



Full wwPDB EM Validation Report ⓘ

Jun 3, 2025 – 12:42 PM EDT

PDB ID : 9D9Z / pdb_00009d9z
EMDB ID : EMD-46686
Title : Structure of human UBR4-KCMF1-CaM E3 ligase complex (Silencing Factor of the Integrated stress response, SiFI)
Authors : Yang, Z.; Rape, M.
Deposited on : 2024-08-21
Resolution : 3.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

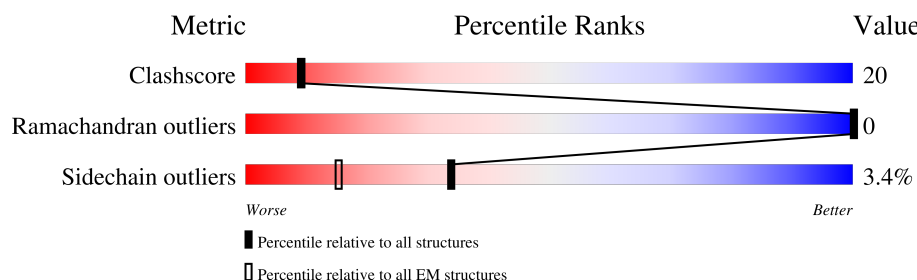
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	5205	<div> <div>50%</div> <div>45%</div> <div>29%</div> <div>25%</div> </div>
1	B	5205	<div> <div>50%</div> <div>46%</div> <div>28%</div> <div>24%</div> </div>
2	C	149	<div> <div>83%</div> <div>51%</div> <div>43%</div> <div>• •</div> </div>
2	D	149	<div> <div>85%</div> <div>47%</div> <div>46%</div> <div>• •</div> </div>
3	E	381	<div> <div>34%</div> <div>30%</div> <div>17%</div> <div>52%</div> </div>
3	F	381	<div> <div>35%</div> <div>29%</div> <div>18%</div> <div>52%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ZN	A	5202	-	-	X	-
4	ZN	B	5202	-	-	X	-
5	CA	D	202	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 66746 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called UBR4 (endogenously FLAG-tagged at the N-terminus),E3 ubiquitin-protein ligase UBR4,E3 ubiquitin-protein ligase UBR4,E3 ubiquitin-protein ligase UBR4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3917	Total	C	N	O	S	0	0
			30658	19475	5230	5749	204		
1	B	3946	Total	C	N	O	S	0	0
			30933	19647	5279	5802	205		

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	144	Total	C	N	O	S	0	0
			1134	696	182	247	9		
2	D	143	Total	C	N	O	S	0	0
			1127	692	181	245	9		

- Molecule 3 is a protein called E3 ubiquitin-protein ligase KCMF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	182	Total	C	N	O	S	0	0
			1435	881	250	288	16		
3	F	182	Total	C	N	O	S	0	0
			1435	881	250	288	16		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	6	Total	Zn	0
			6	6	
4	B	6	Total	Zn	0
			6	6	
4	E	4	Total	Zn	0
			4	4	

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Mol	Chain	Residues	Atoms		AltConf
4	F	4	Total	Zn	0
			4	4	

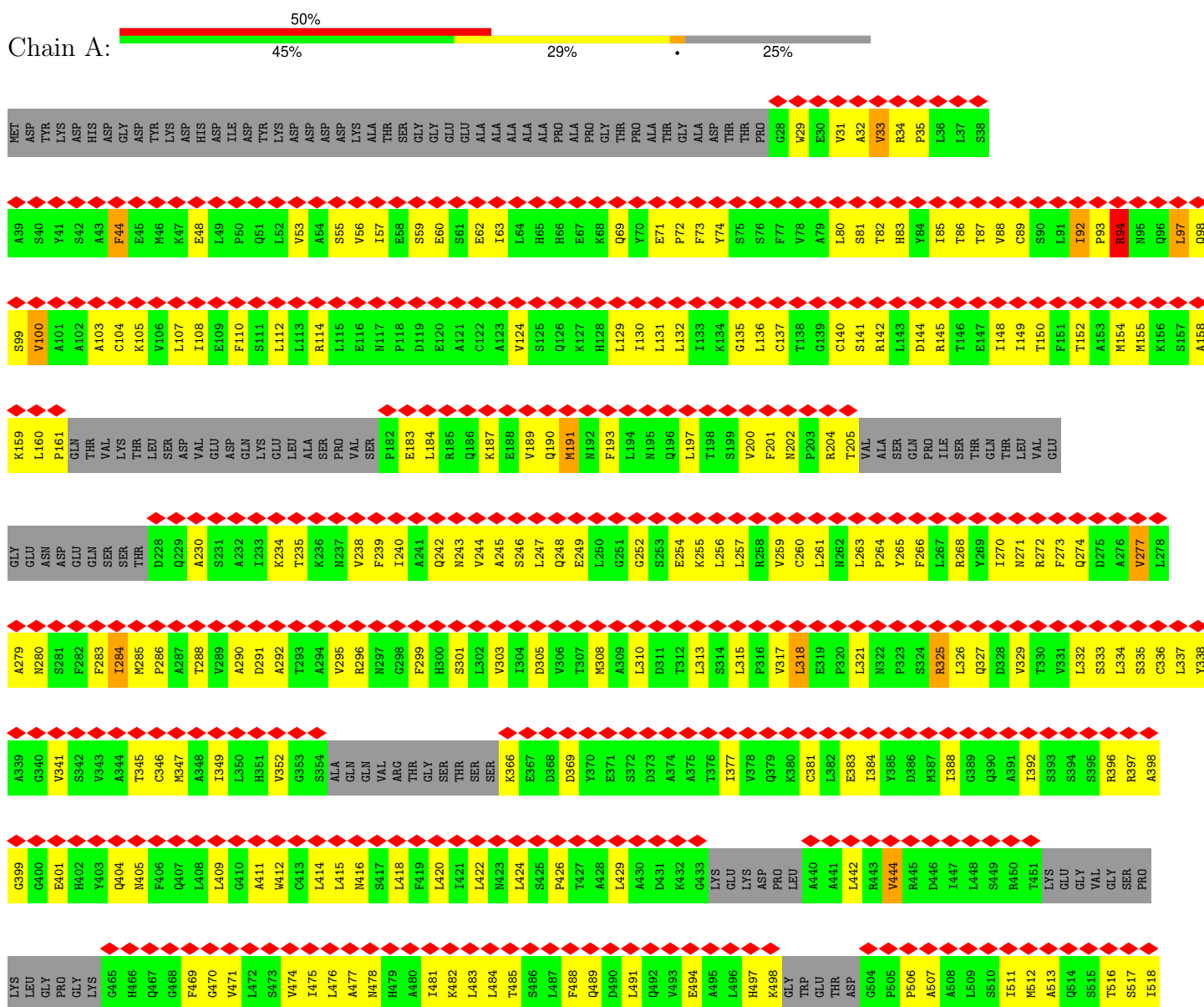
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	C	2	Total	Ca	0
			2	2	
5	D	2	Total	Ca	0
			2	2	

3 Residue-property plots

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

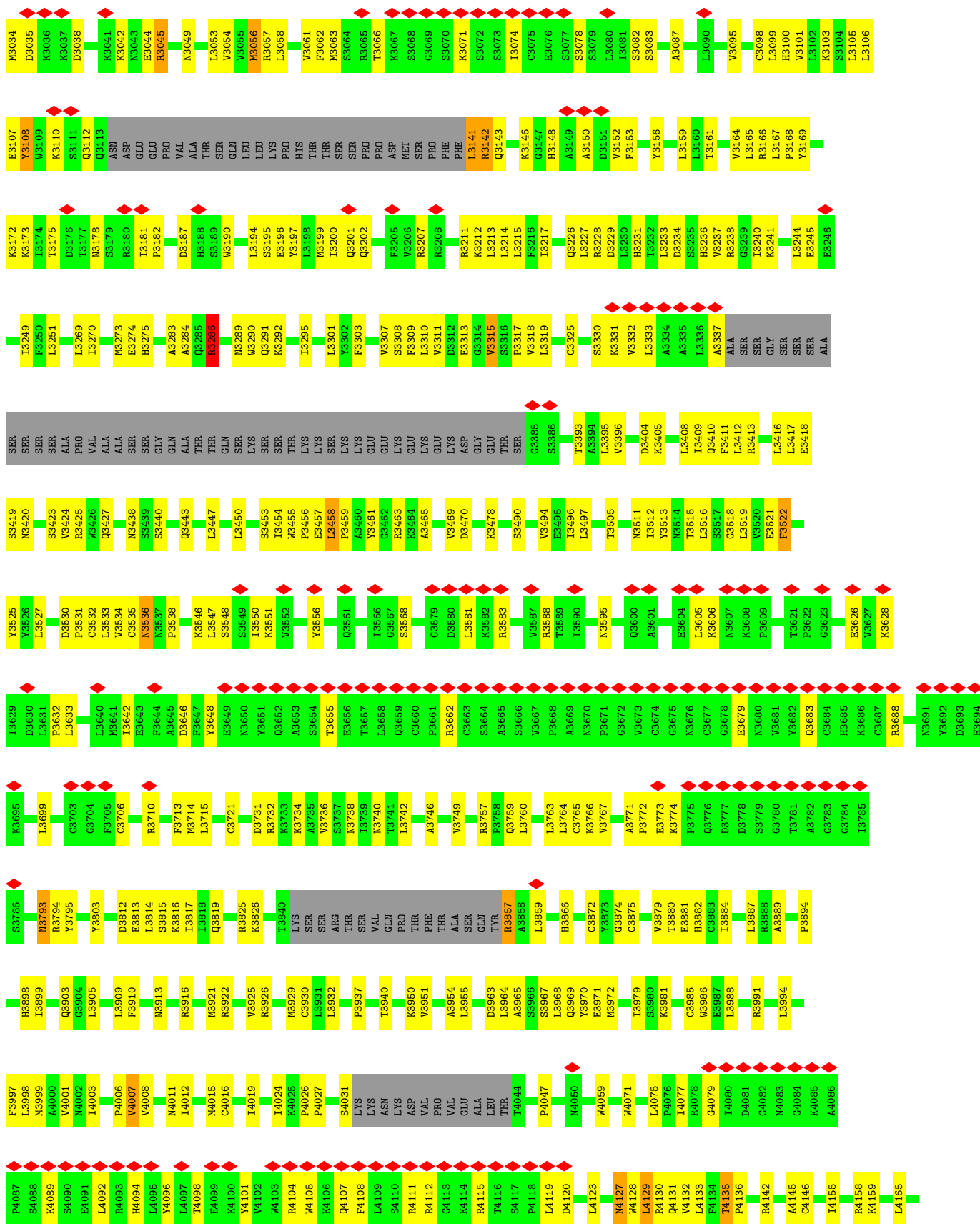
- Molecule 1: UBR4 (endogenously FLAG-tagged at the N-terminus),E3 ubiquitin-protein ligase UBR4,E3 ubiquitin-protein ligase UBR4,E3 ubiquitin-protein ligase UBR4



I1299	M1239	Q1179	Q1119	I1059	L999	E939	Q879	H819	R759	K699	ALA	Q519
E1240	E1240	N1180	S1120	K1060	Q1000	A940	V880	N820	L760	G700	S640	R520
F1241	F1241	F1181	I1121	Q1061	Y1001	S941	Q881	F821	L761	S701	R641	I521
P1242	P1242	N1182	Y1122	G1062	Y1002	E942	H882	T822	L762	S702	D643	Q522
M1243	M1243	E1183	T1123	M1063	F1003	H883	H883	E823	I763	D703	P644	R523
I1244	I1244	E1184	L1124	K1064	L1004	D944	L884	T824	W764	E704	E644	L524
G1245	G1245	GLY	D1125	A1065	I1005	L945	L885	R826	Q765	E705	E645	I525
S1246	S1246	THR	A1126	E1066	L1006	N946	S886	R826	H766	F706	L646	D526
M1247	M1247	GLU	A1127	H1067	W1007	R947	P887	R827	K767	A707	L647	S527
R1248	R1248	LYS	I1128	A1068	R1008	L948	P888	A828	A768	A708	L648	V528
P1190	P1190	P1190	S1129	S1069	I1009	D949	PHE	R829	S769	A709	E649	P529
S1191	S1191	S1191	K1130	S1070	L1010	S950	TRP	L830	A770	A709	L650	L530
K1192	K1192	K1192	Y1131	L1071	G1011	V951	ALA	S831	Q771	L710	M531	M531
E1193	E1193	E1193	Q1132	L1072	I1012	A952	SER	L832	G772	Y711	N532	N532
K1194	K1194	K1194	V1133	E1073	L1013	C953	GLY	F833	D773	H712	GLY	GLY
L1195	L1195	L1195	S1134	L1074	P1014	D954	SER	V834	P774	F713	THR	THR
L1135	L1135	L1135	D1136	A1075	P1015	V955	GLN	Q835	W715	N714	ILE	ILE
Q1197	Q1197	Q1197	L1136	S1076	S1016	L956	ASP	Q836	S716	H715	L655	L534
F1198	F1198	F1198	E1137	T1077	S1017	L957	SER	T836	V776	S716	L656	L535
A1199	A1199	A1199	H1138	T1078	K1017	F957	ASN	R837	P657	L717	L657	T536
A1200	A1200	A1200	F1139	T1079	T1018	S958	SER	Q838	P777	L717	L658	L537
V1201	V1201	V1201	S1140	K1079	Y1019	K959	ARG	E839	E778	V718	L659	L538
L1202	L1202	L1202	K1141	C1080	I1020	L960	ARG	E839	C779	T719	S539	S539
A1203	A1203	A1203	M1142	S1081	N1021	V961	A903	L840	L780	S720	ALA	T540
I1204	I1204	I1204	M1142	V1082	Q1022	K962	T904	S841	K781	D721	ALA	S541
S1205	S1205	S1205	A1143	V1083	L1023	P963	T905	V842	W782	L722	PRO	Y542
A1264	A1264	A1264	ALA	K1084	S1024	D964	P906	H843	W783	Q723	PRO	R543
V1265	V1265	GLY	GLY	Y1085	M1025	D964	L907	H844	D784	S724	PRO	K544
Q1266	Q1266	THR	THR	D1086	M1026	E965	Y908	D845	R785	P725	PRO	A545
A1267	A1267	ASP	ASP	T1087	N1026	L966	H909	A846	F786	N726	PRO	C546
A1268	A1268	PRO	PRO	E1088	S1027	P967	G910	Q847	L787	L727	PRO	V547
H1269	H1269	HIS	HIS	V1089	P1028	A968	F911	M848	S788	Q728	PRO	L548
I1270	I1270	LYS	LYS	V1090	E1029	A969	K912	R849	T789	N729	LEU	Q549
G1271	G1271	S1151	S1151	V1090	M1030	E913	E913	F850	M790	T730	GLY	R550
T1272	T1272	S1152	S1152	E1091	S1031	T971	V914	H851	K791	L731	SER	R550
L1273	L1273	E1153	E1153	E1092	E1032	L972	E915	P852	Q792	L732	SER	Q551
C1274	C1274	I1154	I1154	F1093	E1032	L973	E916	L853	N793	Q733	ARG	R552
S1275	S1275	T1155	T1155	Y1094	D1034	L974	N917	T854	A794	Q734	VAL	K553
Q1276	Q1276	K1156	K1156	A1095	I1035	A975	W918	L855	L795	L735	LYS	G554
T1217	T1217	N1157	N1157	R1096	I1036	A976	S919	A856	Q796	G736	SER	SER
L1218	L1218	L1158	L1158	Q1097	H1037	G977	K920	R857	G797	V737	PRO	MET
V1219	V1219	L1159	L1159	Q1097	T1038	S978	H921	L858	V798	A738	LYS	SER
Q1220	Q1220	P1160	P1160	S1099	T1039	F922	F922	L859	W799	F739	GLN	ASP
N1221	N1221	A1161	A1161	S1100	L1039	S923	S923	L860	P800	F740	ALA	ALA
L1222	L1222	T1162	T1162	F1101	R1040	S923	S924	T861	S801	S741	PRO	SER
P1223	P1223	L1163	L1163	C1102	W1041	D981	S924	T861	S801	S741	GLY	ALA
S1224	S1224	Q1164	Q1164	S1103	S1042	T982	D925	F862	E802	E742	LYS	THR
S1225	S1225	L1165	L1165	T1104	S1043	V983	A926	D863	T803	G743	GLY	SER
V1226	V1226	I1166	I1166	T1104	R1044	R984	V927	Y864	E804	P744	ASN	ASN
Q1227	Q1227	D1167	D1167	D1105	L1045	R985	P928	L865	D805	W745	THR	THR
T1228	T1228	T1168	T1168	C1106	R1046	K986	P928	L866	L806	P746	TYR	TYR
V1229	V1229	Y1169	Y1169	T1107	I1047	E987	P930	R867	N807	L747	GLY	GLY
C1230	C1230	A1170	A1170	T1108	S1048	N988	P930	Q868	V808	V748	ASP	ASP
E1231	E1231	S1171	S1171	I1109	S1049	K989	F932	Q869	E809	I749	PHE	PHE
S1232	S1232	F1172	F1172	L1110	Y1050	N990	Y933	S870	H810	H750	SER	SER
W1233	W1233	T1173	T1173	Q1111	V1051	V991	C934	R871	L811	F751	THR	THR
N1234	N1234	R1174	R1174	L1112	M1052	T992	V935	A872	O812	Q752	GLY	GLY
M1235	M1235	A1175	A1175	H1113	W1053	A993	L936	P873	N813	S753	ASP	ASP
I1236	I1236	Y1176	Y1176	E1114	I1064	E995	S937	H874	L814	L754	PHE	PHE
N1237	N1237	L1177	L1177	I1115	K1055	E995	P938	Y875	L815	S755	SER	SER
T1238	T1238	L1178	L1178	P1116	D1056	A996	L938	L876	L816	V756	THR	THR
				S1117	H1057	C997	F938	F877	T817	L757	GLY	GLY
				L1118	L1058	A998		E878	F818	S758		

P2085	I2025	M1960	C1900	Q1840	E1722	LVS	S1601	V1539	S1479	L1419	V1359
F2086	Y2026	P1961	V1901	A1841	D1723	L1663	L1602	V1540	D1480	S1420	M1360
Y2087	D2027	K1963	L1902	L1842	G1724	C1664	Y1602	M1541	Q1481	A1421	I1361
Z2088	L2028	E1964	S1903	S1843	S1725	F1665	L1604	A1542	L1482	K1422	L1362
T2089	C2029	D1965	P1905	E1844	C1726	F1666	A1604	T1543	D1483	F1423	A1363
N2090	M2030	Y1966	SER	L1845	L1727	T1667	D1605	L1544	V1484	C1424	M1364
D2031	V2031	H1906	H1906	L1846	A1728	T1668	V1606	T1545	T1485	M1425	H1365
A2032	A2032	L1947	C1907	T1847	L1729	T1669	T1607	S1546	Q1486	R1426	A1366
L2033	L2033	ARG	THR	ARG	VAL	GLN	M1608	A1547	E1487	V1427	D1367
S2034	S2034	THR	VAL	VAL	LYS	LYS	A1609	G1548	N1488	L1428	P1368
P2035	P2035	GLY	GLY	GLY	THR	PHE	L1610	Q1549	R1489	K1429	N1369
T2036	T2036	GLY	GLY	GLY	PRO	MET	SER	Q1550	Q1490	F1430	S1370
F2037	F2037	CYS	CYS	ASN	SER	ASN	GLN	A1551	L1491	F1431	G1371
Y2038	Y2038	ARG	ARG	SER	SER	Q1676	ASN	G1552	L1492	T1432	L1372
Z2039	Z2039	E1797	A1913	M1853	GLY	H1677	GLY	H1553	Q1493	K1433	D1373
L2040	L2040	E1798	V1915	M1854	MET	V1678	GLN	L1554	L1494	L1434	E1374
D2041	D2041	L1799	S1915	T1855	SER	H1679	GLY	L1554	L1494	S1375	F1435
P2042	P2042	Q1800	H1916	D1856	THR	Y1680	PRO	L1555	T1496	Q1436	I1376
S2043	S2043	Q1857	E1917	Q1857	MET	C1681	SER	L1556	T1497	L1437	L1377
S2044	S2044	N1801	K1918	L1858	LYS	H1682	HIS	H1557	Y1498	T1438	E1378
K2045	K2045	Q1802	Q1802	GLY	GLY	GLY	LEU	N1558	T1499	E1439	C1380
L2046	L2046	A1803	A1803	SER	SER	T1683	VAL	A1559	V1500	K1440	L1381
R2047	R2047	M1859	M1859	ALA	ALA	C1684	ASP	A1560	R1501	S1441	Q1382
D2048	D2048	P1861	F1805	PHE	PHE	K1685	GLY	V1561	E1502	P1442	Y1383
A2107	A2107	L1862	S1806	GLN	GLN	H1686	GLU	D1562	N1503	N1443	L1384
L2108	L2108	L1863	F1807	SER	SER	V1687	ARG	W1563	S1504	P1444	E1385
V2049	V2049	G1864	A1808	PRO	PRO	ASP	ALA	L1564	Q1505	S1445	K1386
T2050	T2050	S1865	L1926	ILE	ILE	GLY	ILE	S1565	V1506	L1446	Q1387
F2051	F2051	Q1866	P1809	SER	SER	G1691	VAL	R1566	G1507	L1447	L1388
L2118	L2118	E1867	L1810	GLY	GLY	V1692	ASP	C1567	E1508	H1448	E1389
L2119	L2119	Q1868	L1811	SER	SER	C1693	ASP	K1568	G1509	L1449	V1390
M2120	M2120	A1869	A1928	LEU	LEU	V1694	TRP	K1569	V1510	C1450	L1391
L2121	L2121	F1870	L1930	VAL	VAL	C1696	GLU	L1571	C1511	G1451	Q1392
F2123	F2123	E1871	M1814	ARG	ARG	A1697	LEU	S1572	A1512	S1452	L1393
G2124	G2124	L1815	L1815	HIS	HIS	V1695	ALA	Q1573	V1513	L1453	A1394
S2125	S2125	H1872	L1816	ALA	ALA	C1699	VAL	K1574	L1514	A1454	K1395
Y2126	Y2126	R1874	L1816	ALA	ALA	C1700	GLU	L1575	GLU	Q1455	A1396
C2127	C2127	F1877	F1817	THR	THR	H1701	GLU	V1576	G1516	L1456	M1397
Q2128	Q2128	L1875	L1818	SER	SER	K1702	ASP	V1577	T1517	A1457	E1397
T2062	T2062	L1876	M1819	SER	SER	D1703	SER	E1578	L1518	C1458	E1398
M2064	M2064	Y1877	M1876	THR	THR	H1704	GLN	K1579	T1519	V1459	E1399
S2065	S2065	Q1823	L1820	ALA	ALA	E1705	ALA	L1580	P1520	E1460	F1400
C2066	C2066	L1822	A1821	PRO	PRO	E1706	ASP	M1581	M1521	P1461	F1401
A2067	A2067	Q1824	N1825	VAL	VAL	S1707	SER	A1582	A1522	S1402	S1402
Q2068	Q2068	L1824	N1825	THR	THR	Y1708	ASP	ASN	T1523	V1462	D1403
Y2069	Y2069	Q1881	L1945	ILE	ILE	ALA	GLU	VAL	T1524	R1463	R1463
L2070	L2070	Q1882	A1946	SER	SER	LYS	ASP	MET	E1524	L1464	S1404
Y2071	Y2071	T1885	L1886	VAL	VAL	TVR	ASP	HIS	G1405	Q1465	E1406
T2072	T2072	R1886	ALA	ALA	ASP	GLY	LYS	GLY	L1526	A1466	E1406
Q2073	Q2073	Q1887	SER	SER	ASP	GLY	ASN	LYS	A1527	W1467	L1407
L2140	L2140	L1888	VAL	VAL	ASP	S1713	ASN	HIS	N1528	L1468	V1408
M2075	M2075	L1889	GLY	GLY	THR	F1714	V1590	V1590	G1529	L1469	Q1409
E2076	E2076	P1949	SER	SER	SER	F1715	M1591	M1591	D1530	T1470	I1410
Z2077	Z2077	Q1950	S1835	S1835	S1835	C1716	L1592	L1592	G1531	M1471	M1411
A2078	A2078	P1951	A1891	A1891	A1891	D1717	L1593	L1593	T1532	T1472	M1412
S2079	S2079	F1952	H1892	H1892	H1892	C1718	E1594	E1594	G1533	T1473	A1413
S2080	S2080	V1953	R1837	R1837	R1837	G1719	C1595	C1595	F1534	S1474	T1414
A2081	A2081	V1953	A1838	A1838	A1838	A1720	T1596	T1596	P1535	P1475	A1415
Q2082	Q2082	L1894	R1895	R1895	R1895	K1721	C1597	C1597	E1536	P1476	N1416
F2147	F2147	F2022	L1894	L1894	L1894						
P2148	P2148	K2024	R1896	R1896	R1896						
N2150	N2150		L1957	L1957	L1957						
I2151	I2151		T1958	T1958	T1958						
			G1959	G1959	G1959						

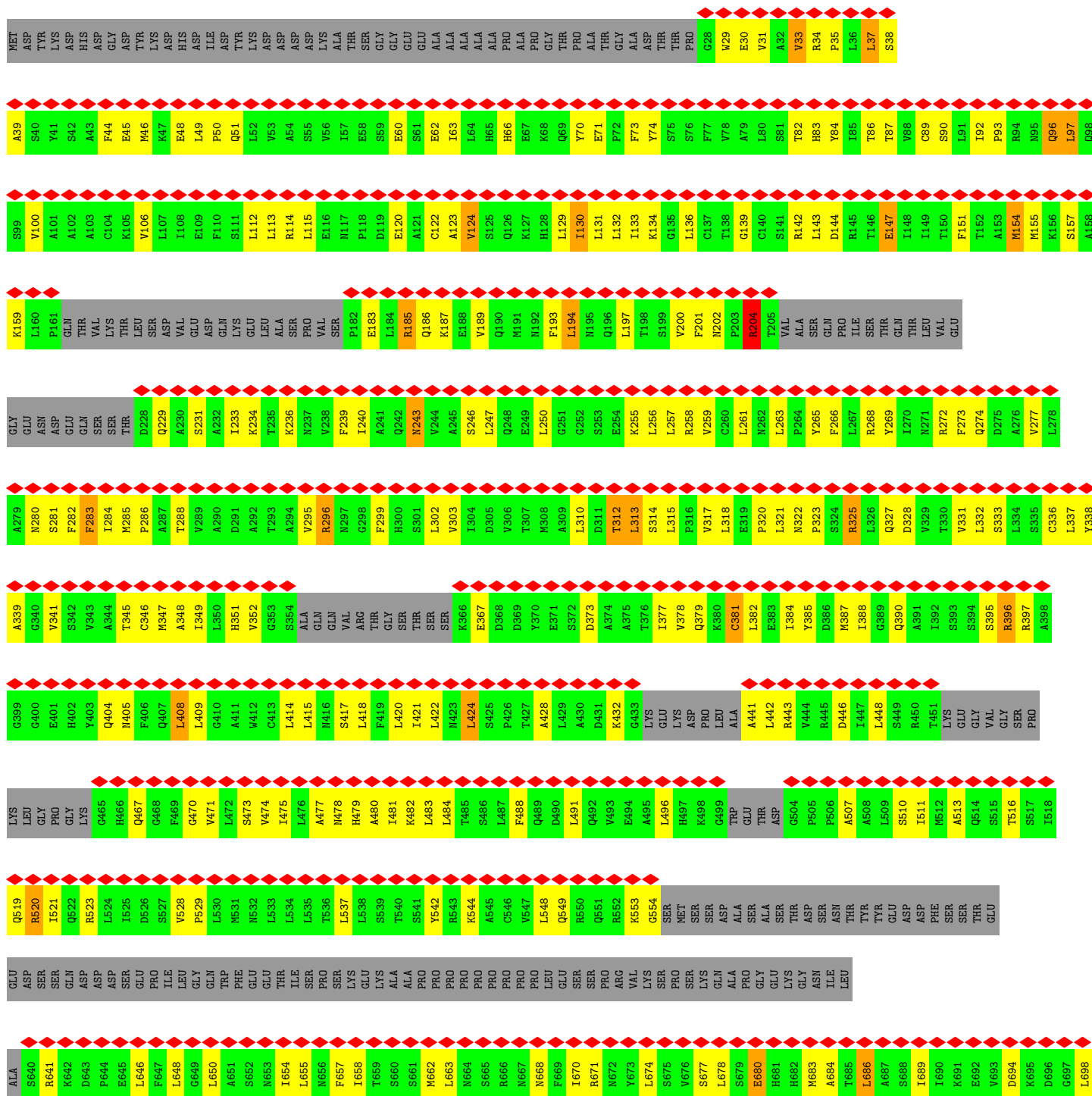






ASP
VAL
ALA
GLY
LEU
LEU
SER
SER
ILE
THR
ASP
PRO
GLU
SER
PHE
LEU
LYS
LYS
LEU
LEU
ASN
SER
VAL
PRO

- Molecule 1: UBR4 (endogenously FLAG-tagged at the N-terminus),E3 ubiquitin-protein ligase UBR4,E3 ubiquitin-protein ligase UBR4,E3 ubiquitin-protein ligase UBR4



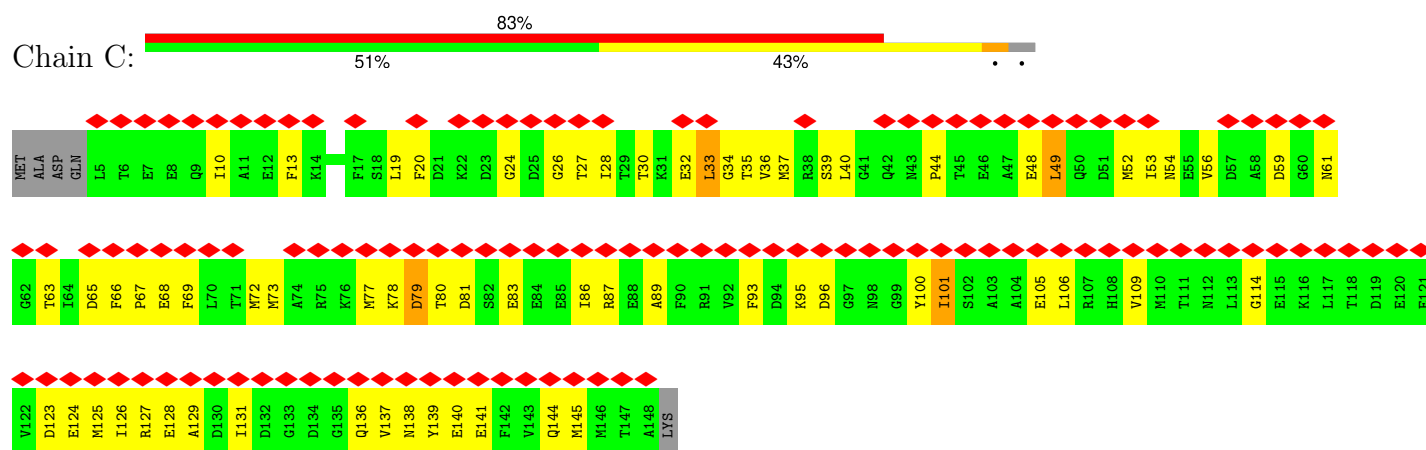
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Y1359	N1360	I1361	L1362	A1363	N1364	H1365	A1366	D1367	P1368	N1369	S1370	G1371	L1372	D1373	E1374	S1375	L1376	L1377	E1378	E1379	C1380	L1381	Q1382	Y1383	L1384	E1385	K1386	Q1387	L1388	E1389	L1390	S1391	L1392	A1393	R1394	K1395	A1396	M1397	E1398	F1399	F1400	F1401	S1402	D1403	S1404	G1405	E1406	L1407	L1408	Q1409	I1410	M1411	M1412	A1413	T1414	A1415	P1416	PRO	LYS	ASP			
I1299	V1300	W1301	S1302	D1303	E1304	M1305	N1306	P1307	P1308	Q1309	V1310	I1311	R1312	T1313	L1314	L1315	P1316	L1317	L1318	L1319	E1320	S1321	S1322	T1323	E1324	S1325	V1326	A1327	E1328	I1329	S1330	M1331	M1332	L1333	L1334	E1335	R1336	I1337	L1338	G1339	P1340	A1341	E1342	S1343	D1344	E1345	F1346	L1347	L1348	R1349	V1350	Y1351	E1352	K1353	L1354	L1355	T1356	G1357	C1358				
M1239	E1240	F1241	P1242	N1243	I1244	G1245	S1246	W1247	R1248	N1249	A1250	F1251	A1252	N1253	D1254	T1255	I1256	P1257	S1258	E1259	S1260	Y1261	I1262	S1263	A1264	V1265	Q1266	A1267	A1268	H1269	L1270	G1271	L1272	L1273	C1274	S1275	Q1276	S1277	L1278	V1279	L1280	A1281	A1282	S1283	L1284	K1285	H1286	T1287	L1288	L1289	S1290	L1291	V1292	R1293	L1294	T1295	G1296	D1297	L1298				
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Q1119	S1120	I1121	Y1122	T1123	L1124	D1125	A1126	A1127	I1128	S1129	K1130	V1131	Q1132	V1133	S1134	L1135	D1136	E1137	H1138	F1139	K1141	M1142	A1143	ALA	GLU	THR	ASP	PRO	HIS	LYS	S1151	S1152	E1153	I1154	T1155	K1156	N1157	L1158	P1159	A1161	T1162	L1163	L1164	L1165	I1166	D1167	T1168	Y1169	A1170	S1171	F1172	T1173	R1174	A1175	Y1176	L1177	L1178						
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L999	Q1000	Y1001	Y1002	F1003	L1004	I1005	L1006	W1007	R1008	I1009	L1010	G1011	I1012	L1013	P1014	P1015	S1016	K1017	T1018	Y1019	I1020	N1021	Q1022	L1023	S1024	M1025	N1026	S1027	P1028	E1029	M1030	S1031	E1032	C1033	D1034	I1035	L1036	H1037	T1038	L1039	R1040	W1041	S1042	S1043	R1044	L1045	R1046	I1047	N1048	S1049	Y1050	V1051	N1052	W1053	I1054	K1055	D1056	H1057	L1058				
E939	A940	S941	E942	D943	D944	L945	N946	R947	L948	D949	S950	Y951	A952	C953	D954	V955	L956	F957	S958	K959	L960	V961	K962	Y963	D964	E965	L966	Y967	A968	A969	L970	T971	A972	L973	L974	A975	A976	G977	S978	Q979	L980	D981	T982	V983	R984	R985	K986	E987	N988	K989	N990	V991	T992	A993	L994	E995	A996	C997	A998				
Q879	V880	Q881	H882	N883	L884	L885	S886	P887	P888	F889	G890	TRP	ALA	GLY	SER	GLN	ASP	SER	ASN	SER	ARG	ARG	A903	T904	T905	P906	L907	Y908	H909	G910	F911	K912	E913	V914	E915	E916	N917	W918	S919	K920	H921	F922	S923	SER	ASP	ALA	VAL	PRO	HIS	P930	R931	F932	Y933	C934	V935	L936	S937	P938					
H819	N820	F821	T822	E823	T824	G825	R826	R827	A828	I829	L830	S831	L832	F833	V834	Q835	I836	I837	Q838	E839	L840	S841	V842	N843	M844	D845	A846	N847	M848	R849	F850	V851	P852	L853	I854	L855	A856	R857	G977	K920	H921	L858	L859	Q922	L860	I861	F862	D863	Y864	L865	L866	H867	Q868	Y869	S870	K871	Q872	M873	L874	L875	L876	F877	E878
R759	L760	L761	L762	I763	W764	Q765	H766	K767	A768	S769	A770	Q771	Q772	D773	P774	D775	P776	P777	E778	C779	L780	K781	V782	W783	D784	R785	F786	L787	S788	T789	M790	K791	Q792	N793	A794	L795	Q796	G797	V798	V799	P800	S801	E802	T803	E804	D805	L806	N807	Y808	E809	H810	L811	Q812	M813	L814	L815	L816	I817	F818				
K699	G700	S701	S702	D703	E704	E705	F706	A707	A708	A709	L710	Y711	H712	F713	N714	H715	S716	L717	V718	T719	S720	D721	L722	Q723	S724	P725	N726	L727	Q728	N729	T730	L731	L732	Q733	Q734	L735	G736	V737	A738	P739	F740	S741	E742	G743	P744	W745	P746	L747	Y748	I749	H750	P751	Q752	S753	L754	S755	V756	L757	S758				

D2213	P2148	Q2082	F2022	G1959	M1899	Q1839	ASP	K1721	ASN	L1599	V1539	SER
M2214	I2149	Q2083	V2023	M1960	C1900	Q1840	GLU	E1722	LYS	M1600	V1540	D1480
V2215	N2150	G2084	F2024	P1961	V1901	A1841	LYS	D1723	L1663	S1601	M1541	Q1481
A2216	I2151	P2085	Y2025	K1963	L1902	L1842	PRO	G1724	C1664	Y1602	A1542	L1482
I2217	K2152	F2086	D2027	S1904	S1903	S1843	LYS	S1725	T1665	L1603	T1543	D1483
R2218	S2153	Y2087	L2028	P1905	P1904	E1844	SER	C1726	F1666	A1604	L1544	V1484
H2219	S2154	V2088	C2029	H1906	S1904	L1845	SER	L1727	T1667	D1605	A1545	I1485
T2220	N2155	T2089	V2030	L1968	H1906	H1846	LEU	A1728	T1668	V1606	S1546	Q1486
A2221	G2157	N2090	D2031	V1969	G1907	T1847	CYS	L1729	T1669	T1607	A1547	E1487
C2222	S2158	L2092	A2032	C1970	R1908	V1848	THR	VAL	Q1670	N1608	G1548	N1488
N2223	K2159	E2093	L2033	G1971	Q1910	K1850	VAL	LYS	K1671	A1609	Q1549	R1489
E2224	T2160	L2094	L2034	L1972	H1911	K1851	GLU	ARG	E1672	Q1550	G1550	Q1490
Q2225	N2095	N2095	P2035	K1973	L1912	A1851	CYS	PRO	F1673	SER	A1551	L1491
Q2226	H2096	C1975	T2036	L1914	A1913	E1853	ARG	GLY	M1674	GLN	G1552	L1492
R2227	E2097	D1976	F2037	S1915	V1914	M1854	GLU	GLY	Q1676	ASN	H1553	Q1493
T2228	D2098	V1977	Y2038	H1916	S1915	T1855	GLY	MET	H1677	GLY	L1554	L1494
N2230	L2099	L1978	L2040	H1917	E1917	Q1857	THR	THR	Y1679	PRO	Q1555	L1495
L2231	K2100	T1979	P2042	K1918	K1919	M1859	SER	GLU	C1681	LYS	H1557	T1497
L2232	S2102	S1981	S2043	S1982	K1920	M1860	SER	ALA	H1680	HIS	A1558	Y1498
C2233	N2103	S1983	K2044	S1983	I1921	P1861	ASP	PHE	T1683	VAL	A1560	V1500
E2235	S2104	G1984	K2045	G1984	T1922	L1863	GLU	GLN	T1684	GLY	V1561	R1501
D2236	Q2105	S1985	T2046	S1985	V1923	Y1866	GLU	SER	M1686	GLU	W1563	N1503
Q2237	V2106	V1986	R2047	L1924	L1924	G1864	A1808	PRO	VAL	ARG	L1564	S1504
S2238	A2107	V1987	D2048	Q1925	Q1925	S1865	P1809	ARG	ASP	ILE	S1565	Q1505
L2239	G2108	D1988	Y2049	L1926	L1926	Q1866	L1810	ILE	GLY	GLU	R1566	V1506
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Q2181	H2117	L1990	L2052	A1928	A1928	G1868	L1812	GLU	G1691	ASP	K1568	E1508
T2183	T2118	P2053	F2053	L1929	L1929	A1869	D1813	SER	V1692	SER	K1569	G1509
T2184	L2119	N2054	M2054	K1930	L1930	F1870	M1814	LEU	C1693	ASP	Y1570	V1510
V2186	Q2120	E2055	E2055	K1931	K1931	E1871	L1815	ARG	T1694	VAL	L1571	G1511
L2188	M2121	E2056	E2056	Q1932	Q1932	N1872	N1816	HIS	V1695	GLU	S1572	A1512
V2189	L2122	G2057	G2057	A1933	A1933	V1873	F1817	SER	G1696	LEU	Q1573	V1513
V2190	F2123	K2058	K2058	D1934	D1934	R1874	M1818	THR	A1697	ALA	K1574	L1514
M2191	F2124	M2059	M2059	S1935	S1935	M1875	M1819	SER	V1699	VAL	N1575	L1515
V2192	S2125	I2060	I2060	S1936	S1936	N1876	D1820	PRO	G1700	GLU	V1576	G1516
L2193	Y2126	I2061	I2061	T1998	T1998	Y1877	A1821	ALA	H1701	GLU	V1577	T1517
P2194	C2127	G2063	G2063	G1999	G1999	S1878	Q1823	ASP	K1702	ASP	E1578	L1518
D2195	Q2128	M2064	M2064	N2000	N2000	G1879	T1822	LYS	D1703	GLN	K1579	P1520
T2196	G2129	S2065	S2065	F2001	F2001	D1880	T1824	LYS	D1703	ALA	L1580	M1521
F2197	K2130	S2066	S2066	I2002	I2002	Q1881	N1825	VAL	H1704	GLU	N1581	H1521
L2198	S2131	Z2067	Z2067	T2003	T2003	Q1882	Q1827	THR	E1705	ASP	ALA	ASN
I2198	F2132	A2067	A2067	K2004	K2004	L1888	F1826	ILE	S1707	SER	VAL	T1523
Q2200	A2133	G2068	G2068	A2005	A2005	I1885	Q1828	GLY	Y1708	ASP	GLU	E1524
E2201	A2134	Y2069	Y2069	V2006	V2006	Q1883	Q1828	ASP	S1707	ASP	GLU	M1525
I2202	T2135	T2071	T2071	L2007	L2007	I1886	S1830	LYS	Y1708	ASP	GLY	L1526
K2203	T2136	T2072	T2072	A1946	A1946	R1886	A1831	VAL	ALA	LEU	LYS	A1527
T2204	S2137	Q2073	Q2073	S1947	S1947	Q1887	V1832	LYS	LYS	CYS	HIS	N1528
L2205	R2138	L2074	L2074	A1948	A1948	L1888	G1833	THR	GLY	GLY	GLY	G1529
P2206	T2139	M2075	M2075	P1949	P1949	I1889	S1834	SER	F1714	M1590	M1591	D1530
A2207	T2140	E2076	E2076	V1950	V1950	A1891	S1835	THR	F1715	L1592	L1592	G1531
K2208	L2141	E2077	E2077	P1951	P1951	H1892	S1836	ALA	C1716	L1593	L1593	T1532
A2209	E2142	A2078	A2078	F1952	F1952	H1892	R1837	VAL	D1717	E1594	E1594	G1533
K2210	V2143	S2079	S2079	V1954	V1954	L1894	R1837	VAL	G1718	C1595	C1595	F1534
I2211	L2144	S2080	S2080	L1955	L1955	R1895	A1838	ALA	A1720	T1596	T1596	F1535
Q2212	Q2145	A2081	A2081	S1956	S1956	V1897	A1898	ALA		C1597	C1597	E1536
	L2146			L1957	L1957	V1897	A1898			Y1598	Y1598	L1537
	F2147			T1958	T1958	A1898						M1538

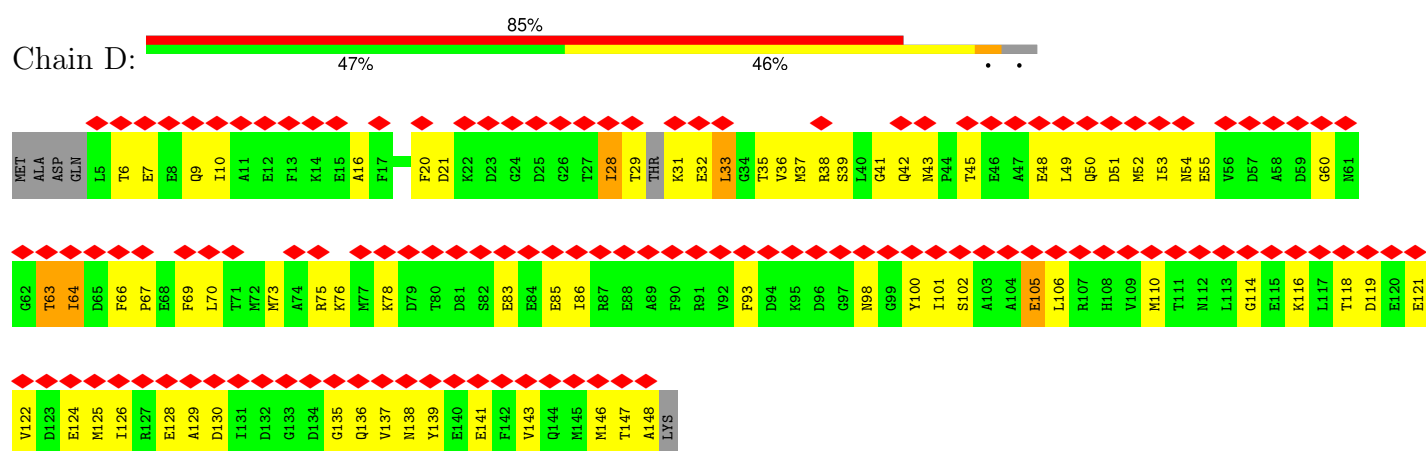




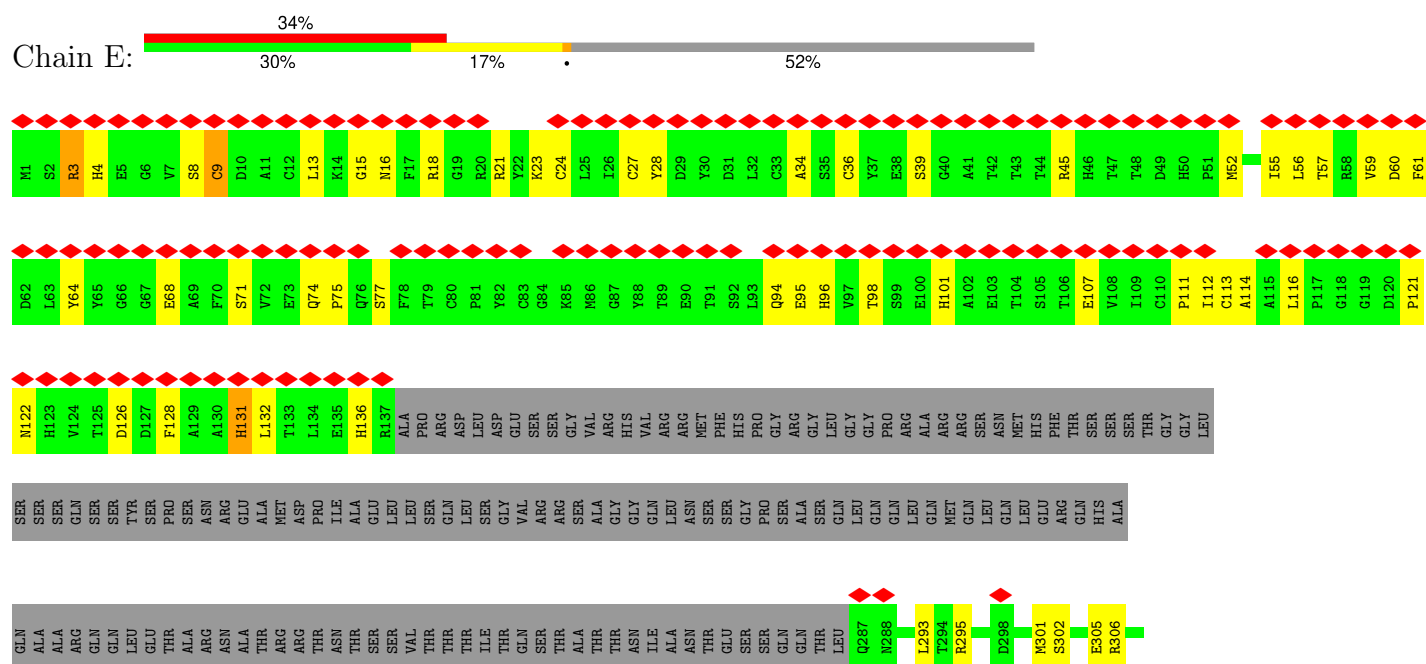
- Molecule 2: Calmodulin-1



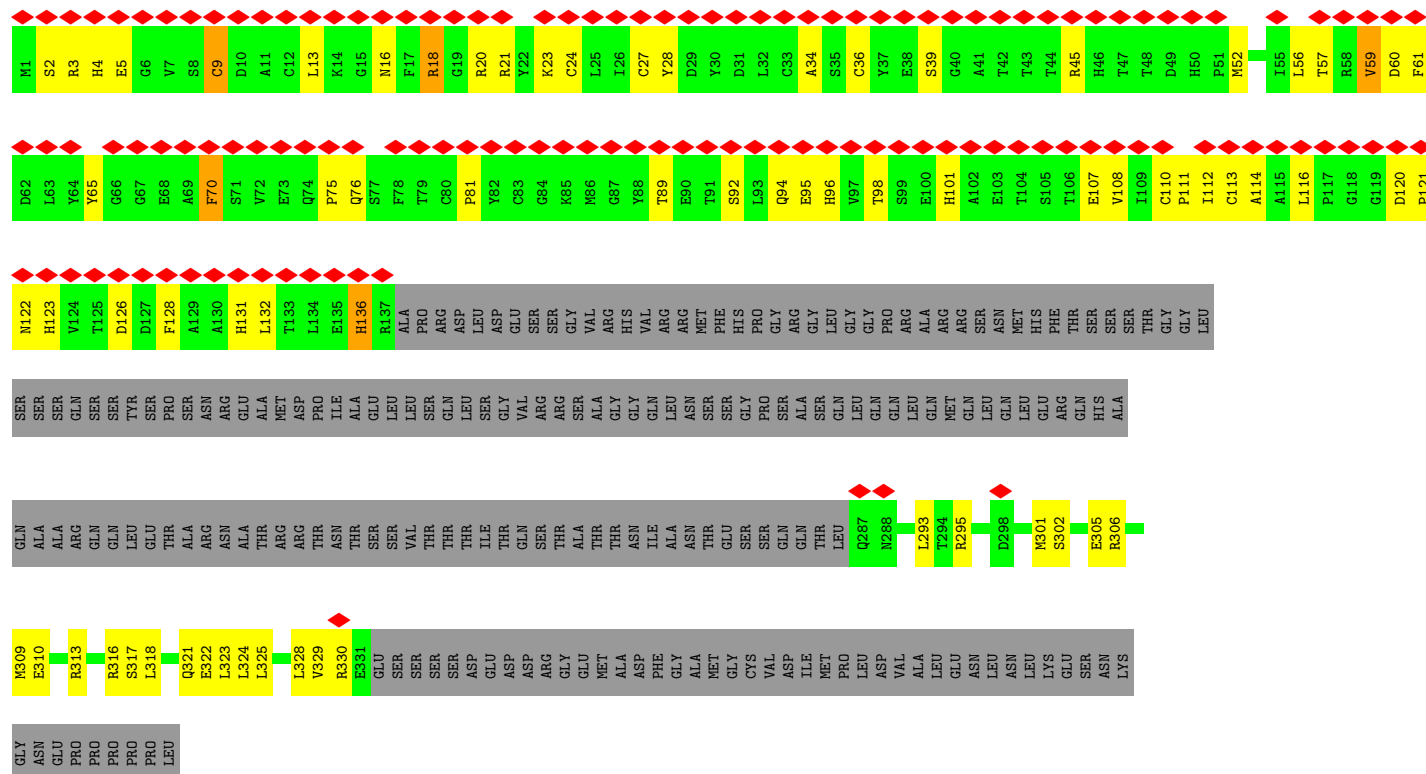
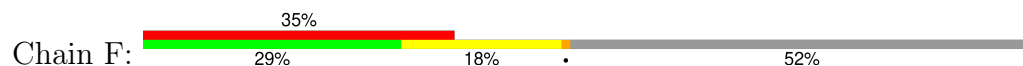
• Molecule 2: Calmodulin-1



• Molecule 3: E3 ubiquitin-protein ligase KCMF1



- Molecule 3: E3 ubiquitin-protein ligase KCMF1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	126380	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.255	Depositor
Minimum map value	-0.578	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.13	Depositor
Map size (\AA)	440.16, 440.16, 440.16	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.048, 1.048, 1.048	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.88	39/31195 (0.1%)	1.04	1/42247 (0.0%)
1	B	0.91	36/31477 (0.1%)	1.10	2/42619 (0.0%)
2	C	0.97	0/1146	1.24	0/1539
2	D	0.98	0/1138	1.25	0/1526
3	E	1.01	12/1463 (0.8%)	0.99	0/1978
3	F	1.00	13/1463 (0.9%)	1.01	0/1978
All	All	0.91	100/67882 (0.1%)	1.08	3/91887 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	19
1	B	0	25
2	D	0	1
3	E	0	1
3	F	0	2
All	All	0	48

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1682	HIS	C-N	-10.20	1.20	1.33
1	B	1993	HIS	C-N	8.77	1.43	1.34
1	A	2290	ASP	C-N	-8.62	1.22	1.33
1	B	1865	SER	C-N	8.21	1.44	1.33
1	A	1894	LEU	C-N	-8.11	1.21	1.33
1	A	1717	ASP	C-N	-8.11	1.23	1.33
1	A	1865	SER	C-N	8.01	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1681	CYS	C-N	-7.75	1.22	1.33
1	B	2318	LYS	C-N	-7.68	1.24	1.33
1	B	2327	TYR	C-N	-7.66	1.22	1.33
1	A	2038	TYR	C-N	7.62	1.44	1.33
1	A	2318	LYS	C-N	-7.62	1.24	1.33
1	A	1860	VAL	C-N	7.60	1.42	1.33
1	B	1860	VAL	C-N	7.54	1.42	1.33
1	B	2038	TYR	C-N	7.51	1.44	1.33
1	B	2076	GLU	C-N	-7.50	1.24	1.33
1	A	2146	LEU	C-N	7.43	1.42	1.33
3	F	9	CYS	C-N	-7.42	1.22	1.33
1	A	2076	GLU	C-N	-7.38	1.24	1.33
3	E	101	HIS	C-N	-7.38	1.24	1.34
1	B	2535	SER	C-N	-7.36	1.24	1.33
1	B	2146	LEU	C-N	7.36	1.42	1.33
3	E	9	CYS	C-N	-7.32	1.22	1.33
3	F	39	SER	C-N	-7.29	1.25	1.33
3	E	59	VAL	C-N	-7.18	1.24	1.34
3	E	39	SER	C-N	-7.18	1.25	1.33
3	F	101	HIS	C-N	-7.12	1.24	1.34
3	E	61	PHE	C-N	-7.06	1.24	1.34
3	F	59	VAL	C-N	-7.05	1.24	1.34
3	F	34	ALA	C-N	-7.03	1.24	1.33
3	F	61	PHE	C-N	-6.96	1.24	1.34
3	E	34	ALA	C-N	-6.84	1.24	1.33
1	A	2251	TYR	C-N	6.75	1.43	1.33
1	A	2294	HIS	C-N	-6.70	1.24	1.33
3	E	98	THR	C-N	-6.70	1.24	1.33
1	B	2026	TYR	C-N	-6.66	1.24	1.33
1	A	2658	ASN	C-N	-6.63	1.25	1.33
3	F	98	THR	C-N	-6.59	1.24	1.33
1	A	1973	LYS	C-N	6.58	1.43	1.33
1	B	1973	LYS	C-N	6.54	1.42	1.33
1	A	2026	TYR	C-N	-6.54	1.24	1.33
1	B	1925	GLN	C-N	6.44	1.43	1.33
1	A	1870	PHE	C-N	-6.26	1.24	1.33
1	B	2392	GLU	C-N	-6.21	1.25	1.33
1	A	2067	ALA	C-N	6.11	1.42	1.33
1	B	1870	PHE	C-N	-6.08	1.25	1.33
1	A	2374	THR	C-N	-6.03	1.25	1.33
1	A	1925	GLN	C-N	6.02	1.43	1.33
1	B	2374	THR	C-N	-5.96	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2242	TYR	C-N	-5.91	1.25	1.33
1	B	2315	GLN	C-N	-5.89	1.26	1.33
1	B	2067	ALA	C-N	5.88	1.42	1.33
1	A	2315	GLN	C-N	-5.87	1.26	1.33
1	A	2366	SER	C-N	-5.87	1.26	1.33
1	B	2366	SER	C-N	-5.86	1.26	1.33
1	B	2177	VAL	C-N	5.78	1.41	1.33
1	B	2313	ASN	C-N	-5.64	1.26	1.33
1	A	1965	ASP	C-N	-5.61	1.25	1.33
1	B	2510	THR	C-N	-5.58	1.26	1.33
3	F	57	THR	C-N	-5.57	1.26	1.33
3	E	57	THR	C-N	-5.55	1.26	1.33
1	A	2177	VAL	C-N	5.49	1.41	1.33
1	B	2699	GLN	C-N	-5.49	1.26	1.33
3	F	36	CYS	C-N	-5.49	1.26	1.33
1	B	1965	ASP	C-N	-5.48	1.25	1.33
1	B	2350	THR	C-N	-5.42	1.26	1.33
1	B	2084	GLY	C-N	5.39	1.40	1.33
1	B	1825	ASN	C-N	5.38	1.41	1.33
1	A	1895	ARG	C-N	-5.38	1.25	1.33
1	A	2350	THR	C-N	-5.38	1.26	1.33
1	A	2577	ALA	C-N	-5.35	1.27	1.33
3	E	36	CYS	C-N	-5.34	1.27	1.33
1	A	2084	GLY	C-N	5.33	1.40	1.33
1	B	1831	ALA	C-N	5.32	1.39	1.33
3	E	95	GLU	C-N	-5.32	1.27	1.33
3	F	96	HIS	C-N	-5.29	1.27	1.33
1	A	1955	LEU	C-N	5.29	1.40	1.33
1	B	2703	ARG	C-N	-5.27	1.27	1.33
1	A	1867	GLU	C-N	5.24	1.40	1.33
3	E	60	ASP	C-N	-5.23	1.27	1.33
1	B	2234	CYS	C-N	-5.21	1.26	1.34
1	B	2091	VAL	C-N	-5.21	1.26	1.33
3	F	60	ASP	C-N	-5.20	1.27	1.33
3	F	95	GLU	C-N	-5.20	1.27	1.33
3	E	96	HIS	C-N	-5.19	1.27	1.33
1	B	2622	ILE	C-N	-5.17	1.27	1.33
1	A	2234	CYS	C-N	-5.16	1.27	1.34
1	A	1864	GLY	C-N	-5.13	1.25	1.33
3	F	110	CYS	C-N	-5.13	1.27	1.34
1	B	2216	ALA	C-N	5.12	1.40	1.33
1	A	2579	SER	C-N	-5.11	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1867	GLU	C-N	5.09	1.40	1.33
1	A	2061	ILE	C-N	-5.09	1.27	1.33
1	B	2343	ASN	C-N	-5.09	1.25	1.33
1	B	2035	PRO	C-N	-5.07	1.27	1.33
1	A	2035	PRO	C-N	-5.05	1.27	1.33
1	A	2359	GLN	C-N	-5.03	1.27	1.33
1	A	2558	SER	C-N	-5.02	1.27	1.33
1	A	2622	ILE	C-N	-5.00	1.27	1.33
1	B	2314	ALA	C-N	-5.00	1.27	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1282	ALA	N-CA-C	-6.39	104.32	111.28
1	B	1131	VAL	N-CA-CB	5.70	117.22	110.55
1	B	529	PRO	N-CA-C	-5.06	102.05	112.47

There are no chirality outliers.

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1008	ARG	Sidechain
1	A	1174	ARG	Sidechain
1	A	1293	ARG	Sidechain
1	A	1394	ARG	Sidechain
1	A	2320	ARG	Sidechain
1	A	2703	ARG	Sidechain
1	A	3045	ARG	Sidechain
1	A	3142	ARG	Sidechain
1	A	3166	ARG	Sidechain
1	A	325	ARG	Sidechain
1	A	3286	ARG	Sidechain
1	A	3732	ARG	Sidechain
1	A	3825	ARG	Sidechain
1	A	3857	ARG	Sidechain
1	A	4319	ARG	Sidechain
1	A	4491	ARG	Sidechain
1	A	849	ARG	Sidechain
1	A	94	ARG	Sidechain
1	A	985	ARG	Sidechain
1	B	1008	ARG	Sidechain
1	B	1312	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	1336	ARG	Sidechain
1	B	1470	ARG	Sidechain
1	B	185	ARG	Sidechain
1	B	1896	ARG	Sidechain
1	B	204	ARG	Sidechain
1	B	2381	ARG	Sidechain
1	B	296	ARG	Sidechain
1	B	2974	ARG	Sidechain
1	B	2989	ARG	Sidechain
1	B	3286	ARG	Sidechain
1	B	3732	ARG	Sidechain
1	B	3836	ARG	Sidechain
1	B	396	ARG	Sidechain
1	B	397	ARG	Sidechain
1	B	4115	ARG	Sidechain
1	B	4256	ARG	Sidechain
1	B	4280	ARG	Sidechain
1	B	4319	ARG	Sidechain
1	B	4607	ARG	Sidechain
1	B	520	ARG	Sidechain
1	B	759	ARG	Sidechain
1	B	849	ARG	Sidechain
1	B	985	ARG	Sidechain
2	D	75	ARG	Sidechain
3	E	3	ARG	Sidechain
3	F	18	ARG	Sidechain
3	F	330	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	30658	0	31020	1288	0
1	B	30933	0	31316	1262	0
2	C	1134	0	1063	68	0
2	D	1127	0	1055	61	0
3	E	1435	0	1344	44	0
3	F	1435	0	1344	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	6	0	0	2	0
4	B	6	0	0	3	0
4	E	4	0	0	0	0
4	F	4	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	2	0
All	All	66746	0	67142	2687	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 20.

All (2687) 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:3270:ILE:CD1	1:B:3632:PRO:HG2	1.66	1.25
1:A:3270:ILE:CD1	1:A:3632:PRO:HG2	1.66	1.23
1:B:3087:ALA:CB	1:B:3181:ILE:HG21	1.73	1.19
1:A:73:PHE:CD1	1:A:159:LYS:HA	1.80	1.15
2:D:98:ASN:HB2	5:D:202:CA:CA	1.06	1.15
1:B:3087:ALA:HB2	1:B:3181:ILE:HG21	1.31	1.11
1:A:3270:ILE:HD13	1:A:3632:PRO:HG2	1.25	1.10
1:A:1450:CYS:HB2	1:A:1505:GLN:HB2	1.33	1.09
1:A:1700:CYS:SG	1:A:1726:CYS:HA	1.92	1.09
1:A:2212:GLN:NE2	1:A:2235:GLU:HA	1.65	1.09
1:B:3087:ALA:HB2	1:B:3181:ILE:HD13	1.36	1.08
1:B:910:GLY:HA2	1:B:933:TYR:HA	1.19	1.08
1:B:1205:GLY:HA3	1:B:1215:GLY:CA	1.83	1.08
1:B:3270:ILE:HD13	1:B:3632:PRO:HG2	1.25	1.07
1:A:1500:VAL:HG22	1:A:1547:ALA:HB2	1.33	1.07
1:B:2564:ASP:OD1	1:B:2631:LYS:HB3	1.55	1.06
1:A:1700:CYS:SG	1:A:1727:LEU:N	2.29	1.04
2:C:106:LEU:HD22	2:C:126:ILE:HD11	1.38	1.04
1:A:3269:LEU:HB3	1:A:3633:LEU:CD1	1.89	1.03
1:B:3269:LEU:HB3	1:B:3633:LEU:CD1	1.89	1.02
1:A:2342:ASN:HB3	1:A:2399:LYS:HA	1.40	1.01
1:A:1870:PHE:CZ	1:A:1924:LEU:HD11	1.97	0.99
1:B:1870:PHE:CZ	1:B:1924:LEU:HD11	1.97	0.99
1:B:1205:GLY:HA3	1:B:1215:GLY:HA2	1.43	0.99
1:A:1873:VAL:HG11	1:A:2233:LEU:HD21	1.45	0.99
1:A:3793:ASN:HA	1:B:3521:GLU:HG3	1.43	0.99
1:B:2698:LYS:HD2	1:B:2998:PRO:HA	1.46	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2173:HIS:CD2	1:A:2253:LEU:HD11	1.99	0.98
1:B:1205:GLY:CA	1:B:1215:GLY:HA3	1.94	0.97
1:B:1901:VAL:HG11	1:B:2217:ILE:HD12	1.45	0.96
1:B:3410:GLN:HG3	1:B:3850:THR:HB	1.47	0.96
1:A:53:VAL:HG11	1:A:99:SER:HB3	1.47	0.96
2:D:50:GLN:O	2:D:53:ILE:HG22	1.65	0.96
1:A:1901:VAL:HG11	1:A:2217:ILE:HD12	1.45	0.95
1:A:2294:HIS:O	1:A:2425:LYS:HE2	1.68	0.94
2:D:101:ILE:HB	2:D:137:VAL:HB	1.48	0.93
1:B:1870:PHE:HZ	1:B:1924:LEU:CD1	1.82	0.93
1:A:1438:THR:HA	1:A:1446:LEU:HD13	1.47	0.93
1:A:1870:PHE:HZ	1:A:1924:LEU:CD1	1.82	0.92
1:B:3087:ALA:HB1	1:B:3181:ILE:HG21	1.53	0.91
1:A:690:ILE:HA	1:A:710:LEU:HD21	1.51	0.91
1:B:1438:THR:HA	1:B:1446:LEU:HD13	1.51	0.91
1:B:1394:ARG:HA	1:B:1397:MET:HE2	1.53	0.91
1:B:2564:ASP:CG	1:B:2631:LYS:HB3	1.96	0.90
1:A:1398:GLU:HA	1:A:1449:LEU:HD21	1.50	0.90
1:B:1486:GLN:HA	1:B:1489:ARG:HD2	1.52	0.90
3:F:94:GLN:HA	3:F:132:LEU:HD13	1.53	0.90
1:A:1870:PHE:HE2	1:A:2239:LEU:HD11	1.37	0.90
3:E:94:GLN:HA	3:E:132:LEU:HD13	1.54	0.90
1:B:3003:ILE:HA	1:B:3006:LEU:HD12	1.54	0.89
2:D:98:ASN:CB	5:D:202:CA:CA	1.79	0.89
1:A:1105:ASP:H	1:A:1110:LEU:HD21	1.37	0.89
1:B:3270:ILE:CD1	1:B:3632:PRO:CG	2.51	0.89
1:A:3521:GLU:HG3	1:B:3793:ASN:HA	1.53	0.89
1:B:281:SER:HB2	1:B:443:ARG:HD2	1.56	0.88
1:B:1166:ILE:HG12	1:B:1291:LEU:HB3	1.56	0.88
1:A:3270:ILE:CD1	1:A:3632:PRO:CG	2.51	0.88
1:B:1159:LEU:HA	1:B:1298:LEU:HD13	1.55	0.88
1:B:134:LYS:HA	1:B:315:LEU:HD21	1.54	0.87
1:A:4231:ASP:HB3	1:A:4234:GLN:HB2	1.56	0.87
1:B:1600:MET:HA	1:B:1603:LEU:HD12	1.55	0.87
1:B:2687:LEU:HD22	1:B:2991:VAL:HG21	1.56	0.87
1:A:2027:ASP:OD1	1:A:2029:CYS:SG	2.33	0.87
3:E:114:ALA:HA	3:E:121:PRO:HA	1.56	0.87
1:A:2040:LEU:HD13	1:A:2085:PRO:HB2	1.57	0.87
1:A:3066:THR:HG21	1:A:3082:SER:HB3	1.57	0.86
1:B:1493:GLN:HG2	1:B:1540:VAL:HG22	1.54	0.86
1:A:1401:PHE:HA	1:A:1406:GLU:HG3	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4306:THR:HG21	1:A:4338:ILE:HG12	1.57	0.86
1:A:3172:LYS:HE3	1:A:3217:ILE:HA	1.57	0.86
1:A:4232:LEU:HD13	1:B:3750:TYR:HB2	1.57	0.86
1:A:1921:ILE:HB	1:A:1948:ALA:HB3	1.57	0.86
2:C:69:PHE:CZ	2:C:73:MET:SD	2.67	0.86
1:A:2040:LEU:CD1	1:A:2085:PRO:HB2	2.06	0.86
1:A:2173:HIS:HD2	1:A:2253:LEU:HD11	1.35	0.86
1:B:2027:ASP:OD1	1:B:2029:CYS:SG	2.33	0.86
2:C:106:LEU:CD2	2:C:126:ILE:HD11	2.05	0.86
1:A:1338:LEU:HD13	1:A:1346:PHE:HA	1.56	0.85
1:A:2375:MET:HG2	1:A:2387:PHE:HE1	1.40	0.85
1:B:2040:LEU:CD1	1:B:2085:PRO:HB2	2.05	0.85
1:A:1112:LEU:HD13	1:A:1179:GLN:HB2	1.57	0.85
1:B:2040:LEU:HD13	1:B:2085:PRO:HB2	1.57	0.85
1:B:3419:SER:O	1:B:3420:ASN:CG	2.19	0.85
1:A:1453:LEU:HB3	1:A:1506:VAL:HG13	1.58	0.85
1:A:687:ALA:HB2	1:A:731:LEU:HD12	1.58	0.85
1:B:1278:LEU:HB3	1:B:1281:ALA:HB2	1.57	0.85
2:C:106:LEU:HD22	2:C:126:ILE:CD1	2.07	0.85
1:A:1960:ASN:HD21	1:A:2012:GLN:HA	1.41	0.85
1:B:4444:MET:HE3	1:B:4447:LEU:HD13	1.58	0.85
1:B:1870:PHE:HZ	1:B:1924:LEU:HD11	1.37	0.84
1:B:910:GLY:CA	1:B:933:TYR:HA	2.04	0.84
1:B:2695:PHE:CE1	1:B:2699:GLN:NE2	2.45	0.84
1:A:1205:GLY:HA2	1:A:1215:GLY:CA	2.07	0.84
1:A:3419:SER:O	1:A:3420:ASN:CG	2.19	0.84
1:B:3419:SER:O	1:B:3420:ASN:OD1	1.96	0.84
3:F:114:ALA:HA	3:F:121:PRO:HA	1.57	0.83
1:A:420:LEU:HD22	1:A:442:LEU:HG	1.61	0.83
1:B:2189:VAL:HG22	1:B:2230:MET:HE1	1.60	0.83
1:B:4705:LEU:HB3	1:B:4754:VAL:HG22	1.60	0.83
1:A:2189:VAL:CG2	1:A:2230:MET:HE1	2.08	0.83
2:C:80:THR:O	2:C:81:ASP:OD1	1.95	0.83
1:B:2189:VAL:CG2	1:B:2230:MET:HE1	2.09	0.83
1:A:73:PHE:HD1	1:A:159:LYS:HA	1.37	0.83
1:A:4444:MET:HE3	1:A:4447:LEU:HD13	1.59	0.83
1:A:3269:LEU:HB3	1:A:3633:LEU:HD11	1.61	0.82
1:A:2189:VAL:HG22	1:A:2230:MET:HE1	1.60	0.82
1:B:1407:LEU:HB3	1:B:1431:PHE:CE1	2.15	0.82
1:B:1407:LEU:HB3	1:B:1431:PHE:HE1	1.45	0.82
1:B:1414:THR:HG23	1:B:1423:PHE:HD2	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3419:SER:O	1:A:3420:ASN:OD1	1.96	0.82
1:A:4328:PRO:HA	1:A:4331:ILE:HD12	1.61	0.82
1:A:3940:THR:HG21	1:A:3985:CYS:HB3	1.60	0.82
1:B:1475:PRO:HD3	1:B:1485:ILE:HD12	1.61	0.81
1:A:349:ILE:HD12	1:A:429:LEU:HD11	1.62	0.81
1:B:1499:ILE:HG23	1:B:1506:VAL:HB	1.61	0.81
3:E:8:SER:HA	3:E:15:GLY:HA2	1.62	0.81
1:A:1417:GLU:HA	1:A:1470:ARG:HD2	1.62	0.81
1:B:2122:LEU:HD22	1:B:2136:ILE:HD11	1.63	0.81
2:C:49:LEU:C	2:C:49:LEU:HD13	2.06	0.81
1:B:1208:ARG:HD2	1:B:1327:ALA:HB3	1.63	0.81
1:B:3270:ILE:HD13	1:B:3632:PRO:CG	2.11	0.81
1:A:3164:VAL:O	1:A:3168:PRO:HD2	1.81	0.81
1:B:2698:LYS:HE3	1:B:3001:GLN:HB3	1.63	0.81
1:B:3516:LEU:HD22	1:B:3799:LEU:HD21	1.63	0.81
1:A:1700:CYS:SG	1:A:1726:CYS:CA	2.69	0.80
1:B:3269:LEU:HB3	1:B:3633:LEU:HD11	1.61	0.80
1:A:1904:SER:H	1:A:1964:GLU:HB3	1.45	0.80
1:A:2368:ILE:HG23	1:A:2377:LEU:HD11	1.62	0.80
1:A:3997:PHE:HB2	1:A:4016:CYS:HB3	1.63	0.80
1:A:124:VAL:HG12	1:A:129:LEU:HG	1.63	0.80
1:A:352:VAL:HB	1:A:426:PRO:HG3	1.64	0.80
1:B:4713:PHE:HE1	1:B:4751:LEU:HD21	1.46	0.80
1:B:2368:ILE:HD11	1:B:2387:PHE:CZ	2.16	0.80
1:A:659:THR:HA	1:A:663:LEU:HD12	1.63	0.80
1:A:712:HIS:HA	1:A:715:HIS:CD2	2.15	0.79
1:A:3760:LEU:HD11	1:A:3803:TYR:HB2	1.63	0.79
1:B:2122:LEU:CD2	1:B:2136:ILE:HD11	2.13	0.79
1:B:1554:LEU:HG	1:B:1804:ASN:OD1	1.82	0.79
1:B:2375:MET:HG2	1:B:2387:PHE:HE1	1.44	0.79
1:A:1030:MET:HB3	1:A:1034:ASP:HB3	1.62	0.79
1:B:263:LEU:HB2	1:B:266:PHE:HB2	1.65	0.79
1:A:131:LEU:HD11	1:A:142:ARG:HD2	1.64	0.79
1:A:4234:GLN:HE22	1:A:4279:GLN:HB3	1.48	0.79
1:A:4335:LEU:HD22	1:A:4511:LEU:HD11	1.63	0.79
1:B:3588:ARG:HD2	1:B:3646:ASP:OD2	1.83	0.79
1:A:1554:LEU:HG	1:A:1802:GLN:HE22	1.48	0.79
1:A:2122:LEU:HD22	1:A:2136:ILE:HD11	1.63	0.79
1:B:2122:LEU:HD22	1:B:2136:ILE:CD1	2.13	0.79
1:A:3872:CYS:SG	1:A:3875:CYS:HB2	2.23	0.78
1:A:1450:CYS:CB	1:A:1505:GLN:HB2	2.11	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3066:THR:HG21	1:B:3082:SER:HB2	1.65	0.78
1:A:313:LEU:HD13	1:A:388:ILE:HD11	1.65	0.78
1:A:2122:LEU:CD2	1:A:2136:ILE:HD11	2.13	0.78
1:A:3588:ARG:HD2	1:A:3646:ASP:OD2	1.82	0.77
1:B:1408:VAL:HA	1:B:1411:MET:HE2	1.66	0.77
1:A:910:GLY:HA2	1:A:933:TYR:HA	1.66	0.77
1:B:3315:VAL:HG22	1:B:3633:LEU:HD21	1.66	0.77
1:B:1412:MET:HB3	1:B:1463:ARG:NE	1.99	0.77
1:B:3004:LEU:HB2	1:B:3058:LEU:HD11	1.64	0.77
1:A:415:LEU:HD11	1:A:484:LEU:HD21	1.67	0.77
1:A:2122:LEU:HD22	1:A:2136:ILE:CD1	2.13	0.77
1:B:4591:LYS:HB2	1:B:4630:LYS:HE3	1.65	0.77
1:A:4635:VAL:HG11	1:A:4685:LYS:HG3	1.67	0.76
2:D:50:GLN:O	2:D:53:ILE:CG2	2.32	0.76
1:A:3270:ILE:HD13	1:A:3632:PRO:CG	2.11	0.76
1:A:793:ASN:HB2	1:A:854:ILE:HG21	1.66	0.76
1:A:984:ARG:HH11	1:A:984:ARG:HB2	1.51	0.76
1:B:1407:LEU:H	1:B:1407:LEU:HD12	1.50	0.76
1:B:352:VAL:HG22	1:B:467:GLN:HG2	1.67	0.76
1:B:2070:ILE:HD12	1:B:2094:ILE:HD11	1.67	0.76
1:A:656:ASN:HB3	1:B:204:ARG:HD3	1.67	0.76
1:B:1218:LEU:HD22	1:B:1376:ILE:HG23	1.68	0.75
1:B:2637:PRO:HD3	1:B:2648:PRO:HG2	1.67	0.75
1:B:4339:ILE:HG21	1:B:4514:TYR:HB3	1.67	0.75
1:A:3167:LEU:HB3	1:A:3168:PRO:HD3	1.66	0.75
1:B:1545:ALA:HB1	1:B:1553:HIS:HB2	1.68	0.75
1:B:2683:MET:HG3	1:B:2999:TYR:HE2	1.51	0.75
1:A:1870:PHE:HZ	1:A:1924:LEU:HD11	1.37	0.75
1:A:1814:MET:HA	1:A:1817:PHE:CE1	2.21	0.75
1:A:3965:ALA:HA	1:A:4011:ASN:HD21	1.52	0.75
1:B:286:PRO:HB3	1:B:295:VAL:HG21	1.68	0.75
1:B:1201:VAL:HG13	1:B:1218:LEU:HB3	1.67	0.75
1:B:1664:CYS:HB2	1:B:1729:LEU:HA	1.66	0.75
1:B:1489:ARG:NH2	1:B:1533:GLY:HA2	2.01	0.75
1:B:910:GLY:HA2	1:B:933:TYR:CA	2.09	0.74
1:B:1904:SER:H	1:B:1964:GLU:HB3	1.52	0.74
1:A:193:PHE:HB2	1:B:881:GLN:HE21	1.50	0.74
1:B:860:LEU:HB2	1:B:1005:ILE:HD13	1.69	0.74
1:A:1994:PRO:HG3	1:A:2002:ILE:HD11	1.68	0.74
1:A:2192:VAL:HG13	1:A:2197:PHE:HE1	1.52	0.74
1:A:3459:PRO:HA	1:A:3879:VAL:HG21	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4238:LEU:HG	1:B:4287:THR:HG21	1.68	0.74
1:B:112:LEU:HD12	1:B:250:LEU:HD12	1.68	0.74
1:B:2682:TYR:HD2	1:B:2977:LEU:HD11	1.53	0.73
1:A:1314:LEU:HD13	1:A:1317:LEU:HD12	1.69	0.73
1:B:3290:TRP:NE1	1:B:3326:ALA:HB2	2.03	0.73
1:A:1518:LEU:HD22	1:A:1537:LEU:HD11	1.68	0.73
1:B:3203:THR:HB	1:B:3206:VAL:HB	1.69	0.73
1:B:3459:PRO:HA	1:B:3879:VAL:HG21	1.69	0.73
1:B:4621:PRO:HB3	1:B:4668:GLY:HA3	1.69	0.73
1:B:1205:GLY:HA2	1:B:1215:GLY:HA3	1.71	0.73
1:A:4713:PHE:HE1	1:A:4751:LEU:HD21	1.53	0.73
1:B:3749:VAL:HG11	1:B:3813:GLU:HG2	1.70	0.73
1:B:1204:ILE:HG21	1:B:1357:GLY:HA3	1.71	0.73
1:A:200:VAL:HB	1:B:715:HIS:CE1	2.23	0.73
1:A:800:PRO:HD2	1:A:853:LEU:HD23	1.70	0.72
1:A:1205:GLY:HA2	1:A:1215:GLY:HA3	1.70	0.72
1:A:1610:LEU:HD13	1:A:1800:GLN:HA	1.71	0.72
1:A:3240:ILE:HD11	1:A:3275:HIS:HB2	1.70	0.72
1:B:3057:ARG:HB2	1:B:3163:MET:HE1	1.68	0.72
1:B:4105:TRP:HZ2	2:D:129:ALA:HB2	1.55	0.72
1:B:3240:ILE:HD11	1:B:3275:HIS:HB2	1.70	0.72
1:B:3256:VAL:HG23	1:B:3849:PRO:HA	1.71	0.72
1:A:261:LEU:HD21	1:A:332:LEU:HB2	1.72	0.72
1:A:3793:ASN:HA	1:B:3521:GLU:CG	2.20	0.72
1:B:1515:LEU:HD12	1:B:1541:MET:HG3	1.71	0.72
1:B:2305:GLY:HA3	1:B:2308:LEU:HB2	1.71	0.72
1:A:1870:PHE:CE1	1:A:1924:LEU:HD11	2.25	0.72
1:A:2212:GLN:HE21	1:A:2235:GLU:HA	1.54	0.72
1:B:4123:LEU:HD13	1:B:4165:LEU:HD22	1.71	0.72
2:C:69:PHE:CE1	2:C:73:MET:SD	2.82	0.72
3:E:107:GLU:HA	3:E:126:ASP:HA	1.71	0.72
1:A:912:LYS:O	1:A:916:GLU:HG3	1.89	0.72
1:B:1561:VAL:HG22	1:B:1810:LEU:HD22	1.71	0.72
1:B:3090:LEU:HD11	1:B:3184:PRO:HB3	1.72	0.72
1:A:73:PHE:CE1	1:A:159:LYS:HA	2.24	0.72
1:A:97:LEU:HD12	1:A:235:THR:HG23	1.72	0.72
1:A:420:LEU:HD21	1:A:444:VAL:HA	1.71	0.72
1:B:3001:GLN:HB2	1:B:3139:PHE:HE2	1.54	0.72
3:F:107:GLU:HA	3:F:126:ASP:HA	1.71	0.72
1:A:284:ILE:HD12	1:A:442:LEU:HD23	1.70	0.72
1:B:921:HIS:CD2	1:B:993:ALA:HB2	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2622:ILE:HD11	1:A:2667:TYR:CG	2.25	0.71
1:A:1863:LEU:HB3	1:A:1940:LEU:HD21	1.71	0.71
1:A:3813:GLU:O	1:A:3817:ILE:HG13	1.90	0.71
1:A:471:VAL:HG21	1:A:641:ARG:H	1.55	0.71
1:A:1854:MET:HE1	1:A:2151:ILE:HG23	1.71	0.71
1:A:2151:ILE:HD11	1:A:2164:LEU:HD11	1.72	0.71
1:A:2212:GLN:CD	1:A:2235:GLU:HA	2.14	0.71
1:A:3955:LEU:HD21	1:A:4012:ILE:HD12	1.73	0.71
1:A:3979:ILE:HG21	1:A:4019:ILE:HG23	1.72	0.71
1:B:2987:GLN:HA	1:B:2990:ASN:HD22	1.54	0.71
1:A:1554:LEU:HD11	1:A:1798:GLU:HB2	1.73	0.71
1:B:1870:PHE:CE1	1:B:1924:LEU:HD11	2.25	0.71
1:B:3547:LEU:HD13	1:B:3715:LEU:HD11	1.73	0.71
1:A:2565:LEU:HD21	1:A:2573:LEU:HD12	1.72	0.71
1:B:1117:SER:O	1:B:1121:ILE:HG13	1.91	0.71
1:B:3087:ALA:CB	1:B:3181:ILE:HD13	2.15	0.71
1:B:2626:VAL:HG21	1:B:2681:ILE:HD13	1.73	0.70
1:B:4048:TYR:HE1	1:B:4076:PRO:HD3	1.54	0.70
1:A:1576:VAL:HA	1:A:1579:LYS:HD2	1.73	0.70
1:A:4314:ILE:HG23	1:A:4487:CYS:SG	2.31	0.70
1:A:135:GLY:HA2	1:A:140:CYS:O	1.90	0.70
1:B:4127:ASN:HD21	1:B:4165:LEU:HD21	1.55	0.70
1:A:4477:GLY:HA3	1:A:4518:VAL:HG11	1.72	0.70
1:A:4011:ASN:O	1:A:4015:MET:HG2	1.90	0.70
1:A:1963:LYS:HD3	1:A:1966:TYR:CE2	2.27	0.70
1:A:3066:THR:HA	1:A:3078:SER:HB2	1.72	0.70
1:B:1538:MET:HG2	1:B:1598:HIS:HB3	1.74	0.70
1:B:1438:THR:OG1	1:B:1446:LEU:HB3	1.91	0.70
1:B:3001:GLN:HB2	1:B:3139:PHE:CE2	2.26	0.70
1:A:494:GLU:HB3	1:A:498:LYS:HD3	1.74	0.69
1:A:3955:LEU:HD22	1:A:4003:ILE:HD12	1.74	0.69
1:A:2308:LEU:HD23	1:A:2330:ASN:HD22	1.57	0.69
1:B:1338:LEU:HD13	1:B:1346:PHE:HA	1.74	0.69
1:B:3270:ILE:HD12	1:B:3632:PRO:HG2	1.72	0.69
1:B:1414:THR:HG23	1:B:1423:PHE:CD2	2.27	0.69
1:A:1335:GLU:HA	1:A:1339:GLY:O	1.93	0.69
1:A:1961:PRO:HB3	1:A:2171:MET:HE1	1.75	0.69
1:A:3518:GLY:HA2	1:B:3770:ALA:HB1	1.73	0.69
1:B:4339:ILE:HA	1:B:4475:MET:HB2	1.75	0.69
1:A:73:PHE:HD1	1:A:158:ALA:O	1.75	0.69
1:B:3556:TYR:O	1:B:3606:LYS:HE3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:VAL:HB	1:B:715:HIS:ND1	2.07	0.69
1:A:3054:VAL:HA	1:A:3057:ARG:HD2	1.75	0.69
1:A:3330:SER:HB3	1:A:3333:LEU:HB3	1.74	0.69
1:A:4705:LEU:HB3	1:A:4754:VAL:HG22	1.73	0.69
1:B:3095:VAL:HG12	1:B:3190:TRP:CZ3	2.27	0.69
1:B:1963:LYS:HD3	1:B:1966:TYR:CE2	2.27	0.69
1:B:4597:LEU:HD11	1:B:4623:LEU:HD12	1.75	0.69
1:B:130:ILE:HG12	1:B:312:THR:HG23	1.74	0.69
1:B:3066:THR:HA	1:B:3078:SER:HB2	1.75	0.69
1:A:2632:LEU:O	1:A:2649:GLY:HA2	1.93	0.68
1:A:193:PHE:HB2	1:B:881:GLN:NE2	2.08	0.68
1:B:1961:PRO:HB3	1:B:2171:MET:HE1	1.75	0.68
1:B:2368:ILE:HG23	1:B:2377:LEU:HD11	1.75	0.68
1:A:797:GLY:HA3	1:A:850:PHE:HB3	1.75	0.68
1:A:3556:TYR:O	1:A:3606:LYS:HE3	1.93	0.68
1:A:329:VAL:HG12	1:A:388:ILE:HG23	1.74	0.68
1:A:1138:HIS:O	1:A:1142:MET:HG2	1.94	0.68
1:A:3812:ASP:O	1:A:3816:LYS:HG3	1.93	0.68
1:A:4238:LEU:HG	1:A:4287:THR:HG21	1.75	0.68
1:B:1191:SER:HB3	1:B:1194:LYS:HG3	1.75	0.68
1:A:845:ASP:HB3	1:A:849:ARG:HH12	1.57	0.68
1:A:286:PRO:HB3	1:A:295:VAL:HG21	1.76	0.68
1:A:1799:LEU:H	1:A:1799:LEU:HD12	1.56	0.68
1:A:2669:THR:HG22	1:A:2970:LEU:HD13	1.76	0.68
1:A:3794:ARG:N	1:B:3521:GLU:OE2	2.20	0.68
1:A:4105:TRP:HZ2	2:C:129:ALA:HB2	1.58	0.68
1:B:1338:LEU:HB3	1:B:1345:GLU:HB2	1.76	0.68
1:A:1142:MET:O	1:A:1143:ALA:C	2.35	0.68
1:A:4335:LEU:HD13	1:A:4511:LEU:HD21	1.75	0.68
1:B:763:ILE:HG22	1:B:767:LYS:HE3	1.74	0.68
1:B:852:PRO:HB2	1:B:855:LEU:HB3	1.76	0.68
1:A:288:THR:HB	1:A:291:ASP:CG	2.19	0.67
1:A:1041:TRP:CZ3	1:A:1044:ARG:HD2	2.28	0.67
1:B:3087:ALA:HA	1:B:3181:ILE:HD12	1.74	0.67
1:A:1047:ILE:HB	1:A:1050:TYR:HD2	1.59	0.67
1:A:1365:HIS:HB3	1:A:1372:LEU:HD12	1.75	0.67
1:A:1173:THR:HG22	1:A:1233:TRP:HZ2	1.60	0.67
1:A:2292:PHE:HE2	1:A:2386:ASP:HB3	1.57	0.67
1:B:4264:GLY:HA2	1:B:4312:VAL:HG11	1.76	0.67
1:A:752:GLN:HE21	1:A:888:PRO:HG3	1.59	0.67
1:A:3143:GLN:HA	1:A:3146:LYS:HE2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1025:MET:HG2	1:B:1026:ASN:N	2.10	0.67
1:B:4522:ARG:HB3	1:B:4572:GLU:HG2	1.77	0.67
1:B:2698:LYS:HE3	1:B:3001:GLN:CB	2.25	0.67
1:B:39:ALA:HB1	1:B:44:PHE:HA	1.76	0.67
1:B:1387:GLN:HG3	1:B:1393:ALA:HB1	1.74	0.67
1:B:1555:GLN:HA	1:B:1558:ASN:HD22	1.59	0.67
1:B:2702:ILE:HD11	1:B:3001:GLN:NE2	2.10	0.67
1:B:3244:LEU:HB3	1:B:3249:ILE:HB	1.76	0.67
1:A:1218:LEU:HD13	1:A:1376:ILE:HG23	1.76	0.67
1:A:2302:GLU:HB2	1:A:2341:SER:HB2	1.76	0.67
1:B:768:ALA:HA	1:B:773:ASP:HB2	1.75	0.67
1:A:1682:HIS:CE1	1:A:2383:ARG:HB2	2.30	0.67
1:A:3244:LEU:HB3	1:A:3249:ILE:HB	1.76	0.67
1:A:3337:ALA:HB1	1:A:3423:SER:HB3	1.77	0.67
1:B:1205:GLY:CA	1:B:1215:GLY:CA	2.56	0.67
1:B:1679:TYR:CD1	1:B:1708:TYR:HA	2.30	0.67
1:A:284:ILE:HG13	1:A:442:LEU:HB3	1.77	0.66
1:A:2013:THR:HG21	1:A:2029:CYS:HB3	1.77	0.66
1:B:265:TYR:HA	1:B:268:ARG:HD3	1.77	0.66
1:B:415:LEU:HD11	1:B:484:LEU:HD21	1.76	0.66
1:B:3241:LYS:O	1:B:3245:GLU:HG2	1.95	0.66
1:B:4094:HIS:O	1:B:4098:THR:HG23	1.95	0.66
1:B:793:ASN:HB2	1:B:854:ILE:HG21	1.78	0.66
1:B:1300:VAL:HG13	1:B:1336:ARG:HD3	1.78	0.66
1:A:2480:VAL:HA	1:A:2524:GLN:CD	2.20	0.66
1:B:1087:VAL:O	1:B:1091:GLU:HG3	1.96	0.66
1:A:4271:LEU:HD22	1:A:4327:THR:HG23	1.77	0.66
1:B:1247:TRP:HA	1:B:1251:PHE:HB2	1.76	0.66
1:B:3994:LEU:HD23	1:B:4060:LEU:HD21	1.78	0.66
1:B:4714:LEU:HD11	1:B:4754:VAL:HG11	1.77	0.66
1:A:763:ILE:HG22	1:A:767:LYS:HE3	1.75	0.66
1:A:1531:GLY:HA3	1:A:1591:MET:HB3	1.77	0.66
1:A:1499:ILE:HG23	1:A:1506:VAL:HB	1.78	0.66
1:A:2636:LYS:HA	1:A:2649:GLY:HA3	1.78	0.66
1:A:3270:ILE:HD12	1:A:3632:PRO:HG2	1.72	0.66
1:B:1863:LEU:HB3	1:B:1940:LEU:HD21	1.76	0.66
1:B:4027:PRO:HD2	3:F:313:ARG:HE	1.59	0.66
1:A:274:GLN:O	1:A:277:VAL:HG22	1.95	0.66
1:A:1428:LEU:HB3	1:A:1491:LEU:HB3	1.78	0.66
1:B:787:LEU:HD12	1:B:832:LEU:HD23	1.78	0.66
1:B:2978:LEU:HD21	1:B:3024:LEU:HD22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2259:PRO:HG3	1:A:2647:LEU:HD12	1.78	0.65
1:A:3241:LYS:O	1:A:3245:GLU:HG2	1.95	0.65
1:A:1350:VAL:O	1:A:1354:LEU:HG	1.96	0.65
1:B:471:VAL:HG21	1:B:641:ARG:HA	1.76	0.65
1:B:3175:THR:HG21	1:B:3184:PRO:HD3	1.79	0.65
1:A:4094:HIS:O	1:A:4098:THR:HG23	1.96	0.65
1:B:33:VAL:O	1:B:37:LEU:HG	1.95	0.65
1:B:2683:MET:HG3	1:B:2999:TYR:CE2	2.31	0.65
1:A:56:VAL:O	1:A:60:GLU:N	2.28	0.65
1:A:1859:MET:HE2	1:A:2230:MET:HB2	1.78	0.65
1:B:3087:ALA:HB2	1:B:3181:ILE:CD1	2.21	0.65
2:D:93:PHE:CE2	2:D:101:ILE:HA	2.31	0.65
1:A:1361:ILE:HA	1:A:1365:HIS:HB2	1.78	0.65
1:B:1408:VAL:HG11	1:B:1459:VAL:HG11	1.78	0.65
1:A:2054:ASN:HA	1:A:2138:ARG:HB3	1.78	0.65
1:A:3536:ASN:O	1:A:3538:PRO:HD3	1.97	0.65
2:D:83:GLU:HA	2:D:86:ILE:HD12	1.79	0.65
1:A:2345:SER:HA	1:A:2399:LYS:HE2	1.78	0.65
1:A:3408:LEU:HD12	1:A:3411:PHE:HE2	1.62	0.65
1:B:1519:THR:HB	1:B:1520:PRO:HD3	1.78	0.65
3:F:111:PRO:HD2	3:F:128:PHE:CE2	2.32	0.65
1:A:3270:ILE:HD12	1:A:3632:PRO:CG	2.26	0.65
1:A:3447:LEU:HA	1:A:3450:LEU:HD12	1.79	0.65
1:B:1098:ILE:HD11	1:B:1161:ALA:HA	1.78	0.65
1:B:1159:LEU:HB3	1:B:1160:PRO:HD3	1.78	0.65
1:B:1681:CYS:SG	4:B:5202:ZN:ZN	1.86	0.65
1:A:911:PHE:HB3	1:A:914:VAL:HB	1.77	0.64
1:A:2978:LEU:O	1:A:2982:LEU:HG	1.97	0.64
1:A:4495:ILE:HG21	1:A:4505:LEU:HD12	1.80	0.64
3:F:24:CYS:HA	3:F:52:MET:SD	2.37	0.64
1:A:507:ALA:O	1:A:523:ARG:NE	2.30	0.64
1:B:3516:LEU:HD23	1:B:3764:LEU:HD21	1.79	0.64
1:A:1415:ALA:HB2	1:A:1467:TRP:HB2	1.78	0.64
1:B:2054:ASN:HA	1:B:2138:ARG:HB3	1.79	0.64
1:B:3408:LEU:HD12	1:B:3411:PHE:HE2	1.61	0.64
1:A:1104:ILE:HG21	1:A:1168:THR:HG23	1.79	0.64
1:A:1500:VAL:CG2	1:A:1547:ALA:HB2	2.21	0.64
1:B:3063:MET:HG2	1:B:3174:ILE:HD11	1.77	0.64
1:A:1570:TYR:HE2	1:A:1576:VAL:HG21	1.62	0.64
1:A:1681:CYS:SG	4:A:5202:ZN:ZN	1.86	0.64
1:A:3211:ARG:HH21	1:A:3228:ARG:HH22	1.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1859:MET:HE2	1:B:2230:MET:HB2	1.78	0.64
1:A:2040:LEU:CD1	1:A:2085:PRO:CB	2.76	0.64
1:A:4487:CYS:HA	1:A:4490:ASN:HD22	1.62	0.64
1:B:337:LEU:O	1:B:341:VAL:HG13	1.97	0.64
1:A:4522:ARG:HB3	1:A:4572:GLU:HG2	1.79	0.64
1:B:3497:LEU:HD11	1:B:3913:ASN:HD21	1.62	0.64
1:B:3803:TYR:HA	1:B:3807:CYS:HB2	1.80	0.64
1:A:93:PRO:O	1:A:97:LEU:N	2.30	0.64
1:A:98:GLN:HG3	1:A:201:PHE:CE1	2.32	0.64
1:B:4713:PHE:CE1	1:B:4751:LEU:HD21	2.30	0.64
3:F:3:ARG:HG2	3:F:18:ARG:HG2	1.79	0.64
1:A:1054:ILE:O	1:A:1058:LEU:HG	1.98	0.63
1:A:1679:TYR:CD1	1:A:1708:TYR:HA	2.33	0.63
1:B:441:ALA:HB1	1:B:443:ARG:HH22	1.62	0.63
1:B:1499:ILE:HG12	1:B:1506:VAL:HG21	1.80	0.63
3:E:24:CYS:HA	3:E:52:MET:SD	2.39	0.63
1:A:1019:TYR:OH	1:A:1038:THR:HA	1.99	0.63
1:A:1474:SER:HA	1:A:1485:ILE:HD12	1.81	0.63
1:A:1570:TYR:CE2	1:A:1576:VAL:HG21	2.32	0.63
1:A:3463:ARG:HE	1:A:3535:CYS:HA	1.63	0.63
1:B:4127:ASN:HD22	3:F:328:LEU:HD22	1.62	0.63
3:E:71:SER:HB2	3:E:74:GLN:HB2	1.80	0.63
1:A:1708:TYR:HB3	1:A:2353:ARG:CZ	2.28	0.63
1:A:1873:VAL:CG1	1:A:2233:LEU:HD21	2.23	0.63
1:B:510:SER:HB3	1:B:513:ALA:HB2	1.80	0.63
1:B:1214:LEU:HD21	1:B:1354:LEU:HD22	1.81	0.63
1:B:1315:LEU:HB3	1:B:1316:PRO:HD3	1.80	0.63
1:B:2686:LEU:HD21	1:B:3002:VAL:HG21	1.79	0.63
1:B:3447:LEU:HA	1:B:3450:LEU:HD12	1.80	0.63
2:C:13:PHE:HB3	2:C:69:PHE:HE2	1.63	0.63
1:B:3270:ILE:HD12	1:B:3632:PRO:CG	2.26	0.63
1:A:73:PHE:CD1	1:A:159:LYS:CA	2.70	0.63
1:A:2692:ALA:HA	1:A:2695:PHE:HD1	1.63	0.63
1:B:867:HIS:HE1	1:B:1012:ILE:HG21	1.63	0.63
3:E:111:PRO:HD2	3:E:128:PHE:CE2	2.33	0.63
1:A:3148:HIS:CE1	1:A:3150:ALA:HB3	2.33	0.63
1:A:2192:VAL:HG13	1:A:2197:PHE:CE1	2.33	0.62
1:B:1464:LEU:HD23	1:B:1517:THR:HG21	1.81	0.62
1:A:104:CYS:HA	1:A:107:LEU:HD12	1.81	0.62
1:A:516:THR:HB	1:A:519:GLN:HG3	1.80	0.62
1:A:2705:LEU:HG	1:A:3005:MET:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1104:ILE:HG23	1:A:1110:LEU:HD11	1.82	0.62
1:A:3497:LEU:HD11	1:A:3913:ASN:HD21	1.62	0.62
1:B:46:MET:O	1:B:50:PRO:HD3	1.99	0.62
1:A:136:LEU:HD22	1:A:239:PHE:HZ	1.63	0.62
1:A:790:MET:HE3	1:A:858:LEU:HG	1.81	0.62
1:A:2665:HIS:CD2	1:A:2704:VAL:HB	2.34	0.62
1:B:303:VAL:HG22	1:B:377:ILE:HG13	1.82	0.62
1:B:1318:LEU:HA	1:B:1327:ALA:HB1	1.82	0.62
1:B:4335:LEU:HA	1:B:4338:ILE:HD12	1.81	0.62
2:D:29:THR:HG23	2:D:31:LYS:HB2	1.81	0.62
2:D:122:VAL:O	2:D:126:ILE:HG12	1.99	0.62
1:B:1550:GLY:O	1:B:1553:HIS:HB3	2.00	0.62
1:A:2291:PHE:CZ	1:A:2350:THR:O	2.52	0.62
1:B:1557:HIS:O	1:B:1561:VAL:HG23	1.99	0.62
1:B:1877:TYR:HB2	1:B:1886:ARG:HG3	1.82	0.62
1:B:3099:LEU:HD11	1:B:3193:PHE:HD1	1.65	0.62
1:B:3273:MET:HE1	1:B:3318:VAL:HG21	1.81	0.62
2:D:102:SER:HB2	2:D:105:GLU:CD	2.25	0.62
1:A:1047:ILE:HG13	1:A:1255:THR:HB	1.80	0.62
1:A:1427:VAL:HG13	1:A:1431:PHE:HE2	1.64	0.62
1:B:1178:LEU:HD11	1:B:1199:ALA:HB2	1.81	0.62
1:B:1204:ILE:HG12	1:B:1357:GLY:HA3	1.80	0.62
1:B:1726:CYS:SG	4:B:5206:ZN:ZN	1.88	0.62
1:B:2040:LEU:CD1	1:B:2085:PRO:CB	2.76	0.62
1:A:184:LEU:HD22	1:A:184:LEU:H	1.64	0.61
1:B:2567:PRO:HG3	1:B:2632:LEU:HD22	1.82	0.61
1:A:3007:THR:C	1:A:3009:ASP:H	2.08	0.61
1:B:3763:LEU:HD13	1:B:3799:LEU:HA	1.82	0.61
1:B:4232:LEU:C	1:B:4234:GLN:H	2.08	0.61
1:B:2701:LEU:HD13	1:B:3002:VAL:CG1	2.29	0.61
1:B:3327:LEU:O	1:B:3392:CYS:SG	2.55	0.61
3:E:112:ILE:HD12	3:E:136:HIS:HB3	1.80	0.61
1:A:2626:VAL:HG21	1:A:2681:ILE:HG21	1.81	0.61
1:B:2356:ILE:HD13	1:B:2377:LEU:HD13	1.81	0.61
2:C:33:LEU:CD2	2:C:72:MET:HE1	2.30	0.61
1:A:4591:LYS:HB2	1:A:4630:LYS:HD2	1.82	0.61
1:B:2517:ALA:HB3	1:B:2522:GLN:HE21	1.65	0.61
2:D:33:LEU:HD13	2:D:64:ILE:HG21	1.82	0.61
1:A:1347:LEU:HB3	1:A:1351:TYR:CE2	2.35	0.61
1:A:1681:CYS:HG	4:A:5202:ZN:ZN	1.13	0.61
1:B:414:LEU:HB3	1:B:480:ALA:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1427:VAL:HG13	1:B:1431:PHE:HE2	1.65	0.61
1:B:2698:LYS:HE2	1:B:3001:GLN:HE21	1.64	0.61
1:B:3532:CYS:SG	1:B:3868:SER:HA	2.40	0.61
1:A:252:GLY:HA2	1:A:255:LYS:HD2	1.83	0.61
1:B:1561:VAL:HG22	1:B:1810:LEU:CD2	2.30	0.61
1:B:4027:PRO:HB2	3:F:313:ARG:HH21	1.65	0.61
1:A:263:LEU:HB2	1:A:266:PHE:HB2	1.83	0.61
1:A:497:HIS:O	1:A:498:LYS:C	2.43	0.61
1:A:1564:LEU:HB2	1:A:1603:LEU:HD11	1.82	0.61
1:A:1682:HIS:HB2	1:A:1705:GLU:HB2	1.81	0.61
1:B:4635:VAL:HG11	1:B:4685:LYS:HG3	1.82	0.61
1:A:471:VAL:O	1:A:475:ILE:HG12	1.99	0.61
1:A:1680:HIS:HB3	1:A:1687:VAL:HG12	1.82	0.61
1:A:2698:LYS:HZ3	1:A:3001:GLN:HB3	1.66	0.61
1:B:806:LEU:HD21	1:B:811:LEU:HB2	1.82	0.61
1:B:3053:LEU:HD13	1:B:3160:LEU:HD12	1.81	0.61
1:B:4488:MET:HE3	1:B:4511:LEU:HB3	1.83	0.61
2:C:49:LEU:C	2:C:49:LEU:CD1	2.74	0.61
1:A:104:CYS:HB3	1:A:136:LEU:HD13	1.82	0.60
1:B:740:PHE:HD1	1:B:778:GLU:HG3	1.66	0.60
1:A:1052:ASN:O	1:A:1053:TRP:C	2.45	0.60
1:A:4594:LEU:O	1:A:4598:LEU:HG	2.01	0.60
1:B:1693:CYS:HB3	1:B:1716:CYS:HB2	1.84	0.60
2:D:50:GLN:C	2:D:53:ILE:HG22	2.26	0.60
2:D:137:VAL:HG13	2:D:141:GLU:HB2	1.83	0.60
1:A:1402:SER:HA	1:A:1452:SER:HB2	1.82	0.60
1:B:3057:ARG:HB2	1:B:3163:MET:CE	2.32	0.60
1:B:1119:GLN:HA	1:B:1122:TYR:CE2	2.36	0.60
1:B:1534:PHE:CD2	1:B:1595:CYS:HB2	2.36	0.60
1:B:2308:LEU:HD13	1:B:2328:VAL:HG11	1.84	0.60
1:A:2483:LEU:HD12	1:A:2524:GLN:HB3	1.82	0.60
1:B:851:VAL:HG11	1:B:995:GLU:HG2	1.84	0.60
2:C:33:LEU:HD21	2:C:72:MET:HE1	1.83	0.60
1:A:1594:GLU:HA	1:A:2477:ARG:HH22	1.66	0.60
1:A:2291:PHE:HZ	1:A:2350:THR:O	1.85	0.60
1:B:273:PHE:CD2	1:B:338:TYR:HB2	2.37	0.60
1:B:1124:LEU:O	1:B:1128:ILE:HG12	2.01	0.60
1:B:1290:SER:HA	1:B:1293:ARG:HD3	1.82	0.60
1:A:963:TYR:HE1	1:A:1013:LEU:HD13	1.66	0.60
1:A:3731:ASP:HA	1:A:3734:LYS:HB3	1.83	0.60
1:B:921:HIS:HD2	1:B:993:ALA:HB2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1340:PRO:HD2	1:B:1343:SER:HB3	1.84	0.60
1:B:3087:ALA:HB2	1:B:3181:ILE:CG2	2.19	0.60
1:A:105:LYS:HG3	1:A:246:SER:HB2	1.83	0.60
1:A:202:ASN:HB3	1:A:204:ARG:NE	2.16	0.60
1:A:2354:ILE:HG12	1:A:2387:PHE:HE2	1.67	0.60
1:A:3187:ASP:H	1:A:3190:TRP:CD1	2.20	0.60
1:A:4278:VAL:O	1:B:3825:ARG:NH1	2.33	0.60
1:A:4594:LEU:HD11	1:A:4620:ILE:HG23	1.83	0.60
1:B:754:LEU:HD22	1:B:807:ASN:HD21	1.65	0.60
1:B:1063:MET:HG2	1:B:1068:ALA:HB2	1.84	0.60
1:B:2368:ILE:HD11	1:B:2387:PHE:CE1	2.37	0.60
1:B:3516:LEU:CD2	1:B:3764:LEU:HD21	2.31	0.60
1:B:4621:PRO:HG3	1:B:4665:ILE:HA	1.82	0.60
1:A:810:HIS:O	1:A:813:MET:HG3	2.01	0.60
1:B:1500:VAL:HG21	1:B:1543:THR:O	2.02	0.60
1:B:1996:LEU:HD11	1:B:2002:ILE:HG13	1.83	0.60
3:F:75:PRO:HD2	3:F:116:LEU:HD23	1.84	0.60
1:A:670:ILE:O	1:A:674:LEU:HG	2.02	0.59
1:A:1519:THR:HB	1:A:1520:PRO:HD3	1.82	0.59
1:A:3273:MET:HE1	1:A:3318:VAL:HG21	1.83	0.59
1:B:1414:THR:HG22	1:B:1424:CYS:SG	2.41	0.59
1:B:2581:ALA:HB2	1:B:2588:LEU:HD22	1.83	0.59
1:A:1171:SER:HA	1:A:1174:ARG:HD2	1.83	0.59
1:B:296:ARG:HH12	1:B:347:MET:HE3	1.67	0.59
1:A:4313:CYS:SG	1:A:4331:ILE:HG12	2.42	0.59
1:B:3894:PRO:O	1:B:3898:HIS:ND1	2.35	0.59
1:A:1607:THR:HB	1:A:2488:SER:HB2	1.84	0.59
1:B:1356:THR:HA	1:B:1400:PHE:CZ	2.36	0.59
1:B:1398:GLU:HA	1:B:1449:LEU:HD21	1.85	0.59
1:B:2682:TYR:CD2	1:B:2977:LEU:HD11	2.36	0.59
1:A:1051:VAL:HG22	1:A:1072:LEU:HD11	1.84	0.59
1:A:2487:GLU:HB2	1:A:2528:LEU:HA	1.84	0.59
1:A:3106:LEU:HG	1:A:3110:LYS:HE3	1.84	0.59
1:B:3723:VAL:HG11	1:B:3824:SER:OG	2.02	0.59
1:B:4682:ILE:HG23	1:B:4687:ILE:HD12	1.84	0.59
2:D:106:LEU:HD11	2:D:110:MET:HE2	1.83	0.59
1:A:1045:LEU:HD12	1:A:1072:LEU:HD11	1.83	0.59
1:A:1429:LYS:O	1:A:1430:PHE:C	2.45	0.59
1:B:4129:LEU:HD23	1:B:4165:LEU:HD23	1.85	0.59
1:B:4314:ILE:HG12	1:B:4484:GLY:HA2	1.85	0.59
1:A:1514:LEU:O	1:A:1518:LEU:HG	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2121:MET:HE2	1:A:2133:ALA:HB1	1.84	0.59
1:A:3201:GLN:HA	1:A:3207:ARG:HH21	1.68	0.59
1:A:4199:TYR:HA	2:C:20:PHE:CZ	2.38	0.59
1:B:151:PHE:HA	1:B:154:MET:HE2	1.84	0.59
1:B:1450:CYS:HB2	1:B:1505:GLN:HB2	1.83	0.59
1:B:2121:MET:HE2	1:B:2133:ALA:HB1	1.84	0.59
1:B:382:LEU:HD12	1:B:475:ILE:HG22	1.83	0.59
1:B:1015:PRO:HB2	1:B:1020:ILE:HD11	1.85	0.59
1:B:1468:LEU:HA	1:B:1471:MET:HE2	1.84	0.59
1:B:2173:HIS:ND1	1:B:2176:LEU:HD22	2.18	0.59
1:B:2698:LYS:HE2	1:B:3001:GLN:NE2	2.17	0.59
1:B:2702:ILE:HG12	1:B:3005:MET:HG2	1.85	0.59
1:B:4271:LEU:HD22	1:B:4274:ARG:HH21	1.67	0.59
1:A:1685:LYS:HA	1:A:2381:ARG:HH22	1.68	0.59
1:B:1515:LEU:CD1	1:B:1541:MET:HG3	2.32	0.59
1:B:1870:PHE:CZ	1:B:1924:LEU:CD1	2.65	0.59
1:A:4316:THR:HA	1:A:4319:ARG:HE	1.67	0.59
1:A:265:TYR:CZ	1:A:301:SER:HB2	2.38	0.58
1:A:2173:HIS:ND1	1:A:2176:LEU:HD22	2.18	0.58
1:B:680:GLU:HB3	1:B:730:THR:HG21	1.84	0.58
1:B:3270:ILE:O	1:B:3274:GLU:HG2	2.03	0.58
1:B:4096:TYR:CE1	2:D:48:GLU:HG2	2.38	0.58
1:B:4620:ILE:HB	1:B:4621:PRO:HD3	1.85	0.58
1:A:688:SER:O	1:A:692:GLU:HG3	2.03	0.58
1:A:2370:ILE:HD11	1:A:2401:LEU:HD11	1.85	0.58
1:B:299:PHE:O	1:B:303:VAL:HG23	2.03	0.58
1:A:1714:PHE:CZ	1:A:1716:CYS:HA	2.38	0.58
1:A:1901:VAL:CG1	1:A:2217:ILE:HD12	2.28	0.58
1:B:3683:GLN:OE1	1:B:3688:ARG:HD2	2.03	0.58
1:B:4325:TYR:HA	1:B:4504:LEU:HD22	1.86	0.58
3:F:302:SER:O	3:F:306:ARG:N	2.34	0.58
1:A:967:TYR:HE2	1:A:1015:PRO:HA	1.66	0.58
1:A:1119:GLN:HA	1:A:1122:TYR:CE2	2.38	0.58
1:A:3240:ILE:HD11	1:A:3275:HIS:CB	2.33	0.58
1:A:3679:GLU:CD	1:A:3683:GLN:HE22	2.11	0.58
1:B:4355:LYS:HE3	1:B:4365:GLY:O	2.04	0.58
1:B:4429:TRP:CE2	1:B:4438:MET:HA	2.38	0.58
1:A:1307:PRO:HB2	1:A:1308:PRO:HD3	1.84	0.58
1:B:3757:ARG:HB3	1:B:3758:PRO:HD3	1.86	0.58
1:A:56:VAL:HA	1:A:59:SER:HB2	1.85	0.58
1:A:1808:ALA:HB3	1:A:1809:PRO:HD3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4089:LYS:HA	1:A:4092:LEU:HD12	1.86	0.58
1:A:1191:SER:HB3	1:A:1194:LYS:HG3	1.85	0.58
1:A:4429:TRP:CE2	1:A:4438:MET:HA	2.38	0.58
1:B:1361:ILE:HA	1:B:1365:HIS:HB2	1.85	0.58
1:B:3679:GLU:CD	1:B:3683:GLN:HE22	2.11	0.58
1:A:3469:VAL:HG21	1:A:3882:HIS:HB3	1.86	0.58
1:B:93:PRO:HB2	1:B:96:GLN:HB2	1.85	0.58
1:B:810:HIS:O	1:B:813:MET:HG3	2.03	0.58
1:B:2978:LEU:HA	1:B:3006:LEU:HD13	1.86	0.58
1:A:53:VAL:O	1:A:57:ILE:HG13	2.03	0.58
1:A:787:LEU:HD12	1:A:832:LEU:HD23	1.85	0.58
1:A:1428:LEU:HD13	1:A:1491:LEU:HB2	1.85	0.58
1:A:2291:PHE:O	1:A:2295:ASN:ND2	2.35	0.58
1:B:1118:LEU:HD12	1:B:1280:LEU:HD23	1.86	0.58
1:B:4221:LEU:O	1:B:4224:GLU:HG3	2.04	0.58
1:A:745:TRP:HE1	1:A:810:HIS:CE1	2.22	0.57
1:A:1090:VAL:HG13	1:A:1127:ALA:HB1	1.85	0.57
1:B:1515:LEU:HD11	1:B:1556:LEU:HD22	1.85	0.57
1:B:2162:PRO:HG2	1:B:2181:GLN:HG2	1.87	0.57
1:B:2548:LEU:HD11	1:B:2580:ILE:HG21	1.85	0.57
1:A:82:THR:HA	1:A:107:LEU:HD13	1.86	0.57
1:A:3683:GLN:OE1	1:A:3688:ARG:HD2	2.03	0.57
1:B:908:TYR:CZ	1:B:931:ARG:HD3	2.39	0.57
1:B:1600:MET:HB3	1:B:2481:SER:HB2	1.84	0.57
1:B:2310:GLN:HG3	1:B:2311:VAL:HG23	1.84	0.57
1:B:4223:LEU:O	1:B:4279:GLN:NE2	2.38	0.57
1:B:4635:VAL:CG1	1:B:4685:LYS:HG3	2.34	0.57
2:C:49:LEU:HD11	2:C:53:ILE:HD12	1.85	0.57
1:A:1203:ALA:HA	1:A:1320:GLU:HG3	1.86	0.57
1:A:1996:LEU:HD13	1:A:2001:PHE:HA	1.86	0.57
1:B:3057:ARG:HD3	1:B:3139:PHE:CD1	2.39	0.57
1:A:1870:PHE:HB3	1:A:1873:VAL:CG2	2.34	0.57
1:A:2657:VAL:HG11	1:A:2693:VAL:O	2.05	0.57
1:A:3547:LEU:HD13	1:A:3715:LEU:HD11	1.84	0.57
1:B:1929:LEU:HD11	1:B:2241:ILE:HD11	1.86	0.57
1:B:3324:SER:O	1:B:3329:GLY:N	2.36	0.57
1:B:39:ALA:CB	1:B:44:PHE:HA	2.35	0.57
1:B:1534:PHE:CE2	1:B:1595:CYS:HB2	2.39	0.57
1:B:3240:ILE:HD11	1:B:3275:HIS:CB	2.33	0.57
1:B:3469:VAL:HG21	1:B:3882:HIS:HB3	1.86	0.57
2:C:95:LYS:HG2	2:C:105:GLU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:PRO:HG3	1:A:854:ILE:HD11	1.85	0.57
1:A:1037:HIS:CE1	1:A:1041:TRP:HE1	2.22	0.57
1:B:1319:LEU:HD21	1:B:1350:VAL:HG13	1.87	0.57
1:B:2354:ILE:HG12	1:B:2387:PHE:HE2	1.68	0.57
1:B:3087:ALA:CA	1:B:3181:ILE:CD1	2.83	0.57
1:A:284:ILE:H	1:A:442:LEU:H	1.52	0.57
1:A:3270:ILE:O	1:A:3274:GLU:HG2	2.03	0.57
1:A:4307:LYS:HD2	1:A:4479:MET:HA	1.85	0.57
1:B:783:TRP:HD1	1:B:821:PHE:HE2	1.53	0.57
1:B:1244:ILE:HG13	1:B:1248:ARG:HB2	1.86	0.57
1:B:1429:LYS:O	1:B:1430:PHE:C	2.45	0.57
1:B:1520:PRO:HA	1:B:1523:THR:HB	1.87	0.57
1:B:2340:ILE:HD13	1:B:2422:ILE:HD11	1.86	0.57
1:A:3894:PRO:O	1:A:3898:HIS:ND1	2.35	0.57
1:B:844:MET:HB3	1:B:848:MET:HE3	1.85	0.57
1:B:1554:LEU:HD12	1:B:1557:HIS:CD2	2.40	0.57
1:B:1681:CYS:HG	4:B:5202:ZN:ZN	1.16	0.57
1:B:3220:SER:HB3	1:B:3223:LYS:HE2	1.87	0.57
1:B:4053:HIS:HB2	1:B:4071:TRP:CD1	2.39	0.57
1:A:189:VAL:HG21	1:B:874:VAL:HG13	1.85	0.57
1:A:1517:THR:O	1:A:1520:PRO:HD2	2.04	0.57
1:B:1268:ALA:O	1:B:1272:THR:HG23	2.05	0.57
1:B:1495:LEU:HA	1:B:1498:TYR:CD2	2.40	0.57
1:B:3087:ALA:CA	1:B:3181:ILE:HD12	2.35	0.57
1:B:4617:LEU:O	1:B:4621:PRO:HD2	2.05	0.57
1:A:1206:SER:HB2	1:A:1319:LEU:HA	1.87	0.57
1:A:1233:TRP:HE3	1:A:1278:LEU:HD13	1.70	0.57
1:A:4355:LYS:HE3	1:A:4365:GLY:O	2.05	0.57
1:B:1133:VAL:HG22	1:B:1246:SER:HB3	1.86	0.57
1:B:1241:PHE:CE1	1:B:1272:THR:HG21	2.39	0.57
1:B:4089:LYS:HA	1:B:4092:LEU:HD12	1.85	0.57
1:A:2308:LEU:HD13	1:A:2328:VAL:HG11	1.86	0.56
1:A:4130:ARG:HB2	1:A:4169:TYR:CE1	2.40	0.56
1:A:4714:LEU:HD11	1:A:4754:VAL:HG11	1.86	0.56
1:B:479:HIS:HA	1:B:482:LYS:HE2	1.87	0.56
1:B:1119:GLN:HA	1:B:1122:TYR:CD2	2.40	0.56
1:A:396:ARG:HH21	1:B:404:GLN:NE2	2.02	0.56
1:A:1101:PHE:CD2	1:A:1168:THR:HG21	2.40	0.56
1:A:1398:GLU:HG3	1:A:1445:SER:HA	1.86	0.56
1:A:3463:ARG:NH2	1:A:3534:VAL:O	2.38	0.56
1:B:516:THR:HB	1:B:519:GLN:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1415:ALA:HB2	1:B:1467:TRP:HB2	1.87	0.56
1:B:2370:ILE:HD11	1:B:2401:LEU:HD11	1.87	0.56
2:D:93:PHE:HE2	2:D:101:ILE:HA	1.69	0.56
3:E:302:SER:O	3:E:306:ARG:N	2.34	0.56
1:A:145:ARG:O	1:A:149:ILE:HG13	2.06	0.56
1:B:470:GLY:H	1:B:473:SER:HB2	1.71	0.56
1:B:4228:LEU:HD22	1:B:4278:VAL:HG11	1.88	0.56
2:C:93:PHE:HB3	2:C:101:ILE:HD12	1.86	0.56
1:A:2027:ASP:CG	1:A:2029:CYS:HG	2.08	0.56
1:A:4598:LEU:O	1:A:4601:ILE:HG23	2.05	0.56
1:B:521:ILE:HG21	1:B:670:ILE:HD11	1.88	0.56
1:A:1169:TYR:HA	1:A:1172:PHE:HD2	1.70	0.56
1:A:1947:SER:C	1:A:3655:THR:HG21	2.30	0.56
1:B:2301:VAL:HG11	1:B:2422:ILE:HG13	1.86	0.56
1:A:1173:THR:HG22	1:A:1233:TRP:CZ2	2.41	0.56
1:A:1481:GLN:HA	1:A:1481:GLN:HE21	1.69	0.56
1:A:1519:THR:HA	1:A:1563:TRP:HZ2	1.69	0.56
1:B:1395:LYS:O	1:B:1399:GLU:HG2	2.06	0.56
1:B:1560:ALA:HA	1:B:1563:TRP:CE3	2.40	0.56
1:B:2977:LEU:HD23	1:B:3006:LEU:HD21	1.88	0.56
1:B:3948:ILE:HA	1:B:3996:LEU:HD21	1.87	0.56
1:A:273:PHE:O	1:A:277:VAL:HG13	2.06	0.56
1:A:2173:HIS:CE1	1:A:2176:LEU:HD22	2.41	0.56
1:A:4699:ILE:HD13	1:A:4747:ASN:HB3	1.87	0.56
1:B:553:LYS:O	1:B:554:GLY:C	2.48	0.56
1:B:3290:TRP:HE1	1:B:3326:ALA:HB2	1.69	0.56
1:B:3951:VAL:HG13	1:B:4012:ILE:HD13	1.87	0.56
1:A:291:ASP:O	1:A:295:VAL:HG23	2.06	0.56
1:A:491:LEU:HD21	1:A:518:ILE:HA	1.88	0.56
1:A:1948:ALA:HB1	1:A:1978:LEU:HD13	1.88	0.56
1:A:2701:LEU:O	1:A:2704:VAL:HG22	2.05	0.56
1:A:1412:MET:HB3	1:A:1463:ARG:CZ	2.36	0.56
1:A:3662:ARG:NH2	1:A:3679:GLU:OE2	2.39	0.56
1:A:4199:TYR:HA	2:C:20:PHE:HZ	1.70	0.56
1:A:4691:ALA:HB1	1:A:4722:ILE:HG23	1.88	0.56
1:B:82:THR:HG23	1:B:136:LEU:HG	1.87	0.56
1:B:4419:LEU:HD13	1:B:4459:LEU:HG	1.87	0.56
2:C:124:GLU:O	2:C:128:GLU:HG2	2.06	0.56
1:A:420:LEU:HD21	1:A:444:VAL:CA	2.35	0.55
1:A:683:MET:SD	1:A:727:LEU:HD23	2.46	0.55
1:A:1159:LEU:HB3	1:A:1160:PRO:HD3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4682:ILE:HG23	1:A:4687:ILE:HD12	1.88	0.55
1:B:2978:LEU:HB2	1:B:3006:LEU:HB3	1.89	0.55
3:E:301:MET:O	3:E:306:ARG:NH1	2.39	0.55
1:A:404:GLN:HE21	1:B:396:ARG:HB2	1.72	0.55
1:A:1058:LEU:HB3	1:A:1063:MET:SD	2.46	0.55
1:A:1899:MET:SD	1:A:2233:LEU:HB2	2.46	0.55
1:A:4489:LEU:HD21	1:A:4532:THR:HG23	1.87	0.55
1:A:4641:TYR:HD1	1:A:4655:ASP:HA	1.71	0.55
1:B:663:LEU:HD23	1:B:674:LEU:CD1	2.36	0.55
1:B:683:MET:HE3	1:B:727:LEU:HD23	1.87	0.55
1:B:827:ARG:HG3	1:B:955:VAL:HG13	1.88	0.55
1:B:967:TYR:CE2	1:B:1015:PRO:HA	2.42	0.55
1:B:1097:GLN:HA	1:B:1097:GLN:HE21	1.71	0.55
1:B:2173:HIS:CE1	1:B:2176:LEU:HD22	2.41	0.55
1:B:3072:SER:C	1:B:3074:ILE:H	2.14	0.55
1:B:3213:LEU:O	1:B:3217:ILE:HG12	2.05	0.55
1:A:183:GLU:H	1:A:183:GLU:CD	2.13	0.55
1:A:2358:THR:HA	1:A:2382:SER:HB2	1.87	0.55
1:B:1572:SER:O	1:B:1573:GLN:C	2.49	0.55
1:B:1603:LEU:HD13	1:B:1807:PHE:CZ	2.41	0.55
1:B:1961:PRO:HB3	1:B:2171:MET:CE	2.37	0.55
1:B:3662:ARG:NH2	1:B:3679:GLU:OE2	2.39	0.55
1:B:3739:ILE:HG12	1:B:3824:SER:HB3	1.88	0.55
1:B:4216:GLU:HG2	1:B:4238:LEU:HB2	1.88	0.55
1:A:1315:LEU:HB3	1:A:1316:PRO:HD3	1.87	0.55
1:A:1556:LEU:HD22	1:A:1559:ALA:HB3	1.89	0.55
1:A:2300:ASP:HA	1:A:2318:LYS:HZ1	1.72	0.55
1:A:2371:PHE:HZ	1:A:2397:ALA:HB2	1.71	0.55
1:B:48:GLU:O	1:B:51:GLN:HB3	2.07	0.55
1:B:284:ILE:H	1:B:441:ALA:HA	1.71	0.55
1:B:1558:ASN:HD21	1:B:1803:ALA:HB1	1.70	0.55
1:B:2263:ILE:HG13	1:B:2266:MET:HE2	1.87	0.55
1:B:2312:TYR:CE2	1:B:2328:VAL:HG13	2.41	0.55
1:B:3729:GLU:HB3	1:B:3733:LYS:HE3	1.88	0.55
1:B:4423:GLU:HB3	1:B:4459:LEU:HD13	1.87	0.55
3:F:28:TYR:CE2	3:F:122:ASN:HB3	2.42	0.55
1:A:204:ARG:O	1:A:205:THR:C	2.50	0.55
1:A:2982:LEU:O	1:A:2985:LEU:HB3	2.06	0.55
1:A:4719:LEU:HB3	1:A:4720:PRO:HD3	1.88	0.55
1:B:1311:ILE:HA	1:B:1334:LEU:HD21	1.87	0.55
1:B:1453:LEU:C	1:B:1455:GLN:H	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2181:GLN:HG3	1:B:2188:LEU:HD11	1.89	0.55
1:B:4613:LEU:O	1:B:4617:LEU:HG	2.06	0.55
1:A:691:LYS:HD3	1:A:735:LEU:HA	1.88	0.55
1:A:1269:HIS:CE1	1:A:1283:SER:HB3	2.42	0.55
1:B:1088:GLU:HA	1:B:1091:GLU:CD	2.32	0.55
1:B:4313:CYS:SG	1:B:4335:LEU:HD21	2.46	0.55
1:A:674:LEU:O	1:A:678:LEU:HG	2.06	0.55
1:A:1875:MET:SD	1:A:1917:GLU:HA	2.47	0.55
1:A:4024:ILE:HD11	3:E:324:LEU:HD12	1.88	0.55
1:B:1901:VAL:CG1	1:B:2217:ILE:HD12	2.28	0.55
1:B:2212:GLN:N	1:B:2233:LEU:O	2.40	0.55
1:B:4239:LYS:HE2	1:B:4286:GLU:OE1	2.06	0.55
1:B:4771:LEU:O	1:B:4774:HIS:HB3	2.07	0.55
1:A:1118:LEU:HD21	1:A:1269:HIS:HB3	1.87	0.55
1:B:973:LEU:HB3	1:B:1002:TYR:OH	2.06	0.55
1:B:2040:LEU:HD11	1:B:2085:PRO:CB	2.37	0.55
1:B:2966:THR:HA	1:B:2969:ARG:HE	1.72	0.55
1:A:261:LEU:CD2	1:A:332:LEU:HB2	2.36	0.55
1:B:246:SER:O	1:B:250:LEU:HG	2.06	0.55
1:B:3409:ILE:HG12	1:B:3450:LEU:HD22	1.88	0.55
2:C:87:ARG:HG3	2:C:139:TYR:CE1	2.42	0.55
1:B:313:LEU:HD12	1:B:384:ILE:HG23	1.89	0.55
1:A:1529:GLY:HA2	1:A:1592:ILE:HD11	1.89	0.54
1:A:1858:LEU:HB2	1:A:2200:GLN:OE1	2.07	0.54
1:A:4131:GLN:O	1:A:4135:THR:HG23	2.07	0.54
1:B:2360:ALA:HB3	1:B:2363:ARG:HB2	1.88	0.54
1:B:3107:GLU:HA	1:B:3110:LYS:HD2	1.89	0.54
1:A:1348:ALA:O	1:A:1352:GLU:HG3	2.07	0.54
1:A:1961:PRO:HB3	1:A:2171:MET:CE	2.37	0.54
1:A:2474:VAL:HA	1:A:2477:ARG:HE	1.71	0.54
1:A:2654:GLU:HG2	1:A:2692:ALA:HB1	1.88	0.54
1:A:4159:LYS:HZ3	1:A:4196:TRP:CD1	2.25	0.54
1:B:1025:MET:HG2	1:B:1026:ASN:H	1.72	0.54
1:B:3001:GLN:NE2	1:B:3138:PRO:HD3	2.22	0.54
2:D:28:ILE:HD12	2:D:33:LEU:HA	1.88	0.54
2:D:76:LYS:HE2	2:D:76:LYS:HA	1.89	0.54
3:F:301:MET:O	3:F:306:ARG:NH1	2.39	0.54
1:A:35:PRO:HB3	1:A:48:GLU:HB3	1.90	0.54
1:A:4107:GLN:O	1:A:4111:ARG:HG2	2.07	0.54
1:B:808:VAL:HG21	1:B:931:ARG:HD2	1.90	0.54
1:A:183:GLU:O	1:A:187:LYS:HD3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:ALA:O	1:A:644:PRO:HB3	2.07	0.54
1:A:1700:CYS:SG	1:A:1726:CYS:C	2.89	0.54
1:A:3738:ASN:O	1:A:3742:LEU:HG	2.07	0.54
1:A:4476:ALA:C	1:A:4521:ASN:HD21	2.15	0.54
1:B:1545:ALA:HB2	1:B:1556:LEU:HD22	1.89	0.54
1:B:1708:TYR:O	1:B:2353:ARG:NH2	2.40	0.54
1:B:1858:LEU:HB2	1:B:2200:GLN:OE1	2.07	0.54
1:B:3881:GLU:HG2	1:B:3921:MET:HG3	1.88	0.54
2:C:78:LYS:HB2	2:C:80:THR:HG23	1.88	0.54
3:E:75:PRO:HD2	3:E:116:LEU:HD23	1.88	0.54
1:A:1000:GLN:HA	1:A:1270:LEU:HD13	1.89	0.54
1:A:1474:SER:HB2	1:A:1485:ILE:HG21	1.89	0.54
1:A:3568:SER:HB3	1:A:3721:CYS:HA	1.90	0.54
1:B:3406:GLU:HG3	1:B:3850:THR:HG21	1.88	0.54
1:B:4212:LEU:HD23	1:B:4215:LYS:HD2	1.89	0.54
1:A:1047:ILE:HB	1:A:1050:TYR:CD2	2.42	0.54
1:A:1870:PHE:CZ	1:A:1924:LEU:CD1	2.66	0.54
1:A:2040:LEU:HD11	1:A:2085:PRO:CB	2.37	0.54
1:A:3095:VAL:HG12	1:A:3190:TRP:CZ3	2.43	0.54
1:A:4313:CYS:HB3	1:A:4331:ILE:HD13	1.88	0.54
1:B:194:LEU:HD13	1:B:197:LEU:HD12	1.90	0.54
1:B:2701:LEU:HD13	1:B:3002:VAL:HG11	1.90	0.54
1:B:3706:CYS:O	1:B:3710:ARG:NH1	2.41	0.54
1:B:4107:GLN:O	1:B:4111:ARG:HG2	2.07	0.54
1:B:4355:LYS:CE	1:B:4365:GLY:O	2.55	0.54
1:A:299:PHE:HZ	1:A:346:CYS:SG	2.31	0.54
1:A:2266:MET:HE1	1:A:2659:ALA:HB2	1.90	0.54
1:A:3409:ILE:HG12	1:A:3450:LEU:HD22	1.88	0.54
1:B:336:CYS:O	1:B:381:CYS:SG	2.65	0.54
1:B:1306:ASN:HD22	1:B:1309:GLN:HB2	1.72	0.54
1:B:2547:LEU:HD12	1:B:2580:ILE:HD11	1.89	0.54
1:B:2695:PHE:HE1	1:B:2699:GLN:NE2	2.02	0.54
1:B:3172:LYS:HE3	1:B:3217:ILE:HA	1.89	0.54
1:B:3198:LEU:HD22	1:B:3207:ARG:HG3	1.89	0.54
1:A:85:ILE:HA	1:A:88:VAL:HG22	1.90	0.54
1:A:4423:GLU:HB3	1:A:4459:LEU:HD13	1.89	0.54
1:B:49:LEU:C	1:B:51:GLN:N	2.63	0.54
1:B:261:LEU:HD11	1:B:328:ASP:HB3	1.90	0.54
1:B:1394:ARG:NH2	1:B:1437:LEU:HD13	2.23	0.54
1:B:2675:ILE:C	1:B:2677:THR:H	2.15	0.54
1:B:4537:LEU:HD21	1:B:4623:LEU:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:27:THR:HA	2:C:61:ASN:HA	1.88	0.54
1:A:239:PHE:HA	1:A:242:GLN:OE1	2.08	0.54
1:A:1022:GLN:O	1:A:1026:ASN:N	2.40	0.54
1:A:1435:PHE:CD1	1:A:1498:TYR:HB3	2.43	0.54
1:A:2261:SER:HB2	1:A:2263:ILE:HG22	1.90	0.54
1:A:2668:CYS:O	1:A:2973:VAL:HG21	2.08	0.54
1:A:3881:GLU:HG2	1:A:3921:MET:HG3	1.89	0.54
1:A:4540:LEU:HB2	1:A:4562:VAL:HG11	1.89	0.54
1:B:1875:MET:SD	1:B:1917:GLU:HA	2.47	0.54
1:A:3706:CYS:O	1:A:3710:ARG:NH1	2.41	0.54
1:B:2023:VAL:HG23	1:B:2046:ILE:HD13	1.89	0.54
1:B:2025:ILE:HD12	1:B:2075:MET:HE3	1.90	0.54
1:B:2698:LYS:HD2	1:B:2998:PRO:CA	2.30	0.54
1:A:2180:VAL:HG22	1:A:2214:MET:HE2	1.90	0.53
1:A:2300:ASP:HA	1:A:2318:LYS:NZ	2.23	0.53
1:A:4105:TRP:CZ2	2:C:129:ALA:HB2	2.42	0.53
1:B:44:PHE:CD1	1:B:84:TYR:HB3	2.43	0.53
1:B:231:SER:HA	1:B:234:LYS:HD2	1.89	0.53
1:B:1384:LEU:HD13	1:B:1397:MET:SD	2.48	0.53
1:B:3532:CYS:SG	1:B:3534:VAL:HB	2.48	0.53
1:B:4423:GLU:CB	1:B:4459:LEU:HD13	2.38	0.53
1:A:1407:LEU:HB3	1:A:1431:PHE:HE1	1.72	0.53
1:A:2025:ILE:HD12	1:A:2075:MET:HE3	1.90	0.53
1:B:30:GLU:O	1:B:33:VAL:HG22	2.08	0.53
1:B:63:ILE:HA	1:B:74:TYR:HD2	1.73	0.53
1:B:783:TRP:CD1	1:B:821:PHE:HE2	2.26	0.53
1:B:1044:ARG:C	1:B:1046:ARG:N	2.63	0.53
1:A:1162:THR:O	1:A:1166:ILE:HG13	2.08	0.53
1:A:2051:PHE:HB3	1:A:2059:ASN:HD21	1.73	0.53
1:A:3512:ILE:O	1:A:3516:LEU:HG	2.08	0.53
1:A:3759:GLN:HE21	1:A:3763:LEU:HG	1.74	0.53
1:B:286:PRO:HB2	1:B:346:CYS:HB2	1.89	0.53
1:B:844:MET:HE2	1:B:844:MET:HA	1.90	0.53
1:B:2352:MET:HE1	1:B:2403:LEU:HD13	1.91	0.53
1:A:3169:TYR:HD1	1:A:3213:LEU:HD13	1.74	0.53
1:B:1805:PHE:HD2	1:B:2494:PRO:HD2	1.73	0.53
2:C:87:ARG:HG3	2:C:139:TYR:HE1	1.73	0.53
1:A:552:ARG:NH2	1:A:643:ASP:HA	2.23	0.53
1:A:2096:HIS:HB3	1:A:2099:LEU:HG	1.91	0.53
2:D:138:ASN:CG	2:D:139:TYR:H	2.17	0.53
1:A:392:ILE:O	1:A:399:GLY:HA2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1015:PRO:HG3	1:A:1041:TRP:CD2	2.44	0.53
1:A:3310:LEU:HA	1:A:3859:LEU:HD23	1.90	0.53
1:B:2332:LYS:HA	3:F:20:ARG:HH22	1.74	0.53
1:B:2702:ILE:HG23	1:B:3005:MET:HG2	1.89	0.53
1:B:4636:GLU:O	1:B:4640:PRO:HD3	2.08	0.53
2:C:30:THR:HB	2:C:53:ILE:HG12	1.90	0.53
3:F:23:LYS:HD3	3:F:114:ALA:HB1	1.90	0.53
1:A:834:VAL:HG13	1:A:966:LEU:HD13	1.90	0.53
1:A:1048:SER:HA	1:A:1051:VAL:HB	1.91	0.53
1:A:1877:TYR:CE1	1:A:1885:ILE:HG21	2.43	0.53
1:A:2187:PRO:HB3	1:A:2214:MET:SD	2.48	0.53
1:A:3315:VAL:HG22	1:A:3633:LEU:HD21	1.90	0.53
1:A:4123:LEU:HD13	1:A:4165:LEU:HD22	1.90	0.53
1:A:4355:LYS:CE	1:A:4365:GLY:O	2.57	0.53
1:B:49:LEU:HB3	1:B:50:PRO:HD3	1.89	0.53
1:B:443:ARG:HB2	1:B:446:ASP:CG	2.33	0.53
1:B:909:HIS:NE2	1:B:937:SER:HB2	2.24	0.53
1:B:3106:LEU:HD12	1:B:3200:ILE:HD11	1.89	0.53
2:C:33:LEU:CD1	2:C:72:MET:HE1	2.38	0.53
3:E:27:CYS:SG	3:E:45:ARG:O	2.67	0.53
1:A:103:ALA:O	1:A:107:LEU:HG	2.09	0.53
1:B:1191:SER:H	1:B:1194:LYS:HD3	1.73	0.53
1:B:1387:GLN:CG	1:B:1393:ALA:HB1	2.37	0.53
1:B:1595:CYS:SG	1:B:1596:THR:N	2.82	0.53
1:B:3547:LEU:O	1:B:3551:LYS:HG3	2.09	0.53
1:A:89:CYS:HB2	1:A:239:PHE:CD2	2.44	0.53
1:A:245:ALA:O	1:A:249:GLU:HG3	2.09	0.53
1:A:839:GLU:O	1:A:842:VAL:HG12	2.09	0.53
1:A:2698:LYS:NZ	1:A:3001:GLN:HB3	2.24	0.53
1:A:3547:LEU:O	1:A:3551:LYS:HG3	2.09	0.53
1:A:4096:TYR:CE1	2:C:48:GLU:HG2	2.44	0.53
1:B:4047:PRO:HA	1:B:4075:LEU:CD2	2.39	0.53
1:A:303:VAL:HG22	1:A:377:ILE:HG13	1.90	0.53
1:A:3746:ALA:HA	1:A:3749:VAL:HG22	1.91	0.53
1:B:136:LEU:O	1:B:243:ASN:ND2	2.42	0.53
1:B:1603:LEU:HD13	1:B:1807:PHE:HZ	1.73	0.53
1:B:3512:ILE:O	1:B:3516:LEU:HG	2.08	0.53
2:C:59:ASP:HB3	2:C:63:THR:HB	1.89	0.53
1:A:1306:ASN:HB3	1:A:1309:GLN:HB3	1.92	0.52
1:A:1525:MET:HA	1:A:1530:ASP:HB2	1.91	0.52
1:A:2352:MET:HE1	1:A:2403:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1010:LEU:HD22	1:B:1037:HIS:CE1	2.44	0.52
1:B:1435:PHE:CD1	1:B:1498:TYR:HB3	2.43	0.52
1:B:1600:MET:HB3	1:B:2481:SER:CB	2.39	0.52
1:B:2698:LYS:CE	1:B:3001:GLN:HE21	2.22	0.52
1:B:3309:PHE:CD2	1:B:3850:THR:HA	2.44	0.52
1:B:3419:SER:HB3	1:B:3425:ARG:HG3	1.92	0.52
1:A:59:SER:HA	1:A:62:GLU:HB2	1.91	0.52
1:A:4665:ILE:O	1:A:4669:ILE:HG13	2.09	0.52
1:B:272:ARG:HD2	1:B:338:TYR:HE1	1.75	0.52
1:B:420:LEU:HD13	1:B:442:LEU:HB2	1.91	0.52
1:B:859:LEU:O	1:B:1009:ILE:HD11	2.09	0.52
1:B:1542:ALA:HB1	1:B:1602:TYR:CG	2.44	0.52
1:B:1930:LEU:HD13	1:B:2219:HIS:HB3	1.91	0.52
1:B:2292:PHE:HA	1:B:2295:ASN:HD22	1.74	0.52
1:B:3997:PHE:HB2	1:B:4016:CYS:HB3	1.90	0.52
1:A:230:ALA:O	1:A:234:LYS:HG3	2.09	0.52
1:A:336:CYS:O	1:A:381:CYS:SG	2.67	0.52
1:A:545:ALA:HB2	1:A:647:PHE:HB2	1.92	0.52
1:A:2073:GLN:HB2	1:A:2088:VAL:HG13	1.91	0.52
1:A:4245:LEU:HD23	1:A:4294:MET:HE1	1.90	0.52
1:A:4644:PHE:HB3	1:A:4722:ILE:HD11	1.90	0.52
1:B:542:TYR:CE2	1:B:689:ILE:HG23	2.44	0.52
1:B:740:PHE:HA	1:B:781:LYS:HG2	1.91	0.52
1:B:1097:GLN:HA	1:B:1097:GLN:NE2	2.24	0.52
1:B:1162:THR:HG22	1:B:1166:ILE:HD11	1.90	0.52
1:B:3042:LYS:HA	1:B:3049:ASN:HB3	1.92	0.52
2:C:138:ASN:HB3	2:C:140:GLU:HG2	1.91	0.52
1:A:1094:PHE:O	1:A:1098:ILE:HG13	2.10	0.52
1:A:1875:MET:HG2	1:A:1877:TYR:CE1	2.44	0.52
1:A:2517:ALA:HB2	1:A:2521:VAL:HB	1.91	0.52
1:B:943:ASP:O	1:B:944:ASP:C	2.52	0.52
1:B:1489:ARG:NH2	1:B:1533:GLY:CA	2.72	0.52
1:B:1845:LEU:HD12	1:B:1850:LYS:HE3	1.92	0.52
1:B:2052:LEU:HG	1:B:2060:ILE:HB	1.91	0.52
1:B:2073:GLN:HB2	1:B:2088:VAL:HG13	1.91	0.52
1:B:2701:LEU:HD12	1:B:3002:VAL:HG21	1.90	0.52
1:B:4195:HIS:CD2	2:D:35:THR:HG21	2.45	0.52
1:A:478:ASN:OD1	1:A:650:LEU:HD13	2.09	0.52
1:A:906:PRO:HG2	1:A:908:TYR:HE2	1.74	0.52
1:B:1819:MET:CE	1:B:2508:LEU:HD12	2.39	0.52
1:B:2291:PHE:HZ	1:B:2350:THR:HB	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1169:TYR:HA	1:A:1172:PHE:CD2	2.44	0.52
1:A:1571:LEU:C	1:A:1573:GLN:N	2.65	0.52
1:A:2292:PHE:CE2	1:A:2386:ASP:HB3	2.40	0.52
1:A:4740:ILE:O	1:A:4744:SER:HB2	2.09	0.52
1:B:4052:ILE:N	1:B:4119:LEU:O	2.43	0.52
2:C:140:GLU:HG3	2:C:141:GLU:HG3	1.91	0.52
1:A:491:LEU:HD23	1:A:517:SER:OG	2.10	0.52
1:A:661:SER:O	1:A:665:SER:HB2	2.09	0.52
1:A:945:LEU:HA	1:A:1053:TRP:CD1	2.45	0.52
1:B:144:ASP:HB2	1:B:147:GLU:HG3	1.91	0.52
1:B:712:HIS:HA	1:B:715:HIS:CD2	2.44	0.52
1:B:3309:PHE:HE1	1:B:3411:PHE:HB3	1.74	0.52
1:B:3408:LEU:HD12	1:B:3411:PHE:CE2	2.44	0.52
1:B:3968:LEU:CD1	1:B:4012:ILE:HD11	2.39	0.52
1:B:4327:THR:HB	1:B:4328:PRO:HD3	1.90	0.52
2:C:100:TYR:CE1	2:C:138:ASN:HB2	2.45	0.52
3:E:4:HIS:O	3:E:16:ASN:HA	2.09	0.52
1:A:844:MET:HA	1:A:844:MET:HE2	1.90	0.52
1:A:2997:ILE:HB	1:A:2998:PRO:HD3	1.90	0.52
1:B:2375:MET:HG2	1:B:2387:PHE:CE1	2.35	0.52
1:B:3513:TYR:CZ	1:B:3525:TYR:HB3	2.44	0.52
1:B:4644:PHE:HB3	1:B:4722:ILE:HD11	1.92	0.52
1:B:4719:LEU:HB3	1:B:4720:PRO:HD3	1.92	0.52
2:C:20:PHE:CD2	2:C:36:VAL:HG22	2.45	0.52
1:A:405:ASN:HB2	1:A:511:ILE:HA	1.92	0.52
1:A:4560:GLU:HA	1:A:4563:LEU:HD12	1.90	0.52
1:A:4723:LEU:HD11	1:A:4760:ILE:HG23	1.91	0.52
1:B:90:SER:HA	1:B:236:LYS:HB2	1.91	0.52
1:B:313:LEU:HD13	1:B:388:ILE:HD11	1.92	0.52
1:B:1542:ALA:HB1	1:B:1602:TYR:CD1	2.45	0.52
1:B:1930:LEU:HB3	1:B:2219:HIS:CD2	2.45	0.52
1:B:2480:VAL:HG13	1:B:2524:GLN:HG3	1.91	0.52
1:B:4077:ILE:HG21	2:D:116:LYS:HE3	1.92	0.52
1:A:345:THR:O	1:A:349:ILE:HG12	2.10	0.52
1:A:470:GLY:O	1:A:474:VAL:HG23	2.10	0.52
1:A:1043:SER:HB3	1:A:1256:ILE:HG21	1.92	0.52
1:A:3950:LYS:HG2	1:A:3971:GLU:OE1	2.10	0.52
1:A:3954:ALA:HB3	1:A:3968:LEU:HD11	1.92	0.52
1:A:4155:ILE:HB	1:A:4158:ARG:HD2	1.92	0.52
1:B:1490:GLN:O	1:B:1494:LEU:HD13	2.09	0.52
1:B:1558:ASN:HD21	1:B:1803:ALA:CB	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3007:THR:HA	1:B:3010:LEU:HG	1.91	0.52
1:B:3793:ASN:OD1	1:B:3795:TYR:HB2	2.10	0.52
1:A:254:GLU:HA	1:A:257:LEU:HD12	1.90	0.51
1:A:1024:SER:HB3	1:A:1074:LEU:HD23	1.92	0.51
1:A:1309:GLN:HA	1:A:1312:ARG:HD2	1.91	0.51
1:A:1499:ILE:HG12	1:A:1506:VAL:HG21	1.92	0.51
1:A:1845:LEU:HD12	1:A:1850:LYS:HE3	1.92	0.51
1:A:3546:LYS:HG2	1:A:3714:MET:SD	2.51	0.51
1:B:723:GLN:HG2	1:B:728:GLN:HG3	1.92	0.51
1:B:1952:PHE:HE1	1:B:1976:HIS:CD2	2.28	0.51
1:B:3936:ASN:HB3	1:B:3939:ALA:HB3	1.92	0.51
1:B:4155:ILE:HB	1:B:4158:ARG:HD2	1.92	0.51
1:B:4224:GLU:HA	1:B:4279:GLN:HE21	1.74	0.51
1:B:4258:PHE:O	1:B:4259:LYS:C	2.51	0.51
2:C:49:LEU:HD13	2:C:49:LEU:O	2.09	0.51
1:A:73:PHE:HB2	1:A:161:PRO:HD3	1.92	0.51
1:A:266:PHE:O	1:A:270:ILE:HG13	2.10	0.51
1:A:3419:SER:HB3	1:A:3425:ARG:HG3	1.92	0.51
1:A:4195:HIS:CD2	2:C:35:THR:HG21	2.44	0.51
1:B:123:ALA:HB1	1:B:154:MET:SD	2.50	0.51
1:B:303:VAL:HG21	1:B:373:ASP:HB3	1.92	0.51
1:B:1214:LEU:O	1:B:1218:LEU:HG	2.10	0.51
1:B:1570:TYR:HA	1:B:1573:GLN:HE21	1.76	0.51
1:B:3063:MET:HG3	1:B:3170:GLN:HB3	1.92	0.51
1:B:3196:GLU:O	1:B:3200:ILE:HG13	2.10	0.51
1:A:80:LEU:HD11	1:A:152:THR:HA	1.92	0.51
1:A:1560:ALA:HA	1:A:1563:TRP:HE3	1.75	0.51
1:A:83:HIS:O	1:A:87:THR:HG23	2.10	0.51
1:A:546:CYS:O	1:A:550:ARG:HG3	2.11	0.51
1:A:549:GLN:O	1:A:553:LYS:HG2	2.09	0.51
1:B:2072:THR:O	1:B:2090:ASN:HB2	2.10	0.51
1:B:3458:LEU:HD11	1:B:3465:ALA:HB1	1.92	0.51
1:B:3766:LYS:HB3	1:B:3795:TYR:CD2	2.45	0.51
2:C:49:LEU:HD11	2:C:53:ILE:CD1	2.40	0.51
3:F:4:HIS:CD2	3:F:21:ARG:HB2	2.44	0.51
1:A:202:ASN:HB3	1:A:204:ARG:CZ	2.41	0.51
1:A:327:GLN:HA	1:A:511:ILE:HD11	1.92	0.51
1:A:539:SER:HB2	1:A:543:ARG:NH1	2.25	0.51
1:A:2094:ILE:HG12	1:A:2143:VAL:HG21	1.93	0.51
1:A:3071:LYS:HD2	1:A:3074:ILE:HB	1.91	0.51
1:A:3404:ASP:OD1	1:A:3404:ASP:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:LEU:HD11	1:B:247:LEU:HD12	1.92	0.51
1:A:491:LEU:CD1	1:A:670:ILE:HD11	2.40	0.51
1:A:1159:LEU:HA	1:A:1298:LEU:HD13	1.91	0.51
1:A:1814:MET:HA	1:A:1817:PHE:HE1	1.70	0.51
1:A:3998:LEU:O	1:A:4001:VAL:HG12	2.10	0.51
1:B:663:LEU:HD23	1:B:674:LEU:HD13	1.93	0.51
1:B:712:HIS:HA	1:B:715:HIS:NE2	2.25	0.51
1:B:1169:TYR:HA	1:B:1172:PHE:CD2	2.46	0.51
1:B:1401:PHE:HD2	1:B:1449:LEU:HD22	1.76	0.51
1:B:1558:ASN:O	1:B:1561:VAL:HB	2.11	0.51
1:B:3194:LEU:HB2	1:B:3214:LEU:HD13	1.93	0.51
1:B:3940:THR:HG21	1:B:3985:CYS:HB3	1.90	0.51
1:B:4130:ARG:HB2	1:B:4169:TYR:CE1	2.46	0.51
1:B:4438:MET:HE3	1:B:4440:ILE:HD11	1.93	0.51
1:A:1515:LEU:HA	1:A:1544:LEU:HD13	1.93	0.51
1:A:4423:GLU:CB	1:A:4459:LEU:HD13	2.41	0.51
1:B:31:VAL:O	1:B:35:PRO:HD2	2.11	0.51
1:B:1403:ASP:OD2	1:B:1404:SER:N	2.44	0.51
1:B:3405:LYS:HB2	1:B:3450:LEU:HD21	1.93	0.51
1:B:3519:LEU:HD13	1:B:3767:VAL:HG11	1.92	0.51
1:B:4286:GLU:HB3	1:B:4290:MET:HE3	1.92	0.51
1:B:4548:GLN:HG3	1:B:4605:PHE:HD1	1.75	0.51
2:D:42:GLN:HB2	2:D:78:LYS:HG2	1.92	0.51
1:A:918:TRP:O	1:A:922:PHE:HB2	2.10	0.51
1:A:1010:LEU:HB3	1:A:1037:HIS:CE1	2.45	0.51
1:A:1468:LEU:HD22	1:A:1518:LEU:HD21	1.92	0.51
1:A:1995:GLN:HB2	1:A:2024:LYS:NZ	2.26	0.51
1:A:3233:LEU:HD13	1:A:3290:TRP:HE3	1.76	0.51
1:A:4077:ILE:HG13	1:A:4079:GLY:H	1.75	0.51
1:A:4258:PHE:HE1	2:C:19:LEU:HD21	1.75	0.51
1:B:1893:VAL:HG12	1:B:2001:PHE:HZ	1.76	0.51
1:B:3292:LYS:O	1:B:3295:ILE:HG22	2.11	0.51
1:A:967:TYR:CE2	1:A:1015:PRO:HA	2.44	0.51
1:A:1010:LEU:HB3	1:A:1037:HIS:HE1	1.75	0.51
1:A:3286:ARG:HH21	1:A:3286:ARG:HG3	1.75	0.51
1:B:443:ARG:HB2	1:B:446:ASP:HB2	1.93	0.51
1:B:1473:THR:O	1:B:1485:ILE:HD13	2.10	0.51
1:B:1698:LYS:HG2	1:B:2289:ILE:HD12	1.92	0.51
1:B:3001:GLN:HG2	1:B:3004:LEU:HD23	1.92	0.51
1:A:44:PHE:HE2	1:A:48:GLU:HB2	1.75	0.51
1:A:1019:TYR:CZ	1:A:1023:LEU:HD21	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4679:LYS:NZ	1:A:4731:ILE:O	2.42	0.51
1:B:63:ILE:HA	1:B:74:TYR:CD2	2.46	0.51
1:B:1417:GLU:HA	1:B:1470:ARG:HD2	1.93	0.51
1:B:2359:GLN:HG2	1:B:2418:ASP:OD1	2.11	0.51
1:B:4232:LEU:C	1:B:4234:GLN:N	2.69	0.51
1:A:4282:LYS:O	1:A:4286:GLU:HG2	2.11	0.50
1:B:765:GLN:NE2	1:B:817:ILE:HG23	2.26	0.50
1:B:1091:GLU:HG2	1:B:1158:LEU:HD13	1.92	0.50
1:B:2296:GLN:HE21	1:B:2347:MET:HE1	1.76	0.50
1:A:396:ARG:HH21	1:B:404:GLN:CD	2.18	0.50
1:A:816:LEU:HD21	1:B:193:PHE:CZ	2.46	0.50
1:A:3007:THR:C	1:A:3009:ASP:N	2.65	0.50
1:B:909:HIS:CE1	1:B:937:SER:HB2	2.46	0.50
1:B:1428:LEU:CD1	1:B:1488:ASN:HA	2.42	0.50
1:B:1960:ASN:HD21	1:B:2012:GLN:HA	1.76	0.50
1:B:2023:VAL:HG21	1:B:2049:VAL:HG21	1.93	0.50
1:B:3307:VAL:O	1:B:3311:VAL:HG13	2.12	0.50
1:B:3330:SER:HA	1:B:3333:LEU:HB2	1.93	0.50
2:C:33:LEU:HD11	2:C:72:MET:HE1	1.91	0.50
1:A:548:LEU:HD11	1:A:647:PHE:CE2	2.46	0.50
1:A:1205:GLY:HA2	1:A:1215:GLY:C	2.36	0.50
1:A:1515:LEU:CA	1:A:1544:LEU:HD13	2.42	0.50
1:A:1682:HIS:CE1	1:A:2383:ARG:HD2	2.45	0.50
1:B:31:VAL:O	1:B:34:ARG:HB3	2.12	0.50
1:B:739:PRO:HB3	1:B:782:VAL:HG23	1.94	0.50
1:B:2327:TYR:CD1	1:B:2359:GLN:HG3	2.46	0.50
1:A:3511:ASN:HB2	1:B:4007:VAL:HG22	1.94	0.50
1:B:49:LEU:C	1:B:51:GLN:H	2.19	0.50
1:B:71:GLU:OE1	1:B:122:CYS:HA	2.11	0.50
1:B:143:LEU:HD13	1:B:151:PHE:CE2	2.47	0.50
1:B:808:VAL:HG11	1:B:908:TYR:HB3	1.94	0.50
1:B:834:VAL:HG11	1:B:961:VAL:HG13	1.93	0.50
1:B:3100:HIS:O	1:B:3103:LYS:HG3	2.11	0.50
3:E:324:LEU:O	3:E:328:LEU:HG	2.10	0.50
1:A:650:LEU:O	1:A:654:ILE:HG13	2.11	0.50
1:A:846:ALA:HB1	1:A:850:PHE:CE2	2.47	0.50
1:A:2385:PHE:HB3	1:A:2387:PHE:CZ	2.46	0.50
1:A:3458:LEU:HD11	1:A:3465:ALA:HB1	1.92	0.50
1:A:4597:LEU:O	1:A:4601:ILE:HG22	2.11	0.50
1:B:2009:PRO:HB2	1:B:2642:LEU:HD21	1.94	0.50
1:B:2049:VAL:HG22	1:B:2063:ILE:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:113:CYS:SG	3:E:136:HIS:CE1	3.04	0.50
1:A:3405:LYS:HB2	1:A:3450:LEU:HD21	1.93	0.50
1:B:83:HIS:O	1:B:87:THR:HG23	2.11	0.50
1:B:864:TYR:HA	1:B:936:LEU:HG	1.94	0.50
1:B:3872:CYS:O	1:B:3873:TYR:C	2.55	0.50
1:B:4749:HIS:O	1:B:4753:GLN:HG3	2.11	0.50
2:C:137:VAL:HG13	2:C:141:GLU:HB2	1.93	0.50
1:A:317:VAL:HG12	1:A:318:LEU:N	2.26	0.50
1:A:491:LEU:HD22	1:A:518:ILE:HG12	1.92	0.50
1:A:723:GLN:HG2	1:A:728:GLN:HG3	1.92	0.50
1:A:786:PHE:CE1	1:A:806:LEU:HD13	2.47	0.50
1:A:873:PRO:HG2	1:A:876:LEU:HB2	1.93	0.50
1:A:1050:TYR:HE2	1:A:1255:THR:HG21	1.77	0.50
1:A:1196:GLN:HG2	1:A:1365:HIS:HE1	1.76	0.50
1:A:2340:ILE:HD12	1:A:2401:LEU:HD23	1.93	0.50
1:A:3000:MET:HE2	1:A:3058:LEU:HD13	1.93	0.50
1:A:3200:ILE:HG22	1:A:3202:GLN:H	1.75	0.50
1:A:3408:LEU:HD12	1:A:3411:PHE:CE2	2.44	0.50
1:A:3937:PRO:HA	1:A:3940:THR:HG22	1.94	0.50
1:B:39:ALA:CB	1:B:44:PHE:CD1	2.95	0.50
1:B:2189:VAL:HG21	1:B:2230:MET:HE1	1.93	0.50
1:B:2667:TYR:O	1:B:2668:CYS:SG	2.69	0.50
1:B:2988:LEU:HD21	1:B:2999:TYR:CD1	2.47	0.50
1:B:3003:ILE:O	1:B:3007:THR:HG23	2.12	0.50
1:B:3404:ASP:OD1	1:B:3404:ASP:N	2.41	0.50
1:B:4035:LYS:O	1:B:4036:ASP:C	2.54	0.50
1:B:4077:ILE:HG22	2:D:114:GLY:O	2.11	0.50
1:B:4768:LEU:HA	1:B:4771:LEU:HD12	1.94	0.50
1:A:1058:LEU:HD23	1:A:1061:GLN:HE22	1.75	0.50
1:A:1427:VAL:HG13	1:A:1431:PHE:CE2	2.47	0.50
1:A:2311:VAL:HG13	3:E:56:LEU:HD11	1.94	0.50
1:A:4108:PHE:O	1:A:4112:ARG:HG3	2.12	0.50
1:B:1057:HIS:O	1:B:1061:GLN:HG3	2.12	0.50
1:B:1450:CYS:CB	1:B:1505:GLN:HB2	2.41	0.50
1:B:1453:LEU:C	1:B:1455:GLN:N	2.69	0.50
1:B:1553:HIS:HD2	1:B:1556:LEU:HD23	1.77	0.50
1:B:3273:MET:O	1:B:3273:MET:HE3	2.11	0.50
2:C:44:PRO:HB2	2:C:48:GLU:HB2	1.94	0.50
2:D:124:GLU:O	2:D:128:GLU:HG2	2.12	0.50
1:A:73:PHE:CD1	1:A:158:ALA:O	2.60	0.50
1:A:418:LEU:HD21	1:A:476:LEU:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:MET:HE2	1:A:683:MET:HA	1.93	0.50
1:A:881:GLN:HA	1:A:885:LEU:HD12	1.92	0.50
1:A:1156:LYS:HG2	1:A:1304:GLU:HG2	1.94	0.50
1:A:1356:THR:HA	1:A:1400:PHE:HE2	1.77	0.50
1:A:3007:THR:HG21	1:A:3062:PHE:CZ	2.46	0.50
1:B:341:VAL:HB	1:B:417:SER:HB2	1.94	0.50
1:B:834:VAL:HG13	1:B:966:LEU:HD13	1.93	0.50
1:B:852:PRO:CB	1:B:855:LEU:HB3	2.41	0.50
1:B:1044:ARG:C	1:B:1046:ARG:H	2.19	0.50
1:B:1162:THR:O	1:B:1166:ILE:HG13	2.12	0.50
1:B:1359:TYR:CD1	1:B:1406:GLU:HB3	2.47	0.50
1:B:1485:ILE:O	1:B:1489:ARG:HG3	2.12	0.50
1:B:1570:TYR:CE2	1:B:1592:ILE:HG13	2.47	0.50
1:B:2246:VAL:HG13	1:B:2250:SER:HB3	1.94	0.50
1:B:2474:VAL:HG22	1:B:2477:ARG:NH2	2.27	0.50
3:F:27:CYS:SG	3:F:45:ARG:O	2.69	0.50
1:A:85:ILE:CG2	1:A:100:VAL:HG13	2.42	0.49
1:A:662:MET:HB3	1:A:674:LEU:HD11	1.94	0.49
1:A:3273:MET:HE3	1:A:3273:MET:O	2.11	0.49
1:A:3307:VAL:C	1:A:3309:PHE:H	2.19	0.49
1:B:37:LEU:HD12	1:B:38:SER:N	2.26	0.49
1:B:1296:GLY:O	1:B:1300:VAL:HG22	2.12	0.49
1:B:1553:HIS:O	1:B:1553:HIS:CG	2.65	0.49
1:B:2103:ASN:C	1:B:2105:GLN:H	2.19	0.49
1:B:2632:LEU:O	1:B:2649:GLY:HA2	2.12	0.49
1:B:2993:GLY:HA3	1:B:3050:GLU:OE1	2.12	0.49
1:B:4108:PHE:O	1:B:4112:ARG:HG3	2.11	0.49
2:C:24:GLY:HA3	2:C:28:ILE:HD12	1.92	0.49
2:D:86:ILE:HD11	2:D:146:MET:HG2	1.94	0.49
1:A:1233:TRP:HH2	1:A:1281:ALA:HB1	1.77	0.49
1:A:1300:VAL:HA	1:A:1336:ARG:NH1	2.27	0.49
1:A:1565:SER:O	1:A:1569:LYS:HG2	2.11	0.49
1:A:3100:HIS:O	1:A:3103:LYS:HG3	2.11	0.49
1:A:4335:LEU:HD13	1:A:4511:LEU:CD2	2.41	0.49
1:B:3000:MET:HE3	1:B:3054:VAL:HG12	1.92	0.49
1:A:535:LEU:HD12	1:A:682:HIS:CD2	2.46	0.49
1:A:914:VAL:HG11	1:A:1001:TYR:HD1	1.76	0.49
1:A:1101:PHE:HA	1:A:1104:ILE:HD13	1.95	0.49
1:A:2047:ARG:HE	1:A:2066:SER:HB3	1.78	0.49
1:A:2335:GLY:HA3	1:A:2405:ILE:O	2.12	0.49
1:A:3951:VAL:HG13	1:A:4012:ILE:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4310:MET:HE3	1:A:4335:LEU:HG	1.95	0.49
1:A:4595:VAL:HA	1:A:4598:LEU:HD12	1.94	0.49
1:B:288:THR:HG22	1:B:432:LYS:HB3	1.93	0.49
1:B:786:PHE:HZ	1:B:806:LEU:HD22	1.77	0.49
1:B:1819:MET:CE	1:B:2508:LEU:CD1	2.91	0.49
1:B:1952:PHE:CD1	1:B:1974:ASP:HB2	2.47	0.49
1:B:2070:ILE:HD12	1:B:2094:ILE:CD1	2.40	0.49
1:A:159:LYS:O	1:A:160:LEU:C	2.52	0.49
1:A:244:VAL:O	1:A:248:GLN:HG2	2.12	0.49
1:A:547:VAL:O	1:A:551:GLN:HG3	2.11	0.49
1:A:1929:LEU:HD21	1:A:2241:ILE:HD11	1.94	0.49
1:A:4413:LYS:HD3	1:A:4456:ILE:HD11	1.94	0.49
1:B:477:ALA:O	1:B:481:ILE:HG12	2.11	0.49
3:F:301:MET:SD	3:F:306:ARG:HG3	2.53	0.49
1:A:397:ARG:O	1:A:398:ALA:HB3	2.12	0.49
1:A:1460:GLU:HB2	1:A:1463:ARG:HB3	1.94	0.49
1:A:1510:VAL:O	1:A:1514:LEU:HG	2.13	0.49
1:A:1567:CYS:SG	1:A:1596:THR:HG23	2.52	0.49
1:A:1870:PHE:CE2	1:A:2239:LEU:HD11	2.30	0.49
1:A:2687:LEU:O	1:A:2688:CYS:C	2.55	0.49
1:B:745:TRP:HE1	1:B:810:HIS:CE1	2.31	0.49
1:B:808:VAL:HG22	1:B:933:TYR:CD2	2.48	0.49
1:B:867:HIS:O	1:B:949:ASP:HB2	2.13	0.49
1:B:1451:GLY:O	1:B:1454:ALA:HB3	2.12	0.49
1:B:1848:VAL:O	1:B:1850:LYS:NZ	2.38	0.49
1:B:3588:ARG:HG3	1:B:3648:TYR:CZ	2.47	0.49
1:B:4476:ALA:HB1	1:B:4515:CYS:HA	1.94	0.49
3:E:301:MET:SD	3:E:306:ARG:HG3	2.53	0.49
1:A:686:LEU:O	1:A:690:ILE:HG13	2.12	0.49
1:A:740:PHE:CD1	1:A:778:GLU:HG3	2.48	0.49
1:A:1241:PHE:HE2	1:A:1269:HIS:CD2	2.30	0.49
1:A:1347:LEU:HD22	1:A:1351:TYR:OH	2.13	0.49
1:A:1925:GLN:HB3	1:A:1943:THR:HB	1.95	0.49
1:A:2626:VAL:HG21	1:A:2681:ILE:HD13	1.93	0.49
1:A:4277:VAL:HG21	1:B:3732:ARG:HH22	1.78	0.49
1:B:1300:VAL:CG1	1:B:1336:ARG:HD3	2.43	0.49
1:B:1388:LEU:HG	1:B:1397:MET:HE1	1.95	0.49
1:B:1486:GLN:HG3	1:B:1489:ARG:HH11	1.78	0.49
1:B:3979:ILE:HG21	1:B:4019:ILE:HG23	1.93	0.49
1:B:4560:GLU:HA	1:B:4563:LEU:HD12	1.93	0.49
1:A:31:VAL:O	1:A:35:PRO:HD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:HIS:CD2	1:A:937:SER:HA	2.48	0.49
1:A:1135:LEU:O	1:A:1139:PHE:HD2	1.96	0.49
1:A:1453:LEU:HB3	1:A:1506:VAL:CG1	2.37	0.49
1:A:2356:ILE:HD13	1:A:2377:LEU:HD13	1.94	0.49
1:A:2363:ARG:HH11	1:A:2416:MET:HE1	1.76	0.49
1:A:3988:LEU:H	1:A:3988:LEU:HD12	1.77	0.49
1:B:2292:PHE:CE2	1:B:2386:ASP:HB3	2.47	0.49
1:B:2295:ASN:HB3	1:B:2423:TYR:HB3	1.94	0.49
1:B:3063:MET:HE2	1:B:3170:GLN:HG2	1.95	0.49
1:B:3221:LYS:HD2	1:B:3224:TYR:HD2	1.76	0.49
1:B:4130:ARG:O	1:B:4134:PHE:HD2	1.96	0.49
2:D:60:GLY:HA2	2:D:64:ILE:HG12	1.94	0.49
3:E:309:MET:O	3:E:313:ARG:HG2	2.12	0.49
1:A:129:LEU:HA	1:A:132:LEU:HD12	1.94	0.49
1:A:531:MET:HE1	1:A:535:LEU:HD11	1.94	0.49
1:A:2405:ILE:HD12	1:A:2417:ILE:HD11	1.95	0.49
1:A:2581:ALA:HB2	1:A:2588:LEU:HD22	1.95	0.49
1:A:3412:LEU:HD22	1:A:3454:ILE:HD12	1.95	0.49
1:A:3872:CYS:SG	1:A:3875:CYS:CB	2.93	0.49
1:A:4692:LEU:HD21	1:A:4740:ILE:HG12	1.94	0.49
1:B:1159:LEU:HD13	1:B:1298:LEU:HB2	1.94	0.49
1:B:2040:LEU:HD11	1:B:2085:PRO:HB3	1.95	0.49
1:B:2052:LEU:HD11	1:B:2060:ILE:HD12	1.95	0.49
1:B:3309:PHE:HD2	1:B:3850:THR:HA	1.77	0.49
1:A:396:ARG:HH21	1:B:404:GLN:HE22	1.61	0.49
1:A:1666:PHE:HA	1:A:1669:THR:OG1	2.13	0.49
1:A:2474:VAL:HG13	1:A:2477:ARG:HH21	1.78	0.49
1:A:2548:LEU:HD11	1:A:2588:LEU:HA	1.95	0.49
1:A:2555:LEU:HD23	1:A:2565:LEU:HD22	1.95	0.49
1:A:3410:GLN:HE21	1:A:3857:ARG:HH11	1.60	0.49
1:A:3548:SER:HA	1:A:3551:LYS:HE2	1.95	0.49
1:A:4228:LEU:HD11	1:B:3829:LEU:HD22	1.95	0.49
1:B:1151:SER:O	1:B:1154:ILE:HG12	2.13	0.49
1:B:1930:LEU:HD13	1:B:2219:HIS:CB	2.42	0.49
1:B:2982:LEU:HD11	1:B:3027:GLN:CB	2.43	0.49
1:B:3735:ALA:O	1:B:3739:ILE:HG13	2.13	0.49
3:F:309:MET:O	3:F:313:ARG:HG2	2.12	0.49
1:A:1351:TYR:HA	1:A:1354:LEU:HD12	1.95	0.49
1:A:3307:VAL:C	1:A:3309:PHE:N	2.71	0.49
1:A:4001:VAL:C	1:A:4003:ILE:N	2.69	0.49
1:B:946:ASN:O	1:B:947:ARG:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1673:PHE:HD1	1:B:1714:PHE:HA	1.78	0.49
1:B:3226:GLN:HA	1:B:3289:ASN:ND2	2.28	0.49
2:C:10:ILE:HG13	2:C:66:PHE:HZ	1.76	0.49
2:D:100:TYR:CD1	2:D:136:GLN:HB2	2.48	0.49
1:A:675:SER:HB3	1:A:722:LEU:HD12	1.95	0.48
1:A:1515:LEU:HB2	1:A:1544:LEU:HB3	1.95	0.48
1:A:1895:ARG:NH2	1:A:2180:VAL:HG11	2.27	0.48
1:A:2373:ARG:NH2	1:A:2393:GLU:OE2	2.45	0.48
1:A:4480:ALA:HB2	1:A:4521:ASN:OD1	2.12	0.48
1:B:1355:ILE:HD13	1:B:1397:MET:HG2	1.93	0.48
1:B:2266:MET:HE1	1:B:2659:ALA:HB2	1.93	0.48
1:B:3412:LEU:HD22	1:B:3454:ILE:HD12	1.95	0.48
1:B:4309:PHE:CE1	1:B:4338:ILE:HD11	2.48	0.48
1:B:4314:ILE:HD11	1:B:4479:MET:HE1	1.95	0.48
1:B:4485:LEU:HD12	1:B:4524:GLN:HG2	1.93	0.48
3:E:3:ARG:HG2	3:E:18:ARG:HG2	1.93	0.48
1:A:92:ILE:HD12	1:A:97:LEU:HA	1.94	0.48
1:A:874:VAL:HG13	1:B:189:VAL:HG11	1.94	0.48
1:A:1383:TYR:O	1:A:1387:GLN:HG2	2.13	0.48
1:A:1515:LEU:CD2	1:A:1555:GLN:HG3	2.43	0.48
1:A:3521:GLU:N	1:B:3791:SER:O	2.46	0.48
1:B:272:ARG:HD2	1:B:338:TYR:CE1	2.47	0.48
1:B:313:LEU:HD21	1:B:332:LEU:HD21	1.95	0.48
1:B:1118:LEU:HD13	1:B:1273:LEU:HB2	1.94	0.48
1:B:1374:GLU:O	1:B:1375:SER:C	2.56	0.48
1:B:1536:GLU:O	1:B:1540:VAL:HG23	2.13	0.48
1:B:1859:MET:HE2	1:B:2230:MET:CB	2.44	0.48
1:B:2676:ASN:C	1:B:2678:ALA:N	2.70	0.48
1:B:3410:GLN:NE2	1:B:3853:ALA:HB2	2.28	0.48
2:C:106:LEU:CD2	2:C:126:ILE:CD1	2.80	0.48
2:D:16:ALA:O	2:D:20:PHE:HD2	1.95	0.48
1:A:334:LEU:HD11	1:A:409:LEU:HD13	1.95	0.48
1:A:1682:HIS:HE1	1:A:2383:ARG:HB2	1.76	0.48
1:A:3108:TYR:O	1:A:3112:GLN:HG2	2.13	0.48
1:A:4602:ASN:HA	1:A:4607:ARG:HE	1.77	0.48
1:B:711:TYR:CD2	1:B:887:PRO:HA	2.48	0.48
1:B:811:LEU:HD23	1:B:933:TYR:HE1	1.77	0.48
1:B:857:ARG:O	1:B:861:ILE:HG13	2.13	0.48
1:B:1384:LEU:HB3	1:B:1430:PHE:CE1	2.47	0.48
1:B:1555:GLN:HA	1:B:1558:ASN:ND2	2.26	0.48
1:B:4101:TYR:OH	2:D:85:GLU:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4238:LEU:CG	1:B:4287:THR:HG21	2.38	0.48
1:A:548:LEU:HD13	1:A:642:LYS:C	2.38	0.48
1:A:1190:PRO:HG2	1:A:1195:LEU:HD21	1.95	0.48
1:A:1459:VAL:HG21	1:A:1464:LEU:HD13	1.95	0.48
1:A:1899:MET:CE	1:A:2233:LEU:HB2	2.43	0.48
1:A:2118:VAL:HA	1:A:2644:PRO:HA	1.94	0.48
1:A:3045:ARG:NH2	1:A:3153:PHE:HB2	2.28	0.48
1:A:3226:GLN:HA	1:A:3289:ASN:ND2	2.27	0.48
1:A:4252:GLU:O	1:A:4256:ARG:HG3	2.13	0.48
1:A:4641:TYR:CD1	1:A:4655:ASP:HA	2.48	0.48
1:B:3095:VAL:HG12	1:B:3190:TRP:HZ3	1.76	0.48
1:B:4020:LEU:O	1:B:4024:ILE:HG13	2.13	0.48
1:B:4258:PHE:O	1:B:4261:ARG:N	2.44	0.48
1:B:4696:LYS:O	1:B:4699:ILE:HG22	2.13	0.48
1:A:422:LEU:HD11	1:A:537:LEU:HD23	1.95	0.48
1:A:1665:THR:O	1:A:1669:THR:HG23	2.13	0.48
1:A:2296:GLN:HE21	1:A:2347:MET:HE1	1.77	0.48
1:A:2320:ARG:HH21	3:E:68:GLU:HB3	1.78	0.48
1:A:3212:LYS:HA	1:A:3215:LEU:HG	1.94	0.48
1:A:3922:ARG:NH1	1:A:3970:TYR:OH	2.46	0.48
1:B:2025:ILE:CD1	1:B:2075:MET:HE3	2.44	0.48
1:B:2301:VAL:HG21	1:B:2422:ILE:HG21	1.95	0.48
1:B:2564:ASP:OD1	1:B:2631:LYS:CB	2.45	0.48
1:B:3309:PHE:CE1	1:B:3411:PHE:HB3	2.48	0.48
1:A:411:ALA:O	1:A:412:TRP:C	2.56	0.48
1:A:1030:MET:HE3	1:A:1035:ILE:HD13	1.96	0.48
1:A:1118:LEU:HA	1:A:1121:ILE:HD12	1.95	0.48
1:A:2189:VAL:HG21	1:A:2230:MET:HE1	1.92	0.48
1:A:2480:VAL:HA	1:A:2524:GLN:HG3	1.95	0.48
1:A:2578:ARG:HD2	1:A:2659:ALA:HA	1.96	0.48
1:A:3161:THR:O	1:A:3165:LEU:HG	2.14	0.48
1:A:3418:GLU:HG2	1:A:3461:TYR:CE1	2.49	0.48
1:A:3521:GLU:CG	1:B:3793:ASN:HA	2.37	0.48
1:B:255:LYS:HG2	1:B:258:ARG:NH2	2.29	0.48
1:B:740:PHE:CD1	1:B:778:GLU:HG3	2.48	0.48
1:B:1009:ILE:O	1:B:1013:LEU:HG	2.14	0.48
1:B:1094:PHE:HB3	1:B:1161:ALA:HB1	1.93	0.48
1:B:4311:ALA:O	1:B:4315:GLU:HG2	2.13	0.48
2:D:20:PHE:CD2	2:D:36:VAL:HG22	2.49	0.48
3:F:112:ILE:HG22	3:F:136:HIS:CE1	2.48	0.48
1:A:349:ILE:CD1	1:A:424:LEU:HD13	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1404:SER:HB2	1:A:1406:GLU:HG2	1.95	0.48
1:A:2300:ASP:HB2	1:A:3583:ARG:HH22	1.79	0.48
1:A:3063:MET:HE1	1:A:3167:LEU:HD12	1.95	0.48
1:A:4071:TRP:O	1:A:4075:LEU:HD12	2.13	0.48
1:B:1427:VAL:HG13	1:B:1431:PHE:CE2	2.47	0.48
1:B:1428:LEU:HD13	1:B:1491:LEU:HB2	1.94	0.48
1:B:1428:LEU:HB3	1:B:1491:LEU:HB3	1.95	0.48
1:B:1457:ALA:H	1:B:1510:VAL:HG22	1.78	0.48
1:B:3308:SER:HA	1:B:3319:LEU:HD13	1.96	0.48
1:A:284:ILE:HG22	1:A:286:PRO:HD2	1.96	0.48
1:A:948:LEU:HG	1:A:953:CYS:SG	2.54	0.48
1:A:4325:TYR:CZ	1:A:4495:ILE:HA	2.48	0.48
1:B:286:PRO:HB3	1:B:295:VAL:CG2	2.41	0.48
1:B:1194:LYS:HA	1:B:1370:SER:C	2.38	0.48
1:B:1256:ILE:HG12	1:B:1259:GLU:H	1.78	0.48
1:B:1551:ALA:O	1:B:1554:LEU:HD22	2.14	0.48
1:B:1924:LEU:HD23	1:B:1944:ARG:HA	1.95	0.48
1:B:1925:GLN:HB2	1:B:1945:LEU:HD21	1.96	0.48
1:B:4071:TRP:O	1:B:4075:LEU:HD12	2.13	0.48
2:C:52:MET:O	2:C:56:VAL:HG22	2.13	0.48
1:A:738:ALA:HB3	1:A:741:SER:HB3	1.96	0.48
1:A:857:ARG:O	1:A:861:ILE:HG13	2.14	0.48
1:A:1027:SER:N	1:A:1028:PRO:HD2	2.29	0.48
1:A:1859:MET:HE2	1:A:2230:MET:CB	2.44	0.48
1:A:2405:ILE:CD1	1:A:2417:ILE:HD11	2.44	0.48
1:A:3930:CYS:HB3	1:A:3981:LYS:HG3	1.95	0.48
1:A:4307:LYS:CD	1:A:4479:MET:HA	2.44	0.48
1:A:4438:MET:HE3	1:A:4440:ILE:HD11	1.95	0.48
1:B:836:ILE:O	1:B:840:LEU:HG	2.14	0.48
1:B:1082:SER:HA	1:B:1085:TYR:HB3	1.96	0.48
1:B:1237:ASN:HA	1:B:1285:LYS:HD2	1.96	0.48
2:C:65:ASP:H	2:C:68:GLU:HB3	1.78	0.48
1:A:913:GLU:CD	1:A:913:GLU:H	2.20	0.48
1:A:1022:GLN:C	1:A:1024:SER:N	2.71	0.48
1:A:1434:LEU:CD1	1:A:1449:LEU:HD12	2.44	0.48
1:A:1601:SER:N	1:A:2481:SER:HB3	2.29	0.48
1:A:1902:LEU:HD21	1:A:1967:LEU:HD13	1.96	0.48
1:A:2517:ALA:HB3	1:A:2522:GLN:HG2	1.94	0.48
1:A:2985:LEU:HD12	1:A:2988:LEU:HD13	1.95	0.48
1:A:3226:GLN:OE1	1:A:3227:LEU:HD22	2.14	0.48
1:A:3532:CYS:O	1:A:3536:ASN:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:LEU:HD13	1:B:201:PHE:HZ	1.79	0.48
1:B:1278:LEU:HB3	1:B:1281:ALA:CB	2.38	0.48
1:B:1895:ARG:HH22	1:B:2180:VAL:HG11	1.78	0.48
1:B:2220:THR:CG2	1:B:2224:GLU:HA	2.44	0.48
1:B:4021:GLN:HG2	1:B:4025:LYS:HE2	1.96	0.48
1:B:4665:ILE:O	1:B:4669:ILE:HG13	2.14	0.48
1:A:1177:LEU:HG	1:A:1233:TRP:CD2	2.48	0.47
1:A:2040:LEU:HD11	1:A:2085:PRO:HB3	1.95	0.47
1:B:296:ARG:HA	1:B:299:PHE:CD2	2.49	0.47
1:B:1319:LEU:HD22	1:B:1354:LEU:HD21	1.96	0.47
1:B:1921:ILE:HD11	1:B:1969:VAL:HG11	1.96	0.47
1:B:2405:ILE:HG13	1:B:2417:ILE:HD11	1.96	0.47
1:B:3516:LEU:HD11	1:B:3760:LEU:HD21	1.95	0.47
1:A:1693:CYS:HB3	1:A:1716:CYS:HB2	1.95	0.47
1:A:4596:MET:O	1:A:4600:GLN:HG2	2.14	0.47
1:B:303:VAL:HG22	1:B:377:ILE:CG1	2.44	0.47
1:B:347:MET:HE2	1:B:351:HIS:HE1	1.80	0.47
1:B:863:ASP:HB2	1:B:1009:ILE:HG12	1.96	0.47
1:B:908:TYR:CD2	1:B:908:TYR:N	2.81	0.47
1:B:1412:MET:HB3	1:B:1463:ARG:HE	1.78	0.47
1:B:3226:GLN:OE1	1:B:3227:LEU:HD22	2.14	0.47
1:A:92:ILE:HG21	1:A:100:VAL:HG21	1.96	0.47
1:A:273:PHE:HD2	1:A:338:TYR:HB2	1.79	0.47
1:A:786:PHE:HE1	1:A:806:LEU:HD13	1.78	0.47
1:A:864:TYR:HA	1:A:936:LEU:HD21	1.97	0.47
1:A:906:PRO:HG2	1:A:908:TYR:CE2	2.49	0.47
1:A:3142:ARG:O	1:A:3146:LYS:HG3	2.14	0.47
1:A:4119:LEU:HD23	3:E:329:VAL:HG21	1.96	0.47
1:B:1831:ALA:O	1:B:2568:GLU:HG2	2.14	0.47
1:B:2405:ILE:CD1	1:B:2417:ILE:HD11	2.44	0.47
1:B:3440:SER:OG	1:B:3443:GLN:OE1	2.20	0.47
1:B:3747:ASP:O	1:B:3750:TYR:HB3	2.14	0.47
1:A:137:CYS:O	1:A:240:ILE:HG23	2.13	0.47
1:A:799:VAL:HB	1:A:851:VAL:HG11	1.96	0.47
1:A:1023:LEU:HD22	1:A:1038:THR:HG23	1.96	0.47
1:A:1176:TYR:CD1	1:A:1281:ALA:HB3	2.50	0.47
1:A:1570:TYR:C	1:A:1570:TYR:CD2	2.93	0.47
1:A:2025:ILE:CD1	1:A:2075:MET:HE3	2.44	0.47
1:A:2704:VAL:O	1:A:2974:ARG:NH2	2.47	0.47
1:A:3175:THR:HA	1:A:3181:ILE:HG13	1.95	0.47
1:B:1500:VAL:HG13	1:B:1547:ALA:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2181:GLN:HG3	1:B:2188:LEU:CD1	2.44	0.47
1:B:2688:CYS:O	1:B:2689:PRO:C	2.56	0.47
1:B:2982:LEU:HD11	1:B:3027:GLN:HG3	1.96	0.47
1:B:3950:LYS:HG2	1:B:3971:GLU:OE1	2.15	0.47
1:B:4745:ILE:CD1	1:B:4771:LEU:HD13	2.45	0.47
2:C:28:ILE:HG22	2:C:32:GLU:HG2	1.96	0.47
3:F:325:LEU:O	3:F:329:VAL:HG23	2.15	0.47
1:A:29:TRP:CD1	1:A:160:LEU:HD21	2.50	0.47
1:A:984:ARG:HG2	1:A:989:LYS:HB2	1.97	0.47
1:A:1825:ASN:HB3	1:A:2475:LEU:HD23	1.96	0.47
1:A:4413:LYS:CD	1:A:4456:ILE:HD11	2.45	0.47
1:B:239:PHE:O	1:B:243:ASN:ND2	2.48	0.47
1:B:345:THR:O	1:B:349:ILE:HG12	2.14	0.47
1:B:1576:VAL:HA	1:B:1579:LYS:HD2	1.96	0.47
1:B:1909:ARG:HB3	1:B:1911:HIS:CD2	2.49	0.47
1:B:3173:LYS:HA	1:B:3216:PHE:HZ	1.78	0.47
1:B:3418:GLU:HG2	1:B:3461:TYR:CE1	2.49	0.47
1:B:3884:ILE:HD11	1:B:3913:ASN:HD22	1.80	0.47
2:C:49:LEU:CD1	2:C:53:ILE:HD12	2.45	0.47
1:A:3588:ARG:HG3	1:A:3648:TYR:CZ	2.49	0.47
1:A:3772:PRO:HG2	1:B:3918:ALA:HA	1.95	0.47
1:A:4424:VAL:HA	1:A:4459:LEU:HD21	1.96	0.47
1:A:4547:GLU:HG2	1:A:4605:PHE:CE2	2.49	0.47
1:B:694:ASP:CG	1:B:750:HIS:HB3	2.40	0.47
1:B:963:TYR:OH	1:B:1013:LEU:HB3	2.15	0.47
1:B:2368:ILE:CD1	1:B:2387:PHE:CZ	2.93	0.47
1:B:3548:SER:HA	1:B:3551:LYS:HE2	1.95	0.47
1:B:4125:HIS:HA	1:B:4165:LEU:HD12	1.96	0.47
1:A:270:ILE:O	1:A:274:GLN:HG3	2.14	0.47
1:A:327:GLN:NE2	1:A:512:MET:SD	2.88	0.47
1:A:710:LEU:HG	1:A:714:ASN:HD21	1.80	0.47
1:A:860:LEU:HB2	1:A:1005:ILE:HD13	1.96	0.47
1:A:1039:LEU:CD2	1:A:1089:ILE:HD13	2.44	0.47
1:A:1159:LEU:CD2	1:A:1305:MET:HB3	2.45	0.47
1:A:1388:LEU:O	1:A:1394:ARG:NE	2.46	0.47
1:A:1708:TYR:HB3	1:A:2353:ARG:NH2	2.30	0.47
1:A:2356:ILE:HG13	1:A:2379:LEU:HD13	1.95	0.47
1:A:3455:TRP:CZ3	1:A:3458:LEU:HD22	2.50	0.47
1:A:3530:ASP:O	1:A:3531:PRO:C	2.58	0.47
1:A:3884:ILE:HD11	1:A:3913:ASN:HD22	1.79	0.47
1:A:4071:TRP:CE2	1:A:4075:LEU:HD11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4307:LYS:NZ	1:A:4478:VAL:HB	2.30	0.47
1:A:4533:LEU:HB2	1:A:4587:LEU:HB3	1.96	0.47
1:B:49:LEU:O	1:B:51:GLN:N	2.48	0.47
1:B:544:LYS:O	1:B:548:LEU:HG	2.14	0.47
1:B:549:GLN:O	1:B:553:LYS:HG2	2.14	0.47
1:B:755:SER:O	1:B:759:ARG:HG3	2.14	0.47
1:B:1094:PHE:CE1	1:B:1162:THR:HA	2.50	0.47
1:B:1909:ARG:HB3	1:B:1911:HIS:NE2	2.30	0.47
1:B:3034:MET:SD	1:B:3034:MET:N	2.87	0.47
1:B:3098:CYS:SG	1:B:3167:LEU:HD22	2.55	0.47
1:B:3417:LEU:HD13	1:B:3461:TYR:CD2	2.50	0.47
1:B:3515:THR:O	1:B:3519:LEU:HG	2.15	0.47
1:B:4109:LEU:CD1	1:B:4114:LYS:HB2	2.45	0.47
1:B:4267:LEU:O	1:B:4271:LEU:HG	2.15	0.47
1:B:4413:LYS:HD3	1:B:4456:ILE:HD11	1.97	0.47
1:B:4615:GLY:HA2	1:B:4618:ARG:HD2	1.97	0.47
1:A:310:LEU:HD11	1:A:383:GLU:HG2	1.97	0.47
1:A:793:ASN:O	1:A:797:GLY:N	2.48	0.47
1:B:45:GLU:O	1:B:46:MET:C	2.58	0.47
1:B:283:PHE:HB3	1:B:443:ARG:NH2	2.30	0.47
1:B:1126:ALA:HB1	1:B:1262:ILE:HG23	1.96	0.47
1:B:1896:ARG:HA	1:B:1955:LEU:O	2.15	0.47
1:B:3969:GLN:O	1:B:3973:LEU:HG	2.15	0.47
1:B:4525:LEU:HB3	1:B:4532:THR:HG21	1.97	0.47
2:C:66:PHE:HB3	2:C:67:PRO:HD3	1.97	0.47
3:F:65:TYR:HB3	3:F:70:PHE:HE2	1.80	0.47
1:A:191:MET:N	1:A:191:MET:SD	2.88	0.47
1:A:271:ASN:N	1:A:271:ASN:HD22	2.13	0.47
1:A:292:ALA:HB1	1:A:346:CYS:HB2	1.95	0.47
1:A:315:LEU:O	1:A:317:VAL:HG23	2.15	0.47
1:A:1048:SER:O	1:A:1049:SER:C	2.55	0.47
1:A:1515:LEU:HD11	1:A:1556:LEU:HD23	1.97	0.47
1:A:1594:GLU:HG2	1:A:1595:CYS:N	2.30	0.47
1:A:1921:ILE:HD11	1:A:1969:VAL:HG11	1.96	0.47
1:A:3284:ALA:HA	1:A:3331:LYS:HD2	1.97	0.47
1:B:285:MET:N	1:B:286:PRO:HD2	2.30	0.47
1:B:733:GLN:HA	1:B:738:ALA:HB2	1.96	0.47
1:B:1356:THR:HA	1:B:1400:PHE:CE2	2.50	0.47
1:B:3190:TRP:CD1	1:B:3190:TRP:H	2.33	0.47
1:B:3848:GLN:HE21	1:B:3849:PRO:HD2	1.80	0.47
1:B:4071:TRP:CE2	1:B:4075:LEU:HD11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:113:CYS:HB3	3:F:120:ASP:O	2.15	0.47
3:F:120:ASP:HB3	3:F:123:HIS:HB2	1.97	0.47
1:A:506:PRO:HG3	1:A:526:ASP:OD2	2.14	0.47
1:A:530:LEU:O	1:A:534:LEU:HG	2.14	0.47
1:A:1570:TYR:CD2	1:A:1592:ILE:HG21	2.50	0.47
1:A:1875:MET:HG2	1:A:1877:TYR:CZ	2.50	0.47
1:A:2122:LEU:HD23	1:A:2136:ILE:HD11	1.96	0.47
1:A:2223:ASN:HB2	1:A:2225:GLN:HG3	1.97	0.47
1:A:2479:VAL:HG21	1:A:2521:VAL:HG13	1.97	0.47
1:A:3292:LYS:O	1:A:3295:ILE:HG22	2.15	0.47
1:A:4006:PRO:HG2	1:B:3507:HIS:O	2.14	0.47
1:A:4135:THR:H	1:A:4142:ARG:HD3	1.79	0.47
1:B:1431:PHE:O	1:B:1435:PHE:HD2	1.98	0.47
1:B:2202:ILE:HG21	1:B:2232:LEU:HD11	1.97	0.47
1:B:2405:ILE:HD12	1:B:2417:ILE:HD11	1.96	0.47
1:B:2701:LEU:HD13	1:B:3002:VAL:HG13	1.95	0.47
1:A:82:THR:HB	1:A:132:LEU:HD22	1.96	0.46
1:A:485:THR:O	1:A:489:GLN:HG2	2.15	0.46
1:A:1233:TRP:HH2	1:A:1281:ALA:CB	2.27	0.46
1:A:1453:LEU:CB	1:A:1506:VAL:HG13	2.38	0.46
1:A:3766:LYS:HB3	1:A:3795:TYR:CE2	2.50	0.46
1:B:3090:LEU:CD1	1:B:3184:PRO:HB3	2.43	0.46
1:B:4112:ARG:NH2	2:D:128:GLU:HB3	2.30	0.46
2:D:70:LEU:O	2:D:73:MET:HG2	2.15	0.46
1:A:260:CYS:O	1:A:263:LEU:HG	2.15	0.46
1:A:317:VAL:O	1:A:318:LEU:HG	2.15	0.46
1:A:318:LEU:HD13	1:A:329:VAL:HG11	1.97	0.46
1:A:1194:LYS:HA	1:A:1370:SER:C	2.41	0.46
1:A:1295:THR:O	1:A:1299:ILE:HG13	2.15	0.46
1:A:1571:LEU:C	1:A:1573:GLN:H	2.23	0.46
1:A:3417:LEU:HD13	1:A:3461:TYR:CD2	2.49	0.46
1:A:3456:PRO:HA	1:A:3496:ILE:HD11	1.96	0.46
1:B:986:LYS:HG3	1:B:1113:HIS:CE1	2.50	0.46
1:B:1963:LYS:HD3	1:B:1966:TYR:CZ	2.50	0.46
1:B:3905:LEU:HD23	1:B:3932:LEU:HD11	1.96	0.46
1:B:4128:TRP:O	1:B:4129:LEU:C	2.57	0.46
1:B:4710:TRP:O	1:B:4714:LEU:HG	2.15	0.46
1:A:1159:LEU:HD23	1:A:1305:MET:HB3	1.98	0.46
1:A:1431:PHE:O	1:A:1435:PHE:HD2	1.98	0.46
1:A:1525:MET:SD	1:A:1534:PHE:HA	2.56	0.46
1:A:2523:GLN:HA	1:A:2526:LYS:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2700:ALA:O	1:A:2704:VAL:HG13	2.14	0.46
1:A:3301:LEU:HD23	1:A:3301:LEU:HA	1.76	0.46
1:A:3419:SER:HB3	1:A:3425:ARG:CG	2.46	0.46
1:A:3749:VAL:HG21	1:A:3817:ILE:HD12	1.97	0.46
1:A:3887:LEU:HD13	1:A:3905:LEU:HD21	1.97	0.46
1:A:4328:PRO:HB2	1:A:4332:PHE:HE2	1.79	0.46
1:B:341:VAL:HB	1:B:417:SER:CB	2.45	0.46
1:B:470:GLY:O	1:B:474:VAL:HG23	2.15	0.46
1:B:765:GLN:HE22	1:B:817:ILE:HG23	1.80	0.46
1:B:1019:TYR:OH	1:B:1038:THR:HA	2.15	0.46
1:B:2053:PHE:O	1:B:2138:ARG:HD2	2.15	0.46
1:B:3456:PRO:HA	1:B:3496:ILE:HD11	1.96	0.46
1:A:273:PHE:CD2	1:A:338:TYR:HB2	2.51	0.46
1:A:471:VAL:HG21	1:A:641:ARG:HG2	1.98	0.46
1:A:847:GLN:HG3	1:A:976:ALA:HB2	1.98	0.46
1:A:1058:LEU:HD23	1:A:1061:GLN:NE2	2.29	0.46
1:A:3527:LEU:HD21	1:A:3757:ARG:HD3	1.97	0.46
1:A:3536:ASN:HD21	1:A:3815:SER:HB2	1.80	0.46
1:A:4101:TYR:HA	1:A:4104:ARG:HB2	1.97	0.46
1:A:4195:HIS:NE2	2:C:35:THR:HG21	2.30	0.46
1:B:274:GLN:O	1:B:277:VAL:HG22	2.16	0.46
1:B:471:VAL:O	1:B:475:ILE:HG12	2.15	0.46
1:B:1159:LEU:CA	1:B:1298:LEU:HD13	2.35	0.46
1:B:2262:VAL:HG13	1:B:2265:ILE:HD12	1.97	0.46
1:B:2509:ALA:HB2	1:B:2528:LEU:HD23	1.97	0.46
1:B:2985:LEU:HD23	1:B:2988:LEU:HD22	1.97	0.46
1:B:3053:LEU:HD13	1:B:3160:LEU:CD1	2.45	0.46
1:B:3419:SER:HB3	1:B:3425:ARG:CG	2.46	0.46
1:B:3455:TRP:CZ3	1:B:3458:LEU:HD22	2.50	0.46
1:B:4128:TRP:CZ2	3:F:328:LEU:HD21	2.51	0.46
1:B:4750:LYS:O	1:B:4754:VAL:HG23	2.15	0.46
1:A:71:GLU:HB2	1:A:72:PRO:HD3	1.97	0.46
1:A:718:VAL:HG12	1:A:763:ILE:HD12	1.97	0.46
1:A:862:PHE:O	1:A:866:LEU:HG	2.15	0.46
1:A:984:ARG:HH11	1:A:984:ARG:CB	2.24	0.46
1:A:1233:TRP:CE3	1:A:1278:LEU:HD13	2.51	0.46
1:A:1963:LYS:HD3	1:A:1966:TYR:CZ	2.50	0.46
1:A:2194:PRO:HG2	1:A:2251:TYR:OH	2.16	0.46
1:B:89:CYS:SG	1:B:239:PHE:CD2	2.97	0.46
1:B:284:ILE:O	1:B:441:ALA:N	2.48	0.46
1:B:387:MET:O	1:B:390:GLN:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:ILE:O	1:B:662:MET:HB2	2.16	0.46
1:B:3001:GLN:NE2	1:B:3138:PRO:CD	2.78	0.46
1:B:3021:LEU:HD12	1:B:3024:LEU:HD23	1.97	0.46
1:B:4632:GLN:HA	1:B:4681:LEU:HD21	1.98	0.46
3:E:302:SER:OG	3:E:305:GLU:HB3	2.16	0.46
3:F:324:LEU:O	3:F:328:LEU:HG	2.16	0.46
1:A:104:CYS:SG	1:A:136:LEU:HD22	2.56	0.46
1:A:349:ILE:HG23	1:A:429:LEU:HD11	1.96	0.46
1:A:735:LEU:HD13	1:A:753:SER:HA	1.96	0.46
1:A:847:GLN:HG3	1:A:976:ALA:CB	2.46	0.46
1:A:1203:ALA:O	1:A:1204:ILE:C	2.57	0.46
1:A:1428:LEU:CD1	1:A:1488:ASN:HA	2.46	0.46
1:B:1561:VAL:CG2	1:B:1810:LEU:HD22	2.43	0.46
1:B:2264:SER:HB3	1:B:2652:HIS:CE1	2.51	0.46
1:B:2307:ASP:HB2	1:B:2336:PHE:HB2	1.97	0.46
1:B:2368:ILE:CG2	1:B:2377:LEU:HD11	2.43	0.46
2:D:6:THR:HG23	2:D:9:GLN:H	1.79	0.46
3:E:28:TYR:CE2	3:E:122:ASN:HB3	2.51	0.46
1:A:280:ASN:HD22	1:A:523:ARG:HH11	1.64	0.46
1:A:283:PHE:HA	1:A:442:LEU:O	2.16	0.46
1:A:963:TYR:OH	1:A:1013:LEU:HB3	2.16	0.46
1:A:3910:PHE:HB2	1:A:3929:MET:HE1	1.97	0.46
1:A:4001:VAL:C	1:A:4003:ILE:H	2.22	0.46
1:A:4232:LEU:HD13	1:B:3750:TYR:CB	2.36	0.46
1:A:4325:TYR:HB3	1:A:4501:GLY:HA2	1.98	0.46
1:B:1105:ASP:HB3	1:B:1108:THR:HB	1.98	0.46
1:B:1561:VAL:HG13	1:B:1810:LEU:HD22	1.97	0.46
1:B:2117:HIS:CD2	1:B:2642:LEU:HD22	2.51	0.46
1:B:2677:THR:HA	1:B:2680:LYS:HD2	1.98	0.46
1:B:4206:LEU:HB2	1:B:4207:PRO:HD3	1.98	0.46
1:B:4745:ILE:HB	1:B:4746:PRO:HD3	1.97	0.46
1:A:664:ASN:HD21	1:B:202:ASN:HB3	1.81	0.46
1:A:917:ASN:HA	1:A:920:LYS:HD2	1.98	0.46
1:A:1101:PHE:O	1:A:1104:ILE:HB	2.14	0.46
1:A:1678:TRP:HB3	1:A:1714:PHE:CD1	2.51	0.46
1:A:3313:GLU:O	1:A:3317:PRO:HD3	2.15	0.46
1:A:3880:THR:O	1:A:3884:ILE:HG12	2.16	0.46
1:A:4281:THR:HG22	1:A:4283:LEU:H	1.81	0.46
1:A:4339:ILE:HD13	1:A:4476:ALA:HB2	1.97	0.46
1:B:62:GLU:O	1:B:66:HIS:HB3	2.15	0.46
1:B:327:GLN:O	1:B:331:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1596:THR:HG22	1:B:2478:LEU:HD13	1.98	0.46
1:B:2291:PHE:CZ	1:B:2350:THR:HB	2.51	0.46
1:B:4101:TYR:HA	1:B:4104:ARG:HB2	1.97	0.46
2:D:51:ASP:HA	2:D:54:ASN:HD22	1.81	0.46
2:D:118:THR:O	2:D:119:ASP:C	2.58	0.46
1:A:110:PHE:CZ	1:A:114:ARG:HD2	2.51	0.46
1:A:506:PRO:HB2	1:A:523:ARG:NH2	2.29	0.46
1:A:1039:LEU:HD22	1:A:1130:LYS:HE2	1.98	0.46
1:A:1515:LEU:HD23	1:A:1555:GLN:HG3	1.98	0.46
1:B:269:TYR:CD1	1:B:339:ALA:HA	2.50	0.46
1:B:484:LEU:O	1:B:488:PHE:HD1	1.99	0.46
1:B:668:ASN:HA	1:B:671:ARG:HB2	1.98	0.46
1:B:1377:LEU:HD12	1:B:1377:LEU:H	1.81	0.46
1:B:2687:LEU:HD13	1:B:2991:VAL:HG11	1.98	0.46
1:B:3046:SER:HB2	1:B:3049:ASN:HD21	1.80	0.46
1:B:3108:TYR:O	1:B:3112:GLN:HG2	2.15	0.46
1:B:4730:ALA:O	1:B:4731:ILE:C	2.59	0.46
2:C:26:GLY:O	2:C:61:ASN:HA	2.16	0.46
1:A:200:VAL:CB	1:B:715:HIS:ND1	2.77	0.46
1:A:511:ILE:HG13	1:A:512:MET:N	2.31	0.46
1:A:1015:PRO:HG3	1:A:1041:TRP:CE2	2.50	0.46
1:A:1132:GLN:HE22	1:A:1293:ARG:HH21	1.62	0.46
1:A:1380:CYS:O	1:A:1380:CYS:SG	2.74	0.46
1:A:1568:LYS:HG2	1:A:1817:PHE:HZ	1.80	0.46
1:A:1877:TYR:HB2	1:A:1886:ARG:HG3	1.98	0.46
1:A:2385:PHE:HB3	1:A:2387:PHE:CE2	2.50	0.46
1:A:2405:ILE:HG13	1:A:2417:ILE:HD11	1.97	0.46
1:B:1345:GLU:CD	1:B:1345:GLU:H	2.24	0.46
1:B:3099:LEU:HB2	1:B:3190:TRP:CZ3	2.51	0.46
1:B:3909:LEU:HD22	1:B:3925:VAL:HG13	1.98	0.46
1:B:4621:PRO:HB3	1:B:4668:GLY:CA	2.44	0.46
1:A:337:LEU:HD11	1:A:414:LEU:HD21	1.98	0.45
1:A:2202:ILE:HG21	1:A:2232:LEU:HD11	1.97	0.45
1:A:3234:ASP:O	1:A:3238:ARG:HG2	2.16	0.45
1:A:3533:LEU:HD12	1:A:3819:GLN:HG2	1.98	0.45
1:B:313:LEU:CD1	1:B:384:ILE:HG23	2.45	0.45
1:B:747:LEU:HB3	1:B:806:LEU:N	2.31	0.45
1:B:858:LEU:HA	1:B:858:LEU:HD23	1.80	0.45
1:B:2356:ILE:HG13	1:B:2379:LEU:HD13	1.98	0.45
2:C:13:PHE:HB3	2:C:69:PHE:CE2	2.47	0.45
2:D:93:PHE:CZ	2:D:101:ILE:HA	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:GLN:O	1:A:193:PHE:HB3	2.16	0.45
1:A:285:MET:N	1:A:286:PRO:CD	2.79	0.45
1:A:1081:SER:HA	1:A:1084:LYS:HD2	1.97	0.45
1:A:1233:TRP:CH2	1:A:1281:ALA:CB	2.99	0.45
1:A:4750:LYS:O	1:A:4754:VAL:HG23	2.17	0.45
1:B:761:LEU:HB3	1:B:779:CYS:SG	2.56	0.45
1:B:1093:TYR:O	1:B:1096:ARG:HG2	2.15	0.45
1:B:1489:ARG:O	1:B:1493:GLN:HG3	2.16	0.45
1:B:3005:MET:HA	1:B:3008:THR:HG23	1.98	0.45
1:A:135:GLY:CA	1:A:140:CYS:O	2.63	0.45
1:A:338:TYR:HA	1:A:341:VAL:HG22	1.97	0.45
1:A:477:ALA:O	1:A:481:ILE:HG12	2.15	0.45
1:A:1023:LEU:CD2	1:A:1038:THR:HG23	2.46	0.45
1:A:1032:GLU:O	1:A:1033:CYS:SG	2.71	0.45
1:A:1087:VAL:O	1:A:1091:GLU:HG3	2.17	0.45
1:A:2101:ASP:HB3	1:A:2106:VAL:HG22	1.98	0.45
1:A:2371:PHE:CZ	1:A:2397:ALA:HB2	2.51	0.45
1:A:4031:SER:N	3:E:310:GLU:OE2	2.50	0.45
1:B:2295:ASN:CB	1:B:2423:TYR:HB3	2.45	0.45
1:B:2626:VAL:HG21	1:B:2681:ILE:HG21	1.98	0.45
1:B:4003:ILE:HG22	1:B:4005:THR:H	1.81	0.45
2:D:20:PHE:HB3	2:D:32:GLU:HB3	1.99	0.45
2:D:39:SER:C	2:D:41:GLY:H	2.25	0.45
2:D:121:GLU:O	2:D:125:MET:HG2	2.16	0.45
1:A:543:ARG:O	1:A:547:VAL:HG23	2.16	0.45
1:A:1959:GLY:O	1:A:1961:PRO:HD3	2.16	0.45
1:A:2092:LEU:HD23	1:A:2094:ILE:HD11	1.97	0.45
1:A:4135:THR:O	1:A:4142:ARG:NH1	2.46	0.45
1:B:827:ARG:NE	1:B:955:VAL:HG22	2.31	0.45
1:B:1240:GLU:CD	1:B:1240:GLU:H	2.24	0.45
1:B:1408:VAL:O	1:B:1412:MET:HG2	2.17	0.45
1:B:1593:LEU:HB3	1:B:2474:VAL:HG11	1.99	0.45
1:B:1902:LEU:HD21	1:B:1967:LEU:HD13	1.98	0.45
1:B:2255:PRO:C	1:B:2257:LEU:N	2.74	0.45
1:B:2636:LYS:HD2	1:B:2653:ILE:HD11	1.98	0.45
1:B:2982:LEU:HD13	1:B:2982:LEU:C	2.41	0.45
3:F:302:SER:OG	3:F:305:GLU:HB3	2.16	0.45
1:A:333:SER:HB2	1:A:388:ILE:CG1	2.46	0.45
1:A:485:THR:HG22	1:A:657:PHE:HD1	1.81	0.45
1:A:1019:TYR:CE2	1:A:1023:LEU:HD11	2.52	0.45
1:A:1039:LEU:HD21	1:A:1089:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1105:ASP:N	1:A:1110:LEU:HD21	2.18	0.45
1:A:3972:MET:HE3	1:A:3972:MET:HB3	1.73	0.45
1:B:34:ARG:HB3	1:B:35:PRO:HD3	1.99	0.45
1:B:255:LYS:HG2	1:B:258:ARG:HH21	1.80	0.45
1:B:1541:MET:HG2	1:B:1556:LEU:HD11	1.99	0.45
1:B:3410:GLN:HG3	1:B:3850:THR:CB	2.33	0.45
1:B:3910:PHE:HB2	1:B:3929:MET:HE1	1.97	0.45
1:A:144:ASP:O	1:A:148:ILE:HG13	2.17	0.45
1:A:1388:LEU:O	1:A:1394:ARG:HB2	2.17	0.45
1:A:1509:GLY:O	1:A:1513:VAL:HG23	2.17	0.45
1:A:3038:ASP:O	1:A:3042:LYS:HG2	2.17	0.45
1:A:3251:LEU:HD12	1:A:3303:PHE:CD2	2.51	0.45
1:A:3626:GLU:OE1	1:A:3628:LYS:HE3	2.17	0.45
1:A:4745:ILE:HB	1:A:4746:PRO:HD3	1.99	0.45
1:B:908:TYR:O	1:B:908:TYR:CG	2.70	0.45
1:B:985:ARG:HH11	1:B:1280:LEU:HD11	1.81	0.45
1:B:1110:LEU:H	1:B:1175:ALA:CB	2.29	0.45
1:B:1174:ARG:O	1:B:1178:LEU:HG	2.16	0.45
1:B:2698:LYS:HG3	1:B:3002:VAL:HG23	1.98	0.45
1:B:4053:HIS:HB2	1:B:4071:TRP:HD1	1.81	0.45
1:B:4711:LYS:HA	1:B:4714:LEU:HD12	1.99	0.45
1:A:44:PHE:CE2	1:A:48:GLU:HB2	2.51	0.45
1:A:136:LEU:O	1:A:243:ASN:ND2	2.49	0.45
1:A:416:ASN:HD22	1:A:416:ASN:N	2.15	0.45
1:A:680:GLU:HB3	1:A:730:THR:HG21	1.99	0.45
1:A:974:LEU:HD23	1:A:1006:LEU:HD23	1.99	0.45
1:A:1163:LEU:HA	1:A:1166:ILE:HD12	1.98	0.45
1:A:2122:LEU:HB2	1:A:2136:ILE:HD12	1.99	0.45
1:A:4170:LEU:O	1:A:4173:LEU:HB3	2.17	0.45
1:A:4313:CYS:HB3	1:A:4331:ILE:CD1	2.47	0.45
1:B:478:ASN:OD1	1:B:650:LEU:HD13	2.17	0.45
1:B:2122:LEU:HD23	1:B:2136:ILE:HD11	1.96	0.45
1:B:2622:ILE:HD11	1:B:2667:TYR:CG	2.52	0.45
1:B:2702:ILE:CD1	1:B:3001:GLN:NE2	2.79	0.45
1:B:3056:MET:HA	1:B:3059:LEU:HD12	1.99	0.45
1:B:3714:MET:HE3	1:B:3714:MET:HB3	1.78	0.45
1:A:279:ALA:O	1:A:280:ASN:C	2.59	0.45
1:A:284:ILE:O	1:A:442:LEU:N	2.50	0.45
1:A:1456:LEU:HD22	1:A:1510:VAL:HG13	1.98	0.45
1:A:3337:ALA:HB3	1:A:3427:GLN:HE21	1.81	0.45
1:A:3909:LEU:HD22	1:A:3925:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4098:THR:HB	2:C:109:VAL:HG13	1.99	0.45
1:A:4310:MET:HG2	1:A:4335:LEU:CD1	2.47	0.45
1:A:4419:LEU:HD13	1:A:4459:LEU:HG	1.97	0.45
1:A:4710:TRP:O	1:A:4714:LEU:HG	2.16	0.45
1:B:678:LEU:HB3	1:B:727:LEU:CD2	2.46	0.45
1:B:686:LEU:HA	1:B:686:LEU:HD23	1.73	0.45
1:B:1077:THR:HA	1:B:1082:SER:HB2	1.98	0.45
1:B:1407:LEU:H	1:B:1407:LEU:CD1	2.25	0.45
1:B:3301:LEU:HD23	1:B:3301:LEU:HA	1.76	0.45
1:B:3461:TYR:O	1:B:3534:VAL:HG11	2.17	0.45
2:D:7:GLU:HA	2:D:10:ILE:HG22	1.99	0.45
1:A:55:SER:O	1:A:59:SER:N	2.36	0.45
1:A:1090:VAL:HG11	1:A:1131:VAL:HG22	1.99	0.45
1:A:1468:LEU:HA	1:A:1471:MET:HE2	1.99	0.45
1:A:1515:LEU:CD1	1:A:1541:MET:HG3	2.47	0.45
1:A:1570:TYR:CG	1:A:1592:ILE:HG21	2.52	0.45
1:A:1807:PHE:O	1:A:1810:LEU:HB3	2.17	0.45
1:A:1924:LEU:HD23	1:A:1944:ARG:HA	1.99	0.45
1:A:2390:THR:O	1:A:2391:ARG:C	2.59	0.45
1:A:2480:VAL:HA	1:A:2524:GLN:CG	2.46	0.45
1:A:2978:LEU:HB2	1:A:3006:LEU:HD13	1.99	0.45
1:A:3194:LEU:HD13	1:A:3214:LEU:HD21	1.97	0.45
1:A:3478:LYS:HD2	1:A:3478:LYS:HA	1.83	0.45
1:B:1204:ILE:CG2	1:B:1357:GLY:HA3	2.43	0.45
1:B:1831:ALA:HB2	1:B:2260:SER:HB3	1.97	0.45
1:B:3887:LEU:HD13	1:B:3905:LEU:HD21	1.98	0.45
1:B:4052:ILE:HG23	3:F:322:GLU:HB3	1.99	0.45
3:E:317:SER:O	3:E:321:GLN:HG3	2.17	0.45
1:A:31:VAL:O	1:A:34:ARG:HB3	2.17	0.45
1:A:488:PHE:HE2	1:A:670:ILE:HD12	1.82	0.45
1:A:1557:HIS:HB2	1:A:1799:LEU:HD23	1.97	0.45
1:A:1610:LEU:HD21	1:A:1799:LEU:HB2	1.99	0.45
1:A:1807:PHE:O	1:A:1811:VAL:HG23	2.17	0.45
1:A:1950:VAL:HG11	1:A:1969:VAL:HG11	1.98	0.45
1:A:2375:MET:HG2	1:A:2387:PHE:CE1	2.32	0.45
1:A:2540:HIS:HB3	1:A:2584:ARG:NE	2.32	0.45
1:A:3148:HIS:CE1	1:A:3152:VAL:H	2.34	0.45
1:A:3229:ASP:HB2	1:A:3289:ASN:HD22	1.82	0.45
1:A:3905:LEU:HD23	1:A:3932:LEU:HD11	1.99	0.45
1:A:4026:PRO:O	1:A:4027:PRO:C	2.59	0.45
1:A:4595:VAL:CG2	1:A:4630:LYS:HA	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:PHE:HB3	1:B:443:ARG:CZ	2.47	0.45
1:B:1047:ILE:O	1:B:1051:VAL:HG23	2.17	0.45
1:B:1498:TYR:O	1:B:1504:SER:HB2	2.17	0.45
1:B:1959:GLY:O	1:B:1961:PRO:HD3	2.16	0.45
1:B:2978:LEU:HD23	1:B:3010:LEU:HD11	1.98	0.45
1:B:3012:GLY:H	1:B:3077:SER:HB2	1.80	0.45
1:B:3226:GLN:HA	1:B:3289:ASN:HD22	1.81	0.45
1:B:3756:HIS:HB2	1:B:3807:CYS:SG	2.57	0.45
1:B:4050:ASN:OD1	2:D:38:ARG:NH2	2.50	0.45
1:A:97:LEU:HD23	1:A:98:GLN:N	2.32	0.44
1:A:3033:GLY:O	1:A:3034:MET:C	2.61	0.44
1:A:3642:ILE:HD13	1:A:3713:PHE:CE1	2.52	0.44
1:A:4570:LEU:HD13	1:A:4622:TYR:CB	2.47	0.44
1:A:4639:LYS:HB3	1:A:4640:PRO:HD3	1.99	0.44
1:B:414:LEU:O	1:B:418:LEU:HG	2.17	0.44
1:B:722:LEU:H	1:B:722:LEU:HD12	1.82	0.44
1:B:1564:LEU:HD13	1:B:1596:THR:HG23	1.98	0.44
1:B:1728:ALA:O	1:B:1729:LEU:C	2.60	0.44
1:B:2695:PHE:CZ	1:B:2699:GLN:NE2	2.84	0.44
1:B:3234:ASP:O	1:B:3238:ARG:HG2	2.16	0.44
1:A:94:ARG:H	1:A:94:ARG:HD2	1.81	0.44
1:A:252:GLY:O	1:A:256:LEU:HG	2.18	0.44
1:A:471:VAL:CG2	1:A:641:ARG:H	2.26	0.44
1:A:738:ALA:O	1:A:785:ARG:NH1	2.50	0.44
1:A:1346:PHE:O	1:A:1350:VAL:HG23	2.17	0.44
1:A:1903:SER:HB2	1:A:1910:GLN:HA	1.99	0.44
1:A:2622:ILE:HD11	1:A:2667:TYR:CB	2.47	0.44
1:A:4120:ASP:OD1	1:A:4120:ASP:N	2.46	0.44
1:A:4332:PHE:HB2	1:A:4507:VAL:HG12	2.00	0.44
1:B:418:LEU:HD11	1:B:477:ALA:HA	1.98	0.44
1:B:1174:ARG:HG2	1:B:1320:GLU:OE2	2.16	0.44
1:B:2122:LEU:HB2	1:B:2136:ILE:HD12	1.99	0.44
1:B:3058:LEU:HD12	1:B:3058:LEU:HA	1.82	0.44
1:B:3099:LEU:HD11	1:B:3193:PHE:CD1	2.51	0.44
1:B:4170:LEU:O	1:B:4173:LEU:HB3	2.17	0.44
1:B:4313:CYS:HB3	1:B:4331:ILE:HG23	1.99	0.44
3:F:24:CYS:CA	3:F:52:MET:SD	3.05	0.44
1:A:202:ASN:CG	1:A:204:ARG:HG3	2.43	0.44
1:A:288:THR:HG22	1:A:290:ALA:H	1.81	0.44
1:A:1180:ASN:O	1:A:1181:PHE:C	2.58	0.44
1:B:115:LEU:HD13	1:B:130:ILE:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:SER:OG	1:B:385:TYR:HA	2.18	0.44
1:B:674:LEU:O	1:B:678:LEU:HG	2.18	0.44
1:B:813:MET:HB2	1:B:813:MET:HE3	1.68	0.44
1:B:1295:THR:HG22	1:B:1299:ILE:HD13	2.00	0.44
1:B:3058:LEU:HG	1:B:3062:PHE:CZ	2.52	0.44
1:B:3642:ILE:HD13	1:B:3713:PHE:CE1	2.52	0.44
1:B:3880:THR:O	1:B:3884:ILE:HG12	2.16	0.44
1:B:4705:LEU:CD1	1:B:4753:GLN:HB2	2.47	0.44
3:E:24:CYS:CA	3:E:52:MET:SD	3.06	0.44
1:A:264:PRO:HG2	1:A:305:ASP:OD2	2.18	0.44
1:A:1381:LEU:HB3	1:A:1426:ARG:NH2	2.32	0.44
1:A:3513:TYR:CD1	1:A:3525:TYR:HD1	2.35	0.44
1:A:3525:TYR:CE2	1:A:3874:GLY:HA2	2.53	0.44
1:A:4746:PRO:O	1:A:4750:LYS:HG3	2.16	0.44
1:B:1664:CYS:HB3	1:B:1667:THR:HG23	1.99	0.44
1:B:2300:ASP:OD2	1:B:2344:ASN:ND2	2.50	0.44
1:B:4093:ARG:NH2	2:D:51:ASP:OD2	2.51	0.44
2:D:60:GLY:H	2:D:63:THR:HB	1.82	0.44
2:D:93:PHE:CE2	2:D:101:ILE:HG12	2.52	0.44
1:A:59:SER:O	1:A:63:ILE:HG13	2.17	0.44
1:A:844:MET:HB3	1:A:848:MET:HE3	1.98	0.44
1:A:1534:PHE:N	1:A:1535:PRO:HD2	2.32	0.44
1:A:1899:MET:HE2	1:A:2233:LEU:HB3	2.00	0.44
1:A:2349:MET:HB2	1:A:2397:ALA:O	2.18	0.44
1:A:3004:LEU:HD22	1:A:3061:VAL:HG11	2.00	0.44
1:A:3273:MET:HG3	1:A:3633:LEU:CD2	2.48	0.44
1:B:382:LEU:HD23	1:B:382:LEU:HA	1.82	0.44
1:B:443:ARG:HB2	1:B:446:ASP:CB	2.47	0.44
1:B:909:HIS:ND1	1:B:934:CYS:O	2.49	0.44
1:B:1859:MET:SD	1:B:2244:ALA:HA	2.58	0.44
1:B:1891:ALA:HB3	1:B:1893:VAL:HG23	1.98	0.44
1:B:1976:HIS:ND1	1:B:1989:HIS:NE2	2.57	0.44
1:B:2129:GLY:HA3	1:B:2161:SER:O	2.17	0.44
1:B:3004:LEU:O	1:B:3008:THR:HG23	2.18	0.44
2:C:13:PHE:CD1	2:C:40:LEU:HD13	2.52	0.44
1:A:284:ILE:HG22	1:A:286:PRO:CD	2.47	0.44
1:A:718:VAL:HG13	1:A:760:LEU:HD23	1.98	0.44
1:A:911:PHE:HD2	1:A:1001:TYR:CD1	2.35	0.44
1:A:1434:LEU:HD11	1:A:1449:LEU:HD12	2.00	0.44
1:A:2309:LEU:O	3:E:77:SER:OG	2.34	0.44
1:A:2522:GLN:O	1:A:2526:LYS:HG3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2692:ALA:HA	1:A:2695:PHE:CD1	2.49	0.44
1:A:3291:GLN:HA	1:A:3395:LEU:HD11	1.99	0.44
1:A:3412:LEU:O	1:A:3416:LEU:HB2	2.18	0.44
1:A:4047:PRO:HA	1:A:4075:LEU:HD23	1.99	0.44
1:B:1414:THR:HG21	1:B:1424:CYS:HA	1.99	0.44
1:B:2048:ASP:OD1	1:B:2049:VAL:N	2.51	0.44
1:B:2215:VAL:HG23	1:B:2231:ILE:HB	1.99	0.44
1:B:2264:SER:HB3	1:B:2652:HIS:NE2	2.32	0.44
1:B:2540:HIS:HB3	1:B:2584:ARG:CZ	2.48	0.44
1:B:2985:LEU:O	1:B:2988:LEU:HB2	2.17	0.44
1:B:3273:MET:HG3	1:B:3633:LEU:CD2	2.48	0.44
1:B:4234:GLN:HE22	1:B:4279:GLN:HB3	1.83	0.44
1:A:405:ASN:ND2	1:A:513:ALA:O	2.51	0.44
1:A:1489:ARG:O	1:A:1493:GLN:HG3	2.18	0.44
1:A:1680:HIS:O	1:A:1706:ILE:HA	2.17	0.44
1:A:1867:GLU:HG2	1:A:2236:ASP:OD2	2.18	0.44
1:A:3087:ALA:HB2	1:A:3181:ILE:HG21	2.00	0.44
1:A:3963:ASP:O	1:A:3964:LEU:C	2.60	0.44
1:B:115:LEU:HD12	1:B:133:ILE:HD12	1.99	0.44
1:B:302:LEU:O	1:B:303:VAL:C	2.61	0.44
1:B:1191:SER:O	1:B:1192:LYS:C	2.61	0.44
1:B:1952:PHE:CZ	1:B:1969:VAL:HG12	2.53	0.44
1:B:2060:ILE:HG12	1:B:2074:LEU:HD12	2.00	0.44
1:B:3251:LEU:HD12	1:B:3303:PHE:CD2	2.52	0.44
1:B:3626:GLU:OE1	1:B:3628:LYS:HE3	2.17	0.44
1:B:3998:LEU:O	1:B:4001:VAL:HG12	2.18	0.44
2:D:86:ILE:CD1	2:D:146:MET:HG2	2.48	0.44
1:A:867:HIS:CD2	1:A:947:ARG:HD2	2.52	0.44
1:A:1098:ILE:O	1:A:1101:PHE:HB2	2.18	0.44
1:A:1378:GLU:HG2	1:A:1426:ARG:HG3	2.00	0.44
1:A:2973:VAL:O	1:A:2976:MET:HG3	2.17	0.44
1:A:3889:ALA:HB2	3:E:293:LEU:HD13	2.00	0.44
1:B:185:ARG:HA	1:B:185:ARG:HE	1.83	0.44
1:B:648:LEU:HD23	1:B:648:LEU:HA	1.69	0.44
1:B:1429:LYS:O	1:B:1432:THR:N	2.51	0.44
1:B:1480:ASP:HB3	1:B:1483:ASP:HB2	2.00	0.44
1:B:2151:ILE:HD12	1:B:2162:PRO:HD2	1.99	0.44
1:B:3087:ALA:CA	1:B:3181:ILE:HD13	2.47	0.44
1:B:3269:LEU:HB3	1:B:3633:LEU:HD12	1.92	0.44
1:B:3305:LEU:HB2	1:B:3323:LEU:HD21	1.99	0.44
1:B:3571:ILE:HG12	1:B:3717:ALA:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4606:VAL:HG13	1:B:4612:VAL:HG12	1.99	0.44
2:D:147:THR:O	2:D:148:ALA:C	2.60	0.44
3:E:301:MET:HE1	3:E:305:GLU:HG2	2.00	0.44
1:A:1039:LEU:HD22	1:A:1130:LYS:CD	2.48	0.44
1:A:1048:SER:O	1:A:1051:VAL:HB	2.18	0.44
1:A:1130:LYS:O	1:A:1131:VAL:C	2.59	0.44
1:A:1299:ILE:HG22	1:A:1336:ARG:HH11	1.83	0.44
1:A:1474:SER:CB	1:A:1485:ILE:HG21	2.48	0.44
1:A:1571:LEU:O	1:A:1573:GLN:N	2.51	0.44
1:A:4115:ARG:NH2	2:C:125:MET:SD	2.91	0.44
1:B:155:MET:C	1:B:157:SER:N	2.74	0.44
1:B:1077:THR:C	1:B:1078:THR:HG1	2.26	0.44
1:B:1355:ILE:HD13	1:B:1397:MET:CG	2.47	0.44
1:B:1468:LEU:O	1:B:1472:THR:HG23	2.17	0.44
1:B:2973:VAL:O	1:B:2977:LEU:HB2	2.18	0.44
1:B:3899:ILE:O	1:B:3903:GLN:HG2	2.18	0.44
1:B:3922:ARG:NH1	1:B:3970:TYR:OH	2.50	0.44
2:C:145:MET:HE3	2:C:145:MET:HB3	1.90	0.44
3:F:301:MET:HE1	3:F:305:GLU:HG2	2.00	0.44
1:A:34:ARG:HB3	1:A:35:PRO:HD3	2.00	0.43
1:A:261:LEU:HD23	1:A:332:LEU:HD13	1.99	0.43
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.86	0.43
1:A:1197:GLY:C	1:A:1372:LEU:HD21	2.43	0.43
1:A:2072:THR:O	1:A:2090:ASN:HB2	2.18	0.43
1:A:2194:PRO:HD3	1:A:2251:TYR:CE1	2.52	0.43
1:A:4101:TYR:CD2	2:C:89:ALA:HB2	2.53	0.43
1:A:4159:LYS:HE2	1:A:4159:LYS:HB3	1.84	0.43
1:B:1000:GLN:HG3	1:B:1270:LEU:HD13	2.00	0.43
1:B:1815:LEU:HD12	1:B:2508:LEU:HD21	1.99	0.43
1:B:1854:MET:HE2	1:B:2152:LYS:N	2.32	0.43
1:B:4127:ASN:ND2	3:F:328:LEU:HD22	2.31	0.43
2:D:37:MET:HG2	2:D:69:PHE:HE1	1.83	0.43
2:D:101:ILE:N	2:D:137:VAL:O	2.48	0.43
1:A:539:SER:O	1:A:543:ARG:HD3	2.18	0.43
1:A:853:LEU:O	1:A:857:ARG:HG2	2.18	0.43
1:A:3083:SER:HB3	1:A:3178:ASN:HD22	1.84	0.43
1:A:3826:LYS:HE2	1:A:3826:LYS:HB3	1.84	0.43
1:A:4419:LEU:HD22	1:A:4459:LEU:HD12	1.99	0.43
1:B:1534:PHE:N	1:B:1535:PRO:HD2	2.33	0.43
1:B:3412:LEU:O	1:B:3416:LEU:HB2	2.18	0.43
1:B:3490:SER:O	1:B:3494:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3746:ALA:HA	1:B:3749:VAL:HG22	1.99	0.43
1:B:3764:LEU:HD23	1:B:3764:LEU:HA	1.83	0.43
1:B:3972:MET:HG3	1:B:4011:ASN:O	2.18	0.43
1:B:4125:HIS:HA	1:B:4165:LEU:CD1	2.48	0.43
1:A:98:GLN:HG3	1:A:201:PHE:CZ	2.54	0.43
1:A:765:GLN:NE2	1:A:817:ILE:HG23	2.33	0.43
1:A:1811:VAL:HA	1:A:1814:MET:HE2	2.00	0.43
1:A:3308:SER:HA	1:A:3319:LEU:HD13	2.00	0.43
1:A:3317:PRO:HG3	1:A:3424:VAL:CG2	2.48	0.43
1:A:4146:CYS:HA	1:A:4186:LEU:HD22	2.00	0.43
1:A:4310:MET:HE3	1:A:4335:LEU:CD2	2.49	0.43
1:A:4360:GLU:CD	1:A:4366:ARG:HH21	2.26	0.43
1:B:280:ASN:HB3	1:B:283:PHE:HE1	1.84	0.43
1:B:3068:SER:HA	1:B:3075:CYS:HB2	2.00	0.43
1:B:4413:LYS:CD	1:B:4456:ILE:HD11	2.48	0.43
3:E:9:CYS:O	3:E:13:LEU:HA	2.18	0.43
3:E:23:LYS:HD3	3:E:114:ALA:HB1	2.00	0.43
1:A:110:PHE:O	1:A:114:ARG:HG2	2.18	0.43
1:A:197:LEU:HD23	1:A:197:LEU:HA	1.84	0.43
1:A:1178:LEU:HD21	1:A:1202:LEU:HD21	2.00	0.43
1:A:1192:LYS:HA	1:A:1195:LEU:HB2	2.00	0.43
1:A:2698:LYS:NZ	1:A:2998:PRO:O	2.52	0.43
1:A:3505:THR:OG1	1:A:3916:ARG:NH1	2.37	0.43
1:A:3595:ASN:HD21	1:A:3605:LEU:HD13	1.83	0.43
1:A:4278:VAL:O	1:B:3825:ARG:HD3	2.18	0.43
1:B:124:VAL:HG21	1:B:129:LEU:HD21	1.99	0.43
1:B:855:LEU:HD23	1:B:1002:TYR:HE2	1.82	0.43
1:B:1177:LEU:HD21	1:B:1233:TRP:HB2	1.99	0.43
1:B:1209:CYS:SG	1:B:1210:LYS:N	2.91	0.43
1:B:1244:ILE:HG12	1:B:1249:ASN:HB3	2.01	0.43
1:B:2675:ILE:C	1:B:2677:THR:N	2.75	0.43
1:B:2997:ILE:HB	1:B:2998:PRO:HD3	2.00	0.43
1:B:3301:LEU:HD21	1:B:3326:ALA:HB3	1.99	0.43
1:B:3889:ALA:HB2	3:F:293:LEU:HD13	1.99	0.43
1:B:4746:PRO:O	1:B:4750:LYS:HG3	2.18	0.43
2:D:130:ASP:OD2	2:D:135:GLY:N	2.48	0.43
3:E:21:ARG:HB3	3:E:55:ILE:HB	2.01	0.43
1:A:34:ARG:O	1:A:35:PRO:C	2.61	0.43
1:A:516:THR:HG22	1:A:518:ILE:H	1.84	0.43
1:A:864:TYR:HA	1:A:936:LEU:CD2	2.48	0.43
1:A:1021:ASN:OD1	1:A:1071:LEU:HD21	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2578:ARG:HD2	1:A:2659:ALA:CB	2.48	0.43
1:A:3173:LYS:HB3	1:A:3173:LYS:HE2	1.76	0.43
1:A:3773:GLU:HB3	1:A:3794:ARG:HE	1.83	0.43
1:A:3899:ILE:O	1:A:3903:GLN:HG2	2.19	0.43
1:A:3986:TRP:CZ2	3:E:316:ARG:HG2	2.54	0.43
1:A:4007:VAL:HG22	1:B:3511:ASN:HB2	2.00	0.43
1:A:4749:HIS:O	1:A:4753:GLN:HG3	2.18	0.43
1:B:428:ALA:O	1:B:432:LYS:HG2	2.18	0.43
1:B:796:GLN:HB2	1:B:798:VAL:HG23	2.00	0.43
1:B:1289:LEU:HD11	1:B:1325:SER:HB2	2.00	0.43
1:B:2038:TYR:C	1:B:2038:TYR:CD2	2.96	0.43
1:B:2984:THR:O	1:B:2987:GLN:N	2.51	0.43
1:B:3033:GLY:C	1:B:3035:ASP:N	2.76	0.43
1:B:3727:GLU:H	1:B:3731:ASP:HB2	1.82	0.43
1:B:4146:CYS:HA	1:B:4186:LEU:HD22	2.01	0.43
1:B:4159:LYS:HZ3	1:B:4196:TRP:CD1	2.36	0.43
2:C:54:ASN:C	2:C:56:VAL:N	2.77	0.43
1:A:773:ASP:HB3	1:A:774:PRO:HD2	1.99	0.43
1:A:872:ALA:O	1:B:186:GLN:NE2	2.52	0.43
1:A:1429:LYS:O	1:A:1432:THR:N	2.51	0.43
1:A:1707:SER:O	1:A:1708:TYR:C	2.62	0.43
1:A:4136:PRO:HB2	1:B:3508:PRO:HB3	2.00	0.43
1:A:4273:LEU:HD12	1:A:4291:LEU:HD12	2.00	0.43
1:B:793:ASN:O	1:B:797:GLY:N	2.52	0.43
1:B:1345:GLU:O	1:B:1349:ARG:HG2	2.18	0.43
1:B:1996:LEU:HD22	1:B:2019:THR:HG21	2.00	0.43
1:B:2683:MET:HE2	1:B:2999:TYR:OH	2.19	0.43
1:B:3001:GLN:HG3	1:B:3139:PHE:CZ	2.54	0.43
1:B:3301:LEU:HD21	1:B:3326:ALA:CB	2.48	0.43
2:C:100:TYR:CD1	2:C:136:GLN:HB3	2.54	0.43
1:A:270:ILE:HG12	1:A:335:SER:CB	2.48	0.43
1:A:317:VAL:HG12	1:A:318:LEU:H	1.82	0.43
1:A:420:LEU:O	1:A:424:LEU:HG	2.19	0.43
1:A:1332:ASN:HA	1:A:1335:GLU:CD	2.44	0.43
1:A:1521:MET:HB2	1:A:1537:LEU:HD21	1.99	0.43
1:A:1606:VAL:O	1:A:1610:LEU:HG	2.19	0.43
1:A:2305:GLY:HA2	1:A:2339:GLU:H	1.83	0.43
1:A:2340:ILE:HD13	1:A:2422:ILE:HD11	2.00	0.43
1:A:2363:ARG:NH1	1:A:2416:MET:HE1	2.34	0.43
1:A:2698:LYS:NZ	1:A:3002:VAL:HG23	2.33	0.43
1:A:3057:ARG:HG3	1:A:3141:LEU:HG	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4128:TRP:HA	1:A:4131:GLN:HG2	2.01	0.43
1:A:4318:LYS:HA	1:A:4491:ARG:HH22	1.83	0.43
1:A:4491:ARG:O	1:A:4495:ILE:HG13	2.19	0.43
1:B:66:HIS:NE2	1:B:71:GLU:HG2	2.33	0.43
1:B:257:LEU:HD23	1:B:257:LEU:HA	1.59	0.43
1:B:1038:THR:O	1:B:1039:LEU:C	2.61	0.43
1:B:1077:THR:HG23	1:B:1082:SER:H	1.84	0.43
1:B:1191:SER:N	1:B:1194:LYS:HD3	2.32	0.43
1:B:1388:LEU:C	1:B:1390:SER:H	2.26	0.43
1:B:3540:VAL:HB	1:B:3718:LYS:HD2	1.99	0.43
1:B:4024:ILE:HD11	3:F:324:LEU:HD12	2.00	0.43
1:B:4414:ILE:HD11	1:B:4451:ALA:HB1	2.01	0.43
1:B:4601:ILE:HD11	1:B:4620:ILE:CD1	2.49	0.43
1:A:124:VAL:HG11	1:A:129:LEU:CD2	2.48	0.43
1:A:296:ARG:HA	1:A:299:PHE:CE2	2.54	0.43
1:A:404:GLN:OE1	1:A:404:GLN:HA	2.17	0.43
1:A:659:THR:HA	1:A:663:LEU:CD1	2.40	0.43
1:A:817:ILE:HG22	1:A:821:PHE:CE2	2.53	0.43
1:A:1281:ALA:HA	1:A:1284:LEU:CG	2.49	0.43
1:A:1394:ARG:HH11	1:A:1443:ASN:HD21	1.65	0.43
1:A:2661:VAL:HG11	1:A:2701:LEU:HG	2.01	0.43
1:A:2688:CYS:O	1:A:2689:PRO:C	2.61	0.43
1:A:3207:ARG:O	1:A:3211:ARG:HG3	2.18	0.43
1:B:321:LEU:HD12	1:B:395:SER:CB	2.49	0.43
1:B:862:PHE:CE1	1:B:866:LEU:HD11	2.53	0.43
1:B:2493:GLY:O	1:B:2498:LYS:HE3	2.19	0.43
1:B:2544:ASP:HA	1:B:2580:ILE:HD12	2.00	0.43
1:B:2564:ASP:OD2	1:B:2631:LYS:O	2.37	0.43
1:B:3095:VAL:HG11	1:B:3186:PHE:HE1	1.84	0.43
2:D:38:ARG:HD2	2:D:43:ASN:HA	2.00	0.43
1:A:255:LYS:O	1:A:259:VAL:HG23	2.19	0.43
1:A:732:LEU:HD21	1:A:760:LEU:HD12	2.00	0.43
1:A:1298:LEU:HA	1:A:1301:TRP:NE1	2.34	0.43
1:A:2023:VAL:HG21	1:A:2049:VAL:HG21	2.01	0.43
1:A:2368:ILE:HD11	1:A:2387:PHE:CZ	2.54	0.43
1:A:3490:SER:O	1:A:3494:VAL:HG23	2.18	0.43
1:A:4600:GLN:O	1:A:4601:ILE:C	2.62	0.43
1:B:282:PHE:HB3	1:B:420:LEU:HD11	1.99	0.43
1:B:1359:TYR:CE1	1:B:1406:GLU:HB3	2.53	0.43
1:B:1407:LEU:HB3	1:B:1431:PHE:CZ	2.51	0.43
1:B:1560:ALA:HB1	1:B:1599:ILE:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2027:ASP:CG	1:B:2029:CYS:SG	3.00	0.43
1:B:2622:ILE:HD11	1:B:2667:TYR:CB	2.47	0.43
1:B:3310:LEU:HG	1:B:3851:PHE:HB3	2.01	0.43
1:B:3409:ILE:HD13	1:B:3454:ILE:HD11	2.01	0.43
1:B:3460:ALA:O	1:B:3868:SER:N	2.40	0.43
1:B:3525:TYR:HE2	1:B:3874:GLY:HA2	1.84	0.43
3:F:317:SER:O	3:F:321:GLN:HG3	2.17	0.43
1:A:329:VAL:CG1	1:A:388:ILE:HD12	2.49	0.43
1:A:547:VAL:HA	1:A:550:ARG:HH11	1.83	0.43
1:A:811:LEU:HD23	1:A:933:TYR:HE1	1.84	0.43
1:A:852:PRO:O	1:A:853:LEU:C	2.61	0.43
1:A:1281:ALA:HB2	1:A:1284:LEU:HD12	2.01	0.43
1:A:2683:MET:HE3	1:A:2683:MET:HB2	1.90	0.43
1:A:2698:LYS:O	1:A:2702:ILE:HG13	2.19	0.43
1:A:3007:THR:O	1:A:3009:ASP:N	2.52	0.43
1:A:4477:GLY:CA	1:A:4518:VAL:HG11	2.46	0.43
1:B:29:TRP:CE3	1:B:73:PHE:HZ	2.37	0.43
1:B:194:LEU:HD13	1:B:194:LEU:HA	1.89	0.43
1:B:405:ASN:O	1:B:409:LEU:HG	2.19	0.43
1:B:801:SER:O	1:B:805:ASP:N	2.52	0.43
1:B:1514:LEU:O	1:B:1518:LEU:HG	2.19	0.43
1:B:2263:ILE:HG12	1:B:2655:ALA:HB1	2.00	0.43
1:B:3294:CYS:HB3	1:B:3301:LEU:HG	1.99	0.43
1:B:3295:ILE:HD12	1:B:3295:ILE:HA	1.93	0.43
1:B:4598:LEU:HD11	1:B:4634:LEU:HB2	2.00	0.43
1:B:4606:VAL:HG11	1:B:4616:LEU:HD22	2.00	0.43
1:B:4751:LEU:HD23	1:B:4751:LEU:HA	1.77	0.43
1:A:248:GLN:HB3	1:B:496:LEU:HD11	2.01	0.42
1:A:280:ASN:HB2	1:A:412:TRP:HE1	1.84	0.42
1:A:405:ASN:CB	1:A:511:ILE:HA	2.49	0.42
1:A:484:LEU:O	1:A:488:PHE:HD1	2.02	0.42
1:A:864:TYR:HD2	1:A:865:LEU:HD23	1.84	0.42
1:A:973:LEU:HD23	1:A:973:LEU:HA	1.85	0.42
1:A:1345:GLU:H	1:A:1345:GLU:CD	2.27	0.42
1:A:1859:MET:N	1:A:2200:GLN:OE1	2.43	0.42
1:A:2698:LYS:HG2	1:A:2998:PRO:HA	2.00	0.42
1:A:3021:LEU:O	1:A:3025:LEU:HG	2.18	0.42
1:A:3699:LEU:HD23	1:A:3706:CYS:HB2	2.01	0.42
1:A:4101:TYR:CE2	2:C:89:ALA:HB2	2.54	0.42
1:A:4622:TYR:HA	1:A:4670:LYS:HE3	2.00	0.42
1:B:256:LEU:HD12	1:B:317:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:TYR:HB3	1:B:302:LEU:HD13	2.01	0.42
1:B:654:ILE:O	1:B:658:ILE:HG13	2.19	0.42
1:B:881:GLN:HA	1:B:885:LEU:HD12	2.00	0.42
1:B:1032:GLU:O	1:B:1035:ILE:HB	2.19	0.42
1:B:1405:GLY:O	1:B:1409:GLN:HG2	2.18	0.42
1:B:2192:VAL:HG13	1:B:2197:PHE:HE1	1.82	0.42
1:B:3396:VAL:HG11	1:B:3438:ASN:CB	2.49	0.42
1:B:3986:TRP:CZ2	3:F:316:ARG:HG2	2.54	0.42
1:A:666:ARG:HA	1:A:671:ARG:HE	1.84	0.42
1:A:1269:HIS:ND1	1:A:1283:SER:HB3	2.35	0.42
1:A:1288:LEU:O	1:A:1292:VAL:HG23	2.18	0.42
1:A:1324:GLU:HA	1:A:1327:ALA:HB2	2.01	0.42
1:A:3440:SER:OG	1:A:3443:GLN:OE1	2.20	0.42
1:A:4003:ILE:HB	1:A:4008:VAL:HG11	2.01	0.42
1:A:4199:TYR:HE1	2:C:39:SER:HA	1.84	0.42
1:A:4727:ARG:O	1:A:4731:ILE:HG13	2.19	0.42
1:A:4744:SER:O	1:A:4748:LEU:HG	2.19	0.42
1:B:474:VAL:HG11	1:B:646:LEU:HG	1.99	0.42
1:B:866:LEU:HD13	1:B:1013:LEU:HD21	2.01	0.42
1:B:1177:LEU:HD23	1:B:1177:LEU:HA	1.84	0.42
1:B:1387:GLN:HB3	1:B:1397:MET:SD	2.59	0.42
1:B:1701:HIS:HB2	1:B:1706:ILE:HD11	2.01	0.42
1:B:3021:LEU:O	1:B:3025:LEU:HG	2.19	0.42
1:B:3525:TYR:CE2	1:B:3874:GLY:HA2	2.54	0.42
1:B:4360:GLU:CD	1:B:4366:ARG:HH21	2.25	0.42
2:D:45:THR:OG1	2:D:48:GLU:HG3	2.19	0.42
3:F:2:SER:H	3:F:59:VAL:HG21	1.84	0.42
1:A:718:VAL:HG13	1:A:760:LEU:CD2	2.49	0.42
1:A:1377:LEU:H	1:A:1377:LEU:HD12	1.84	0.42
1:A:2023:VAL:HG23	1:A:2046:ILE:HD13	2.02	0.42
1:A:3095:VAL:HG12	1:A:3190:TRP:CH2	2.54	0.42
1:A:3515:THR:HG21	1:A:3764:LEU:HD22	2.01	0.42
1:A:3736:VAL:HG12	1:A:3740:ASN:HD21	1.85	0.42
1:A:4570:LEU:HD13	1:A:4622:TYR:HB2	2.01	0.42
1:B:1097:GLN:HE21	1:B:1097:GLN:CA	2.31	0.42
1:B:1560:ALA:HB1	1:B:1599:ILE:CG2	2.49	0.42
1:B:1575:ASN:O	1:B:1579:LYS:HG3	2.20	0.42
1:B:2151:ILE:HD11	1:B:2164:LEU:HD21	2.01	0.42
1:B:2379:LEU:HD23	1:B:2379:LEU:H	1.84	0.42
1:B:3527:LEU:HD11	1:B:3757:ARG:HB2	2.00	0.42
1:B:3647:PHE:HB2	1:B:3649:GLU:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:318:LEU:O	3:E:322:GLU:HG2	2.20	0.42
1:A:240:ILE:O	1:A:244:VAL:HG23	2.19	0.42
1:A:296:ARG:HA	1:A:299:PHE:CZ	2.54	0.42
1:A:317:VAL:C	1:A:318:LEU:HG	2.44	0.42
1:A:699:LYS:O	1:A:703:ASP:HB2	2.19	0.42
1:A:1556:LEU:HD21	1:A:1563:TRP:CZ3	2.54	0.42
1:A:2071:TYR:CE1	1:A:2091:VAL:HG22	2.55	0.42
1:A:2355:GLN:HB2	1:A:2384:TRP:CE2	2.55	0.42
1:A:2695:PHE:O	1:A:2698:LYS:HB3	2.19	0.42
1:A:3023:ASN:O	1:A:3027:GLN:HG2	2.19	0.42
1:A:4281:THR:HB	1:A:4284:ILE:HG12	2.00	0.42
1:A:4484:GLY:O	1:A:4485:LEU:C	2.62	0.42
1:B:154:MET:O	1:B:157:SER:OG	2.34	0.42
1:B:183:GLU:O	1:B:187:LYS:HG2	2.19	0.42
1:B:488:PHE:HE2	1:B:670:ILE:HD12	1.84	0.42
1:B:881:GLN:HA	1:B:885:LEU:HB2	2.01	0.42
1:B:1014:PRO:HB3	1:B:1057:HIS:CD2	2.55	0.42
1:B:1110:LEU:O	1:B:1175:ALA:HB1	2.20	0.42
1:B:1912:LEU:HB2	1:B:1926:LEU:HD11	2.02	0.42
1:B:2192:VAL:HG13	1:B:2197:PHE:CE1	2.54	0.42
1:B:3595:ASN:HD21	1:B:3605:LEU:HD13	1.83	0.42
1:B:4372:TYR:HD1	1:B:4376:GLU:OE2	2.02	0.42
2:D:66:PHE:HB3	2:D:67:PRO:HD3	2.01	0.42
1:A:856:ALA:HB1	1:A:1001:TYR:HD2	1.85	0.42
1:A:1057:HIS:HA	1:A:1060:LYS:HD2	2.01	0.42
1:A:1176:TYR:CZ	1:A:1280:LEU:HB2	2.55	0.42
1:A:1817:PHE:CE2	1:A:1818:LEU:HG	2.55	0.42
1:A:1854:MET:HE2	1:A:2152:LYS:H	1.83	0.42
1:A:3409:ILE:HD13	1:A:3454:ILE:HD11	2.01	0.42
1:A:4659:LEU:HG	1:A:4721:PHE:HB3	2.01	0.42
1:A:4716:ARG:HA	1:A:4717:PRO:HD3	1.94	0.42
1:B:1473:THR:O	1:B:1485:ILE:HG21	2.19	0.42
1:B:1867:GLU:HG2	1:B:2236:ASP:OD2	2.18	0.42
1:B:2009:PRO:CB	1:B:2642:LEU:HD21	2.50	0.42
1:B:4513:SER:O	1:B:4517:LYS:HG2	2.19	0.42
3:E:4:HIS:CD2	3:E:21:ARG:HB2	2.55	0.42
3:E:113:CYS:SG	3:E:131:HIS:CE1	3.13	0.42
1:A:926:ALA:O	1:A:928:PRO:HD3	2.19	0.42
1:A:2178:CYS:HB3	1:A:2214:MET:HE1	2.02	0.42
1:A:3195:SER:HG	1:A:3231:HIS:CE1	2.34	0.42
1:A:3997:PHE:HZ	1:A:4128:TRP:CE3	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:LEU:HD23	1:B:136:LEU:HA	1.82	0.42
1:B:313:LEU:HD21	1:B:332:LEU:CD2	2.49	0.42
1:B:352:VAL:HG21	1:B:424:LEU:HD13	2.02	0.42
1:B:1545:ALA:HB2	1:B:1556:LEU:CD2	2.48	0.42
1:B:1597:CYS:SG	1:B:2477:ARG:HB2	2.59	0.42
1:B:2405:ILE:CG1	1:B:2417:ILE:HD11	2.49	0.42
1:B:4119:LEU:HD11	3:F:329:VAL:HG11	2.00	0.42
1:B:4346:VAL:HG21	1:B:4425:TYR:CD1	2.55	0.42
3:E:111:PRO:HD2	3:E:128:PHE:CZ	2.54	0.42
3:E:295:ARG:HG2	3:E:295:ARG:O	2.19	0.42
3:F:295:ARG:HG2	3:F:295:ARG:O	2.19	0.42
3:F:318:LEU:O	3:F:322:GLU:HG2	2.20	0.42
1:A:112:LEU:HD13	1:A:252:GLY:HA3	2.02	0.42
1:A:273:PHE:CE1	1:A:334:LEU:HB3	2.54	0.42
1:A:415:LEU:HD21	1:A:484:LEU:HD11	2.01	0.42
1:A:1219:VAL:O	1:A:1227:GLN:NE2	2.53	0.42
1:A:1233:TRP:CH2	1:A:1281:ALA:HB1	2.54	0.42
1:A:1345:GLU:O	1:A:1349:ARG:HG2	2.19	0.42
1:A:2263:ILE:HA	1:A:2575:ILE:HD11	2.02	0.42
1:A:2266:MET:SD	1:A:2575:ILE:HG12	2.60	0.42
1:A:3295:ILE:HD12	1:A:3295:ILE:HA	1.84	0.42
1:A:3550:ILE:HD11	1:A:3715:LEU:HD12	2.01	0.42
1:A:3884:ILE:HD11	1:A:3913:ASN:ND2	2.34	0.42
1:B:30:GLU:H	1:B:30:GLU:HG3	1.66	0.42
1:B:131:LEU:HD11	1:B:142:ARG:HG3	2.01	0.42
1:B:2137:SER:O	1:B:2141:LEU:N	2.51	0.42
1:B:3269:LEU:HB3	1:B:3633:LEU:HD13	1.90	0.42
1:B:4491:ARG:O	1:B:4495:ILE:HG13	2.20	0.42
2:C:123:ASP:O	2:C:127:ARG:HG2	2.20	0.42
3:F:111:PRO:HD2	3:F:128:PHE:CZ	2.55	0.42
1:A:1090:VAL:HG21	1:A:1131:VAL:HG13	2.02	0.42
1:A:1138:HIS:HA	1:A:1141:LYS:HD3	2.02	0.42
1:A:1912:LEU:HB2	1:A:1926:LEU:HD11	2.02	0.42
1:A:2049:VAL:HG22	1:A:2063:ILE:HG12	2.01	0.42
1:A:2551:ALA:HA	1:A:2573:LEU:HD22	2.01	0.42
1:A:4414:ILE:HD11	1:A:4451:ALA:HB1	2.02	0.42
1:B:115:LEU:CD1	1:B:130:ILE:HG13	2.50	0.42
1:B:255:LYS:O	1:B:259:VAL:HG23	2.20	0.42
1:B:919:SER:HA	1:B:922:PHE:CD2	2.54	0.42
1:B:943:ASP:OD2	1:B:943:ASP:N	2.52	0.42
1:B:2300:ASP:OD1	1:B:2300:ASP:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2701:LEU:HD12	1:B:3002:VAL:CG2	2.50	0.42
2:C:34:GLY:HA2	2:C:37:MET:HE2	2.01	0.42
2:C:95:LYS:HE2	2:C:109:VAL:HG23	2.02	0.42
1:A:94:ARG:O	1:A:97:LEU:HB3	2.19	0.42
1:A:130:ILE:HD12	1:A:308:MET:HG3	2.02	0.42
1:A:150:THR:O	1:A:154:MET:HG3	2.20	0.42
1:A:1848:VAL:O	1:A:1850:LYS:NZ	2.38	0.42
1:A:2042:PRO:HD3	1:A:2088:VAL:O	2.20	0.42
1:A:3749:VAL:HG23	1:A:3814:LEU:HD13	2.02	0.42
1:A:3773:GLU:O	1:A:3774:LYS:C	2.63	0.42
1:B:414:LEU:HD12	1:B:483:LEU:HD12	2.01	0.42
1:B:1591:MET:O	1:B:1594:GLU:HG2	2.20	0.42
1:B:1693:CYS:N	1:B:1716:CYS:SG	2.92	0.42
1:B:2551:ALA:HA	1:B:2573:LEU:HD22	2.01	0.42
1:B:2686:LEU:HD11	1:B:3002:VAL:HG11	2.02	0.42
1:B:3050:GLU:O	1:B:3054:VAL:HG23	2.19	0.42
1:B:3061:VAL:O	1:B:3065:ARG:N	2.44	0.42
1:B:3076:GLU:H	1:B:3076:GLU:HG3	1.73	0.42
1:B:3233:LEU:HD13	1:B:3290:TRP:HE3	1.85	0.42
1:B:3699:LEU:HD23	1:B:3706:CYS:HB2	2.01	0.42
1:B:3922:ARG:O	1:B:3926:ARG:HG3	2.20	0.42
1:B:4224:GLU:HA	1:B:4279:GLN:NE2	2.35	0.42
1:B:4510:LYS:HE2	1:B:4514:TYR:OH	2.19	0.42
2:D:28:ILE:H	2:D:28:ILE:HG12	1.48	0.42
3:E:3:ARG:HG2	3:E:18:ARG:CG	2.50	0.42
1:A:124:VAL:HG11	1:A:129:LEU:HD23	2.02	0.42
1:A:336:CYS:SG	1:A:384:ILE:HD12	2.59	0.42
1:A:699:LYS:O	1:A:704:GLU:HG3	2.20	0.42
1:A:2405:ILE:CG1	1:A:2417:ILE:HD11	2.50	0.42
1:A:3269:LEU:HB3	1:A:3633:LEU:HD13	1.91	0.42
1:A:4328:PRO:O	1:A:4331:ILE:HB	2.19	0.42
1:A:4372:TYR:HD1	1:A:4376:GLU:OE2	2.02	0.42
1:A:4748:LEU:HB2	1:A:4768:LEU:HD21	2.02	0.42
1:B:159:LYS:HA	1:B:159:LYS:HD2	1.85	0.42
1:B:321:LEU:HD23	1:B:321:LEU:HA	1.87	0.42
1:B:1307:PRO:HB2	1:B:1308:PRO:HD3	2.01	0.42
1:B:1486:GLN:HG3	1:B:1489:ARG:NH1	2.35	0.42
1:B:1554:LEU:HA	1:B:1557:HIS:CD2	2.54	0.42
1:B:1563:TRP:HD1	1:B:1566:ARG:HH11	1.68	0.42
1:B:2369:GLU:HA	1:B:2373:ARG:O	2.20	0.42
1:B:2379:LEU:HB3	1:B:2385:PHE:HZ	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3054:VAL:HG13	1:B:3057:ARG:HD2	2.02	0.42
1:B:4273:LEU:HD22	1:B:4284:ILE:CG2	2.49	0.42
1:A:184:LEU:HD22	1:A:184:LEU:N	2.32	0.41
1:A:1046:ARG:HD2	1:A:1046:ARG:HA	1.88	0.41
1:A:3453:SER:O	1:A:3456:PRO:HD2	2.20	0.41
1:B:100:VAL:HG12	1:B:239:PHE:HE1	1.85	0.41
1:B:3988:LEU:HD12	1:B:3988:LEU:H	1.85	0.41
1:B:4309:PHE:CD1	1:B:4338:ILE:HD11	2.54	0.41
2:C:73:MET:O	2:C:77:MET:N	2.46	0.41
3:F:9:CYS:O	3:F:13:LEU:HA	2.19	0.41
3:F:81:PRO:HB2	3:F:108:VAL:HB	2.02	0.41
1:A:29:TRP:HA	1:A:32:ALA:HB3	2.01	0.41
1:A:292:ALA:O	1:A:296:ARG:HG3	2.19	0.41
1:A:643:ASP:HA	1:A:644:PRO:HD2	1.96	0.41
1:A:768:ALA:HA	1:A:773:ASP:HB2	2.01	0.41
1:A:853:LEU:HD13	1:A:998:ALA:HB2	2.02	0.41
1:A:1382:GLN:N	1:A:1426:ARG:HH21	2.18	0.41
1:A:1682:HIS:HA	1:A:2381:ARG:NH2	2.35	0.41
1:A:2038:TYR:C	1:A:2038:TYR:CD2	2.96	0.41
1:A:2118:VAL:HG11	1:A:2174:PRO:HB3	2.03	0.41
1:A:3167:LEU:HB3	1:A:3168:PRO:CD	2.43	0.41
1:A:3396:VAL:HG11	1:A:3438:ASN:CB	2.49	0.41
1:A:3771:ALA:HB1	1:B:3919:ALA:HB2	2.02	0.41
1:A:3922:ARG:O	1:A:3926:ARG:HG3	2.20	0.41
1:A:4492:LEU:HD23	1:A:4492:LEU:HA	1.87	0.41
1:A:4710:TRP:HZ3	1:A:4751:LEU:HD23	1.86	0.41
1:B:943:ASP:HB3	1:B:1255:THR:HG21	2.01	0.41
1:B:1679:TYR:HB2	1:B:1692:VAL:HG22	2.02	0.41
1:B:1805:PHE:CD2	1:B:2494:PRO:HD2	2.52	0.41
1:B:2046:ILE:HG23	1:B:2063:ILE:HG23	2.01	0.41
1:B:2118:VAL:HG11	1:B:2174:PRO:HB3	2.02	0.41
1:B:2259:PRO:HB2	1:B:2651:THR:HG21	2.00	0.41
1:B:2593:GLU:HG3	1:B:2667:TYR:OH	2.20	0.41
1:B:3729:GLU:HA	1:B:3732:ARG:HB3	2.02	0.41
1:B:3884:ILE:HD11	1:B:3913:ASN:ND2	2.34	0.41
1:B:4307:LYS:HG2	1:B:4478:VAL:CG1	2.50	0.41
1:B:4695:MET:HE1	1:B:4748:LEU:HD21	2.01	0.41
1:A:73:PHE:HD2	1:A:74:TYR:HD1	1.67	0.41
1:A:366:LYS:HA	1:A:369:ASP:CG	2.45	0.41
1:A:694:ASP:CB	1:A:750:HIS:HB3	2.50	0.41
1:A:995:GLU:O	1:A:999:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1060:LYS:O	1:A:1061:GLN:C	2.63	0.41
1:A:1194:LYS:HA	1:A:1370:SER:O	2.20	0.41
1:A:1201:VAL:HG13	1:A:1218:LEU:HB3	2.02	0.41
1:A:2639:ASN:HB3	1:A:2642:LEU:HG	2.01	0.41
1:A:3053:LEU:HA	1:A:3056:MET:HE2	2.01	0.41
1:A:3099:LEU:HD22	1:A:3190:TRP:CE2	2.55	0.41
1:A:3470:ASP:OD1	3:E:293:LEU:HG	2.21	0.41
1:A:3964:LEU:HA	1:A:3967:SER:HB2	2.02	0.41
1:A:3991:ARG:HA	1:A:4059:TRP:CZ3	2.55	0.41
1:A:4699:ILE:HA	1:A:4700:PRO:HD3	1.94	0.41
1:B:320:PRO:O	1:B:325:ARG:NH1	2.49	0.41
1:B:321:LEU:HD12	1:B:395:SER:HB2	2.03	0.41
1:B:655:LEU:HD23	1:B:655:LEU:HA	1.75	0.41
1:B:1243:ASN:OD1	1:B:1243:ASN:N	2.53	0.41
1:B:1678:TRP:CD1	1:B:1678:TRP:H	2.39	0.41
1:B:1859:MET:N	1:B:2200:GLN:OE1	2.43	0.41
1:B:2187:PRO:HB3	1:B:2214:MET:SD	2.59	0.41
1:B:3320:LEU:HD23	1:B:3320:LEU:HA	1.92	0.41
1:B:3387:GLN:HG2	1:B:3388:GLU:N	2.35	0.41
1:B:4108:PHE:HA	1:B:4111:ARG:CG	2.50	0.41
1:B:4363:LEU:HD21	1:B:4444:MET:HG3	2.00	0.41
2:C:10:ILE:HG13	2:C:66:PHE:CZ	2.55	0.41
3:F:5:GLU:HA	3:F:16:ASN:OD1	2.21	0.41
1:A:29:TRP:O	1:A:33:VAL:HG13	2.19	0.41
1:A:1204:ILE:HD11	1:A:1357:GLY:CA	2.50	0.41
1:A:1232:SER:O	1:A:1236:ILE:HG13	2.21	0.41
1:A:1679:TYR:CE1	1:A:1708:TYR:HA	2.55	0.41
1:A:2479:VAL:HG21	1:A:2521:VAL:HG22	2.02	0.41
1:A:2517:ALA:CB	1:A:2521:VAL:HB	2.50	0.41
1:A:3181:ILE:HA	1:A:3182:PRO:HD3	1.88	0.41
1:A:3311:VAL:HB	1:A:3315:VAL:HB	2.03	0.41
1:A:4132:VAL:CG1	1:A:4145:ALA:HB2	2.50	0.41
1:A:4244:LEU:O	1:A:4248:PHE:HD1	2.03	0.41
1:B:139:GLY:HA2	1:B:240:ILE:HD11	2.02	0.41
1:B:310:LEU:HA	1:B:313:LEU:HB2	2.03	0.41
1:B:310:LEU:O	1:B:314:SER:N	2.50	0.41
1:B:422:LEU:HD11	1:B:537:LEU:HG	2.02	0.41
1:B:1132:GLN:HE22	1:B:1293:ARG:HH21	1.69	0.41
1:B:1244:ILE:HG21	1:B:1249:ASN:HB3	2.01	0.41
1:B:1428:LEU:HB3	1:B:1491:LEU:CB	2.51	0.41
1:B:1600:MET:HG2	1:B:2478:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2025:ILE:HD13	1:B:2075:MET:CE	2.50	0.41
1:B:3102:LEU:O	1:B:3197:TYR:OH	2.31	0.41
1:B:4129:LEU:HD12	1:B:4129:LEU:HA	1.85	0.41
1:B:4187:TYR:O	1:B:4191:ILE:HG12	2.21	0.41
1:B:4331:ILE:O	1:B:4335:LEU:HG	2.21	0.41
2:C:131:ILE:HD11	2:C:144:GLN:HG2	2.03	0.41
1:A:108:ILE:O	1:A:112:LEU:HG	2.20	0.41
1:A:418:LEU:O	1:A:422:LEU:HG	2.21	0.41
1:A:1178:LEU:CD2	1:A:1202:LEU:HD21	2.50	0.41
1:A:1294:LEU:O	1:A:1298:LEU:HG	2.20	0.41
1:A:2025:ILE:HD13	1:A:2075:MET:CE	2.50	0.41
1:A:3142:ARG:HA	1:A:3142:ARG:HD3	1.85	0.41
1:A:4767:LEU:O	1:A:4771:LEU:HG	2.21	0.41
1:B:114:ARG:HD3	1:B:114:ARG:HA	1.68	0.41
1:B:694:ASP:OD2	1:B:750:HIS:HB3	2.20	0.41
1:B:808:VAL:HG11	1:B:908:TYR:CB	2.49	0.41
1:B:936:LEU:HD13	1:B:1008:ARG:NH2	2.35	0.41
1:B:1374:GLU:OE1	1:B:1423:PHE:HB2	2.21	0.41
1:B:2058:LYS:HB2	1:B:2074:LEU:HD11	2.01	0.41
1:B:2564:ASP:OD1	1:B:2631:LYS:HD3	2.20	0.41
1:B:2985:LEU:HA	1:B:2988:LEU:HD13	2.02	0.41
1:B:3311:VAL:HG23	1:B:3312:ASP:O	2.20	0.41
1:B:3396:VAL:HG11	1:B:3438:ASN:HB3	2.02	0.41
1:B:3512:ILE:HD11	1:B:3761:GLU:HG2	2.02	0.41
1:B:3901:VAL:HG11	1:B:3939:ALA:HB2	2.02	0.41
1:B:4244:LEU:O	1:B:4248:PHE:HD1	2.03	0.41
1:B:4727:ARG:NE	1:B:4766:ASN:HB3	2.35	0.41
1:A:418:LEU:HD11	1:A:477:ALA:HA	2.01	0.41
1:A:481:ILE:O	1:A:485:THR:HG23	2.20	0.41
1:A:548:LEU:HD22	1:A:642:LYS:HA	2.02	0.41
1:A:693:VAL:HG21	1:A:710:LEU:HD22	2.02	0.41
1:A:834:VAL:HG11	1:A:961:VAL:HG13	2.03	0.41
1:A:921:HIS:HB2	1:A:993:ALA:HB2	2.03	0.41
1:A:1178:LEU:HA	1:A:1181:PHE:CE2	2.55	0.41
1:A:1255:THR:OG1	1:A:1256:ILE:N	2.54	0.41
1:A:1536:GLU:O	1:A:1540:VAL:HG23	2.20	0.41
1:A:1556:LEU:HD13	1:A:1560:ALA:HB2	2.01	0.41
1:A:2054:ASN:HB3	1:A:2060:ILE:HD11	2.02	0.41
1:A:3053:LEU:HD22	1:A:3156:TYR:CD1	2.55	0.41
1:A:3463:ARG:NH2	1:A:3538:PRO:HA	2.35	0.41
1:A:3519:LEU:CD1	1:A:3767:VAL:HG11	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4108:PHE:HA	1:A:4111:ARG:CG	2.50	0.41
1:A:4694:TYR:CD1	1:A:4694:TYR:C	2.98	0.41
1:B:229:GLN:O	1:B:233:ILE:HG13	2.20	0.41
1:B:916:GLU:O	1:B:920:LYS:HG3	2.20	0.41
1:B:1388:LEU:HD23	1:B:1394:ARG:HG3	2.02	0.41
1:B:1475:PRO:HG2	1:B:1481:GLN:HB2	2.01	0.41
1:B:1590:VAL:HA	1:B:1593:LEU:HD13	2.01	0.41
1:B:2414:VAL:HG11	1:B:2416:MET:HE3	2.02	0.41
1:B:3087:ALA:CB	1:B:3181:ILE:CD1	2.89	0.41
1:A:325:ARG:O	1:A:326:LEU:C	2.64	0.41
1:A:414:LEU:HD12	1:A:483:LEU:HD12	2.01	0.41
1:A:942:GLU:HB3	1:A:947:ARG:NE	2.35	0.41
1:A:1268:ALA:O	1:A:1272:THR:HG23	2.20	0.41
1:A:1384:LEU:HD22	1:A:1384:LEU:HA	1.95	0.41
1:A:1729:LEU:HD23	1:A:1729:LEU:HA	1.90	0.41
1:A:1798:GLU:H	1:A:1798:GLU:CD	2.28	0.41
1:A:2311:VAL:HG11	3:E:64:TYR:CD1	2.56	0.41
1:A:3049:ASN:HB3	1:A:3156:TYR:OH	2.19	0.41
1:A:3283:ALA:HB1	1:A:3325:CYS:CB	2.50	0.41
1:A:4303:GLU:HB2	1:A:4475:MET:SD	2.60	0.41
1:A:4336:CYS:HB3	1:A:4514:TYR:HE2	1.85	0.41
1:A:4713:PHE:CE1	1:A:4751:LEU:HD21	2.44	0.41
1:B:1486:GLN:O	1:B:1490:GLN:HG3	2.20	0.41
1:B:1859:MET:CE	1:B:2230:MET:HB2	2.50	0.41
1:B:2094:ILE:HD13	1:B:2124:PHE:CZ	2.56	0.41
1:B:2687:LEU:O	1:B:2688:CYS:C	2.63	0.41
1:B:3003:ILE:O	1:B:3006:LEU:HB2	2.21	0.41
1:B:3105:LEU:HB2	1:B:3197:TYR:OH	2.21	0.41
1:B:3287:THR:OG1	1:B:3330:SER:HB3	2.20	0.41
1:B:3306:GLN:O	1:B:3309:PHE:HB2	2.21	0.41
1:B:3928:LEU:O	1:B:3932:LEU:HG	2.21	0.41
1:B:4562:VAL:O	1:B:4566:MET:HG3	2.20	0.41
1:B:4616:LEU:O	1:B:4620:ILE:HG13	2.21	0.41
2:C:83:GLU:HA	2:C:86:ILE:HB	2.03	0.41
1:A:108:ILE:HD11	1:A:243:ASN:HB3	2.03	0.41
1:A:925:ASP:N	1:A:925:ASP:OD1	2.54	0.41
1:A:1001:TYR:O	1:A:1005:ILE:HG13	2.21	0.41
1:A:1395:LYS:O	1:A:1399:GLU:HG2	2.21	0.41
1:A:1976:HIS:ND1	1:A:1989:HIS:NE2	2.57	0.41
1:A:2246:VAL:O	1:A:2250:SER:OG	2.37	0.41
1:A:2686:LEU:HD13	1:A:2999:TYR:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2975:LEU:HD11	1:A:3020:ALA:CB	2.51	0.41
1:A:3107:GLU:HA	1:A:3110:LYS:HD2	2.02	0.41
1:A:3450:LEU:O	1:A:3454:ILE:HG13	2.21	0.41
1:A:3522:PHE:HD1	1:A:3522:PHE:H	1.67	0.41
1:A:4759:GLY:O	1:A:4763:LEU:HG	2.21	0.41
1:B:132:LEU:HD21	1:B:143:LEU:CD1	2.50	0.41
1:B:1001:TYR:CE2	1:B:1005:ILE:HD11	2.56	0.41
1:B:1169:TYR:O	1:B:1173:THR:HG23	2.21	0.41
1:B:2044:SER:OG	1:B:2065:SER:HB2	2.20	0.41
1:B:2298:LEU:N	1:B:2422:ILE:O	2.43	0.41
1:B:3236:HIS:O	1:B:3240:ILE:HG12	2.21	0.41
1:B:3320:LEU:HD12	1:B:3424:VAL:HG13	2.03	0.41
1:B:4570:LEU:HD13	1:B:4622:TYR:HB3	2.03	0.41
2:D:121:GLU:O	2:D:122:VAL:C	2.60	0.41
3:F:89:THR:N	3:F:92:SER:OG	2.50	0.41
1:A:86:THR:CG2	1:A:141:SER:HB3	2.51	0.41
1:A:469:PHE:CZ	1:A:474:VAL:HG22	2.55	0.41
1:A:884:LEU:C	1:A:886:SER:H	2.29	0.41
1:A:1039:LEU:HB3	1:A:1130:LYS:HD2	2.03	0.41
1:A:1041:TRP:HA	1:A:1044:ARG:HG3	2.03	0.41
1:A:1133:VAL:HG22	1:A:1247:TRP:CE2	2.56	0.41
1:A:1210:LYS:HE3	1:A:1210:LYS:HB2	1.93	0.41
1:A:1515:LEU:HD11	1:A:1556:LEU:CD2	2.50	0.41
1:A:1952:PHE:HE1	1:A:1976:HIS:CD2	2.39	0.41
1:A:2229:THR:CG2	1:A:2241:ILE:HG23	2.51	0.41
1:A:2250:SER:O	1:A:2254:GLN:HG3	2.21	0.41
1:A:2301:VAL:HG13	1:A:2340:ILE:HG23	2.02	0.41
1:A:2311:VAL:HG11	3:E:64:TYR:CG	2.56	0.41
1:A:2324:THR:C	1:A:2326:MET:H	2.29	0.41
1:A:2506:GLN:HG3	1:A:2546:ALA:HB1	2.02	0.41
1:A:3053:LEU:HD22	1:A:3156:TYR:CE1	2.56	0.41
1:A:3098:CYS:O	1:A:3101:VAL:HG12	2.21	0.41
1:A:3105:LEU:HB2	1:A:3197:TYR:OH	2.21	0.41
1:A:3236:HIS:O	1:A:3240:ILE:HG12	2.21	0.41
1:A:3413:ARG:NH1	1:A:3457:GLU:OE1	2.41	0.41
1:A:3951:VAL:HA	1:A:3968:LEU:HD22	2.03	0.41
1:A:4077:ILE:HG22	2:C:114:GLY:O	2.21	0.41
1:A:4717:PRO:O	1:A:4720:PRO:HD2	2.21	0.41
1:B:120:GLU:H	1:B:120:GLU:HG3	1.59	0.41
1:B:348:ALA:CB	1:B:421:ILE:HG23	2.51	0.41
1:B:945:LEU:HG	1:B:946:ASN:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1213:THR:O	1:B:1217:THR:HG23	2.20	0.41
1:B:2173:HIS:HE2	1:B:2253:LEU:HD11	1.86	0.41
1:B:2255:PRO:C	1:B:2257:LEU:H	2.29	0.41
1:B:2620:SER:C	1:B:2622:ILE:N	2.78	0.41
1:B:3031:GLU:O	1:B:3052:HIS:NE2	2.54	0.41
1:B:3453:SER:O	1:B:3456:PRO:HD2	2.20	0.41
1:B:4205:VAL:HG11	1:B:4248:PHE:CE2	2.56	0.41
1:B:4476:ALA:C	1:B:4521:ASN:HD21	2.25	0.41
2:D:106:LEU:O	2:D:110:MET:HG2	2.21	0.41
3:F:3:ARG:HG2	3:F:18:ARG:CG	2.49	0.41
3:F:94:GLN:HG3	3:F:132:LEU:HB3	2.03	0.41
1:A:478:ASN:O	1:A:482:LYS:HG3	2.20	0.41
1:A:659:THR:O	1:A:663:LEU:HB2	2.21	0.41
1:A:740:PHE:CD2	1:A:781:LYS:HG2	2.56	0.41
1:A:1051:VAL:HG13	1:A:1072:LEU:HG	2.02	0.41
1:A:1218:LEU:HD22	1:A:1376:ILE:HA	2.02	0.41
1:A:1240:GLU:H	1:A:1240:GLU:CD	2.29	0.41
1:A:1428:LEU:HD12	1:A:1488:ASN:HA	2.01	0.41
1:A:1664:CYS:SG	1:A:1666:PHE:HB3	2.61	0.41
1:A:1929:LEU:HD11	1:A:2241:ILE:HD11	2.02	0.41
1:A:2054:ASN:OD1	1:A:2058:LYS:N	2.53	0.41
1:A:4132:VAL:O	1:A:4133:LEU:C	2.64	0.41
1:A:4343:GLU:HB3	1:A:4426:LYS:NZ	2.36	0.41
1:B:268:ARG:HB3	1:B:272:ARG:HH21	1.85	0.41
1:B:1035:ILE:HD13	1:B:1035:ILE:HA	1.91	0.41
1:B:1870:PHE:HE2	1:B:2239:LEU:HD11	1.86	0.41
1:B:2191:MET:HB3	1:B:2198:LEU:HB2	2.03	0.41
1:B:2198:LEU:HD23	1:B:2198:LEU:HA	1.88	0.41
1:B:3000:MET:HE2	1:B:3000:MET:HB2	1.79	0.41
1:B:3095:VAL:HG11	1:B:3186:PHE:CE1	2.56	0.41
1:B:3439:SER:HB3	1:B:3443:GLN:HB2	2.03	0.41
1:B:3450:LEU:O	1:B:3454:ILE:HG13	2.21	0.41
1:B:3470:ASP:OD1	3:F:293:LEU:HG	2.20	0.41
1:B:3729:GLU:O	1:B:3730:GLU:C	2.64	0.41
1:B:4723:LEU:HD13	1:B:4763:LEU:HB2	2.01	0.41
2:C:79:ASP:OD1	2:C:79:ASP:N	2.54	0.41
1:A:73:PHE:CE1	1:A:155:MET:SD	3.14	0.40
1:A:484:LEU:HD22	1:A:530:LEU:HD11	2.03	0.40
1:A:1118:LEU:HD13	1:A:1273:LEU:HG	2.03	0.40
1:A:1499:ILE:HG22	1:A:1511:CYS:SG	2.60	0.40
1:A:1819:MET:HA	1:A:1822:ILE:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2173:HIS:CD2	1:A:2253:LEU:CD1	2.87	0.40
1:A:2410:ASP:HA	1:A:2411:PRO:HD3	1.94	0.40
1:A:3044:GLU:O	1:A:3049:ASN:ND2	2.53	0.40
1:A:3968:LEU:O	1:A:3969:GLN:C	2.63	0.40
1:A:4195:HIS:NE2	2:C:35:THR:CG2	2.85	0.40
1:A:4714:LEU:HD11	1:A:4754:VAL:CG1	2.49	0.40
1:B:129:LEU:HD23	1:B:129:LEU:HA	1.88	0.40
1:B:337:LEU:HD12	1:B:337:LEU:HA	1.94	0.40
1:B:484:LEU:HB3	1:B:657:PHE:CZ	2.56	0.40
1:B:491:LEU:HD13	1:B:521:ILE:HG13	2.03	0.40
1:B:1104:ILE:HG23	1:B:1110:LEU:CD1	2.51	0.40
1:B:1236:ILE:CG2	1:B:1282:ALA:HB2	2.51	0.40
1:B:1845:LEU:HA	1:B:2194:PRO:HA	2.02	0.40
1:B:2316:GLN:HE22	3:F:76:GLN:CD	2.29	0.40
1:B:3179:SER:O	1:B:3180:ARG:C	2.65	0.40
1:B:3298:ASP:HB3	1:B:3398:GLN:CD	2.45	0.40
1:B:4031:SER:HB3	3:F:310:GLU:OE2	2.21	0.40
1:B:4059:TRP:CE3	3:F:323:LEU:HD21	2.56	0.40
1:B:4307:LYS:HG2	1:B:4478:VAL:HG13	2.01	0.40
1:A:112:LEU:HD11	1:A:247:LEU:HD12	2.04	0.40
1:A:234:LYS:O	1:A:238:VAL:HG23	2.21	0.40
1:A:317:VAL:O	1:A:318:LEU:C	2.63	0.40
1:A:671:ARG:HB3	1:A:722:LEU:HD11	2.03	0.40
1:A:741:SER:OG	1:A:785:ARG:NH1	2.54	0.40
1:A:1025:MET:HE2	1:A:1025:MET:HB3	1.88	0.40
1:A:1137:GLU:HG2	1:A:1141:LYS:HD2	2.04	0.40
1:A:1204:ILE:HG21	1:A:1218:LEU:HD12	2.03	0.40
1:A:1392:GLN:CD	1:A:1392:GLN:H	2.28	0.40
1:A:1996:LEU:HB3	1:A:2000:ASN:HB3	2.03	0.40
1:A:2060:ILE:HG12	1:A:2074:LEU:HD12	2.03	0.40
1:A:2369:GLU:HA	1:A:2373:ARG:O	2.20	0.40
1:A:4059:TRP:CE3	3:E:323:LEU:HD21	2.56	0.40
1:A:4127:ASN:C	1:A:4129:LEU:N	2.78	0.40
1:A:4187:TYR:O	1:A:4191:ILE:HG12	2.21	0.40
1:A:4201:ALA:HA	1:A:4205:VAL:HG12	2.03	0.40
1:A:4280:ARG:NH1	1:A:4285:ASP:OD2	2.52	0.40
1:A:4363:LEU:HD21	1:A:4444:MET:HG3	2.02	0.40
1:B:322:ASN:O	1:B:323:PRO:C	2.63	0.40
1:B:336:CYS:O	1:B:337:LEU:C	2.63	0.40
1:B:684:ALA:HA	1:B:734:GLN:HG3	2.03	0.40
1:B:905:THR:HG22	1:B:906:PRO:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1079:LYS:C	1:B:1081:SER:H	2.28	0.40
1:B:2042:PRO:HD3	1:B:2088:VAL:O	2.21	0.40
1:B:2220:THR:HG23	1:B:2224:GLU:HA	2.02	0.40
1:B:3289:ASN:HA	1:B:3292:LYS:NZ	2.36	0.40
1:B:3295:ILE:HD13	1:B:3395:LEU:HD23	2.03	0.40
1:B:3742:LEU:HD13	1:B:3820:LYS:HG2	2.03	0.40
1:B:4273:LEU:O	1:B:4280:ARG:NH2	2.53	0.40
1:B:4716:ARG:HA	1:B:4717:PRO:HD3	1.92	0.40
2:D:50:GLN:HA	2:D:53:ILE:HG22	2.03	0.40
3:F:65:TYR:HB3	3:F:70:PHE:CE2	2.56	0.40
1:A:81:SER:O	1:A:85:ILE:HG13	2.21	0.40
1:A:793:ASN:HB3	1:A:854:ILE:HG13	2.02	0.40
1:A:864:TYR:C	1:A:866:LEU:H	2.30	0.40
1:A:1055:LYS:O	1:A:1059:ILE:HG13	2.22	0.40
1:A:1063:MET:SD	1:A:1068:ALA:HB2	2.62	0.40
1:A:1806:SER:C	1:A:1809:PRO:HD2	2.47	0.40
1:A:3196:GLU:HA	1:A:3199:MET:HG2	2.02	0.40
1:A:4325:TYR:CE1	1:A:4495:ILE:HA	2.56	0.40
1:B:507:ALA:O	1:B:523:ARG:NE	2.51	0.40
1:B:791:LYS:HD3	1:B:836:ILE:HG12	2.03	0.40
1:B:833:PHE:HE1	1:B:858:LEU:HD22	1.87	0.40
1:B:855:LEU:CD2	1:B:1002:TYR:HE2	2.34	0.40
1:B:1110:LEU:H	1:B:1175:ALA:HB2	1.86	0.40
1:B:1242:PRO:HB2	1:B:1251:PHE:HZ	1.87	0.40
1:B:1528:ASN:HD22	1:B:1528:ASN:H	1.68	0.40
1:B:1822:ILE:CG2	1:B:1826:PHE:CE2	3.04	0.40
1:B:2702:ILE:HA	1:B:3005:MET:HG2	2.03	0.40
1:B:3013:GLU:HG2	1:B:3077:SER:HB3	2.03	0.40
1:B:3106:LEU:HG	1:B:3110:LYS:HE3	2.02	0.40
1:B:3177:THR:OG1	1:B:3178:ASN:N	2.55	0.40
1:B:3304:LEU:HD23	1:B:3304:LEU:HA	1.93	0.40
1:B:4132:VAL:HA	1:B:4135:THR:HG23	2.02	0.40
1:B:4596:MET:O	1:B:4600:GLN:HG2	2.21	0.40
1:A:193:PHE:CZ	1:B:816:LEU:HD21	2.56	0.40
1:A:545:ALA:HB1	1:A:648:LEU:HG	2.04	0.40
1:A:718:VAL:HG13	1:A:760:LEU:HG	2.03	0.40
1:A:918:TRP:HA	1:A:918:TRP:CE3	2.56	0.40
1:A:1176:TYR:CD1	1:A:1281:ALA:CB	3.05	0.40
1:A:1219:VAL:O	1:A:1222:LEU:HB2	2.20	0.40
1:A:1312:ARG:O	1:A:1316:PRO:HD3	2.21	0.40
1:A:1447:LEU:HA	1:A:1505:GLN:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2302:GLU:HG3	1:A:2343:ASN:HD21	1.86	0.40
1:A:4251:VAL:HB	1:A:4254:ILE:HD12	2.02	0.40
1:B:408:LEU:HD13	1:B:520:ARG:HB3	2.04	0.40
1:B:952:ALA:O	1:B:956:LEU:HG	2.21	0.40
1:B:1109:ILE:HG23	1:B:1178:LEU:HD12	2.03	0.40
1:B:1127:ALA:O	1:B:1131:VAL:HG22	2.21	0.40
1:B:1314:LEU:HA	1:B:1317:LEU:HD12	2.02	0.40
1:B:1474:SER:HA	1:B:1485:ILE:CD1	2.51	0.40
1:B:2680:LYS:O	1:B:2684:GLN:HG3	2.22	0.40
1:B:2702:ILE:HD11	1:B:3001:GLN:CD	2.46	0.40
1:B:3556:TYR:O	1:B:3606:LYS:CE	2.67	0.40
1:B:3893:ASN:HB3	1:B:3896:LEU:HB2	2.03	0.40
1:B:4274:ARG:HB2	1:B:4288:GLN:HE22	1.86	0.40
1:B:4303:GLU:O	1:B:4307:LYS:HG3	2.21	0.40
1:B:4325:TYR:O	1:B:4329:VAL:HG23	2.22	0.40
1:B:4609:ASN:HB3	1:B:4612:VAL:HB	2.02	0.40
2:D:52:MET:O	2:D:55:GLU:HB3	2.21	0.40
1:A:268:ARG:O	1:A:272:ARG:HG3	2.22	0.40
1:A:659:THR:HA	1:A:663:LEU:HB2	2.02	0.40
1:A:1416:ASN:O	1:A:1470:ARG:NH1	2.52	0.40
1:A:3034:MET:HG2	1:A:3035:ASP:N	2.36	0.40
1:A:3393:THR:HA	1:A:3396:VAL:HG12	2.04	0.40
1:A:4601:ILE:HA	1:A:4606:VAL:HG11	2.02	0.40
1:B:31:VAL:O	1:B:35:PRO:CD	2.69	0.40
1:B:60:GLU:HG3	1:B:106:VAL:HG13	2.02	0.40
1:B:747:LEU:HD11	1:B:793:ASN:ND2	2.37	0.40
1:B:1424:CYS:O	1:B:1428:LEU:HG	2.21	0.40
1:B:1666:PHE:HA	1:B:1669:THR:OG1	2.21	0.40
1:B:2311:VAL:HG13	3:F:56:LEU:HD11	2.02	0.40
1:B:2686:LEU:CD2	1:B:3002:VAL:HG21	2.49	0.40
1:B:3789:SER:O	1:B:3797:LEU:HD11	2.21	0.40
1:B:4062:ARG:HB2	1:B:4062:ARG:NH1	2.37	0.40
1:B:4316:THR:O	1:B:4319:ARG:HB2	2.21	0.40
2:D:67:PRO:HA	2:D:70:LEU:HB3	2.04	0.40
2:D:137:VAL:CG1	2:D:141:GLU:HB2	2.50	0.40
2:D:143:VAL:O	2:D:147:THR:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3853/5205 (74%)	3738 (97%)	115 (3%)	0	100	100
1	B	3884/5205 (75%)	3762 (97%)	122 (3%)	0	100	100
2	C	142/149 (95%)	136 (96%)	6 (4%)	0	100	100
2	D	139/149 (93%)	132 (95%)	7 (5%)	0	100	100
3	E	178/381 (47%)	175 (98%)	3 (2%)	0	100	100
3	F	178/381 (47%)	170 (96%)	8 (4%)	0	100	100
All	All	8374/11470 (73%)	8113 (97%)	261 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3438/4542 (76%)	3329 (97%)	109 (3%)	34	59
1	B	3474/4542 (76%)	3347 (96%)	127 (4%)	29	54
2	C	123/127 (97%)	118 (96%)	5 (4%)	26	51
2	D	122/127 (96%)	115 (94%)	7 (6%)	17	43
3	E	162/330 (49%)	161 (99%)	1 (1%)	84	90
3	F	162/330 (49%)	159 (98%)	3 (2%)	52	71
All	All	7481/9998 (75%)	7229 (97%)	252 (3%)	34	57

All (252) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	VAL
1	A	44	PHE
1	A	69	GLN
1	A	92	ILE
1	A	94	ARG
1	A	97	LEU
1	A	100	VAL
1	A	191	MET
1	A	277	VAL
1	A	284	ILE
1	A	318	LEU
1	A	347	MET
1	A	401	GLU
1	A	444	VAL
1	A	530	LEU
1	A	686	LEU
1	A	722	LEU
1	A	771	GLN
1	A	799	VAL
1	A	807	ASN
1	A	813	MET
1	A	830	LEU
1	A	909	HIS
1	A	911	PHE
1	A	913	GLU
1	A	937	SER
1	A	984	ARG
1	A	1040	ARG
1	A	1045	LEU
1	A	1046	ARG
1	A	1061	GLN
1	A	1063	MET
1	A	1072	LEU
1	A	1113	HIS
1	A	1131	VAL
1	A	1154	ILE
1	A	1159	LEU
1	A	1173	THR
1	A	1177	LEU
1	A	1214	LEU
1	A	1244	ILE
1	A	1301	TRP

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Mol	Chain	Res	Type
1	A	1303	ASP
1	A	1318	LEU
1	A	1384	LEU
1	A	1471	MET
1	A	1481	GLN
1	A	1484	VAL
1	A	1485	ILE
1	A	1486	GLN
1	A	1496	THR
1	A	1500	VAL
1	A	1528	ASN
1	A	1553	HIS
1	A	1554	LEU
1	A	1556	LEU
1	A	1594	GLU
1	A	1607	THR
1	A	1690	VAL
1	A	1714	PHE
1	A	1894	LEU
1	A	1906	HIS
1	A	1950	VAL
1	A	1956	SER
1	A	2180	VAL
1	A	2184	THR
1	A	2204	THR
1	A	2301	VAL
1	A	2475	LEU
1	A	2488	SER
1	A	2667	TYR
1	A	2695	PHE
1	A	2698	LYS
1	A	2984	THR
1	A	2994	VAL
1	A	3056	MET
1	A	3108	TYR
1	A	3141	LEU
1	A	3159	LEU
1	A	3237	VAL
1	A	3286	ARG
1	A	3315	VAL
1	A	3332	VAL
1	A	3458	LEU

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Mol	Chain	Res	Type
1	A	3522	PHE
1	A	3536	ASN
1	A	3581	LEU
1	A	3765	CYS
1	A	3793	ASN
1	A	3866	HIS
1	A	3994	LEU
1	A	3999	MET
1	A	4007	VAL
1	A	4127	ASN
1	A	4129	LEU
1	A	4135	THR
1	A	4230	THR
1	A	4277	VAL
1	A	4309	PHE
1	A	4310	MET
1	A	4316	THR
1	A	4335	LEU
1	A	4400	LEU
1	A	4447	LEU
1	A	4478	VAL
1	A	4505	LEU
1	A	4520	VAL
1	A	4601	ILE
1	A	4616	LEU
1	B	33	VAL
1	B	37	LEU
1	B	70	TYR
1	B	86	THR
1	B	92	ILE
1	B	96	GLN
1	B	97	LEU
1	B	113	LEU
1	B	124	VAL
1	B	130	ILE
1	B	147	GLU
1	B	154	MET
1	B	194	LEU
1	B	200	VAL
1	B	204	ARG
1	B	243	ASN
1	B	283	PHE

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Mol	Chain	Res	Type
1	B	312	THR
1	B	313	LEU
1	B	318	LEU
1	B	325	ARG
1	B	367	GLU
1	B	378	VAL
1	B	379	GLN
1	B	381	CYS
1	B	408	LEU
1	B	424	LEU
1	B	448	LEU
1	B	511	ILE
1	B	528	VAL
1	B	677	SER
1	B	680	GLU
1	B	686	LEU
1	B	698	LEU
1	B	703	ASP
1	B	717	LEU
1	B	727	LEU
1	B	799	VAL
1	B	813	MET
1	B	830	LEU
1	B	844	MET
1	B	867	HIS
1	B	909	HIS
1	B	911	PHE
1	B	922	PHE
1	B	936	LEU
1	B	939	GLU
1	B	943	ASP
1	B	948	LEU
1	B	981	ASP
1	B	992	THR
1	B	1036	LEU
1	B	1040	ARG
1	B	1045	LEU
1	B	1057	HIS
1	B	1112	LEU
1	B	1131	VAL
1	B	1204	ILE
1	B	1212	ASN

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Mol	Chain	Res	Type
1	B	1240	GLU
1	B	1299	ILE
1	B	1318	LEU
1	B	1326	VAL
1	B	1334	LEU
1	B	1338	LEU
1	B	1358	CYS
1	B	1387	GLN
1	B	1392	GLN
1	B	1470	ARG
1	B	1474	SER
1	B	1486	GLN
1	B	1528	ASN
1	B	1536	GLU
1	B	1549	GLN
1	B	1553	HIS
1	B	1554	LEU
1	B	1557	HIS
1	B	1595	CYS
1	B	1597	CYS
1	B	1664	CYS
1	B	1800	GLN
1	B	1805	PHE
1	B	1817	PHE
1	B	1873	VAL
1	B	1934	ASP
1	B	2300	ASP
1	B	2301	VAL
1	B	2673	ASP
1	B	2676	ASN
1	B	2974	ARG
1	B	2982	LEU
1	B	2985	LEU
1	B	2995	ARG
1	B	3001	GLN
1	B	3002	VAL
1	B	3003	ILE
1	B	3005	MET
1	B	3034	MET
1	B	3038	ASP
1	B	3045	ARG
1	B	3049	ASN

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Mol	Chain	Res	Type
1	B	3050	GLU
1	B	3098	CYS
1	B	3197	TYR
1	B	3285	GLN
1	B	3286	ARG
1	B	3328	CYS
1	B	3458	LEU
1	B	3543	CYS
1	B	3581	LEU
1	B	3968	LEU
1	B	4135	THR
1	B	4228	LEU
1	B	4230	THR
1	B	4276	LEU
1	B	4277	VAL
1	B	4279	GLN
1	B	4297	ASP
1	B	4329	VAL
1	B	4331	ILE
1	B	4400	LEU
1	B	4447	LEU
1	B	4593	GLN
1	B	4612	VAL
1	B	4634	LEU
1	B	4752	GLU
1	B	4773	GLU
2	C	33	LEU
2	C	49	LEU
2	C	79	ASP
2	C	96	ASP
2	C	101	ILE
2	D	21	ASP
2	D	28	ILE
2	D	33	LEU
2	D	49	LEU
2	D	63	THR
2	D	64	ILE
2	D	105	GLU
3	E	131	HIS
3	F	70	PHE
3	F	131	HIS
3	F	136	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (140) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	98	GLN
1	A	196	GLN
1	A	229	GLN
1	A	243	ASN
1	A	271	ASN
1	A	274	GLN
1	A	327	GLN
1	A	402	HIS
1	A	407	GLN
1	A	466	HIS
1	A	479	HIS
1	A	664	ASN
1	A	712	HIS
1	A	714	ASN
1	A	729	ASN
1	A	792	GLN
1	A	867	HIS
1	A	868	GLN
1	A	879	GLN
1	A	881	GLN
1	A	917	ASN
1	A	1067	HIS
1	A	1182	ASN
1	A	1227	GLN
1	A	1253	ASN
1	A	1364	ASN
1	A	1365	HIS
1	A	1418	ASN
1	A	1481	GLN
1	A	1486	GLN
1	A	1493	GLN
1	A	1553	HIS
1	A	1598	HIS
1	A	1682	HIS
1	A	1802	GLN
1	A	1892	HIS
1	A	1916	HIS
1	A	2296	GLN
1	A	2343	ASN
1	A	2990	ASN

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Mol	Chain	Res	Type
1	A	3023	ASN
1	A	3148	HIS
1	A	3178	ASN
1	A	3321	GLN
1	A	3397	ASN
1	A	3410	GLN
1	A	3491	GLN
1	A	3536	ASN
1	A	3591	ASN
1	A	3639	ASN
1	A	3683	GLN
1	A	3740	ASN
1	A	3759	GLN
1	A	3835	GLN
1	A	4011	ASN
1	A	4127	ASN
1	A	4161	GLN
1	A	4234	GLN
1	A	4279	GLN
1	A	4490	ASN
1	A	4602	ASN
1	B	69	GLN
1	B	83	HIS
1	B	98	GLN
1	B	192	ASN
1	B	229	GLN
1	B	243	ASN
1	B	262	ASN
1	B	274	GLN
1	B	379	GLN
1	B	407	GLN
1	B	656	ASN
1	B	729	ASN
1	B	867	HIS
1	B	881	GLN
1	B	882	HIS
1	B	921	HIS
1	B	979	GLN
1	B	1022	GLN
1	B	1097	GLN
1	B	1111	GLN
1	B	1113	HIS

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Mol	Chain	Res	Type
1	B	1132	GLN
1	B	1227	GLN
1	B	1234	ASN
1	B	1266	GLN
1	B	1306	ASN
1	B	1309	GLN
1	B	1364	ASN
1	B	1387	GLN
1	B	1418	ASN
1	B	1486	GLN
1	B	1493	GLN
1	B	1528	ASN
1	B	1553	HIS
1	B	1558	ASN
1	B	1573	GLN
1	B	1800	GLN
1	B	1925	GLN
1	B	2182	GLN
1	B	2219	HIS
1	B	2258	GLN
1	B	2294	HIS
1	B	2296	GLN
1	B	2316	GLN
1	B	2319	HIS
1	B	2522	GLN
1	B	2524	GLN
1	B	2699	GLN
1	B	2983	GLN
1	B	2990	ASN
1	B	3001	GLN
1	B	3049	ASN
1	B	3209	GLN
1	B	3397	ASN
1	B	3438	ASN
1	B	3491	GLN
1	B	3591	ASN
1	B	3639	ASN
1	B	3683	GLN
1	B	3740	ASN
1	B	3756	HIS
1	B	3835	GLN
1	B	3848	GLN

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Mol	Chain	Res	Type
1	B	4002	ASN
1	B	4021	GLN
1	B	4233	GLN
1	B	4490	ASN
1	B	4602	ASN
1	B	4766	ASN
2	C	43	ASN
2	C	54	ASN
2	C	98	ASN
2	C	138	ASN
2	D	54	ASN
2	D	61	ASN
2	D	98	ASN
3	F	74	GLN
3	F	76	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

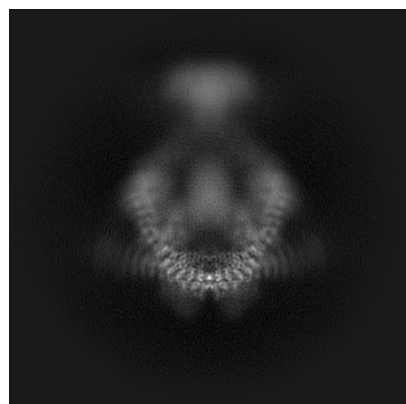
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46686. These allow visual inspection of the internal detail of the map and identification of artifacts.

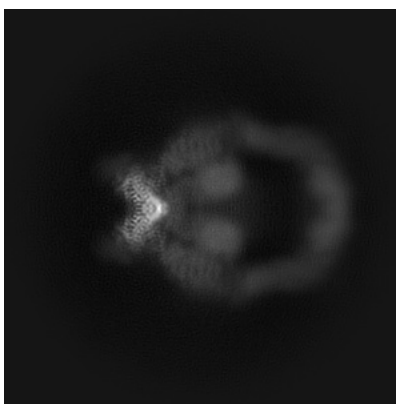
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

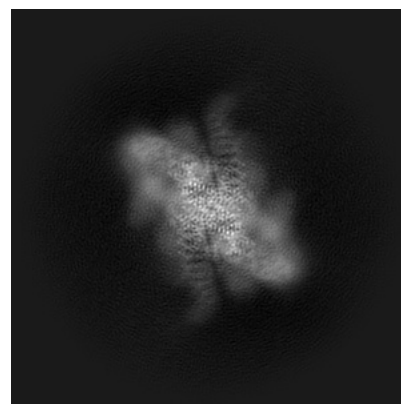
6.1.1 Primary map



X

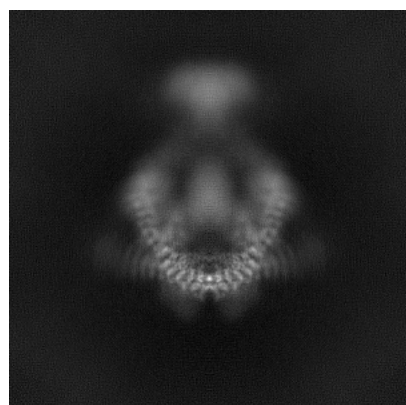


Y

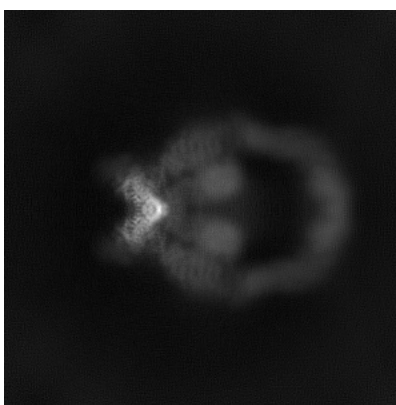


Z

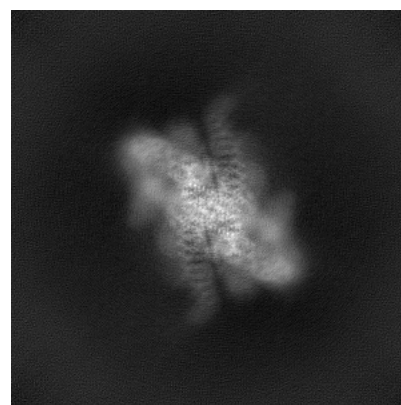
6.1.2 Raw map



X



Y

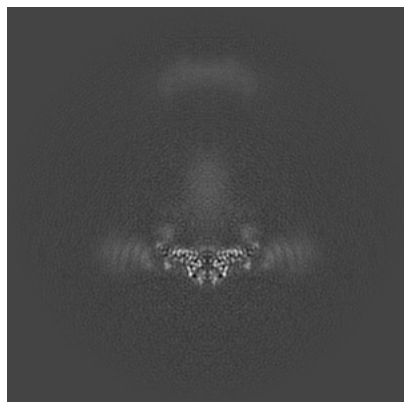


Z

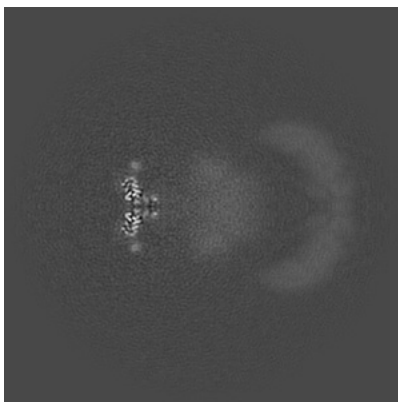
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

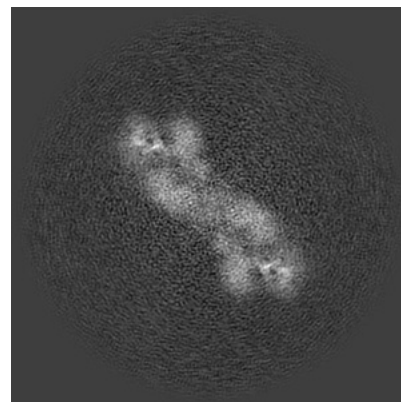
6.2.1 Primary map



X Index: 210



Y Index: 210

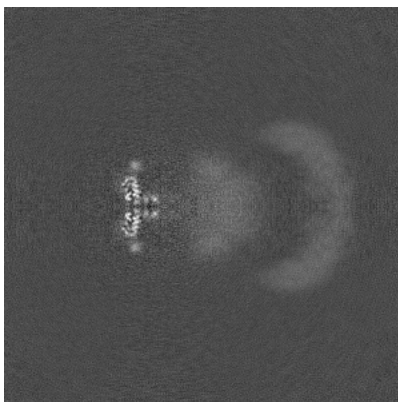


Z Index: 210

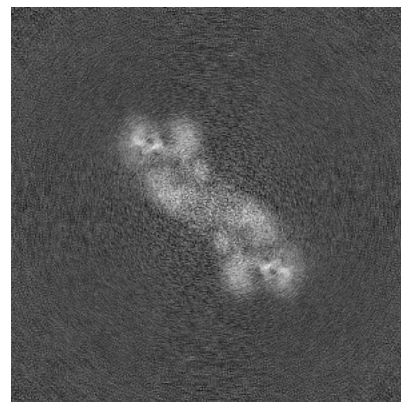
6.2.2 Raw map



X Index: 210



Y Index: 210



Z Index: 210

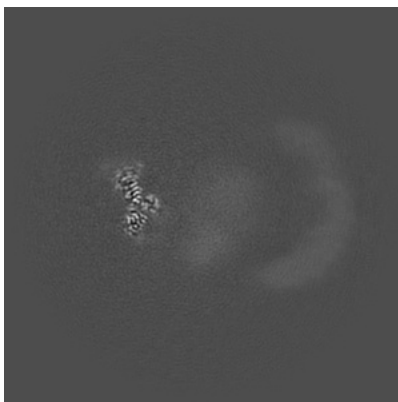
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

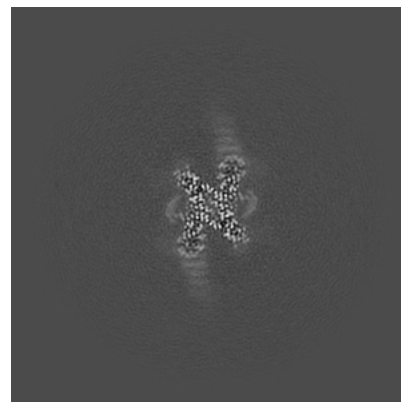
6.3.1 Primary map



X Index: 193

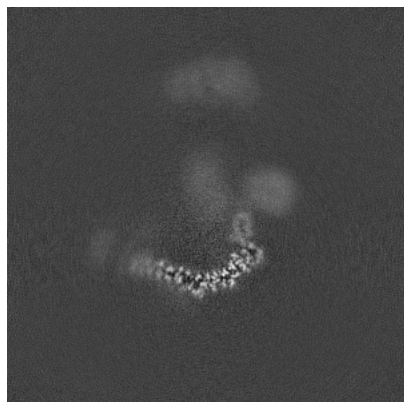


Y Index: 221

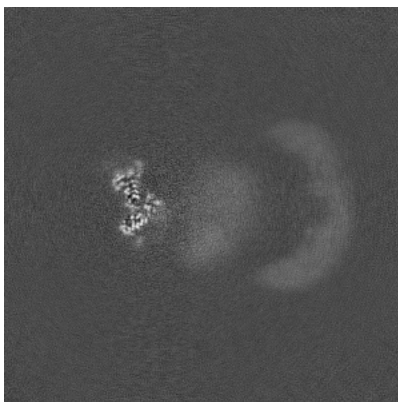


Z Index: 140

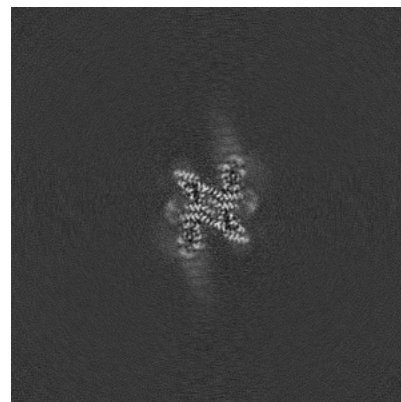
6.3.2 Raw map



X Index: 188



Y Index: 218

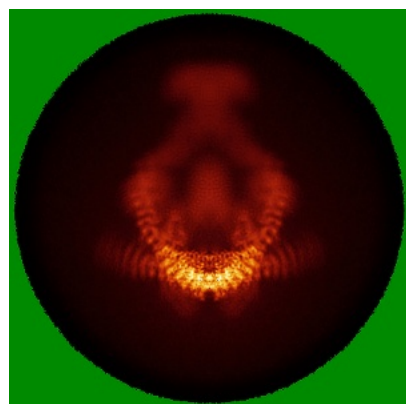


Z Index: 138

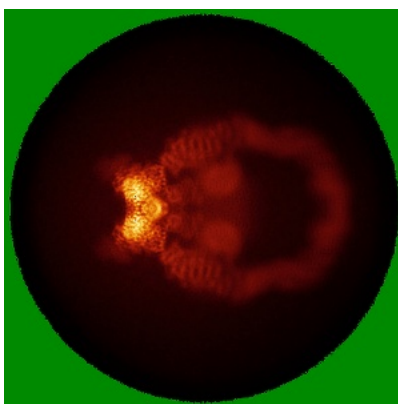
The images above show the largest variance slices of the map in three orthogonal directions.

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

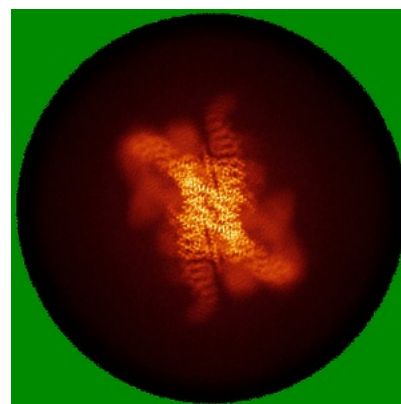
6.4.1 Primary map



X

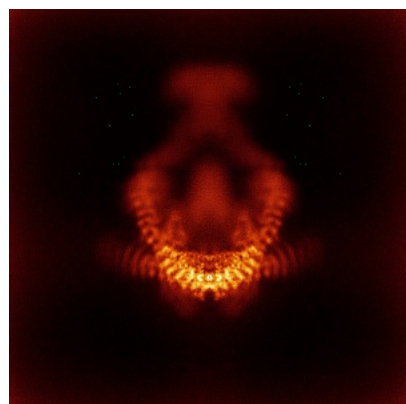


Y

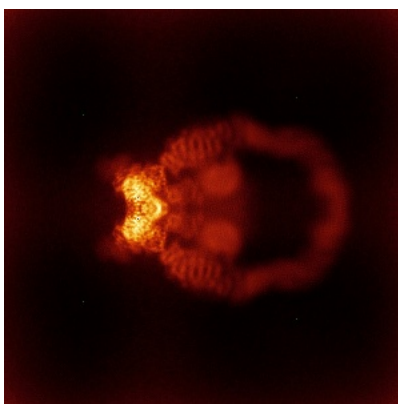


Z

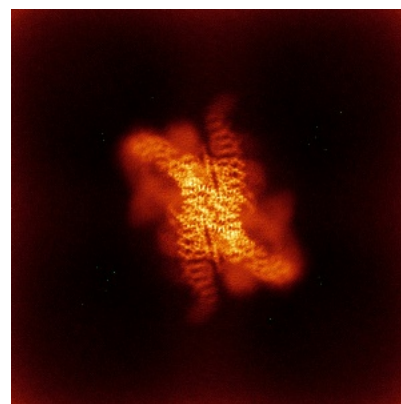
6.4.2 Raw map



X



Y

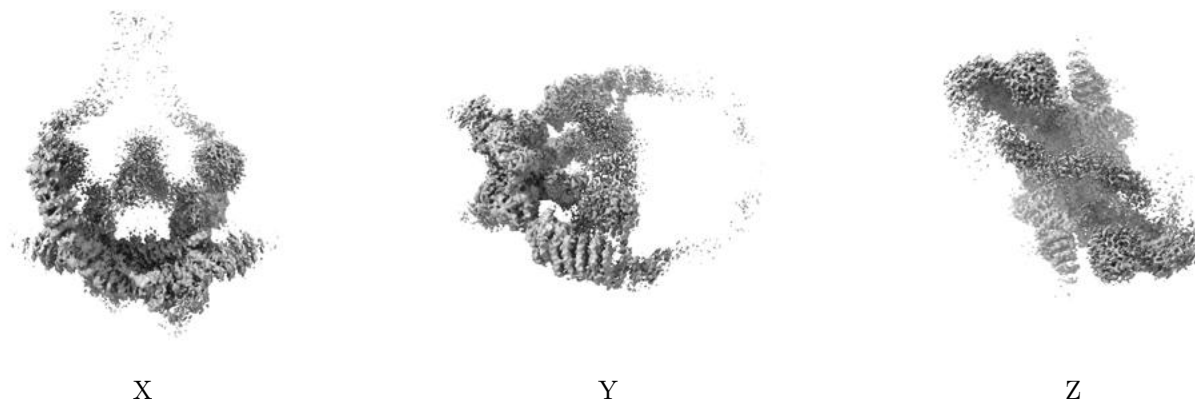


Z

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

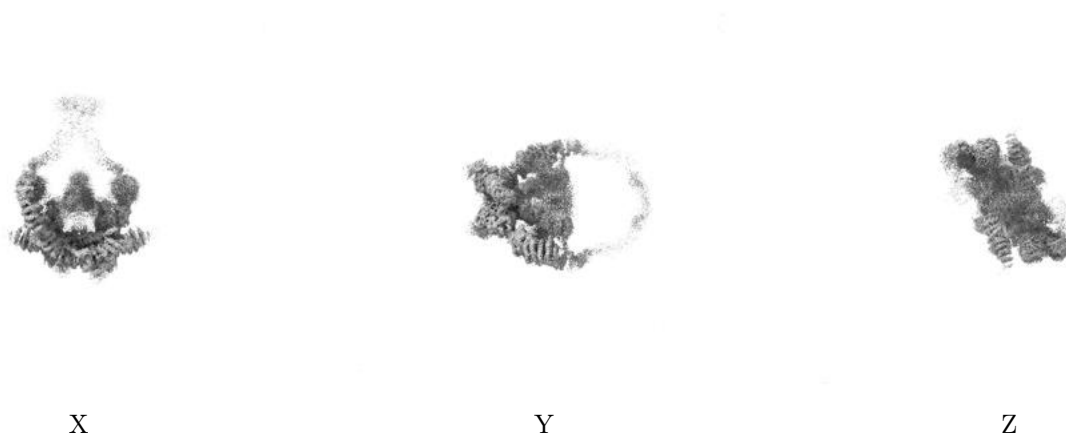
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

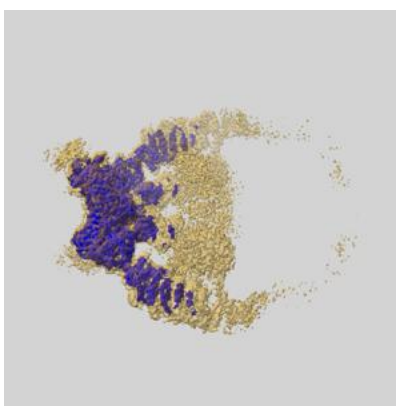
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

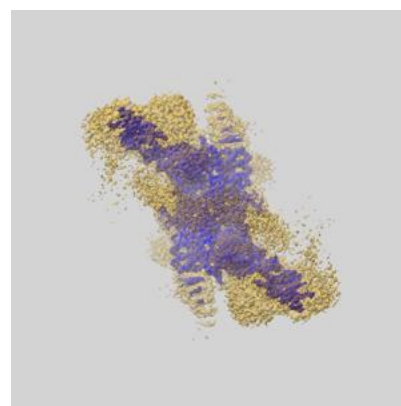
6.6.1 emd_46686_msk_1.map [i](#)



X



Y

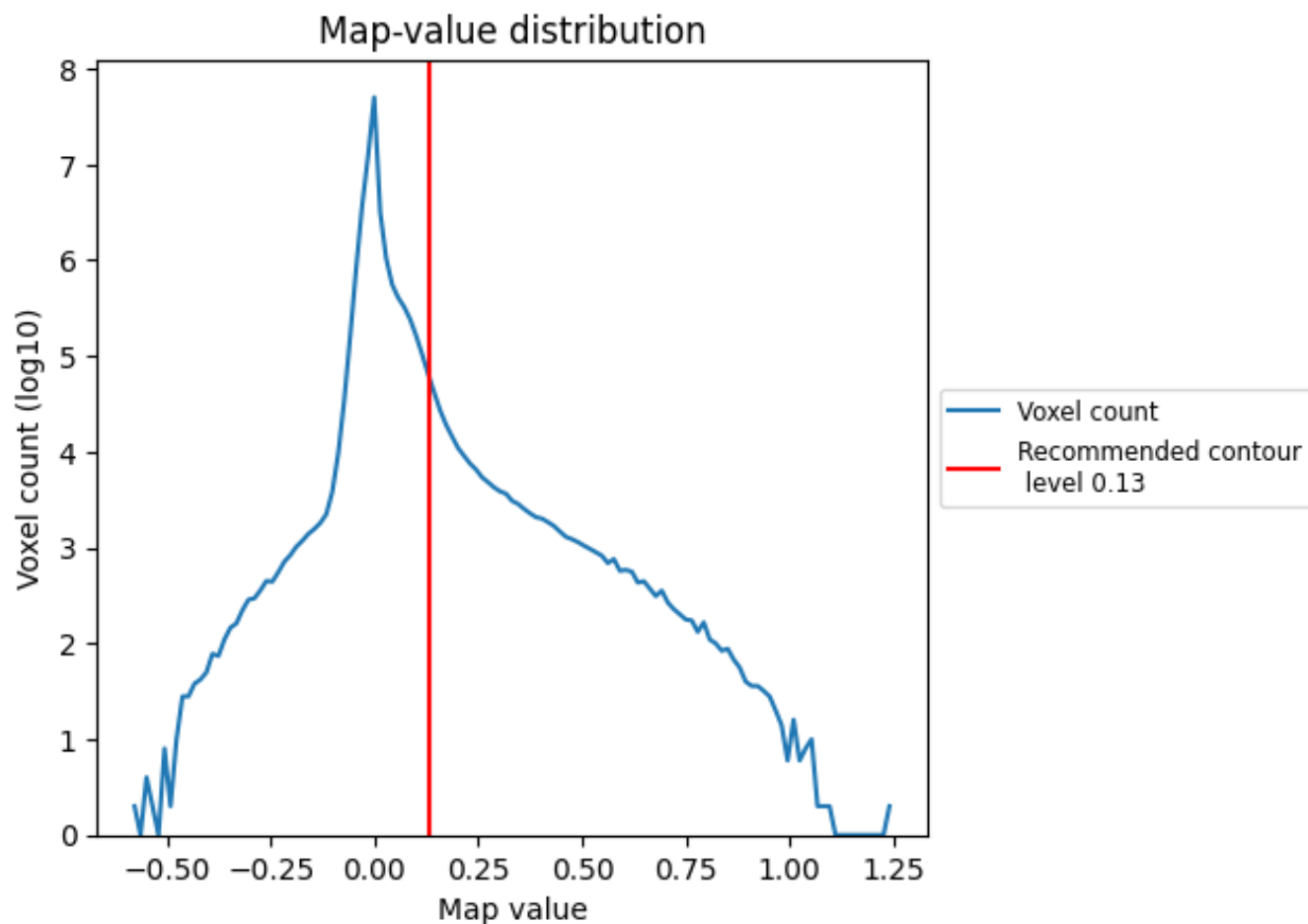


Z

7 Map analysis [i](#)

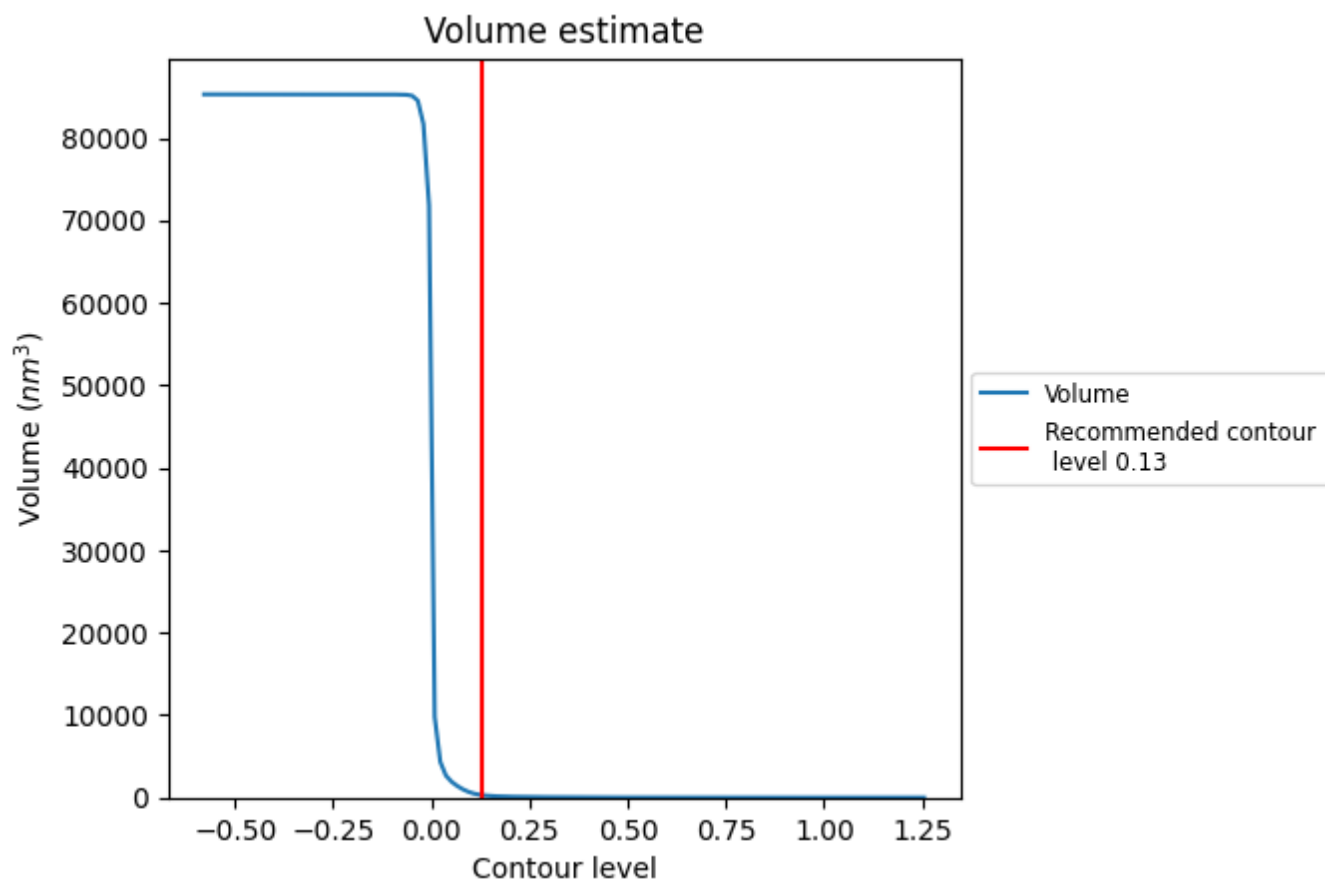
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

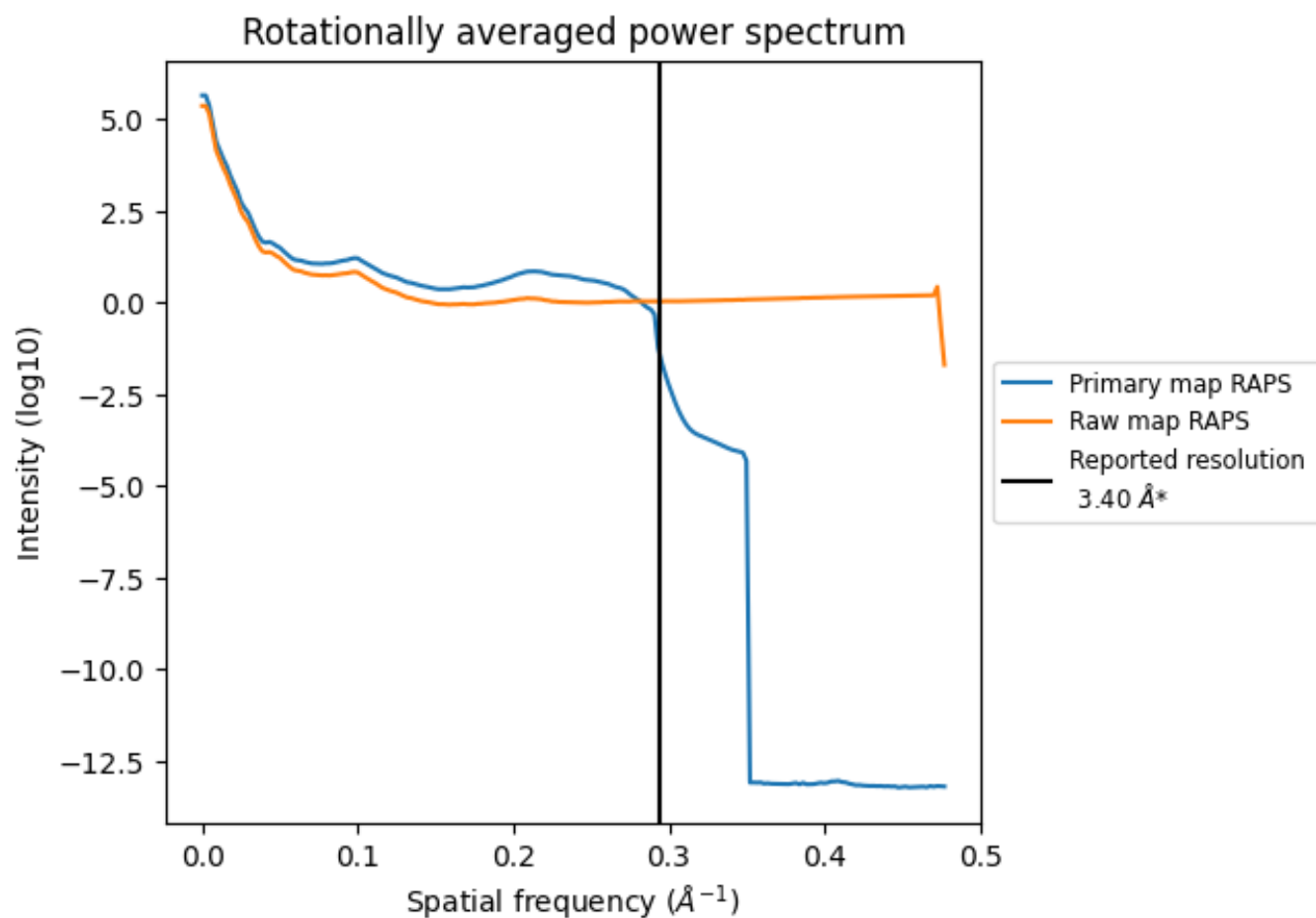
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 296 nm^3 ; this corresponds to an approximate mass of 268 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

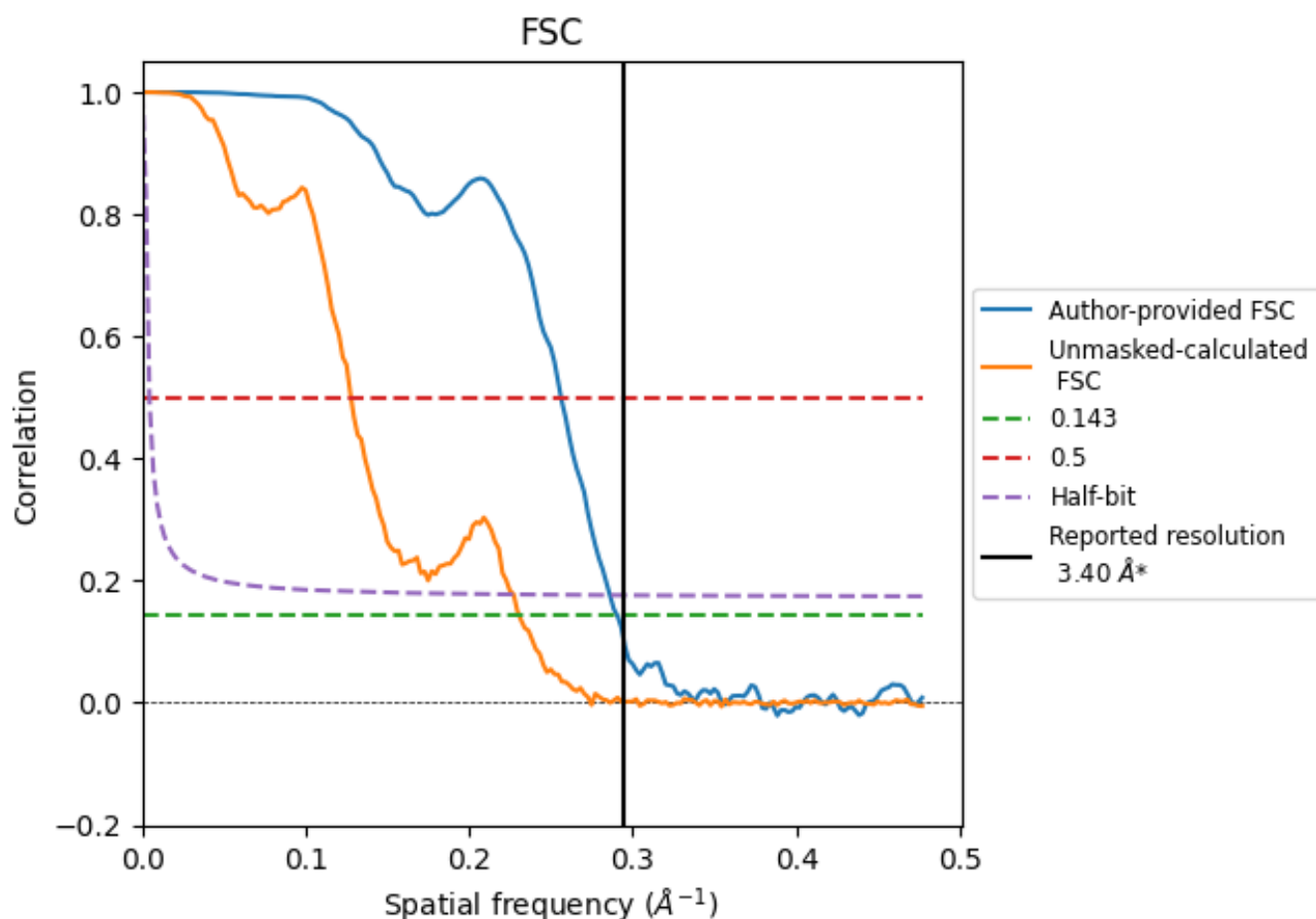


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

8.2 Resolution estimates [i](#)

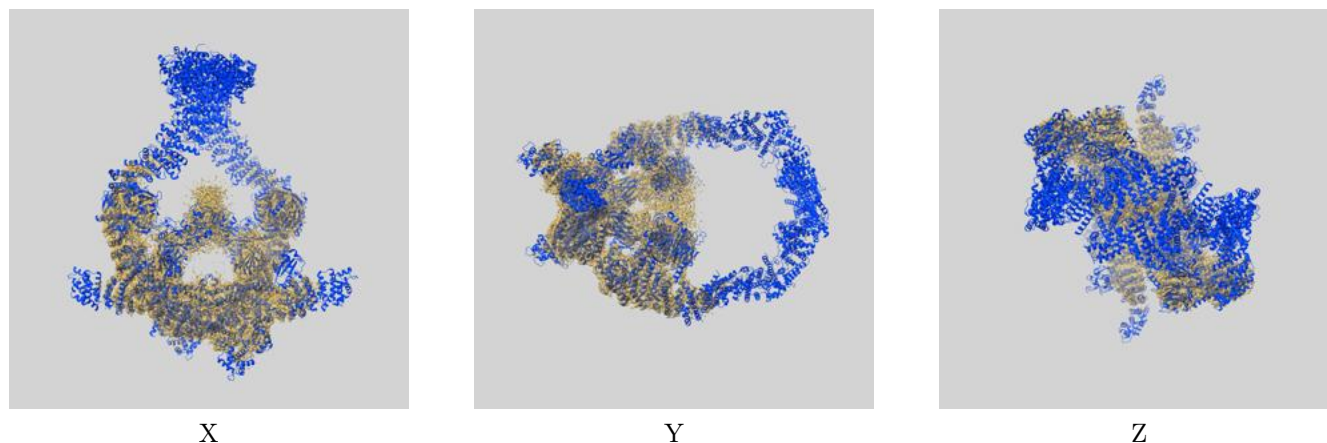
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.44	3.90	3.50
Unmasked-calculated*	4.34	7.83	4.40

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.34 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

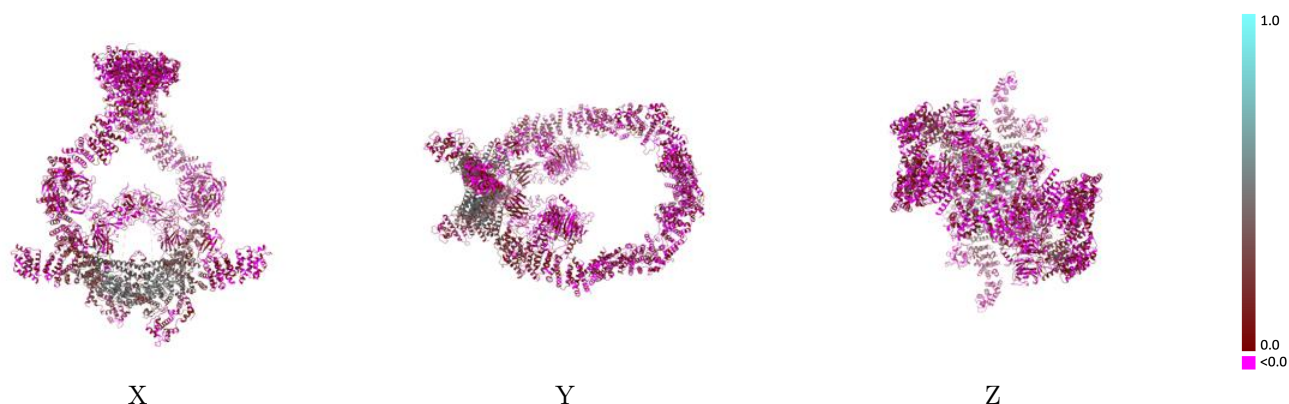
This section contains information regarding the fit between EMDB map EMD-46686 and PDB model 9D9Z. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



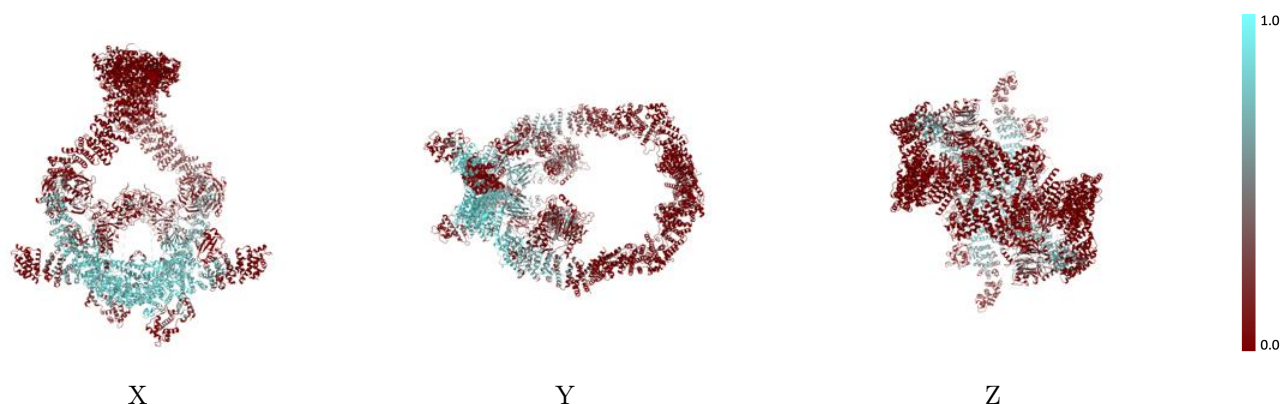
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



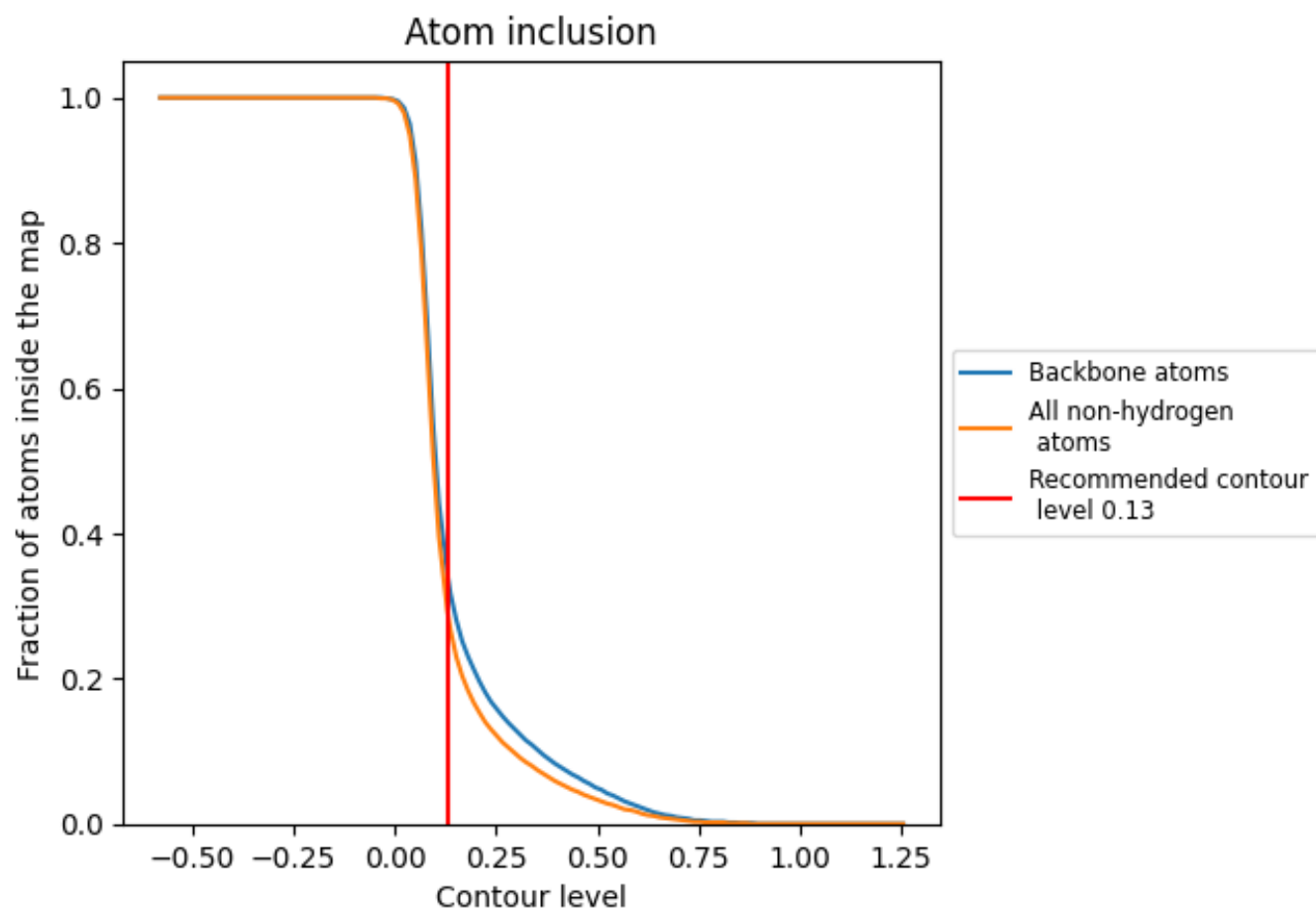
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.13).

9.4 Atom inclusion [i](#)



At the recommended contour level, 34% of all backbone atoms, 29% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.2930	<div></div> 0.1100
A	<div></div> 0.3000	<div></div> 0.1120
B	<div></div> 0.2990	<div></div> 0.1130
C	<div></div> 0.1500	<div></div> 0.0740
D	<div></div> 0.1350	<div></div> 0.0820
E	<div></div> 0.2720	<div></div> 0.0850
F	<div></div> 0.2740	<div></div> 0.0890

1.0

0.0

<0.0