:B:1485:SER:HA	1:B:1488:TYR:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1568:ASN:N	1:B:1568:ASN:OD1	2.51	0.44
1:B:180:LEU:HD23	1:B:183:GLU:OE1	2.17	0.44
1:B:1906:THR:O	1:B:1910:GLU:HB2	2.18	0.44
1:B:2083:LEU:HD22	1:B:2184:TYR:HD2	1.82	0.44
1:B:901:MSE:HE1	1:B:2535:THR:CG2	2.47	0.44
1:B:2536:LEU:HA	1:B:2539:LEU:HB2	1.99	0.44
1:B:2817:LEU:HA	1:B:2820:MSE:HE2	1.99	0.44
1:B:2936:TYR:HD2	1:B:3979:LEU:CD2	2.28	0.44
1:B:3103:ILE:HD11	1:B:3138:ILE:HG21	2.00	0.44
1:B:3243:ILE:HG22	1:B:3278:GLN:HE21	1.83	0.44
1:B:3631:LYS:HG3	1:B:3685:PRO:HG2	1.99	0.44
1:B:3720:ALA:HB3	1:B:3741:ARG:O	2.17	0.44
1:B:3771:MSE:O	1:B:3774:ILE:HB	2.17	0.44
1:B:4013:TRP:CE3	1:B:4014:LYS:HB2	2.53	0.44
1:B:4074:PHE:O	1:B:4077:TYR:HB3	2.17	0.44
1:B:3984:MSE:SE	1:B:4108:MSE:HE2	2.68	0.44
1:B:612:LEU:O	1:B:615:ALA:HB3	2.18	0.44
1:B:625:ASN:HA	1:B:666:PHE:CE1	2.53	0.44
1:B:886:TRP:HH2	1:B:958:MSE:HB2	1.82	0.44
1:B:894:PHE:O	1:B:940:PHE:CZ	2.71	0.44
1:A:1076:LEU:HD23	1:A:1076:LEU:HA	1.65	0.44
1:A:1072:ALA:HB1	1:A:1076:LEU:HG	2.00	0.44
1:A:82:ARG:HD2	1:A:114:VAL:CG1	2.48	0.44
1:A:1387:GLY:HA2	1:A:1392:MSE:HG3	1.99	0.44
1:A:1582:LEU:HA	1:A:1582:LEU:HD23	1.77	0.44
1:A:1722:PHE:HE2	1:A:1754:GLN:HA	1.81	0.44
1:A:1946:ASN:O	1:A:1949:ILE:N	2.31	0.44
1:A:2028:LEU:HB2	1:A:2030:TYR:HE2	1.82	0.44
1:A:2068:ARG:O	1:A:2070:GLU:N	2.50	0.44
1:A:2453:GLU:HA	1:A:2456:ASN:ND2	2.33	0.44
1:A:2936:TYR:CD2	1:A:3979:LEU:HD11	2.52	0.44
1:A:321:LYS:C	1:A:325:ASN:HD22	2.20	0.44
1:A:3247:ARG:HB2	1:A:3278:GLN:NE2	2.32	0.44
1:A:452:LYS:O	1:A:455:LEU:HG	2.17	0.44
1:A:760:LEU:CD2	1:A:803:SER:HB3	2.47	0.44
1:A:948:MSE:N	1:A:949:PRO:HD3	2.33	0.44
1:B:1087:ARG:NE	1:B:1134:LEU:HD22	2.33	0.44
1:B:1424:THR:O	1:B:1426:GLN:N	2.51	0.44
1:B:175:TYR:HB3	1:B:226:GLY:HA3	1.98	0.44
1:B:1913:LYS:HB2	1:B:1916:ILE:HB	2.00	0.44
1:B:197:PHE:O	1:B:201:LEU:HG	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2177:ASN:HB2	1:B:2182:ILE:HG23	1.99	0.44
1:B:2211:LEU:H	1:B:2211:LEU:HG	1.49	0.44
1:B:2224:PHE:CE2	1:B:2259:LYS:HD3	2.53	0.44
1:B:2318:ALA:O	1:B:2322:VAL:HB	2.18	0.44
1:B:2505:VAL:O	1:B:2508:GLN:N	2.50	0.44
1:B:320:LEU:O	1:B:323:VAL:HB	2.17	0.44
1:B:3413:TYR:CD1	1:B:3449:LYS:HB3	2.53	0.44
1:B:3699:LEU:HA	1:B:3699:LEU:HD12	1.83	0.44
1:B:563:LEU:O	1:B:566:ASP:HB2	2.18	0.44
1:B:571:SER:HB2	1:B:605:THR:H	1.83	0.44
1:B:638:GLN:NE2	1:B:667:TYR:HB3	2.32	0.44
1:B:653:LEU:HD23	1:B:653:LEU:HA	1.50	0.44
1:B:727:ALA:O	1:B:731:THR:HG23	2.18	0.44
1:B:78:PHE:O	1:B:81:CYS:N	2.51	0.44
1:B:966:PHE:CE1	1:B:969:LEU:HD13	2.53	0.44
1:A:1022:ASP:CG	1:A:1023:SER:H	2.21	0.44
1:A:1032:CYS:HB3	1:A:1036:PHE:CE2	2.52	0.44
1:A:993:HIS:ND1	1:A:1038:LYS:HE2	2.33	0.44
1:A:2183:HIS:HE1	1:A:2237:ILE:HD13	1.82	0.44
1:A:2271:SER:HB2	1:A:2314:GLU:CG	2.47	0.44
1:A:2461:PHE:CE1	1:A:2462:VAL:HG23	2.52	0.44
1:A:271:GLY:O	1:A:274:LEU:HD12	2.18	0.44
1:A:294:PHE:HZ	1:A:341:PHE:CZ	2.36	0.44
1:A:3155:VAL:HG11	1:A:3159:ARG:NH1	2.32	0.44
1:A:3186:ARG:HA	1:A:3189:PHE:CD2	2.52	0.44
1:A:3266:SER:HB2	1:A:3271:ASP:OD1	2.17	0.44
1:A:3276:TRP:HB3	1:A:3280:TYR:CE2	2.52	0.44
1:A:3455:LYS:H	1:A:3455:LYS:HG3	1.62	0.44
1:A:366:TYR:C	1:A:369:PHE:HB3	2.36	0.44
1:A:3857:LEU:HG	1:A:3859:TYR:CD2	2.53	0.44
1:A:82:ARG:HH21	1:A:83:GLU:HG3	1.83	0.44
1:B:1334:LYS:HD3	1:B:1334:LYS:HA	1.45	0.44
1:B:1369:MSE:SE	1:B:1418:HIS:ND1	3.01	0.44
1:B:1471:GLN:OE1	1:B:1471:GLN:N	2.51	0.44
1:B:1684:LEU:HA	1:B:1684:LEU:HD23	1.71	0.44
1:B:1761:LEU:HD13	1:B:1860:GLU:OE1	2.18	0.44
1:B:1999:GLU:HB3	1:B:2051:SER:HB3	2.00	0.44
1:B:2093:CYS:CA	1:B:2096:PRO:HD2	2.48	0.44
1:B:2164:TRP:C	1:B:2167:PRO:HD2	2.38	0.44
1:B:2232:ARG:O	1:B:2234:ASN:N	2.51	0.44
1:B:2213:ASN:CG	1:B:2250:SER:HB2	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2854:PHE:HZ	1:B:2881:LEU:HB2	1.81	0.44
1:B:2886:GLN:HG3	1:B:2887:PRO:HD3	1.99	0.44
1:B:2916:LEU:HB3	1:B:2917:PRO:HD3	2.00	0.44
1:B:3475:TYR:HB2	1:B:3479:THR:H	1.83	0.44
1:B:3636:PHE:C	1:B:3638:LYS:N	2.71	0.44
1:B:3819:THR:HG1	1:B:3889:ARG:NH1	2.10	0.44
1:B:3974:MSE:HB3	1:B:3976:GLU:CB	2.48	0.44
1:B:3975:LYS:HE3	1:B:3975:LYS:HB2	1.81	0.44
1:B:848:LEU:HD12	1:B:848:LEU:HA	1.78	0.44
1:B:928:VAL:HG23	1:B:929:ALA:N	2.33	0.44
1:A:1014:LEU:HD23	1:A:1028:PHE:HE2	1.83	0.44
1:A:1733:THR:HG23	1:A:1881:TYR:CE2	2.53	0.44
1:A:2021:GLY:N	1:A:2022:PRO:HD2	2.32	0.44
1:A:2004:TYR:CD1	1:A:2054:TYR:HB3	2.52	0.44
1:A:3720:ALA:HB3	1:A:3741:ARG:O	2.18	0.44
1:A:3960:PRO:HG2	1:A:3961:PHE:CE2	2.52	0.44
1:A:446:PHE:N	1:A:447:PRO:CD	2.81	0.44
1:A:447:PRO:HD2	1:A:448:GLN:H	1.82	0.44
1:B:1017:ILE:HD12	1:B:1025:LEU:HD23	2.00	0.44
1:B:1070:PRO:O	1:B:1073:PHE:CE2	2.71	0.44
1:B:1368:LEU:HA	1:B:1371:VAL:CG1	2.48	0.44
1:B:1937:ARG:O	1:B:1941:HIS:HB2	2.18	0.44
1:B:2028:LEU:HB2	1:B:2030:TYR:HE2	1.81	0.44
1:B:2164:TRP:CH2	1:B:2190:VAL:HG12	2.53	0.44
1:B:2316:TYR:CE2	1:B:2317:ALA:HB2	2.53	0.44
1:B:2473:MSE:O	1:B:2477:LEU:HG	2.17	0.44
1:B:271:GLY:O	1:B:274:LEU:HD12	2.18	0.44
1:B:290:TYR:O	1:B:294:PHE:HB3	2.17	0.44
1:B:2983:ASP:O	1:B:2986:PRO:HD2	2.18	0.44
1:B:3109:SER:O	1:B:3112:GLN:HB3	2.17	0.44
1:B:856:VAL:HG21	1:B:3110:PHE:CZ	2.53	0.44
1:B:3842:TRP:HA	1:B:3845:LYS:HB2	2.00	0.44
1:B:393:LYS:O	1:B:397:LEU:HB2	2.18	0.44
1:B:12:LEU:HD21	1:B:41:GLU:HB2	2.00	0.44
1:B:13:LEU:HD22	1:B:61:ARG:HD2	2.00	0.44
1:B:927:LYS:HE3	1:B:928:VAL:CG1	2.47	0.44
1:A:1017:ILE:HB	1:A:1025:LEU:HB2	2.00	0.43
1:A:1073:PHE:HD1	1:A:1074:LYS:N	2.06	0.43
1:A:1163:LEU:HA	1:A:1260:LEU:HD21	2.00	0.43
1:A:12:LEU:HD21	1:A:41:GLU:HB2	2.00	0.43
1:A:1471:GLN:O	1:A:1475:LEU:CB	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1804:MSE:HE1	1:A:1822:ARG:HH11	1.82	0.43
1:A:1762:MSE:SE	1:A:1896:ILE:HG12	2.67	0.43
1:A:1945:TYR:O	1:A:1948:ALA:HB3	2.18	0.43
1:A:266:ALA:HB2	1:A:308:LEU:HG	1.99	0.43
1:A:3092:LEU:HD22	1:A:3192:LYS:HE3	2.00	0.43
1:A:3259:LEU:HD21	1:A:3279:SER:HB2	1.99	0.43
1:A:360:SER:O	1:A:363:ILE:HB	2.18	0.43
1:A:3887:PHE:HZ	1:A:3904:PHE:CE2	2.36	0.43
1:A:3908:HIS:O	1:A:3911:ILE:HG12	2.17	0.43
1:A:3915:HIS:CD2	1:A:3920:ILE:HD12	2.53	0.43
1:A:3810:VAL:O	1:A:3929:MSE:HG3	2.18	0.43
1:A:3961:PHE:CZ	1:A:3963:LEU:HD13	2.53	0.43
1:A:646:VAL:HG11	1:A:710:PHE:CG	2.54	0.43
1:A:764:PRO:HB2	1:A:848:LEU:HD11	2.00	0.43
1:A:992:ILE:CD1	1:A:1035:GLU:HB2	2.48	0.43
1:B:1015:ASP:HA	1:B:1018:VAL:CG2	2.47	0.43
1:B:1079:SER:O	1:B:1082:PHE:HB3	2.17	0.43
1:B:1153:LEU:HB3	1:B:1154:PRO:HD3	2.01	0.43
1:B:1218:SER:OG	1:B:1219:PHE:N	2.51	0.43
1:B:13:LEU:HA	1:B:16:GLN:HG2	2.00	0.43
1:B:1876:ILE:O	1:B:1876:ILE:HG12	2.17	0.43
1:B:217:LEU:HB3	1:B:264:ARG:HG3	2.00	0.43
1:B:2554:PHE:O	1:B:2557:LEU:HB2	2.18	0.43
1:B:280:SER:O	1:B:322:GLN:HG2	2.17	0.43
1:B:2923:TRP:CD1	1:B:2931:ARG:HD3	2.53	0.43
1:B:2979:GLN:H	1:B:2979:GLN:CD	2.22	0.43
1:B:3107:ILE:HG22	1:B:3111:MSE:HE2	1.98	0.43
1:B:3454:LEU:HD21	1:B:3461:ALA:HB2	1.99	0.43
1:B:3610:TYR:O	1:B:3613:MSE:HB3	2.18	0.43
1:B:3631:LYS:HB2	1:B:3685:PRO:HB2	2.00	0.43
1:B:3872:ARG:NH1	1:B:3965:ARG:HH12	2.16	0.43
1:B:70:ARG:HG3	1:B:78:PHE:CB	2.48	0.43
1:B:733:LEU:O	1:B:737:PRO:HG3	2.18	0.43
1:A:1073:PHE:CE1	1:A:3745:GLU:HA	2.53	0.43
1:A:1067:ALA:HA	1:A:1079:SER:HB2	2.00	0.43
1:A:1354:GLU:C	1:A:1356:TRP:H	2.21	0.43
1:A:1583:MSE:HE1	1:A:1640:GLU:OE2	2.17	0.43
1:A:1733:THR:N	1:A:1734:PRO:HD3	2.33	0.43
1:A:1747:LEU:HD13	1:A:1880:MSE:HE1	2.00	0.43
1:A:1950:SER:O	1:A:2000:ARG:NH1	2.51	0.43
1:A:2373:PRO:HA	1:A:2378:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2415:LEU:HD11	1:A:2419:ASP:OD2	2.17	0.43
1:A:2795:GLN:O	1:A:2799:GLN:HG2	2.18	0.43
1:A:2860:ASP:HB3	1:A:2868:LEU:HD22	2.00	0.43
1:A:2963:SER:O	1:A:2967:GLU:HG2	2.18	0.43
1:A:3547:THR:HB	1:A:3548:GLY:O	2.18	0.43
1:A:3921:GLY:C	1:A:3923:ARG:N	2.71	0.43
1:A:733:LEU:H	1:A:733:LEU:HG	1.61	0.43
1:A:681:LYS:HD2	1:A:746:ARG:NE	2.33	0.43
1:A:739:ASN:OD1	1:A:776:TRP:HA	2.19	0.43
1:A:784:VAL:O	1:A:787:PRO:HD2	2.18	0.43
1:B:1010:LEU:HA	1:B:1013:ILE:HG12	1.99	0.43
1:B:1039:TRP:CG	1:B:1055:ASN:HB2	2.53	0.43
1:B:1087:ARG:HD3	1:B:1134:LEU:CB	2.38	0.43
1:B:1945:TYR:O	1:B:1946:ASN:C	2.56	0.43
1:B:1945:TYR:O	1:B:1948:ALA:N	2.50	0.43
1:B:2110:PRO:HB2	1:B:2111:PRO:HD3	1.99	0.43
1:B:2286:PRO:HB2	1:B:2289:ASP:CA	2.40	0.43
1:B:2464:HIS:H	1:B:2465:PRO:CD	2.31	0.43
1:B:2927:ALA:HB2	1:B:2930:TYR:CD2	2.52	0.43
1:B:3110:PHE:CD1	1:B:3111:MSE:N	2.86	0.43
1:B:358:GLU:CG	1:B:359:LEU:N	2.81	0.43
1:B:3847:SER:HA	1:B:3857:LEU:HD22	2.00	0.43
1:B:3880:ALA:O	1:B:3884:LYS:HG3	2.18	0.43
1:B:4113:ASP:O	1:B:4116:ILE:N	2.47	0.43
1:B:451:PRO:O	1:B:454:GLN:HB3	2.18	0.43
1:B:572:VAL:HG13	1:B:573:LEU:N	2.33	0.43
1:A:1365:ASN:O	1:A:1369:MSE:HG2	2.17	0.43
1:A:1577:LEU:HD12	1:A:1578:ALA:HB2	2.01	0.43
1:A:1996:VAL:HG21	1:A:2047:THR:CB	2.48	0.43
1:A:2358:ASP:O	1:A:2361:ILE:HG22	2.18	0.43
1:A:3033:GLU:HB3	1:A:3038:GLU:OE1	2.19	0.43
1:A:342:MSE:O	1:A:345:PHE:HB2	2.18	0.43
1:A:348:ILE:HG23	1:A:357:LYS:HE3	1.99	0.43
1:A:3829:LEU:HA	1:A:3829:LEU:HD12	1.70	0.43
1:A:929:ALA:O	1:A:933:LEU:HB2	2.18	0.43
1:A:939:MSE:O	1:A:942:LEU:HB3	2.19	0.43
1:A:966:PHE:CE1	1:A:988:VAL:HG12	2.54	0.43
1:B:1107:TYR:CD2	1:B:1131:ILE:HD12	2.53	0.43
1:B:1147:LYS:O	1:B:1151:ARG:NE	2.52	0.43
1:B:1356:TRP:HA	1:B:1356:TRP:CE3	2.52	0.43
1:B:1550:VAL:HG23	1:B:1551:ILE:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1722:PHE:HB3	1:B:1723:PRO:HD3	1.99	0.43
1:B:2126:MSE:HE2	1:B:2156:VAL:CG2	2.48	0.43
1:B:2171:LEU:HG	1:B:2177:ASN:ND2	2.30	0.43
1:B:2323:LEU:CD2	1:B:2345:VAL:HG21	2.48	0.43
1:B:2408:MSE:HA	1:B:2408:MSE:CE	2.41	0.43
1:B:275:PHE:O	1:B:277:LEU:N	2.52	0.43
1:B:2788:SER:HA	1:B:2791:ILE:HG13	2.01	0.43
1:B:2923:TRP:CD1	1:B:2926:LEU:HD21	2.53	0.43
1:B:3008:TRP:H	1:B:3050:LYS:HG2	1.83	0.43
1:B:352:VAL:HG23	1:B:357:LYS:HG2	2.01	0.43
1:B:2937:ASP:OD1	1:B:3976:GLU:HA	2.18	0.43
1:B:554:ASN:O	1:B:558:GLU:OE2	2.37	0.43
1:B:620:PHE:HE2	1:B:641:PHE:CE2	2.37	0.43
1:B:717:LYS:HA	1:B:717:LYS:HD3	1.84	0.43
1:B:785:MSE:HB3	1:B:785:MSE:HE2	1.68	0.43
1:A:1087:ARG:HD3	1:A:1134:LEU:CD2	2.45	0.43
1:A:1652:ILE:CD1	1:A:1713:VAL:HG13	2.48	0.43
1:A:2915:ARG:O	1:A:2938:VAL:HG21	2.19	0.43
1:A:3008:TRP:N	1:A:3050:LYS:HG2	2.33	0.43
1:A:3583:LEU:HA	1:A:3583:LEU:HD23	1.85	0.43
1:A:732:PHE:HB2	1:A:733:LEU:CD2	2.48	0.43
1:B:139:ARG:HG3	1:B:173:LYS:HZ2	1.84	0.43
1:B:1633:TRP:NE1	1:B:1697:PRO:HG2	2.33	0.43
1:B:1856:THR:O	1:B:1860:GLU:HB2	2.18	0.43
1:B:2356:MSE:SE	1:B:2360:PHE:CZ	3.21	0.43
1:B:2926:LEU:HD12	1:B:3123:GLN:CD	2.38	0.43
1:B:3271:ASP:OD2	1:B:3272:TRP:CD1	2.72	0.43
1:B:3498:TRP:NE1	1:B:3502:MSE:SE	2.99	0.43
1:B:3480:LEU:HD22	1:B:3516:HIS:HB3	1.99	0.43
1:B:3682:GLU:C	1:B:3685:PRO:HD2	2.38	0.43
1:B:389:ILE:HG22	1:B:390:GLN:N	2.33	0.43
1:B:3904:PHE:HE1	1:B:3967:PHE:HE1	1.66	0.43
1:B:485:GLN:O	1:B:488:ILE:HG12	2.19	0.43
1:B:575:ILE:HD12	1:B:604:PRO:O	2.18	0.43
1:B:74:ASN:HB3	1:B:75:SER:H	1.45	0.43
1:B:910:PHE:CE2	1:B:941:MSE:SE	3.22	0.43
1:B:981:ARG:HA	1:B:984:TYR:CD2	2.52	0.43
1:A:1056:THR:OG1	1:A:1057:LYS:N	2.51	0.43
1:A:1014:LEU:HB2	1:A:1078:ALA:HA	2.01	0.43
1:A:1087:ARG:NE	1:A:1134:LEU:HD22	2.32	0.43
1:A:1645:VAL:HG12	1:A:1646:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1942:CYS:HB2	1:A:1990:PHE:CD1	2.54	0.43
1:A:226:GLY:O	1:A:230:LEU:HD23	2.19	0.43
1:A:2359:LYS:O	1:A:2362:VAL:HG22	2.18	0.43
1:A:2365:ASN:HB2	1:A:2400:VAL:HG13	1.99	0.43
1:A:2461:PHE:HE1	1:A:2469:CYS:SG	2.42	0.43
1:A:2463:SER:O	1:A:2464:HIS:ND1	2.51	0.43
1:A:2794:LEU:HA	1:A:2797:VAL:CG2	2.46	0.43
1:A:241:ASP:HB2	1:A:282:PHE:CE2	2.53	0.43
1:A:3052:LEU:HD23	1:A:3188:PHE:CZ	2.54	0.43
1:A:3253:SER:HA	1:A:3256:MSE:HB2	2.00	0.43
1:A:3683:CYS:SG	1:A:3736:LYS:NZ	2.90	0.43
1:A:3759:ARG:C	1:A:3761:ASP:H	2.21	0.43
1:A:448:GLN:O	1:A:449:TYR:CD1	2.71	0.43
1:A:572:VAL:HG13	1:A:573:LEU:N	2.29	0.43
1:A:963:LYS:HB3	1:A:1009:LEU:CD1	2.48	0.43
1:B:1401:ASN:O	1:B:1404:LYS:HB3	2.19	0.43
1:B:1916:ILE:O	1:B:1920:TYR:CD1	2.71	0.43
1:B:2040:MSE:HE2	1:B:2040:MSE:HB3	1.96	0.43
1:B:2066:PHE:HB3	1:B:2067:ARG:HG2	2.00	0.43
1:B:2311:ARG:HG3	1:B:2363:CYS:CB	2.43	0.43
1:B:2908:LYS:NZ	1:B:2986:PRO:CG	2.81	0.43
1:B:273:ARG:HA	1:B:318:SER:OG	2.19	0.43
1:B:3443:PRO:C	1:B:3445:LEU:H	2.21	0.43
1:B:3656:LEU:O	1:B:3659:PHE:HB2	2.19	0.43
1:B:3908:HIS:CD2	1:B:3967:PHE:CZ	3.06	0.43
1:B:657:SER:C	1:B:733:LEU:HD13	2.38	0.43
1:B:714:VAL:O	1:B:717:LYS:N	2.52	0.43
1:A:1332:TYR:CZ	1:A:1386:ILE:HG22	2.54	0.43
1:A:1565:GLU:HG2	1:A:1566:THR:HG23	2.00	0.43
1:A:1687:HIS:HB3	1:A:1691:GLN:HE22	1.83	0.43
1:A:185:HIS:O	1:A:186:PRO:C	2.56	0.43
1:A:2012:ARG:HA	1:A:2012:ARG:HD3	1.69	0.43
1:A:2227:LYS:HZ2	1:A:2232:ARG:C	2.21	0.43
1:A:2216:LEU:HD22	1:A:2249:LEU:HD21	2.01	0.43
1:A:224:LEU:HD13	1:A:248:ILE:HD13	2.01	0.43
1:A:2473:MSE:O	1:A:2477:LEU:HG	2.17	0.43
1:A:2538:ARG:NH1	1:A:2566:THR:H	2.08	0.43
1:A:2804:ILE:O	1:A:2806:LYS:N	2.46	0.43
1:A:3506:LEU:HD11	1:A:3555:VAL:HG13	2.00	0.43
1:A:3835:PRO:HB2	1:A:3836:PRO:HD3	2.00	0.43
1:A:3842:TRP:CZ3	1:A:3843:LEU:HD23	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:PRO:CA	1:A:476:ARG:HH22	2.18	0.43
1:A:680:ILE:HG12	1:A:701:TYR:HD1	1.79	0.43
1:B:112:THR:O	1:B:116:THR:OG1	2.25	0.43
1:B:1165:LEU:O	1:B:1168:LEU:N	2.50	0.43
1:B:1174:ALA:O	1:B:1178:ARG:HB2	2.18	0.43
1:B:1256:TRP:O	1:B:1259:LEU:N	2.51	0.43
1:B:1266:CYS:O	1:B:1270:PHE:CD2	2.72	0.43
1:B:1354:GLU:C	1:B:1356:TRP:H	2.22	0.43
1:B:390:GLN:NE2	1:B:1724:MSE:HB2	2.33	0.43
1:B:1885:PRO:O	1:B:1886:LYS:C	2.57	0.43
1:B:1920:TYR:O	1:B:1923:PHE:HB3	2.18	0.43
1:B:2083:LEU:HD13	1:B:2184:TYR:HE2	1.83	0.43
1:B:2482:ASP:CG	1:B:2485:ARG:HH21	2.21	0.43
1:B:2517:LEU:HA	1:B:2520:ILE:HG22	2.00	0.43
1:B:2557:LEU:HB3	1:B:2561:PHE:CZ	2.53	0.43
1:B:2936:TYR:CD2	1:B:3979:LEU:HD11	2.54	0.43
1:B:334:HIS:ND1	1:B:338:LEU:HD21	2.33	0.43
1:B:3564:GLN:C	1:B:3566:GLY:H	2.22	0.43
1:B:3572:ILE:CA	1:B:3575:LEU:HB3	2.49	0.43
1:B:3789:ARG:HB3	1:B:3938:ILE:CG2	2.49	0.43
1:B:3944:HIS:NE2	1:B:3948:SER:O	2.51	0.43
1:B:4075:ARG:O	1:B:4078:VAL:HG22	2.19	0.43
1:B:553:VAL:HB	1:B:637:LYS:NZ	2.31	0.43
1:B:669:LEU:HA	1:B:669:LEU:HD23	1.74	0.43
1:B:913:ARG:CB	1:B:934:LEU:HD12	2.48	0.43
1:A:2239:LYS:NZ	2:K:109:UNK:O	2.35	0.43
2:S:212:UNK:O	2:S:215:UNK:N	2.52	0.43
1:A:1112:ALA:HA	1:A:1115:HIS:CE1	2.54	0.43
1:A:1153:LEU:HB3	1:A:1154:PRO:HD3	2.00	0.43
1:A:1253:THR:HB	1:A:1254:LEU:HG	2.00	0.43
1:A:1330:TYR:CE1	1:A:1334:LYS:HE3	2.53	0.43
1:A:1433:ALA:HB1	1:A:1437:TYR:CZ	2.53	0.43
1:A:1808:ASP:CB	1:A:1814:PHE:HB3	2.30	0.43
1:A:2009:LYS:O	1:A:2010:GLU:HG3	2.18	0.43
1:A:2192:THR:HA	1:A:2195:SER:OG	2.19	0.43
1:A:257:ARG:N	1:A:258:PRO:CD	2.81	0.43
1:A:2876:VAL:HG22	1:A:3035:PHE:CZ	2.53	0.43
1:A:3272:TRP:CE3	1:A:3307:LEU:HD21	2.53	0.43
1:A:3283:LEU:HG	1:A:3300:VAL:CG2	2.48	0.43
1:A:3344:GLU:HB2	1:A:3348:LEU:CD1	2.48	0.43
1:A:3359:ILE:CG2	1:A:3391:ALA:HB3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3427:GLU:OE1	1:A:3435:ASP:HB3	2.19	0.43
1:A:3445:LEU:O	1:A:3449:LYS:NZ	2.42	0.43
1:A:474:VAL:HG21	1:A:1564:SER:OG	2.19	0.43
1:A:562:HIS:O	1:A:562:HIS:ND1	2.50	0.43
1:A:742:GLU:HB3	1:A:783:HIS:CG	2.54	0.43
1:B:963:LYS:CG	1:B:1009:LEU:HD11	2.49	0.43
1:B:1091:GLU:CG	1:B:1137:ILE:HD13	2.49	0.43
1:B:1214:GLU:O	1:B:1218:SER:OG	2.23	0.43
1:B:1349:LEU:HA	1:B:1353:PRO:CD	2.45	0.43
1:B:1353:PRO:HA	1:B:1358:LEU:CB	2.48	0.43
1:B:1725:GLN:O	1:B:1725:GLN:HG2	2.18	0.43
1:B:1991:PRO:HA	1:B:1994:VAL:HG12	2.00	0.43
1:B:1989:ASN:HB3	1:B:2040:MSE:HE2	2.01	0.43
1:B:2071:GLN:HA	1:B:2074:PRO:HG2	2.01	0.43
1:B:2257:PHE:CD1	1:B:2299:TYR:HB3	2.54	0.43
1:B:2437:ASP:O	1:B:2440:TYR:HB3	2.18	0.43
1:B:2515:PRO:HG2	1:B:2518:GLN:HE22	1.84	0.43
1:B:2548:PRO:O	1:B:2550:ILE:HG13	2.19	0.43
1:B:2987:THR:OG1	1:B:2991:LYS:HB2	2.19	0.43
1:B:3179:TRP:HZ2	1:B:3258:LEU:HG	1.83	0.43
1:B:3287:ARG:NH1	1:B:3328:ILE:HA	2.33	0.43
1:B:3319:ASN:O	1:B:3323:PHE:CD2	2.71	0.43
1:B:3498:TRP:HE1	1:B:3502:MSE:CG	2.32	0.43
1:B:3499:ILE:HD13	1:B:3499:ILE:HA	1.76	0.43
1:B:3630:ARG:O	1:B:3634:GLN:N	2.50	0.43
1:B:3696:ARG:HB2	1:B:3699:LEU:CB	2.48	0.43
1:B:744:ASP:C	1:B:746:ARG:N	2.70	0.43
1:B:767:GLU:HG3	1:B:851:ILE:HD11	2.01	0.43
1:B:892:LEU:HD23	1:B:907:LEU:HD13	2.01	0.43
1:A:1116:ALA:CB	1:A:1164:CYS:HB3	2.49	0.43
1:A:1508:LYS:NZ	1:A:1516:GLU:HG3	2.33	0.43
1:A:175:TYR:CZ	1:A:204:LEU:HD11	2.54	0.43
1:A:2312:TYR:O	1:A:2315:VAL:HG22	2.19	0.43
1:A:2837:LEU:HG	1:A:2837:LEU:H	1.51	0.43
1:A:3252:PHE:HA	1:A:3282:ARG:CZ	2.48	0.43
1:A:342:MSE:O	1:A:342:MSE:HG2	2.17	0.43
1:A:3884:LYS:N	1:A:3970:LEU:HD12	2.34	0.43
1:A:3955:VAL:O	1:A:3955:VAL:HG13	2.18	0.43
1:A:4066:LEU:CD2	1:A:4075:ARG:HG3	2.45	0.43
1:A:568:PHE:HZ	1:A:653:LEU:HG	1.84	0.43
1:A:595:ASP:CG	1:A:1026:ARG:HG3	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:798:GLY:O	1:A:801:LYS:HE2	2.19	0.43
1:A:901:MSE:HE1	1:A:2539:LEU:HD21	2.00	0.43
1:A:937:MSE:HA	1:A:940:PHE:CD1	2.53	0.43
1:A:984:TYR:O	1:A:988:VAL:HG13	2.19	0.43
1:B:1038:LYS:HA	1:B:1038:LYS:HD2	1.85	0.43
1:B:993:HIS:CB	1:B:1038:LYS:HG2	2.37	0.43
1:B:14:ARG:O	1:B:18:THR:HG23	2.18	0.43
1:B:1871:MSE:CA	1:B:1874:TYR:HB2	2.45	0.43
1:B:2138:VAL:HA	1:B:2141:ASN:ND2	2.34	0.43
1:B:224:LEU:O	1:B:228:SER:OG	2.34	0.43
1:B:2276:LEU:O	1:B:2279:ILE:HB	2.18	0.43
1:B:197:PHE:CE1	1:B:230:LEU:HD22	2.53	0.43
1:B:2401:VAL:O	1:B:2405:VAL:HG13	2.19	0.43
1:B:2433:LYS:O	1:B:2436:LEU:N	2.44	0.43
1:B:2443:MSE:HB3	1:B:2480:ILE:CG1	2.43	0.43
1:B:2510:LEU:HG	1:B:2522:ARG:HE	1.84	0.43
1:B:2575:PRO:HG3	1:B:2789:SER:OG	2.18	0.43
1:B:2989:ALA:HA	1:B:2992:ASP:HB2	1.99	0.43
1:B:3329:LEU:HA	1:B:3329:LEU:HD23	1.80	0.43
1:B:3503:VAL:HG21	1:B:3535:ILE:C	2.39	0.43
1:B:3531:TYR:CD2	1:B:3707:GLY:HA3	2.53	0.43
1:B:3788:LEU:HD12	1:B:3788:LEU:HA	1.74	0.43
1:B:458:CYS:HA	1:B:461:ILE:HD12	2.01	0.43
1:B:766:ALA:HB1	1:B:768:VAL:HG23	2.00	0.43
1:B:948:MSE:N	1:B:949:PRO:HD3	2.34	0.43
1:A:996:THR:O	1:A:1042:LYS:HG2	2.19	0.43
1:A:175:TYR:HA	1:A:178:LEU:HD12	2.00	0.43
1:A:1883:ARG:HG3	1:A:1884:LEU:N	2.33	0.43
1:A:1949:ILE:CD1	1:A:1952:ILE:HG21	2.48	0.43
1:A:2379:MSE:SE	1:A:2404:ARG:HD3	2.69	0.43
1:A:2439:ILE:O	1:A:2441:LYS:N	2.52	0.43
1:A:3155:VAL:N	1:A:3156:PRO:CD	2.82	0.43
1:A:3314:SER:HB2	1:A:3315:TYR:O	2.19	0.43
1:A:3495:PHE:HA	1:A:3498:TRP:CZ2	2.54	0.43
1:A:3651:LEU:HA	1:A:3654:MSE:HE3	2.01	0.43
1:A:514:VAL:CG1	1:A:610:ALA:HB1	2.49	0.43
1:A:763:THR:N	1:A:764:PRO:HD3	2.34	0.43
1:A:745:VAL:HG11	1:A:776:TRP:CZ2	2.54	0.43
1:A:905:ILE:O	1:A:906:PHE:HB2	2.18	0.43
1:A:981:ARG:CG	1:A:982:GLN:N	2.81	0.43
1:B:103:TYR:O	1:B:106:GLU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1222:ASN:O	1:B:1225:GLU:HB2	2.18	0.43
1:B:125:ILE:H	1:B:126:PRO:HD2	1.84	0.43
1:B:130:LEU:HD12	1:B:130:LEU:HA	1.65	0.43
1:B:173:LYS:O	1:B:174:VAL:C	2.57	0.43
1:B:2253:TYR:HA	1:B:2256:ILE:HB	2.01	0.43
1:B:2526:SER:O	1:B:2530:ARG:HB3	2.19	0.43
1:B:2841:ASN:HD22	1:B:2871:LEU:HD23	1.84	0.43
1:B:2943:PHE:CE2	1:B:2944:THR:HG23	2.54	0.43
1:B:3262:LEU:HD12	1:B:3266:SER:OG	2.18	0.43
1:B:3424:LEU:CD1	1:B:3439:LEU:HD11	2.49	0.43
1:B:3480:LEU:HB3	1:B:3516:HIS:HB2	2.01	0.43
1:B:3525:TYR:O	1:B:3529:ILE:HB	2.19	0.43
1:B:3174:ASP:OD2	1:B:3783:GLN:HG3	2.19	0.43
1:B:385:TYR:HA	1:B:388:LEU:HB3	2.00	0.43
1:B:3984:MSE:O	1:B:3987:ALA:HB3	2.18	0.43
1:B:4020:MSE:HE3	1:B:4027:TRP:HE1	1.84	0.43
1:B:892:LEU:HD11	1:B:958:MSE:CG	2.49	0.43
1:B:933:LEU:HD11	1:B:2795:GLN:OE1	2.19	0.43
1:A:1133:HIS:ND1	1:A:1136:ARG:HD2	2.34	0.43
1:A:184:VAL:O	1:A:185:HIS:CG	2.72	0.43
1:A:2399:GLU:HA	1:A:2402:LEU:HD23	2.01	0.43
1:A:3167:ARG:HG2	1:A:3186:ARG:NH2	2.33	0.43
1:A:3141:PHE:CE1	1:A:3193:ILE:HG13	2.49	0.43
1:A:3617:LEU:CD1	1:A:3644:PHE:HD2	2.30	0.43
1:A:3908:HIS:CD2	1:A:3912:CYS:SG	3.12	0.43
1:A:3917:ILE:O	1:A:4048:LYS:HE2	2.19	0.43
1:A:3951:GLN:NE2	1:A:4068:HIS:CE1	2.87	0.43
1:A:4074:PHE:O	1:A:4077:TYR:HB3	2.19	0.43
1:A:435:LEU:O	1:A:439:VAL:HG23	2.19	0.43
1:A:47:SER:O	1:A:51:LEU:HB2	2.19	0.43
1:A:634:LEU:HD22	1:A:667:TYR:CD1	2.53	0.43
1:A:70:ARG:CD	1:A:82:ARG:HD3	2.38	0.43
1:A:939:MSE:HA	1:A:939:MSE:HE3	2.01	0.43
1:B:1017:ILE:HA	1:B:1021:VAL:O	2.18	0.43
1:B:1027:ASP:O	1:B:1031:ARG:HG2	2.19	0.43
1:B:1296:PHE:CE1	1:B:1362:ASP:HB2	2.53	0.43
1:B:1296:PHE:CZ	1:B:1362:ASP:HB2	2.54	0.43
1:B:1449:ALA:O	1:B:1453:SER:OG	2.28	0.43
1:B:1874:TYR:CE1	1:B:1881:TYR:CG	3.06	0.43
1:B:2167:PRO:CB	1:B:2171:LEU:HD22	2.47	0.43
1:B:2461:PHE:HA	1:B:2464:HIS:ND1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2871:LEU:O	1:B:2873:PRO:HD3	2.19	0.43
1:B:2879:GLY:CA	1:B:2886:GLN:HG2	2.31	0.43
1:B:3020:ASP:OD2	1:B:3024:PRO:HA	2.18	0.43
1:B:3179:TRP:CG	1:B:3179:TRP:O	2.71	0.43
1:B:3266:SER:HB3	1:B:3271:ASP:HB2	2.01	0.43
1:B:348:ILE:O	1:B:364:ARG:HD3	2.19	0.43
1:B:3575:LEU:HB2	1:B:3686:TRP:CZ3	2.54	0.43
1:B:3830:SER:O	1:B:3833:ARG:N	2.50	0.43
1:B:2858:ILE:HG23	1:B:3894:PRO:HG3	2.00	0.43
1:B:396:PHE:CE1	1:B:397:LEU:HG	2.54	0.43
1:B:3989:ARG:HE	1:B:4100:GLU:HB3	1.83	0.43
1:B:4003:ASP:O	1:B:4006:VAL:HG22	2.19	0.43
1:B:408:TYR:O	1:B:411:PRO:HD2	2.19	0.43
1:B:560:LEU:HA	1:B:563:LEU:HD12	2.00	0.43
1:B:719:LYS:HE3	1:B:750:PRO:HB2	2.01	0.43
1:A:971:ARG:HD2	1:A:1024:THR:OG1	2.18	0.42
1:A:1073:PHE:HD1	1:A:1074:LYS:CG	2.31	0.42
1:A:1305:ASP:OD1	1:A:1334:LYS:HD2	2.18	0.42
1:A:1913:LYS:O	1:A:1915:LEU:N	2.52	0.42
1:A:194:GLU:HA	1:A:197:PHE:CD2	2.51	0.42
1:A:2299:TYR:O	1:A:2302:ALA:HB3	2.19	0.42
1:A:2645:UNK:HA	1:A:2649:UNK:O	2.20	0.42
1:A:3049:LEU:HA	1:A:3188:PHE:HZ	1.82	0.42
1:A:3076:ALA:HB1	1:A:3080:LEU:CD1	2.48	0.42
1:A:3144:PHE:HZ	1:A:3193:ILE:HD11	1.84	0.42
1:A:3619:ASP:O	1:A:3625:LEU:HB2	2.19	0.42
1:A:3675:LYS:N	1:A:3676:PRO:HD2	2.33	0.42
1:A:3690:PHE:CD1	1:A:3692:VAL:HG23	2.54	0.42
1:A:3906:SER:O	1:A:3910:LEU:HD13	2.18	0.42
1:A:3955:VAL:CG1	1:A:4027:TRP:HE1	2.25	0.42
1:A:4113:ASP:HB3	1:A:4116:ILE:HG13	2.00	0.42
1:A:446:PHE:CD1	1:A:446:PHE:N	2.75	0.42
1:A:892:LEU:HG	1:A:958:MSE:SE	2.69	0.42
1:B:1033:ILE:HD11	1:B:1089:PHE:HE2	1.84	0.42
1:B:1455:CYS:HA	1:B:1458:LEU:HD12	2.00	0.42
1:B:146:GLU:HG3	1:B:149:ILE:HD12	2.00	0.42
1:B:1574:ASN:CG	1:B:1582:LEU:HD21	2.40	0.42
1:B:1718:ILE:CG2	1:B:1750:LEU:HD11	2.40	0.42
1:B:1812:LEU:HD13	1:B:1814:PHE:HD2	1.84	0.42
1:B:1981:LEU:HA	1:B:1984:LEU:CD2	2.48	0.42
1:B:2452:ARG:O	1:B:2455:LEU:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2804:ILE:O	1:B:2806:LYS:N	2.50	0.42
1:B:3104:GLN:O	1:B:3107:ILE:HB	2.19	0.42
1:B:856:VAL:HG11	1:B:3110:PHE:CZ	2.54	0.42
1:B:3252:PHE:CE2	1:B:3289:ARG:NH2	2.87	0.42
1:B:3390:GLN:O	1:B:3394:GLU:HB2	2.18	0.42
1:B:3483:MSE:O	1:B:3486:GLU:HG2	2.19	0.42
1:B:3525:TYR:HA	1:B:3529:ILE:CG2	2.49	0.42
1:B:381:VAL:HB	1:B:384:MSE:SE	2.68	0.42
1:B:3985:VAL:O	1:B:3988:LEU:N	2.51	0.42
1:B:4077:TYR:CG	1:B:4119:ARG:NH2	2.87	0.42
1:B:4093:GLU:O	1:B:4095:GLU:HG2	2.19	0.42
1:B:432:THR:HB	1:B:433:PRO:CD	2.48	0.42
1:B:963:LYS:O	1:B:967:PRO:HD3	2.20	0.42
1:B:993:HIS:C	1:B:993:HIS:ND1	2.73	0.42
1:A:1812:LEU:O	1:A:1815:THR:HG23	2.19	0.42
1:A:361:ILE:HG21	1:A:1858:LEU:HD23	2.01	0.42
1:A:1882:SER:O	1:A:1885:PRO:HD2	2.19	0.42
1:A:2070:GLU:CG	1:A:2072:ARG:HG3	2.33	0.42
1:A:2251:ILE:HG23	1:A:2288:TYR:HD2	1.84	0.42
1:A:2358:ASP:HB3	1:A:2389:PHE:CE1	2.54	0.42
1:A:2552:VAL:HG22	1:A:2553:HIS:ND1	2.35	0.42
1:A:262:LEU:H	1:A:262:LEU:HG	1.62	0.42
1:A:2943:PHE:O	1:A:2945:SER:N	2.45	0.42
1:A:293:LEU:HA	1:A:296:VAL:HG12	2.00	0.42
1:A:3174:ASP:HA	1:A:3249:GLN:NE2	2.34	0.42
1:A:3397:GLN:HE21	1:A:3413:TYR:HD1	1.63	0.42
1:A:3435:ASP:O	1:A:3439:LEU:HB2	2.18	0.42
1:A:3583:LEU:HD22	1:A:3587:ASP:OD2	2.19	0.42
1:A:349:ILE:HD12	1:A:368:LEU:HD12	1.99	0.42
1:A:3806:LEU:HG	1:A:3807:GLU:N	2.33	0.42
1:B:1157:PHE:HB3	1:B:1169:VAL:HG22	2.02	0.42
1:B:1263:ALA:HB1	1:B:1267:TYR:HE1	1.84	0.42
1:B:1389:VAL:O	1:B:1389:VAL:HG12	2.19	0.42
1:B:138:PHE:HD2	1:B:173:LYS:CE	2.25	0.42
1:B:1583:MSE:HE2	1:B:1639:LEU:C	2.40	0.42
1:B:1727:ARG:O	1:B:1730:PRO:HD2	2.19	0.42
1:B:1992:VAL:HG11	1:B:2044:ASP:OD1	2.19	0.42
1:B:2125:TRP:CZ3	1:B:2129:LEU:HD21	2.55	0.42
1:B:2255:LEU:HD12	1:B:2258:GLU:HB2	2.01	0.42
1:B:2291:GLN:O	1:B:2294:ILE:N	2.53	0.42
1:B:2325:LEU:O	1:B:2329:TYR:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2320:ALA:CA	1:B:2367:VAL:HG23	2.49	0.42
1:B:2776:ARG:H	1:B:2776:ARG:HG2	1.59	0.42
1:B:3047:SER:HB2	1:B:3050:LYS:CE	2.48	0.42
1:B:346:TYR:HA	1:B:349:ILE:HD12	2.01	0.42
1:B:3470:GLN:HG2	1:B:3474:ARG:HH11	1.83	0.42
1:B:367:GLY:C	1:B:369:PHE:N	2.69	0.42
1:B:3987:ALA:O	1:B:3991:PHE:HD1	2.01	0.42
1:B:4019:LYS:HA	1:B:4019:LYS:HE2	2.01	0.42
1:B:44:LEU:H	1:B:44:LEU:HG	1.71	0.42
1:B:487:LEU:CD2	1:B:530:LEU:HB2	2.49	0.42
1:B:560:LEU:HB2	1:B:616:LYS:HG2	2.01	0.42
1:B:775:GLU:O	1:B:779:TYR:CD2	2.70	0.42
1:B:970:LEU:CD2	1:B:1031:ARG:NH2	2.78	0.42
2:S:212:UNK:C	2:S:214:UNK:N	2.82	0.42
1:A:131:LEU:HD23	1:A:135:LEU:HD11	2.02	0.42
1:A:1345:THR:HG22	1:A:1349:LEU:HD12	2.01	0.42
1:A:143:LEU:CD1	1:A:143:LEU:H	2.25	0.42
1:A:1798:LEU:O	1:A:1802:TYR:HB2	2.19	0.42
1:A:1955:VAL:HA	1:A:2003:LYS:HZ2	1.85	0.42
1:A:2167:PRO:HA	1:A:2171:LEU:H	1.84	0.42
1:A:2300:PHE:HZ	1:A:2341:LEU:HD22	1.83	0.42
1:A:14:ARG:HH12	1:A:2392:VAL:HG11	1.83	0.42
1:A:2462:VAL:HG13	1:A:2470:ARG:HE	1.84	0.42
1:A:3069:MSE:HA	1:A:3072:GLU:HB3	2.02	0.42
1:A:3465:PHE:HD1	1:A:3483:MSE:SE	2.52	0.42
1:A:3557:ARG:O	1:A:3560:SER:HB3	2.19	0.42
1:A:3587:ASP:HB3	1:A:4022:LYS:HZ2	1.85	0.42
1:A:3640:PHE:O	1:A:3644:PHE:CG	2.72	0.42
1:A:3568:ILE:HG21	1:A:3699:LEU:HD21	2.01	0.42
1:A:3972:LEU:HD12	1:A:3974:MSE:HE3	2.01	0.42
1:A:568:PHE:O	1:A:571:SER:N	2.52	0.42
1:A:658:THR:HA	1:A:733:LEU:CD2	2.38	0.42
1:A:901:MSE:SE	1:A:2536:LEU:HD21	2.69	0.42
1:B:1163:LEU:CD2	1:B:1260:LEU:HD11	2.47	0.42
1:B:1353:PRO:HG3	1:B:1358:LEU:HB3	2.02	0.42
1:B:2012:ARG:HA	1:B:2012:ARG:HD3	1.79	0.42
1:B:2171:LEU:CD2	1:B:2177:ASN:HD21	2.32	0.42
1:B:2424:MSE:HA	1:B:2436:LEU:HD12	2.01	0.42
1:B:2928:LYS:HB3	1:B:3784:ARG:CG	2.49	0.42
1:B:294:PHE:CE2	1:B:298:LEU:HD21	2.55	0.42
1:B:3624:GLY:O	1:B:3625:LEU:HD23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3754:GLY:HA2	1:B:3800:LEU:HB2	2.02	0.42
1:B:3946:PHE:HE2	1:B:4048:LYS:HD2	1.84	0.42
1:B:403:GLY:O	1:B:405:ASP:N	2.52	0.42
1:B:557:SER:O	1:B:560:LEU:HG	2.19	0.42
1:B:808:GLU:CD	1:B:3114:TYR:HB3	2.40	0.42
1:B:892:LEU:HD11	1:B:958:MSE:CB	2.49	0.42
1:B:932:GLU:O	1:B:935:HIS:HB3	2.18	0.42
1:A:1475:LEU:O	1:A:1479:VAL:HG23	2.20	0.42
1:A:153:PHE:HA	1:A:156:PHE:CD2	2.54	0.42
1:A:1632:TRP:N	1:A:1632:TRP:CD1	2.86	0.42
1:A:177:LEU:HA	1:A:180:LEU:HD12	2.01	0.42
1:A:1968:SER:O	1:A:1971:PRO:HD2	2.19	0.42
1:A:1999:GLU:OE1	1:A:2051:SER:HB2	2.20	0.42
1:A:2023:SER:HB2	1:A:2024:TYR:CE1	2.54	0.42
1:A:2386:LEU:HA	1:A:2386:LEU:HD23	1.75	0.42
1:A:2473:MSE:HE2	1:A:2473:MSE:HB3	1.90	0.42
1:A:2797:VAL:HG12	1:A:2800:ARG:NH1	2.34	0.42
1:A:2926:LEU:HD22	1:A:2931:ARG:NE	2.34	0.42
1:A:3247:ARG:NE	1:A:3278:GLN:OE1	2.50	0.42
1:A:3272:TRP:CZ3	1:A:3307:LEU:HD11	2.55	0.42
1:A:3315:TYR:CG	1:A:3316:LEU:N	2.88	0.42
1:A:438:LEU:HA	1:A:438:LEU:HD12	1.87	0.42
1:A:560:LEU:CB	1:A:616:LYS:HZ3	2.05	0.42
1:B:1064:TYR:CD1	1:B:1106:ILE:HD11	2.55	0.42
1:B:1300:SER:O	1:B:1304:HIS:ND1	2.35	0.42
1:B:1493:PRO:O	1:B:1497:ARG:HG2	2.20	0.42
1:B:1596:VAL:HG13	1:B:1597:LEU:H	1.83	0.42
1:B:1608:ARG:NE	1:B:1608:ARG:O	2.51	0.42
1:B:2360:PHE:O	1:B:2364:LEU:HG	2.19	0.42
1:B:2379:MSE:HE1	1:B:2404:ARG:CD	2.42	0.42
1:B:2424:MSE:HA	1:B:2436:LEU:CD1	2.49	0.42
1:B:3005:LEU:O	1:B:3254:LEU:HD21	2.20	0.42
1:B:3118:ASP:N	1:B:3118:ASP:OD1	2.51	0.42
1:B:3251:ASN:ND2	1:B:3254:LEU:HD13	2.35	0.42
1:B:3324:ARG:O	1:B:3328:ILE:HG13	2.20	0.42
1:B:3479:THR:O	1:B:3483:MSE:CB	2.63	0.42
1:B:3570:ASP:HA	1:B:3573:ASN:HB3	2.02	0.42
1:B:3612:ARG:O	1:B:3615:ALA:HB3	2.19	0.42
1:B:3704:GLN:HG3	1:B:3796:MSE:SE	2.68	0.42
1:B:3775:LEU:HD13	1:B:3781:CYS:SG	2.59	0.42
1:B:3705:TYR:HD2	1:B:3792:SER:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3819:THR:O	1:B:3823:GLU:HG2	2.18	0.42
1:B:3501:HIS:ND1	1:B:4008:GLU:OE1	2.52	0.42
1:B:436:GLU:O	1:B:439:VAL:HB	2.20	0.42
1:B:493:LYS:HB3	1:B:494:PRO:HD2	2.00	0.42
1:B:742:GLU:HA	1:B:745:VAL:HG23	2.01	0.42
1:B:766:ALA:C	1:B:768:VAL:H	2.17	0.42
1:B:88:PHE:HB3	1:B:92:PHE:CZ	2.55	0.42
1:B:971:ARG:O	1:B:974:CYS:HB3	2.19	0.42
1:A:1019:ASP:HB2	1:A:1021:VAL:HG23	2.00	0.42
1:A:1238:GLN:HG3	1:A:1298:LEU:HD21	2.01	0.42
1:A:1469:PRO:HG3	1:A:1510:LEU:HD21	2.00	0.42
1:A:1718:ILE:CG2	1:A:1750:LEU:HD11	2.48	0.42
1:A:1970:LYS:HZ3	1:A:2017:GLY:HA3	1.85	0.42
1:A:2136:PRO:C	1:A:2139:PRO:HD2	2.39	0.42
1:A:2322:VAL:HG12	1:A:2323:LEU:N	2.35	0.42
1:A:2367:VAL:O	1:A:2371:PHE:HE1	2.03	0.42
1:A:2357:GLU:CD	1:A:2388:LYS:HZ1	2.22	0.42
1:A:2408:MSE:O	1:A:2409:THR:OG1	2.31	0.42
1:A:2548:PRO:O	1:A:2550:ILE:HG13	2.18	0.42
1:A:2869:LEU:HD23	1:A:2893:LEU:HA	2.01	0.42
1:A:866:ILE:HG21	1:A:3129:LEU:HD22	2.02	0.42
1:A:2961:ALA:HB3	1:A:3254:LEU:CD1	2.49	0.42
1:A:3343:SER:O	1:A:3345:PRO:HD3	2.19	0.42
1:A:367:GLY:O	1:A:369:PHE:N	2.52	0.42
1:A:3766:GLN:O	1:A:3770:VAL:HG23	2.20	0.42
1:A:4037:ASN:O	1:A:4037:ASN:ND2	2.53	0.42
1:A:463:LYS:O	1:A:466:LEU:HB3	2.19	0.42
1:A:481:THR:O	1:A:485:GLN:HG2	2.18	0.42
1:A:560:LEU:HA	1:A:563:LEU:HD12	2.01	0.42
1:A:736:LEU:HA	1:A:739:ASN:HB2	2.02	0.42
1:A:678:LYS:HB2	1:A:743:LEU:HD13	2.02	0.42
1:A:924:ARG:H	1:A:924:ARG:HG2	1.74	0.42
1:B:1726:SER:O	1:B:1729:PHE:HB3	2.19	0.42
1:B:177:LEU:H	1:B:177:LEU:HG	1.63	0.42
1:B:1890:HIS:HE1	1:B:1941:HIS:CD2	2.38	0.42
1:B:1952:ILE:HG12	1:B:1953:CYS:N	2.35	0.42
1:B:224:LEU:HD13	1:B:248:ILE:HD13	2.00	0.42
1:B:2555:LEU:HD12	1:B:2556:SER:N	2.32	0.42
1:B:2646:UNK:HA	1:B:2778:GLY:HA3	2.00	0.42
1:B:2794:LEU:HA	1:B:2794:LEU:HD23	1.80	0.42
1:B:2957:LEU:HD21	1:B:4101:GLU:CG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3119:VAL:HG21	1:B:3899:ALA:CB	2.48	0.42
1:B:356:ASN:CG	1:B:1859:ASN:H	2.23	0.42
1:B:3629:ARG:NH2	1:B:3638:LYS:HZ1	2.17	0.42
1:B:3631:LYS:HD2	1:B:3681:LYS:O	2.19	0.42
1:B:3824:GLU:O	1:B:3829:LEU:HD13	2.19	0.42
1:B:3850:HIS:H	1:B:3850:HIS:CD2	2.37	0.42
1:B:3791:TYR:OH	1:B:3942:PHE:CE2	2.70	0.42
1:B:575:ILE:HG13	1:B:579:LEU:HD13	2.01	0.42
1:B:957:PRO:O	1:B:961:LEU:HB2	2.20	0.42
1:A:1700:THR:OG1	1:A:1701:SER:N	2.48	0.42
1:A:172:GLU:HG3	1:A:173:LYS:N	2.35	0.42
1:A:402:THR:HB	1:A:1763:THR:HB	2.02	0.42
1:A:154:SER:OG	1:A:181:LEU:HD13	2.19	0.42
1:A:1915:LEU:HD12	1:A:1916:ILE:N	2.34	0.42
1:A:1890:HIS:CB	1:A:1937:ARG:HD2	2.46	0.42
1:A:1970:LYS:NZ	1:A:2017:GLY:CA	2.83	0.42
1:A:2311:ARG:O	1:A:2311:ARG:HG2	2.19	0.42
1:A:899:ARG:HH22	1:A:2570:PRO:HB2	1.83	0.42
1:A:2813:PHE:HA	1:A:2816:ILE:CG2	2.47	0.42
1:A:3034:PRO:C	1:A:3036:TYR:H	2.23	0.42
1:A:3101:TYR:HE2	1:A:3102:TYR:CE1	2.38	0.42
1:A:3198:THR:OG1	1:A:3199:PRO:HD3	2.19	0.42
1:A:3530:VAL:HG11	1:A:3700:GLU:O	2.18	0.42
1:A:3771:MSE:O	1:A:3775:LEU:HG	2.20	0.42
1:A:3923:ARG:CG	1:A:3962:ARG:HH22	2.00	0.42
1:A:396:PHE:CZ	1:A:437:HIS:CD2	3.07	0.42
1:A:655:LEU:HA	1:A:658:THR:OG1	2.18	0.42
1:A:774:GLU:OE2	1:A:854:ARG:HB2	2.19	0.42
1:A:952:GLY:C	1:A:954:GLY:H	2.23	0.42
1:B:1166:LEU:HB3	1:B:1170:LYS:HZ1	1.83	0.42
1:B:1270:PHE:HZ	1:B:1347:THR:C	2.23	0.42
1:B:1437:TYR:O	1:B:1439:PRO:HD2	2.20	0.42
1:B:1718:ILE:HG23	1:B:1750:LEU:CD1	2.40	0.42
1:B:1751:GLU:H	1:B:1751:GLU:HG3	1.57	0.42
1:B:1763:THR:N	1:B:1864:ASP:OD2	2.52	0.42
1:B:1889:VAL:HG22	1:B:1900:PHE:CE2	2.54	0.42
1:B:1927:MSE:C	1:B:1929:GLY:N	2.72	0.42
1:B:2074:PRO:HB2	1:B:2075:THR:H	1.75	0.42
1:B:2168:LEU:HG	1:B:2168:LEU:H	1.56	0.42
1:B:2602:UNK:CB	1:B:2790:LEU:HD23	2.49	0.42
1:B:2823:PHE:CG	1:B:2824:LYS:N	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2900:LEU:HD12	1:B:2905:LEU:HD21	2.02	0.42
1:B:3034:PRO:C	1:B:3036:TYR:H	2.23	0.42
1:B:3039:THR:O	1:B:3042:PRO:HD2	2.19	0.42
1:B:3141:PHE:HZ	1:B:3192:LYS:CB	2.31	0.42
1:B:3167:ARG:NH1	1:B:3167:ARG:CG	2.71	0.42
1:B:3255:ALA:HB1	1:B:3282:ARG:CZ	2.49	0.42
1:B:3585:PHE:CD1	1:B:3613:MSE:HE1	2.53	0.42
1:B:3588:TRP:NE1	1:B:3609:MSE:O	2.39	0.42
1:B:3763:ARG:HH21	1:B:4009:PRO:HG3	1.85	0.42
1:B:627:VAL:CG1	1:B:628:GLU:N	2.81	0.42
1:B:890:LYS:HD3	1:B:890:LYS:HA	1.85	0.42
1:B:898:PHE:HD2	1:B:2566:THR:OG1	2.02	0.42
1:A:1002:GLU:O	1:A:1005:ASP:OD2	2.38	0.42
1:A:1069:HIS:H	1:A:1070:PRO:CD	2.32	0.42
1:A:1093:GLU:HB3	1:A:1096:VAL:CG1	2.50	0.42
1:A:1360:LYS:HG3	1:A:1360:LYS:H	1.52	0.42
1:A:1372:LEU:HG	1:A:1418:HIS:HE1	1.85	0.42
1:A:136:GLN:HG2	1:A:139:ARG:HH11	1.84	0.42
1:A:170:VAL:CG2	1:A:173:LYS:HD3	2.47	0.42
1:A:1817:GLN:NE2	1:A:1821:ASP:HB2	2.35	0.42
1:A:1960:LYS:HB2	1:A:1998:MSE:SE	2.70	0.42
1:A:2065:ARG:HB3	1:A:2125:TRP:HD1	1.82	0.42
1:A:2292:CYS:CB	1:A:2300:PHE:HB2	2.38	0.42
1:A:197:PHE:CZ	1:A:230:LEU:HD22	2.54	0.42
1:A:2375:ALA:HB1	1:A:2411:LEU:CD2	2.49	0.42
1:A:2384:PHE:C	1:A:2387:PRO:HD2	2.39	0.42
1:A:2411:LEU:HG	1:A:2412:TYR:N	2.34	0.42
1:A:2433:LYS:O	1:A:2436:LEU:N	2.46	0.42
1:A:2434:VAL:O	1:A:2438:ILE:HG13	2.19	0.42
1:A:2990:GLU:O	1:A:2994:TRP:CD1	2.72	0.42
1:A:3181:ASP:HA	1:A:3184:THR:HG23	2.02	0.42
1:A:3450:MSE:O	1:A:3454:LEU:HG	2.20	0.42
1:A:3503:VAL:HG21	1:A:3535:ILE:C	2.40	0.42
1:A:3513:ALA:O	1:A:3518:VAL:HB	2.20	0.42
1:A:3575:LEU:O	1:A:3686:TRP:HH2	2.03	0.42
1:A:3619:ASP:N	1:A:3620:PRO:HD2	2.34	0.42
1:A:3745:GLU:O	1:A:3745:GLU:HG2	2.20	0.42
1:A:3839:TYR:CE2	1:A:3843:LEU:HD11	2.54	0.42
1:A:3955:VAL:HG22	1:A:3957:GLU:HG3	2.01	0.42
1:A:580:ASP:O	1:A:584:GLU:N	2.53	0.42
1:A:649:PHE:C	1:A:651:TYR:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:GLU:OE1	1:A:783:HIS:CD2	2.72	0.42
1:A:929:ALA:O	1:A:933:LEU:CB	2.67	0.42
1:A:927:LYS:HE2	1:A:976:VAL:HG12	2.02	0.42
1:B:963:LYS:HG3	1:B:1009:LEU:HD11	2.00	0.42
1:B:1580:LEU:HD13	1:B:1639:LEU:HB3	2.00	0.42
1:B:1655:ILE:HD12	1:B:1655:ILE:H	1.85	0.42
1:B:1679:LEU:O	1:B:1683:LYS:HG3	2.19	0.42
1:B:1756:PRO:C	1:B:1758:LEU:N	2.71	0.42
1:B:2255:LEU:HD13	1:B:2258:GLU:OE1	2.20	0.42
1:B:2405:VAL:HB	1:B:2439:ILE:CD1	2.49	0.42
1:B:2411:LEU:HG	1:B:2412:TYR:N	2.35	0.42
1:B:2474:TYR:O	1:B:2478:MSE:HG3	2.19	0.42
1:B:2520:ILE:HG13	1:B:2524:PHE:CE2	2.55	0.42
1:B:2637:UNK:O	1:B:2641:UNK:CB	2.67	0.42
1:B:2933:ILE:HG22	1:B:2937:ASP:OD2	2.20	0.42
1:B:3258:LEU:HA	1:B:3258:LEU:HD22	1.75	0.42
1:B:3427:GLU:HG3	1:B:3439:LEU:HD13	2.01	0.42
1:B:3522:THR:OG1	1:B:3558:ILE:HD11	2.20	0.42
1:B:3816:LEU:HD23	1:B:3816:LEU:HA	1.84	0.42
1:B:558:GLU:HA	1:B:561:ASN:ND2	2.35	0.42
1:B:576:VAL:HG13	1:B:601:TRP:CE3	2.41	0.42
1:B:38:LEU:HD13	1:B:62:ASP:OD2	2.20	0.42
2:S:114:UNK:O	2:S:116:UNK:N	2.53	0.42
1:A:1463:LEU:O	1:A:1467:ILE:HG12	2.20	0.42
1:A:1498:GLN:C	1:A:1501:PRO:HD2	2.40	0.42
1:A:1608:ARG:NE	1:A:1608:ARG:O	2.52	0.42
1:A:1655:ILE:HD13	1:A:1681:ASP:CB	2.45	0.42
1:A:1889:VAL:HG22	1:A:1900:PHE:CG	2.54	0.42
1:A:2066:PHE:CD1	1:A:2128:PHE:HE1	2.38	0.42
1:A:2210:VAL:HG13	1:A:2211:LEU:HG	2.01	0.42
1:A:2300:PHE:CE2	1:A:2341:LEU:HB2	2.54	0.42
1:A:2943:PHE:CE1	1:A:2984:GLY:HA2	2.55	0.42
1:A:35:ILE:HG21	1:A:84:GLU:HB3	2.02	0.42
1:A:3690:PHE:HD1	1:A:3692:VAL:HG23	1.84	0.42
1:A:3872:ARG:HD2	1:A:3965:ARG:NH1	2.35	0.42
1:A:3982:SER:HB3	1:A:3986:HIS:HE1	1.83	0.42
1:A:453:MSE:SE	1:A:456:VAL:HG11	2.70	0.42
1:A:781:ASP:OD2	1:A:862:LEU:HD21	2.20	0.42
1:A:961:LEU:HA	1:A:961:LEU:HD13	1.81	0.42
1:B:107:ILE:O	1:B:110:THR:HB	2.20	0.42
1:B:1551:ILE:HA	1:B:1554:SER:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1686:LEU:CD2	1:B:1727:ARG:NH1	2.83	0.42
1:B:1861:SER:O	1:B:1864:ASP:HB3	2.20	0.42
1:B:2135:ASN:N	1:B:2136:PRO:HD3	2.35	0.42
1:B:2166:SER:O	1:B:2170:GLN:CB	2.50	0.42
1:B:2171:LEU:CG	1:B:2177:ASN:HD21	2.29	0.42
1:B:2326:ILE:HA	1:B:2326:ILE:HD13	1.89	0.42
1:B:2443:MSE:N	1:B:2444:PRO:HD2	2.35	0.42
1:B:2531:LEU:HA	1:B:2531:LEU:HD12	1.89	0.42
1:B:2541:ALA:O	1:B:2545:LEU:HG	2.20	0.42
1:B:2905:LEU:HB2	1:B:2906:PRO:CD	2.50	0.42
1:B:2875:ALA:HB2	1:B:2921:LEU:HD23	2.01	0.42
1:B:3283:LEU:HD13	1:B:3287:ARG:CZ	2.50	0.42
1:B:3283:LEU:HD13	1:B:3287:ARG:NE	2.34	0.42
1:B:3529:ILE:HG22	1:B:3529:ILE:O	2.19	0.42
1:B:3694:PHE:CD2	1:B:3697:ASN:HA	2.54	0.42
1:B:3577:GLN:HG3	1:B:3800:LEU:CD2	2.50	0.42
1:B:3885:ARG:O	1:B:3888:VAL:HG12	2.20	0.42
1:B:617:PRO:HB3	1:B:659:ARG:CD	2.50	0.42
1:B:792:ILE:O	1:B:796:LEU:HG	2.19	0.42
1:B:886:TRP:CH2	1:B:958:MSE:HB2	2.54	0.42
1:B:980:THR:HG22	1:B:984:TYR:CE2	2.52	0.42
1:A:971:ARG:HD2	1:A:1024:THR:CB	2.50	0.42
1:A:1127:CYS:O	1:A:1131:ILE:HG23	2.20	0.42
1:A:1279:LEU:HG	1:A:1292:LYS:NZ	2.33	0.42
1:A:1651:LYS:HB2	1:A:1684:LEU:CD1	2.50	0.42
1:A:1686:LEU:HD23	1:A:1727:ARG:CZ	2.50	0.42
1:A:1939:LEU:O	1:A:1942:CYS:N	2.53	0.42
1:A:1981:LEU:O	1:A:1984:LEU:HG	2.19	0.42
1:A:2166:SER:N	1:A:2167:PRO:CD	2.82	0.42
1:A:2154:GLU:N	1:A:2199:LEU:HD22	2.34	0.42
1:A:2233:HIS:HA	1:A:2236:GLU:CD	2.40	0.42
1:A:2913:LYS:HG3	1:A:2914:ALA:H	1.82	0.42
1:A:3454:LEU:HD21	1:A:3461:ALA:HB2	2.01	0.42
1:A:3789:ARG:HH22	1:A:3806:LEU:CD2	2.23	0.42
1:A:403:GLY:C	1:A:405:ASP:N	2.71	0.42
1:A:575:ILE:HD13	1:A:603:ILE:HB	2.01	0.42
1:A:758:LEU:HA	1:A:758:LEU:HD12	1.91	0.42
1:B:1007:VAL:HA	1:B:1010:LEU:HD11	2.02	0.42
1:B:1017:ILE:HB	1:B:1025:LEU:CB	2.47	0.42
1:B:1349:LEU:CD2	1:B:1353:PRO:HG2	2.49	0.42
1:B:1467:ILE:HG13	1:B:1468:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2327:LEU:HA	1:B:2330:VAL:HG12	2.01	0.42
1:B:2877:SER:O	1:B:2880:CYS:N	2.36	0.42
1:B:3053:LEU:HD23	1:B:3053:LEU:HA	1.55	0.42
1:B:3293:CYS:HA	1:B:3297:VAL:CG2	2.50	0.42
1:B:62:ASP:O	1:B:66:LEU:HD23	2.20	0.42
1:B:642:PHE:HE2	1:B:710:PHE:HE2	1.66	0.42
1:B:992:ILE:HA	1:B:995:PHE:CE2	2.54	0.42
1:A:1015:ASP:HA	1:A:1018:VAL:HG22	2.01	0.42
1:A:1083:ASN:HD21	1:A:1104:LEU:CD2	2.32	0.42
1:A:1303:MSE:HB2	1:A:1371:VAL:HG23	2.01	0.42
1:A:147:PHE:CD2	1:A:148:LYS:HG3	2.55	0.42
1:A:1715:GLU:O	1:A:1719:VAL:HG23	2.19	0.42
1:A:2035:THR:HG22	1:A:2076:VAL:HG13	2.02	0.42
1:A:2276:LEU:O	1:A:2279:ILE:HB	2.19	0.42
1:A:2387:PRO:O	1:A:2390:HIS:HB3	2.20	0.42
1:A:2472:GLN:O	1:A:2476:ILE:HG12	2.19	0.42
1:A:2520:ILE:HD12	1:A:2607:UNK:CB	2.50	0.42
1:A:2538:ARG:NH1	1:A:2565:MSE:HG3	2.35	0.42
1:A:2843:PHE:HE2	1:A:2853:PRO:HG3	1.85	0.42
1:A:281:GLN:HA	1:A:326:MSE:SE	2.70	0.42
1:A:3280:TYR:CG	1:A:3328:ILE:HD11	2.55	0.42
1:A:356:ASN:CG	1:A:1859:ASN:HB2	2.40	0.42
1:A:393:LYS:HA	1:A:396:PHE:CE1	2.54	0.42
1:A:429:GLU:N	1:A:429:GLU:OE1	2.53	0.42
1:A:436:GLU:OE2	1:A:475:LEU:HD11	2.19	0.42
1:A:654:ILE:HG23	1:A:722:LYS:NZ	2.35	0.42
1:A:846:ILE:HG23	1:A:854:ARG:NH1	2.35	0.42
1:B:1335:CYS:HA	1:B:1338:VAL:HG12	2.01	0.42
1:B:149:ILE:O	1:B:152:LEU:HG	2.20	0.42
1:B:1681:ASP:HB2	1:B:1717:LEU:CD2	2.50	0.42
1:B:1809:ASP:N	1:B:1810:PRO:HD3	2.35	0.42
1:B:2385:LEU:HG	1:B:2389:PHE:CZ	2.55	0.42
1:B:2398:LEU:O	1:B:2402:LEU:HD23	2.20	0.42
1:B:3148:GLN:HE22	1:B:3160:LEU:HD22	1.85	0.42
1:B:3283:LEU:HG	1:B:3300:VAL:CG2	2.49	0.42
1:B:3978:GLY:O	1:B:3979:LEU:HD23	2.19	0.42
1:B:446:PHE:HD2	1:B:533:HIS:CG	2.37	0.42
1:B:617:PRO:HB3	1:B:659:ARG:HD2	2.02	0.42
1:B:913:ARG:O	1:B:917:LEU:HG	2.20	0.42
1:B:977:ASP:HB3	1:B:980:THR:HG22	2.02	0.42
1:A:1080:LEU:HD23	1:A:1128:CYS:SG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1060:PHE:CD2	1:A:1099:PHE:HZ	2.38	0.41
1:A:82:ARG:NH1	1:A:114:VAL:HG13	2.35	0.41
1:A:1747:LEU:O	1:A:1748:ASP:C	2.58	0.41
1:A:1763:THR:N	1:A:1864:ASP:OD2	2.43	0.41
1:A:2082:GLU:HB2	1:A:2086:ASP:CB	2.50	0.41
1:A:2534:ASN:HB3	1:A:2537:ASP:HB2	2.01	0.41
1:A:279:ALA:HA	1:A:282:PHE:CD2	2.55	0.41
1:A:2943:PHE:CD1	1:A:2944:THR:N	2.79	0.41
1:A:3386:SER:O	1:A:3390:GLN:HB2	2.19	0.41
1:A:345:PHE:O	1:A:348:ILE:N	2.53	0.41
1:A:381:VAL:HB	1:A:384:MSE:SE	2.70	0.41
1:A:3995:PRO:O	1:A:3999:THR:OG1	2.17	0.41
1:A:398:THR:HA	1:A:400:THR:HG22	2.02	0.41
1:A:417:VAL:O	1:A:420:VAL:HG12	2.20	0.41
1:A:489:ARG:HA	1:A:612:LEU:HB2	2.02	0.41
1:A:513:GLU:OE1	1:A:653:LEU:HD11	2.19	0.41
1:B:2047:THR:O	1:B:2050:GLN:HB2	2.20	0.41
1:B:2190:VAL:HG21	1:B:2241:LEU:CD1	2.47	0.41
1:B:2843:PHE:HE2	1:B:2853:PRO:HG3	1.84	0.41
1:B:3585:PHE:O	1:B:3589:SER:OG	2.30	0.41
1:B:368:LEU:HD13	1:B:388:LEU:HD23	2.00	0.41
1:B:3577:GLN:HA	1:B:3800:LEU:HD22	2.02	0.41
1:B:454:GLN:CG	1:B:533:HIS:HE1	2.29	0.41
1:A:100:ILE:HG22	1:A:100:ILE:O	2.20	0.41
1:A:997:ASN:HA	1:A:1042:LYS:HD3	2.03	0.41
1:A:1503:LEU:HA	1:A:1503:LEU:HD23	1.88	0.41
1:A:1569:THR:O	1:A:1573:LYS:CB	2.67	0.41
1:A:1711:ARG:HG3	1:A:1712:ARG:N	2.35	0.41
1:A:1722:PHE:O	1:A:1725:GLN:HB3	2.20	0.41
1:A:2263:LYS:HB3	1:A:2264:ASP:H	1.61	0.41
1:A:2458:VAL:HG12	1:A:2473:MSE:HG3	2.01	0.41
1:A:2482:ASP:HB2	1:A:2485:ARG:NH2	2.35	0.41
1:A:2502:ALA:O	1:A:2506:LEU:HG	2.19	0.41
1:A:3351:ILE:HG23	1:A:3355:LYS:CE	2.49	0.41
1:A:3454:LEU:HD21	1:A:3461:ALA:CB	2.50	0.41
1:A:3505:LEU:HD12	1:A:3509:ASP:CB	2.45	0.41
1:A:560:LEU:HA	1:A:563:LEU:CG	2.50	0.41
1:B:1354:GLU:C	1:B:1356:TRP:N	2.74	0.41
1:B:2010:GLU:C	1:B:2012:ARG:N	2.73	0.41
1:B:2166:SER:N	1:B:2167:PRO:HD2	2.35	0.41
1:B:2193:ILE:HD12	1:B:2245:TRP:CZ2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2277:LEU:O	1:B:2280:VAL:HB	2.20	0.41
1:B:2337:LEU:HD12	1:B:2337:LEU:HA	1.86	0.41
1:B:2359:LYS:O	1:B:2362:VAL:HG22	2.20	0.41
1:B:2365:ASN:HA	1:B:2368:THR:HB	2.00	0.41
1:B:2473:MSE:HB3	1:B:2473:MSE:HE2	1.82	0.41
1:B:271:GLY:HA2	1:B:274:LEU:HD11	2.02	0.41
1:B:2837:LEU:HD13	1:B:2868:LEU:N	2.35	0.41
1:B:2886:GLN:H	1:B:2886:GLN:HG3	1.48	0.41
1:B:3241:LYS:O	1:B:3243:ILE:N	2.41	0.41
1:B:389:ILE:HG23	1:B:434:VAL:HG21	2.00	0.41
1:B:3929:MSE:HB3	1:B:3938:ILE:HD12	2.02	0.41
1:B:43:VAL:O	1:B:45:SER:N	2.52	0.41
1:A:1163:LEU:HD23	1:A:1260:LEU:HD11	2.03	0.41
1:A:1251:GLN:O	1:A:1255:CYS:HB2	2.20	0.41
1:A:1582:LEU:O	1:A:1583:MSE:C	2.59	0.41
1:A:1684:LEU:HA	1:A:1684:LEU:HD23	1.82	0.41
1:A:1695:LEU:O	1:A:1700:THR:HB	2.20	0.41
1:A:2103:HIS:HA	1:A:2106:ARG:HB2	2.02	0.41
1:A:2168:LEU:HD13	1:A:2214:ARG:NH2	2.35	0.41
1:A:2462:VAL:HA	1:A:2465:PRO:HD3	2.02	0.41
1:A:2443:MSE:CE	1:A:2476:ILE:HB	2.34	0.41
1:A:2841:ASN:HD22	1:A:2871:LEU:HG	1.86	0.41
1:A:3011:LEU:O	1:A:3011:LEU:HD13	2.19	0.41
1:A:3056:GLU:HA	1:A:3092:LEU:HD11	2.02	0.41
1:A:349:ILE:HG12	1:A:364:ARG:HB2	2.01	0.41
1:A:3621:LYS:HB3	1:A:3638:LYS:HE2	2.02	0.41
1:A:398:THR:C	1:A:400:THR:N	2.74	0.41
1:A:513:GLU:OE2	1:A:655:LEU:HD23	2.21	0.41
1:A:592:GLU:HB3	1:A:601:TRP:HZ2	1.84	0.41
1:A:922:SER:OG	1:A:925:GLN:OE1	2.19	0.41
1:A:955:ALA:O	1:A:959:TYR:HB3	2.19	0.41
1:A:999:LYS:HD2	1:A:1001:PHE:CE2	2.55	0.41
1:B:1025:LEU:HD12	1:B:1028:PHE:HD2	1.84	0.41
1:B:113:SER:O	1:B:116:THR:HB	2.20	0.41
1:B:1164:CYS:O	1:B:1164:CYS:SG	2.77	0.41
1:B:1648:LEU:O	1:B:1652:ILE:HD12	2.20	0.41
1:B:162:LEU:HD21	1:B:196:LEU:HD13	2.01	0.41
1:B:2160:TYR:HA	1:B:2163:HIS:CD2	2.55	0.41
1:B:2213:ASN:CB	1:B:2250:SER:HB2	2.50	0.41
1:B:2367:VAL:HG22	1:B:2371:PHE:CE1	2.55	0.41
1:B:2396:LEU:H	1:B:2396:LEU:HD12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:GLN:C	1:B:260:ILE:HG13	2.41	0.41
1:B:2647:UNK:HA	1:B:2775:TYR:HD1	1.85	0.41
1:B:2806:LYS:HD3	1:B:2855:VAL:CG1	2.43	0.41
1:B:19:LEU:HB2	1:B:34:LEU:HD13	2.02	0.41
1:B:61:ARG:O	1:B:65:LEU:CB	2.54	0.41
1:B:646:VAL:HG11	1:B:710:PHE:CZ	2.54	0.41
1:B:850:GLU:CD	1:B:854:ARG:HH21	2.21	0.41
1:A:1060:PHE:HB3	1:A:1064:TYR:CE2	2.56	0.41
1:A:166:ILE:HG22	1:A:167:PRO:HD2	2.02	0.41
1:A:1640:GLU:HG2	1:A:1691:GLN:HG2	2.01	0.41
1:A:1729:PHE:HZ	1:A:1870:LYS:HZ3	1.69	0.41
1:A:1997:PRO:HA	1:A:2000:ARG:N	2.36	0.41
1:A:2813:PHE:O	1:A:2816:ILE:HG22	2.20	0.41
1:A:3151:LEU:HA	1:A:3152:SER:HA	1.85	0.41
1:A:449:TYR:CD2	1:A:454:GLN:HA	2.55	0.41
1:A:51:LEU:H	1:A:51:LEU:HG	1.62	0.41
1:A:488:ILE:HD12	1:A:616:LYS:HD3	2.02	0.41
1:A:741:ILE:HB	1:A:744:ASP:CG	2.40	0.41
1:A:851:ILE:O	1:A:855:VAL:HG23	2.19	0.41
1:B:1006:THR:O	1:B:1010:LEU:HG	2.21	0.41
1:B:1092:GLU:O	1:B:1093:GLU:HB2	2.20	0.41
1:B:1289:SER:OG	1:B:1289:SER:O	2.39	0.41
1:B:1735:ARG:O	1:B:1736:PHE:HB2	2.20	0.41
1:B:1761:LEU:HD23	1:B:1762:MSE:N	2.36	0.41
1:B:1931:ASN:OD1	1:B:1932:GLN:N	2.53	0.41
1:B:1945:TYR:HD1	1:B:1948:ALA:HB3	1.86	0.41
1:B:2003:LYS:HA	1:B:2006:GLU:HB2	2.03	0.41
1:B:2066:PHE:HB3	1:B:2067:ARG:HA	2.02	0.41
1:B:2386:LEU:HA	1:B:2386:LEU:HD23	1.80	0.41
1:B:2870:SER:C	1:B:2872:ASP:N	2.71	0.41
1:B:2995:GLU:O	1:B:2998:SER:HB3	2.20	0.41
1:B:3778:ASP:OD1	1:B:3780:ALA:N	2.53	0.41
1:B:3944:HIS:CG	1:B:3949:ALA:HA	2.55	0.41
1:B:3953:LEU:HD13	1:B:4069:GLU:HB3	2.01	0.41
1:B:4028:ILE:HA	1:B:4031:ILE:HD12	2.02	0.41
1:A:1025:LEU:HD12	1:A:1025:LEU:HA	1.78	0.41
1:A:2083:LEU:HA	1:A:2083:LEU:HD23	1.81	0.41
1:A:2163:HIS:O	1:A:2167:PRO:HD3	2.21	0.41
1:A:2239:LYS:HE2	1:A:2240:THR:CG2	2.45	0.41
1:A:249:PHE:HZ	1:A:272:LEU:HD12	1.86	0.41
1:A:2512:ASP:HB2	1:A:2515:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3002:TYR:CE1	1:A:3003:ASN:HB3	2.55	0.41
1:A:3048:LYS:HZ3	1:A:3089:LEU:HB3	1.85	0.41
1:A:3135:LEU:O	1:A:3138:ILE:HB	2.20	0.41
1:A:3640:PHE:HB3	1:A:3644:PHE:CD2	2.56	0.41
1:A:3687:MSE:C	1:A:3689:ASP:N	2.70	0.41
1:A:3710:LYS:HA	1:A:3710:LYS:HD3	1.95	0.41
1:A:703:CYS:O	1:A:707:PHE:CD1	2.73	0.41
1:B:1076:LEU:HA	1:B:1076:LEU:HD23	1.75	0.41
1:B:1255:CYS:SG	1:B:1333:SER:HB3	2.60	0.41
1:B:1366:THR:O	1:B:1369:MSE:HB2	2.20	0.41
1:B:1608:ARG:HD3	1:B:1631:SER:H	1.86	0.41
1:B:567:GLU:OE2	1:B:1798:LEU:HD22	2.21	0.41
1:B:2129:LEU:HD13	1:B:2156:VAL:CG1	2.51	0.41
1:B:2427:ARG:HB3	1:B:2433:LYS:HB2	2.02	0.41
1:B:2634:UNK:O	1:B:2637:UNK:N	2.53	0.41
1:B:2789:SER:O	1:B:2793:PRO:HD3	2.21	0.41
1:B:2970:LYS:HE3	1:B:2974:GLU:OE2	2.21	0.41
1:B:3026:ASP:O	1:B:3030:ILE:HG13	2.20	0.41
1:B:3072:GLU:HA	1:B:3076:ALA:HA	2.03	0.41
1:B:31:GLY:O	1:B:34:LEU:HB3	2.20	0.41
1:B:3006:ALA:HB2	1:B:3254:LEU:HD11	2.03	0.41
1:B:368:LEU:C	1:B:372:PRO:HG2	2.41	0.41
1:B:3974:MSE:CB	1:B:3976:GLU:HB3	2.49	0.41
1:B:394:GLN:O	1:B:398:THR:HG23	2.20	0.41
1:B:476:ARG:HA	1:B:479:ILE:CG1	2.50	0.41
1:B:633:ILE:HG23	1:B:637:LYS:CE	2.51	0.41
1:B:906:PHE:O	1:B:909:VAL:HB	2.21	0.41
1:A:1014:LEU:O	1:A:1078:ALA:HB2	2.19	0.41
1:A:1116:ALA:HB2	1:A:1164:CYS:HB3	2.03	0.41
1:A:1220:LEU:HD13	1:A:1274:ARG:CG	2.49	0.41
1:A:1359:LEU:HD11	1:A:1365:ASN:OD1	2.20	0.41
1:A:197:PHE:CE2	1:A:230:LEU:HD22	2.56	0.41
1:A:2412:TYR:HD2	1:A:2416:LYS:NZ	2.17	0.41
1:A:246:ARG:CA	1:A:249:PHE:HD2	2.32	0.41
1:A:2520:ILE:HG23	1:A:2521:ILE:N	2.36	0.41
1:A:2858:ILE:CD1	1:A:2888:VAL:HB	2.51	0.41
1:A:2887:PRO:HG3	1:A:2921:LEU:HD13	2.03	0.41
1:A:2962:ARG:HH22	1:A:3006:ALA:HB1	1.85	0.41
1:A:3614:TYR:CD1	1:A:3618:GLY:HA3	2.56	0.41
1:A:3622:ALA:HB1	1:A:3623:PRO:HD2	2.02	0.41
1:A:3723:ASP:HB2	1:A:3741:ARG:NE	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3766:GLN:O	1:A:3769:GLN:HG2	2.21	0.41
1:A:3920:ILE:HG13	1:A:3923:ARG:HD3	2.02	0.41
1:A:2936:TYR:HD2	1:A:3979:LEU:HD21	1.83	0.41
1:A:504:GLU:O	1:A:508:HIS:CG	2.74	0.41
1:A:752:LEU:O	1:A:756:PHE:HD1	2.02	0.41
1:A:75:SER:HA	1:A:79:ARG:HG3	2.01	0.41
1:A:923:ASP:O	1:A:927:LYS:HE3	2.20	0.41
1:B:989:MSE:SE	1:B:1030:GLY:O	2.89	0.41
1:B:717:LYS:HZ3	1:B:1121:LEU:HD11	1.83	0.41
1:B:168:ASP:O	1:B:170:VAL:N	2.47	0.41
1:B:1880:MSE:O	1:B:1883:ARG:N	2.51	0.41
1:B:204:LEU:HG	1:B:204:LEU:H	1.53	0.41
1:B:204:LEU:HD22	1:B:219:VAL:CG1	2.46	0.41
1:B:2066:PHE:CD1	1:B:2128:PHE:HE1	2.39	0.41
1:B:2164:TRP:CZ3	1:B:2186:VAL:HG23	2.55	0.41
1:B:2542:LEU:HD13	1:B:2546:TYR:CE2	2.56	0.41
1:B:3329:LEU:O	1:B:3332:THR:OG1	2.32	0.41
1:B:3494:GLN:O	1:B:3498:TRP:CZ3	2.73	0.41
1:B:3736:LYS:HB3	1:B:3752:VAL:HB	2.02	0.41
1:B:3772:ASN:HA	1:B:3775:LEU:HG	2.02	0.41
1:B:431:TYR:CA	1:B:434:VAL:HG12	2.44	0.41
1:B:527:TYR:CD1	1:B:531:PHE:HZ	2.38	0.41
1:A:1165:LEU:O	1:A:1166:LEU:C	2.59	0.41
1:A:1168:LEU:O	1:A:1171:TRP:HB3	2.21	0.41
1:A:1364:CYS:C	1:A:1366:THR:N	2.74	0.41
1:A:1500:LEU:HB3	1:A:1501:PRO:HD3	2.03	0.41
1:A:160:LEU:O	1:A:164:LYS:HG2	2.20	0.41
1:A:1816:ARG:HD3	1:A:1819:PHE:HE1	1.86	0.41
1:A:1949:ILE:HD12	1:A:1949:ILE:HA	1.88	0.41
1:A:1992:VAL:HG23	1:A:1993:GLU:N	2.35	0.41
1:A:2040:MSE:HA	1:A:2043:PHE:CD1	2.55	0.41
1:A:2070:GLU:HB2	1:A:2072:ARG:N	2.36	0.41
1:A:217:LEU:N	1:A:218:PRO:HD2	2.36	0.41
1:A:2219:LEU:HB3	1:A:2238:ILE:HG21	2.02	0.41
1:A:2238:ILE:O	1:A:2242:VAL:HG23	2.21	0.41
1:A:2344:LEU:O	1:A:2347:LYS:HB2	2.21	0.41
1:A:2541:ALA:O	1:A:2545:LEU:HG	2.20	0.41
1:A:2824:LYS:HB3	1:A:2825:THR:H	1.69	0.41
1:A:2863:CYS:O	1:A:2865:HIS:N	2.54	0.41
1:A:2920:VAL:O	1:A:2923:TRP:HB3	2.21	0.41
1:A:3033:GLU:OE2	1:A:3079:GLU:CD	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3356:ALA:HB1	1:A:3384:HIS:HB3	2.02	0.41
1:A:3502:MSE:CE	1:A:3517:SER:HB3	2.51	0.41
1:A:3529:ILE:HG22	1:A:3529:ILE:O	2.21	0.41
1:A:3676:PRO:CG	1:A:3677:PRO:HD3	2.50	0.41
1:A:3928:PHE:O	1:A:3928:PHE:CD1	2.74	0.41
1:A:396:PHE:CE1	1:A:437:HIS:CD2	3.08	0.41
1:A:474:VAL:HG11	1:A:1564:SER:CB	2.50	0.41
1:A:481:THR:HG22	1:A:482:VAL:N	2.35	0.41
1:A:560:LEU:O	1:A:563:LEU:N	2.54	0.41
1:A:704:PHE:HA	1:A:707:PHE:CG	2.56	0.41
1:A:508:HIS:CD2	1:A:725:LEU:HD13	2.55	0.41
1:A:959:TYR:O	1:A:963:LYS:CB	2.62	0.41
1:A:980:THR:CG2	1:A:984:TYR:CE1	3.01	0.41
1:B:989:MSE:CG	1:B:1031:ARG:NH1	2.83	0.41
1:B:1273:GLU:HG2	1:B:1276:VAL:HB	2.02	0.41
1:B:1513:GLY:O	1:B:1517:LEU:HG	2.19	0.41
1:B:1909:ASN:ND2	1:B:1909:ASN:N	2.69	0.41
1:B:1911:LEU:HD22	1:B:1916:ILE:HG21	2.03	0.41
1:B:1946:ASN:ND2	1:B:1993:GLU:OE2	2.40	0.41
1:B:1996:VAL:HG23	1:B:1997:PRO:CD	2.51	0.41
1:B:2062:ALA:O	1:B:2066:PHE:N	2.53	0.41
1:B:2412:TYR:CG	1:B:2412:TYR:O	2.73	0.41
1:B:2565:MSE:SE	1:B:2565:MSE:O	2.88	0.41
1:B:2787:HIS:HB3	1:B:2790:LEU:HD12	2.02	0.41
1:B:2870:SER:HA	1:B:2897:LEU:CD2	2.51	0.41
1:B:2975:ALA:C	1:B:2977:ASN:N	2.74	0.41
1:B:2925:GLU:HB3	1:B:3121:LEU:HD21	2.02	0.41
1:B:3136:THR:O	1:B:3140:GLU:CB	2.68	0.41
1:B:3259:LEU:HD11	1:B:3275:SER:O	2.21	0.41
1:B:3291:GLN:O	1:B:3294:SER:OG	2.39	0.41
1:B:3492:CYS:HB2	1:B:3713:PRO:HG3	2.03	0.41
1:B:4002:MSE:O	1:B:4006:VAL:HG13	2.21	0.41
1:B:4082:ARG:HG3	1:B:4091:ALA:CB	2.37	0.41
1:B:752:LEU:HA	1:B:755:ALA:CB	2.50	0.41
1:A:1111:LEU:N	1:A:1111:LEU:HD12	2.35	0.41
1:A:1894:SER:C	1:A:1896:ILE:H	2.24	0.41
1:A:2138:VAL:HB	1:A:2139:PRO:HD3	2.03	0.41
1:A:2330:VAL:CG2	1:A:2338:GLU:HB3	2.35	0.41
1:A:2423:VAL:HG22	1:A:2424:MSE:N	2.36	0.41
1:A:2640:UNK:O	1:A:2641:UNK:C	2.68	0.41
1:A:265:TYR:C	1:A:268:PRO:HD2	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2999:LEU:HD12	1:A:3002:TYR:HE2	1.86	0.41
1:A:3048:LYS:HE2	1:A:3048:LYS:HB3	1.68	0.41
1:A:3190:LEU:O	1:A:3194:GLU:HB2	2.21	0.41
1:A:4070:LYS:HB3	1:A:4073:ALA:HB3	2.02	0.41
1:B:1463:LEU:O	1:B:1463:LEU:HD23	2.21	0.41
1:B:1548:GLY:O	1:B:1552:HIS:ND1	2.53	0.41
1:B:1606:ARG:NH1	1:B:1806:ARG:HB3	2.36	0.41
1:B:1880:MSE:CE	1:B:1884:LEU:HD11	2.51	0.41
1:B:1874:TYR:HD2	1:B:1885:PRO:HG3	1.85	0.41
1:B:2009:LYS:CG	1:B:2010:GLU:H	2.34	0.41
1:B:2083:LEU:HD23	1:B:2083:LEU:HA	1.82	0.41
1:B:2164:TRP:CE3	1:B:2215:LEU:HG	2.55	0.41
1:B:2367:VAL:O	1:B:2371:PHE:HE1	2.04	0.41
1:B:2371:PHE:CG	1:B:2372:PRO:HD3	2.56	0.41
1:B:2440:TYR:CE2	1:B:2443:MSE:SE	3.24	0.41
1:B:2943:PHE:C	1:B:2945:SER:N	2.73	0.41
1:B:3031:TRP:CD2	1:B:3034:PRO:HD3	2.56	0.41
1:B:3148:GLN:NE2	1:B:3197:LEU:HD12	2.36	0.41
1:B:3839:TYR:CE1	1:B:3867:THR:HB	2.29	0.41
1:B:46:SER:H	1:B:51:LEU:CD1	2.34	0.41
1:B:476:ARG:HA	1:B:479:ILE:HG13	2.03	0.41
1:B:634:LEU:CB	1:B:638:GLN:HE22	2.32	0.41
1:B:70:ARG:NH2	1:B:79:ARG:HG2	2.35	0.41
1:B:911:LEU:O	1:B:915:THR:HG23	2.20	0.41
1:A:1005:ASP:HB2	1:A:1006:THR:H	1.63	0.41
1:A:995:PHE:HZ	1:A:1006:THR:HG1	1.69	0.41
1:A:1013:ILE:HG21	1:A:1028:PHE:HB2	2.02	0.41
1:A:1147:LYS:CD	1:A:1180:GLN:HG2	2.50	0.41
1:A:1369:MSE:CE	1:A:1418:HIS:HB2	2.51	0.41
1:A:1431:LEU:HD11	1:A:1479:VAL:HG22	2.01	0.41
1:A:1938:ARG:O	1:A:1941:HIS:HB3	2.21	0.41
1:A:2439:ILE:HG12	1:A:2442:MSE:CE	2.51	0.41
1:A:2445:LYS:HD3	1:A:2445:LYS:HA	1.78	0.41
1:A:2514:ASN:H	1:A:2515:PRO:HD3	1.86	0.41
1:A:2884:LEU:HD12	1:A:2884:LEU:H	1.86	0.41
1:A:2943:PHE:HE1	1:A:2984:GLY:HA2	1.86	0.41
1:A:3425:ARG:NH1	1:A:3999:THR:CG2	2.84	0.41
1:A:3567:VAL:HG22	1:A:3571:PHE:CZ	2.56	0.41
1:A:3736:LYS:HD2	1:A:3752:VAL:HG21	2.03	0.41
1:A:3779:SER:O	1:A:3782:SER:N	2.54	0.41
1:A:3972:LEU:HD12	1:A:3974:MSE:CE	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ILE:O	1:B:104:SER:HB3	2.20	0.41
1:B:1145:LEU:HD13	1:B:1149:LYS:HD3	2.02	0.41
1:B:1359:LEU:O	1:B:1362:ASP:OD1	2.39	0.41
1:B:1374:GLN:HA	1:B:1374:GLN:OE1	2.21	0.41
1:B:1583:MSE:HE3	1:B:1643:MSE:SE	2.70	0.41
1:B:1949:ILE:O	1:B:1952:ILE:HG22	2.20	0.41
1:B:1981:LEU:HA	1:B:1984:LEU:HD23	2.01	0.41
1:B:2386:LEU:HD12	1:B:2404:ARG:HE	1.84	0.41
1:B:3147:LYS:O	1:B:3151:LEU:HG	2.20	0.41
1:B:3155:VAL:HG21	1:B:3159:ARG:HH21	1.83	0.41
1:B:3231:ILE:HG23	1:B:3235:LYS:HE3	2.02	0.41
1:B:3319:ASN:ND2	1:B:3400:SER:HA	2.35	0.41
1:B:3632:PHE:HE2	1:B:3683:CYS:SG	2.43	0.41
1:B:3575:LEU:CD2	1:B:3687:MSE:SE	3.18	0.41
1:B:3705:TYR:CD2	1:B:3792:SER:HB2	2.56	0.41
1:B:4106:CYS:O	1:B:4108:MSE:N	2.54	0.41
1:B:804:ALA:O	1:B:806:SER:N	2.53	0.41
1:B:922:SER:C	1:B:924:ARG:N	2.74	0.41
1:B:978:GLN:N	1:B:981:ARG:HD3	2.34	0.41
1:A:1069:HIS:N	1:A:1070:PRO:CD	2.84	0.41
1:A:1385:ASN:O	1:A:1388:ASP:N	2.46	0.41
1:A:15:LEU:HA	1:A:2359:LYS:NZ	2.36	0.41
1:A:1874:TYR:CD2	1:A:1885:PRO:HG3	2.56	0.41
1:A:178:LEU:HB3	1:A:197:PHE:CE1	2.56	0.41
1:A:2165:LEU:HD11	1:A:2211:LEU:HD22	2.03	0.41
1:A:2239:LYS:CD	1:A:2279:ILE:HD12	2.49	0.41
1:A:2646:UNK:CB	1:A:2779:ASP:HA	2.51	0.41
1:A:2797:VAL:HG23	1:A:2798:ALA:N	2.36	0.41
1:A:2876:VAL:HG13	1:A:3035:PHE:CE1	2.56	0.41
1:A:295:GLU:HA	1:A:298:LEU:HB2	2.02	0.41
1:A:298:LEU:O	1:A:301:CYS:HB3	2.21	0.41
1:A:3027:LEU:HB3	1:A:3031:TRP:CZ2	2.56	0.41
1:A:3311:ASN:HB3	1:A:3312:VAL:H	1.62	0.41
1:A:3356:ALA:HB2	1:A:3384:HIS:HB3	2.03	0.41
1:A:340:TYR:O	1:A:344:GLN:HG3	2.21	0.41
1:A:3741:ARG:HG2	1:A:3741:ARG:HH11	1.84	0.41
1:A:3850:HIS:H	1:A:3850:HIS:CD2	2.39	0.41
1:A:3887:PHE:O	1:A:3890:MSE:HG2	2.20	0.41
1:B:1165:LEU:O	1:B:1166:LEU:C	2.60	0.41
1:B:1338:VAL:HA	1:B:1341:ILE:HD12	2.03	0.41
1:B:153:PHE:CD1	1:B:154:SER:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1752:LEU:C	1:B:1754:GLN:H	2.23	0.41
1:B:185:HIS:N	1:B:186:PRO:HD2	2.27	0.41
1:B:2009:LYS:HE2	1:B:2012:ARG:HH11	1.86	0.41
1:B:214:GLU:HB3	1:B:215:PRO:HD2	2.02	0.41
1:B:2220:MSE:O	1:B:2221:LYS:C	2.59	0.41
1:B:175:TYR:CD2	1:B:222:GLY:HA3	2.54	0.41
1:B:2849:SER:O	1:B:2850:PHE:CD1	2.74	0.41
1:B:3151:LEU:HA	1:B:3152:SER:HA	1.73	0.41
1:B:3186:ARG:HH11	1:B:3186:ARG:HG3	1.85	0.41
1:B:3292:GLY:HA2	1:B:3296:GLN:HG2	2.03	0.41
1:B:3503:VAL:HG22	1:B:3539:SER:CB	2.51	0.41
1:B:3694:PHE:O	1:B:3697:ASN:N	2.54	0.41
1:B:3950:THR:OG1	1:B:4065:LEU:HD22	2.20	0.41
1:B:553:VAL:O	1:B:556:SER:HB3	2.21	0.41
1:B:613:HIS:CG	1:B:614:PRO:HD3	2.56	0.41
1:B:806:SER:O	1:B:808:GLU:N	2.54	0.41
1:B:850:GLU:CD	1:B:854:ARG:NH2	2.75	0.41
1:A:960:GLN:CG	1:A:1009:LEU:HD21	2.44	0.41
1:A:1342:MSE:HE3	1:A:1402:LEU:HD23	2.03	0.41
1:A:1678:LEU:O	1:A:1681:ASP:OD1	2.38	0.41
1:A:1692:ALA:HA	1:A:1695:LEU:HD12	2.02	0.41
1:A:1955:VAL:HA	1:A:2003:LYS:NZ	2.36	0.41
1:A:2256:ILE:CD1	1:A:2276:LEU:HD11	2.49	0.41
1:A:2442:MSE:O	1:A:2451:LEU:HD21	2.21	0.41
1:A:2536:LEU:HA	1:A:2536:LEU:HD23	1.81	0.41
1:A:2826:LEU:O	1:A:2830:ASN:HB2	2.21	0.41
1:A:3174:ASP:N	1:A:3175:PRO:CD	2.84	0.41
1:A:3301:LEU:HB2	1:A:3328:ILE:HG21	2.03	0.41
1:A:3454:LEU:C	1:A:3456:LEU:H	2.25	0.41
1:A:3629:ARG:O	1:A:3686:TRP:NE1	2.51	0.41
1:A:3630:ARG:HA	1:A:3686:TRP:NE1	2.36	0.41
1:A:3683:CYS:O	1:A:3687:MSE:HB2	2.21	0.41
1:A:34:LEU:HD11	1:A:38:LEU:HD11	2.03	0.41
1:A:591:GLN:HB3	1:A:1026:ARG:HD3	2.03	0.41
1:A:617:PRO:O	1:A:659:ARG:HD2	2.21	0.41
1:A:671:SER:O	1:A:675:ARG:HB2	2.21	0.41
1:A:776:TRP:CE2	1:A:780:ILE:HD12	2.55	0.41
1:A:846:ILE:HG23	1:A:854:ARG:HH12	1.86	0.41
1:B:1010:LEU:HD12	1:B:1011:GLU:H	1.85	0.41
1:B:115:TYR:O	1:B:118:ASP:HB3	2.21	0.41
1:B:1452:VAL:HG11	1:B:1502:SER:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:LYS:O	1:B:159:GLU:HG3	2.21	0.41
1:B:2044:ASP:O	1:B:2048:GLY:HA3	2.20	0.41
1:B:2795:GLN:O	1:B:2799:GLN:HG2	2.21	0.41
1:B:2915:ARG:O	1:B:2938:VAL:HG21	2.21	0.41
1:B:2991:LYS:O	1:B:2995:GLU:HG2	2.21	0.41
1:B:3593:ARG:HD3	1:B:3663:THR:HG21	2.03	0.41
1:B:3600:PRO:C	1:B:3602:ASN:N	2.75	0.41
1:B:3601:VAL:O	1:B:3605:ASN:HB2	2.21	0.41
1:B:3654:MSE:SE	1:B:3659:PHE:CB	3.17	0.41
1:B:3839:TYR:HB2	1:B:3871:PHE:CZ	2.56	0.41
1:B:3920:ILE:CG1	1:B:3923:ARG:HD2	2.35	0.41
1:B:710:PHE:O	1:B:711:GLY:C	2.59	0.41
1:B:892:LEU:CD2	1:B:907:LEU:HD13	2.50	0.41
1:A:127:ALA:O	1:A:131:LEU:CB	2.69	0.40
1:A:1462:GLY:O	1:A:1464:LEU:N	2.54	0.40
1:A:1507:CYS:SG	1:A:1508:LYS:HG2	2.61	0.40
1:A:1710:LEU:HD23	1:A:1710:LEU:HA	1.68	0.40
1:A:1960:LYS:HG2	1:A:1963:GLN:OE1	2.20	0.40
1:A:197:PHE:O	1:A:201:LEU:HG	2.21	0.40
1:A:2120:ARG:NE	1:A:2120:ARG:HA	2.36	0.40
1:A:225:LYS:O	1:A:228:SER:OG	2.31	0.40
1:A:2775:TYR:N	1:A:2775:TYR:CD1	2.89	0.40
1:A:2576:MSE:HE3	1:A:2788:SER:HB2	2.02	0.40
1:A:3024:PRO:N	1:A:3025:PRO:CD	2.84	0.40
1:A:3076:ALA:O	1:A:3080:LEU:HG	2.21	0.40
1:A:3065:ILE:HD13	1:A:3089:LEU:HD21	2.02	0.40
1:A:3008:TRP:HB2	1:A:3257:LYS:NZ	2.36	0.40
1:A:3503:VAL:HG13	1:A:3504:ALA:H	1.87	0.40
1:A:3636:PHE:O	1:A:3640:PHE:HB2	2.21	0.40
1:A:3664:ASN:O	1:A:3668:LEU:HB2	2.21	0.40
1:A:4059:ILE:HD13	1:A:4059:ILE:HG21	1.82	0.40
1:A:4066:LEU:HG	1:A:4075:ARG:CA	2.44	0.40
1:A:797:ASP:OD1	1:A:800:LEU:HD12	2.21	0.40
1:A:913:ARG:HE	1:A:916:GLU:CD	2.24	0.40
1:B:1032:CYS:O	1:B:1035:GLU:N	2.54	0.40
1:B:1142:HIS:C	1:B:1144:SER:N	2.73	0.40
1:B:1291:LEU:HB3	1:B:1292:LYS:H	1.65	0.40
1:B:1426:GLN:O	1:B:1430:GLU:HG3	2.21	0.40
1:B:1651:LYS:HB3	1:B:1680:ALA:HB1	2.02	0.40
1:B:2042:GLN:HG3	1:B:2046:SER:HB3	2.03	0.40
1:B:2226:PRO:HA	1:B:2229:ALA:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2298:GLU:HB3	1:B:2301:GLN:HB3	2.03	0.40
1:B:2368:THR:HA	1:B:2371:PHE:CE1	2.56	0.40
1:B:2374:LEU:O	1:B:2374:LEU:HD12	2.21	0.40
1:B:2374:LEU:H	1:B:2378:PHE:HE1	1.69	0.40
1:B:2481:HIS:CE1	1:B:2485:ARG:HD3	2.56	0.40
1:B:2852:PRO:O	1:B:2855:VAL:HB	2.22	0.40
1:B:281:GLN:HG3	1:B:326:MSE:HE1	2.02	0.40
1:B:4058:VAL:HG12	1:B:4061:CYS:HB3	2.03	0.40
1:B:783:HIS:C	1:B:785:MSE:H	2.24	0.40
1:B:805:LEU:H	1:B:805:LEU:HG	1.71	0.40
1:B:952:GLY:C	1:B:954:GLY:H	2.25	0.40
1:B:979:VAL:O	1:B:982:GLN:HB3	2.21	0.40
1:A:1350:ASN:OD1	1:A:1405:ALA:HA	2.20	0.40
1:A:1797:LEU:HA	1:A:1797:LEU:HD23	1.83	0.40
1:A:2296:SER:OG	1:A:2297:SER:N	2.52	0.40
1:A:2260:PHE:CE2	1:A:2303:LEU:HA	2.57	0.40
1:A:2308:SER:HA	1:A:2352:HIS:NE2	2.36	0.40
1:A:2424:MSE:HA	1:A:2436:LEU:CD1	2.51	0.40
1:A:979:VAL:HG21	1:A:2656:UNK:HA	2.02	0.40
1:A:2882:ALA:HB1	1:A:2885:GLN:HB2	2.03	0.40
1:A:3052:LEU:HG	1:A:3092:LEU:CD2	2.50	0.40
1:A:3125:ARG:HA	1:A:3125:ARG:HD3	1.57	0.40
1:A:3811:THR:O	1:A:3814:ASP:N	2.54	0.40
1:A:385:TYR:CZ	1:A:424:LEU:HD21	2.56	0.40
1:A:3880:ALA:HB1	1:A:3884:LYS:NZ	2.36	0.40
1:A:463:LYS:O	1:A:466:LEU:N	2.54	0.40
1:A:513:GLU:HA	1:A:653:LEU:HD21	2.03	0.40
1:A:654:ILE:CG2	1:A:729:CYS:HB2	2.51	0.40
1:A:757:LYS:HA	1:A:760:LEU:HD11	2.01	0.40
1:A:766:ALA:O	1:A:768:VAL:HG23	2.22	0.40
1:A:971:ARG:CG	1:A:972:LEU:H	2.27	0.40
1:B:104:SER:HA	1:B:107:ILE:HD12	2.02	0.40
1:B:1087:ARG:CD	1:B:1134:LEU:HB3	2.40	0.40
1:B:82:ARG:HD2	1:B:114:VAL:HG13	2.03	0.40
1:B:1229:CYS:SG	1:B:1282:LEU:HG	2.61	0.40
1:B:1357:LYS:HG3	1:B:1360:LYS:HZ1	1.86	0.40
1:B:1419:LEU:HD23	1:B:1419:LEU:HA	1.81	0.40
1:B:1465:HIS:HA	1:B:1469:PRO:CD	2.51	0.40
1:B:2077:HIS:O	1:B:2081:LEU:HG	2.21	0.40
1:B:2200:ALA:O	1:B:2204:GLY:N	2.55	0.40
1:B:2349:LEU:HA	1:B:2364:LEU:HD13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2480:ILE:HA	1:B:2480:ILE:HD12	1.83	0.40
1:B:280:SER:C	1:B:322:GLN:HG2	2.42	0.40
1:B:2939:LEU:HD11	1:B:2994:TRP:CZ3	2.56	0.40
1:B:2960:GLU:HG2	1:B:3289:ARG:HH22	1.86	0.40
1:B:3602:ASN:O	1:B:3606:ILE:HB	2.21	0.40
1:B:3824:GLU:HG2	1:B:3882:LEU:HD21	2.03	0.40
1:B:4063:GLU:O	1:B:4066:LEU:HB2	2.20	0.40
1:B:487:LEU:O	1:B:490:ILE:HG22	2.20	0.40
1:B:491:CYS:HB2	1:B:527:TYR:CD1	2.56	0.40
1:B:560:LEU:O	1:B:563:LEU:N	2.54	0.40
1:B:560:LEU:HA	1:B:563:LEU:CG	2.52	0.40
1:B:593:ASN:ND2	1:B:1084:ASN:HB2	2.37	0.40
1:B:86:LEU:HD13	1:B:134:LEU:CD2	2.52	0.40
1:B:934:LEU:HD21	1:B:962:TYR:OH	2.22	0.40
1:A:1424:THR:HA	1:A:1427:SER:HB2	2.02	0.40
1:A:1597:LEU:HA	1:A:1600:MSE:HB2	2.03	0.40
1:A:1604:SER:OG	1:A:1605:PHE:N	2.54	0.40
1:A:178:LEU:HD13	1:A:197:PHE:CE1	2.57	0.40
1:A:2420:PHE:CZ	1:A:2424:MSE:HG3	2.57	0.40
1:A:2531:LEU:HA	1:A:2531:LEU:HD12	1.91	0.40
1:A:257:ARG:N	1:A:258:PRO:HD2	2.37	0.40
1:A:294:PHE:CG	1:A:295:GLU:N	2.89	0.40
1:A:2960:GLU:O	1:A:2965:TYR:CD1	2.74	0.40
1:A:294:PHE:O	1:A:297:LEU:HG	2.21	0.40
1:A:2989:ALA:O	1:A:2993:PHE:N	2.49	0.40
1:A:3173:MSE:HB3	1:A:3174:ASP:H	1.58	0.40
1:A:2960:GLU:CG	1:A:3289:ARG:HH22	2.34	0.40
1:A:3495:PHE:CE1	1:A:3521:ILE:HA	2.56	0.40
1:A:3762:GLN:HE21	1:A:3763:ARG:HH11	1.67	0.40
1:A:3771:MSE:SE	1:A:3991:PHE:CE1	3.24	0.40
1:A:4062:ASP:C	1:A:4066:LEU:HD22	2.42	0.40
1:B:1014:LEU:HD23	1:B:1028:PHE:HE2	1.86	0.40
1:B:1741:ASP:HB3	1:B:1745:LYS:HE3	2.03	0.40
1:B:2088:LEU:HG	1:B:2095:ALA:H	1.87	0.40
1:B:2065:ARG:CZ	1:B:2097:LEU:HD21	2.52	0.40
1:B:2957:LEU:HD22	1:B:3989:ARG:NH2	2.36	0.40
1:B:3356:ALA:CB	1:B:3384:HIS:HB3	2.51	0.40
1:B:3447:VAL:HG21	1:B:3475:TYR:CE2	2.56	0.40
1:B:3479:THR:HG23	1:B:3480:LEU:HD23	2.03	0.40
1:B:3606:ILE:HG22	1:B:3610:TYR:CE2	2.56	0.40
1:B:3896:ALA:HA	1:B:3899:ALA:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3907:SER:HB2	1:B:3937:VAL:H	1.86	0.40
1:B:3964:THR:O	1:B:3967:PHE:HB3	2.21	0.40
1:B:3974:MSE:HA	1:B:3975:LYS:CB	2.47	0.40
1:B:4055:ASN:HA	1:B:4056:PRO:HD3	1.91	0.40
1:B:480:SER:O	1:B:484:HIS:HB2	2.21	0.40
1:B:542:ASP:HA	1:B:545:LEU:HD12	2.04	0.40
1:B:661:PRO:CG	1:B:733:LEU:HA	2.51	0.40
1:B:667:TYR:O	1:B:669:LEU:N	2.39	0.40
1:B:676:ASN:O	1:B:680:ILE:HG13	2.21	0.40
1:B:75:SER:HA	1:B:79:ARG:HG3	2.03	0.40
1:B:932:GLU:HB3	1:B:2794:LEU:CD1	2.45	0.40
1:A:1056:THR:O	1:A:1059:LEU:HB2	2.22	0.40
1:A:1106:ILE:HA	1:A:1109:GLU:HB3	2.04	0.40
1:A:1084:ASN:ND2	1:A:1131:ILE:HG22	2.33	0.40
1:A:136:GLN:HG2	1:A:139:ARG:NH1	2.37	0.40
1:A:1492:ALA:HB1	1:A:1493:PRO:HD2	2.02	0.40
1:A:1524:LEU:HG	1:A:1559:PHE:CD1	2.56	0.40
1:A:1583:MSE:HB3	1:A:1584:GLN:H	1.70	0.40
1:A:2142:ILE:O	1:A:2145:PHE:HB2	2.22	0.40
1:A:2640:UNK:O	1:A:2643:UNK:N	2.54	0.40
1:A:286:LEU:HD22	1:A:290:TYR:HD2	1.87	0.40
1:A:3011:LEU:HD11	1:A:3043:TYR:C	2.42	0.40
1:A:3448:GLU:O	1:A:3451:LEU:HB2	2.21	0.40
1:A:3425:ARG:NH2	1:A:3467:ARG:HH12	2.18	0.40
1:A:3812:LEU:HD22	1:A:3928:PHE:CE1	2.57	0.40
1:A:3930:VAL:HA	1:A:3937:VAL:HA	2.02	0.40
1:A:396:PHE:CE1	1:A:437:HIS:NE2	2.90	0.40
1:B:1128:CYS:O	1:B:1131:ILE:HG23	2.21	0.40
1:B:1682:THR:CB	1:B:1724:MSE:SE	3.18	0.40
1:B:2007:ILE:HD13	1:B:2007:ILE:HG21	1.72	0.40
1:B:2065:ARG:HD3	1:B:2100:LEU:HD11	2.02	0.40
1:B:2485:ARG:HH11	1:B:2530:ARG:NH2	2.18	0.40
1:B:262:LEU:HD22	1:B:306:VAL:CG1	2.51	0.40
1:B:2813:PHE:CD1	1:B:2814:SER:N	2.90	0.40
1:B:3176:MSE:HG2	1:B:3249:GLN:HG2	2.03	0.40
1:B:3230:LEU:O	1:B:3234:CYS:HB2	2.22	0.40
1:B:3564:GLN:C	1:B:3566:GLY:N	2.73	0.40
1:B:3736:LYS:HB2	1:B:3736:LYS:HE3	1.87	0.40
1:B:3860:LYS:O	1:B:3864:ARG:HG3	2.22	0.40
1:B:3959:MSE:SE	1:B:4124:TRP:CZ3	3.25	0.40
1:B:3981:TYR:HE1	1:B:4105:LYS:N	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:MSE:HE3	1:B:410:MSE:HB3	1.84	0.40
1:B:435:LEU:HD12	1:B:436:GLU:N	2.36	0.40
1:B:484:HIS:O	1:B:488:ILE:HG23	2.22	0.40
1:B:506:GLU:O	1:B:509:ARG:HG2	2.20	0.40
1:B:544:ILE:O	1:B:546:ALA:N	2.55	0.40
1:B:611:ASN:O	1:B:614:PRO:HD2	2.20	0.40
1:B:742:GLU:HB3	1:B:783:HIS:CD2	2.56	0.40
1:B:763:THR:HB	1:B:770:LEU:HD23	2.02	0.40
1:A:1639:LEU:HD12	1:A:1640:GLU:N	2.37	0.40
1:A:1727:ARG:O	1:A:1730:PRO:HD2	2.21	0.40
1:A:1602:ASP:HB2	1:A:1810:PRO:CB	2.52	0.40
1:A:1916:ILE:HG23	1:A:1920:TYR:HE1	1.85	0.40
1:A:2065:ARG:CZ	1:A:2097:LEU:HD21	2.50	0.40
1:A:2307:MSE:O	1:A:2310:VAL:O	2.40	0.40
1:A:2325:LEU:HD12	1:A:2325:LEU:HA	1.82	0.40
1:A:2926:LEU:HB2	1:A:3123:GLN:CD	2.42	0.40
1:A:3042:PRO:HA	1:A:3045:ILE:CG1	2.49	0.40
1:A:3144:PHE:CZ	1:A:3193:ILE:HD11	2.57	0.40
1:A:323:VAL:O	1:A:327:VAL:CB	2.66	0.40
1:A:2960:GLU:HG2	1:A:3252:PHE:CB	2.51	0.40
1:A:3251:ASN:HD21	1:A:3254:LEU:HD22	1.87	0.40
1:A:2929:LEU:HD21	1:A:3784:ARG:HB3	2.04	0.40
1:A:882:SER:HB2	1:A:3892:THR:CB	2.52	0.40
1:A:3933:GLU:C	1:A:3935:GLY:H	2.24	0.40
1:A:442:GLN:OE1	1:A:457:CYS:HB3	2.22	0.40
1:B:1017:ILE:HD12	1:B:1025:LEU:CD2	2.52	0.40
1:B:101:ALA:O	1:B:104:SER:OG	2.17	0.40
1:B:1353:PRO:HA	1:B:1358:LEU:HB3	2.03	0.40
1:B:1571:LEU:HD13	1:B:1599:GLY:O	2.21	0.40
1:B:1737:ASN:C	1:B:1739:TYR:N	2.73	0.40
1:B:1762:MSE:CB	1:B:1896:ILE:HG12	2.48	0.40
1:B:1916:ILE:HG23	1:B:1920:TYR:HE1	1.85	0.40
1:B:2379:MSE:HE3	1:B:2383:PHE:HD1	1.87	0.40
1:B:2461:PHE:CE1	1:B:2462:VAL:HG23	2.57	0.40
1:B:2894:GLU:CD	1:B:3973:PRO:HG2	2.41	0.40
1:B:2950:LYS:O	1:B:2954:GLN:HB2	2.22	0.40
1:B:3159:ARG:C	1:B:3161:LEU:H	2.25	0.40
1:B:350:ARG:NH1	1:B:387:GLU:CD	2.74	0.40
1:B:3605:ASN:HB3	1:B:3609:MSE:CE	2.52	0.40
1:B:376:ILE:HG13	1:B:381:VAL:HG21	2.03	0.40
1:B:3775:LEU:HB3	1:B:3781:CYS:SG	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3870:SER:OG	1:B:3871:PHE:N	2.54	0.40
1:B:509:ARG:HB3	1:B:729:CYS:SG	2.62	0.40
1:B:567:GLU:HB3	1:B:606:SER:HB2	2.04	0.40
1:B:869:ASN:O	1:B:873:VAL:HG23	2.21	0.40
1:B:971:ARG:CG	1:B:972:LEU:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3631/4128 (88%)	2664 (73%)	724 (20%)	243 (7%)	1	21
1	B	3631/4128 (88%)	2657 (73%)	723 (20%)	251 (7%)	1	20
2	K	1/194 (0%)	1 (100%)	0	0	100	100
2	S	1/194 (0%)	1 (100%)	0	0	100	100
All	All	7264/8644 (84%)	5323 (73%)	1447 (20%)	494 (7%)	1	21

All (494) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	ALA
1	A	76	ILE
1	A	147	PHE
1	A	167	PRO
1	A	184	VAL
1	A	185	HIS
1	A	276	ALA
1	A	325	ASN
1	A	405	ASP
1	A	428	PRO

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Mol	Chain	Res	Type
1	A	430	VAL
1	A	544	ILE
1	A	546	ALA
1	A	566	ASP
1	A	635	PRO
1	A	650	SER
1	A	742	GLU
1	A	755	ALA
1	A	767	GLU
1	A	885	ALA
1	A	897	PRO
1	A	903	PRO
1	A	905	ILE
1	A	958	MSE
1	A	1001	PHE
1	A	1005	ASP
1	A	1053	PRO
1	A	1094	SER
1	A	1110	SER
1	A	1141	LYS
1	A	1143	VAL
1	A	1271	ILE
1	A	1324	PRO
1	A	1425	ALA
1	A	1583	MSE
1	A	1591	LYS
1	A	1593	VAL
1	A	1733	THR
1	A	1746	PHE
1	A	1762	MSE
1	A	1978	PHE
1	A	2003	LYS
1	A	2012	ARG
1	A	2029	SER
1	A	2030	TYR
1	A	2058	ASP
1	A	2068	ARG
1	A	2069	ARG
1	A	2074	PRO
1	A	2075	THR
1	A	2126	MSE
1	A	2155	GLU

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Mol	Chain	Res	Type
1	A	2177	ASN
1	A	2248	CYS
1	A	2261	SER
1	A	2286	PRO
1	A	2287	PRO
1	A	2290	PRO
1	A	2357	GLU
1	A	2373	PRO
1	A	2424	MSE
1	A	2464	HIS
1	A	2785	ILE
1	A	2878	ALA
1	A	2926	LEU
1	A	2927	ALA
1	A	3173	MSE
1	A	3313	SER
1	A	3345	PRO
1	A	3576	ASP
1	A	3600	PRO
1	A	3603	LYS
1	A	3688	SER
1	A	3716	HIS
1	A	3835	PRO
1	A	3933	GLU
1	B	76	ILE
1	B	167	PRO
1	B	184	VAL
1	B	185	HIS
1	B	238	MSE
1	B	260	ILE
1	B	276	ALA
1	B	395	MSE
1	B	405	ASP
1	B	430	VAL
1	B	540	MSE
1	B	546	ALA
1	B	566	ASP
1	B	635	PRO
1	B	670	LEU
1	B	742	GLU
1	B	746	ARG
1	B	767	GLU

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Mol	Chain	Res	Type
1	B	784	VAL
1	B	871	LEU
1	B	885	ALA
1	B	897	PRO
1	B	903	PRO
1	B	923	ASP
1	B	1001	PHE
1	B	1005	ASP
1	B	1073	PHE
1	B	1093	GLU
1	B	1110	SER
1	B	1119	LYS
1	B	1122	GLY
1	B	1141	LYS
1	B	1143	VAL
1	B	1214	GLU
1	B	1271	ILE
1	B	1324	PRO
1	B	1408	MSE
1	B	1591	LYS
1	B	1762	MSE
1	B	1957	ASN
1	B	1974	ASN
1	B	1978	PHE
1	B	2012	ARG
1	B	2029	SER
1	B	2058	ASP
1	B	2068	ARG
1	B	2069	ARG
1	B	2074	PRO
1	B	2075	THR
1	B	2155	GLU
1	B	2156	VAL
1	B	2177	ASN
1	B	2248	CYS
1	B	2261	SER
1	B	2263	LYS
1	B	2286	PRO
1	B	2287	PRO
1	B	2290	PRO
1	B	2373	PRO
1	B	2424	MSE

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Mol	Chain	Res	Type
1	B	2785	ILE
1	B	2878	ALA
1	B	2884	LEU
1	B	3240	MSE
1	B	3241	LYS
1	B	3313	SER
1	B	3340	ALA
1	B	3600	PRO
1	B	3603	LYS
1	B	3688	SER
1	B	3711	PRO
1	B	3835	PRO
1	A	97	GLY
1	A	169	THR
1	A	170	VAL
1	A	186	PRO
1	A	187	SER
1	A	260	ILE
1	A	602	MSE
1	A	608	PRO
1	A	746	ARG
1	A	772	ALA
1	A	871	LEU
1	A	923	ASP
1	A	957	PRO
1	A	1000	LYS
1	A	1075	ARG
1	A	1093	GLU
1	A	1112	ALA
1	A	1119	LYS
1	A	1122	GLY
1	A	1169	VAL
1	A	1214	GLU
1	A	1231	GLN
1	A	1237	ALA
1	A	1290	LEU
1	A	1590	THR
1	A	1700	THR
1	A	1724	MSE
1	A	1745	LYS
1	A	1934	LEU
1	A	1957	ASN

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Mol	Chain	Res	Type
1	A	1963	GLN
1	A	2002	LYS
1	A	2011	ALA
1	A	2016	ASN
1	A	2072	ARG
1	A	2168	LEU
1	A	2282	ALA
1	A	2423	VAL
1	A	2514	ASN
1	A	2824	LYS
1	A	2884	LEU
1	A	3311	ASN
1	A	3312	VAL
1	A	3340	ALA
1	A	3456	LEU
1	A	3575	LEU
1	A	3678	GLY
1	A	3973	PRO
1	B	325	ASN
1	B	394	GLN
1	B	428	PRO
1	B	545	LEU
1	B	654	ILE
1	B	671	SER
1	B	712	LYS
1	B	755	ALA
1	B	958	MSE
1	B	1053	PRO
1	B	1075	ARG
1	B	1094	SER
1	B	1290	LEU
1	B	1420	ARG
1	B	1425	ALA
1	B	1709	GLU
1	B	1733	THR
1	B	1811	ARG
1	B	2002	LYS
1	B	2030	TYR
1	B	2072	ARG
1	B	2168	LEU
1	B	2423	VAL
1	B	2570	PRO

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Mol	Chain	Res	Type
1	B	2801	ASP
1	B	2824	LYS
1	B	2871	LEU
1	B	2926	LEU
1	B	2944	THR
1	B	3064	PHE
1	B	3242	MSE
1	B	3345	PRO
1	B	3403	CYS
1	B	3456	LEU
1	B	3499	ILE
1	B	3678	GLY
1	B	3826	ALA
1	B	3933	GLU
1	A	28	ALA
1	A	30	ALA
1	A	48	PRO
1	A	404	ASP
1	A	425	ASP
1	A	604	PRO
1	A	628	GLU
1	A	654	ILE
1	A	1045	THR
1	A	1077	GLY
1	A	1238	GLN
1	A	1289	SER
1	A	1408	MSE
1	A	1420	ARG
1	A	1722	PHE
1	A	1811	ARG
1	A	1962	TYR
1	A	2034	SER
1	A	2096	PRO
1	A	2206	PRO
1	A	2263	LYS
1	A	2280	VAL
1	A	2371	PHE
1	A	2823	PHE
1	A	2914	ALA
1	A	3314	SER
1	A	3545	THR
1	A	3598	LYS

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Mol	Chain	Res	Type
1	A	3796	MSE
1	A	3826	ALA
1	A	3857	LEU
1	A	3978	GLY
1	B	27	ALA
1	B	48	PRO
1	B	101	ALA
1	B	125	ILE
1	B	144	MSE
1	B	186	PRO
1	B	257	ARG
1	B	368	LEU
1	B	404	ASP
1	B	425	ASP
1	B	513	GLU
1	B	650	SER
1	B	957	PRO
1	B	1215	GLU
1	B	1231	GLN
1	B	1237	ALA
1	B	1238	GLN
1	B	1492	ALA
1	B	1565	GLU
1	B	1583	MSE
1	B	1700	THR
1	B	1722	PHE
1	B	1917	LYS
1	B	2003	LYS
1	B	2011	ALA
1	B	2080	VAL
1	B	2096	PRO
1	B	2206	PRO
1	B	2357	GLU
1	B	2371	PHE
1	B	2465	PRO
1	B	2514	ASN
1	B	2575	PRO
1	B	2795	GLN
1	B	2823	PHE
1	B	2927	ALA
1	B	3174	ASP
1	B	3311	ASN

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Mol	Chain	Res	Type
1	B	3601	VAL
1	B	3716	HIS
1	B	3796	MSE
1	B	4120	THR
1	A	27	ALA
1	A	125	ILE
1	A	257	ARG
1	A	277	LEU
1	A	515	ARG
1	A	543	SER
1	A	712	LYS
1	A	784	VAL
1	A	878	GLU
1	A	949	PRO
1	A	1073	PHE
1	A	1463	LEU
1	A	1492	ALA
1	A	1565	GLU
1	A	1647	ALA
1	A	1723	PRO
1	A	2010	GLU
1	A	2080	VAL
1	A	2176	ASN
1	A	2542	LEU
1	A	2795	GLN
1	A	2871	LEU
1	A	2873	PRO
1	A	2879	GLY
1	A	3064	PHE
1	A	3240	MSE
1	A	3443	PRO
1	A	3472	ILE
1	A	3760	GLN
1	A	3860	LYS
1	B	49	ALA
1	B	69	VAL
1	B	169	THR
1	B	277	LEU
1	B	411	PRO
1	B	604	PRO
1	B	910	PHE
1	B	947	GLN

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Mol	Chain	Res	Type
1	B	1000	LYS
1	B	1045	THR
1	B	1069	HIS
1	B	1077	GLY
1	B	1112	ALA
1	B	1348	LEU
1	B	1590	THR
1	B	1723	PRO
1	B	1757	MSE
1	B	1891	ALA
1	B	1895	LYS
1	B	1934	LEU
1	B	1962	TYR
1	B	1987	ARG
1	B	2098	THR
1	B	2464	HIS
1	B	3075	LYS
1	B	3486	GLU
1	B	3497	SER
1	B	3637	GLY
1	B	3654	MSE
1	B	3720	ALA
1	B	3760	GLN
1	B	3847	SER
1	B	3860	LYS
1	B	3973	PRO
1	A	368	LEU
1	A	540	MSE
1	A	598	PRO
1	A	634	LEU
1	A	900	GLU
1	A	1069	HIS
1	A	1364	CYS
1	A	1510	LEU
1	A	1891	ALA
1	A	1895	LYS
1	A	2448	PRO
1	A	2465	PRO
1	A	2569	SER
1	A	2805	ALA
1	A	3091	LEU
1	A	3654	MSE

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Mol	Chain	Res	Type
1	A	3720	ALA
1	A	3732	LEU
1	A	4058	VAL
1	B	30	ALA
1	B	74	ASN
1	B	745	VAL
1	B	763	THR
1	B	878	GLU
1	B	997	ASN
1	B	1071	ASN
1	B	1169	VAL
1	B	1247	PRO
1	B	1346	THR
1	B	1423	ILE
1	B	1593	VAL
1	B	1631	SER
1	B	1701	SER
1	B	1707	LEU
1	B	1812	LEU
1	B	1963	GLN
1	B	2016	ASN
1	B	2280	VAL
1	B	2289	ASP
1	B	2292	CYS
1	B	2879	GLY
1	B	2914	ALA
1	B	3129	LEU
1	B	3243	ILE
1	B	3312	VAL
1	B	3472	ILE
1	B	3978	GLY
1	A	74	ASN
1	A	298	LEU
1	A	627	VAL
1	A	763	THR
1	A	1520	ALA
1	A	2289	ASP
1	A	2942	ILE
1	A	3117	ILE
1	A	3317	SER
1	A	3499	ILE
1	A	3711	PRO

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Mol	Chain	Res	Type
1	A	3981	TYR
1	B	187	SER
1	B	298	LEU
1	B	323	VAL
1	B	427	VAL
1	B	627	VAL
1	B	718	MSE
1	B	748	TYR
1	B	1364	CYS
1	B	1738	ASN
1	B	2291	GLN
1	B	2873	PRO
1	B	2976	LEU
1	B	3443	PRO
1	B	4068	HIS
1	A	256	ILE
1	A	411	PRO
1	A	553	VAL
1	A	1637	SER
1	A	2076	VAL
1	A	2505	VAL
1	A	2552	VAL
1	A	2575	PRO
1	A	3025	PRO
1	A	3601	VAL
1	B	50	VAL
1	B	67	VAL
1	B	170	VAL
1	B	2552	VAL
1	B	4058	VAL
1	A	50	VAL
1	A	69	VAL
1	A	1382	ILE
1	A	2156	VAL
1	A	3174	ASP
1	B	948	MSE
1	B	1382	ILE
1	B	2448	PRO
1	B	3331	GLY
1	A	67	VAL
1	A	381	VAL
1	A	447	PRO

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Mol	Chain	Res	Type
1	A	2059	PRO
1	A	2230	VAL
1	A	2324	GLY
1	A	3919	GLY
1	B	381	VAL
1	B	495	VAL
1	B	2230	VAL
1	B	2569	SER
1	B	3919	GLY
1	A	1247	PRO
1	A	1729	PHE
1	B	174	VAL
1	B	544	ILE
1	B	884	VAL
1	B	905	ILE
1	B	1637	SER
1	B	2804	ILE
1	A	1468	LEU
1	A	3178	ILE
1	B	256	ILE
1	B	2802	PRO
1	B	2942	ILE

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	3259/3384 (96%)	3089 (95%)	170 (5%)	27	61
1	B	3259/3384 (96%)	3084 (95%)	175 (5%)	26	60
2	K	-	1 (100%)	0	100	100
2	S	-	1 (100%)	0	100	100
All	All	6520/6768 (96%)	6175 (95%)	345 (5%)	26	61

All (345) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	LEU
1	A	156	PHE
1	A	274	LEU
1	A	277	LEU
1	A	294	PHE
1	A	326	MSE
1	A	342	MSE
1	A	360	SER
1	A	361	ILE
1	A	368	LEU
1	A	392	CYS
1	A	393	LYS
1	A	396	PHE
1	A	405	ASP
1	A	420	VAL
1	A	444	ASP
1	A	445	SER
1	A	446	PHE
1	A	556	SER
1	A	559	SER
1	A	564	LEU
1	A	595	ASP
1	A	603	ILE
1	A	612	LEU
1	A	620	PHE
1	A	625	ASN
1	A	630	CYS
1	A	631	ARG
1	A	754	MSE
1	A	763	THR
1	A	793	LEU
1	A	858	MSE
1	A	866	ILE
1	A	879	MSE
1	A	884	VAL
1	A	891	ARG
1	A	898	PHE
1	A	907	LEU
1	A	924	ARG
1	A	939	MSE
1	A	963	LYS
1	A	965	THR
1	A	966	PHE

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Mol	Chain	Res	Type
1	A	970	LEU
1	A	975	ASP
1	A	983	LEU
1	A	988	VAL
1	A	989	MSE
1	A	993	HIS
1	A	1005	ASP
1	A	1010	LEU
1	A	1014	LEU
1	A	1017	ILE
1	A	1024	THR
1	A	1068	LEU
1	A	1070	PRO
1	A	1105	VAL
1	A	1107	TYR
1	A	1108	MSE
1	A	1121	LEU
1	A	1131	ILE
1	A	1180	GLN
1	A	1288	SER
1	A	1291	LEU
1	A	1347	THR
1	A	1364	CYS
1	A	1372	LEU
1	A	1403	MSE
1	A	1430	GLU
1	A	1444	ASP
1	A	1507	CYS
1	A	1526	GLU
1	A	1583	MSE
1	A	1590	THR
1	A	1592	MSE
1	A	1597	LEU
1	A	1600	MSE
1	A	1640	GLU
1	A	1643	MSE
1	A	1721	HIS
1	A	1737	ASN
1	A	1743	MSE
1	A	1757	MSE
1	A	1758	LEU
1	A	1759	LEU

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Mol	Chain	Res	Type
1	A	1761	LEU
1	A	1812	LEU
1	A	1883	ARG
1	A	1886	LYS
1	A	1919	CYS
1	A	1942	CYS
1	A	1947	CYS
1	A	1950	SER
1	A	1959	LEU
1	A	1986	ARG
1	A	1993	GLU
1	A	1998	MSE
1	A	2012	ARG
1	A	2104	MSE
1	A	2155	GLU
1	A	2189	ILE
1	A	2239	LYS
1	A	2241	LEU
1	A	2245	TRP
1	A	2277	LEU
1	A	2287	PRO
1	A	2307	MSE
1	A	2330	VAL
1	A	2337	LEU
1	A	2338	GLU
1	A	2355	THR
1	A	2362	VAL
1	A	2370	SER
1	A	2402	LEU
1	A	2404	ARG
1	A	2473	MSE
1	A	2555	LEU
1	A	2568	MSE
1	A	2574	ASN
1	A	2788	SER
1	A	2886	GLN
1	A	2890	ILE
1	A	2921	LEU
1	A	2943	PHE
1	A	2991	LYS
1	A	3011	LEU
1	A	3050	LYS

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Mol	Chain	Res	Type
1	A	3051	LEU
1	A	3084	GLN
1	A	3145	ILE
1	A	3173	MSE
1	A	3256	MSE
1	A	3278	GLN
1	A	3283	LEU
1	A	3326	GLN
1	A	3416	LEU
1	A	3451	LEU
1	A	3481	SER
1	A	3509	ASP
1	A	3518	VAL
1	A	3575	LEU
1	A	3636	PHE
1	A	3641	ASP
1	A	3670	MSE
1	A	3687	MSE
1	A	3706	ASP
1	A	3729	MSE
1	A	3771	MSE
1	A	3781	CYS
1	A	3810	VAL
1	A	3811	THR
1	A	3813	LYS
1	A	3824	GLU
1	A	3831	ASP
1	A	3846	MSE
1	A	3883	LEU
1	A	3893	SER
1	A	3895	GLU
1	A	3926	ASN
1	A	3928	PHE
1	A	3929	MSE
1	A	3944	HIS
1	A	3959	MSE
1	A	3963	LEU
1	A	3964	THR
1	A	3967	PHE
1	A	4066	LEU
1	A	4078	VAL
1	A	4104	VAL

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Mol	Chain	Res	Type
1	A	4128	MSE
1	B	42	CYS
1	B	111	CYS
1	B	143	LEU
1	B	145	ASP
1	B	156	PHE
1	B	274	LEU
1	B	298	LEU
1	B	322	GLN
1	B	360	SER
1	B	361	ILE
1	B	368	LEU
1	B	389	ILE
1	B	393	LYS
1	B	395	MSE
1	B	396	PHE
1	B	405	ASP
1	B	408	TYR
1	B	410	MSE
1	B	420	VAL
1	B	444	ASP
1	B	446	PHE
1	B	487	LEU
1	B	491	CYS
1	B	559	SER
1	B	564	LEU
1	B	603	ILE
1	B	612	LEU
1	B	620	PHE
1	B	633	ILE
1	B	653	LEU
1	B	666	PHE
1	B	733	LEU
1	B	741	ILE
1	B	763	THR
1	B	793	LEU
1	B	865	GLN
1	B	898	PHE
1	B	901	MSE
1	B	924	ARG
1	B	963	LYS
1	B	965	THR

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Mol	Chain	Res	Type
1	B	966	PHE
1	B	970	LEU
1	B	989	MSE
1	B	993	HIS
1	B	1000	LYS
1	B	1005	ASP
1	B	1009	LEU
1	B	1010	LEU
1	B	1017	ILE
1	B	1024	THR
1	B	1036	PHE
1	B	1070	PRO
1	B	1108	MSE
1	B	1121	LEU
1	B	1131	ILE
1	B	1287	GLN
1	B	1347	THR
1	B	1354	GLU
1	B	1372	LEU
1	B	1392	MSE
1	B	1399	CYS
1	B	1430	GLU
1	B	1471	GLN
1	B	1507	CYS
1	B	1583	MSE
1	B	1590	THR
1	B	1597	LEU
1	B	1602	ASP
1	B	1639	LEU
1	B	1725	GLN
1	B	1733	THR
1	B	1743	MSE
1	B	1758	LEU
1	B	1759	LEU
1	B	1761	LEU
1	B	1802	TYR
1	B	1812	LEU
1	B	1819	PHE
1	B	1858	LEU
1	B	1909	ASN
1	B	1927	MSE
1	B	1930	GLU

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Mol	Chain	Res	Type
1	B	1942	CYS
1	B	1950	SER
1	B	1959	LEU
1	B	1973	LYS
1	B	1974	ASN
1	B	1976	LEU
1	B	1986	ARG
1	B	1993	GLU
1	B	1998	MSE
1	B	1999	GLU
1	B	2012	ARG
1	B	2023	SER
1	B	2104	MSE
1	B	2126	MSE
1	B	2155	GLU
1	B	2239	LYS
1	B	2245	TRP
1	B	2265	PRO
1	B	2277	LEU
1	B	2287	PRO
1	B	2325	LEU
1	B	2330	VAL
1	B	2338	GLU
1	B	2355	THR
1	B	2362	VAL
1	B	2370	SER
1	B	2374	LEU
1	B	2402	LEU
1	B	2481	HIS
1	B	2555	LEU
1	B	2559	THR
1	B	2576	MSE
1	B	2776	ARG
1	B	2788	SER
1	B	2820	MSE
1	B	2865	HIS
1	B	2886	GLN
1	B	2890	ILE
1	B	2921	LEU
1	B	2929	LEU
1	B	2943	PHE
1	B	2991	LYS

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Mol	Chain	Res	Type
1	B	3044	MSE
1	B	3050	LYS
1	B	3051	LEU
1	B	3058	ASP
1	B	3118	ASP
1	B	3120	LEU
1	B	3133	GLN
1	B	3145	ILE
1	B	3155	VAL
1	B	3238	MSE
1	B	3242	MSE
1	B	3258	LEU
1	B	3282	ARG
1	B	3283	LEU
1	B	3311	ASN
1	B	3397	GLN
1	B	3403	CYS
1	B	3416	LEU
1	B	3450	MSE
1	B	3451	LEU
1	B	3467	ARG
1	B	3509	ASP
1	B	3518	VAL
1	B	3636	PHE
1	B	3641	ASP
1	B	3763	ARG
1	B	3782	SER
1	B	3796	MSE
1	B	3810	VAL
1	B	3813	LYS
1	B	3820	MSE
1	B	3835	PRO
1	B	3846	MSE
1	B	3856	MSE
1	B	3858	MSE
1	B	3883	LEU
1	B	3895	GLU
1	B	3904	PHE
1	B	3926	ASN
1	B	3944	HIS
1	B	3959	MSE
1	B	3963	LEU

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Mol	Chain	Res	Type
1	B	3970	LEU
1	B	4016	PHE
1	B	4020	MSE
1	B	4029	GLN
1	B	4066	LEU
1	B	4090	ARG
1	B	4104	VAL
1	B	4119	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	ASN
1	A	334	HIS
1	A	508	HIS
1	A	783	HIS
1	A	1069	HIS
1	A	1083	ASN
1	A	1146	ASN
1	A	1385	ASN
1	A	1418	HIS
1	A	1457	GLN
1	A	1459	HIS
1	A	1476	HIS
1	A	1574	ASN
1	A	1687	HIS
1	A	1725	GLN
1	A	1754	GLN
1	A	1890	HIS
1	A	2170	GLN
1	A	2177	ASN
1	A	2183	HIS
1	A	2234	ASN
1	A	2426	HIS
1	A	2518	GLN
1	A	3003	ASN
1	A	3081	HIS
1	A	3122	HIS
1	A	3251	ASN
1	A	3291	GLN
1	A	3319	ASN
1	A	3501	HIS

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Mol	Chain	Res	Type
1	A	3524	ASN
1	A	3762	GLN
1	A	3927	ASN
1	A	3951	GLN
1	A	4068	HIS
1	B	390	GLN
1	B	409	GLN
1	B	437	HIS
1	B	442	GLN
1	B	508	HIS
1	B	593	ASN
1	B	990	GLN
1	B	993	HIS
1	B	1055	ASN
1	B	1238	GLN
1	B	1350	ASN
1	B	1476	HIS
1	B	1574	ASN
1	B	1687	HIS
1	B	1866	GLN
1	B	1890	HIS
1	B	1897	ASN
1	B	1974	ASN
1	B	2077	HIS
1	B	2177	ASN
1	B	2348	GLN
1	B	2365	ASN
1	B	2481	HIS
1	B	2518	GLN
1	B	3251	ASN
1	B	3459	ASN
1	B	3494	GLN
1	B	3524	ASN
1	B	3772	ASN
1	B	3908	HIS
1	B	3926	ASN
1	B	4018	GLN
1	B	4110	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	1
2	K	1
2	S	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	133:UNK	C	201:UNK	N	46.74
1	S	133:UNK	C	201:UNK	N	41.40
1	B	3794:VAL	C	3795:PRO	N	1.18
1	A	1069:HIS	C	1070:PRO	N	1.15

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	3551/4128 (86%)	0.27	237 (6%)	19 15	83, 248, 332, 443	0
1	B	3551/4128 (86%)	0.32	249 (7%)	17 14	117, 251, 358, 507	0
2	K	0/194	-	-	-	-	-
2	S	0/194	-	-	-	-	-
All	All	7102/8644 (82%)	0.29	486 (6%)	18 15	83, 249, 343, 507	0

All (486) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	122	LYS	12.9
1	B	1355	GLY	9.7
1	B	31	GLY	9.6
1	B	145	ASP	9.5
1	A	126	PRO	8.8
1	B	586	GLN	8.6
1	A	123	CYS	8.6
1	A	1290	LEU	8.3
1	A	1286	ALA	8.1
1	B	3026	ASP	7.9
1	A	1763	THR	7.9
1	A	121	ALA	7.6
1	A	1287	GLN	7.4
1	B	30	ALA	7.1
1	A	1289	SER	7.0
1	B	3023	ASN	7.0
1	A	1285	GLU	6.7
1	A	1523	GLY	6.7
1	B	215	PRO	6.7
1	B	3358	ARG	6.7
1	A	2910	VAL	6.6
1	B	3025	PRO	6.4

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Mol	Chain	Res	Type	RSRZ
1	B	1357	LYS	6.4
1	B	153	PHE	6.4
1	A	215	PRO	6.4
1	B	24	ARG	6.3
1	B	3033	GLU	6.3
1	B	25	CYS	6.3
1	A	953	GLN	6.2
1	A	589	GLY	6.1
1	A	590	GLU	6.1
1	B	22	ALA	6.0
1	A	2906	PRO	6.0
1	A	2898	LEU	5.8
1	A	1761	LEU	5.8
1	B	2263	LYS	5.8
1	B	3029	LYS	5.7
1	B	3027	LEU	5.7
1	A	2905	LEU	5.7
1	B	3028	ASN	5.6
1	A	2202	PRO	5.6
1	B	3515	GLN	5.6
1	A	124	LYS	5.5
1	B	100	ILE	5.4
1	A	125	ILE	5.4
1	A	3029	LYS	5.3
1	A	2113	GLY	5.3
1	B	32	HIS	5.1
1	A	2250	SER	5.0
1	B	280	SER	5.0
1	A	503	SER	5.0
1	A	3152	SER	5.0
1	A	3403	CYS	5.0
1	A	2900	LEU	5.0
1	B	2900	LEU	4.9
1	A	2897	LEU	4.9
1	B	3153	SER	4.9
1	B	26	GLY	4.8
1	A	950	GLU	4.8
1	B	2430	GLU	4.6
1	B	257	ARG	4.6
1	A	237	SER	4.6
1	B	10	CYS	4.6
1	A	1288	SER	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	1044	ILE	4.6
1	B	3675	LYS	4.6
1	B	3528	ALA	4.6
1	B	253	LEU	4.5
1	B	23	ASP	4.5
1	A	2821	ASP	4.5
1	A	951	GLY	4.5
1	A	670	LEU	4.5
1	B	3024	PRO	4.5
1	B	495	VAL	4.5
1	B	1763	THR	4.4
1	B	3406	ALA	4.4
1	A	127	ALA	4.4
1	B	1761	LEU	4.4
1	B	125	ILE	4.4
1	B	3359	ILE	4.4
1	A	3402	SER	4.4
1	A	3311	ASN	4.3
1	B	123	CYS	4.3
1	B	3976	GLU	4.3
1	A	3510	GLN	4.3
1	A	280	SER	4.3
1	B	1286	ALA	4.2
1	A	2183	HIS	4.2
1	B	582	THR	4.2
1	A	128	LEU	4.2
1	B	3020	ASP	4.2
1	B	3623	PRO	4.2
1	A	2985	GLU	4.2
1	B	3074	GLN	4.1
1	A	2203	THR	4.1
1	B	3152	SER	4.1
1	A	3357	ARG	4.1
1	A	1589	ASN	4.1
1	B	2116	ASP	4.1
1	A	2782	ASP	4.1
1	A	952	GLY	4.0
1	B	72	SER	4.0
1	B	216	LYS	4.0
1	B	3499	ILE	4.0
1	B	1354	GLU	4.0
1	A	3308	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	3272	TRP	4.0
1	A	216	LYS	4.0
1	B	279	ALA	3.9
1	B	126	PRO	3.9
1	A	1284	THR	3.9
1	B	27	ALA	3.9
1	A	171	LEU	3.9
1	A	2868	LEU	3.9
1	A	671	SER	3.9
1	B	122	LYS	3.9
1	A	3269	ARG	3.9
1	A	897	PRO	3.9
1	A	3478	GLU	3.8
1	A	1357	LYS	3.8
1	A	3196	LYS	3.8
1	A	3509	ASP	3.8
1	A	956	PRO	3.7
1	B	1856	THR	3.7
1	A	1673	THR	3.7
1	A	1489	LYS	3.7
1	B	154	SER	3.7
1	B	4039	TYR	3.7
1	A	506	GLU	3.7
1	A	3358	ARG	3.7
1	A	153	PHE	3.6
1	A	2984	GLY	3.6
1	A	3150	ASN	3.6
1	B	2942	ILE	3.6
1	B	542	ASP	3.6
1	A	2986	PRO	3.6
1	A	588	VAL	3.6
1	B	631	ARG	3.6
1	B	116	THR	3.6
1	B	1043	GLN	3.6
1	A	3317	SER	3.5
1	B	3676	PRO	3.5
1	B	1287	GLN	3.5
1	A	3199	PRO	3.5
1	A	129	ASP	3.5
1	A	2201	THR	3.5
1	A	2527	HIS	3.5
1	A	3149	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	157	TYR	3.5
1	A	3515	GLN	3.5
1	B	1356	TRP	3.5
1	B	3405	PRO	3.5
1	A	591	GLN	3.4
1	B	3936	GLY	3.4
1	B	1671	VAL	3.4
1	B	2067	ARG	3.4
1	B	4082	ARG	3.4
1	B	668	LYS	3.3
1	A	3026	ASP	3.3
1	A	1435	ASN	3.3
1	B	1290	LEU	3.3
1	B	2981	TRP	3.3
1	A	2978	LYS	3.3
1	A	3098	ARG	3.3
1	A	1586	SER	3.3
1	A	1526	GLU	3.3
1	B	3035	PHE	3.3
1	A	2308	SER	3.3
1	B	2090	ARG	3.2
1	B	3624	GLY	3.2
1	A	252	VAL	3.2
1	A	2197	THR	3.2
1	B	92	PHE	3.2
1	B	3056	GLU	3.2
1	B	213	ARG	3.2
1	B	2464	HIS	3.2
1	B	628	GLU	3.2
1	A	3102	TYR	3.2
1	B	1437	TYR	3.2
1	A	3153	SER	3.2
1	A	2988	GLU	3.2
1	A	604	PRO	3.2
1	A	1604	SER	3.2
1	B	2175	GLU	3.2
1	A	214	GLU	3.2
1	A	1436	LEU	3.2
1	B	3355	LYS	3.1
1	A	120	ALA	3.1
1	B	3550	LYS	3.1
1	B	2533	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	3514	VAL	3.1
1	A	892	LEU	3.1
1	B	585	ILE	3.1
1	A	739	ASN	3.1
1	A	2068	ARG	3.1
1	B	2980	ASP	3.1
1	B	3809	THR	3.1
1	A	2444	PRO	3.1
1	B	3540	TYR	3.1
1	B	3510	GLN	3.1
1	A	157	TYR	3.0
1	A	2867	ALA	3.0
1	A	2980	ASP	3.0
1	A	505	SER	3.0
1	B	950	GLU	3.0
1	B	190	ILE	3.0
1	B	3822	GLN	3.0
1	A	2899	ARG	3.0
1	B	2264	ASP	3.0
1	B	71	LYS	3.0
1	B	124	LYS	3.0
1	B	4081	ALA	3.0
1	B	3841	ASP	3.0
1	B	265	TYR	3.0
1	A	2267	SER	2.9
1	B	1284	THR	2.9
1	A	513	GLU	2.9
1	A	213	ARG	2.9
1	B	1548	GLY	2.9
1	B	3674	SER	2.9
1	B	1672	PHE	2.9
1	A	896	VAL	2.9
1	B	103	TYR	2.9
1	A	3976	GLU	2.9
1	B	627	VAL	2.9
1	A	1699	PHE	2.9
1	B	3486	GLU	2.9
1	A	1522	GLY	2.9
1	A	2907	ALA	2.9
1	B	35	ILE	2.9
1	A	3700	GLU	2.9
1	B	86	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	2496	GLN	2.9
1	A	18	THR	2.8
1	A	2208	ASP	2.8
1	B	14	ARG	2.8
1	B	2078	ASP	2.8
1	A	355	ASN	2.8
1	A	1488	TYR	2.8
1	A	3273	LEU	2.8
1	B	34	LEU	2.8
1	A	3404	GLY	2.8
1	A	3624	GLY	2.8
1	B	104	SER	2.8
1	B	2427	ARG	2.8
1	A	81	CYS	2.8
1	B	3380	ARG	2.8
1	B	3879	PRO	2.8
1	B	38	LEU	2.8
1	B	472	GLY	2.8
1	B	2822	LYS	2.7
1	B	2930	TYR	2.7
1	B	2899	ARG	2.7
1	B	3830	SER	2.7
1	B	3341	LEU	2.7
1	A	809	THR	2.7
1	B	101	ALA	2.7
1	B	1822	ARG	2.7
1	B	146	GLU	2.7
1	A	781	ASP	2.7
1	A	1698	PHE	2.7
1	A	3312	VAL	2.7
1	B	3070	HIS	2.7
1	B	2465	PRO	2.7
1	B	115	TYR	2.7
1	A	1558	TYR	2.7
1	B	262	LEU	2.7
1	A	3318	LYS	2.7
1	B	877	ASP	2.7
1	B	1816	ARG	2.7
1	B	2081	LEU	2.7
1	A	3633	ILE	2.7
1	A	3875	GLU	2.7
1	A	259	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	2898	LEU	2.7
1	A	3603	LYS	2.6
1	B	908	ASP	2.6
1	B	330	ASN	2.6
1	B	1101	PHE	2.6
1	A	543	SER	2.6
1	A	2781	PRO	2.6
1	B	59	PHE	2.6
1	B	21	ALA	2.6
1	A	782	ARG	2.6
1	A	890	LYS	2.6
1	B	2905	LEU	2.6
1	B	2411	LEU	2.6
1	A	2263	LYS	2.6
1	B	99	LYS	2.6
1	A	2975	ALA	2.6
1	B	252	VAL	2.6
1	B	95	LYS	2.6
1	B	3580	ASN	2.6
1	B	1799	GLU	2.6
1	B	494	PRO	2.6
1	B	2390	HIS	2.6
1	B	3875	GLU	2.6
1	A	2259	LYS	2.5
1	A	2979	GLN	2.5
1	B	2412	TYR	2.5
1	A	2421	VAL	2.5
1	A	3828	TYR	2.5
1	B	4115	ASN	2.5
1	A	3879	PRO	2.5
1	B	3828	TYR	2.5
1	B	583	LEU	2.5
1	B	2084	GLU	2.5
1	B	3549	HIS	2.5
1	B	1732	GLY	2.5
1	B	3432	SER	2.5
1	A	1907	GLU	2.5
1	B	3553	GLU	2.5
1	A	587	THR	2.5
1	B	20	SER	2.5
1	B	2077	HIS	2.5
1	B	2821	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	3393	GLU	2.5
1	B	1255	CYS	2.5
1	A	3405	PRO	2.5
1	B	1509	GLN	2.5
1	B	3105	ASN	2.5
1	B	3489	SER	2.5
1	A	3052	LEU	2.5
1	B	11	SER	2.5
1	B	2461	PHE	2.4
1	A	799	TYR	2.4
1	B	28	ALA	2.4
1	B	183	GLU	2.4
1	B	2176	ASN	2.4
1	A	2440	TYR	2.4
1	A	3105	ASN	2.4
1	A	2114	GLU	2.4
1	A	2195	SER	2.4
1	A	3627	ALA	2.4
1	A	2869	LEU	2.4
1	B	82	ARG	2.4
1	A	3252	PHE	2.4
1	B	1426	GLN	2.4
1	A	80	GLU	2.4
1	A	1788	ARG	2.4
1	B	167	PRO	2.4
1	A	585	ILE	2.4
1	B	1002	GLU	2.4
1	A	262	LEU	2.4
1	A	3300	VAL	2.4
1	B	1350	ASN	2.4
1	B	1589	ASN	2.4
1	A	3708	ARG	2.4
1	B	2986	PRO	2.4
1	A	3326	GLN	2.4
1	B	117	LYS	2.4
1	A	3629	ARG	2.4
1	A	2893	LEU	2.3
1	B	2488	GLU	2.4
1	B	2904	GLU	2.4
1	A	593	ASN	2.3
1	B	676	ASN	2.3
1	B	2486	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	3698	GLU	2.3
1	B	516	THR	2.3
1	A	1277	GLY	2.3
1	B	191	ASN	2.3
1	A	3406	ALA	2.3
1	A	580	ASP	2.3
1	A	3159	ARG	2.3
1	A	514	VAL	2.3
1	A	3695	LEU	2.3
1	B	1051	LYS	2.3
1	B	867	ASN	2.3
1	B	150	GLY	2.3
1	B	4118	GLY	2.3
1	B	2943	PHE	2.3
1	B	3346	ALA	2.3
1	B	3407	ALA	2.3
1	A	2909	ARG	2.3
1	B	3488	SER	2.3
1	B	136	GLN	2.3
1	B	3627	ALA	2.3
1	B	2201	THR	2.3
1	B	3350	GLU	2.3
1	A	3610	TYR	2.3
1	B	63	PHE	2.3
1	B	1138	ILE	2.3
1	B	3622	ALA	2.3
1	B	1020	PRO	2.3
1	A	1465	HIS	2.3
1	B	1512	SER	2.3
1	B	3199	PRO	2.3
1	A	4092	GLN	2.3
1	A	3443	PRO	2.3
1	A	672	ILE	2.3
1	A	1088	GLU	2.3
1	B	3625	LEU	2.3
1	B	2308	SER	2.3
1	A	2464	HIS	2.3
1	A	2082	GLU	2.3
1	A	2067	ARG	2.3
1	A	3630	ARG	2.2
1	B	2491	THR	2.2
1	B	3500	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	2492	ASP	2.2
1	A	2939	LEU	2.2
1	A	3604	LYS	2.2
1	B	579	LEU	2.2
1	B	1442	GLN	2.2
1	A	507	ASP	2.2
1	B	868	LYS	2.2
1	B	68	PHE	2.2
1	A	119	ARG	2.2
1	A	27	ALA	2.2
1	A	586	GLN	2.2
1	B	3617	LEU	2.2
1	B	3546	SER	2.2
1	A	62	ASP	2.2
1	B	2184	TYR	2.2
1	A	582	THR	2.2
1	A	194	GLU	2.2
1	A	3104	GLN	2.2
1	A	1463	LEU	2.2
1	B	1818	SER	2.2
1	B	2391	GLY	2.2
1	A	3197	LEU	2.2
1	A	3849	LYS	2.2
1	B	493	LYS	2.2
1	A	3696	ARG	2.2
1	B	132	ILE	2.2
1	A	2093	CYS	2.1
1	B	81	CYS	2.1
1	B	3150	ASN	2.1
1	A	356	ASN	2.1
1	B	3629	ARG	2.1
1	B	29	LEU	2.1
1	A	2461	PHE	2.1
1	A	2112	GLN	2.1
1	A	3074	GLN	2.1
1	A	130	LEU	2.1
1	A	1506	SER	2.1
1	A	3674	SER	2.1
1	B	1031	ARG	2.1
1	A	3282	ARG	2.1
1	B	341	PHE	2.1
1	B	1436	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	3551	ASN	2.1
1	A	3058	ASP	2.1
1	B	47	SER	2.1
1	B	2174	SER	2.1
1	B	3544	ASP	2.1
1	A	3439	LEU	2.1
1	B	3506	LEU	2.1
1	A	2903	ALA	2.1
1	A	3310	ASN	2.1
1	A	3400	SER	2.1
1	B	60	SER	2.1
1	A	634	LEU	2.1
1	B	258	PRO	2.1
1	B	1052	SER	2.1
1	A	3699	LEU	2.1
1	A	2009	LYS	2.1
1	A	2842	ARG	2.1
1	A	1437	TYR	2.1
1	A	3007	GLU	2.1
1	B	37	GLY	2.1
1	A	3356	ALA	2.1
1	A	3493	TRP	2.1
1	A	3382	PHE	2.1
1	A	3636	PHE	2.1
1	A	28	ALA	2.0
1	A	512	GLY	2.0
1	B	1360	LYS	2.0
1	B	1471	GLN	2.0
1	A	4093	GLU	2.0
1	A	3479	THR	2.0
1	A	2493	ASN	2.0
1	A	16	GLN	2.0
1	B	4110	GLN	2.0
1	A	1557	GLU	2.0
1	B	1161	ALA	2.0
1	A	3008	TRP	2.0
1	A	3267	LYS	2.0
1	B	336	ASN	2.0
1	B	3327	ASN	2.0
1	B	4067	GLY	2.0
1	B	3507	ASP	2.0
1	B	413	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	3476	PRO	2.0
1	A	3546	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.