



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:31 PM UTC

PDB ID : 5UAQ / pdb_00005uaq
Title : Escherichia coli RNA polymerase RpoB H526Y mutant
Authors : Molodtsov, V.; Scharf, N.T.; Stefan, M.A.; Garcia, G.A.; Murakami, K.S.
Deposited on : 2016-12-19
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

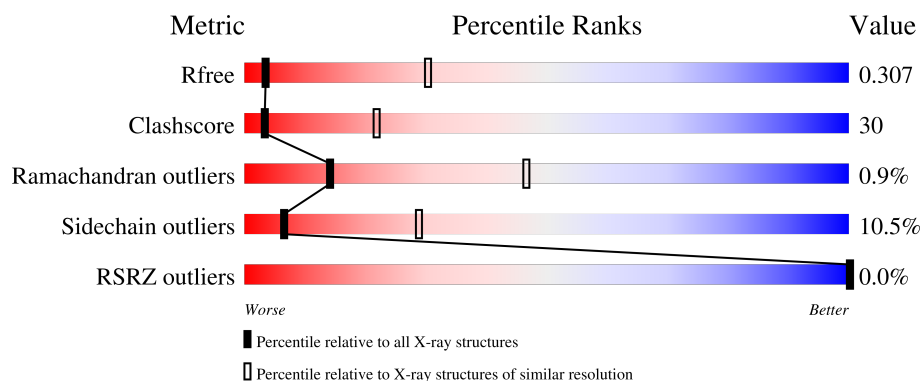
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	329	
1	B	329	
1	G	329	
1	H	329	
2	C	1342	

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Mol	Chain	Length	Quality of chain
2	I	1342	48% 45% 6%
3	D	1407	35% 40% 8% 17%
3	J	1407	36% 39% 7% 18%
4	E	91	63% 32% • •
4	K	91	% 49% 36% • 13%
5	F	613	38% 34% • 24%
5	L	613	35% 37% 5% 23%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 55699 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2403	1505	421	469	8			
1	B	217	Total	C	N	O	S	0	0	0
			1672	1044	295	327	6			
1	G	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	H	217	Total	C	N	O	S	0	0	0
			1667	1041	293	327	6			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10572	6634	1839	2056	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10568	6632	1838	2055	43			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	526	TYR	HIS	engineered mutation	UNP P0A8V2
I	526	TYR	HIS	engineered mutation	UNP P0A8V2

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1166	Total	C	N	O	S	0	0	0
			9107	5723	1634	1704	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9029	5676	1620	1687	46			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	467	Total	C	N	O	S	0	0	0
			3806	2385	677	721	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		
6	J	1	Total	Mg	0	0
			1	1		

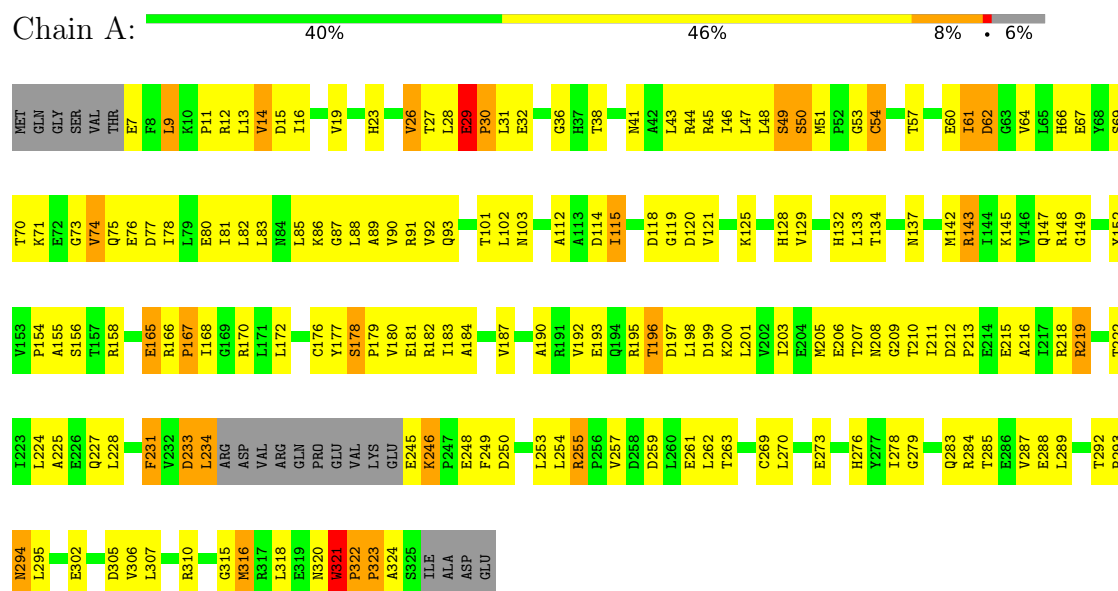
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	2	Total	Zn	0	0
			2	2		
7	J	2	Total	Zn	0	0
			2	2		

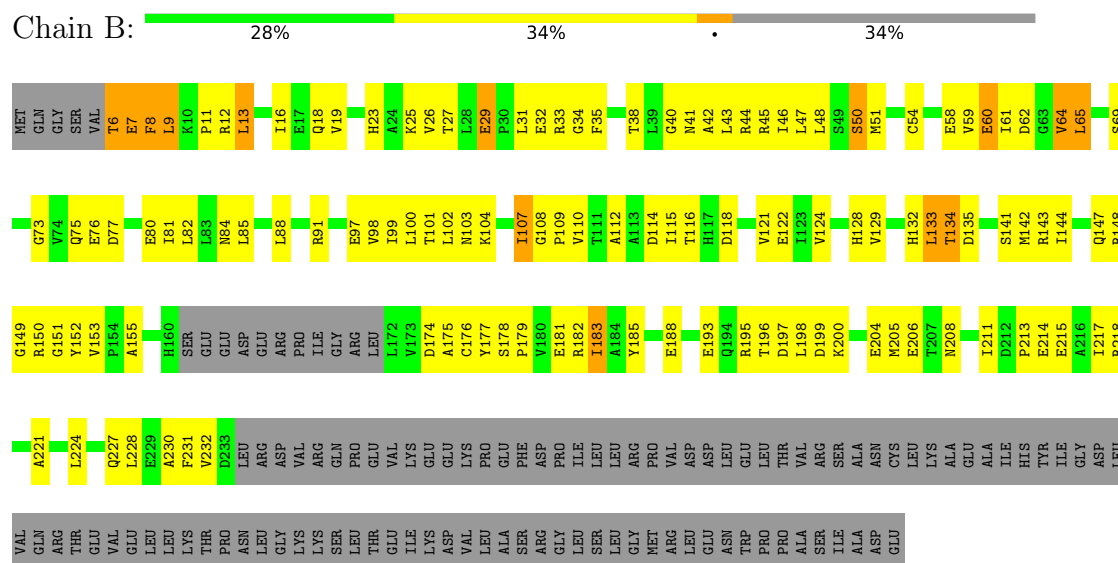
3 Residue-property plots

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 electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

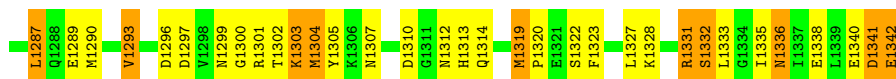
• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha

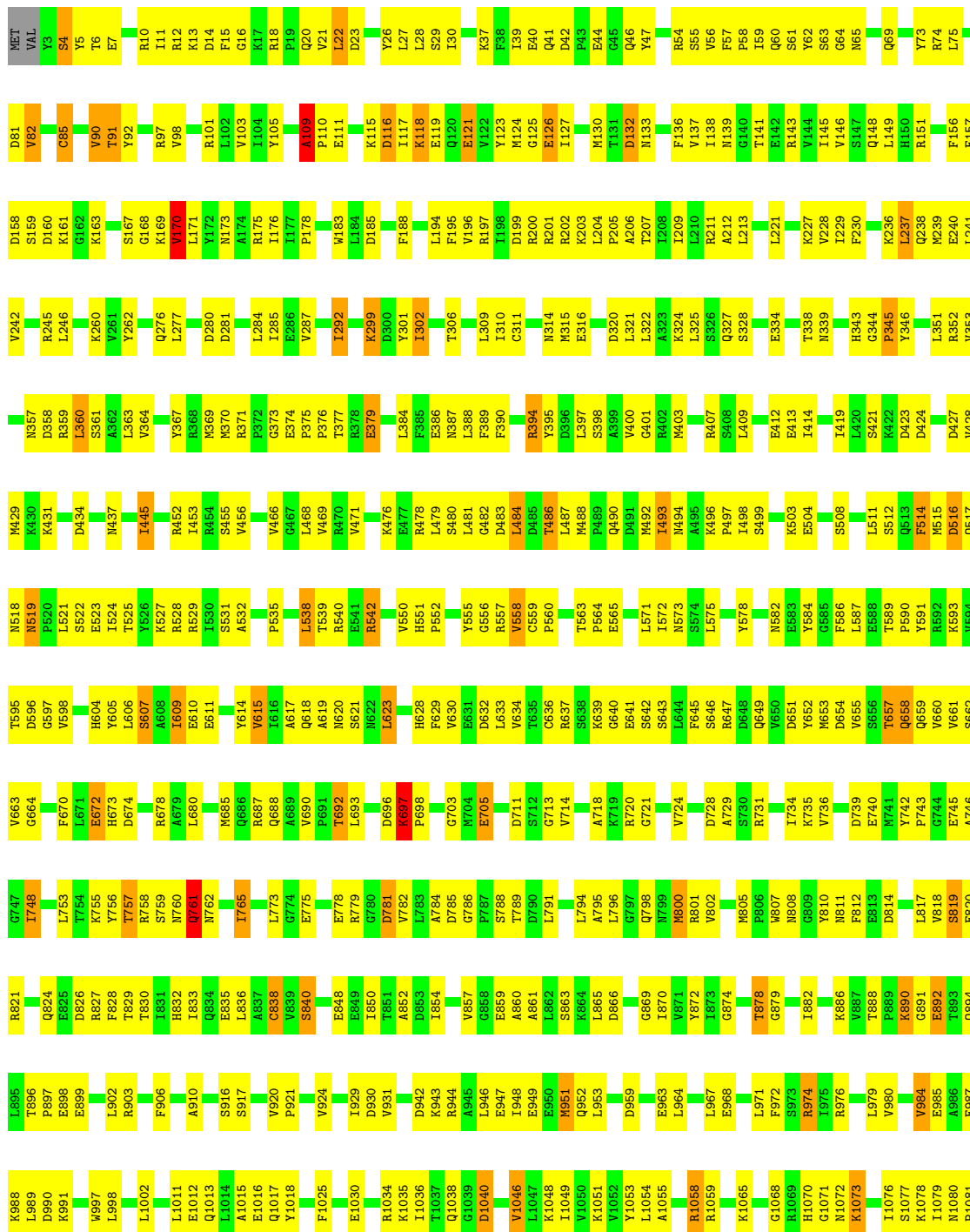


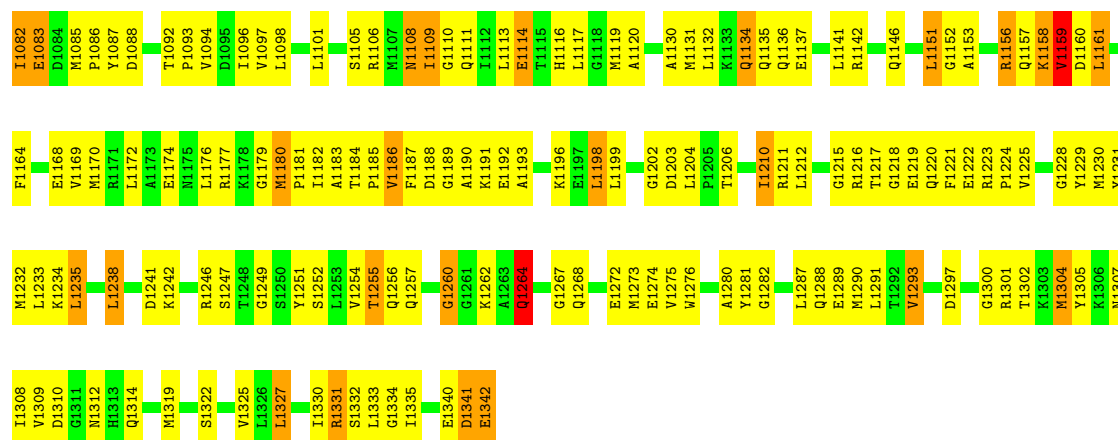
D1214	G1215	T1216	T1217	F1221	R1222	R1223	P1224	V1225	G1228	Y1229	M1230	Y1231	L1235	M1236	H1237	L1238	V1239	D1240	D1241	K1242	M1243	R1246	S1247	T1248	G1249	S1250	I1251	S1252	V1253	V1254	T1255	Q1256	Q1257	K1262	A1263	Q1264	F1265	G1266	G1267	Q1268	E1272	M1273	V1274	V1275	M1276	A1277	L1278	E1279	A1280	Y1281	G1282	A1283	A1284																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
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A679	L680	M681	Q682	A683	N684	H685	R686	R687	T692	L693	R694	A695	P696	R697	E698	L699	V700	G701	G702	G703	W704	S638	K639	G640	E641	S642	F645	S646	R647	Q649	V650	D651	Y652	M653	D654	V655	S656	T657	Q658	Q659	V660	V661	S662	A665	S666	L667	F670	L671	L672	H673	A676	N677	R678																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
K755	Y756	T757	R758	W759	Q761	N762	T763	T764	T765	M768	L773	G774	E775	F776	R779	G780	D781	V782	L783	A784	S788	T789	D790	L791	G792	E793	L794	A795	L796	G797	Q798	N799	R800	R801	V802	W803	E804	R805	P806	W807	N808	N811	F812	E813	D814	S815	L816	L817	W818	S819	E820	R821	Q824																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
E825	D826	R827	F828	T829	W830	I831	H832	R833	Q834	E835	L836	A837	C838	W839	S840	G841	K842	R843	A844	R845	L846	M851	Q852	L853	S854	K858	D859	L860	S861	E862	W863	R864	D865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000	L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	L1029	L1030	L1031	L1032	L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1047	L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060	L1061	L1062	L1063	L1064	L1065	L1066	L1067	L1068	L1069	L1070	L1071	L1072	L1073	L1074	L1075	L1076	L1077	L1078	L1079	L1080	L1081	L1082	L1083	L1084	L1085	L1086	L1087	L1088	L1089	L1090	L1091	L1092	L1093	L1094	L1095	L1096	L1097	L1098	L1099	L1100	L1101	L1102	L1103	L1104	L1105	L1106	L1107	L1108	L1109	L1110	L1111	L1112	L1113	L1114	L1115	L1116	L1117	L1118	L1119	L1120	L1121	L1122	L1123	L1124	L1125	L1126	L1127	L1128	L1129	L1130	L1131	L1132	L1133	L1134	L1135	L1136	L1137	L1138	L1139	L1140	L1141	L1142	L1143	L1144	L1145	L1146	L1147	L1148	L1149	L1150	L1151	L1152	L1153	L1154	L1155	L1156	L1157	L1158	L1159	L1160	L1161	L1162	L1163	L1164	L1165	L1166	L1167	L1168	L1169	L1170	L1171	L1172	L1173	L1174	L1175	L1176	L1177	L1178	L1179	L1180	L1181	L1182	L1183	L1184	L1185	L1186	L1187	L1188	L1189	L1190	L1191	L1192	L1193	L1194	L1195	L1196	L1197	L1198	L1199	L1200	L1201	L1202	L1203	L1204	L1205	L1206	L1207	L1208	L1209	L1210	L1211	L1212	L1213	L1214	L1215	L1216	L1217	L1218	L1219	L1220	L1221	L1222	L1223	L1224	L1225	L1226	L1227	L1228	L1229	L1230	L1231	L1232	L1233	L1234	L1235	L1236	L1237	L1238	L1239	L1240	L1241	L1242	L1243	L1244	L1245	L1246	L1247	L1248	L1249	L1250	L1251	L1252	L1253	L1254	L1255	L1256	L1257	L1258	L1259	L1260	L1261	L1262	L1263	L1264	L1265	L1266	L1267	L1268	L1269	L1270	L1271	L1272	L1273	L1274	L1275	L1276	L1277	L1278	L1279	L1280	L1281	L1282	L1283	L1284	L1285	L1286	L1287	L1288	L1289	L1290	L1291	L1292	L1293	L1294	L1295	L1296	L1297	L1298	L1299	L1300	L1301	L1302	L1303	L1304	L1305	L1306	L1307	L1308	L1309	L1310	L1311	L1312	L1313	L1314	L1315	L1316	L1317	L1318	L1319	L1320	L1321	L1322	L1323	L1324	L1325	L1326	L1327	L1328	L1329	L1330	L1331	L1332	L1333	L1334	L1335	L1336	L1337	L1338	L1339	L1340	L1341	L1342	L1343	L1344	L1345	L1346	L1347	L1348	L1349	L1350	L1351	L1352	L1353	L1354	L1355	L1356	L1357	L1358	L1359	L1360	L1361	L1362	L1363	L1364	L1365	L1366	L1367	L1368	L1369	L1370	L1371	L1372	L1373	L1374	L1375	L1376	L1377	L1378	L1379	L1380	L1381	L1382	L1383	L1384	L1385	L1386	L1387	L1388	L1389	L1390	L1391	L1392	L1393	L1394	L1395	L1396	L1397	L1398	L1399	L1400	L1401	L1402	L1403	L1404	L1405	L1406	L1407	L1408	L1409	L1410	L1411	L1412	L1413	L1414	L1415	L1416	L1417	L1418	L1419	L1420	L1421	L1422	L1423	L1424	L1425	L1426	L1427	L1428	L1429	L1430	L1431	L1432	L1433	L1434	L1435	L1436	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447	L1448	L1449	L1450	L1451	L1452	L1453	L1454	L1455	L1456	L1457	L1458	L1459	L1460	L1461	L1462	L1463	L1464	L1465	L1466	L1467	L1468	L1469	L1470	L1471	L1472	L1473	L1474	L1475	L1476	L1477	L1478	L1479	L1480	L1481	L1482	L1483	L1484	L1485	L1486	L1487	L1488	L1489	L1490	L1491	L1492	L1493	L1494	L1495	L1496	L1497	L1498	L1499	L1500	L1501	L1502	L1503	L1504	L1505	L1506	L1507	L1508	L1509	L1510	L1511	L1512	L1513	L1514	L1515	L1516	L1517	L1518	L1519	L1520	L1521	L1522	L1523	L1524	L1525	L1526	L1527	L1528	L1529	L1530	L1531	L1532	L1533	L1534	L1535	L1536	L1537	L1538	L1539	L1540	L1541	L1542	L1543	L1544	L1545	L1546	L1547	L1548	L1549	L1550	L1551	L1552	L1553	L1554	L1555	L1556	L1557	L1558	L1559	L1560	L1561	L1562	L1563	L1564	L1565	L1566	L1567	L1568	L1569	L1570	L1571	L1572	L1573	L1574	L1575	L1576	L1577	L1578	L1579	L1580	L1581	L1582	L1583	L1584	L1585	L1586	L1587	L1588	L1589	L1590	L1591	L1592	L1593	L1594	L1595	L1596	L1597	L1598	L1599	L1600	L1601	L1602	L1603	L1604	L1605	L1606	L1607	L1608	L1609	L1610	L1611	L1612	L1613	L1614	L1615	L1616	L1617	L1618	L1619	L1620	L1621	L1622	L1623	L1624	L1625	L1626	L1627	L1628	L1629	L1630	L1631	L1632	L1633	L1634	L1635	L1636	L1637	L1638	L1639	L1640	L1641	L1642	L1643	L1644	L1645	L1646	L1647	L1648	L1649	L1650	L1651	L1652	L1653	L1654	L1655	L1656	L1657	L1658	L1659	L1660	L1661	L1662	L1663	L1664	L1665	L1666	L1667	L1668	L1669	L1670	L1671	L1672	L1673	L1674	L1675	L1676	L1677	L1678	L1679	L1680



● Molecule 2: DNA-directed RNA polymerase subunit beta

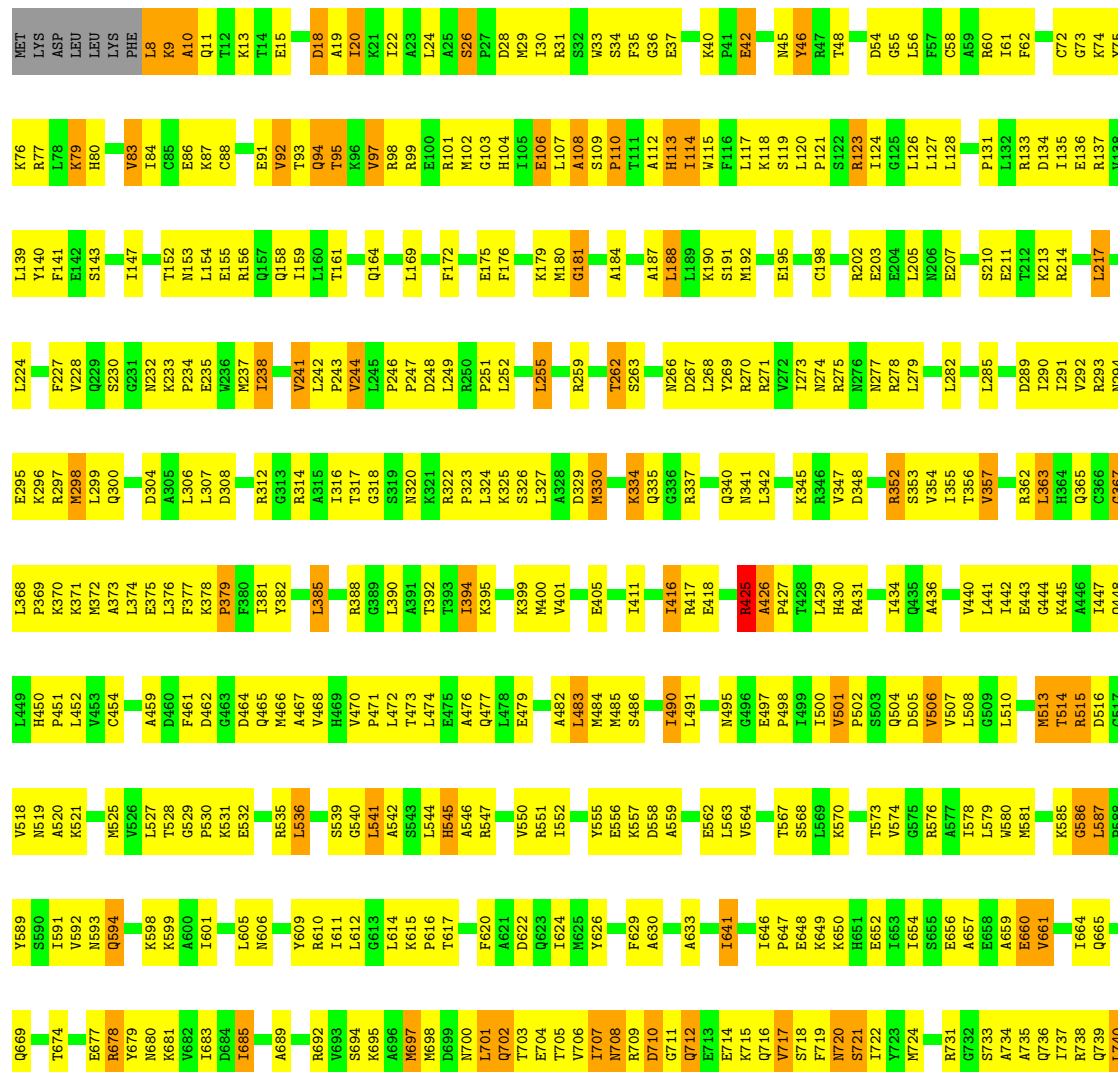
Chain I: 48% 45% 6%





• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D: 35% 40% 8% 17%





V582	V497	S428	E350	D267	V130	ASP
T583	L498	T429	T351	Y268	Q131	ALA
R584	K499	Y430		L269	C132	ASP
E585	I500	A431		V270	S133	ASP
R586	A501		T354	N271	V134	LEU
I587	K502	W433		S272		MET
R588		W434	Q357	M273	Y137	LEU
Q589	I505	I435	V358	R274	F138	ALA
I590	S506	R436	K359	V275	E139	GLU
	M507	Q437	D360	M276		ASN
	E508		I361	M277	Y143	THR
K597		S442	N362	D278		ALA
L598	G512		R363	R279	Y148	ASP
R599	D513	Q446	R364	V280		GLU
H600	D514	A447	N365	R281	V151	ASP
P601	E515	R448	S366	E219		ALA
S602	E516	T449	I367	K220	E154	ALA
R603	D516	T450	R284	F221		GLU
S604	S517	I450	R285	A222	R157	ALA
E605	H518	R451	G368	E223	L158	ALA
L519	H519	E369	E370	L224	S159	ALA
V606	L520	I452	A371	R225	D160	GLN
L607	G520	M456	A372	A226	L161	VAL
R608	L530	T457	R373			LEU
S609	P531	E458	R374	C294	G164	SER
F610	L532	T459		K295	F165	SER
L611	D533	I460	N383	K296	V166	VAL
		M461	L384	M297	D167	GLU
	T536	K462	R385	P298		GLU
L640		L463	L386	K299	PRO	SER
		R464	V387	K300	ASN	GLU
T544		R465	I388	N301	ALA	ILE
		I466	S389	F302	GLU	GLY
V547	M470		I390	K236	ARG	
	L471	L472	K393	ALA	T94	
T552	Q472	E473	Y394	LYS	T95	
	E473		T395	GLY	D96	
E555	M474		N396	SER	P97	
A556	G475		R397	HIS	V98	
K557	R476		S312	A243	R99	
V558	E477		D313	T244	M100	
L559	P478		L399	A245	Y101	
R560	T479		Q400	Q246	M102	
M561	E480		W315	E247	R103	
	E481		F316	E248	E104	
	E482		N317	I249	M105	
T565	L483		A318	L250		
D566	L484		A319	K251	T112	
M567	A484		E407			
N568	E485		G408	E254	G115	
	R486		M409			
Y571	M487		L330	K257	D118	
T572	L488		S334	Q258	I119	
L573	M489			F259		
E574	P490		L341	R260	R122	
E575	E491		Q342	L261	I123	
V576	D492		K343	V262	E124	
G577	K493		L344	F263		
	I494		Q345	K264	GLU	
	R495		Q346	Q265	ASP	
F580			K426	F266	I127	
D581			F427		N128	
					GLU	
					GLU	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	185.36Å 206.28Å 308.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 3.60 29.90 – 3.60	Depositor EDS
% Data completeness (in resolution range)	93.7 (29.90-3.60) 93.5 (29.90-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 3.56Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.246 , 0.305 0.248 , 0.307	Depositor DCC
R_{free} test set	2000 reflections (1.46%)	wwPDB-VP
Wilson B-factor (Å ²)	142.2	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 109.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	55699	wwPDB-VP
Average B, all atoms (Å ²)	157.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.87	0/2435	1.28	20/3300 (0.6%)
1	B	0.77	0/1692	1.17	3/2293 (0.1%)
1	G	0.59	0/1751	1.22	7/2373 (0.3%)
1	H	0.57	0/1686	1.08	7/2285 (0.3%)
2	C	1.23	5/10741 (0.0%)	1.37	70/14492 (0.5%)
2	I	0.82	0/10737	1.13	26/14487 (0.2%)
3	D	1.27	3/9246 (0.0%)	1.39	41/12478 (0.3%)
3	J	1.07	2/9168 (0.0%)	1.25	29/12374 (0.2%)
4	E	0.68	0/693	0.95	0/935
4	K	0.35	0/629	0.75	0/847
5	F	0.92	0/3857	1.21	9/5184 (0.2%)
5	L	0.81	1/3872 (0.0%)	1.09	2/5205 (0.0%)
All	All	1.02	11/56507 (0.0%)	1.25	214/76253 (0.3%)

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	2
1	G	0	1
2	C	0	11
2	I	0	2
3	D	0	12
3	J	0	9
5	F	0	1
5	L	0	1
All	All	0	39

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	811	ASN	CB-CG	-8.81	1.30	1.52
3	J	307	LEU	CG-CD2	-6.91	1.29	1.52
2	C	1076	ILE	CB-CG2	-6.62	1.30	1.52
3	D	426	ALA	C-N	-5.64	1.20	1.33
2	C	1079	ILE	C-N	5.62	1.45	1.33
2	C	1096	ILE	CB-CG2	-5.56	1.34	1.52
3	J	145	VAL	CB-CG2	-5.52	1.34	1.52
2	C	592	ARG	CB-CG	-5.34	1.36	1.52
3	D	114	ILE	CG1-CD1	-5.18	1.31	1.51
3	D	1256	ILE	CG1-CD1	-5.10	1.31	1.51
5	L	96	ASP	C-N	-5.04	1.22	1.33

All (214) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	109	ALA	CA-C-N	15.51	136.53	119.93
2	I	109	ALA	C-N-CA	15.51	136.53	119.93
2	C	109	ALA	CA-C-N	14.05	134.97	119.93
2	C	109	ALA	C-N-CA	14.05	134.97	119.93
2	C	762	ASN	CA-C-N	-9.17	104.69	122.02
2	C	762	ASN	C-N-CA	-9.17	104.69	122.02
5	F	602	SER	N-CA-C	-8.89	91.87	110.80
1	A	322	PRO	CA-C-N	8.82	128.96	120.31
1	A	322	PRO	C-N-CA	8.82	128.96	120.31
1	A	323	PRO	CA-C-O	-8.75	111.27	122.12
3	D	515	ARG	N-CA-C	-8.70	95.47	108.79
2	C	1287	LEU	CB-CG-CD2	-7.93	86.92	110.70
3	D	888	CYS	CA-CB-SG	-7.79	96.47	114.40
2	I	373	GLY	CA-C-N	7.69	131.08	120.39
2	I	373	GLY	C-N-CA	7.69	131.08	120.39
3	D	114	ILE	CG1-CB-CG2	-7.62	87.84	110.70
3	D	123	ARG	CG-CD-NE	-7.60	95.27	112.00
1	A	323	PRO	CA-C-N	7.25	134.74	121.70
1	A	323	PRO	C-N-CA	7.25	134.74	121.70
2	C	1264	GLN	N-CA-C	-6.91	96.38	108.20
3	D	470	VAL	CB-CA-C	-6.83	103.40	110.71
3	J	162	GLU	CA-CB-CG	6.83	127.76	114.10
5	L	602	SER	N-CA-C	-6.82	96.28	110.80
3	J	198	CYS	CA-CB-SG	-6.76	98.85	114.40
5	F	379	MET	CA-CB-CG	-6.74	100.62	114.10
1	G	54	CYS	CA-CB-SG	-6.72	98.94	114.40
1	H	29	GLU	N-CA-C	6.68	116.00	108.25
2	C	1303	LYS	CA-CB-CG	6.66	127.43	114.10

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1106	ARG	CA-C-N	-6.64	112.65	122.41
2	C	1106	ARG	C-N-CA	-6.64	112.65	122.41
1	G	195	ARG	N-CA-CB	6.59	121.62	110.49
2	I	1241	ASP	N-CA-C	-6.58	96.78	110.80
3	D	385	LEU	CA-C-N	-6.53	111.76	122.54
3	D	385	LEU	C-N-CA	-6.53	111.76	122.54
2	I	1235	LEU	CA-C-N	-6.46	113.20	122.77
2	I	1235	LEU	C-N-CA	-6.46	113.20	122.77
3	J	355	ILE	CA-C-N	6.40	133.76	121.54
3	J	355	ILE	C-N-CA	6.40	133.76	121.54
3	D	241	VAL	CB-CA-C	-6.36	101.14	110.81
2	C	800	MET	CB-CG-SD	-6.35	93.64	112.70
1	H	53	GLY	N-CA-C	6.34	119.83	110.63
2	I	1255	THR	CA-C-N	-6.34	112.54	121.99
2	I	1255	THR	C-N-CA	-6.34	112.54	121.99
3	D	907	HIS	N-CA-CB	-6.33	101.31	110.36
2	C	1235	LEU	CA-C-N	-6.31	113.42	122.77
2	C	1235	LEU	C-N-CA	-6.31	113.42	122.77
3	J	1247	LYS	CB-CG-CD	-6.28	96.85	111.30
3	J	888	CYS	CA-CB-SG	-6.20	100.13	114.40
2	C	454	ARG	CG-CD-NE	-6.17	98.42	112.00
3	D	541	LEU	CA-CB-CG	-6.14	94.81	116.30
3	D	838	ARG	CB-CG-CD	6.13	125.39	111.30
3	J	189	LEU	CA-CB-CG	-6.13	94.86	116.30
3	D	357	VAL	N-CA-C	6.10	122.03	109.34
2	I	1327	LEU	CA-CB-CG	-6.08	95.04	116.30
1	G	211	ILE	N-CA-C	6.06	117.75	108.71
2	C	512	SER	CA-C-N	-6.05	112.41	122.21
2	C	512	SER	C-N-CA	-6.05	112.41	122.21
3	D	376	LEU	CB-CG-CD2	-6.04	92.59	110.70
3	D	486	SER	CA-CB-OG	-6.03	99.03	111.10
3	J	515	ARG	N-CA-C	-6.02	99.58	108.79
2	C	1281	TYR	CA-C-N	-6.01	109.62	121.41
2	C	1281	TYR	C-N-CA	-6.01	109.62	121.41
3	D	118	LYS	N-CA-C	6.01	120.74	113.17
2	C	1157	GLN	N-CA-C	5.97	117.79	111.28
2	I	1159	VAL	CA-C-N	5.95	132.90	121.54
2	I	1159	VAL	C-N-CA	5.95	132.90	121.54
1	A	321	TRP	N-CA-C	5.93	118.50	110.31
2	C	1103	VAL	N-CA-C	5.93	121.69	108.88
2	C	49	LEU	CA-CB-CG	-5.92	95.57	116.30
2	C	813	GLU	CA-CB-CG	-5.91	102.28	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	831	ILE	N-CA-C	5.90	116.36	107.80
2	C	61	SER	CA-C-N	-5.85	113.81	122.41
2	C	61	SER	C-N-CA	-5.85	113.81	122.41
3	J	48	THR	CA-C-N	-5.84	110.63	122.31
3	J	48	THR	C-N-CA	-5.84	110.63	122.31
2	C	512	SER	N-CA-C	5.83	118.23	108.73
2	C	517	GLN	CA-C-N	5.82	132.66	121.54
2	C	517	GLN	C-N-CA	5.82	132.66	121.54
3	J	566	LYS	N-CA-CB	5.81	121.64	111.13
2	C	1136	GLN	CA-CB-CG	-5.80	102.50	114.10
3	D	721	SER	CB-CA-C	-5.80	101.69	110.92
2	I	531	SER	N-CA-C	5.79	118.91	108.48
2	I	1304	MET	CB-CG-SD	-5.79	95.32	112.70
1	G	142	MET	CA-CB-CG	-5.79	102.52	114.10
3	D	238	ILE	CA-CB-CG1	-5.75	100.62	110.40
2	C	42	ASP	C-N-CD	-5.75	101.43	125.00
3	D	426	ALA	N-CA-C	5.75	119.99	112.17
3	J	900	GLY	CA-C-N	-5.74	111.56	121.66
3	J	900	GLY	C-N-CA	-5.74	111.56	121.66
1	A	48	LEU	CA-C-N	-5.73	110.60	121.54
1	A	48	LEU	C-N-CA	-5.73	110.60	121.54
3	D	262	THR	CB-CA-C	-5.72	98.15	110.45
1	A	316	MET	CA-CB-CG	-5.71	102.67	114.10
1	A	54	CYS	CA-CB-SG	-5.71	101.28	114.40
3	D	800	LEU	CD1-CG-CD2	-5.70	98.26	110.80
3	J	62	PHE	CA-C-N	-5.66	112.98	121.87
3	J	62	PHE	C-N-CA	-5.66	112.98	121.87
3	J	503	SER	CA-C-N	-5.65	110.75	121.54
3	J	503	SER	C-N-CA	-5.65	110.75	121.54
2	C	818	VAL	CA-CB-CG2	-5.65	100.80	110.40
1	B	9	LEU	CA-C-N	5.64	143.04	121.95
1	B	9	LEU	C-N-CA	5.64	143.04	121.95
2	C	1059	ARG	N-CA-CB	5.63	120.00	110.49
2	I	1264	GLN	N-CA-C	-5.61	98.61	108.20
3	J	271	ARG	CB-CG-CD	-5.60	98.43	111.30
2	C	1335	ILE	N-CA-C	5.58	116.34	108.36
3	D	1246	VAL	N-CA-C	5.58	116.34	108.36
1	G	68	TYR	CB-CA-C	5.58	119.89	110.79
1	A	294	ASN	N-CA-C	5.57	122.66	110.80
5	L	422	ARG	CA-CB-CG	-5.57	102.97	114.10
3	D	137	ARG	CG-CD-NE	-5.56	99.77	112.00
1	H	29	GLU	CA-C-N	5.55	140.32	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	29	GLU	C-N-CA	5.55	140.32	127.00
2	C	796	LEU	CB-CG-CD2	-5.53	94.10	110.70
2	I	126	GLU	CA-CB-CG	-5.53	103.04	114.10
1	H	29	GLU	C-N-CD	-5.52	108.45	120.60
2	I	658	GLN	CA-CB-CG	-5.52	103.06	114.10
2	C	1265	PHE	CA-CB-CG	-5.51	108.29	113.80
3	J	829	GLY	N-CA-C	-5.51	100.12	113.18
3	D	188	LEU	CB-CG-CD2	-5.50	94.20	110.70
5	F	510	PRO	N-CA-C	-5.50	102.56	111.19
3	J	117	LEU	CB-CG-CD1	-5.49	94.25	110.70
1	B	11	PRO	N-CA-C	5.48	123.76	112.47
2	C	482	GLY	N-CA-C	5.44	126.08	113.18
2	C	1319	MET	N-CA-C	5.44	118.12	109.64
2	C	200	ARG	CA-CB-CG	-5.44	103.23	114.10
2	C	200	ARG	CG-CD-NE	-5.44	100.04	112.00
2	C	1079	ILE	CB-CG1-CD1	-5.43	102.39	113.80
3	D	370	LYS	CA-CB-CG	5.43	124.96	114.10
2	C	1119	MET	CB-CG-SD	-5.43	96.41	112.70
2	C	1161	LEU	CA-CB-CG	-5.41	97.35	116.30
1	A	29	GLU	C-N-CD	-5.41	102.81	125.00
1	H	95	LYS	CA-CB-CG	5.41	124.92	114.10
3	D	42	GLU	CA-CB-CG	5.41	124.92	114.10
1	G	142	MET	CB-CG-SD	5.41	128.92	112.70
2	C	697	LYS	N-CA-C	-5.39	97.89	109.81
3	J	1261	LEU	CB-CG-CD2	-5.39	94.54	110.70
3	D	904	ALA	N-CA-C	-5.38	106.55	113.01
3	D	472	LEU	CB-CA-C	-5.38	102.37	112.00
1	G	48	LEU	CA-CB-CG	-5.36	97.53	116.30
2	C	1058	ARG	CA-C-N	-5.36	111.31	121.54
2	C	1058	ARG	C-N-CA	-5.36	111.31	121.54
2	I	838	CYS	CA-CB-SG	-5.35	102.09	114.40
1	A	29	GLU	CA-C-N	5.34	126.52	119.84
1	A	29	GLU	C-N-CA	5.34	126.52	119.84
5	F	580	PHE	CA-C-N	5.33	131.71	121.54
5	F	580	PHE	C-N-CA	5.33	131.71	121.54
2	C	1160	ASP	CA-C-N	5.30	135.54	126.32
2	C	1160	ASP	C-N-CA	5.30	135.54	126.32
3	D	123	ARG	CB-CG-CD	5.29	123.47	111.30
2	C	1157	GLN	CA-C-N	5.29	131.65	121.54
2	C	1157	GLN	C-N-CA	5.29	131.65	121.54
2	C	1336	ASN	CB-CA-C	-5.29	102.08	110.81
2	I	1260	GLY	N-CA-C	-5.29	102.72	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1040	ASP	N-CA-CB	-5.28	102.20	109.97
3	D	271	ARG	NE-CZ-NH1	-5.28	116.22	121.50
2	C	513	GLN	CB-CA-C	-5.28	98.46	110.07
3	J	434	ILE	CG1-CB-CG2	-5.27	94.90	110.70
3	J	487	THR	CA-C-N	-5.24	111.36	121.58
3	J	487	THR	C-N-CA	-5.24	111.36	121.58
2	C	1239	VAL	CA-C-N	-5.23	114.23	122.08
2	C	1239	VAL	C-N-CA	-5.23	114.23	122.08
2	C	1256	GLN	CA-CB-CG	-5.23	103.64	114.10
3	D	1244	GLN	CB-CG-CD	5.23	121.49	112.60
2	C	112	GLY	N-CA-C	-5.23	102.82	110.87
2	C	1060	ILE	CA-C-N	-5.23	113.34	122.38
2	C	1060	ILE	C-N-CA	-5.23	113.34	122.38
2	C	1255	THR	CB-CA-C	-5.23	100.15	109.71
2	I	1058	ARG	CA-C-N	-5.22	111.58	121.54
2	I	1058	ARG	C-N-CA	-5.22	111.58	121.54
2	C	1241	ASP	N-CA-C	-5.21	99.71	110.80
3	D	585	LYS	N-CA-C	5.19	116.20	108.31
1	A	294	ASN	CA-C-N	-5.16	115.87	123.00
1	A	294	ASN	C-N-CA	-5.16	115.87	123.00
2	C	542	ARG	CA-C-N	-5.15	114.46	122.09
2	C	542	ARG	C-N-CA	-5.15	114.46	122.09
1	A	255	ARG	CB-CG-CD	-5.15	99.45	111.30
3	D	352	ARG	CG-CD-NE	-5.15	100.67	112.00
3	J	1344	LEU	CA-CB-CG	-5.15	98.27	116.30
3	J	253	VAL	N-CA-C	5.15	120.00	108.88
3	D	262	THR	N-CA-C	5.15	116.89	109.07
3	D	585	LYS	CB-CA-C	-5.14	110.63	116.54
3	D	570	LYS	CA-CB-CG	5.13	124.36	114.10
1	H	228	LEU	CA-CB-CG	-5.13	98.33	116.30
3	D	705	THR	N-CA-C	-5.13	102.32	109.96
2	C	152	SER	CB-CA-C	-5.12	101.42	109.52
2	C	812	PHE	CA-C-N	-5.12	111.77	121.54
2	C	812	PHE	C-N-CA	-5.12	111.77	121.54
2	C	390	PHE	CA-CB-CG	-5.11	108.69	113.80
5	F	508	GLU	CA-CB-CG	-5.11	103.88	114.10
2	I	761	GLN	CA-C-N	5.10	130.88	121.70
2	I	761	GLN	C-N-CA	5.10	130.88	121.70
3	D	860	ARG	CA-C-N	-5.09	115.64	122.42
3	D	860	ARG	C-N-CA	-5.09	115.64	122.42
5	F	462	LYS	CA-CB-CG	5.09	124.28	114.10
3	D	119	SER	N-CA-C	-5.09	102.85	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	263	SER	CB-CA-C	-5.09	99.25	109.68
2	C	699	LEU	CA-CB-CG	-5.08	98.52	116.30
2	C	1335	ILE	CA-CB-CG2	-5.07	101.88	110.50
2	C	540	ARG	NE-CZ-NH1	-5.06	116.44	121.50
2	C	1070	HIS	CA-C-N	-5.05	113.83	121.51
2	C	1070	HIS	C-N-CA	-5.05	113.83	121.51
3	J	293	ARG	CA-CB-CG	-5.05	104.00	114.10
3	D	298	MET	CA-CB-CG	-5.04	104.01	114.10
2	I	731	ARG	N-CA-CB	-5.03	103.43	111.43
3	J	357	VAL	N-CA-C	5.03	119.80	109.34
1	A	289	LEU	CA-C-N	-5.03	112.56	120.60
1	A	289	LEU	C-N-CA	-5.03	112.56	120.60
1	A	143	ARG	CG-CD-NE	5.02	123.05	112.00
2	C	1304	MET	CB-CG-SD	-5.02	97.64	112.70
5	F	544	THR	CA-C-N	-5.02	113.16	120.29
5	F	544	THR	C-N-CA	-5.02	113.16	120.29
2	I	237	LEU	N-CA-C	5.02	121.49	110.80
3	D	176	PHE	N-CA-C	-5.01	100.19	108.75

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	321	TRP	Peptide
1	A	49	SER	Mainchain
2	C	1077	SER	Mainchain
2	C	109	ALA	Peptide
2	C	1107	MET	Mainchain
2	C	1164	PHE	Mainchain
2	C	1332	SER	Mainchain
2	C	236	LYS	Peptide
2	C	473	ARG	Mainchain
2	C	560	PRO	Mainchain
2	C	573	ASN	Mainchain
2	C	683	ALA	Mainchain
2	C	686	GLN	Mainchain
3	D	113	HIS	Mainchain
3	D	1184	ASP	Peptide
3	D	1296	GLY	Peptide
3	D	1310	THR	Mainchain
3	D	181	GLY	Mainchain
3	D	308	ASP	Mainchain

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Mol	Chain	Res	Type	Group
3	D	367	GLY	Mainchain
3	D	379	PRO	Mainchain
3	D	425	ARG	Mainchain
3	D	483	LEU	Mainchain
3	D	914	ALA	Mainchain
3	D	921	GLN	Mainchain
5	F	601	PRO	Peptide
1	G	171	LEU	Peptide
2	I	109	ALA	Peptide
2	I	236	LYS	Peptide
3	J	102	MET	Mainchain
3	J	1184	ASP	Peptide
3	J	1296	GLY	Peptide
3	J	1305	ASP	Mainchain
3	J	143	SER	Mainchain
3	J	186	GLN	Mainchain
3	J	248	ASP	Mainchain
3	J	299	LEU	Mainchain
3	J	475	GLU	Mainchain
5	L	601	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2403	0	2453	202	0
1	B	1672	0	1694	120	0
1	G	1730	0	1756	149	0
1	H	1667	0	1689	127	1
2	C	10572	0	10584	698	3
2	I	10568	0	10578	636	0
3	D	9107	0	9308	652	0
3	J	9029	0	9225	612	0
4	E	691	0	695	23	0
4	K	627	0	634	27	0
5	F	3806	0	3873	226	2
5	L	3821	0	3884	211	0
6	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	1	0	0	0	0
7	D	2	0	0	0	0
7	J	2	0	0	0	0
All	All	55699	0	56373	3395	3

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 30.

All (3395) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:THR:O	1:A:28:LEU:HD12	1.10	1.23
2:I:27:LEU:O	2:I:528:ARG:NH1	1.78	1.17
1:A:27:THR:O	1:A:28:LEU:CD1	1.93	1.17
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.36	1.08
3:D:1280:VAL:HG11	3:D:1304:ARG:HH21	1.16	1.08
2:C:1131:MET:HE2	2:C:1141:LEU:HD12	1.35	1.07
1:A:27:THR:C	1:A:28:LEU:HD12	1.78	1.07
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.36	1.07
1:A:12:ARG:H	1:A:30:PRO:CG	1.67	1.06
2:C:758:ARG:HH22	2:C:761:GLN:HG3	1.22	1.04
1:A:45:ARG:HG2	1:B:38:THR:HB	1.40	1.04
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.40	1.04
2:C:324:LYS:O	2:C:327:GLN:NE2	1.89	1.03
2:C:1142:ARG:HD3	2:C:1161:LEU:HD11	1.43	1.01
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.42	1.00
1:A:12:ARG:H	1:A:30:PRO:HG3	1.22	1.00
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.23	0.99
2:I:560:PRO:O	3:J:780:ARG:NH2	1.96	0.99
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.00	0.98
5:F:490:PRO:HG2	5:F:493:LYS:HE3	1.46	0.97
1:A:27:THR:C	1:A:28:LEU:CD1	2.36	0.96
2:I:821:ARG:HH21	2:I:1082:ILE:HG21	1.27	0.96
2:C:131:THR:HG22	2:C:135:THR:H	1.27	0.96
3:J:418:GLU:HG3	4:K:45:LYS:H	1.30	0.95
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.28	0.95
3:D:56:LEU:H	3:D:56:LEU:HD12	1.29	0.95
2:C:142:GLU:HB2	2:C:760:ASN:HD21	1.30	0.94
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.46	0.94
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.30	0.93
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.51	0.92
2:I:886:LYS:HE3	2:I:916:SER:HB3	1.52	0.92
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.52	0.92
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.53	0.91
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.49	0.91
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.51	0.91
2:I:890:LYS:NZ	2:I:891:GLY:O	2.02	0.91
1:A:11:PRO:HA	1:A:30:PRO:CG	2.01	0.90
1:A:12:ARG:N	1:A:30:PRO:HG3	1.86	0.90
3:J:1368:ASP:OD1	3:J:1371:ARG:NH2	2.04	0.90
3:D:1293:GLU:HG2	3:J:1227:HIS:HB2	1.51	0.90
2:C:120:GLN:HG3	2:C:121:GLU:HG3	1.51	0.90
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.54	0.90
5:F:278:ASP:OD1	5:F:281:ARG:NH1	2.04	0.90
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.53	0.89
1:A:11:PRO:HA	1:A:30:PRO:HB2	1.54	0.89
1:A:11:PRO:CA	1:A:30:PRO:HG2	2.03	0.89
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.54	0.89
3:D:42:GLU:OE2	5:F:451:ARG:NH2	2.05	0.89
2:I:18:ARG:NH1	2:I:621:SER:O	2.05	0.89
2:I:523:GLU:HG2	2:I:527:LYS:HE3	1.55	0.88
2:I:202:ARG:HD3	2:I:369:MET:HG2	1.54	0.88
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.37	0.88
3:D:1291:GLU:OE1	3:J:1302:TYR:OH	1.91	0.88
1:A:16:ILE:HG23	1:A:26:VAL:HG12	1.55	0.87
2:C:930:ASP:OD2	2:C:931:VAL:N	2.08	0.86
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.57	0.86
2:C:758:ARG:NH2	2:C:761:GLN:HG3	1.91	0.86
2:C:1297:ASP:OD1	2:C:1300:GLY:N	2.08	0.86
1:G:231:PHE:HD1	1:H:218:ARG:HG2	1.40	0.86
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.40	0.85
5:L:132:CYS:SG	5:L:257:LYS:NZ	2.48	0.85
5:L:492:ASP:HB2	5:L:495:ARG:HH12	1.41	0.85
1:H:101:THR:HG22	1:H:116:THR:HB	1.58	0.85
3:D:817:HIS:CE1	3:D:860:ARG:HE	1.93	0.85
3:D:1341:ARG:NH1	3:D:1343:GLU:OE2	2.09	0.85
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.10	0.85
2:I:183:TRP:HB2	2:I:199:ASP:HA	1.59	0.85
5:L:244:THR:O	5:L:247:GLU:HG2	1.77	0.85
2:I:1307:ASN:HB3	2:I:1312:ASN:O	1.75	0.85
1:A:11:PRO:HA	1:A:30:PRO:CB	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:102:MET:HE3	3:J:246:PRO:HD3	1.59	0.84
3:J:799:ARG:NH1	3:J:1146:GLU:OE1	2.09	0.84
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.58	0.84
1:B:16:ILE:HG23	1:B:26:VAL:HG22	1.57	0.84
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.59	0.83
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.26	0.83
2:I:1287:LEU:HD22	3:J:1357:ILE:HD11	1.61	0.83
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.58	0.83
3:D:11:GLN:HG2	3:D:15:GLU:HG3	1.60	0.83
3:D:1203:ARG:HH22	3:D:1205:GLU:HG2	1.40	0.83
2:I:344:GLY:O	2:I:346:TYR:N	2.10	0.83
1:A:12:ARG:N	1:A:30:PRO:CG	2.40	0.83
1:B:48:LEU:HD21	3:D:535:ARG:HG3	1.61	0.83
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.43	0.83
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.60	0.82
2:I:452:ARG:NH1	2:I:584:TYR:O	2.12	0.82
2:I:478:ARG:HH12	2:I:482:GLY:HA2	1.42	0.82
1:A:60:GLU:CD	1:A:143:ARG:HH21	1.88	0.82
2:I:1131:MET:HE2	2:I:1141:LEU:HD12	1.60	0.82
2:C:1149:TYR:HD1	2:C:1159:VAL:HG11	1.44	0.82
3:D:75:TYR:OH	3:D:86:GLU:OE1	1.95	0.82
5:F:121:LYS:NZ	5:F:421:TYR:OH	2.10	0.82
1:A:7:GLU:O	1:B:150:ARG:NH2	2.12	0.82
1:B:41:ASN:OD1	1:B:44:ARG:NH1	2.10	0.82
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.60	0.82
2:I:930:ASP:OD2	2:I:931:VAL:N	2.12	0.82
1:A:29:GLU:O	1:A:31:LEU:N	2.13	0.81
3:D:128:LEU:HA	3:D:192:MET:HE1	1.61	0.81
3:D:557:LYS:HA	3:D:563:LEU:HA	1.62	0.81
5:F:470:MET:SD	5:F:486:ARG:NH1	2.53	0.81
5:L:466:ILE:HD11	5:L:487:MET:HE3	1.62	0.81
3:J:1203:ARG:HH12	3:J:1205:GLU:HG2	1.45	0.81
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.63	0.81
3:J:1280:VAL:HG11	3:J:1304:ARG:NH2	1.95	0.81
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.62	0.81
3:D:930:LEU:HD22	3:D:1244:GLN:HG3	1.63	0.81
5:L:231:THR:HG23	5:L:249:ILE:HG12	1.63	0.81
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.62	0.80
3:J:1171:GLY:HA2	3:J:1193:TRP:HZ3	1.44	0.80
3:J:514:THR:OG1	3:J:594:GLN:O	1.98	0.80
1:G:41:ASN:ND2	2:I:1216:ARG:O	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.62	0.80
3:D:1368:ASP:OD1	3:D:1371:ARG:NH2	2.15	0.80
2:I:1312:ASN:HD21	2:I:1314:GLN:NE2	1.79	0.80
2:I:757:THR:HG23	2:I:765:ILE:HG23	1.64	0.80
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.64	0.80
1:A:11:PRO:HA	1:A:30:PRO:HG2	1.59	0.79
1:A:89:ALA:H	1:A:125:LYS:HD3	1.47	0.79
1:A:228:LEU:HD22	1:B:221:ALA:HB1	1.64	0.79
3:D:327:LEU:HA	3:D:330:MET:HG3	1.62	0.79
2:I:761:GLN:HG2	2:I:762:ASN:OD1	1.82	0.79
2:I:860:ALA:O	2:I:863:SER:OG	2.01	0.79
5:L:105:MET:HE1	5:L:385:ARG:HG2	1.64	0.79
1:G:12:ARG:HD2	1:H:230:ALA:HB1	1.62	0.79
2:C:721:GLY:N	2:C:740:GLU:OE1	2.13	0.79
3:D:515:ARG:NH2	3:D:717:VAL:O	2.16	0.79
4:K:25:ARG:NH1	4:K:65:ASP:OD1	2.15	0.79
1:B:16:ILE:HG12	1:B:26:VAL:HG13	1.65	0.79
2:C:1212:LEU:HD22	2:C:1225:VAL:HG21	1.65	0.79
3:D:1227:HIS:CD2	3:J:1293:GLU:HG2	2.16	0.79
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.15	0.79
3:D:721:SER:HA	3:D:724:MET:HE2	1.65	0.79
3:J:810:THR:HG21	3:J:893:GLY:HA3	1.65	0.79
2:I:949:GLU:HG2	2:I:1036:ILE:HG22	1.65	0.78
1:G:41:ASN:HD22	1:H:41:ASN:HD22	1.32	0.78
1:H:23:HIS:ND1	1:H:206:GLU:HG2	1.97	0.78
5:F:582:VAL:HG12	5:F:586:ARG:HG2	1.65	0.78
2:I:1114:GLU:OE1	2:I:1230:MET:HA	1.82	0.78
5:F:483:LEU:H	5:F:483:LEU:HD12	1.46	0.78
2:I:30:ILE:HD12	2:I:30:ILE:H	1.48	0.78
1:A:7:GLU:HG3	1:B:150:ARG:HE	1.49	0.78
1:A:14:VAL:HG22	1:A:15:ASP:H	1.48	0.78
2:I:1073:LYS:HE3	3:J:462:ASP:HB2	1.64	0.78
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.18	0.78
3:J:518:VAL:HG11	3:J:707:ILE:HD13	1.64	0.78
1:B:76:GLU:OE2	1:B:132:HIS:N	2.13	0.78
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	1.66	0.78
2:C:133:ASN:O	2:C:527:LYS:NZ	2.17	0.78
1:H:196:THR:HG23	3:J:443:GLU:HG3	1.64	0.78
3:D:1140:ARG:NH2	3:D:1236:GLU:HG2	1.99	0.77
1:H:59:VAL:O	1:H:171:LEU:N	2.16	0.77
2:I:703:GLY:N	2:I:705:GLU:OE2	2.16	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:HIS:HB2	1:A:205:MET:O	1.85	0.77
3:D:587:LEU:HD23	3:D:591:ILE:HG21	1.66	0.77
5:F:492:ASP:HB2	5:F:495:ARG:HH12	1.48	0.77
3:J:518:VAL:O	3:J:547:ARG:NH1	2.18	0.77
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.66	0.77
5:F:573:LEU:HD23	5:F:573:LEU:H	1.49	0.77
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.67	0.77
5:L:585:GLU:OE2	5:L:588:ARG:NH1	2.18	0.77
1:A:261:GLU:CD	2:C:859:GLU:H	1.93	0.76
2:C:131:THR:HG23	2:C:133:ASN:H	1.50	0.76
3:D:418:GLU:HG3	4:E:45:LYS:H	1.50	0.76
1:A:187:VAL:HG12	1:A:201:LEU:HD13	1.68	0.76
1:A:45:ARG:NH2	2:C:1216:ARG:HA	1.99	0.76
3:D:83:VAL:HG13	3:D:92:VAL:HG13	1.65	0.76
3:J:905:ARG:HH11	4:K:16:ARG:HD2	1.51	0.76
3:D:109:SER:HB2	3:D:296:LYS:HE2	1.68	0.76
3:D:1280:VAL:HG11	3:D:1304:ARG:NH2	1.99	0.76
2:I:1072:ASN:OD1	2:I:1072:ASN:N	2.14	0.76
3:J:1263:LYS:HE2	3:J:1279:GLN:HE21	1.50	0.76
2:C:705:GLU:HB2	2:C:794:LEU:H	1.50	0.76
3:D:1160:SER:OG	3:D:1203:ARG:NH1	2.18	0.76
2:I:637:ARG:HA	2:I:642:SER:HA	1.66	0.76
2:C:4:SER:OG	2:C:5:TYR:N	2.16	0.76
2:C:1299:ASN:HD22	2:C:1303:LYS:HE2	1.49	0.76
3:J:1252:HIS:O	3:J:1255:VAL:HG13	1.85	0.76
1:B:6:THR:N	1:B:7:GLU:OE2	2.17	0.76
3:D:1289:ASN:OD1	3:D:1290:ARG:NH1	2.19	0.76
1:G:161:SER:O	1:G:163:GLU:N	2.18	0.76
1:A:118:ASP:HB3	1:A:121:VAL:HG23	1.68	0.75
2:I:1272:GLU:HB2	3:J:342:LEU:O	1.87	0.75
2:C:759:SER:OG	2:C:763:THR:N	2.18	0.75
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.67	0.75
3:J:1368:ASP:HA	3:J:1371:ARG:HH12	1.49	0.75
5:F:466:ILE:HD11	5:F:487:MET:HE3	1.67	0.75
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.68	0.75
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.69	0.75
5:L:572:THR:HG23	5:L:575:GLU:HB2	1.67	0.75
2:C:69:GLN:NE2	2:C:101:ARG:HD2	2.00	0.75
2:C:142:GLU:HB2	2:C:760:ASN:ND2	2.02	0.75
2:C:42:ASP:OD2	2:C:44:GLU:HG2	1.86	0.75
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:42:ASP:OD2	2:C:44:GLU:O	2.05	0.75
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.69	0.75
3:D:30:ILE:HG23	3:D:243:PRO:HG3	1.69	0.75
3:D:97:VAL:HG12	3:D:101:ARG:HG3	1.69	0.75
2:I:1117:LEU:HD21	2:I:1182:ILE:HD12	1.68	0.75
1:A:61:ILE:HG23	1:A:142:MET:HB3	1.69	0.75
2:C:1164:PHE:N	2:C:1168:GLU:OE1	2.18	0.75
3:J:140:TYR:OH	3:J:312:ARG:NH2	2.20	0.75
2:C:16:GLY:O	2:C:1156:ARG:HG2	1.87	0.74
2:C:149:LEU:HD12	2:C:452:ARG:O	1.86	0.74
2:C:1293:VAL:HG11	2:C:1304:MET:HE2	1.68	0.74
3:J:523:GLU:OE2	3:J:547:ARG:NH1	2.18	0.74
3:D:798:ARG:NH1	3:D:802:ASP:OD2	2.20	0.74
5:L:395:THR:OG1	5:L:396:ASN:N	2.16	0.74
2:I:292:ILE:HB	2:I:322:LEU:HD11	1.68	0.74
2:I:929:ILE:HD13	2:I:1055:ALA:HB2	1.69	0.74
2:I:1184:THR:HG23	2:I:1189:GLY:HA3	1.68	0.74
2:C:511:LEU:HD12	2:C:511:LEU:N	2.02	0.74
2:C:759:SER:O	2:C:761:GLN:N	2.19	0.74
3:D:1280:VAL:HG21	3:D:1304:ARG:NE	2.01	0.74
2:C:615:VAL:HG13	2:C:651:ASP:H	1.51	0.74
3:D:888:CYS:SG	3:D:889:ASP:N	2.61	0.74
2:I:109:ALA:HB1	2:I:110:PRO:C	2.13	0.74
2:I:1302:THR:HG22	5:L:531:PRO:HB3	1.70	0.74
3:J:362:ARG:H	3:J:365:GLN:HE21	1.33	0.74
2:C:1114:GLU:OE1	2:C:1230:MET:HA	1.88	0.74
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.68	0.74
1:G:9:LEU:O	1:H:227:GLN:NE2	2.21	0.74
2:C:142:GLU:CB	2:C:760:ASN:HD21	1.99	0.74
2:C:878:THR:OG1	2:C:879:GLY:N	2.19	0.74
3:D:98:ARG:HB3	3:D:248:ASP:OD2	1.88	0.74
3:D:363:LEU:HA	3:D:450:HIS:CD2	2.23	0.74
1:A:12:ARG:H	1:A:30:PRO:HG2	1.53	0.74
3:D:45:ASN:HB3	3:D:48:THR:O	1.89	0.73
2:I:1101:LEU:HD12	3:J:505:ASP:OD2	1.87	0.73
3:J:1159:ILE:HA	3:J:1206:ARG:HB3	1.70	0.73
5:L:343:LYS:H	5:L:343:LYS:HD2	1.52	0.73
1:B:149:GLY:HA3	1:B:177:TYR:CD2	2.23	0.73
2:C:86:GLN:HA	2:C:140:GLY:HA2	1.69	0.73
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.69	0.73
2:C:1289:GLU:OE2	3:D:473:THR:HG22	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:73:GLY:O	3:D:76:LYS:NZ	2.17	0.73
5:L:305:LEU:HB3	5:L:315:TRP:HB3	1.70	0.73
5:L:362:ASN:HB2	5:L:365:MET:HE2	1.70	0.73
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.69	0.73
3:D:847:ASP:HA	3:D:860:ARG:H	1.53	0.73
1:G:194:GLN:O	1:G:195:ARG:HG2	1.88	0.73
2:I:148:GLN:NE2	2:I:535:PRO:O	2.18	0.73
1:H:50:SER:HA	1:H:150:ARG:O	1.88	0.73
1:A:166:ARG:O	1:A:168:ILE:N	2.22	0.73
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.70	0.73
2:I:207:THR:HG21	2:I:351:LEU:HG	1.70	0.73
2:I:724:VAL:HA	2:I:734:ILE:HD13	1.71	0.73
2:I:758:ARG:HH22	2:I:761:GLN:HG3	1.54	0.73
1:A:87:GLY:O	1:A:125:LYS:NZ	2.21	0.73
2:C:131:THR:CG2	2:C:135:THR:H	2.02	0.73
3:D:1183:SER:OG	3:J:206:ASN:ND2	2.22	0.72
3:J:152:THR:OG1	3:J:153:ASN:N	2.22	0.72
3:J:403:ARG:HB3	3:J:405:GLU:HG3	1.71	0.72
5:L:97:PRO:HA	5:L:100:MET:HG3	1.70	0.72
1:A:32:GLU:HA	1:A:198:LEU:HD22	1.71	0.72
2:C:74:ARG:HH12	2:C:121:GLU:CD	1.96	0.72
3:D:314:ARG:NH2	3:D:323:PRO:HG3	2.04	0.72
2:C:812:PHE:CE2	3:D:451:PRO:HB3	2.24	0.72
5:F:134:VAL:HA	5:F:273:MET:HE1	1.71	0.72
2:I:819:SER:HB2	2:I:1085:MET:SD	2.29	0.72
3:J:435:GLN:HB2	3:J:457:TYR:OH	1.89	0.72
3:D:399:LYS:NZ	5:F:611:LEU:O	2.23	0.72
2:C:30:ILE:H	2:C:30:ILE:HD12	1.53	0.72
2:C:242:VAL:HB	2:C:245:ARG:HD2	1.70	0.72
2:I:125:GLY:HA2	2:I:499:SER:HB2	1.71	0.72
2:I:942:ASP:OD2	2:I:1048:LYS:NZ	2.23	0.72
1:B:82:LEU:HA	1:B:85:LEU:HD12	1.71	0.72
2:I:1312:ASN:ND2	2:I:1314:GLN:HE21	1.82	0.72
1:A:36:GLY:HA3	1:A:187:VAL:HG11	1.71	0.72
3:D:72:CYS:HB3	3:D:88:CYS:SG	2.29	0.72
5:F:395:THR:OG1	5:F:396:ASN:N	2.23	0.72
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.72	0.72
3:J:576:ARG:NH1	3:J:593:ASN:O	2.21	0.72
3:D:598:LYS:O	3:D:601:ILE:HG22	1.89	0.72
3:J:905:ARG:NH1	3:J:910:ASN:HD21	1.88	0.72
5:L:512:GLY:O	5:L:514:ASP:N	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:79:LEU:HD21	2:I:756:TYR:OH	1.89	0.72
1:H:89:ALA:HB3	1:H:124:VAL:HG12	1.70	0.72
5:L:387:VAL:HG22	5:L:435:ILE:HD13	1.71	0.72
3:J:810:THR:CG2	3:J:893:GLY:HA3	2.20	0.71
5:L:386:LEU:O	5:L:389:SER:OG	2.05	0.71
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.23	0.71
2:C:617:ALA:HA	2:C:636:CYS:SG	2.29	0.71
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.72	0.71
2:I:836:LEU:HD13	2:I:1054:LEU:HD13	1.70	0.71
3:J:1309:ILE:HG13	3:J:1310:THR:N	2.05	0.71
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.23	0.71
2:C:1202:GLY:O	2:C:1203:ASP:HB2	1.90	0.71
3:J:650:LYS:NZ	3:J:765:GLU:OE2	2.24	0.71
2:C:90:VAL:HG12	2:C:91:THR:H	1.55	0.71
2:C:696:ASP:HB2	2:C:798:GLN:CG	2.19	0.71
2:I:1268:GLN:HE22	3:J:352:ARG:NH1	1.88	0.71
3:J:56:LEU:HD12	3:J:56:LEU:H	1.56	0.71
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.73	0.71
2:I:660:VAL:HG13	2:I:661:VAL:HG13	1.71	0.71
2:C:1284:ALA:HB1	3:D:1356:LEU:HD22	1.70	0.71
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.71	0.71
3:J:706:VAL:HG12	3:J:715:LYS:HB3	1.72	0.71
1:A:83:LEU:HD23	2:C:694:ARG:HE	1.54	0.71
2:C:703:GLY:N	2:C:705:GLU:OE2	2.23	0.71
5:L:281:ARG:HG2	5:L:285:ARG:HD2	1.73	0.71
2:C:980:VAL:HA	2:C:984:VAL:HA	1.72	0.71
2:C:987:GLU:HG2	2:C:991:LYS:HE3	1.71	0.71
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.73	0.71
3:D:35:PHE:HD1	3:D:101:ARG:HB3	1.55	0.71
3:D:355:ILE:HG22	3:D:447:ILE:HB	1.72	0.71
1:G:49:SER:OG	1:G:50:SER:N	2.23	0.71
1:G:102:LEU:HD23	1:G:115:ILE:HG12	1.71	0.71
2:I:578:TYR:HB3	2:I:590:PRO:HG2	1.71	0.70
5:L:601:PRO:HA	5:L:604:SER:HB2	1.74	0.70
1:A:13:LEU:H	1:A:13:LEU:HD23	1.56	0.70
2:C:700:VAL:HG13	2:C:1117:LEU:HD22	1.72	0.70
1:H:102:LEU:HB2	1:H:142:MET:H	1.56	0.70
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.31	0.70
2:I:1333:LEU:HD22	3:J:307:LEU:HD22	1.73	0.70
3:J:798:ARG:NH1	3:J:802:ASP:OD2	2.23	0.70
1:A:310:ARG:O	5:F:608:ARG:NH1	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:ARG:O	1:B:13:LEU:HG	1.91	0.70
3:D:1273:ASP:HB3	3:D:1276:GLU:HG3	1.73	0.70
1:G:66:HIS:CE1	2:I:874:GLY:HA2	2.26	0.70
5:L:512:GLY:C	5:L:514:ASP:H	2.00	0.70
1:A:29:GLU:HB3	1:A:30:PRO:CD	2.21	0.70
2:I:810:TYR:CD2	3:J:359:PRO:HG2	2.27	0.70
2:I:1223:ARG:NH1	3:J:721:SER:OG	2.24	0.70
5:F:227:GLN:HE22	5:F:251:LYS:HZ1	1.40	0.70
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.74	0.70
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.22	0.70
2:C:1080:ASN:HB3	2:C:1085:MET:HE3	1.72	0.70
3:D:516:ASP:HA	3:D:545:HIS:HB2	1.74	0.70
5:F:601:PRO:HA	5:F:604:SER:HB2	1.72	0.70
3:J:1177:ILE:HD12	3:J:1186:TYR:HB3	1.74	0.70
3:J:1239:ASP:OD1	3:J:1242:ARG:NH2	2.25	0.70
1:A:172:LEU:H	1:A:172:LEU:HD12	1.55	0.70
2:C:864:LYS:HZ3	2:C:877:VAL:HG12	1.57	0.70
3:J:557:LYS:HA	3:J:563:LEU:HA	1.73	0.70
5:L:412:LEU:HB2	5:L:435:ILE:HD11	1.73	0.70
3:D:902:ASP:OD1	3:D:903:LEU:N	2.25	0.70
5:F:277:MET:HG3	5:F:362:ASN:ND2	2.07	0.70
5:L:483:LEU:HD12	5:L:483:LEU:H	1.57	0.70
2:C:1151:LEU:HD11	2:C:1198:LEU:HD23	1.73	0.69
3:D:854:ALA:HB2	3:J:1372:ARG:HB2	1.74	0.69
1:A:51:MET:HE1	1:A:216:ALA:HA	1.74	0.69
5:F:97:PRO:HA	5:F:100:MET:HG3	1.73	0.69
5:F:600:HIS:CD2	5:F:601:PRO:HD2	2.26	0.69
2:I:521:LEU:HA	2:I:524:ILE:HG22	1.75	0.69
5:L:547:VAL:HG23	5:L:603:ARG:HH11	1.57	0.69
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.23	0.69
3:D:866:GLU:OE2	3:D:901:ARG:NH2	2.24	0.69
3:D:1167:LYS:HD3	3:D:1174:ARG:HD2	1.72	0.69
3:J:425:ARG:NH1	3:J:459:ALA:HA	2.07	0.69
3:J:210:SER:O	3:J:214:ARG:HG2	1.92	0.69
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.28	0.69
2:C:8:LYS:HE3	2:C:1171:ARG:CZ	2.23	0.69
3:D:1159:ILE:HA	3:D:1206:ARG:HB3	1.72	0.69
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.73	0.69
1:H:60:GLU:HG3	1:H:143:ARG:O	1.92	0.69
3:J:360:TYR:OH	3:J:448:GLN:OE1	2.05	0.69
3:D:248:ASP:O	3:D:251:PRO:HG3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:708:ASN:HB3	3:D:712:GLN:O	1.92	0.69
3:J:202:ARG:NH2	3:J:225:GLU:OE1	2.25	0.69
3:J:848:VAL:HG23	3:J:858:VAL:HG13	1.74	0.69
3:J:1341:ARG:NH1	3:J:1343:GLU:OE2	2.26	0.69
2:C:453:ILE:HD12	2:C:587:LEU:HD21	1.73	0.69
3:D:709:ARG:C	3:D:711:GLY:H	2.01	0.69
3:D:1149:ARG:CZ	3:D:1153:PRO:HG2	2.22	0.69
1:B:205:MET:HE3	1:B:213:PRO:HB3	1.73	0.69
2:C:582:ASN:HB3	2:C:586:PHE:H	1.57	0.69
1:G:218:ARG:HG3	1:H:231:PHE:O	1.93	0.69
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.73	0.68
1:G:92:VAL:O	1:G:148:ARG:NH2	2.25	0.68
1:G:134:THR:HG23	1:G:135:ASP:H	1.56	0.68
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.28	0.68
1:A:31:LEU:HB2	1:A:199:ASP:O	1.94	0.68
1:B:98:VAL:HG11	1:B:121:VAL:HG22	1.74	0.68
3:D:293:ARG:NH1	5:F:104:GLU:OE2	2.27	0.68
1:A:27:THR:C	1:A:28:LEU:HD13	2.18	0.68
3:D:674:THR:OG1	3:D:677:GLU:HB2	1.94	0.68
5:F:247:GLU:HA	5:F:250:LEU:HD12	1.74	0.68
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.76	0.68
2:C:618:GLN:HG3	2:C:619:ALA:N	2.05	0.68
3:J:1344:LEU:HB3	3:J:1350:ASN:ND2	2.08	0.68
5:L:101:TYR:O	5:L:104:GLU:N	2.26	0.68
5:L:281:ARG:O	5:L:285:ARG:HG3	1.93	0.68
2:C:886:LYS:HE3	2:C:916:SER:HB3	1.75	0.68
3:D:74:LYS:HD2	3:D:87:LYS:HD3	1.75	0.68
3:D:817:HIS:CE1	3:D:860:ARG:NE	2.61	0.68
3:J:1137:GLY:O	3:J:1140:ARG:HB3	1.93	0.68
1:B:48:LEU:HD12	1:B:183:ILE:HD11	1.73	0.68
2:C:12:ARG:HH21	2:C:793:GLU:CD	2.01	0.68
3:D:1266:ILE:HD12	3:D:1273:ASP:O	1.94	0.68
3:D:1295:ASN:CB	3:D:1298:VAL:HB	2.24	0.68
2:C:563:THR:OG1	2:C:564:PRO:HD2	1.93	0.68
1:H:61:ILE:HB	1:H:64:VAL:O	1.94	0.68
3:J:98:ARG:HB3	3:J:248:ASP:OD2	1.94	0.68
3:J:362:ARG:H	3:J:365:GLN:NE2	1.91	0.68
1:A:227:GLN:NE2	1:B:9:LEU:O	2.27	0.68
2:C:296:VAL:HB	2:C:336:LEU:HD12	1.75	0.68
3:D:709:ARG:O	3:D:711:GLY:N	2.27	0.68
5:F:306:PHE:HE1	5:F:315:TRP:CD2	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:79:LEU:HD23	1:G:79:LEU:H	1.59	0.68
2:I:890:LYS:HE2	2:I:891:GLY:H	1.58	0.68
1:B:29:GLU:HB3	1:B:200:LYS:HG3	1.74	0.68
2:C:27:LEU:O	2:C:528:ARG:NH1	2.27	0.68
2:C:363:LEU:HB3	2:C:381:ALA:HB1	1.74	0.68
2:C:557:ARG:HH21	2:C:607:SER:C	2.01	0.68
2:C:1211:ARG:HD3	2:C:1213:TYR:OH	1.94	0.68
3:D:824:PRO:HD3	3:D:835:LEU:HB2	1.74	0.68
3:J:817:HIS:CE1	3:J:860:ARG:HE	2.12	0.68
4:K:70:GLN:NE2	4:K:74:GLU:OE2	2.16	0.68
2:I:724:VAL:HG23	2:I:775:GLU:O	1.94	0.67
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.77	0.67
2:C:656:SER:OG	2:C:657:THR:N	2.22	0.67
3:D:1290:ARG:HG2	3:D:1298:VAL:HG12	1.75	0.67
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.76	0.67
3:J:847:ASP:OD1	3:J:847:ASP:N	2.23	0.67
1:A:7:GLU:OE1	1:B:150:ARG:NH2	2.28	0.67
1:A:73:GLY:O	1:A:134:THR:HG22	1.95	0.67
1:A:155:ALA:HA	1:A:158:ARG:HG3	1.76	0.67
3:D:262:THR:OG1	3:D:263:SER:N	2.24	0.67
1:G:45:ARG:HH22	1:H:37:HIS:HB3	1.59	0.67
2:I:517:GLN:NE2	2:I:687:ARG:O	2.26	0.67
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.75	0.67
1:A:45:ARG:HG2	1:B:38:THR:CB	2.21	0.67
2:C:4:SER:H	2:C:7:GLU:CD	2.01	0.67
3:J:75:TYR:CE2	3:J:83:VAL:HG21	2.28	0.67
3:J:773:PHE:O	3:J:776:THR:HB	1.95	0.67
2:C:268:ARG:HH21	2:C:270:THR:HG21	1.60	0.67
3:D:210:SER:O	3:D:214:ARG:HG2	1.95	0.67
2:I:478:ARG:NH1	2:I:482:GLY:HA2	2.10	0.67
2:I:607:SER:N	2:I:610:GLU:OE1	2.27	0.67
1:G:75:GLN:HA	2:I:729:ALA:N	2.09	0.67
2:I:1080:ASN:HB3	2:I:1085:MET:HE3	1.75	0.67
2:I:1158:LYS:O	2:I:1159:VAL:HG13	1.94	0.67
3:J:1179:PRO:HD2	3:J:1184:ASP:HA	1.77	0.67
2:C:494:ASN:HD22	2:C:497:PRO:HD3	1.58	0.67
5:F:479:THR:HG23	5:F:481:GLU:H	1.58	0.67
2:C:520:PRO:HG3	2:C:714:VAL:HG21	1.77	0.67
2:C:1242:LYS:HD2	3:D:465:GLN:OE1	1.94	0.67
2:I:629:PHE:O	2:I:647:ARG:NH2	2.28	0.67
3:J:700:ASN:O	3:J:704:GLU:HB2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1263:LYS:CE	3:J:1279:GLN:HE21	2.08	0.67
5:F:105:MET:HE1	5:F:385:ARG:HG2	1.75	0.67
1:G:22:THR:O	1:G:207:THR:N	2.27	0.67
1:H:67:GLU:O	1:H:78:ILE:HB	1.95	0.67
2:C:109:ALA:HB1	2:C:110:PRO:C	2.19	0.66
2:C:1238:LEU:H	2:C:1238:LEU:HD12	1.60	0.66
3:D:694:SER:OG	3:D:738:ARG:NE	2.28	0.66
2:I:818:VAL:O	2:I:1079:ILE:HD12	1.95	0.66
3:D:706:VAL:HG12	3:D:715:LYS:HB3	1.75	0.66
5:F:461:ASN:HB3	5:F:465:ARG:NH2	2.11	0.66
1:B:214:GLU:OE2	1:B:218:ARG:NH2	2.26	0.66
2:C:269:ILE:HA	2:C:273:HIS:ND1	2.10	0.66
2:I:55:SER:OG	2:I:56:VAL:N	2.28	0.66
2:I:555:TYR:OH	2:I:654:ASP:OD1	2.11	0.66
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.35	0.66
1:G:231:PHE:HA	1:H:218:ARG:NH1	2.10	0.66
2:I:1280:ALA:HB3	3:J:431:ARG:HB3	1.77	0.66
3:J:1215:GLU:N	3:J:1215:GLU:OE2	2.28	0.66
1:G:52:PRO:HG2	1:G:219:ARG:HE	1.60	0.66
1:G:231:PHE:CD1	1:H:218:ARG:HG2	2.29	0.66
3:J:614:LEU:HD23	4:K:7:GLN:HB2	1.78	0.66
3:J:743:MET:HB2	3:J:759:ILE:O	1.96	0.66
3:J:902:ASP:OD1	3:J:903:LEU:N	2.29	0.66
3:D:56:LEU:HD12	3:D:56:LEU:N	2.04	0.66
5:F:139:GLU:HG2	5:F:351:THR:HA	1.77	0.66
5:L:134:VAL:HA	5:L:273:MET:HE1	1.77	0.66
3:D:77:ARG:HB3	3:D:80:HIS:CE1	2.31	0.66
3:D:362:ARG:H	3:D:365:GLN:HE21	1.43	0.66
1:G:76:GLU:OE1	1:G:132:HIS:N	2.21	0.66
2:I:886:LYS:CE	2:I:916:SER:HB3	2.26	0.66
3:D:77:ARG:HB3	3:D:80:HIS:ND1	2.10	0.66
3:D:392:THR:HG21	5:F:606:VAL:HA	1.78	0.66
1:H:54:CYS:SG	1:H:148:ARG:HG2	2.36	0.66
5:L:139:GLU:HG2	5:L:351:THR:HA	1.77	0.66
5:L:461:ASN:O	5:L:465:ARG:HG2	1.95	0.66
1:B:64:VAL:HG21	1:B:69:SER:HB3	1.78	0.66
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.14	0.66
3:J:349:TYR:HE2	3:J:379:PRO:HG2	1.61	0.66
2:C:3:TYR:CE1	2:C:11:ILE:HD11	2.32	0.65
2:C:1158:LYS:O	2:C:1159:VAL:HG13	1.95	0.65
3:D:708:ASN:OD1	3:D:708:ASN:N	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:371:LYS:HA	5:L:374:ARG:NH1	2.12	0.65
2:C:566:GLY:O	2:C:569:ILE:HG13	1.96	0.65
2:C:816:ILE:O	2:C:1076:ILE:HD12	1.96	0.65
3:J:218:THR:HG21	3:J:1275:LEU:HD11	1.78	0.65
1:A:66:HIS:CE1	1:A:69:SER:HB3	2.31	0.65
2:C:1101:LEU:HD12	3:D:505:ASP:OD2	1.96	0.65
2:I:1246:ARG:NE	3:J:348:ASP:OD1	2.30	0.65
3:J:1358:PRO:HB3	3:J:1366:HIS:CG	2.31	0.65
1:A:45:ARG:NH2	2:C:1215:GLY:O	2.26	0.65
2:C:125:GLY:HA2	2:C:499:SER:HB2	1.78	0.65
1:G:12:ARG:HG2	1:G:13:LEU:HD23	1.76	0.65
2:I:14:ASP:N	2:I:1157:GLN:OE1	2.28	0.65
2:I:176:ILE:HD11	2:I:428:VAL:HG21	1.77	0.65
1:A:41:ASN:ND2	2:C:1216:ARG:O	2.29	0.65
1:G:12:ARG:HA	1:H:231:PHE:CZ	2.32	0.65
3:J:491:LEU:HD23	3:J:498:PRO:HA	1.77	0.65
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.79	0.65
2:C:316:GLU:H	2:C:316:GLU:CD	2.04	0.65
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.78	0.65
3:D:1372:ARG:O	3:D:1375:ALA:HB3	1.96	0.65
2:I:1134:GLN:HB3	2:I:1136:GLN:HG2	1.77	0.65
1:A:29:GLU:N	1:A:30:PRO:HD2	2.12	0.65
3:D:109:SER:CB	3:D:296:LYS:HE2	2.26	0.65
1:G:118:ASP:HB3	1:G:121:VAL:HG23	1.79	0.65
3:J:416:ILE:HG12	3:J:441:LEU:CD2	2.26	0.65
3:J:514:THR:HB	3:J:576:ARG:HG2	1.78	0.65
1:A:156:SER:HB2	2:C:1059:ARG:HH22	1.61	0.65
3:D:827:GLU:HB3	3:D:832:LYS:HD2	1.78	0.65
1:G:102:LEU:HD22	1:G:103:ASN:H	1.60	0.65
3:J:436:ALA:HB3	3:J:485:MET:HA	1.79	0.65
3:J:518:VAL:CG1	3:J:707:ILE:HD13	2.27	0.65
3:J:1140:ARG:NE	3:J:1144:LEU:HD11	2.11	0.65
2:C:483:ASP:HB2	2:C:486:THR:CG2	2.26	0.65
3:D:24:LEU:HD23	3:D:232:ASN:ND2	2.11	0.65
3:D:298:MET:SD	5:F:402:LEU:HB3	2.37	0.65
3:D:418:GLU:H	4:E:45:LYS:HZ2	1.45	0.65
2:I:755:LYS:O	2:I:757:THR:HG22	1.97	0.65
2:I:758:ARG:NH2	2:I:761:GLN:HG3	2.10	0.65
3:J:1289:ASN:OD1	3:J:1290:ARG:NH1	2.30	0.65
5:L:571:TYR:CD1	5:L:575:GLU:HG2	2.31	0.65
1:B:100:LEU:HD21	1:B:121:VAL:HG11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:891:GLY:O	2:C:892:GLU:HG3	1.97	0.64
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.79	0.64
2:I:866:ASP:HA	2:I:872:TYR:OH	1.97	0.64
2:C:42:ASP:OD2	2:C:44:GLU:N	2.30	0.64
2:I:1196:LYS:HA	2:I:1199:LEU:HD12	1.79	0.64
3:J:290:ILE:H	3:J:290:ILE:HD12	1.62	0.64
3:J:901:ARG:HD2	3:J:906:GLY:O	1.97	0.64
3:J:1193:TRP:HB2	3:J:1194:ARG:NH1	2.12	0.64
5:F:490:PRO:HB2	5:F:493:LYS:HG3	1.79	0.64
2:I:57:PHE:HD1	2:I:58:PRO:HA	1.63	0.64
3:D:1179:PRO:HD2	3:D:1184:ASP:HA	1.79	0.64
3:J:258:GLY:HA3	5:L:499:LYS:HD3	1.79	0.64
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.77	0.64
3:J:1159:ILE:HD12	3:J:1206:ARG:HD2	1.77	0.64
3:D:768:ASN:N	3:D:771:GLN:OE1	2.26	0.64
5:F:512:GLY:O	5:F:514:ASP:N	2.30	0.64
3:J:1140:ARG:HE	3:J:1144:LEU:HD11	1.61	0.64
1:B:81:ILE:O	1:B:85:LEU:HG	1.97	0.64
2:C:522:SER:O	2:C:525:THR:HG22	1.97	0.64
1:G:45:ARG:HG2	1:H:38:THR:HB	1.78	0.64
2:I:890:LYS:HE2	2:I:891:GLY:N	2.13	0.64
2:I:1065:LYS:HE2	3:J:462:ASP:O	1.98	0.64
3:J:544:LEU:O	3:J:574:VAL:HB	1.97	0.64
3:J:1140:ARG:NH2	3:J:1236:GLU:HG2	2.12	0.64
4:K:4:VAL:HG13	4:K:5:THR:HG23	1.78	0.64
5:L:573:LEU:HD23	5:L:573:LEU:H	1.63	0.64
1:A:263:THR:N	1:A:302:GLU:OE2	2.26	0.64
2:C:1101:LEU:O	3:D:731:ARG:HD3	1.97	0.64
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.79	0.64
1:G:45:ARG:HD3	2:I:1083:GLU:HB3	1.79	0.64
1:A:71:LYS:HB3	1:A:74:VAL:CG1	2.27	0.64
1:A:261:GLU:OE1	2:C:859:GLU:N	2.28	0.64
1:G:95:LYS:NZ	1:G:118:ASP:OD2	2.30	0.64
3:J:709:ARG:O	3:J:711:GLY:N	2.31	0.64
4:K:71:GLU:HA	4:K:74:GLU:HG3	1.80	0.64
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.80	0.64
3:J:367:GLY:HA3	3:J:448:GLN:HB2	1.79	0.64
5:L:457:ILE:HA	5:L:460:ILE:HD12	1.80	0.64
1:A:71:LYS:HB3	1:A:74:VAL:HG11	1.80	0.63
2:C:14:ASP:HA	2:C:1183:ALA:HB3	1.80	0.63
2:C:670:PHE:CE2	2:C:1113:LEU:HB3	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:317:THR:HG22	3:D:322:ARG:O	1.98	0.63
5:F:244:THR:O	5:F:247:GLU:HG2	1.99	0.63
2:I:1268:GLN:OE1	3:J:352:ARG:HG2	1.98	0.63
3:J:527:LEU:HD23	3:J:532:GLU:HG3	1.79	0.63
3:J:598:LYS:O	3:J:601:ILE:HG22	1.98	0.63
1:B:54:CYS:SG	1:B:148:ARG:HG2	2.38	0.63
2:C:156:PHE:CE2	2:C:158:ASP:HB2	2.34	0.63
2:I:759:SER:O	2:I:761:GLN:N	2.26	0.63
3:J:216:LYS:HA	3:J:219:LYS:HE3	1.80	0.63
3:D:425:ARG:HH12	3:D:464:ASP:CG	2.06	0.63
1:G:179:PRO:HA	1:G:208:ASN:ND2	2.13	0.63
5:F:582:VAL:CG1	5:F:586:ARG:HG2	2.27	0.63
2:I:906:PHE:CE2	5:L:608:ARG:HG3	2.34	0.63
2:I:1217:THR:OG1	2:I:1219:GLU:HG2	1.98	0.63
3:J:115:TRP:CZ2	3:J:1329:THR:HG23	2.34	0.63
2:C:582:ASN:HB3	2:C:586:PHE:N	2.12	0.63
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.62	0.63
3:D:901:ARG:HA	3:D:908:ILE:HA	1.79	0.63
3:D:1143:ASP:OD1	3:D:1148:ARG:NH1	2.32	0.63
2:C:974:ARG:HD2	2:C:1014:LEU:HD21	1.79	0.63
3:D:1160:SER:HG	3:D:1203:ARG:HH12	1.45	0.63
3:J:470:VAL:HG12	3:J:472:LEU:HD23	1.80	0.63
3:J:1326:GLN:OE1	3:J:1330:ARG:NH2	2.31	0.63
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.79	0.63
3:D:892:PHE:H	3:D:1281:GLU:HG2	1.63	0.63
2:I:161:LYS:HA	2:I:170:VAL:HA	1.81	0.63
1:B:50:SER:HA	1:B:150:ARG:O	1.99	0.63
2:C:158:ASP:OD1	2:C:159:SER:N	2.32	0.63
3:D:242:LEU:HD23	3:D:242:LEU:C	2.24	0.63
2:I:987:GLU:HG2	2:I:991:LYS:HE3	1.81	0.63
5:L:164:GLY:O	5:L:260:ARG:HB2	1.99	0.63
2:C:1146:GLN:NE2	2:C:1150:ASP:OD2	2.33	0.62
2:C:1319:MET:HG3	2:C:1320:PRO:HD2	1.81	0.62
3:D:102:MET:HE3	3:D:246:PRO:HD3	1.81	0.62
1:G:11:PRO:HB3	1:G:30:PRO:O	1.98	0.62
1:G:14:VAL:HG13	1:G:15:ASP:H	1.64	0.62
2:I:518:ASN:O	2:I:522:SER:HB3	1.99	0.62
1:G:118:ASP:HB3	1:G:121:VAL:CG2	2.29	0.62
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.33	0.62
3:D:156:ARG:NH2	3:D:191:SER:OG	2.32	0.62
3:D:1282:TYR:O	3:D:1285:VAL:HG12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:821:ARG:NH2	2:I:1082:ILE:HG21	2.08	0.62
1:A:118:ASP:H	1:A:121:VAL:HB	1.64	0.62
1:A:152:TYR:CZ	2:C:824:GLN:HA	2.34	0.62
3:D:1177:ILE:HD12	3:D:1186:TYR:HB3	1.81	0.62
5:L:274:ARG:NH2	5:L:369:GLU:OE2	2.32	0.62
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.81	0.62
5:L:540:LEU:HD12	5:L:610:PHE:CD1	2.34	0.62
2:C:748:ILE:HD11	2:C:967:LEU:HD12	1.80	0.62
3:D:388:ARG:HB2	3:D:390:LEU:HD13	1.80	0.62
1:H:118:ASP:HB2	1:H:121:VAL:CG2	2.29	0.62
2:I:968:GLU:HG3	2:I:1018:TYR:HE1	1.63	0.62
3:J:746:LEU:HD22	3:J:754:ILE:HD11	1.81	0.62
1:A:12:ARG:HG3	1:B:230:ALA:HB1	1.82	0.62
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.28	0.62
2:C:1024:GLU:HA	2:C:1027:LYS:HD3	1.81	0.62
3:D:1198:VAL:HB	3:D:1210:ILE:HA	1.82	0.62
5:L:561:MET:HA	5:L:567:MET:HE1	1.81	0.62
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.82	0.62
5:L:119:ILE:HA	5:L:122:ARG:HD3	1.82	0.62
2:C:131:THR:HG23	2:C:133:ASN:N	2.15	0.62
2:C:814:ASP:OD2	2:C:1106:ARG:NH1	2.21	0.62
3:D:1318:SER:OG	3:D:1342:ASP:OD2	2.11	0.62
1:H:48:LEU:HD21	3:J:535:ARG:HG3	1.82	0.62
2:I:801:ARG:HG2	2:I:1094:VAL:HG23	1.81	0.62
2:C:23:ASP:OD1	2:C:23:ASP:N	2.32	0.62
3:D:1293:GLU:H	3:J:1226:VAL:HB	1.64	0.62
5:F:354:THR:O	5:F:358:VAL:HG23	1.98	0.62
3:J:620:PHE:CE1	3:J:624:ILE:HD11	2.35	0.62
3:J:1270:GLY:HA3	3:J:1298:VAL:HG22	1.81	0.62
1:B:73:GLY:HA2	1:B:134:THR:HG22	1.82	0.61
2:C:593:LYS:HE3	2:C:595:THR:HG22	1.82	0.61
2:C:878:THR:N	2:C:881:ASP:OD2	2.24	0.61
5:F:461:ASN:HB3	5:F:465:ARG:HH21	1.64	0.61
2:I:227:LYS:O	2:I:245:ARG:NH2	2.33	0.61
2:C:13:LYS:NZ	2:C:1148:ALA:O	2.32	0.61
2:C:836:LEU:HD12	2:C:836:LEU:N	2.15	0.61
3:D:697:MET:SD	3:D:741:ALA:HB3	2.40	0.61
2:C:710:VAL:HG13	2:C:717:VAL:HG21	1.82	0.61
3:D:190:LYS:HD3	3:D:235:GLU:HG2	1.81	0.61
1:G:60:GLU:O	1:G:142:MET:HB2	2.00	0.61
2:I:658:GLN:O	2:I:661:VAL:HG22	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1273:MET:HG2	2:I:1276:TRP:CZ3	2.35	0.61
5:F:316:PHE:HZ	5:F:334:SER:HA	1.64	0.61
2:I:896:THR:HB	2:I:897:PRO:HD2	1.81	0.61
3:J:1309:ILE:HG13	3:J:1310:THR:H	1.66	0.61
1:B:59:VAL:HG22	1:B:144:ILE:HG13	1.81	0.61
3:D:891:ASP:HA	3:D:1281:GLU:HG3	1.82	0.61
3:J:418:GLU:H	4:K:45:LYS:NZ	1.98	0.61
1:A:54:CYS:HA	1:A:148:ARG:HA	1.83	0.61
3:D:1149:ARG:NH2	3:D:1153:PRO:HG2	2.16	0.61
1:G:66:HIS:NE2	2:I:929:ILE:HA	2.14	0.61
2:I:1246:ARG:HG2	2:I:1247:SER:N	2.15	0.61
3:J:30:ILE:HG23	3:J:243:PRO:HG3	1.82	0.61
3:J:502:PRO:HB3	3:J:506:VAL:HG21	1.83	0.61
3:D:316:ILE:HA	3:D:323:PRO:HA	1.82	0.61
1:A:218:ARG:HG3	1:B:231:PHE:O	2.01	0.61
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.83	0.61
3:J:115:TRP:CE2	3:J:1329:THR:HG23	2.36	0.61
2:C:601:ASP:OD1	2:C:601:ASP:N	2.32	0.61
3:J:647:PRO:CG	3:J:697:MET:HB3	2.30	0.61
1:A:190:ALA:H	1:A:199:ASP:HA	1.66	0.61
2:C:488:MET:O	2:C:490:GLN:N	2.32	0.61
1:G:152:TYR:HD1	1:G:176:CYS:HB3	1.65	0.61
2:I:466:VAL:O	2:I:469:VAL:HG22	2.01	0.61
5:L:426:LYS:HE2	5:L:428:SER:OG	2.01	0.61
5:L:493:LYS:HA	5:L:496:LYS:HE2	1.81	0.61
1:B:153:VAL:HB	1:B:175:ALA:HB3	1.82	0.60
2:C:667:LEU:HD21	2:C:704:MET:HB2	1.82	0.60
3:D:762:ASN:OD1	3:D:764:ARG:N	2.33	0.60
3:J:361:LEU:HD13	3:J:366:CYS:HA	1.82	0.60
2:C:379:GLU:CD	2:C:379:GLU:H	2.08	0.60
1:H:33:ARG:HD2	2:I:1081:PRO:HG3	1.84	0.60
2:I:848:GLU:OE1	2:I:886:LYS:NZ	2.34	0.60
3:D:833:GLU:OE2	3:D:1247:LYS:NZ	2.35	0.60
2:I:346:TYR:OH	2:I:437:ASN:OD1	2.02	0.60
2:I:697:LYS:HA	2:I:795:ALA:HB2	1.83	0.60
2:I:1297:ASP:OD1	2:I:1300:GLY:N	2.25	0.60
3:J:418:GLU:H	4:K:45:LYS:HZ2	1.47	0.60
2:C:156:PHE:CZ	2:C:158:ASP:HB2	2.37	0.60
2:C:510:GLN:OE1	2:C:534:GLY:HA2	2.00	0.60
2:C:1246:ARG:NH2	3:D:348:ASP:OD1	2.34	0.60
3:D:147:ILE:HG13	3:D:147:ILE:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:514:THR:O	3:D:514:THR:OG1	2.19	0.60
3:D:854:ALA:CB	3:J:1372:ARG:HE	2.14	0.60
3:D:1280:VAL:CG1	3:D:1304:ARG:HH21	2.04	0.60
3:J:128:LEU:HA	3:J:192:MET:HE1	1.82	0.60
3:J:697:MET:SD	3:J:741:ALA:HB3	2.41	0.60
5:L:226:ALA:O	5:L:229:VAL:HG22	2.01	0.60
2:C:256:GLU:HB3	2:C:261:VAL:HG13	1.82	0.60
2:C:268:ARG:NH2	2:C:270:THR:HG21	2.17	0.60
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.37	0.60
3:J:709:ARG:C	3:J:711:GLY:H	2.08	0.60
3:J:138:VAL:HG21	3:J:145:VAL:HB	1.83	0.60
1:B:107:ILE:HG23	1:B:135:ASP:HA	1.82	0.60
2:C:138:ILE:HG22	2:C:139:ASN:N	2.16	0.60
3:D:342:LEU:HD11	3:D:1324:SER:HB3	1.82	0.60
3:D:375:GLU:OE2	3:D:378:LYS:HD2	2.02	0.60
2:I:1222:GLU:OE2	3:J:537:TYR:OH	2.19	0.60
2:I:1247:SER:HB3	3:J:375:GLU:O	2.01	0.60
3:J:536:LEU:HD13	3:J:541:LEU:HB2	1.83	0.60
3:J:888:CYS:SG	3:J:889:ASP:N	2.75	0.60
3:D:115:TRP:CE2	3:D:1329:THR:HG23	2.37	0.60
2:I:42:ASP:OD2	2:I:46:GLN:HB3	2.02	0.60
2:I:519:ASN:HD21	2:I:796:LEU:HD23	1.67	0.60
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.66	0.60
2:I:1293:VAL:HG11	2:I:1304:MET:HE2	1.84	0.60
5:L:299:LYS:HA	5:L:302:PHE:HB3	1.83	0.60
1:A:249:PHE:HB2	1:A:253:LEU:HD12	1.82	0.60
2:C:122:VAL:HG23	5:F:472:GLN:HG3	1.83	0.60
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.37	0.60
2:C:701:GLY:O	2:C:1184:THR:N	2.25	0.60
3:D:810:THR:CG2	3:D:893:GLY:HA3	2.32	0.60
1:A:61:ILE:HG22	1:A:62:ASP:H	1.66	0.60
1:B:151:GLY:O	1:B:177:TYR:HB2	2.02	0.60
2:C:150:HIS:CD2	2:C:454:ARG:HE	2.20	0.60
2:C:498:ILE:H	2:C:498:ILE:HD12	1.66	0.60
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.36	0.60
3:D:363:LEU:HG	3:D:363:LEU:O	2.02	0.60
3:D:641:ILE:O	3:D:641:ILE:HD13	2.02	0.60
2:I:407:ARG:HH21	2:I:414:ILE:HG22	1.65	0.60
2:I:674:ASP:OD1	2:I:1109:ILE:N	2.34	0.60
3:J:495:ASN:ND2	3:J:497:GLU:HB2	2.17	0.60
3:D:1309:ILE:HG13	3:D:1310:THR:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:65:LEU:H	1:G:65:LEU:CD2	2.15	0.59
1:G:228:LEU:HD22	1:H:221:ALA:HB1	1.84	0.59
2:I:557:ARG:HH21	2:I:607:SER:C	2.09	0.59
2:I:591:TYR:HD2	2:I:606:LEU:HD13	1.66	0.59
5:L:233:ASP:O	5:L:236:LYS:HE2	2.02	0.59
5:L:245:ALA:O	5:L:249:ILE:HG13	2.01	0.59
5:L:486:ARG:CZ	5:L:486:ARG:HB2	2.31	0.59
1:B:33:ARG:HH11	2:C:1081:PRO:HG3	1.67	0.59
1:B:73:GLY:HA2	1:B:134:THR:CG2	2.32	0.59
3:D:77:ARG:HG3	3:D:79:LYS:H	1.67	0.59
5:F:599:ARG:O	5:F:604:SER:OG	2.18	0.59
1:G:45:ARG:NH1	1:H:34:GLY:O	2.34	0.59
3:J:810:THR:HG23	3:J:811:GLU:H	1.67	0.59
3:J:1344:LEU:O	3:J:1345:ARG:HB2	2.02	0.59
5:L:127:ILE:O	5:L:130:VAL:HG22	2.02	0.59
2:C:1142:ARG:NH2	2:C:1165:SER:HB2	2.17	0.59
2:C:1313:HIS:HB2	3:D:474:LEU:HD13	1.83	0.59
3:D:1295:ASN:CG	3:D:1298:VAL:HB	2.27	0.59
1:G:172:LEU:HD12	1:G:172:LEU:H	1.67	0.59
2:I:4:SER:OG	2:I:5:TYR:N	2.35	0.59
2:I:1013:GLN:O	2:I:1017:GLN:HG2	2.02	0.59
2:I:1073:LYS:HE3	3:J:462:ASP:CB	2.32	0.59
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.68	0.59
1:A:9:LEU:HD13	1:A:32:GLU:OE2	2.03	0.59
1:B:34:GLY:N	1:B:199:ASP:OD2	2.29	0.59
1:B:62:ASP:OD1	1:B:142:MET:HE2	2.02	0.59
2:C:615:VAL:HG13	2:C:651:ASP:N	2.17	0.59
3:D:1171:GLY:HA2	3:D:1193:TRP:HZ3	1.67	0.59
3:D:1270:GLY:HA3	3:D:1298:VAL:HG22	1.85	0.59
1:H:18:GLN:HA	1:H:24:ALA:HA	1.83	0.59
2:I:159:SER:O	2:I:160:ASP:HB2	2.01	0.59
3:J:1318:SER:OG	3:J:1342:ASP:OD2	2.17	0.59
1:B:182:ARG:NH1	3:D:581:MET:SD	2.75	0.59
5:F:227:GLN:HG2	5:F:252:LEU:HA	1.84	0.59
5:F:532:LEU:O	5:F:536:THR:HG23	2.02	0.59
2:I:878:THR:OG1	2:I:879:GLY:N	2.34	0.59
3:J:527:LEU:HD21	3:J:536:LEU:HG	1.83	0.59
1:A:53:GLY:O	1:A:149:GLY:N	2.27	0.59
1:B:153:VAL:O	1:B:175:ALA:N	2.34	0.59
1:B:197:ASP:O	1:B:198:LEU:HD13	2.02	0.59
3:D:665:GLN:HG3	3:D:669:GLN:HE21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:483:ASP:HB2	2:C:486:THR:HG22	1.83	0.59
2:C:617:ALA:HB3	2:C:653:MET:HG3	1.83	0.59
2:C:1268:GLN:HG2	3:D:467:ALA:HB1	1.84	0.59
5:F:601:PRO:CA	5:F:604:SER:HB2	2.33	0.59
1:H:7:GLU:CD	1:H:8:PHE:H	2.10	0.59
1:H:113:ALA:HB2	1:H:126:PRO:HB3	1.83	0.59
2:I:778:GLU:O	2:I:781:ASP:HB2	2.03	0.59
1:A:11:PRO:CB	1:A:30:PRO:HG2	2.33	0.59
5:F:124:GLU:HA	5:F:127:ILE:HD11	1.83	0.59
1:H:58:GLU:HA	1:H:171:LEU:O	2.03	0.59
2:I:389:PHE:HA	2:I:395:TYR:CD1	2.37	0.59
2:I:523:GLU:OE2	2:I:527:LYS:NZ	2.27	0.59
2:I:692:THR:OG1	2:I:827:ARG:O	2.20	0.59
5:L:479:THR:HG23	5:L:481:GLU:H	1.68	0.59
2:C:519:ASN:C	2:C:519:ASN:OD1	2.45	0.59
1:G:65:LEU:H	1:G:65:LEU:HD22	1.68	0.59
1:H:197:ASP:O	1:H:198:LEU:HD13	2.03	0.59
3:D:527:LEU:HB2	3:D:550:VAL:HG12	1.85	0.58
1:H:29:GLU:HB3	1:H:200:LYS:HG3	1.85	0.58
3:J:416:ILE:HG12	3:J:441:LEU:HD21	1.83	0.58
3:J:516:ASP:HA	3:J:545:HIS:HB2	1.83	0.58
3:J:551:ARG:HA	3:J:568:SER:O	2.03	0.58
3:J:1344:LEU:HA	3:J:1349:GLU:HG3	1.85	0.58
5:L:231:THR:CG2	5:L:249:ILE:HG12	2.33	0.58
5:L:476:ARG:HG3	5:L:477:GLU:N	2.15	0.58
2:C:673:HIS:HB3	2:C:1109:ILE:CG2	2.31	0.58
1:H:62:ASP:OD1	1:H:142:MET:HE2	2.02	0.58
2:I:632:ASP:O	2:I:647:ARG:HB2	2.02	0.58
3:J:30:ILE:CG2	3:J:243:PRO:HG3	2.32	0.58
3:J:930:LEU:HD11	3:J:1241:TYR:CE2	2.38	0.58
1:A:201:LEU:HG	1:A:203:ILE:HG13	1.85	0.58
3:J:335:GLN:HG2	3:J:343:LEU:HD13	1.85	0.58
5:L:544:THR:HG22	5:L:607:LEU:HD21	1.85	0.58
3:D:97:VAL:HG11	3:D:101:ARG:CZ	2.34	0.58
2:I:143:ARG:NH2	2:I:512:SER:O	2.37	0.58
2:I:314:ASN:O	2:I:352:ARG:NH1	2.29	0.58
3:J:62:PHE:CD1	3:J:247:PRO:HD3	2.38	0.58
3:J:532:GLU:HA	3:J:535:ARG:HB3	1.86	0.58
3:J:155:GLU:N	3:J:158:GLN:OE1	2.33	0.58
3:J:843:VAL:HG11	3:J:897:HIS:O	2.03	0.58
5:L:225:ARG:O	5:L:229:VAL:HG13	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:83:VAL:HA	4:E:86:ILE:HG12	1.86	0.58
2:I:696:ASP:HB2	2:I:798:GLN:CG	2.32	0.58
3:J:1219:ASP:O	3:J:1222:ARG:N	2.36	0.58
3:J:1368:ASP:HA	3:J:1371:ARG:NH1	2.19	0.58
2:C:732:ILE:HD13	2:C:783:LEU:HD12	1.84	0.58
2:C:873:ILE:HG13	2:C:944:ARG:HH22	1.68	0.58
2:C:1192:GLU:OE2	3:D:764:ARG:NH1	2.36	0.58
3:D:612:LEU:N	3:D:612:LEU:HD12	2.18	0.58
5:F:281:ARG:HG2	5:F:285:ARG:HD2	1.85	0.58
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.85	0.58
1:G:22:THR:HB	1:G:207:THR:O	2.04	0.58
1:A:29:GLU:CB	1:A:30:PRO:CD	2.79	0.58
2:C:1246:ARG:HG2	2:C:1247:SER:N	2.18	0.58
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.85	0.58
3:D:707:ILE:HD11	3:D:716:GLN:HG2	1.85	0.58
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.85	0.58
1:H:179:PRO:HA	1:H:208:ASN:ND2	2.19	0.58
2:I:1030:GLU:OE2	2:I:1034:ARG:NH2	2.37	0.58
2:I:1120:ALA:HB1	2:I:1198:LEU:HD12	1.85	0.58
3:J:259:ARG:CZ	5:L:505:ILE:HD11	2.34	0.58
3:J:403:ARG:NE	3:J:405:GLU:OE2	2.24	0.58
2:C:49:LEU:HB2	2:C:73:TYR:CZ	2.39	0.58
2:C:151:ARG:CZ	2:C:445:ILE:HD11	2.33	0.58
2:C:169:LYS:HE2	2:C:190:PRO:O	2.03	0.58
5:F:137:TYR:CE2	5:F:273:MET:HG2	2.38	0.58
5:F:512:GLY:C	5:F:514:ASP:H	2.12	0.58
1:G:69:SER:O	1:G:78:ILE:HG12	2.03	0.58
2:C:994:ARG:HD2	2:C:997:TRP:CH2	2.39	0.58
2:C:1302:THR:HG22	5:F:531:PRO:HB3	1.86	0.58
3:D:839:VAL:CG1	3:D:864:LEU:HD12	2.34	0.58
2:I:810:TYR:CZ	3:J:359:PRO:HD2	2.39	0.58
2:I:1281:TYR:CE1	3:J:484:MET:HE3	2.39	0.58
2:C:229:ILE:HB	2:C:240:GLU:HB2	1.86	0.57
3:D:622:ASP:HB3	3:D:626:TYR:HE2	1.69	0.57
3:J:94:GLN:O	3:J:97:VAL:HG23	2.04	0.57
2:C:119:GLU:HB2	2:C:489:PRO:HD2	1.87	0.57
2:C:158:ASP:CG	2:C:159:SER:H	2.12	0.57
2:C:799:ASN:C	2:C:799:ASN:HD22	2.12	0.57
1:G:52:PRO:HG2	1:G:219:ARG:HH21	1.67	0.57
2:I:206:ALA:O	2:I:209:ILE:HG22	2.04	0.57
2:I:836:LEU:N	2:I:836:LEU:HD12	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1156:LEU:HD22	3:J:1156:LEU:N	2.19	0.57
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	2.18	0.57
1:A:11:PRO:CA	1:A:30:PRO:CG	2.70	0.57
2:C:835:GLU:C	2:C:836:LEU:HD12	2.29	0.57
2:C:1253:LEU:O	2:C:1253:LEU:HD22	2.04	0.57
2:I:1260:GLY:HA2	2:I:1264:GLN:O	2.04	0.57
5:L:557:LYS:NZ	5:L:561:MET:HE1	2.18	0.57
1:B:151:GLY:O	1:B:177:TYR:HD2	1.88	0.57
3:D:274:ASN:OD1	5:F:446:GLN:NE2	2.38	0.57
5:F:137:TYR:CD2	5:F:273:MET:HG2	2.39	0.57
1:H:191:ARG:HH12	3:J:370:LYS:HZ3	1.51	0.57
2:I:371:ARG:HB3	2:I:374:GLU:OE2	2.04	0.57
3:J:298:MET:SD	5:L:402:LEU:HB3	2.44	0.57
3:J:600:ALA:O	3:J:603:LYS:HG2	2.05	0.57
3:J:747:MET:HE2	3:J:775:SER:HA	1.85	0.57
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.37	0.57
1:B:64:VAL:HG12	1:B:65:LEU:H	1.70	0.57
2:C:568:ASN:HB2	2:C:571:LEU:HB2	1.86	0.57
2:C:1268:GLN:HE22	3:D:352:ARG:NH1	2.02	0.57
3:D:356:THR:OG1	3:D:357:VAL:N	2.38	0.57
3:D:559:ALA:HB3	3:D:562:GLU:HB3	1.85	0.57
3:J:308:ASP:OD2	3:J:311:ARG:NE	2.38	0.57
3:J:425:ARG:HG2	3:J:426:ALA:H	1.68	0.57
5:L:390:ILE:O	5:L:393:LYS:HB2	2.05	0.57
2:C:798:GLN:OE1	2:C:827:ARG:HB2	2.05	0.57
5:F:461:ASN:O	5:F:465:ARG:HG2	2.04	0.57
5:F:487:MET:HA	5:F:487:MET:HE2	1.86	0.57
1:G:230:ALA:HB3	1:G:231:PHE:CE2	2.39	0.57
2:I:10:ARG:HA	2:I:1172:LEU:HD23	1.87	0.57
2:I:12:ARG:NH2	2:I:698:PRO:O	2.25	0.57
2:I:185:ASP:HB2	2:I:197:ARG:HG3	1.87	0.57
2:C:98:VAL:C	2:C:121:GLU:HA	2.30	0.57
2:C:468:LEU:O	2:C:471:VAL:HG12	2.04	0.57
2:C:936:ARG:HE	2:C:1047:LEU:HD23	1.70	0.57
3:D:518:VAL:CG1	3:D:707:ILE:HD13	2.33	0.57
1:H:99:ILE:HD12	1:H:145:LYS:HB2	1.87	0.57
2:I:1101:LEU:O	3:J:731:ARG:HD3	2.05	0.57
3:J:1280:VAL:HG11	3:J:1304:ARG:HE	1.70	0.57
2:C:1238:LEU:HD12	2:C:1238:LEU:N	2.18	0.57
3:D:210:SER:HB2	3:D:213:LYS:HB2	1.86	0.57
3:D:555:TYR:O	3:D:586:GLY:O	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:503:GLU:HG3	5:F:504:PRO:HD2	1.87	0.57
1:G:75:GLN:O	2:I:729:ALA:HB2	2.04	0.57
1:H:99:ILE:HG13	1:H:144:ILE:O	2.05	0.57
2:I:145:ILE:HB	2:I:456:VAL:HG22	1.86	0.57
3:J:72:CYS:HB3	3:J:88:CYS:SG	2.45	0.57
3:J:1343:GLU:HG3	3:J:1373:ARG:NH2	2.20	0.57
2:C:596:ASP:OD2	2:C:597:GLY:N	2.36	0.57
3:D:19:ALA:HB2	3:D:1373:ARG:HH22	1.68	0.57
3:D:94:GLN:O	3:D:97:VAL:HG23	2.04	0.57
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.70	0.57
1:A:249:PHE:C	5:F:605:GLU:OE2	2.48	0.57
2:C:62:TYR:C	2:C:64:GLY:H	2.13	0.57
2:C:980:VAL:O	2:C:984:VAL:HB	2.05	0.57
3:D:388:ARG:HB2	3:D:390:LEU:CD1	2.35	0.57
3:D:854:ALA:HB2	3:J:1372:ARG:CB	2.34	0.57
2:I:480:SER:HB3	2:I:481:LEU:HD22	1.86	0.57
2:I:606:LEU:HD23	2:I:611:GLU:HA	1.86	0.57
2:I:1246:ARG:NH2	2:I:1249:GLY:H	2.03	0.57
2:I:1334:GLY:O	3:J:25:ALA:HB3	2.05	0.57
5:L:421:TYR:CE2	5:L:422:ARG:HD2	2.40	0.57
2:I:170:VAL:HG23	2:I:171:LEU:N	2.20	0.56
1:B:197:ASP:C	1:B:198:LEU:HD22	2.30	0.56
2:C:170:VAL:O	2:C:171:LEU:HG	2.05	0.56
2:C:886:LYS:CE	2:C:916:SER:HB3	2.35	0.56
5:F:226:ALA:O	5:F:229:VAL:HG22	2.05	0.56
5:F:379:MET:O	5:F:379:MET:HG3	2.01	0.56
2:I:239:MET:O	2:I:284:LEU:HD12	2.03	0.56
2:I:593:LYS:HE3	2:I:595:THR:HG22	1.87	0.56
2:I:655:VAL:N	2:I:659:GLN:OE1	2.37	0.56
2:I:1223:ARG:NH2	3:J:719:PHE:O	2.39	0.56
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.40	0.56
3:J:45:ASN:O	3:J:46:TYR:HD2	1.87	0.56
1:A:23:HIS:HB2	1:A:206:GLU:HA	1.87	0.56
2:C:62:TYR:O	2:C:64:GLY:N	2.38	0.56
2:C:495:ALA:HB3	5:F:471:LEU:HD13	1.85	0.56
2:C:1305:TYR:OH	5:F:532:LEU:HG	2.05	0.56
3:D:133:ARG:NH1	3:D:136:GLU:OE1	2.38	0.56
3:D:224:LEU:O	3:D:228:VAL:HG23	2.04	0.56
3:D:299:LEU:O	3:D:299:LEU:HG	2.02	0.56
3:D:357:VAL:HG22	3:D:461:PHE:CE1	2.39	0.56
3:D:657:ALA:O	3:D:661:VAL:HG12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:817:HIS:HE1	3:D:860:ARG:HE	1.45	0.56
5:F:343:LYS:H	5:F:343:LYS:HD2	1.70	0.56
2:I:40:GLU:O	2:I:73:TYR:OH	2.23	0.56
2:I:468:LEU:O	2:I:471:VAL:HG12	2.06	0.56
3:J:536:LEU:O	3:J:539:SER:OG	2.24	0.56
3:J:1203:ARG:NH1	3:J:1205:GLU:HG2	2.18	0.56
1:A:23:HIS:CB	1:A:206:GLU:HA	2.35	0.56
1:B:82:LEU:O	1:B:85:LEU:HB2	2.05	0.56
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.86	0.56
1:G:38:THR:HG23	1:H:42:ALA:HA	1.88	0.56
2:I:615:VAL:HG13	2:I:651:ASP:H	1.69	0.56
2:I:818:VAL:HG22	2:I:1096:ILE:HG12	1.87	0.56
2:I:1276:TRP:CE2	3:J:801:VAL:HG21	2.41	0.56
3:J:425:ARG:HH11	3:J:459:ALA:HA	1.69	0.56
3:J:1343:GLU:HB3	3:J:1345:ARG:HD3	1.87	0.56
1:G:9:LEU:HD23	1:G:10:LYS:N	2.20	0.56
1:G:73:GLY:N	2:I:728:ASP:OD2	2.35	0.56
2:I:101:ARG:HH21	2:I:118:LYS:HE3	1.71	0.56
2:I:870:ILE:HB	2:I:944:ARG:HD3	1.86	0.56
2:I:1252:SER:O	2:I:1256:GLN:HA	2.06	0.56
3:J:735:ALA:O	3:J:739:GLN:HG3	2.06	0.56
3:J:741:ALA:O	3:J:762:ASN:ND2	2.39	0.56
3:J:1230:THR:O	3:J:1234:VAL:HG22	2.05	0.56
1:B:112:ALA:HB2	1:B:128:HIS:HB3	1.86	0.56
2:C:301:TYR:HB2	2:C:311:CYS:SG	2.46	0.56
2:C:887:VAL:HB	2:C:913:VAL:HG21	1.87	0.56
2:C:905:ILE:O	5:F:599:ARG:NH1	2.27	0.56
1:G:102:LEU:O	1:G:141:SER:HB2	2.06	0.56
1:H:56:VAL:HG22	1:H:144:ILE:HD11	1.87	0.56
1:H:191:ARG:HH12	3:J:370:LYS:NZ	2.03	0.56
2:I:888:THR:HG23	2:I:916:SER:OG	2.06	0.56
2:I:1297:ASP:O	2:I:1301:ARG:HG2	2.05	0.56
2:C:561:ILE:O	2:C:680:LEU:HD12	2.05	0.56
3:D:1167:LYS:NZ	3:D:1170:LYS:HB2	2.20	0.56
5:F:225:ARG:O	5:F:229:VAL:HG13	2.05	0.56
2:I:158:ASP:OD1	2:I:159:SER:N	2.37	0.56
3:J:620:PHE:O	3:J:624:ILE:HG13	2.06	0.56
3:J:930:LEU:HD11	3:J:1241:TYR:CZ	2.41	0.56
1:A:261:GLU:CD	2:C:859:GLU:HB2	2.31	0.56
2:C:22:LEU:HD13	2:C:23:ASP:N	2.21	0.56
2:C:211:ARG:HD3	2:C:357:ASN:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:768:MET:O	2:C:784:ALA:HB1	2.06	0.56
3:D:425:ARG:NH1	3:D:459:ALA:HA	2.21	0.56
1:H:60:GLU:CD	1:H:143:ARG:H	2.12	0.56
2:I:720:ARG:HA	2:I:779:ARG:HG3	1.86	0.56
2:I:1282:GLY:O	3:J:1360:GLY:HA3	2.06	0.56
1:A:36:GLY:CA	1:A:187:VAL:HG11	2.36	0.56
2:C:170:VAL:HG23	2:C:171:LEU:N	2.21	0.56
2:C:828:PHE:HB3	2:C:1060:ILE:HD12	1.88	0.56
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.87	0.56
3:D:650:LYS:HE2	3:D:654:ILE:HD11	1.87	0.56
3:D:700:ASN:O	3:D:704:GLU:HB2	2.06	0.56
2:I:124:MET:HB3	2:I:493:ILE:HD11	1.87	0.56
2:I:136:PHE:O	2:I:143:ARG:N	2.33	0.56
2:I:538:LEU:HA	2:I:542:ARG:CZ	2.35	0.56
2:I:673:HIS:HB3	2:I:1109:ILE:CG2	2.32	0.56
2:I:891:GLY:O	2:I:892:GLU:HG3	2.06	0.56
3:J:621:ALA:HA	3:J:624:ILE:HD12	1.87	0.56
5:L:580:PHE:C	5:L:582:VAL:H	2.14	0.56
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.88	0.56
2:C:397:LEU:H	2:C:397:LEU:HD12	1.71	0.56
2:C:466:VAL:O	2:C:470:ARG:HG2	2.05	0.56
2:C:1080:ASN:CB	2:C:1085:MET:HE3	2.35	0.56
3:D:347:VAL:HG12	3:D:348:ASP:O	2.05	0.56
3:D:1140:ARG:HH21	3:D:1236:GLU:CG	2.15	0.56
1:H:44:ARG:CG	1:H:183:ILE:HD13	2.36	0.56
2:I:138:ILE:HG22	2:I:139:ASN:N	2.19	0.56
2:I:814:ASP:OD2	2:I:1106:ARG:NH1	2.38	0.56
3:J:127:LEU:O	3:J:220:ARG:NH2	2.39	0.56
3:J:518:VAL:HG23	3:J:547:ARG:HH22	1.70	0.56
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.88	0.55
2:C:1299:ASN:HD22	2:C:1303:LYS:CE	2.18	0.55
2:I:494:ASN:HD22	2:I:497:PRO:HD3	1.71	0.55
2:I:1305:TYR:OH	5:L:532:LEU:HG	2.07	0.55
3:J:789:LYS:HE3	3:J:931:THR:O	2.05	0.55
3:J:849:LEU:HB3	3:J:853:THR:HG23	1.87	0.55
3:J:1358:PRO:HB3	3:J:1366:HIS:CD2	2.41	0.55
1:A:49:SER:OG	1:A:50:SER:N	2.38	0.55
1:A:152:TYR:CD1	2:C:824:GLN:HG2	2.41	0.55
1:B:60:GLU:HG3	1:B:143:ARG:O	2.06	0.55
3:D:140:TYR:HB3	5:F:100:MET:SD	2.46	0.55
5:F:492:ASP:HB2	5:F:495:ARG:NH1	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:191:ARG:NH1	1:G:198:LEU:H	2.04	0.55
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.87	0.55
2:I:1132:LEU:HD22	2:I:1177:ARG:NH1	2.21	0.55
3:J:156:ARG:NH2	3:J:191:SER:OG	2.37	0.55
5:L:547:VAL:HG23	5:L:603:ARG:NH1	2.21	0.55
1:A:269:CYS:O	1:A:273:GLU:HG2	2.06	0.55
1:A:279:GLY:HA3	1:A:321:TRP:CZ2	2.42	0.55
1:B:99:ILE:HG13	1:B:144:ILE:O	2.05	0.55
2:C:228:VAL:HB	2:C:335:THR:OG1	2.06	0.55
2:C:607:SER:OG	2:C:608:ALA:N	2.32	0.55
2:C:1254:VAL:O	3:D:99:ARG:NH2	2.37	0.55
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.88	0.55
1:H:60:GLU:HG2	1:H:143:ARG:HB2	1.87	0.55
2:I:324:LYS:O	2:I:327:GLN:NE2	2.40	0.55
2:I:807:TRP:CE3	2:I:808:ASN:HB2	2.41	0.55
2:I:898:GLU:OE1	2:I:898:GLU:N	2.37	0.55
2:I:1085:MET:HB2	2:I:1093:PRO:HB3	1.87	0.55
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	1.88	0.55
3:J:45:ASN:HB3	3:J:48:THR:O	2.06	0.55
1:B:155:ALA:N	1:B:174:ASP:OD1	2.39	0.55
2:C:202:ARG:HH11	2:C:369:MET:HG2	1.71	0.55
2:C:1076:ILE:HD11	2:C:1078:LYS:O	2.06	0.55
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.42	0.55
3:D:536:LEU:HD12	3:D:542:ALA:HB2	1.89	0.55
5:F:285:ARG:HA	5:F:288:MET:HE2	1.88	0.55
3:J:418:GLU:HB2	4:K:45:LYS:HB2	1.88	0.55
1:A:12:ARG:N	1:A:30:PRO:HG2	2.12	0.55
2:C:55:SER:OG	2:C:56:VAL:N	2.39	0.55
2:C:490:GLN:CD	5:F:472:GLN:NE2	2.64	0.55
2:C:637:ARG:HA	2:C:642:SER:HA	1.87	0.55
2:I:1331:ARG:HG2	3:J:33:TRP:CH2	2.42	0.55
2:C:224:PHE:CD2	2:C:347:ILE:HG13	2.41	0.55
2:C:758:ARG:HH22	2:C:761:GLN:CG	2.08	0.55
5:F:354:THR:N	5:F:357:GLN:OE1	2.40	0.55
2:I:4:SER:HB3	2:I:7:GLU:CD	2.31	0.55
2:I:151:ARG:NE	2:I:445:ILE:HD11	2.21	0.55
3:J:356:THR:OG1	3:J:357:VAL:N	2.34	0.55
5:L:266:PHE:O	5:L:269:LEU:HB2	2.06	0.55
3:D:314:ARG:HH22	3:D:323:PRO:HG3	1.69	0.55
3:D:418:GLU:H	4:E:45:LYS:NZ	2.04	0.55
3:J:490:ILE:O	3:J:499:ILE:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:825:VAL:C	3:J:826:ILE:HG13	2.32	0.55
3:J:1159:ILE:CA	3:J:1206:ARG:HB3	2.36	0.55
3:J:1327:GLU:OE2	3:J:1329:THR:HB	2.06	0.55
1:A:60:GLU:HB2	1:A:170:ARG:HG2	1.88	0.55
2:C:1151:LEU:HD23	2:C:1197:GLU:OE2	2.07	0.55
3:D:152:THR:OG1	3:D:153:ASN:N	2.38	0.55
5:F:166:VAL:O	5:F:167:ASP:HB2	2.07	0.55
1:H:60:GLU:OE1	1:H:142:MET:HB2	2.06	0.55
2:I:156:PHE:CE1	2:I:445:ILE:HG13	2.42	0.55
2:I:498:ILE:H	2:I:498:ILE:HD12	1.71	0.55
2:I:678:ARG:NH1	2:I:1071:GLY:O	2.37	0.55
2:I:968:GLU:HG3	2:I:1018:TYR:CE1	2.41	0.55
3:J:568:SER:OG	3:J:569:LEU:N	2.37	0.55
5:L:314:THR:O	5:L:318:ALA:HB3	2.07	0.55
3:D:425:ARG:HG2	3:D:426:ALA:H	1.71	0.55
3:D:515:ARG:O	3:D:545:HIS:HB3	2.07	0.55
3:D:1277:GLY:O	3:D:1278:GLU:HG2	2.07	0.55
1:G:150:ARG:NH1	1:H:7:GLU:O	2.32	0.55
2:I:421:SER:N	2:I:424:ASP:OD2	2.37	0.55
3:J:492:SER:HB2	3:J:499:ILE:HD13	1.88	0.55
3:J:1174:ARG:NH2	3:J:1187:GLU:OE2	2.40	0.55
2:C:297:VAL:HG12	2:C:315:MET:O	2.06	0.55
2:C:1184:THR:HG23	2:C:1189:GLY:HA3	1.89	0.55
3:D:58:CYS:SG	3:D:60:ARG:N	2.80	0.55
3:D:188:LEU:O	3:D:191:SER:OG	2.25	0.55
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.42	0.55
2:I:1077:SER:HA	3:J:356:THR:OG1	2.06	0.55
2:I:1184:THR:HG23	2:I:1189:GLY:CA	2.36	0.55
2:I:1333:LEU:HD22	3:J:307:LEU:CD2	2.37	0.55
3:J:411:ILE:O	3:J:414:GLU:HB2	2.06	0.55
3:J:845:ALA:CB	3:J:881:LYS:HD2	2.37	0.55
1:B:35:PHE:HA	1:B:38:THR:HG22	1.89	0.54
1:B:43:LEU:HD21	1:B:221:ALA:HB2	1.89	0.54
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.89	0.54
3:D:114:ILE:HD13	3:D:304:ASP:CG	2.32	0.54
3:D:121:PRO:HD2	3:D:123:ARG:NH2	2.22	0.54
3:D:355:ILE:HD13	3:D:466:MET:HG3	1.89	0.54
5:F:484:ALA:HB1	5:F:491:GLU:HG3	1.88	0.54
1:H:82:LEU:HD23	1:H:85:LEU:HD12	1.89	0.54
2:I:133:ASN:OD1	2:I:713:GLY:HA3	2.07	0.54
2:I:397:LEU:O	2:I:398:SER:OG	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1356:LEU:O	3:J:1366:HIS:HE1	1.89	0.54
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.88	0.54
1:A:234:LEU:HB2	1:B:218:ARG:NH2	2.22	0.54
2:C:1124:ILE:HG21	2:C:1180:MET:HG3	1.89	0.54
3:D:518:VAL:HG11	3:D:707:ILE:HD13	1.89	0.54
3:D:1347:LEU:O	3:D:1348:LYS:C	2.50	0.54
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.88	0.54
2:I:514:PHE:HE2	2:I:760:ASN:HB3	1.72	0.54
2:I:557:ARG:NH2	2:I:607:SER:O	2.40	0.54
2:I:615:VAL:HG21	2:I:645:PHE:CD2	2.42	0.54
2:I:1132:LEU:HD22	2:I:1177:ARG:HH12	1.71	0.54
3:J:1191:PRO:HB2	3:J:1194:ARG:HD3	1.89	0.54
3:J:1280:VAL:CG1	3:J:1304:ARG:HH21	2.09	0.54
4:K:15:ASN:O	4:K:16:ARG:HB3	2.08	0.54
1:A:158:ARG:HH21	1:A:172:LEU:HB3	1.73	0.54
2:C:189:ASP:OD1	2:C:193:ASN:N	2.22	0.54
2:C:518:ASN:OD1	2:C:519:ASN:N	2.40	0.54
2:C:705:GLU:H	2:C:705:GLU:CD	2.14	0.54
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.41	0.54
2:C:1281:TYR:CE2	3:D:431:ARG:HG3	2.43	0.54
3:D:1165:PHE:HE1	3:D:1200:GLU:HB3	1.72	0.54
5:F:316:PHE:O	5:F:320:ILE:HG13	2.07	0.54
1:H:16:ILE:HG13	1:H:26:VAL:HG22	1.89	0.54
1:H:40:GLY:HA3	1:H:185:TYR:CD1	2.42	0.54
3:J:97:VAL:HG11	3:J:101:ARG:NH2	2.22	0.54
3:J:418:GLU:HG3	4:K:45:LYS:N	2.11	0.54
1:A:83:LEU:CD2	2:C:694:ARG:HE	2.21	0.54
2:C:175:ARG:NH1	2:C:183:TRP:HZ3	2.06	0.54
2:C:496:LYS:HD2	2:C:496:LYS:C	2.32	0.54
2:C:1253:LEU:HD13	2:C:1253:LEU:C	2.32	0.54
3:D:244:VAL:HA	3:D:269:TYR:OH	2.07	0.54
3:D:491:LEU:HD23	3:D:498:PRO:HA	1.89	0.54
1:G:152:TYR:CD1	1:G:176:CYS:HB3	2.41	0.54
1:G:153:VAL:O	1:G:175:ALA:N	2.38	0.54
1:H:61:ILE:HG22	1:H:64:VAL:H	1.72	0.54
3:J:804:ALA:O	3:J:805:GLN:C	2.51	0.54
3:J:1194:ARG:N	3:J:1194:ARG:HD2	2.22	0.54
1:A:90:VAL:HG22	1:A:91:ARG:H	1.73	0.54
2:C:247:ARG:HH12	2:C:271:ALA:HB2	1.72	0.54
2:C:801:ARG:HB2	2:C:1229:TYR:CZ	2.43	0.54
5:F:316:PHE:CZ	5:F:334:SER:HA	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:569:THR:OG1	5:F:570:ASP:N	2.30	0.54
2:I:617:ALA:HA	2:I:636:CYS:SG	2.47	0.54
2:I:1275:VAL:HG22	2:I:1287:LEU:HD11	1.89	0.54
2:I:1281:TYR:HE1	3:J:484:MET:HE3	1.71	0.54
3:J:97:VAL:HG11	3:J:101:ARG:CZ	2.37	0.54
3:J:481:ARG:NH1	4:K:3:ARG:O	2.40	0.54
4:K:35:LYS:NZ	4:K:71:GLU:OE2	2.38	0.54
5:L:316:PHE:HZ	5:L:334:SER:HA	1.72	0.54
1:A:75:GLN:C	2:C:729:ALA:HB2	2.33	0.54
1:B:196:THR:HG23	3:D:443:GLU:HG3	1.90	0.54
2:C:149:LEU:HD13	2:C:453:ILE:HG12	1.89	0.54
2:C:262:TYR:CZ	2:C:282:VAL:HG21	2.43	0.54
2:C:866:ASP:HA	2:C:872:TYR:OH	2.07	0.54
3:D:19:ALA:O	3:D:20:ILE:HG13	2.07	0.54
3:D:24:LEU:HB2	3:D:232:ASN:OD1	2.08	0.54
3:D:322:ARG:NH1	3:D:322:ARG:HB2	2.22	0.54
3:D:369:PRO:HB3	3:D:444:GLY:O	2.07	0.54
3:D:702:GLN:O	3:D:718:SER:N	2.22	0.54
1:G:77:ASP:OD2	2:I:755:LYS:NZ	2.36	0.54
1:G:102:LEU:HD13	1:G:103:ASN:N	2.23	0.54
2:I:4:SER:HB3	2:I:7:GLU:OE2	2.08	0.54
1:B:19:VAL:HB	1:B:23:HIS:HD2	1.70	0.54
1:B:134:THR:HG23	1:B:135:ASP:N	2.22	0.54
3:D:291:ILE:O	3:D:292:VAL:C	2.47	0.54
3:D:378:LYS:NZ	3:D:382:TYR:OH	2.36	0.54
3:D:520:ALA:HB3	3:D:546:ALA:HB2	1.88	0.54
2:I:146:VAL:O	2:I:511:LEU:HD23	2.08	0.54
3:J:474:LEU:O	3:J:477:GLN:N	2.41	0.54
4:K:22:VAL:HG13	4:K:64:LEU:HD12	1.90	0.54
1:A:316:MET:SD	5:F:600:HIS:ND1	2.81	0.54
2:C:97:ARG:HH22	5:F:475:GLY:HA3	1.73	0.54
1:H:219:ARG:O	1:H:223:ILE:HG13	2.07	0.54
2:I:158:ASP:CG	2:I:159:SER:H	2.14	0.54
3:J:58:CYS:SG	3:J:59:ALA:N	2.80	0.54
4:K:53:GLU:HB3	4:K:59:ILE:HG13	1.88	0.54
1:A:44:ARG:HG3	1:A:183:ILE:HG22	1.89	0.54
2:C:886:LYS:H	2:C:917:SER:HB3	1.73	0.54
2:C:1281:TYR:OH	3:D:431:ARG:O	2.24	0.54
4:E:60:ASN:ND2	4:E:63:ILE:HD13	2.22	0.54
3:J:536:LEU:HD12	3:J:542:ALA:HB2	1.89	0.54
3:J:620:PHE:CD1	3:J:624:ILE:HD11	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:460:ILE:O	5:L:463:LEU:HB2	2.08	0.54
3:D:362:ARG:H	3:D:365:GLN:NE2	2.06	0.54
5:F:343:LYS:O	5:F:347:ILE:HG13	2.08	0.54
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.90	0.54
2:I:673:HIS:CB	2:I:1109:ILE:HG22	2.36	0.54
3:J:905:ARG:CZ	3:J:910:ASN:HD21	2.20	0.54
2:C:726:TYR:CE2	2:C:728:ASP:HB2	2.43	0.53
3:D:40:LYS:O	3:D:55:GLY:HA2	2.08	0.53
3:D:825:VAL:C	3:D:826:ILE:HG13	2.33	0.53
3:D:1158:GLU:HB3	3:D:1186:TYR:CE1	2.43	0.53
5:F:128:ASN:HA	5:F:131:GLN:HE21	1.73	0.53
5:F:470:MET:CE	5:F:486:ARG:HH12	2.21	0.53
1:G:166:ARG:O	1:G:167:PRO:C	2.51	0.53
2:I:412:GLU:HB3	2:I:413:GLU:OE1	2.08	0.53
3:J:425:ARG:HH12	3:J:464:ASP:CG	2.16	0.53
3:J:1371:ARG:HB3	3:J:1371:ARG:CZ	2.39	0.53
5:L:248:GLU:HG2	5:L:251:LYS:NZ	2.23	0.53
1:A:207:THR:HG22	1:A:208:ASN:N	2.23	0.53
2:C:1336:ASN:CG	3:D:29:MET:HE3	2.33	0.53
3:D:293:ARG:O	3:D:296:LYS:N	2.41	0.53
3:D:580:TRP:CZ3	3:D:589:TYR:HA	2.44	0.53
3:D:712:GLN:H	3:D:712:GLN:CD	2.15	0.53
3:D:824:PRO:HD3	3:D:835:LEU:HD13	1.91	0.53
1:G:67:GLU:O	1:G:78:ILE:HB	2.08	0.53
2:I:808:ASN:H	3:J:633:ALA:HB2	1.72	0.53
2:I:1116:HIS:HE1	3:J:641:ILE:N	2.01	0.53
3:J:442:ILE:HG22	3:J:443:GLU:O	2.08	0.53
3:J:623:GLN:O	3:J:627:THR:HG22	2.08	0.53
4:K:59:ILE:HD13	4:K:63:ILE:HG21	1.91	0.53
5:L:161:LEU:C	5:L:262:VAL:HG23	2.33	0.53
5:L:561:MET:HG2	5:L:576:VAL:HG22	1.91	0.53
1:A:47:LEU:HD13	1:A:183:ILE:HG12	1.90	0.53
1:A:88:LEU:HD12	1:A:125:LYS:HD3	1.89	0.53
1:A:250:ASP:HB2	5:F:601:PRO:HB3	1.90	0.53
1:B:25:LYS:HG3	1:B:204:GLU:HB2	1.90	0.53
2:C:412:GLU:HB3	2:C:413:GLU:OE1	2.09	0.53
2:C:985:GLU:HG2	2:C:988:LYS:HD2	1.89	0.53
3:D:30:ILE:CG2	3:D:243:PRO:HG3	2.38	0.53
3:D:744:ARG:O	3:D:759:ILE:HB	2.08	0.53
5:F:231:THR:CG2	5:F:249:ILE:HG12	2.37	0.53
1:H:103:ASN:HA	1:H:141:SER:HB2	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:301:TYR:HB2	2:I:311:CYS:SG	2.48	0.53
2:I:1142:ARG:HD3	2:I:1161:LEU:HD11	1.91	0.53
3:J:1169:THR:CG2	3:J:1192:LYS:HD3	2.37	0.53
1:B:175:ALA:HB1	1:B:177:TYR:CZ	2.44	0.53
2:C:176:ILE:HD11	2:C:428:VAL:HG21	1.91	0.53
3:D:808:VAL:HG12	3:D:809:VAL:N	2.23	0.53
3:D:872:LEU:HD22	3:D:877:VAL:HG11	1.91	0.53
2:I:143:ARG:HH21	2:I:512:SER:C	2.15	0.53
2:I:632:ASP:HA	2:I:647:ARG:HD2	1.90	0.53
2:I:963:GLU:O	2:I:967:LEU:HB2	2.08	0.53
3:J:58:CYS:SG	3:J:60:ARG:N	2.79	0.53
3:J:647:PRO:HD3	3:J:697:MET:HB3	1.91	0.53
5:L:285:ARG:HA	5:L:288:MET:HE2	1.90	0.53
2:C:529:ARG:O	2:C:530:ILE:HD13	2.08	0.53
2:C:667:LEU:CD2	2:C:704:MET:HB2	2.38	0.53
2:C:755:LYS:O	2:C:757:THR:HG23	2.09	0.53
2:C:1136:GLN:HE21	2:C:1140:LYS:HZ3	1.56	0.53
2:C:1257:GLN:HE22	3:D:340:GLN:HE21	1.56	0.53
2:C:1281:TYR:HE2	3:D:431:ARG:HG3	1.73	0.53
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.43	0.53
3:D:114:ILE:HB	3:D:304:ASP:OD1	2.08	0.53
3:D:124:ILE:HG12	3:D:237:MET:SD	2.48	0.53
3:D:1372:ARG:HE	3:J:854:ALA:HB2	1.74	0.53
5:F:230:VAL:O	5:F:234:THR:HG23	2.08	0.53
1:G:13:LEU:HA	1:G:28:LEU:HA	1.89	0.53
1:G:31:LEU:HB2	1:G:199:ASP:HB2	1.90	0.53
2:I:990:ASP:HA	2:I:997:TRP:HZ2	1.73	0.53
3:J:1157:ALA:O	3:J:1207:GLY:N	2.39	0.53
2:C:344:GLY:HA3	2:C:346:TYR:CE2	2.44	0.53
3:D:262:THR:O	5:F:507:MET:HB2	2.09	0.53
3:D:930:LEU:HD11	3:D:1241:TYR:CE2	2.43	0.53
5:F:124:GLU:O	5:F:127:ILE:HG13	2.09	0.53
5:F:133:SER:OG	5:F:364:ARG:HD2	2.08	0.53
1:G:77:ASP:OD2	2:I:729:ALA:HB1	2.09	0.53
1:G:167:PRO:HB2	1:G:170:ARG:HB2	1.90	0.53
2:I:195:PHE:HE1	2:I:205:PRO:HG3	1.73	0.53
3:J:263:SER:OG	3:J:264:ASP:N	2.41	0.53
3:J:440:VAL:O	3:J:442:ILE:HG12	2.08	0.53
3:J:795:TYR:CE2	3:J:799:ARG:NE	2.77	0.53
3:J:832:LYS:HD3	3:J:1242:ARG:HH12	1.72	0.53
3:J:1138:LEU:HB3	3:J:1139:PRO:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:GLY:HA3	1:B:177:TYR:CE2	2.43	0.53
2:C:799:ASN:C	2:C:799:ASN:ND2	2.65	0.53
4:E:60:ASN:HD21	4:E:63:ILE:HD13	1.73	0.53
2:I:57:PHE:CD1	2:I:58:PRO:HA	2.42	0.53
2:I:202:ARG:HH11	2:I:369:MET:CG	2.21	0.53
2:I:478:ARG:NH2	2:I:487:LEU:HD13	2.24	0.53
2:I:1202:GLY:O	2:I:1203:ASP:HB2	2.08	0.53
2:I:1211:ARG:O	2:I:1212:LEU:HD12	2.09	0.53
3:J:123:ARG:HH22	3:J:1334:GLU:HG3	1.73	0.53
3:J:123:ARG:HD2	3:J:1337:VAL:HG11	1.91	0.53
3:J:572:THR:HG21	3:J:589:TYR:OH	2.08	0.53
1:A:11:PRO:HD3	1:B:227:GLN:OE1	2.08	0.53
2:C:42:ASP:OD2	2:C:44:GLU:C	2.51	0.53
3:D:131:PRO:HG2	3:D:134:ASP:HB2	1.91	0.53
5:F:281:ARG:O	5:F:285:ARG:HG3	2.09	0.53
1:G:182:ARG:NH2	1:G:206:GLU:OE2	2.42	0.53
3:J:363:LEU:HG	3:J:363:LEU:O	2.08	0.53
2:C:724:VAL:HG23	2:C:775:GLU:O	2.09	0.53
2:C:1305:TYR:HE1	3:D:379:PRO:HG3	1.73	0.53
3:D:62:PHE:O	3:D:101:ARG:HD2	2.09	0.53
2:I:379:GLU:CD	2:I:379:GLU:H	2.15	0.53
3:J:28:ASP:OD1	3:J:31:ARG:NH1	2.41	0.53
3:J:93:THR:HG22	3:J:94:GLN:H	1.74	0.53
3:J:161:THR:HG22	3:J:164:GLN:CD	2.34	0.53
3:J:1140:ARG:NH2	3:J:1144:LEU:HD21	2.24	0.53
2:C:720:ARG:NE	2:C:736:VAL:HG11	2.24	0.53
2:C:1124:ILE:HB	2:C:1180:MET:HB2	1.91	0.53
2:C:1247:SER:HB3	3:D:375:GLU:O	2.09	0.53
3:D:26:SER:OG	3:D:28:ASP:N	2.42	0.53
3:D:35:PHE:CD1	3:D:101:ARG:HB3	2.41	0.53
3:D:56:LEU:H	3:D:56:LEU:CD1	2.14	0.53
3:D:552:ILE:HG21	3:D:589:TYR:CE1	2.44	0.53
3:D:709:ARG:C	3:D:711:GLY:N	2.67	0.53
3:D:1349:GLU:OE2	3:D:1349:GLU:N	2.36	0.53
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.44	0.53
3:J:1259:GLN:NE2	3:J:1262:ARG:HH12	2.06	0.53
2:C:42:ASP:CG	2:C:44:GLU:HG2	2.33	0.52
2:C:746:ALA:HA	2:C:974:ARG:HH21	1.74	0.52
2:C:813:GLU:HB2	3:D:461:PHE:HB2	1.91	0.52
3:D:521:LYS:NZ	3:D:540:GLY:O	2.20	0.52
3:D:1226:VAL:O	3:D:1230:THR:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:445:ASP:OD2	5:F:451:ARG:HD2	2.09	0.52
1:G:60:GLU:HB2	1:G:170:ARG:NH1	2.23	0.52
2:I:582:ASN:HB3	2:I:586:PHE:N	2.24	0.52
2:I:698:PRO:HG3	2:I:1231:TYR:CE2	2.44	0.52
2:I:739:ASP:OD1	2:I:739:ASP:N	2.42	0.52
3:J:514:THR:HG23	3:J:596:LEU:HB2	1.89	0.52
3:J:1157:ALA:HB2	3:J:1210:ILE:HD11	1.90	0.52
5:L:571:TYR:HD1	5:L:575:GLU:HG2	1.74	0.52
1:B:196:THR:HG23	3:D:443:GLU:CD	2.35	0.52
2:C:4:SER:HB3	2:C:7:GLU:CD	2.34	0.52
3:D:140:TYR:O	3:D:297:ARG:NH1	2.42	0.52
3:D:1156:LEU:HD22	3:D:1156:LEU:N	2.24	0.52
3:D:1163:VAL:HG23	3:D:1177:ILE:HA	1.90	0.52
3:D:1266:ILE:HB	3:D:1274:PHE:O	2.09	0.52
5:F:315:TRP:CH2	5:F:341:LEU:HD11	2.44	0.52
5:F:580:PHE:C	5:F:582:VAL:H	2.17	0.52
1:G:68:TYR:HE1	2:I:929:ILE:HG21	1.72	0.52
3:J:421:VAL:HG22	3:J:439:PRO:HG3	1.91	0.52
5:L:364:ARG:HA	5:L:367:ILE:HD12	1.91	0.52
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.91	0.52
5:L:601:PRO:CA	5:L:604:SER:HB2	2.39	0.52
2:C:69:GLN:HG3	2:C:101:ARG:HB3	1.91	0.52
2:C:378:ARG:NH1	2:C:382:GLU:OE2	2.41	0.52
2:C:1272:GLU:HB2	3:D:342:LEU:O	2.09	0.52
2:C:1284:ALA:N	3:D:479:GLU:OE1	2.42	0.52
3:D:195:GLU:O	3:D:198:CYS:HB2	2.09	0.52
3:D:1309:ILE:HG13	3:D:1310:THR:H	1.74	0.52
5:F:114:GLU:HG3	5:F:115:GLY:N	2.24	0.52
5:F:486:ARG:HB2	5:F:486:ARG:CZ	2.38	0.52
2:I:4:SER:H	2:I:7:GLU:CD	2.17	0.52
3:J:708:ASN:HB3	3:J:712:GLN:O	2.09	0.52
3:J:1179:PRO:CD	3:J:1184:ASP:HA	2.40	0.52
2:C:29:SER:O	2:C:30:ILE:C	2.52	0.52
2:C:490:GLN:NE2	5:F:472:GLN:HE22	2.08	0.52
2:C:797:GLY:N	2:C:1231:TYR:OH	2.40	0.52
2:C:1193:ALA:O	2:C:1197:GLU:N	2.32	0.52
3:D:77:ARG:HG3	3:D:79:LYS:HB3	1.90	0.52
2:I:16:GLY:O	2:I:1156:ARG:HG2	2.10	0.52
2:I:1106:ARG:HD2	2:I:1106:ARG:H	1.75	0.52
3:J:123:ARG:NH2	3:J:1334:GLU:HG3	2.24	0.52
1:B:61:ILE:HB	1:B:64:VAL:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3:TYR:HE1	2:C:11:ILE:HD11	1.74	0.52
2:C:799:ASN:ND2	2:C:799:ASN:O	2.41	0.52
2:C:992:LEU:HD23	2:C:992:LEU:H	1.75	0.52
3:D:1179:PRO:CD	3:D:1184:ASP:HA	2.40	0.52
5:F:376:LYS:O	5:F:380:VAL:HG23	2.10	0.52
2:I:514:PHE:CE2	2:I:760:ASN:HB3	2.45	0.52
3:J:201:LEU:HD13	3:J:221:ILE:HB	1.92	0.52
3:J:808:VAL:HG12	3:J:809:VAL:N	2.23	0.52
5:L:137:TYR:CD2	5:L:273:MET:HE2	2.44	0.52
1:A:125:LYS:HE2	1:A:128:HIS:CG	2.44	0.52
2:C:62:TYR:CZ	2:C:476:LYS:HB3	2.44	0.52
2:C:906:PHE:CE2	5:F:608:ARG:HG3	2.45	0.52
3:D:179:LYS:HB2	3:D:184:ALA:HB2	1.91	0.52
3:D:442:ILE:HG22	3:D:443:GLU:O	2.09	0.52
4:E:15:ASN:O	4:E:16:ARG:HB3	2.09	0.52
1:G:182:ARG:O	1:G:183:ILE:HD12	2.10	0.52
2:I:127:ILE:HG13	2:I:127:ILE:O	2.09	0.52
2:I:515:MET:HG2	2:I:515:MET:O	2.09	0.52
2:I:517:GLN:CD	2:I:688:GLN:HA	2.34	0.52
2:I:1234:LYS:HE2	2:I:1238:LEU:HD23	1.91	0.52
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.90	0.52
1:A:145:LYS:NZ	1:A:147:GLN:OE1	2.43	0.52
1:B:215:GLU:HA	1:B:218:ARG:HD2	1.91	0.52
2:C:300:ASP:OD1	2:C:312:ALA:HA	2.09	0.52
2:C:681:MET:O	2:C:685:MET:HE2	2.09	0.52
3:D:436:ALA:HB3	3:D:485:MET:HA	1.92	0.52
3:D:674:THR:HG1	3:D:677:GLU:HB2	1.75	0.52
1:H:195:ARG:HB3	1:H:198:LEU:HD21	1.92	0.52
1:H:197:ASP:C	1:H:198:LEU:HD22	2.34	0.52
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.92	0.52
2:I:670:PHE:HA	2:I:672:GLU:OE2	2.09	0.52
2:I:972:PHE:CZ	2:I:998:LEU:HD11	2.45	0.52
3:J:299:LEU:O	3:J:300:GLN:C	2.53	0.52
1:B:188:GLU:HG3	1:B:200:LYS:HB3	1.92	0.52
3:D:45:ASN:O	3:D:46:TYR:HB3	2.09	0.52
3:D:473:THR:HG23	3:D:476:ALA:H	1.75	0.52
3:D:528:THR:O	3:D:551:ARG:HB3	2.09	0.52
3:D:674:THR:N	3:D:677:GLU:OE1	2.37	0.52
2:I:598:VAL:HG13	2:I:628:HIS:HE1	1.75	0.52
2:I:1035:LYS:O	2:I:1038:GLN:HG2	2.10	0.52
3:J:613:GLY:O	3:J:617:THR:OG1	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ASP:O	1:B:81:ILE:HG13	2.10	0.52
2:C:397:LEU:O	2:C:398:SER:OG	2.24	0.52
2:C:692:THR:OG1	2:C:693:LEU:N	2.42	0.52
3:D:31:ARG:NE	3:D:106:GLU:OE2	2.41	0.52
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.91	0.52
5:F:479:THR:HG23	5:F:481:GLU:N	2.25	0.52
2:I:325:LEU:O	2:I:328:SER:OG	2.28	0.52
3:J:147:ILE:HD11	3:J:179:LYS:HZ3	1.75	0.52
3:J:412:LEU:HA	3:J:415:VAL:HG22	1.91	0.52
1:A:187:VAL:CG1	1:A:201:LEU:HD13	2.39	0.52
2:C:189:ASP:OD1	2:C:192:ASP:N	2.43	0.52
3:D:273:ILE:O	3:D:274:ASN:C	2.52	0.52
3:D:789:LYS:NZ	3:D:931:THR:O	2.42	0.52
3:D:847:ASP:CA	3:D:860:ARG:H	2.20	0.52
2:I:582:ASN:HB3	2:I:586:PHE:H	1.75	0.52
2:C:146:VAL:HG13	2:C:529:ARG:HB3	1.92	0.51
2:C:759:SER:HG	2:C:763:THR:N	2.07	0.51
3:D:270:ARG:NH2	5:F:449:THR:HG23	2.25	0.51
3:D:279:LEU:HD23	3:D:279:LEU:C	2.35	0.51
3:D:1291:GLU:HG2	3:D:1297:LYS:HD3	1.91	0.51
2:I:299:LYS:HG2	2:I:334:GLU:OE1	2.11	0.51
2:I:551:HIS:CG	2:I:552:PRO:HD2	2.45	0.51
2:I:564:PRO:HD2	2:I:572:ILE:HB	1.92	0.51
2:I:1134:GLN:C	2:I:1135:GLN:HG2	2.35	0.51
2:I:1210:ILE:O	2:I:1224:PRO:HA	2.09	0.51
3:J:518:VAL:HA	3:J:547:ARG:CZ	2.40	0.51
3:J:850:LYS:HG2	3:J:857:LEU:HD23	1.92	0.51
5:L:448:ARG:NH2	5:L:500:ILE:O	2.43	0.51
1:B:60:GLU:OE1	1:B:142:MET:HB2	2.10	0.51
2:C:268:ARG:HH21	2:C:270:THR:CG2	2.23	0.51
2:C:553:THR:O	2:C:557:ARG:HD2	2.11	0.51
3:D:290:ILE:H	3:D:290:ILE:HD12	1.75	0.51
1:H:134:THR:HG23	1:H:135:ASP:N	2.24	0.51
3:J:471:PRO:HB3	3:J:476:ALA:HB1	1.92	0.51
3:J:817:HIS:CD2	3:J:860:ARG:HH21	2.28	0.51
3:J:1344:LEU:HB3	3:J:1350:ASN:HD21	1.73	0.51
5:L:431:ALA:O	5:L:434:TRP:N	2.43	0.51
1:A:250:ASP:HB2	5:F:601:PRO:CB	2.40	0.51
2:C:201:ARG:NH2	2:C:370:MET:O	2.37	0.51
2:C:543:ALA:O	2:C:548:ARG:NH1	2.43	0.51
2:C:1246:ARG:NH2	2:C:1249:GLY:H	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:109:SER:O	3:D:110:PRO:C	2.52	0.51
3:D:805:GLN:OE1	3:D:1348:LYS:HD3	2.10	0.51
1:G:112:ALA:HB2	1:G:128:HIS:HB3	1.92	0.51
3:J:664:ILE:HG22	3:J:678:ARG:HG2	1.93	0.51
3:J:925:GLU:HB3	3:J:926:PRO:HD3	1.93	0.51
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.91	0.51
1:A:155:ALA:CA	1:A:158:ARG:HG3	2.40	0.51
1:B:179:PRO:HA	1:B:208:ASN:ND2	2.24	0.51
2:C:358:ASP:OD1	2:C:360:LEU:N	2.44	0.51
2:C:1137:GLU:HG2	2:C:1140:LYS:HG2	1.92	0.51
2:C:1279:GLU:HG2	3:D:1357:ILE:HD13	1.92	0.51
5:F:227:GLN:HE22	5:F:251:LYS:NZ	2.06	0.51
5:F:315:TRP:HZ2	5:F:341:LEU:HD21	1.74	0.51
5:F:513:ASP:C	5:F:515:GLU:H	2.17	0.51
1:H:62:ASP:OD1	1:H:142:MET:HB3	2.11	0.51
2:I:891:GLY:C	2:I:892:GLU:HG3	2.35	0.51
3:J:77:ARG:HG3	3:J:79:LYS:H	1.76	0.51
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.09	0.51
1:B:104:LYS:HG2	1:B:114:ASP:CG	2.36	0.51
5:F:164:GLY:O	5:F:260:ARG:HB2	2.11	0.51
2:I:241:LEU:HD21	2:I:246:LEU:HD11	1.92	0.51
2:I:397:LEU:HD12	2:I:397:LEU:N	2.26	0.51
2:I:812:PHE:CE2	3:J:451:PRO:HB3	2.46	0.51
1:A:91:ARG:HD3	1:A:210:THR:O	2.10	0.51
3:D:318:GLY:C	3:D:320:ASN:H	2.18	0.51
5:F:101:TYR:O	5:F:104:GLU:N	2.42	0.51
2:I:26:TYR:CZ	2:I:28:LEU:HB2	2.46	0.51
2:I:197:ARG:NH2	2:I:203:LYS:HB2	2.26	0.51
2:I:1046:VAL:HG21	2:I:1049:ILE:HD11	1.92	0.51
3:J:54:ASP:OD1	3:J:54:ASP:N	2.42	0.51
3:J:1149:ARG:HG3	3:J:1216:ALA:HB2	1.91	0.51
2:C:158:ASP:HB3	2:C:173:ASN:OD1	2.11	0.51
1:G:9:LEU:HD12	1:G:195:ARG:NH2	2.25	0.51
1:H:153:VAL:O	1:H:175:ALA:N	2.43	0.51
2:I:302:ILE:HG22	2:I:309:LEU:HA	1.93	0.51
3:J:56:LEU:HD12	3:J:56:LEU:N	2.24	0.51
3:J:114:ILE:HB	3:J:304:ASP:OD1	2.11	0.51
3:J:405:GLU:O	3:J:408:VAL:HG22	2.10	0.51
3:J:470:VAL:HG12	3:J:472:LEU:CD2	2.41	0.51
2:C:14:ASP:OD2	2:C:1156:ARG:NE	2.42	0.51
2:C:1152:GLY:O	2:C:1153:ALA:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1257:VAL:HG22	3:D:1260:MET:HE2	1.91	0.51
2:I:943:LYS:O	2:I:947:GLU:HG3	2.11	0.51
2:C:195:PHE:CD1	2:C:203:LYS:HG2	2.46	0.51
2:C:231:GLU:HG2	2:C:332:ARG:NH2	2.26	0.51
3:D:45:ASN:O	3:D:46:TYR:HD2	1.93	0.51
3:D:377:PHE:O	3:D:378:LYS:C	2.54	0.51
3:D:849:LEU:HD13	3:D:849:LEU:H	1.76	0.51
3:D:1165:PHE:CE1	3:D:1200:GLU:HB3	2.46	0.51
3:D:1203:ARG:NH2	3:D:1205:GLU:HG2	2.19	0.51
5:F:396:ASN:C	5:F:398:GLY:H	2.19	0.51
3:J:320:ASN:OD1	3:J:322:ARG:HB3	2.11	0.51
3:J:1158:GLU:HB3	3:J:1186:TYR:CE1	2.46	0.51
1:B:6:THR:O	1:B:6:THR:OG1	2.21	0.51
2:C:894:GLN:O	2:C:894:GLN:HG3	2.11	0.51
3:D:34:SER:HB2	3:D:104:HIS:HB3	1.93	0.51
3:D:75:TYR:HD2	3:D:80:HIS:CD2	2.29	0.51
3:D:556:GLU:O	3:D:564:VAL:N	2.28	0.51
3:J:682:VAL:O	3:J:685:ILE:HG12	2.10	0.51
3:D:22:ILE:O	3:D:1339:GLY:HA2	2.11	0.50
3:D:495:ASN:N	3:D:495:ASN:OD1	2.43	0.50
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.93	0.50
4:E:50:ALA:O	4:E:54:ILE:HG12	2.11	0.50
5:F:387:VAL:HG11	5:F:409:ASN:OD1	2.11	0.50
2:I:1281:TYR:OH	3:J:434:ILE:O	2.29	0.50
1:A:57:THR:HG22	1:A:158:ARG:NH2	2.26	0.50
1:A:75:GLN:HA	2:C:729:ALA:N	2.26	0.50
2:C:91:THR:HG21	2:C:503:LYS:HE2	1.93	0.50
2:C:229:ILE:HG21	2:C:240:GLU:OE2	2.12	0.50
2:C:452:ARG:NH1	2:C:584:TYR:O	2.43	0.50
2:C:1085:MET:HA	2:C:1085:MET:HE2	1.92	0.50
2:C:1112:ILE:O	2:C:1115:THR:N	2.44	0.50
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.76	0.50
2:C:1267:GLY:HA3	3:D:347:VAL:O	2.12	0.50
3:D:664:ILE:HG21	3:D:681:LYS:HG2	1.93	0.50
2:I:238:GLN:HB3	2:I:284:LEU:HD11	1.93	0.50
2:I:921:PRO:O	2:I:924:VAL:HG22	2.11	0.50
3:J:1261:LEU:HD13	3:J:1304:ARG:HD2	1.93	0.50
3:J:1286:LYS:HD2	3:J:1290:ARG:NH2	2.27	0.50
5:L:557:LYS:HZ2	5:L:561:MET:HE1	1.75	0.50
1:A:207:THR:HG22	1:A:209:GLY:H	1.76	0.50
1:A:228:LEU:HA	1:A:231:PHE:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:397:LEU:HD12	2:C:397:LEU:N	2.26	0.50
3:D:574:VAL:O	3:D:578:ILE:HG13	2.11	0.50
1:G:65:LEU:HD22	1:G:65:LEU:N	2.26	0.50
2:I:623:LEU:HA	2:I:630:VAL:HG23	1.92	0.50
2:I:757:THR:O	2:I:833:ILE:HD12	2.11	0.50
3:J:746:LEU:HD23	3:J:758:PRO:HG3	1.93	0.50
5:L:456:MET:HE1	5:L:497:VAL:HG13	1.93	0.50
1:A:152:TYR:OH	2:C:824:GLN:HA	2.11	0.50
2:C:323:ALA:O	2:C:327:GLN:HG3	2.12	0.50
2:C:618:GLN:OE1	3:D:770:LEU:HD13	2.12	0.50
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.93	0.50
3:D:844:THR:OG1	3:D:860:ARG:O	2.20	0.50
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.93	0.50
1:G:88:LEU:HB2	1:G:128:HIS:CD2	2.46	0.50
2:I:101:ARG:HE	2:I:118:LYS:HD2	1.77	0.50
3:J:255:LEU:HB2	3:J:259:ARG:O	2.12	0.50
5:L:161:LEU:O	5:L:262:VAL:HG23	2.11	0.50
2:C:886:LYS:NZ	2:C:916:SER:HB3	2.26	0.50
2:C:1268:GLN:OE1	3:D:352:ARG:HG2	2.12	0.50
5:F:120:ALA:HA	5:F:123:ILE:HD12	1.93	0.50
1:H:19:VAL:HB	1:H:23:HIS:CD2	2.46	0.50
1:H:118:ASP:HB2	1:H:121:VAL:HG23	1.93	0.50
2:I:745:GLU:N	2:I:1017:GLN:HG3	2.26	0.50
3:J:355:ILE:HG21	3:J:466:MET:HG3	1.93	0.50
2:C:887:VAL:HB	2:C:913:VAL:HG22	1.92	0.50
3:D:514:THR:OG1	3:D:594:GLN:O	2.30	0.50
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.47	0.50
3:D:1184:ASP:O	3:D:1186:TYR:N	2.45	0.50
5:F:125:ASP:OD1	5:F:125:ASP:N	2.43	0.50
5:F:292:VAL:HG13	5:F:297:MET:O	2.11	0.50
5:F:478:PRO:HB2	5:F:483:LEU:CD1	2.41	0.50
5:F:478:PRO:HB2	5:F:483:LEU:HD11	1.92	0.50
2:I:157:PHE:CZ	2:I:431:LYS:HG2	2.47	0.50
2:I:556:GLY:HA2	2:I:659:GLN:O	2.12	0.50
3:J:205:LEU:HD23	3:J:217:LEU:HG	1.94	0.50
3:J:516:ASP:N	3:J:516:ASP:OD1	2.44	0.50
1:A:114:ASP:N	1:A:114:ASP:OD1	2.44	0.50
3:D:817:HIS:NE2	3:D:860:ARG:NH2	2.59	0.50
3:D:905:ARG:NH1	4:E:10:VAL:HG11	2.27	0.50
1:G:226:GLU:CD	1:H:10:LYS:HE2	2.37	0.50
1:H:78:ILE:O	1:H:82:LEU:HG	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.93	0.50
3:J:77:ARG:HB3	3:J:80:HIS:CE1	2.47	0.50
3:J:1246:VAL:HG12	3:J:1248:ILE:HG13	1.92	0.50
3:J:1266:ILE:HD12	3:J:1273:ASP:O	2.12	0.50
1:A:224:LEU:HD23	1:A:224:LEU:C	2.36	0.50
1:B:16:ILE:HG12	1:B:26:VAL:CG1	2.41	0.50
2:C:18:ARG:NH1	2:C:621:SER:O	2.45	0.50
2:C:209:ILE:O	2:C:213:LEU:HG	2.12	0.50
2:C:891:GLY:C	2:C:892:GLU:HG3	2.37	0.50
2:C:1149:TYR:HE2	2:C:1180:MET:SD	2.35	0.50
2:C:1160:ASP:CG	2:C:1161:LEU:N	2.67	0.50
2:C:1328:LYS:O	2:C:1332:SER:N	2.45	0.50
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.93	0.50
3:D:1371:ARG:CZ	3:D:1371:ARG:HB3	2.42	0.50
5:L:289:LYS:HE3	5:L:293:GLU:HG2	1.93	0.50
1:A:76:GLU:N	1:A:76:GLU:OE2	2.45	0.50
1:A:177:TYR:O	1:A:178:SER:HB2	2.11	0.50
2:C:566:GLY:H	2:C:569:ILE:CG1	2.23	0.50
3:D:528:THR:HG22	3:D:532:GLU:CD	2.37	0.50
3:D:847:ASP:OD1	3:D:847:ASP:N	2.33	0.50
3:D:1183:SER:OG	3:D:1185:PRO:HD3	2.12	0.50
3:D:1347:LEU:HG	3:D:1357:ILE:HG23	1.93	0.50
1:G:99:ILE:HA	1:G:144:ILE:O	2.12	0.50
2:I:62:TYR:C	2:I:64:GLY:H	2.19	0.50
3:J:349:TYR:CD1	3:J:472:LEU:HD11	2.47	0.50
3:J:481:ARG:O	3:J:485:MET:HB2	2.12	0.50
3:J:800:LEU:O	3:J:803:VAL:HG12	2.12	0.50
3:J:1293:GLU:OE1	3:J:1294:ALA:N	2.38	0.50
2:C:538:LEU:HD22	2:C:543:ALA:HB2	1.93	0.49
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.94	0.49
2:C:1103:VAL:HG22	2:C:1111:GLN:NE2	2.27	0.49
2:C:1131:MET:CE	2:C:1141:LEU:HD12	2.26	0.49
5:F:281:ARG:HA	5:F:284:GLU:OE1	2.11	0.49
2:I:521:LEU:O	2:I:525:THR:N	2.40	0.49
2:I:866:ASP:HA	2:I:872:TYR:CZ	2.46	0.49
3:J:244:VAL:HA	3:J:269:TYR:OH	2.11	0.49
3:J:377:PHE:O	3:J:378:LYS:C	2.54	0.49
5:L:265:GLN:O	5:L:269:LEU:HG	2.12	0.49
1:A:318:LEU:HD11	5:F:600:HIS:NE2	2.28	0.49
2:C:1131:MET:HE1	2:C:1141:LEU:HA	1.93	0.49
2:C:1151:LEU:CD1	2:C:1198:LEU:HD23	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1197:GLU:O	2:C:1200:LYS:HB2	2.11	0.49
3:D:93:THR:HG22	3:D:94:GLN:H	1.77	0.49
5:F:484:ALA:HB1	5:F:491:GLU:CG	2.43	0.49
2:I:23:ASP:OD1	2:I:23:ASP:N	2.44	0.49
2:I:358:ASP:OD1	2:I:360:LEU:HB3	2.12	0.49
2:I:1199:LEU:HD13	2:I:1206:THR:HA	1.94	0.49
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.94	0.49
3:J:491:LEU:HD22	3:J:496:GLY:O	2.12	0.49
5:L:407:GLU:HG3	5:L:442:SER:OG	2.12	0.49
5:L:572:THR:O	5:L:576:VAL:HG23	2.12	0.49
1:A:102:LEU:HB2	1:A:115:ILE:HG23	1.94	0.49
1:B:149:GLY:HA3	1:B:177:TYR:CG	2.47	0.49
2:C:312:ALA:HB3	2:C:315:MET:HE3	1.94	0.49
2:C:490:GLN:HG3	5:F:472:GLN:OE1	2.11	0.49
3:D:870:ASP:O	3:D:874:GLU:HG2	2.12	0.49
3:D:1159:ILE:CA	3:D:1206:ARG:HB3	2.41	0.49
2:I:478:ARG:CZ	2:I:487:LEU:HD13	2.42	0.49
2:I:794:LEU:CD2	2:I:796:LEU:HD11	2.43	0.49
3:J:1280:VAL:O	3:J:1284:ARG:HB3	2.13	0.49
1:A:29:GLU:CB	1:A:30:PRO:HD3	2.38	0.49
3:D:450:HIS:HE1	3:D:452:LEU:HD12	1.76	0.49
3:D:1280:VAL:O	3:D:1284:ARG:HB3	2.12	0.49
3:D:1333:THR:O	3:D:1336:ALA:N	2.46	0.49
5:F:276:MET:O	5:F:280:VAL:HG23	2.12	0.49
1:G:136:GLU:C	1:G:138:ALA:H	2.20	0.49
2:I:1070:HIS:CD2	2:I:1111:GLN:HA	2.47	0.49
2:I:1312:ASN:OD1	2:I:1314:GLN:HG3	2.13	0.49
3:J:642:ASP:HA	3:J:764:ARG:HH21	1.75	0.49
3:J:903:LEU:HD23	3:J:905:ARG:HD3	1.93	0.49
5:L:248:GLU:HA	5:L:251:LYS:HE3	1.95	0.49
5:L:479:THR:HG22	5:L:482:GLU:HB2	1.94	0.49
5:L:606:VAL:HG22	5:L:607:LEU:HD12	1.95	0.49
2:C:446:ASP:OD1	2:C:547:VAL:HG12	2.11	0.49
2:C:490:GLN:CD	5:F:472:GLN:HE22	2.21	0.49
2:C:615:VAL:HG22	2:C:650:VAL:HA	1.94	0.49
3:D:19:ALA:CB	3:D:1373:ARG:HH22	2.26	0.49
3:D:839:VAL:HG12	3:D:839:VAL:O	2.12	0.49
3:D:1154:ALA:N	3:D:1214:PRO:O	2.34	0.49
3:D:1227:HIS:CG	3:J:1293:GLU:HG2	2.47	0.49
5:F:119:ILE:HA	5:F:122:ARG:HD3	1.95	0.49
1:H:73:GLY:HA2	1:H:134:THR:CG2	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:188:LEU:O	3:J:191:SER:OG	2.28	0.49
3:J:597:GLY:O	3:J:601:ILE:HB	2.12	0.49
3:J:844:THR:HB	3:J:860:ARG:O	2.12	0.49
2:C:516:ASP:OD1	2:C:517:GLN:N	2.44	0.49
2:C:801:ARG:O	2:C:1095:ASP:HB2	2.12	0.49
2:C:896:THR:OG1	2:C:899:GLU:HG3	2.11	0.49
3:D:367:GLY:N	3:D:448:GLN:O	2.42	0.49
3:D:733:SER:O	3:D:734:ALA:C	2.56	0.49
5:F:314:THR:O	5:F:318:ALA:HB3	2.12	0.49
1:H:47:LEU:HD13	1:H:183:ILE:HG21	1.93	0.49
1:H:47:LEU:HD22	1:H:180:VAL:HG11	1.94	0.49
2:I:1132:LEU:HB3	2:I:1177:ARG:NH2	2.27	0.49
3:J:545:HIS:NE2	3:J:719:PHE:HE1	2.11	0.49
2:C:98:VAL:O	2:C:121:GLU:HA	2.13	0.49
2:C:596:ASP:OD2	2:C:598:VAL:HG23	2.12	0.49
2:C:1136:GLN:O	2:C:1137:GLU:HB3	2.11	0.49
2:C:1237:HIS:O	2:C:1238:LEU:C	2.56	0.49
3:D:502:PRO:HB3	3:D:506:VAL:HG11	1.95	0.49
1:G:23:HIS:ND1	1:G:205:MET:O	2.45	0.49
1:G:228:LEU:HD21	1:H:224:LEU:HD23	1.94	0.49
1:G:228:LEU:O	1:G:231:PHE:HD2	1.95	0.49
2:I:658:GLN:NE2	2:I:1186:VAL:HG23	2.27	0.49
2:I:807:TRP:HB2	2:I:1097:VAL:HG11	1.95	0.49
5:L:601:PRO:HB3	5:L:608:ARG:NH2	2.28	0.49
1:A:46:ILE:HD11	1:B:38:THR:HG21	1.95	0.49
2:C:208:ILE:HD11	2:C:365:GLU:HB3	1.95	0.49
2:C:605:TYR:C	2:C:606:LEU:HD12	2.38	0.49
2:C:1158:LYS:C	2:C:1159:VAL:HG22	2.37	0.49
3:D:227:PHE:O	3:D:230:SER:HB3	2.12	0.49
5:F:340:ALA:HA	5:F:343:LYS:NZ	2.28	0.49
1:H:19:VAL:HB	1:H:23:HIS:HD2	1.77	0.49
1:H:133:LEU:HD12	1:H:133:LEU:HA	1.64	0.49
2:I:1130:ALA:O	2:I:1134:GLN:N	2.46	0.49
2:I:1152:GLY:O	2:I:1153:ALA:HB2	2.13	0.49
3:J:85:CYS:HB3	3:J:88:CYS:O	2.11	0.49
3:J:454:CYS:SG	3:J:461:PHE:CZ	3.06	0.49
3:J:1165:PHE:HD2	3:J:1173:ARG:CD	2.26	0.49
3:J:1184:ASP:O	3:J:1186:TYR:N	2.46	0.49
4:K:59:ILE:HD12	4:K:64:LEU:HD21	1.95	0.49
5:L:289:LYS:HA	5:L:293:GLU:OE1	2.13	0.49
1:B:91:ARG:HG3	1:B:122:GLU:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:191:LYS:O	2:C:192:ASP:HB2	2.13	0.49
2:C:478:ARG:HG2	2:C:492:MET:HG2	1.95	0.49
2:C:718:ALA:HB2	2:C:783:LEU:CD2	2.43	0.49
2:C:759:SER:C	2:C:761:GLN:N	2.70	0.49
2:C:1284:ALA:CB	3:D:1356:LEU:HD22	2.41	0.49
3:D:34:SER:OG	3:D:104:HIS:ND1	2.37	0.49
3:D:1283:SER:O	3:D:1286:LYS:N	2.45	0.49
1:G:75:GLN:HA	2:I:729:ALA:H	1.78	0.49
1:G:160:HIS:CG	1:G:161:SER:N	2.80	0.49
1:H:59:VAL:HG22	1:H:144:ILE:HG13	1.95	0.49
1:H:60:GLU:CG	1:H:143:ARG:HB2	2.42	0.49
2:I:20:GLN:HG2	2:I:1156:ARG:NH2	2.27	0.49
2:I:90:VAL:HG12	2:I:91:THR:H	1.77	0.49
2:I:98:VAL:HB	2:I:124:MET:HE3	1.94	0.49
2:I:175:ARG:NH1	2:I:200:ARG:HH12	2.11	0.49
3:J:334:LYS:HB3	5:L:516:ASP:OD2	2.13	0.49
5:L:148:TYR:HE1	5:L:158:LEU:HD21	1.77	0.49
5:L:261:LEU:H	5:L:261:LEU:HD12	1.78	0.49
5:L:603:ARG:NH1	5:L:603:ARG:HA	2.27	0.49
1:A:321:TRP:HA	1:A:322:PRO:HA	1.64	0.49
1:B:100:LEU:HD11	1:B:121:VAL:HG21	1.94	0.49
2:C:959:ASP:O	2:C:963:GLU:HG2	2.12	0.49
2:C:1212:LEU:HD22	2:C:1225:VAL:CG2	2.41	0.49
3:D:843:VAL:HG11	3:D:897:HIS:O	2.12	0.49
5:F:512:GLY:C	5:F:514:ASP:N	2.71	0.49
1:H:64:VAL:HG12	1:H:65:LEU:H	1.77	0.49
2:I:139:ASN:O	2:I:141:THR:HG23	2.12	0.49
2:I:674:ASP:OD1	2:I:1110:GLY:N	2.25	0.49
2:I:1219:GLU:OE2	3:J:538:ARG:NH1	2.31	0.49
2:I:1220:GLN:HG2	2:I:1221:PHE:H	1.77	0.49
3:J:322:ARG:HB2	3:J:322:ARG:NH1	2.27	0.49
5:L:230:VAL:O	5:L:234:THR:HG23	2.13	0.49
1:A:262:LEU:HD21	1:A:306:VAL:HG11	1.95	0.48
1:B:60:GLU:CD	1:B:142:MET:HB2	2.38	0.48
2:C:90:VAL:HG12	2:C:91:THR:N	2.27	0.48
2:C:866:ASP:HA	2:C:872:TYR:CZ	2.48	0.48
2:C:1238:LEU:H	2:C:1238:LEU:CD1	2.16	0.48
2:C:1333:LEU:HD21	3:D:327:LEU:HB2	1.95	0.48
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.28	0.48
1:G:64:VAL:HG12	1:G:66:HIS:H	1.78	0.48
1:H:185:TYR:HB2	1:H:201:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:367:TYR:CE2	2:I:376:PRO:HA	2.48	0.48
2:I:745:GLU:H	2:I:1017:GLN:HG3	1.78	0.48
2:I:814:ASP:CG	2:I:1106:ARG:HH12	2.19	0.48
3:J:848:VAL:CG2	3:J:858:VAL:HG13	2.42	0.48
1:A:195:ARG:HG2	1:A:198:LEU:HG	1.94	0.48
2:C:4:SER:HB3	2:C:7:GLU:OE2	2.14	0.48
2:C:1079:ILE:O	2:C:1079:ILE:HG23	2.13	0.48
2:C:1129:ASN:OD1	2:C:1177:ARG:NH2	2.34	0.48
3:D:198:CYS:O	3:D:202:ARG:HG3	2.12	0.48
3:D:318:GLY:O	3:D:320:ASN:N	2.46	0.48
3:D:510:LEU:HD22	3:D:601:ILE:HD11	1.96	0.48
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.29	0.48
1:G:67:GLU:HG3	1:G:171:LEU:HG	1.94	0.48
1:H:82:LEU:HD22	1:H:173:VAL:HG22	1.94	0.48
1:H:112:ALA:HB2	1:H:128:HIS:HB3	1.94	0.48
2:I:15:PHE:CE1	2:I:1151:LEU:HD13	2.48	0.48
3:J:79:LYS:HG3	3:J:80:HIS:N	2.28	0.48
3:J:291:ILE:HD13	5:L:409:ASN:HB3	1.95	0.48
5:L:299:LYS:O	5:L:303:ILE:HG12	2.13	0.48
5:L:555:GLU:OE2	5:L:597:LYS:NZ	2.39	0.48
1:A:283:GLN:O	1:A:315:GLY:HA2	2.14	0.48
2:C:139:ASN:O	2:C:141:THR:N	2.46	0.48
2:C:185:ASP:O	2:C:196:VAL:HA	2.14	0.48
2:C:285:ILE:HD11	2:C:287:VAL:HG12	1.95	0.48
2:C:557:ARG:NH2	2:C:608:ALA:HA	2.28	0.48
2:C:1283:ALA:HB1	3:D:479:GLU:OE2	2.13	0.48
3:D:827:GLU:C	3:D:829:GLY:H	2.21	0.48
4:E:53:GLU:OE1	4:E:59:ILE:HG13	2.14	0.48
5:F:532:LEU:H	5:F:532:LEU:HD12	1.79	0.48
1:G:91:ARG:HG3	1:G:122:GLU:HB3	1.95	0.48
1:G:105:SER:HB2	1:G:138:ALA:O	2.12	0.48
1:H:179:PRO:HA	1:H:208:ASN:HD21	1.78	0.48
2:I:137:VAL:HA	2:I:141:THR:O	2.13	0.48
2:I:786:GLY:N	2:I:789:THR:OG1	2.46	0.48
2:I:801:ARG:HD3	2:I:1094:VAL:HA	1.96	0.48
3:J:45:ASN:O	3:J:46:TYR:CD2	2.66	0.48
3:J:293:ARG:NH1	5:L:104:GLU:OE2	2.46	0.48
3:J:395:LYS:O	3:J:398:LYS:HB3	2.14	0.48
5:L:456:MET:O	5:L:459:THR:HB	2.13	0.48
5:L:474:MET:HE3	5:L:474:MET:HB3	1.74	0.48
1:B:152:TYR:HE1	1:B:176:CYS:HB3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1116:HIS:O	2:C:1119:MET:HB3	2.14	0.48
3:D:905:ARG:HH21	3:D:907:HIS:CB	2.25	0.48
4:E:35:LYS:NZ	4:E:71:GLU:OE2	2.34	0.48
5:F:277:MET:HG3	5:F:362:ASN:HD21	1.77	0.48
5:F:280:VAL:HG22	5:F:347:ILE:HD13	1.94	0.48
2:I:976:ARG:HD2	2:I:989:LEU:HD23	1.95	0.48
3:J:361:LEU:HD22	3:J:365:GLN:HG3	1.94	0.48
1:A:233:ASP:C	1:A:234:LEU:HD22	2.38	0.48
1:B:23:HIS:ND1	1:B:206:GLU:HG2	2.28	0.48
1:B:211:ILE:HD11	1:B:215:GLU:OE2	2.13	0.48
2:C:20:GLN:HG3	2:C:20:GLN:O	2.14	0.48
2:C:325:LEU:O	2:C:328:SER:OG	2.31	0.48
2:C:518:ASN:O	2:C:519:ASN:HB2	2.12	0.48
3:D:266:ASN:O	3:D:267:ASP:C	2.54	0.48
3:D:293:ARG:O	3:D:294:ASN:C	2.57	0.48
2:I:132:ASP:OD1	2:I:132:ASP:N	2.38	0.48
2:I:178:PRO:HB3	2:I:395:TYR:CZ	2.48	0.48
2:I:629:PHE:CE2	2:I:634:VAL:HG11	2.49	0.48
2:I:658:GLN:NE2	2:I:1186:VAL:H	2.11	0.48
2:I:705:GLU:CD	2:I:705:GLU:H	2.20	0.48
2:I:1085:MET:HE2	2:I:1085:MET:HA	1.95	0.48
3:J:1290:ARG:HG2	3:J:1298:VAL:HG12	1.95	0.48
5:L:166:VAL:O	5:L:167:ASP:HB2	2.12	0.48
1:B:206:GLU:OE2	3:D:531:LYS:HE2	2.14	0.48
2:C:40:GLU:O	2:C:73:TYR:OH	2.32	0.48
2:C:685:MET:SD	2:C:1073:LYS:HG3	2.54	0.48
3:D:9:LYS:HE2	3:D:9:LYS:HB3	1.66	0.48
3:D:36:GLY:HA3	3:D:61:ILE:HG23	1.95	0.48
5:F:483:LEU:HD12	5:F:483:LEU:N	2.22	0.48
5:F:557:LYS:HG3	5:F:561:MET:HE1	1.94	0.48
5:F:583:THR:HG22	5:F:584:ARG:HG2	1.95	0.48
1:G:153:VAL:N	1:G:175:ALA:O	2.33	0.48
2:I:800:MET:O	2:I:1229:TYR:HA	2.13	0.48
3:J:337:ARG:HH11	3:J:1327:GLU:HA	1.79	0.48
3:J:681:LYS:O	3:J:684:ASP:HB2	2.14	0.48
5:L:276:MET:O	5:L:280:VAL:HG23	2.14	0.48
2:C:158:ASP:CG	2:C:159:SER:N	2.71	0.48
2:C:524:ILE:HD12	2:C:712:SER:HB2	1.94	0.48
2:C:1017:GLN:O	2:C:1021:LEU:HG	2.14	0.48
3:D:278:ARG:NH1	3:D:295:GLU:OE1	2.39	0.48
3:D:490:ILE:HG12	3:D:491:LEU:HG	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:516:ASP:OD1	3:D:516:ASP:N	2.44	0.48
3:D:720:ASN:OD1	3:D:722:ILE:HG22	2.13	0.48
3:D:1221:LEU:HD11	3:D:1304:ARG:O	2.14	0.48
5:F:277:MET:HE3	5:F:281:ARG:HH21	1.79	0.48
5:F:561:MET:HG2	5:F:576:VAL:HG22	1.95	0.48
1:G:190:ALA:HB2	1:G:200:LYS:CB	2.32	0.48
2:I:742:TYR:HD2	2:I:743:PRO:HD2	1.78	0.48
2:I:1179:GLY:O	2:I:1181:PRO:HD3	2.13	0.48
3:J:515:ARG:HH21	3:J:717:VAL:HG23	1.79	0.48
3:J:516:ASP:HB3	3:J:573:THR:HG21	1.96	0.48
3:J:708:ASN:OD1	3:J:708:ASN:N	2.46	0.48
3:J:797:THR:O	3:J:801:VAL:HG13	2.12	0.48
2:C:10:ARG:CZ	2:C:697:LYS:HD3	2.44	0.48
2:C:886:LYS:O	2:C:916:SER:N	2.47	0.48
2:C:1120:ALA:HB2	2:C:1199:LEU:HG	1.96	0.48
3:D:244:VAL:HG23	3:D:244:VAL:O	2.14	0.48
5:F:114:GLU:HG3	5:F:115:GLY:H	1.78	0.48
3:J:457:TYR:CE2	3:J:466:MET:HE1	2.49	0.48
3:J:556:GLU:HG2	3:J:558:ASP:HB2	1.96	0.48
5:L:394:TYR:OH	5:L:436:ARG:HD2	2.12	0.48
1:A:61:ILE:HG23	1:A:142:MET:CB	2.39	0.48
1:A:166:ARG:O	1:A:166:ARG:HD2	2.14	0.48
2:C:1065:LYS:HE2	3:D:462:ASP:O	2.14	0.48
3:D:580:TRP:O	3:D:580:TRP:CG	2.67	0.48
5:F:489:MET:O	5:F:491:GLU:HB3	2.14	0.48
1:G:10:LYS:HE2	1:H:229:GLU:OE1	2.14	0.48
1:G:64:VAL:CG1	1:G:69:SER:HB2	2.44	0.48
2:I:195:PHE:CD1	2:I:205:PRO:HA	2.49	0.48
2:I:685:MET:HA	2:I:688:GLN:HE21	1.78	0.48
3:J:113:HIS:CE1	3:J:115:TRP:HB2	2.49	0.48
3:J:186:GLN:HG3	3:J:238:ILE:HB	1.96	0.48
5:L:137:TYR:CE2	5:L:273:MET:HG2	2.49	0.48
1:B:108:GLY:O	1:B:133:LEU:HB2	2.13	0.48
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.29	0.48
2:C:108:GLU:OE1	2:C:108:GLU:HA	2.13	0.48
2:C:685:MET:HB2	2:C:685:MET:HE3	1.33	0.48
2:C:805:MET:O	2:C:805:MET:HG3	2.14	0.48
3:D:706:VAL:HG12	3:D:715:LYS:CB	2.44	0.48
5:F:600:HIS:CG	5:F:601:PRO:HD2	2.48	0.48
2:I:496:LYS:HB3	2:I:497:PRO:HD3	1.96	0.48
2:I:1242:LYS:HD2	3:J:465:GLN:OE1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:544:LEU:O	3:J:575:GLY:N	2.47	0.48
3:J:1265:THR:HG22	3:J:1277:GLY:HA2	1.96	0.48
5:L:157:ARG:NH2	5:L:159:SER:OG	2.47	0.48
5:L:343:LYS:HA	5:L:346:GLN:HB3	1.95	0.48
1:A:176:CYS:O	1:A:177:TYR:C	2.57	0.47
2:C:1070:HIS:CD2	2:C:1111:GLN:HA	2.48	0.47
2:C:1176:LEU:HD23	2:C:1176:LEU:HA	1.38	0.47
2:C:1341:ASP:HB3	3:D:18:ASP:OD2	2.14	0.47
3:D:695:LYS:HA	3:D:695:LYS:HD3	1.44	0.47
3:D:1138:LEU:HB3	3:D:1139:PRO:HD3	1.95	0.47
3:D:1206:ARG:NH2	3:D:1223:LEU:O	2.47	0.47
5:F:453:PRO:O	5:F:456:MET:HB2	2.14	0.47
2:I:169:LYS:O	2:I:170:VAL:HG22	2.14	0.47
2:I:213:LEU:HA	2:I:213:LEU:HD23	1.56	0.47
3:J:77:ARG:HB3	3:J:80:HIS:ND1	2.28	0.47
3:J:102:MET:HE2	3:J:102:MET:HB3	1.58	0.47
3:J:239:LEU:HA	3:J:239:LEU:HD23	1.60	0.47
3:J:742:GLY:O	3:J:762:ASN:HB3	2.14	0.47
5:L:598:LEU:O	5:L:604:SER:OG	2.31	0.47
2:C:41:GLN:NE2	2:C:73:TYR:O	2.46	0.47
2:C:123:TYR:HB3	5:F:472:GLN:HB2	1.96	0.47
2:C:587:LEU:HD23	2:C:587:LEU:HA	1.73	0.47
2:C:590:PRO:HG3	2:C:605:TYR:CE2	2.49	0.47
3:D:1295:ASN:HB2	3:D:1298:VAL:HB	1.94	0.47
4:E:25:ARG:HD3	4:E:64:LEU:HD13	1.96	0.47
5:F:277:MET:HE3	5:F:281:ARG:NH2	2.29	0.47
2:I:123:TYR:OH	2:I:126:GLU:HG3	2.13	0.47
2:I:151:ARG:HE	2:I:445:ILE:HD11	1.78	0.47
2:I:494:ASN:HD22	2:I:497:PRO:CD	2.28	0.47
2:I:658:GLN:O	2:I:660:VAL:N	2.47	0.47
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.95	0.47
3:J:598:LYS:N	3:J:728:SER:O	2.33	0.47
2:C:619:ALA:HA	2:C:654:ASP:HB2	1.96	0.47
2:C:811:ASN:HA	2:C:815:SER:HB2	1.94	0.47
5:F:227:GLN:NE2	5:F:251:LYS:HZ1	2.09	0.47
1:G:19:VAL:HG12	1:G:20:SER:N	2.27	0.47
2:I:367:TYR:HD1	2:I:384:LEU:HD22	1.78	0.47
2:I:403:MET:SD	2:I:403:MET:C	2.98	0.47
2:I:736:VAL:HG23	2:I:748:ILE:HA	1.96	0.47
2:I:1085:MET:CB	2:I:1093:PRO:HB3	2.43	0.47
3:J:1257:VAL:O	3:J:1258:ARG:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1356:LEU:O	3:J:1366:HIS:CE1	2.67	0.47
5:L:515:GLU:HG2	5:L:516:ASP:N	2.29	0.47
1:B:101:THR:HG22	1:B:116:THR:HB	1.97	0.47
2:C:302:ILE:O	2:C:330:HIS:NE2	2.36	0.47
2:C:486:THR:HG23	2:C:487:LEU:H	1.79	0.47
2:C:593:LYS:HG3	2:C:595:THR:HG23	1.96	0.47
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.73	0.47
5:F:386:LEU:O	5:F:389:SER:OG	2.27	0.47
2:I:518:ASN:CG	2:I:519:ASN:N	2.72	0.47
2:I:785:ASP:HB3	2:I:789:THR:OG1	2.14	0.47
2:I:1331:ARG:HG2	3:J:33:TRP:CZ3	2.49	0.47
3:J:770:LEU:O	3:J:774:ILE:HG13	2.15	0.47
3:J:1226:VAL:O	3:J:1230:THR:HG22	2.14	0.47
2:C:129:LEU:HD23	2:C:129:LEU:HA	1.64	0.47
2:C:225:PHE:CE2	2:C:347:ILE:HB	2.49	0.47
2:C:623:LEU:HA	2:C:630:VAL:HG23	1.96	0.47
2:C:821:ARG:HG3	2:C:825:GLU:OE1	2.15	0.47
2:C:1148:ALA:HB1	2:C:1180:MET:HE2	1.95	0.47
3:D:482:ALA:C	3:D:483:LEU:HG	2.39	0.47
1:G:29:GLU:HB3	1:G:30:PRO:HD3	1.96	0.47
1:G:97:GLU:HB3	1:G:147:GLN:HA	1.97	0.47
2:I:74:ARG:NH1	2:I:121:GLU:OE2	2.46	0.47
2:I:692:THR:OG1	2:I:693:LEU:N	2.47	0.47
2:I:720:ARG:HH21	2:I:736:VAL:HG11	1.79	0.47
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.96	0.47
3:J:658:GLU:O	3:J:661:VAL:HG13	2.14	0.47
3:J:884:SER:OG	3:J:885:VAL:N	2.48	0.47
1:A:233:ASP:O	1:A:234:LEU:HD22	2.14	0.47
1:A:307:LEU:HA	1:A:307:LEU:HD23	1.53	0.47
2:C:250:THR:HA	2:C:268:ARG:HA	1.97	0.47
2:C:650:VAL:HG23	2:C:650:VAL:O	2.14	0.47
2:C:1142:ARG:CD	2:C:1161:LEU:HD11	2.31	0.47
2:C:1252:SER:HB3	2:C:1255:THR:O	2.14	0.47
2:C:1296:ASP:OD2	3:D:345:LYS:NZ	2.47	0.47
3:D:40:LYS:HB2	3:D:54:ASP:O	2.14	0.47
3:D:268:LEU:HD23	3:D:268:LEU:HA	1.62	0.47
3:D:739:GLN:OE1	3:D:744:ARG:NE	2.48	0.47
3:D:744:ARG:O	3:D:744:ARG:HG3	2.15	0.47
3:D:1146:GLU:HA	3:D:1146:GLU:OE2	2.15	0.47
3:D:1221:LEU:O	3:D:1221:LEU:HD22	2.15	0.47
5:F:112:THR:OG1	5:F:114:GLU:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:13:LYS:O	2:I:1183:ALA:N	2.31	0.47
2:I:197:ARG:NH1	2:I:201:ARG:O	2.45	0.47
2:I:557:ARG:NE	2:I:587:LEU:O	2.41	0.47
2:I:902:LEU:HD21	5:L:611:LEU:HG	1.95	0.47
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.97	0.47
3:J:1286:LYS:HD2	3:J:1290:ARG:HH21	1.78	0.47
5:L:137:TYR:HD2	5:L:273:MET:HE2	1.79	0.47
1:A:246:LYS:HB2	1:A:248:GLU:OE2	2.15	0.47
2:C:62:TYR:C	2:C:64:GLY:N	2.71	0.47
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.50	0.47
2:C:870:ILE:HG22	2:C:944:ARG:NH1	2.29	0.47
2:C:1112:ILE:O	2:C:1113:LEU:C	2.56	0.47
2:C:1120:ALA:HB1	2:C:1198:LEU:HD13	1.96	0.47
3:D:35:PHE:CE1	3:D:101:ARG:HD3	2.50	0.47
3:D:238:ILE:HG23	3:D:238:ILE:HD12	1.67	0.47
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.96	0.47
3:D:648:GLU:OE2	3:D:649:LYS:HE2	2.14	0.47
3:D:1175:LEU:O	3:D:1187:GLU:HA	2.14	0.47
3:D:1181:ASP:CB	3:J:202:ARG:HD3	2.45	0.47
5:F:163:THR:O	5:F:260:ARG:NH2	2.48	0.47
5:F:276:MET:O	5:F:279:ARG:HB2	2.14	0.47
5:F:372:ALA:O	5:F:376:LYS:HG3	2.14	0.47
1:G:37:HIS:HB3	1:H:45:ARG:NH1	2.30	0.47
2:I:242:VAL:HG21	2:I:245:ARG:NH1	2.30	0.47
2:I:344:GLY:O	2:I:346:TYR:CG	2.68	0.47
2:I:528:ARG:NH2	2:I:575:LEU:HD23	2.29	0.47
2:I:835:GLU:OE2	2:I:1051:LYS:HD3	2.14	0.47
2:I:870:ILE:HG22	2:I:944:ARG:NH1	2.29	0.47
2:I:985:GLU:HG2	2:I:988:LYS:HD2	1.97	0.47
3:J:895:CYS:O	3:J:898:CYS:N	2.43	0.47
5:L:390:ILE:HD11	5:L:432:THR:HG23	1.97	0.47
5:L:463:LEU:HD23	5:L:463:LEU:HA	1.68	0.47
5:L:489:MET:CE	5:L:493:LYS:HD2	2.44	0.47
5:L:603:ARG:HA	5:L:603:ARG:CZ	2.44	0.47
1:A:27:THR:HA	1:A:201:LEU:O	2.14	0.47
1:A:102:LEU:HD22	1:A:103:ASN:N	2.30	0.47
1:A:284:ARG:HG3	1:A:288:GLU:OE1	2.15	0.47
2:C:1023:HIS:O	2:C:1027:LYS:HG2	2.14	0.47
2:C:1099:ASN:HD21	3:D:505:ASP:CG	2.22	0.47
3:D:46:TYR:CD1	5:F:452:ILE:HG22	2.50	0.47
5:F:100:MET:HE2	5:F:100:MET:HB3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:379:MET:HG2	5:F:416:VAL:CG2	2.45	0.47
5:F:548:LEU:O	5:F:556:ALA:HB2	2.14	0.47
1:G:66:HIS:HE1	2:I:874:GLY:HA2	1.76	0.47
1:G:79:LEU:HD21	2:I:756:TYR:HH	1.79	0.47
2:I:221:LEU:HD23	2:I:221:LEU:HA	1.63	0.47
2:I:854:ILE:O	2:I:857:VAL:HG22	2.15	0.47
3:J:425:ARG:HD2	3:J:459:ALA:HB2	1.95	0.47
3:J:495:ASN:O	3:J:497:GLU:N	2.48	0.47
3:J:647:PRO:HG3	3:J:697:MET:CB	2.40	0.47
3:J:1280:VAL:HG11	3:J:1304:ARG:CZ	2.44	0.47
1:B:109:PRO:HA	1:B:132:HIS:HA	1.97	0.47
2:C:1331:ARG:HG2	3:D:33:TRP:CH2	2.50	0.47
3:D:810:THR:HG21	3:D:893:GLY:HA3	1.97	0.47
2:I:1309:VAL:HA	3:J:383:GLY:HA3	1.97	0.47
3:J:113:HIS:O	3:J:114:ILE:C	2.57	0.47
3:J:287:ALA:HB1	3:J:288:PRO:HD2	1.95	0.47
3:J:316:ILE:HA	3:J:323:PRO:HA	1.96	0.47
3:J:915:ILE:O	3:J:919:ALA:N	2.45	0.47
2:C:53:PHE:CD1	2:C:468:LEU:HD11	2.49	0.47
2:C:496:LYS:HE3	2:C:497:PRO:HD3	1.97	0.47
2:C:680:LEU:O	2:C:681:MET:C	2.58	0.47
2:C:696:ASP:O	2:C:697:LYS:HB3	2.15	0.47
3:D:37:GLU:O	3:D:61:ILE:HD11	2.14	0.47
3:D:238:ILE:HA	3:D:238:ILE:HD13	1.38	0.47
3:D:1167:LYS:HZ1	3:D:1170:LYS:HB2	1.80	0.47
1:H:18:GLN:NE2	1:H:20:SER:O	2.48	0.47
2:I:62:TYR:O	2:I:64:GLY:N	2.47	0.47
2:I:81:ASP:O	2:I:85:CYS:HB2	2.15	0.47
2:I:185:ASP:HB2	2:I:197:ARG:O	2.15	0.47
2:I:753:LEU:HD21	2:I:784:ALA:CB	2.45	0.47
5:L:306:PHE:HE1	5:L:315:TRP:CH2	2.33	0.47
1:A:12:ARG:NH1	1:A:13:LEU:HD21	2.29	0.46
1:A:316:MET:CB	5:F:600:HIS:CE1	2.98	0.46
2:C:28:LEU:HA	2:C:28:LEU:HD23	1.40	0.46
2:C:356:THR:HG21	2:C:362:ALA:HA	1.97	0.46
2:C:1290:MET:HE2	2:C:1290:MET:HB2	1.72	0.46
3:D:768:ASN:OD1	3:D:771:GLN:OE1	2.33	0.46
3:D:1237:VAL:CG1	3:D:1253:ILE:HD13	2.46	0.46
3:D:1291:GLU:CD	3:J:1302:TYR:OH	2.58	0.46
3:D:1365:TYR:O	3:D:1366:HIS:C	2.58	0.46
2:I:44:GLU:HA	2:I:54:ARG:NH1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:397:LEU:HB3	2:I:401:GLY:HA3	1.97	0.46
2:I:1059:ARG:O	2:I:1234:LYS:NZ	2.43	0.46
3:J:850:LYS:HB3	3:J:851:PRO:HD2	1.98	0.46
1:B:188:GLU:O	1:B:200:LYS:N	2.29	0.46
2:C:157:PHE:CZ	2:C:431:LYS:HG2	2.50	0.46
2:C:169:LYS:O	2:C:170:VAL:HG22	2.15	0.46
2:C:239:MET:O	2:C:284:LEU:HD12	2.15	0.46
2:C:300:ASP:OD1	2:C:313:ALA:N	2.48	0.46
2:C:397:LEU:HB3	2:C:401:GLY:HA3	1.98	0.46
2:C:484:LEU:HD12	2:C:485:ASP:H	1.80	0.46
3:D:112:ALA:HA	3:D:238:ILE:CD1	2.46	0.46
3:D:318:GLY:C	3:D:320:ASN:N	2.73	0.46
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.97	0.46
3:D:519:ASN:OD1	3:D:709:ARG:NH1	2.48	0.46
1:H:110:VAL:HG23	1:H:131:CYS:O	2.15	0.46
1:H:155:ALA:N	1:H:174:ASP:OD1	2.43	0.46
2:I:130:MET:HE3	2:I:136:PHE:CE2	2.49	0.46
2:I:409:LEU:HA	2:I:409:LEU:HD23	1.57	0.46
2:I:802:VAL:HG21	2:I:1098:LEU:HD22	1.96	0.46
2:I:1289:GLU:OE2	3:J:473:THR:HG22	2.16	0.46
3:J:654:ILE:O	3:J:658:GLU:HB2	2.15	0.46
3:J:804:ALA:O	3:J:806:ASP:N	2.48	0.46
3:J:1234:VAL:HG23	3:J:1235:ASN:N	2.30	0.46
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.80	0.46
5:L:305:LEU:HD13	5:L:315:TRP:HA	1.96	0.46
1:A:7:GLU:HG3	1:B:150:ARG:NE	2.26	0.46
1:A:14:VAL:HG22	1:A:15:ASP:N	2.26	0.46
1:A:16:ILE:CG2	1:A:26:VAL:HG12	2.37	0.46
1:A:50:SER:HB2	1:B:8:PHE:HZ	1.79	0.46
1:A:179:PRO:HB3	1:A:211:ILE:HB	1.96	0.46
1:A:255:ARG:HB2	1:A:278:ILE:HD12	1.98	0.46
2:C:1009:ASN:O	2:C:1012:GLU:HB3	2.16	0.46
2:C:1136:GLN:NE2	2:C:1140:LYS:NZ	2.64	0.46
3:D:1291:GLU:CD	3:J:1302:TYR:HH	2.18	0.46
1:H:220:ALA:HA	1:H:223:ILE:HD12	1.97	0.46
2:I:344:GLY:C	2:I:346:TYR:N	2.73	0.46
2:I:517:GLN:O	2:I:517:GLN:HG2	2.14	0.46
2:I:617:ALA:N	2:I:652:TYR:O	2.30	0.46
2:I:657:THR:HG23	2:I:658:GLN:HG3	1.97	0.46
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.97	0.46
3:J:117:LEU:HD12	3:J:117:LEU:HA	1.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:121:PRO:O	3:J:122:SER:C	2.52	0.46
3:J:521:LYS:HE3	3:J:541:LEU:O	2.15	0.46
3:J:647:PRO:CD	3:J:697:MET:HB3	2.45	0.46
3:J:1280:VAL:HG11	3:J:1304:ARG:NE	2.30	0.46
5:L:101:TYR:O	5:L:102:MET:C	2.57	0.46
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.80	0.46
5:L:470:MET:C	5:L:478:PRO:HD3	2.41	0.46
1:A:77:ASP:O	1:A:80:GLU:N	2.48	0.46
1:B:41:ASN:ND2	2:C:1217:THR:HA	2.31	0.46
2:C:128:PRO:HG2	2:C:506:PHE:CD1	2.50	0.46
2:C:705:GLU:HB2	2:C:794:LEU:N	2.27	0.46
2:C:953:LEU:HA	2:C:953:LEU:HD12	1.52	0.46
3:D:45:ASN:O	3:D:46:TYR:CB	2.63	0.46
1:G:98:VAL:HG22	1:G:99:ILE:H	1.79	0.46
1:G:166:ARG:N	1:G:167:PRO:HD2	2.30	0.46
2:I:607:SER:OG	2:I:609:ILE:HG13	2.15	0.46
2:I:653:MET:HG2	2:I:654:ASP:N	2.30	0.46
2:I:830:THR:HG22	2:I:1058:ARG:O	2.15	0.46
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.14	0.46
3:J:746:LEU:CD2	3:J:758:PRO:HG3	2.45	0.46
5:L:296:LYS:HD3	5:L:296:LYS:HA	1.71	0.46
1:B:118:ASP:HB2	1:B:121:VAL:CG2	2.46	0.46
2:C:131:THR:HG21	2:C:135:THR:OG1	2.15	0.46
2:C:247:ARG:HB2	2:C:274:ILE:CD1	2.45	0.46
2:C:262:TYR:HE1	2:C:280:ASP:OD2	1.98	0.46
2:C:676:ALA:O	2:C:677:ASN:C	2.58	0.46
2:C:976:ARG:HD2	2:C:989:LEU:HD23	1.98	0.46
5:F:253:SER:O	5:F:257:LYS:N	2.47	0.46
5:F:466:ILE:HG22	5:F:470:MET:HG3	1.97	0.46
1:H:7:GLU:CD	1:H:8:PHE:N	2.73	0.46
1:H:22:THR:OG1	1:H:207:THR:O	2.33	0.46
3:J:914:ALA:O	3:J:918:ILE:HG23	2.15	0.46
5:L:316:PHE:O	5:L:320:ILE:HG13	2.16	0.46
1:A:47:LEU:O	1:A:180:VAL:HG21	2.15	0.46
1:A:166:ARG:N	1:A:167:PRO:HD2	2.30	0.46
2:C:4:SER:O	2:C:7:GLU:HB2	2.16	0.46
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.98	0.46
2:C:704:MET:O	2:C:707:ALA:N	2.48	0.46
2:C:911:SER:OG	2:C:913:VAL:HG12	2.16	0.46
2:C:1164:PHE:O	2:C:1168:GLU:HB2	2.14	0.46
1:H:44:ARG:HG2	1:H:183:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:27:LEU:HG	2:I:711:ASP:OD2	2.16	0.46
2:I:183:TRP:HB2	2:I:199:ASP:CA	2.39	0.46
2:I:571:LEU:HA	2:I:571:LEU:HD23	1.56	0.46
2:I:796:LEU:H	2:I:796:LEU:HD12	1.81	0.46
2:I:1273:MET:HA	2:I:1276:TRP:CE3	2.50	0.46
3:J:16:GLU:HB3	3:J:17:PHE:HD2	1.79	0.46
3:J:24:LEU:HD23	3:J:232:ASN:ND2	2.31	0.46
3:J:282:LEU:HD23	3:J:282:LEU:HA	1.71	0.46
3:J:827:GLU:C	3:J:829:GLY:H	2.22	0.46
3:J:905:ARG:NH1	3:J:910:ASN:ND2	2.59	0.46
3:J:1261:LEU:HD12	3:J:1261:LEU:C	2.40	0.46
5:L:315:TRP:O	5:L:319:ALA:HB3	2.16	0.46
1:A:152:TYR:CE1	2:C:824:GLN:HG2	2.51	0.46
2:C:171:LEU:HD23	2:C:171:LEU:HA	1.68	0.46
2:C:564:PRO:HD2	2:C:572:ILE:HB	1.98	0.46
2:C:960:LEU:HB3	2:C:1025:PHE:CE2	2.50	0.46
2:C:1174:GLU:OE2	2:C:1177:ARG:NH1	2.48	0.46
3:D:614:LEU:O	3:D:615:LYS:C	2.59	0.46
3:D:614:LEU:O	3:D:617:THR:N	2.49	0.46
3:D:620:PHE:O	3:D:624:ILE:HG13	2.16	0.46
3:D:812:ASP:HB2	3:D:911:LYS:NZ	2.30	0.46
3:D:1181:ASP:HB2	3:J:202:ARG:HD3	1.97	0.46
3:D:1251:LYS:O	3:D:1254:GLU:N	2.49	0.46
1:G:58:GLU:OE1	1:G:145:LYS:HD2	2.16	0.46
2:I:59:ILE:HG23	2:I:476:LYS:HE3	1.98	0.46
2:I:468:LEU:HD23	2:I:468:LEU:HA	1.40	0.46
2:I:593:LYS:HA	2:I:652:TYR:CD2	2.51	0.46
2:I:796:LEU:O	2:I:1233:LEU:HD12	2.16	0.46
2:I:1238:LEU:HD12	2:I:1238:LEU:N	2.28	0.46
3:J:190:LYS:HD3	3:J:235:GLU:HG2	1.96	0.46
3:J:544:LEU:HD12	3:J:544:LEU:HA	1.69	0.46
3:J:885:VAL:O	3:J:1258:ARG:HD2	2.14	0.46
2:C:163:LYS:HE3	2:C:163:LYS:HB3	1.85	0.46
2:C:1332:SER:OG	3:D:327:LEU:HD13	2.15	0.46
3:D:37:GLU:HA	3:D:104:HIS:CE1	2.50	0.46
3:D:722:ILE:HG21	3:D:722:ILE:HD13	1.46	0.46
3:D:846:GLU:HA	3:D:860:ARG:CD	2.45	0.46
2:I:395:TYR:HE2	2:I:397:LEU:HD11	1.81	0.46
2:I:832:HIS:CE1	2:I:1058:ARG:HD2	2.51	0.46
2:I:1101:LEU:HD23	2:I:1101:LEU:HA	1.65	0.46
2:I:1157:GLN:O	2:I:1158:LYS:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:707:ILE:HD11	3:J:716:GLN:HG2	1.98	0.46
3:J:709:ARG:C	3:J:711:GLY:N	2.74	0.46
4:K:30:MET:HE1	4:K:49:ILE:HB	1.97	0.46
5:L:515:GLU:HG2	5:L:516:ASP:H	1.81	0.46
1:A:82:LEU:HD23	1:A:82:LEU:HA	1.58	0.46
1:A:90:VAL:HG22	1:A:91:ARG:N	2.30	0.46
1:A:322:PRO:HA	1:A:323:PRO:HD3	1.77	0.46
2:C:34:SER:OG	2:C:457:GLY:N	2.44	0.46
2:C:958:LYS:O	2:C:961:SER:OG	2.30	0.46
3:D:400:MET:HB3	3:D:400:MET:HE2	1.52	0.46
3:D:1240:VAL:O	3:D:1244:GLN:HG2	2.16	0.46
4:E:66:VAL:HG22	4:E:69:ARG:HH21	1.81	0.46
5:F:161:LEU:C	5:F:262:VAL:HG23	2.41	0.46
5:F:384:LEU:HD22	5:F:409:ASN:ND2	2.31	0.46
5:F:524:GLU:O	5:F:524:GLU:HG3	2.16	0.46
1:G:29:GLU:O	1:G:199:ASP:O	2.34	0.46
1:H:88:LEU:HA	1:H:88:LEU:HD12	1.72	0.46
2:I:367:TYR:CE1	2:I:371:ARG:HD2	2.51	0.46
2:I:756:TYR:HD1	2:I:756:TYR:H	1.61	0.46
2:I:810:TYR:CE2	3:J:359:PRO:HG2	2.50	0.46
3:J:112:ALA:HA	3:J:238:ILE:CD1	2.46	0.46
3:J:474:LEU:HA	3:J:477:GLN:HG3	1.97	0.46
3:J:740:LEU:HD12	3:J:740:LEU:HA	1.54	0.46
3:J:827:GLU:O	3:J:829:GLY:N	2.34	0.46
3:J:1219:ASP:O	3:J:1220:ILE:C	2.58	0.46
5:L:139:GLU:CG	5:L:351:THR:HA	2.44	0.46
5:L:518:HIS:O	5:L:519:LEU:C	2.58	0.46
1:A:60:GLU:OE1	1:A:143:ARG:NE	2.38	0.46
1:A:181:GLU:HB3	1:A:206:GLU:HG3	1.98	0.46
2:C:525:THR:HG21	2:C:687:ARG:CD	2.42	0.46
3:D:211:GLU:OE2	3:D:214:ARG:NH1	2.48	0.46
3:D:362:ARG:HA	3:D:626:TYR:OH	2.15	0.46
3:D:441:LEU:HA	3:D:441:LEU:HD13	1.63	0.46
5:F:396:ASN:C	5:F:398:GLY:N	2.74	0.46
2:I:421:SER:O	2:I:424:ASP:N	2.47	0.46
2:I:596:ASP:CG	2:I:597:GLY:H	2.23	0.46
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.81	0.46
3:J:865:HIS:ND1	3:J:867:GLN:HB2	2.31	0.46
5:L:119:ILE:O	5:L:122:ARG:HB2	2.16	0.46
5:L:513:ASP:C	5:L:515:GLU:H	2.24	0.46
1:A:75:GLN:HG3	1:A:76:GLU:OE2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:896:THR:HB	2:C:897:PRO:HD2	1.96	0.45
3:D:530:PRO:O	3:D:531:LYS:C	2.57	0.45
3:D:615:LYS:HB2	3:D:616:PRO:HD3	1.98	0.45
3:D:859:PRO:HG2	3:D:862:THR:HG21	1.98	0.45
4:E:40:PRO:O	4:E:52:ARG:NH2	2.49	0.45
1:G:187:VAL:HG22	1:G:201:LEU:HD13	1.98	0.45
1:H:99:ILE:HA	1:H:144:ILE:O	2.17	0.45
2:I:28:LEU:HD21	2:I:524:ILE:HG13	1.97	0.45
2:I:517:GLN:O	2:I:518:ASN:C	2.60	0.45
2:I:886:LYS:O	2:I:916:SER:N	2.48	0.45
2:I:1291:LEU:HD21	3:J:1351:VAL:HG13	1.98	0.45
3:J:147:ILE:HD11	3:J:179:LYS:NZ	2.31	0.45
3:J:165:TYR:CE2	3:J:169:LEU:HD12	2.51	0.45
3:J:886:VAL:HA	3:J:1258:ARG:HB2	1.98	0.45
3:J:899:TYR:O	3:J:1251:LYS:HD3	2.16	0.45
3:J:1297:LYS:NZ	3:J:1299:GLY:HA3	2.30	0.45
4:K:26:ARG:NH2	4:K:36:ASP:O	2.49	0.45
5:L:399:LEU:HD12	5:L:399:LEU:HA	1.63	0.45
5:L:532:LEU:H	5:L:532:LEU:HD12	1.81	0.45
2:C:120:GLN:CG	2:C:121:GLU:HG3	2.36	0.45
2:C:273:HIS:HA	2:C:276:GLN:OE1	2.15	0.45
2:C:448:LEU:HD23	2:C:448:LEU:HA	1.75	0.45
2:C:883:LEU:HA	2:C:883:LEU:HD23	1.73	0.45
3:D:796:LEU:HG	3:D:800:LEU:HD22	1.99	0.45
1:H:149:GLY:HA3	1:H:177:TYR:CD2	2.51	0.45
2:I:97:ARG:HB3	2:I:121:GLU:CB	2.46	0.45
2:I:598:VAL:HG13	2:I:628:HIS:CE1	2.51	0.45
2:I:972:PHE:CE2	2:I:998:LEU:HD11	2.50	0.45
2:I:1012:GLU:HG3	2:I:1016:GLU:OE2	2.16	0.45
3:J:97:VAL:HG12	3:J:101:ARG:HG3	1.98	0.45
3:J:349:TYR:CE1	3:J:472:LEU:HD11	2.51	0.45
3:J:368:LEU:HD23	3:J:368:LEU:C	2.41	0.45
3:J:381:ILE:HG21	3:J:401:VAL:HG11	1.97	0.45
1:A:261:GLU:OE2	2:C:859:GLU:HB2	2.17	0.45
2:C:74:ARG:O	2:C:96:LEU:HD12	2.16	0.45
2:C:178:PRO:HB3	2:C:395:TYR:CZ	2.52	0.45
2:C:699:LEU:HD23	2:C:699:LEU:HA	1.40	0.45
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.98	0.45
3:D:112:ALA:HB3	3:D:300:GLN:NE2	2.31	0.45
3:D:612:LEU:HB3	3:D:616:PRO:HG2	1.97	0.45
3:D:689:ALA:O	3:D:692:ARG:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:875:ASN:OD1	3:D:875:ASN:N	2.49	0.45
3:D:1258:ARG:NH2	3:D:1281:GLU:OE1	2.48	0.45
3:D:1291:GLU:C	3:D:1292:LEU:HD12	2.41	0.45
2:I:421:SER:HG	2:I:424:ASP:CG	2.24	0.45
2:I:488:MET:HE3	2:I:488:MET:HB2	1.70	0.45
2:I:504:GLU:OE2	2:I:508:SER:HB2	2.16	0.45
2:I:538:LEU:HA	2:I:542:ARG:NE	2.31	0.45
2:I:758:ARG:HH22	2:I:761:GLN:HE21	1.63	0.45
2:I:1273:MET:HE3	2:I:1273:MET:HB2	1.81	0.45
3:J:275:ARG:HD3	3:J:298:MET:HB3	1.97	0.45
1:B:152:TYR:CE1	1:B:176:CYS:HB3	2.52	0.45
1:B:205:MET:HE2	1:B:205:MET:HB3	1.62	0.45
2:C:400:VAL:H	2:C:400:VAL:HG23	1.46	0.45
2:C:720:ARG:NH2	2:C:736:VAL:HG21	2.31	0.45
3:D:184:ALA:O	3:D:187:ALA:HB3	2.17	0.45
3:D:317:THR:CG2	3:D:320:ASN:HB3	2.42	0.45
3:D:810:THR:HG22	3:D:893:GLY:HA3	1.98	0.45
3:D:1356:LEU:HA	3:D:1356:LEU:HD23	1.40	0.45
1:G:152:TYR:CD2	2:I:824:GLN:HG2	2.52	0.45
2:I:228:VAL:HG22	2:I:245:ARG:HE	1.80	0.45
2:I:397:LEU:HD12	2:I:397:LEU:H	1.81	0.45
2:I:798:GLN:OE1	2:I:828:PHE:HD1	1.99	0.45
2:I:1159:VAL:HB	2:I:1160:ASP:H	1.58	0.45
2:I:1281:TYR:OH	3:J:431:ARG:O	2.33	0.45
3:J:1262:ARG:HD2	3:J:1279:GLN:HE22	1.81	0.45
5:L:143:TYR:OH	5:L:265:GLN:OE1	2.12	0.45
5:L:357:GLN:H	5:L:357:GLN:HG3	1.52	0.45
5:L:470:MET:HA	5:L:473:GLU:HB3	1.98	0.45
5:L:577:GLY:O	5:L:581:ASP:N	2.50	0.45
1:A:233:ASP:O	1:A:234:LEU:HD13	2.17	0.45
1:B:84:ASN:ND2	1:B:129:VAL:O	2.45	0.45
2:C:5:TYR:CZ	2:C:776:PRO:HB2	2.51	0.45
2:C:1030:GLU:OE1	2:C:1033:ARG:NH2	2.50	0.45
2:C:1172:LEU:C	2:C:1172:LEU:HD22	2.42	0.45
3:D:127:LEU:HD12	3:D:127:LEU:HA	1.46	0.45
3:D:282:LEU:HA	3:D:282:LEU:HD23	1.52	0.45
3:D:372:MET:HE1	3:D:468:VAL:HG21	1.97	0.45
3:D:1140:ARG:NH2	3:D:1144:LEU:HD21	2.31	0.45
5:F:466:ILE:CD1	5:F:487:MET:HE3	2.41	0.45
1:H:60:GLU:OE2	1:H:143:ARG:NH1	2.50	0.45
1:H:105:SER:HB3	1:H:137:ASN:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:952:GLN:OE1	2:I:1036:ILE:HG23	2.16	0.45
3:J:585:LYS:HD3	3:J:585:LYS:HA	1.68	0.45
3:J:859:PRO:HG2	3:J:862:THR:HG21	1.97	0.45
5:L:419:PHE:CD1	5:L:430:TYR:CD2	3.05	0.45
5:L:533:ASP:O	5:L:536:THR:N	2.49	0.45
1:A:197:ASP:O	1:A:198:LEU:HD23	2.17	0.45
2:C:5:TYR:HD1	2:C:8:LYS:HD3	1.82	0.45
2:C:388:LEU:HD23	2:C:388:LEU:HA	1.72	0.45
2:C:738:GLU:HA	2:C:741:MET:HE2	1.98	0.45
2:C:1035:LYS:O	2:C:1038:GLN:HG2	2.17	0.45
3:D:107:LEU:HD22	3:D:299:LEU:HD21	1.98	0.45
3:D:205:LEU:C	3:D:205:LEU:HD13	2.41	0.45
3:D:285:LEU:HD12	3:D:285:LEU:N	2.32	0.45
3:D:471:PRO:HG2	3:D:471:PRO:O	2.16	0.45
3:D:846:GLU:HA	3:D:860:ARG:HD3	1.97	0.45
3:D:1233:ILE:O	3:D:1234:VAL:C	2.58	0.45
5:F:127:ILE:O	5:F:128:ASN:C	2.58	0.45
5:F:234:THR:HG21	5:F:248:GLU:OE2	2.16	0.45
5:F:309:ASN:HD21	5:F:312:SER:HB3	1.81	0.45
5:F:311:THR:HG21	5:F:348:GLU:OE2	2.17	0.45
1:G:154:PRO:HB3	2:I:1059:ARG:NH2	2.32	0.45
2:I:697:LYS:HE2	2:I:697:LYS:HB3	1.79	0.45
2:I:1068:GLY:HA3	2:I:1072:ASN:HD21	1.82	0.45
2:I:1212:LEU:O	2:I:1221:PHE:N	2.46	0.45
3:J:549:LYS:HE2	3:J:571:ASP:OD2	2.17	0.45
3:J:799:ARG:HB3	3:J:1309:ILE:HD12	1.98	0.45
5:L:390:ILE:HG21	5:L:390:ILE:HD13	1.74	0.45
2:C:474:ALA:O	2:C:477:GLU:HB3	2.17	0.45
2:C:606:LEU:HD12	2:C:606:LEU:N	2.32	0.45
2:C:1161:LEU:HD12	2:C:1161:LEU:HA	1.26	0.45
3:D:24:LEU:HA	3:D:24:LEU:HD13	1.74	0.45
3:D:605:LEU:HA	3:D:605:LEU:HD23	1.77	0.45
3:D:819:GLY:O	3:D:1227:HIS:HE1	1.99	0.45
5:F:433:TRP:O	5:F:437:GLN:HB3	2.17	0.45
2:I:62:TYR:C	2:I:64:GLY:N	2.74	0.45
2:I:511:LEU:N	2:I:511:LEU:HD12	2.32	0.45
2:I:886:LYS:H	2:I:917:SER:HB3	1.82	0.45
2:I:967:LEU:HD12	2:I:967:LEU:HA	1.84	0.45
2:I:1077:SER:OG	2:I:1078:LYS:N	2.50	0.45
3:J:31:ARG:NH2	3:J:106:GLU:OE2	2.46	0.45
3:J:215:LYS:O	3:J:218:THR:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:521:LYS:NZ	3:J:540:GLY:O	2.24	0.45
4:K:36:ASP:HB2	4:K:37:PRO:HD2	1.99	0.45
5:L:519:LEU:C	5:L:519:LEU:HD23	2.42	0.45
1:B:9:LEU:HB3	1:B:32:GLU:HG2	1.99	0.45
2:C:22:LEU:HD22	2:C:22:LEU:HA	1.82	0.45
2:C:145:ILE:CG2	2:C:456:VAL:HG22	2.47	0.45
2:C:224:PHE:CG	2:C:347:ILE:HG13	2.52	0.45
2:C:1002:LEU:N	2:C:1008:GLN:OE1	2.49	0.45
2:C:1223:ARG:NH2	3:D:719:PHE:O	2.50	0.45
3:D:154:LEU:N	3:D:154:LEU:HD12	2.31	0.45
3:D:532:GLU:HA	3:D:535:ARG:HB3	1.98	0.45
3:D:740:LEU:HD12	3:D:740:LEU:HA	1.47	0.45
3:D:796:LEU:HD12	3:D:796:LEU:HA	1.61	0.45
3:D:836:ARG:HG3	3:D:869:CYS:HB3	1.98	0.45
5:F:364:ARG:HA	5:F:367:ILE:HD12	1.97	0.45
1:H:82:LEU:HD22	1:H:173:VAL:CG2	2.47	0.45
2:I:852:ALA:HB2	2:I:869:GLY:HA2	1.98	0.45
3:J:93:THR:HG22	3:J:94:GLN:N	2.31	0.45
3:J:450:HIS:HE1	3:J:452:LEU:HG	1.82	0.45
3:J:701:LEU:HD22	3:J:701:LEU:HA	1.57	0.45
5:L:96:ASP:O	5:L:98:VAL:N	2.49	0.45
1:A:85:LEU:O	1:A:86:LYS:C	2.58	0.45
2:C:60:GLN:H	2:C:60:GLN:HG2	1.31	0.45
2:C:159:SER:O	2:C:160:ASP:HB2	2.16	0.45
2:C:445:ILE:HG22	2:C:446:ASP:OD1	2.16	0.45
2:C:697:LYS:HB3	2:C:697:LYS:HE2	1.40	0.45
2:C:1246:ARG:CZ	2:C:1249:GLY:H	2.30	0.45
3:D:143:SER:C	3:D:180:MET:HE3	2.42	0.45
3:D:371:LYS:O	3:D:372:MET:C	2.54	0.45
3:D:508:LEU:HD12	3:D:508:LEU:HA	1.62	0.45
3:D:544:LEU:HA	3:D:544:LEU:HD12	1.57	0.45
3:D:622:ASP:HB3	3:D:626:TYR:CE2	2.51	0.45
3:D:630:ALA:O	3:D:633:ALA:HB3	2.17	0.45
3:D:820:ILE:HG22	3:D:1227:HIS:ND1	2.32	0.45
5:F:502:LYS:HE3	5:F:502:LYS:HB2	1.40	0.45
1:G:41:ASN:HD22	1:H:41:ASN:ND2	2.09	0.45
1:G:68:TYR:CE1	2:I:929:ILE:HG21	2.50	0.45
1:G:89:ALA:HB3	1:G:124:VAL:HG12	1.99	0.45
1:G:110:VAL:CG2	1:G:133:LEU:HD23	2.47	0.45
1:G:135:ASP:OD1	1:G:136:GLU:N	2.50	0.45
2:I:496:LYS:C	2:I:496:LYS:HD2	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:968:GLU:CG	2:I:1018:TYR:HE1	2.29	0.45
3:J:1337:VAL:HG23	3:J:1338:ALA:N	2.32	0.45
4:K:26:ARG:NE	4:K:53:GLU:OE1	2.49	0.45
5:L:507:MET:HG2	5:L:520:GLY:CA	2.47	0.45
1:A:132:HIS:CD2	1:A:132:HIS:N	2.84	0.45
2:C:104:ILE:HD12	2:C:115:LYS:O	2.16	0.45
2:C:325:LEU:O	2:C:330:HIS:HB2	2.17	0.45
2:C:447:HIS:CE1	2:C:553:THR:HG21	2.51	0.45
2:C:850:ILE:HG23	2:C:850:ILE:HD12	1.54	0.45
3:D:707:ILE:N	3:D:714:GLU:O	2.48	0.45
1:G:23:HIS:ND1	1:G:206:GLU:HG2	2.31	0.45
1:G:27:THR:C	1:G:28:LEU:HD12	2.42	0.45
1:G:37:HIS:HB3	1:H:45:ARG:NH2	2.31	0.45
1:G:57:THR:HG22	1:G:58:GLU:HG2	1.99	0.45
2:I:1164:PHE:N	2:I:1168:GLU:OE1	2.49	0.45
3:J:438:GLU:OE2	3:J:481:ARG:NH2	2.34	0.45
1:A:89:ALA:HB3	1:A:125:LYS:HD2	1.99	0.44
1:A:227:GLN:HE22	1:B:9:LEU:C	2.23	0.44
1:B:100:LEU:HG	1:B:118:ASP:OD2	2.18	0.44
1:B:196:THR:HG23	3:D:443:GLU:CG	2.47	0.44
2:C:102:LEU:O	2:C:116:ASP:HA	2.17	0.44
2:C:230:PHE:O	2:C:332:ARG:HA	2.17	0.44
3:D:45:ASN:O	3:D:46:TYR:CD2	2.70	0.44
3:D:385:LEU:HA	3:D:385:LEU:HD23	1.78	0.44
3:D:474:LEU:HD23	4:E:28:ARG:HG2	1.99	0.44
3:D:484:MET:HB3	3:D:484:MET:HE2	1.65	0.44
3:D:704:GLU:O	3:D:706:VAL:HG22	2.16	0.44
3:D:854:ALA:HB2	3:J:1372:ARG:HE	1.81	0.44
3:D:907:HIS:CE1	4:E:11:GLU:OE2	2.70	0.44
3:D:1165:PHE:HD2	3:D:1173:ARG:CD	2.30	0.44
3:D:1278:GLU:OE1	3:D:1278:GLU:HA	2.16	0.44
1:H:65:LEU:O	1:H:171:LEU:HD11	2.18	0.44
3:J:645:VAL:HB	3:J:701:LEU:HD23	1.99	0.44
3:J:749:LYS:HD3	3:J:753:SER:HB2	1.98	0.44
3:J:814:CYS:HB3	3:J:890:THR:OG1	2.17	0.44
3:J:839:VAL:O	3:J:839:VAL:HG12	2.16	0.44
3:J:839:VAL:HG12	3:J:864:LEU:HD12	1.98	0.44
3:J:1266:ILE:H	3:J:1266:ILE:HG13	1.42	0.44
3:J:1280:VAL:CG1	3:J:1304:ARG:HE	2.30	0.44
5:L:405:ILE:HD13	5:L:405:ILE:HG21	1.43	0.44
5:L:446:GLN:HE21	5:L:446:GLN:HB3	1.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LEU:O	1:A:31:LEU:CD1	2.66	0.44
1:A:233:ASP:OD2	1:A:233:ASP:N	2.30	0.44
1:A:250:ASP:OD2	5:F:605:GLU:HA	2.17	0.44
1:B:147:GLN:HG3	1:B:148:ARG:H	1.81	0.44
2:C:150:HIS:CG	2:C:454:ARG:HH21	2.35	0.44
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.99	0.44
2:C:484:LEU:CD1	2:C:485:ASP:H	2.30	0.44
2:C:1262:LYS:HD3	2:C:1262:LYS:HA	1.64	0.44
3:D:665:GLN:HG3	3:D:669:GLN:NE2	2.32	0.44
3:D:845:ALA:CB	3:D:881:LYS:HD2	2.47	0.44
3:D:903:LEU:HD13	3:D:909:ILE:HD13	1.99	0.44
5:F:561:MET:HA	5:F:567:MET:HE1	1.98	0.44
1:G:77:ASP:O	1:G:81:ILE:HG13	2.17	0.44
1:H:31:LEU:HA	1:H:31:LEU:HD13	1.67	0.44
2:I:98:VAL:CG2	2:I:124:MET:HE3	2.48	0.44
2:I:389:PHE:CD2	2:I:389:PHE:N	2.85	0.44
2:I:478:ARG:HG2	2:I:492:MET:HG2	2.00	0.44
2:I:483:ASP:HB2	2:I:486:THR:CG2	2.48	0.44
2:I:1176:LEU:HD13	2:I:1180:MET:HG2	2.00	0.44
3:J:266:ASN:O	3:J:267:ASP:C	2.57	0.44
3:J:269:TYR:O	3:J:273:ILE:HG13	2.16	0.44
3:J:283:LEU:HD23	3:J:283:LEU:HA	1.67	0.44
3:J:388:ARG:HB2	3:J:390:LEU:HD13	2.00	0.44
3:J:744:ARG:O	3:J:759:ILE:HB	2.17	0.44
1:B:217:ILE:O	1:B:218:ARG:C	2.61	0.44
2:C:39:ILE:HG23	2:C:39:ILE:O	2.18	0.44
2:C:496:LYS:HE3	2:C:496:LYS:HB3	1.48	0.44
2:C:1087:TYR:HE1	2:C:1215:GLY:HA2	1.81	0.44
3:D:113:HIS:CE1	3:D:307:LEU:HD13	2.52	0.44
3:D:241:VAL:HG12	3:D:242:LEU:N	2.32	0.44
3:D:325:LYS:HG3	3:D:329:ASP:HB2	2.00	0.44
3:D:664:ILE:HG23	3:D:664:ILE:HD12	1.74	0.44
3:D:1151:LYS:O	3:D:1153:PRO:HD3	2.18	0.44
3:D:1216:ALA:HB1	3:D:1218:HIS:HD2	1.81	0.44
3:D:1279:GLN:H	3:D:1279:GLN:HG2	1.60	0.44
3:D:1322:ALA:HB1	3:D:1326:GLN:NE2	2.32	0.44
5:F:269:LEU:HA	5:F:269:LEU:HD23	1.60	0.44
1:G:101:THR:O	1:G:103:ASN:ND2	2.50	0.44
2:I:44:GLU:HA	2:I:54:ARG:HH12	1.81	0.44
2:I:338:THR:HG22	2:I:345:PRO:HB3	1.99	0.44
3:J:264:ASP:N	3:J:264:ASP:OD2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:349:TYR:CE2	3:J:379:PRO:HG2	2.48	0.44
3:J:480:ALA:O	3:J:485:MET:N	2.50	0.44
3:J:749:LYS:HG2	3:J:753:SER:O	2.18	0.44
3:J:1165:PHE:HD2	3:J:1173:ARG:NE	2.14	0.44
3:J:1251:LYS:O	3:J:1252:HIS:C	2.61	0.44
5:L:157:ARG:CZ	5:L:159:SER:OG	2.65	0.44
1:A:285:THR:HG23	1:A:288:GLU:H	1.83	0.44
1:A:292:THR:OG1	1:A:295:LEU:HD12	2.17	0.44
2:C:98:VAL:HG21	2:C:124:MET:HE3	1.99	0.44
2:C:1136:GLN:NE2	2:C:1140:LYS:HZ3	2.13	0.44
2:C:1276:TRP:CZ2	3:D:801:VAL:HG21	2.52	0.44
3:D:102:MET:HE2	3:D:102:MET:HB3	1.52	0.44
3:D:184:ALA:O	3:D:188:LEU:N	2.42	0.44
3:D:274:ASN:O	3:D:275:ARG:C	2.60	0.44
3:D:1270:GLY:O	3:D:1298:VAL:HG11	2.17	0.44
1:G:20:SER:O	1:G:21:SER:C	2.59	0.44
1:G:37:HIS:HB3	1:H:45:ARG:CZ	2.47	0.44
1:G:65:LEU:CD2	1:G:65:LEU:N	2.80	0.44
2:I:15:PHE:CD2	2:I:1190:ALA:HB2	2.51	0.44
2:I:22:LEU:HD22	2:I:22:LEU:HA	1.74	0.44
2:I:386:GLU:HA	2:I:390:PHE:HD2	1.81	0.44
2:I:496:LYS:HB3	2:I:496:LYS:HE3	1.81	0.44
2:I:746:ALA:HA	2:I:974:ARG:HH21	1.82	0.44
2:I:1211:ARG:HE	2:I:1220:GLN:NE2	2.15	0.44
3:J:396:ALA:O	3:J:400:MET:HG3	2.18	0.44
3:J:1257:VAL:HG22	3:J:1260:MET:HE2	1.98	0.44
1:A:73:GLY:C	1:A:134:THR:HG22	2.42	0.44
1:B:33:ARG:NH1	2:C:1081:PRO:HG3	2.32	0.44
1:B:46:ILE:O	1:B:47:LEU:C	2.59	0.44
2:C:541:GLU:H	2:C:541:GLU:CD	2.22	0.44
2:C:694:ARG:HB2	2:C:798:GLN:NE2	2.33	0.44
2:C:797:GLY:C	2:C:1231:TYR:CE1	2.96	0.44
2:C:815:SER:HB3	2:C:1077:SER:HB3	2.00	0.44
3:D:161:THR:HG22	3:D:164:GLN:CD	2.42	0.44
3:D:606:ASN:OD1	3:D:610:ARG:NE	2.51	0.44
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.98	0.44
3:D:1268:ASN:HB2	3:D:1301:THR:OG1	2.17	0.44
5:F:557:LYS:O	5:F:561:MET:HB2	2.18	0.44
1:G:60:GLU:CD	1:G:143:ARG:HH12	2.26	0.44
2:I:42:ASP:OD2	2:I:44:GLU:HG2	2.18	0.44
2:I:69:GLN:HE21	2:I:101:ARG:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:82:VAL:HG22	2:I:92:TYR:CZ	2.51	0.44
2:I:188:PHE:CE1	2:I:194:LEU:HD13	2.53	0.44
2:I:211:ARG:HD3	2:I:357:ASN:O	2.17	0.44
2:I:429:MET:HE2	2:I:429:MET:HB3	1.82	0.44
2:I:558:VAL:HG13	2:I:573:ASN:HB3	1.98	0.44
2:I:805:MET:HE3	2:I:805:MET:HB2	1.88	0.44
3:J:24:LEU:HA	3:J:24:LEU:HD13	1.51	0.44
5:L:151:VAL:HG11	5:L:158:LEU:CD2	2.47	0.44
1:A:93:GLN:HB2	1:A:120:ASP:OD2	2.18	0.44
1:A:118:ASP:OD2	1:A:119:GLY:N	2.50	0.44
2:C:616:ILE:O	2:C:636:CYS:HB3	2.17	0.44
2:C:833:ILE:HD13	2:C:929:ILE:HD11	2.00	0.44
2:C:1253:LEU:HD22	2:C:1253:LEU:C	2.43	0.44
3:D:355:ILE:O	3:D:355:ILE:HG13	2.18	0.44
3:D:372:MET:HE2	3:D:372:MET:HB3	1.59	0.44
3:D:434:ILE:HG21	3:D:434:ILE:HD13	1.71	0.44
3:D:767:LEU:HD12	3:D:767:LEU:N	2.32	0.44
3:D:1219:ASP:O	3:D:1220:ILE:C	2.59	0.44
5:F:383:ASN:HB2	5:F:412:LEU:HD21	2.00	0.44
1:G:61:ILE:CG1	1:G:171:LEU:HD23	2.48	0.44
2:I:158:ASP:CG	2:I:159:SER:N	2.76	0.44
2:I:209:ILE:O	2:I:212:ALA:N	2.51	0.44
2:I:607:SER:N	2:I:610:GLU:HB2	2.33	0.44
2:I:670:PHE:CE2	2:I:1113:LEU:HB3	2.52	0.44
2:I:1011:LEU:O	2:I:1015:ALA:N	2.43	0.44
3:J:395:LYS:HE2	5:L:536:THR:HG21	2.00	0.44
3:J:1289:ASN:OD1	3:J:1290:ARG:CZ	2.66	0.44
2:C:1117:LEU:HD21	2:C:1182:ILE:HD12	2.00	0.44
2:C:1240:ASP:HB3	3:D:445:LYS:CD	2.43	0.44
3:D:139:LEU:HA	3:D:139:LEU:HD23	1.42	0.44
3:D:515:ARG:HH21	3:D:717:VAL:HG23	1.83	0.44
3:D:1290:ARG:HA	3:D:1290:ARG:HD3	1.81	0.44
5:F:295:CYS:SG	5:F:333:VAL:HB	2.58	0.44
5:F:561:MET:HB2	5:F:561:MET:HE3	1.67	0.44
2:I:1220:GLN:HG2	2:I:1221:PHE:N	2.33	0.44
3:J:19:ALA:HA	3:J:1344:LEU:HD12	1.98	0.44
3:J:75:TYR:N	3:J:75:TYR:CD1	2.86	0.44
3:J:308:ASP:CG	3:J:311:ARG:HE	2.25	0.44
3:J:452:LEU:HA	3:J:452:LEU:HD23	1.73	0.44
3:J:490:ILE:HG21	3:J:490:ILE:HD13	1.69	0.44
3:J:682:VAL:HA	3:J:685:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:770:LEU:HA	3:J:770:LEU:HD12	1.66	0.44
5:L:95:THR:O	5:L:96:ASP:C	2.61	0.44
1:A:118:ASP:CG	1:A:119:GLY:N	2.76	0.44
1:A:179:PRO:O	1:A:207:THR:HG23	2.17	0.44
2:C:33:ASP:O	2:C:34:SER:C	2.60	0.44
2:C:49:LEU:HB2	2:C:73:TYR:OH	2.17	0.44
2:C:247:ARG:HH21	2:C:274:ILE:HG21	1.83	0.44
2:C:1253:LEU:HD13	2:C:1254:VAL:N	2.33	0.44
3:D:113:HIS:O	3:D:114:ILE:C	2.59	0.44
3:D:141:PHE:C	3:D:180:MET:HE2	2.42	0.44
5:F:127:ILE:O	5:F:130:VAL:N	2.51	0.44
5:F:412:LEU:HA	5:F:412:LEU:HD12	1.73	0.44
5:F:474:MET:HE3	5:F:474:MET:HB3	1.92	0.44
5:F:511:ILE:O	5:F:511:ILE:HG23	2.17	0.44
1:G:96:ASP:O	1:G:148:ARG:HG3	2.18	0.44
1:H:103:ASN:HA	1:H:141:SER:CB	2.47	0.44
2:I:277:LEU:O	2:I:281:ASP:N	2.51	0.44
2:I:367:TYR:CD2	2:I:376:PRO:HA	2.52	0.44
2:I:532:ALA:HB1	2:I:538:LEU:HD11	2.00	0.44
2:I:614:TYR:CD1	2:I:652:TYR:CE1	3.05	0.44
2:I:953:LEU:HD12	2:I:953:LEU:HA	1.56	0.44
2:I:971:LEU:CD2	2:I:1018:TYR:HB2	2.48	0.44
2:I:980:VAL:O	2:I:984:VAL:HB	2.17	0.44
3:J:860:ARG:HB3	3:J:861:ASN:H	1.68	0.44
3:J:1149:ARG:CZ	3:J:1153:PRO:HG2	2.48	0.44
3:J:1332:LEU:HD13	3:J:1332:LEU:HA	1.77	0.44
5:L:166:VAL:HG23	5:L:258:GLN:O	2.18	0.44
5:L:220:LYS:O	5:L:223:GLU:HB3	2.18	0.44
5:L:484:ALA:HB1	5:L:491:GLU:CG	2.48	0.44
1:B:183:ILE:O	1:B:183:ILE:HD12	2.18	0.44
2:C:805:MET:HE1	2:C:1221:PHE:CZ	2.53	0.44
3:D:26:SER:HB3	3:D:29:MET:HB2	2.00	0.44
3:D:581:MET:HE2	3:D:581:MET:HB3	1.73	0.44
3:D:703:THR:HA	3:D:717:VAL:HA	2.00	0.44
5:F:227:GLN:CG	5:F:252:LEU:HA	2.48	0.44
5:F:253:SER:O	5:F:254:GLU:C	2.61	0.44
1:H:228:LEU:HA	1:H:228:LEU:HD23	1.59	0.44
2:I:361:SER:O	2:I:364:VAL:HB	2.18	0.44
2:I:494:ASN:ND2	2:I:497:PRO:HD3	2.33	0.44
2:I:796:LEU:HD12	2:I:796:LEU:N	2.33	0.44
2:I:1252:SER:HB3	2:I:1255:THR:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1287:LEU:O	2:I:1288:GLN:C	2.60	0.44
3:J:201:LEU:HD12	3:J:221:ILE:HD13	2.00	0.44
3:J:518:VAL:HG23	3:J:547:ARG:NH2	2.33	0.44
3:J:706:VAL:HG12	3:J:715:LYS:CB	2.46	0.44
3:J:797:THR:CG2	3:J:924:GLY:HA3	2.36	0.44
3:J:805:GLN:HB3	3:J:806:ASP:H	1.61	0.44
5:L:357:GLN:HA	5:L:360:ASP:HB2	1.99	0.44
5:L:384:LEU:HD23	5:L:384:LEU:HA	1.55	0.44
1:A:137:ASN:OD1	1:A:137:ASN:N	2.51	0.43
2:C:1195:ILE:HG21	2:C:1195:ILE:HD13	1.70	0.43
2:C:1223:ARG:HH11	2:C:1223:ARG:HD3	1.67	0.43
2:C:1336:ASN:HD21	2:C:1338:GLU:CD	2.26	0.43
3:D:381:ILE:HD13	3:D:381:ILE:HG21	1.67	0.43
3:D:1171:GLY:HA2	3:D:1193:TRP:CZ3	2.51	0.43
3:D:1257:VAL:O	3:D:1260:MET:N	2.51	0.43
3:D:1332:LEU:N	3:D:1332:LEU:HD22	2.32	0.43
3:D:1344:LEU:HD12	3:D:1344:LEU:N	2.33	0.43
5:F:584:ARG:HA	5:F:584:ARG:HH11	1.83	0.43
1:G:170:ARG:C	1:G:171:LEU:HD13	2.43	0.43
2:I:672:GLU:HG2	2:I:1187:PHE:HA	2.00	0.43
2:I:1158:LYS:C	2:I:1159:VAL:HG22	2.43	0.43
5:L:161:LEU:HA	5:L:161:LEU:HD12	1.68	0.43
1:B:181:GLU:OE2	1:B:208:ASN:HA	2.18	0.43
2:C:479:LEU:HA	2:C:479:LEU:HD23	1.73	0.43
2:C:490:GLN:HG3	5:F:472:GLN:CD	2.43	0.43
2:C:819:SER:HB2	2:C:1085:MET:SD	2.57	0.43
2:C:987:GLU:O	2:C:991:LYS:HG3	2.18	0.43
2:C:1142:ARG:HH22	2:C:1165:SER:HB2	1.81	0.43
3:D:400:MET:HE3	3:D:405:GLU:OE1	2.18	0.43
3:D:733:SER:O	3:D:736:GLN:N	2.50	0.43
3:D:1169:THR:OG1	3:D:1192:LYS:HD3	2.18	0.43
3:D:1375:ALA:HB1	3:J:853:THR:HG21	2.00	0.43
1:G:35:PHE:CE1	1:H:46:ILE:HG12	2.53	0.43
1:G:66:HIS:HB2	1:G:69:SER:OG	2.18	0.43
1:H:30:PRO:C	1:H:31:LEU:HD22	2.43	0.43
1:H:57:THR:OG1	1:H:147:GLN:HB3	2.17	0.43
2:I:42:ASP:CG	2:I:46:GLN:HB3	2.43	0.43
2:I:168:GLY:C	2:I:170:VAL:H	2.26	0.43
2:I:276:GLN:O	2:I:280:ASP:N	2.43	0.43
2:I:409:LEU:HD13	2:I:427:ASP:HB3	2.00	0.43
2:I:1087:TYR:OH	2:I:1218:GLY:HA2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1232:MET:HE2	2:I:1232:MET:HB3	1.76	0.43
2:I:1252:SER:HB3	2:I:1257:GLN:H	1.83	0.43
2:I:1268:GLN:HG2	3:J:467:ALA:HB1	2.00	0.43
2:I:1301:ARG:O	2:I:1304:MET:HB3	2.18	0.43
3:J:265:LEU:HA	3:J:265:LEU:HD23	1.67	0.43
3:J:474:LEU:O	3:J:475:GLU:C	2.60	0.43
3:J:1206:ARG:NH2	3:J:1223:LEU:HD13	2.34	0.43
5:L:251:LYS:HA	5:L:254:GLU:HG2	1.99	0.43
5:L:281:ARG:HA	5:L:284:GLU:OE1	2.18	0.43
1:A:165:GLU:C	1:A:167:PRO:HD2	2.43	0.43
1:B:44:ARG:HG3	1:B:183:ILE:HB	2.00	0.43
2:C:208:ILE:O	2:C:362:ALA:HB1	2.19	0.43
2:C:571:LEU:HA	2:C:571:LEU:HD23	1.66	0.43
2:C:1312:ASN:HD21	2:C:1314:GLN:HG3	1.83	0.43
3:D:474:LEU:HA	3:D:474:LEU:HD12	1.60	0.43
3:D:500:ILE:HG22	3:D:500:ILE:O	2.17	0.43
5:F:513:ASP:C	5:F:515:GLU:N	2.76	0.43
1:G:133:LEU:HA	1:G:133:LEU:HD13	1.79	0.43
2:I:22:LEU:HD13	2:I:23:ASP:N	2.34	0.43
2:I:387:ASN:O	2:I:394:ARG:HB2	2.19	0.43
2:I:455:SER:O	2:I:456:VAL:C	2.61	0.43
2:I:640:GLY:O	2:I:641:GLU:HG3	2.18	0.43
2:I:1267:GLY:HA3	3:J:347:VAL:O	2.18	0.43
3:J:1290:ARG:HA	3:J:1290:ARG:HD3	1.78	0.43
3:J:1357:ILE:O	3:J:1359:ALA:N	2.47	0.43
1:A:255:ARG:HD3	1:A:259:ASP:OD2	2.18	0.43
1:B:100:LEU:O	1:B:143:ARG:HA	2.18	0.43
3:D:255:LEU:N	3:D:259:ARG:O	2.48	0.43
3:D:298:MET:HE1	5:F:402:LEU:O	2.18	0.43
3:D:505:ASP:HB2	3:D:629:PHE:HE1	1.83	0.43
3:D:795:TYR:HE2	3:D:799:ARG:NE	2.15	0.43
3:D:891:ASP:CA	3:D:1281:GLU:HG3	2.47	0.43
3:D:910:ASN:ND2	4:E:15:ASN:O	2.50	0.43
3:D:1248:ILE:HG21	3:D:1248:ILE:HD13	1.75	0.43
3:D:1255:VAL:O	3:D:1256:ILE:C	2.59	0.43
3:D:1372:ARG:NE	3:J:854:ALA:HB2	2.33	0.43
5:F:552:THR:H	5:F:552:THR:HG23	1.59	0.43
2:I:158:ASP:HB3	2:I:173:ASN:OD1	2.18	0.43
2:I:538:LEU:HA	2:I:542:ARG:NH2	2.33	0.43
2:I:1287:LEU:O	2:I:1290:MET:N	2.51	0.43
3:J:35:PHE:HD1	3:J:101:ARG:HD3	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:75:TYR:CD2	3:J:83:VAL:HG21	2.54	0.43
3:J:268:LEU:HB3	3:J:306:LEU:HD23	2.00	0.43
3:J:1257:VAL:O	3:J:1260:MET:N	2.51	0.43
5:L:461:ASN:O	5:L:462:LYS:C	2.61	0.43
5:L:502:LYS:HE3	5:L:502:LYS:HB2	1.32	0.43
2:C:370:MET:HE3	2:C:370:MET:HB3	1.88	0.43
2:C:819:SER:HB2	2:C:1085:MET:HG3	2.00	0.43
2:C:1086:PRO:O	2:C:1094:VAL:HG12	2.18	0.43
2:C:1109:ILE:HD12	2:C:1109:ILE:HA	1.59	0.43
2:C:1196:LYS:CD	2:C:1206:THR:HG23	2.29	0.43
3:D:306:LEU:O	3:D:326:SER:HB2	2.18	0.43
3:D:425:ARG:NH1	3:D:464:ASP:CG	2.76	0.43
3:D:541:LEU:HA	3:D:541:LEU:HD23	1.44	0.43
5:F:306:PHE:CE1	5:F:315:TRP:CD2	3.00	0.43
5:F:472:GLN:CD	5:F:472:GLN:C	2.86	0.43
1:G:59:VAL:HG13	1:G:143:ARG:O	2.19	0.43
2:I:6:THR:HG21	2:I:782:VAL:HG23	1.99	0.43
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.53	0.43
2:I:607:SER:H	2:I:610:GLU:CD	2.26	0.43
2:I:619:ALA:HA	2:I:653:MET:HE3	1.99	0.43
2:I:1142:ARG:HH12	2:I:1169:VAL:HG21	1.81	0.43
3:J:41:PRO:HB3	3:J:270:ARG:HG3	2.00	0.43
3:J:385:LEU:HA	3:J:385:LEU:HD23	1.43	0.43
3:J:426:ALA:CB	3:J:427:PRO:HD3	2.44	0.43
5:L:611:LEU:HD23	5:L:611:LEU:HA	1.56	0.43
2:C:756:TYR:CD1	2:C:756:TYR:N	2.86	0.43
2:C:1101:LEU:HD23	2:C:1101:LEU:HA	1.58	0.43
2:C:1137:GLU:HG2	2:C:1140:LYS:CG	2.49	0.43
3:D:97:VAL:HG12	3:D:101:ARG:CG	2.45	0.43
3:D:278:ARG:HH11	3:D:295:GLU:CD	2.25	0.43
3:D:813:ASP:HA	3:D:897:HIS:HB2	2.01	0.43
3:D:1237:VAL:HG11	3:D:1253:ILE:HD13	2.00	0.43
5:F:103:ARG:HH11	5:F:103:ARG:HD3	1.64	0.43
1:G:47:LEU:O	1:G:180:VAL:HG11	2.19	0.43
2:I:1176:LEU:HD22	2:I:1181:PRO:HD2	2.00	0.43
3:J:118:LYS:HA	3:J:118:LYS:HD2	1.62	0.43
3:J:189:LEU:HD23	3:J:189:LEU:HA	1.77	0.43
2:C:88:ARG:HG2	2:C:90:VAL:CG2	2.49	0.43
2:C:409:LEU:HD23	2:C:409:LEU:HA	1.65	0.43
2:C:992:LEU:HG	2:C:997:TRP:HE1	1.84	0.43
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1239:VAL:HG13	2:C:1240:ASP:N	2.33	0.43
3:D:108:ALA:CB	3:D:279:LEU:HD22	2.49	0.43
3:D:108:ALA:HB3	3:D:279:LEU:HD22	1.99	0.43
3:D:647:PRO:HG3	3:D:697:MET:CB	2.47	0.43
3:D:717:VAL:H	3:D:717:VAL:HG22	1.54	0.43
3:D:755:ILE:HG22	3:D:757:THR:H	1.83	0.43
5:F:593:LYS:O	5:F:597:LYS:N	2.50	0.43
1:H:107:ILE:HG23	1:H:135:ASP:HA	1.99	0.43
2:I:156:PHE:CZ	2:I:445:ILE:HG13	2.54	0.43
2:I:690:VAL:HG12	2:I:1234:LYS:O	2.18	0.43
2:I:705:GLU:HB2	2:I:794:LEU:H	1.83	0.43
2:I:1087:TYR:CE1	2:I:1215:GLY:HA2	2.53	0.43
3:J:299:LEU:O	3:J:302:ALA:N	2.51	0.43
1:A:92:VAL:HA	1:A:120:ASP:O	2.18	0.43
2:C:13:LYS:HZ2	2:C:1149:TYR:HA	1.84	0.43
2:C:404:LYS:HD2	2:C:404:LYS:HA	1.75	0.43
2:C:544:GLY:O	2:C:548:ARG:HG3	2.19	0.43
2:C:551:HIS:CE1	2:C:553:THR:HG23	2.53	0.43
2:C:830:THR:HG22	2:C:1058:ARG:O	2.19	0.43
2:C:1113:LEU:O	2:C:1114:GLU:C	2.61	0.43
3:D:502:PRO:HB3	3:D:506:VAL:CG1	2.48	0.43
1:G:219:ARG:HH11	1:G:219:ARG:HD3	1.67	0.43
1:H:83:LEU:HD12	1:H:86:LYS:HE2	2.01	0.43
2:I:159:SER:O	2:I:171:LEU:O	2.37	0.43
2:I:818:VAL:O	2:I:1079:ILE:HA	2.19	0.43
3:J:143:SER:C	3:J:180:MET:HE3	2.43	0.43
3:J:1140:ARG:HH21	3:J:1236:GLU:CG	2.22	0.43
3:J:1171:GLY:HA2	3:J:1193:TRP:CZ3	2.35	0.43
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.99	0.43
5:L:383:ASN:O	5:L:384:LEU:C	2.62	0.43
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.49	0.43
5:L:576:VAL:HG12	5:L:587:ILE:CD1	2.49	0.43
1:A:102:LEU:HD23	1:A:115:ILE:HA	2.01	0.43
1:A:196:THR:OG1	1:A:197:ASP:N	2.50	0.43
1:A:320:ASN:O	1:A:323:PRO:HD3	2.18	0.43
2:C:120:GLN:HE21	2:C:120:GLN:HB2	1.64	0.43
2:C:469:VAL:O	2:C:472:GLU:HB3	2.18	0.43
2:C:760:ASN:O	2:C:761:GLN:O	2.37	0.43
2:C:1273:MET:HB2	2:C:1273:MET:HE3	1.83	0.43
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.52	0.43
2:C:1307:ASN:HB3	2:C:1312:ASN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:24:LEU:HB2	3:D:232:ASN:CG	2.44	0.43
3:D:341:ASN:HB2	3:D:1352:ILE:HD13	2.00	0.43
3:D:411:ILE:HD12	3:D:411:ILE:HG23	1.69	0.43
5:F:503:GLU:CG	5:F:504:PRO:HD2	2.48	0.43
1:G:152:TYR:CE2	2:I:824:GLN:HG2	2.54	0.43
2:I:518:ASN:O	2:I:519:ASN:HB3	2.18	0.43
2:I:598:VAL:HG22	2:I:628:HIS:CE1	2.54	0.43
2:I:1053:TYR:CD1	2:I:1053:TYR:N	2.87	0.43
2:I:1211:ARG:HB2	2:I:1220:GLN:HE21	1.83	0.43
3:J:343:LEU:HD12	3:J:343:LEU:HA	1.80	0.43
5:L:295:CYS:CB	5:L:330:LEU:HD23	2.49	0.43
1:A:92:VAL:HA	1:A:120:ASP:HB3	2.00	0.43
1:A:118:ASP:HB3	1:A:121:VAL:CG2	2.45	0.43
1:A:225:ALA:HA	1:A:228:LEU:HD12	2.00	0.43
2:C:517:GLN:O	2:C:517:GLN:HG2	2.16	0.43
2:C:979:LEU:HD12	2:C:979:LEU:HA	1.72	0.43
2:C:1042:LEU:HD13	2:C:1046:VAL:HG22	2.01	0.43
3:D:135:ILE:HG21	3:D:135:ILE:HD13	1.65	0.43
3:D:352:ARG:HB3	3:D:467:ALA:HA	2.01	0.43
3:D:748:ALA:HA	3:D:754:ILE:HA	2.00	0.43
3:D:848:VAL:HG23	3:D:858:VAL:HG13	2.01	0.43
3:D:905:ARG:HH12	4:E:10:VAL:HG11	1.82	0.43
3:D:908:ILE:HD13	3:D:909:ILE:N	2.34	0.43
3:D:1292:LEU:HA	3:J:1226:VAL:HG21	2.01	0.43
5:F:105:MET:HE2	5:F:105:MET:HB2	1.70	0.43
5:F:470:MET:HE3	5:F:470:MET:HB3	1.85	0.43
5:F:601:PRO:HA	5:F:604:SER:H	1.84	0.43
1:G:52:PRO:HG2	1:G:219:ARG:NE	2.29	0.43
1:H:82:LEU:HA	1:H:85:LEU:HD12	2.00	0.43
2:I:149:LEU:HA	2:I:149:LEU:HD12	1.62	0.43
2:I:1262:LYS:HA	2:I:1262:LYS:HD3	1.83	0.43
2:I:1331:ARG:HA	2:I:1335:ILE:O	2.19	0.43
2:I:1334:GLY:O	3:J:25:ALA:CB	2.66	0.43
3:J:364:HIS:CE1	3:J:365:GLN:OE1	2.72	0.43
3:J:1355:ARG:HE	3:J:1355:ARG:HB3	1.52	0.43
5:L:297:MET:HG2	5:L:298:PRO:N	2.31	0.43
1:A:257:VAL:HG22	1:A:276:HIS:O	2.19	0.42
1:A:270:LEU:HD23	1:A:270:LEU:HA	1.82	0.42
2:C:493:ILE:H	2:C:493:ILE:HG22	1.49	0.42
2:C:557:ARG:HH21	2:C:608:ALA:N	2.16	0.42
2:C:632:ASP:O	2:C:647:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:653:MET:HG2	2:C:654:ASP:N	2.34	0.42
2:C:870:ILE:HB	2:C:944:ARG:HD3	2.01	0.42
2:C:967:LEU:HD12	2:C:967:LEU:HA	1.48	0.42
2:C:1209:GLN:HA	2:C:1225:VAL:O	2.19	0.42
2:C:1268:GLN:HE22	3:D:352:ARG:HH11	1.65	0.42
3:D:93:THR:HG22	3:D:94:GLN:N	2.34	0.42
3:D:416:ILE:O	3:D:417:ARG:C	2.62	0.42
3:D:915:ILE:H	3:D:915:ILE:HG12	1.64	0.42
5:F:290:LEU:HB3	5:F:333:VAL:HG21	2.01	0.42
5:F:399:LEU:HA	5:F:399:LEU:HD12	1.32	0.42
5:F:599:ARG:C	5:F:604:SER:OG	2.62	0.42
2:I:607:SER:H	2:I:610:GLU:HB2	1.83	0.42
2:I:745:GLU:HG3	2:I:1017:GLN:HB3	2.01	0.42
2:I:1038:GLN:O	2:I:1038:GLN:HG3	2.19	0.42
2:I:1276:TRP:CZ2	3:J:801:VAL:HG21	2.54	0.42
3:J:26:SER:HB2	3:J:236:TRP:CZ2	2.53	0.42
3:J:182:ALA:O	3:J:183:GLU:C	2.61	0.42
3:J:495:ASN:N	3:J:495:ASN:OD1	2.52	0.42
3:J:1262:ARG:O	3:J:1280:VAL:HG23	2.19	0.42
4:K:50:ALA:O	4:K:54:ILE:HG12	2.19	0.42
5:L:123:ILE:HD13	5:L:123:ILE:HG21	1.80	0.42
5:L:341:LEU:O	5:L:344:LEU:HB3	2.19	0.42
5:L:350:GLU:H	5:L:350:GLU:HG3	1.54	0.42
5:L:354:THR:O	5:L:358:VAL:HG23	2.19	0.42
2:C:235:ASN:OD1	2:C:236:LYS:HG2	2.19	0.42
2:C:263:VAL:HG12	2:C:264:GLU:O	2.19	0.42
2:C:490:GLN:O	2:C:492:MET:N	2.52	0.42
2:C:591:TYR:CE1	2:C:616:ILE:HG21	2.54	0.42
3:D:322:ARG:HB2	3:D:322:ARG:CZ	2.48	0.42
5:F:105:MET:SD	5:F:105:MET:C	3.02	0.42
5:F:227:GLN:NE2	5:F:251:LYS:NZ	2.66	0.42
5:F:597:LYS:O	5:F:603:ARG:HG3	2.19	0.42
5:F:611:LEU:HA	5:F:611:LEU:HD23	1.82	0.42
2:I:161:LYS:H	2:I:161:LYS:HG2	1.63	0.42
2:I:194:LEU:HD12	2:I:194:LEU:HA	1.80	0.42
2:I:515:MET:O	2:I:515:MET:CG	2.67	0.42
2:I:798:GLN:NE2	2:I:827:ARG:O	2.49	0.42
2:I:894:GLN:HG3	2:I:894:GLN:O	2.18	0.42
2:I:1210:ILE:HG22	2:I:1211:ARG:H	1.84	0.42
3:J:647:PRO:HG3	3:J:697:MET:N	2.34	0.42
3:J:903:LEU:HD12	3:J:903:LEU:HA	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1366:HIS:O	3:J:1367:GLN:C	2.62	0.42
5:L:271:ASN:O	5:L:275:VAL:HG23	2.19	0.42
5:L:572:THR:HG23	5:L:575:GLU:CB	2.43	0.42
2:C:189:ASP:CG	2:C:191:LYS:H	2.27	0.42
2:C:397:LEU:C	2:C:398:SER:HG	2.24	0.42
3:D:528:THR:HG23	3:D:529:GLY:N	2.35	0.42
3:D:544:LEU:O	3:D:574:VAL:HB	2.19	0.42
3:D:647:PRO:CG	3:D:697:MET:HB3	2.50	0.42
3:D:825:VAL:HG22	3:D:833:GLU:N	2.35	0.42
3:D:1306:LEU:C	3:D:1307:LEU:HD12	2.45	0.42
5:F:101:TYR:O	5:F:102:MET:C	2.62	0.42
5:F:560:ARG:O	5:F:563:PHE:O	2.37	0.42
2:I:315:MET:HE3	2:I:315:MET:HB2	1.94	0.42
2:I:643:SER:HG	2:I:645:PHE:HE1	1.68	0.42
2:I:757:THR:OG1	2:I:758:ARG:N	2.52	0.42
2:I:964:LEU:HD22	2:I:1025:PHE:CG	2.55	0.42
2:I:1308:ILE:HD12	3:J:380:PHE:CZ	2.53	0.42
3:J:127:LEU:HD12	3:J:127:LEU:HA	1.47	0.42
3:J:317:THR:HG22	3:J:322:ARG:O	2.19	0.42
3:J:438:GLU:HA	3:J:439:PRO:HD3	1.86	0.42
3:J:596:LEU:HD12	3:J:601:ILE:HG13	2.01	0.42
3:J:1205:GLU:O	3:J:1208:ASP:HB2	2.19	0.42
5:L:165:PHE:HD1	5:L:259:PHE:HA	1.84	0.42
5:L:245:ALA:C	5:L:249:ILE:HG13	2.45	0.42
1:A:187:VAL:HG23	1:A:187:VAL:O	2.20	0.42
1:A:212:ASP:HA	1:A:213:PRO:HD3	1.93	0.42
2:C:1067:ALA:HB2	2:C:1073:LYS:HA	2.00	0.42
2:C:1275:VAL:O	2:C:1276:TRP:C	2.57	0.42
3:D:707:ILE:O	3:D:714:GLU:N	2.52	0.42
3:D:1238:GLN:O	3:D:1239:ASP:C	2.62	0.42
5:F:463:LEU:HD23	5:F:463:LEU:HA	1.80	0.42
1:G:12:ARG:HA	1:H:231:PHE:HZ	1.81	0.42
1:H:51:MET:HB3	1:H:178:SER:CB	2.50	0.42
2:I:146:VAL:HG13	2:I:529:ARG:HB3	2.01	0.42
2:I:230:PHE:HE1	2:I:287:VAL:HG21	1.85	0.42
2:I:388:LEU:HD23	2:I:388:LEU:HA	1.76	0.42
2:I:735:LYS:HA	2:I:748:ILE:HG22	2.02	0.42
2:I:920:VAL:HG13	2:I:1054:LEU:HD21	2.01	0.42
2:I:1225:VAL:HA	3:J:638:SER:CB	2.49	0.42
3:J:294:ASN:HD22	5:L:406:GLN:NE2	2.18	0.42
3:J:810:THR:HG23	3:J:811:GLU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:853:THR:C	3:J:855:ASP:H	2.27	0.42
1:B:31:LEU:HD13	1:B:31:LEU:HA	1.85	0.42
2:C:975:ILE:HG13	2:C:1014:LEU:HD22	2.01	0.42
2:C:1322:SER:OG	2:C:1323:PHE:N	2.52	0.42
3:D:141:PHE:CE1	3:D:181:GLY:HA3	2.54	0.42
3:D:495:ASN:O	3:D:497:GLU:N	2.53	0.42
5:F:121:LYS:HA	5:F:121:LYS:HD3	1.83	0.42
5:F:357:GLN:H	5:F:357:GLN:HG3	1.58	0.42
5:F:442:SER:O	5:F:443:ILE:C	2.61	0.42
1:G:52:PRO:CG	1:G:219:ARG:HH21	2.32	0.42
2:I:516:ASP:C	2:I:518:ASN:H	2.27	0.42
2:I:1132:LEU:HB3	2:I:1177:ARG:CZ	2.49	0.42
3:J:83:VAL:HG13	3:J:92:VAL:HG13	2.01	0.42
3:J:125:GLY:O	3:J:128:LEU:N	2.52	0.42
3:J:517:CYS:HA	3:J:716:GLN:HE22	1.84	0.42
3:J:525:MET:HE3	3:J:525:MET:HB2	1.92	0.42
3:J:844:THR:HG21	3:J:858:VAL:HG21	2.00	0.42
3:J:1356:LEU:HA	3:J:1356:LEU:HD23	1.67	0.42
5:L:452:ILE:HG21	5:L:452:ILE:HD13	1.69	0.42
1:A:249:PHE:CE2	1:A:254:LEU:HG	2.55	0.42
2:C:147:SER:OG	2:C:455:SER:HB3	2.19	0.42
2:C:468:LEU:HA	2:C:468:LEU:HD23	1.77	0.42
2:C:557:ARG:NH2	2:C:607:SER:C	2.72	0.42
2:C:671:LEU:C	2:C:673:HIS:N	2.78	0.42
3:D:88:CYS:SG	3:D:88:CYS:O	2.77	0.42
3:D:426:ALA:CB	3:D:427:PRO:HD3	2.48	0.42
3:D:461:PHE:HD2	3:D:461:PHE:HA	1.64	0.42
3:D:491:LEU:HD23	3:D:491:LEU:HA	1.71	0.42
3:D:825:VAL:O	3:D:826:ILE:C	2.63	0.42
3:D:1357:ILE:C	3:D:1359:ALA:H	2.27	0.42
5:F:95:THR:OG1	5:F:96:ASP:N	2.52	0.42
5:F:396:ASN:O	5:F:398:GLY:N	2.53	0.42
1:G:39:LEU:HD23	1:G:39:LEU:HA	1.70	0.42
2:I:196:VAL:HG12	2:I:204:LEU:O	2.19	0.42
2:I:229:ILE:HB	2:I:240:GLU:HB2	2.01	0.42
2:I:374:GLU:HA	2:I:375:PRO:HD3	1.81	0.42
2:I:1105:SER:HB2	3:J:731:ARG:HG2	2.01	0.42
2:I:1164:PHE:O	2:I:1168:GLU:HB2	2.19	0.42
3:J:599:LYS:HD3	3:J:599:LYS:HA	1.36	0.42
3:J:832:LYS:HD3	3:J:1242:ARG:NH1	2.34	0.42
1:B:109:PRO:HG3	1:B:132:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:LEU:C	1:B:230:ALA:N	2.77	0.42
2:C:478:ARG:HH12	2:C:482:GLY:HA2	1.85	0.42
2:C:678:ARG:CZ	2:C:1106:ARG:HG2	2.50	0.42
2:C:700:VAL:HG11	2:C:1114:GLU:HG2	2.00	0.42
2:C:745:GLU:N	2:C:1017:GLN:HG3	2.34	0.42
2:C:794:LEU:HD21	2:C:796:LEU:HD11	2.02	0.42
3:D:188:LEU:HA	3:D:188:LEU:HD23	1.87	0.42
3:D:262:THR:O	3:D:262:THR:HG23	2.18	0.42
3:D:559:ALA:HB3	3:D:562:GLU:O	2.20	0.42
3:D:576:ARG:NH1	3:D:593:ASN:O	2.52	0.42
3:D:831:VAL:O	3:D:831:VAL:HG13	2.20	0.42
3:D:1342:ASP:OD1	3:D:1343:GLU:N	2.53	0.42
2:I:46:GLN:OE1	2:I:47:TYR:N	2.52	0.42
2:I:338:THR:CG2	2:I:345:PRO:HB3	2.50	0.42
2:I:1217:THR:C	2:I:1219:GLU:H	2.28	0.42
3:J:102:MET:HE2	3:J:244:VAL:O	2.20	0.42
3:J:146:VAL:HG23	3:J:158:GLN:O	2.19	0.42
3:J:557:LYS:O	3:J:559:ALA:N	2.52	0.42
3:J:660:GLU:O	3:J:664:ILE:HG12	2.20	0.42
3:J:698:MET:O	3:J:702:GLN:HB3	2.20	0.42
3:J:797:THR:HG22	3:J:924:GLY:CA	2.35	0.42
3:J:1179:PRO:HG2	3:J:1183:SER:O	2.19	0.42
5:L:482:GLU:O	5:L:486:ARG:NH2	2.53	0.42
1:A:219:ARG:O	1:A:222:THR:HB	2.20	0.42
1:B:153:VAL:CG2	1:B:177:TYR:HE2	2.32	0.42
2:C:48:GLY:N	2:C:461:GLU:OE1	2.52	0.42
2:C:499:SER:O	2:C:503:LYS:HB2	2.20	0.42
2:C:679:ALA:O	2:C:680:LEU:C	2.60	0.42
2:C:865:LEU:HD23	2:C:865:LEU:HA	1.70	0.42
2:C:1164:PHE:HB2	2:C:1168:GLU:CD	2.45	0.42
2:C:1319:MET:O	2:C:1320:PRO:C	2.62	0.42
3:D:74:LYS:HD3	3:D:75:TYR:HE1	1.85	0.42
3:D:227:PHE:CE1	3:D:234:PRO:HG3	2.54	0.42
3:D:249:LEU:HD23	3:D:249:LEU:HA	1.71	0.42
3:D:337:ARG:HB3	3:D:1324:SER:O	2.20	0.42
3:D:357:VAL:HG22	3:D:461:PHE:CD1	2.55	0.42
3:D:411:ILE:HA	3:D:411:ILE:HD13	1.78	0.42
3:D:609:TYR:HA	3:D:617:THR:OG1	2.20	0.42
3:D:770:LEU:HD12	3:D:770:LEU:HA	1.52	0.42
2:I:819:SER:HB2	2:I:1085:MET:CG	2.49	0.42
3:J:189:LEU:HD22	3:J:234:PRO:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:278:ARG:O	3:J:279:LEU:C	2.62	0.42
3:J:1150:PRO:O	3:J:1153:PRO:HG3	2.20	0.42
5:L:148:TYR:CE1	5:L:158:LEU:HD21	2.55	0.42
5:L:219:GLU:O	5:L:222:ALA:HB3	2.19	0.42
5:L:261:LEU:HD12	5:L:261:LEU:N	2.35	0.42
5:L:603:ARG:H	5:L:603:ARG:HG2	1.47	0.42
1:A:78:ILE:HA	1:A:78:ILE:HD13	1.79	0.42
1:A:208:ASN:N	1:A:208:ASN:OD1	2.44	0.42
1:B:12:ARG:O	1:B:29:GLU:O	2.37	0.42
1:B:195:ARG:HB3	1:B:198:LEU:HD21	2.02	0.42
2:C:52:ALA:HB2	2:C:461:GLU:HG3	2.01	0.42
2:C:169:LYS:O	2:C:169:LYS:HG2	2.20	0.42
2:C:269:ILE:HG23	2:C:273:HIS:CB	2.48	0.42
2:C:629:PHE:CD2	2:C:634:VAL:HG11	2.55	0.42
2:C:790:ASP:O	2:C:791:LEU:C	2.63	0.42
2:C:871:VAL:HG22	2:C:872:TYR:O	2.19	0.42
2:C:1222:GLU:C	2:C:1223:ARG:HG3	2.44	0.42
3:D:79:LYS:HG3	3:D:80:HIS:N	2.35	0.42
3:D:289:ASP:O	3:D:290:ILE:C	2.60	0.42
3:D:497:GLU:HA	3:D:498:PRO:HD3	1.95	0.42
3:D:515:ARG:CZ	3:D:719:PHE:CE2	3.02	0.42
3:D:528:THR:HG22	3:D:532:GLU:OE1	2.20	0.42
5:F:551:LEU:HA	5:F:551:LEU:HD23	1.79	0.42
1:H:62:ASP:CG	1:H:141:SER:O	2.63	0.42
1:H:109:PRO:HA	1:H:132:HIS:HA	2.02	0.42
1:H:205:MET:HE2	1:H:205:MET:HB3	1.75	0.42
1:H:214:GLU:HG2	1:H:218:ARG:HE	1.85	0.42
2:I:75:LEU:HD13	2:I:75:LEU:HA	1.55	0.42
2:I:241:LEU:HD12	2:I:241:LEU:HA	1.71	0.42
2:I:563:THR:OG1	2:I:564:PRO:HD2	2.20	0.42
2:I:718:ALA:HB3	2:I:781:ASP:H	1.85	0.42
2:I:836:LEU:CD1	2:I:1054:LEU:HD13	2.46	0.42
3:J:64:PRO:HG3	3:J:90:VAL:CG1	2.49	0.42
3:J:161:THR:O	3:J:162:GLU:C	2.63	0.42
3:J:211:GLU:OE2	3:J:214:ARG:NH2	2.53	0.42
3:J:888:CYS:HB2	3:J:898:CYS:SG	2.59	0.42
3:J:1266:ILE:HB	3:J:1274:PHE:O	2.20	0.42
5:L:599:ARG:O	5:L:604:SER:OG	2.37	0.42
1:A:101:THR:HG22	1:A:103:ASN:HD21	1.85	0.42
1:A:192:VAL:O	1:A:193:GLU:C	2.62	0.42
1:B:51:MET:HB3	1:B:178:SER:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:LEU:HA	1:B:85:LEU:HD23	1.61	0.42
2:C:5:TYR:HB2	2:C:781:ASP:OD1	2.20	0.42
2:C:100:LEU:HA	2:C:100:LEU:HD23	1.70	0.42
2:C:318:SER:OG	2:C:320:ASP:OD2	2.36	0.42
2:C:503:LYS:HZ3	2:C:503:LYS:HG3	1.70	0.42
2:C:718:ALA:HB2	2:C:783:LEU:HD21	2.02	0.42
2:C:1144:PHE:O	2:C:1147:ARG:HB2	2.18	0.42
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.84	0.42
3:D:22:ILE:HD13	3:D:22:ILE:HG21	1.79	0.42
3:D:214:ARG:HA	3:D:217:LEU:HB2	2.02	0.42
3:D:277:ASN:O	3:D:278:ARG:C	2.63	0.42
3:D:737:ILE:O	3:D:740:LEU:N	2.49	0.42
3:D:1177:ILE:HG13	3:D:1186:TYR:O	2.20	0.42
5:F:306:PHE:HE1	5:F:315:TRP:CE2	2.37	0.42
5:F:373:ARG:O	5:F:374:ARG:C	2.61	0.42
5:F:462:LYS:HE3	5:F:488:LEU:HD11	2.01	0.42
5:F:560:ARG:O	5:F:567:MET:HE2	2.20	0.42
1:H:134:THR:HG23	1:H:135:ASP:H	1.83	0.42
2:I:260:LYS:HE3	2:I:262:TYR:CE1	2.55	0.42
2:I:721:GLY:N	2:I:740:GLU:OE1	2.40	0.42
2:I:903:ARG:NH2	2:I:910:ALA:HB2	2.35	0.42
2:I:1170:MET:HE3	2:I:1170:MET:HB3	1.90	0.42
2:I:1233:LEU:HD22	2:I:1233:LEU:N	2.34	0.42
3:J:489:ASN:HA	3:J:904:ALA:HB1	2.01	0.42
3:J:504:GLN:O	3:J:505:ASP:C	2.61	0.42
5:L:363:ARG:O	5:L:367:ILE:HG13	2.20	0.42
5:L:373:ARG:O	5:L:374:ARG:C	2.63	0.42
5:L:470:MET:HE3	5:L:478:PRO:HB3	2.02	0.42
5:L:483:LEU:H	5:L:483:LEU:CD1	2.30	0.42
1:B:42:ALA:O	1:B:43:LEU:C	2.63	0.41
2:C:179:TYR:H	2:C:397:LEU:HA	1.85	0.41
3:D:8:LEU:HD23	3:D:9:LYS:H	1.84	0.41
3:D:18:ASP:HB2	3:D:1373:ARG:NH1	2.35	0.41
3:D:354:VAL:HG12	3:D:355:ILE:N	2.35	0.41
3:D:490:ILE:HG21	3:D:490:ILE:HD13	1.68	0.41
3:D:1342:ASP:OD1	3:D:1344:LEU:N	2.48	0.41
5:F:518:HIS:O	5:F:519:LEU:C	2.63	0.41
1:G:190:ALA:O	1:G:198:LEU:HB2	2.20	0.41
1:G:231:PHE:HA	1:H:218:ARG:HH11	1.81	0.41
1:H:23:HIS:CE1	1:H:206:GLU:HG2	2.54	0.41
2:I:971:LEU:HD22	2:I:1018:TYR:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1136:GLN:O	2:I:1137:GLU:HB3	2.20	0.41
2:I:1161:LEU:HD12	2:I:1161:LEU:HA	1.67	0.41
2:I:1319:MET:HE2	2:I:1319:MET:HB3	1.65	0.41
3:J:132:LEU:O	3:J:132:LEU:HD22	2.20	0.41
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.84	0.41
3:J:482:ALA:O	3:J:488:ASN:ND2	2.54	0.41
3:J:484:MET:HE2	3:J:484:MET:HB3	1.65	0.41
3:J:694:SER:O	3:J:698:MET:HB2	2.20	0.41
3:J:702:GLN:HG2	3:J:703:THR:N	2.30	0.41
5:L:431:ALA:O	5:L:432:THR:C	2.63	0.41
1:A:67:GLU:H	1:A:67:GLU:HG2	1.45	0.41
1:A:190:ALA:HB2	1:A:200:LYS:CB	2.41	0.41
1:B:102:LEU:HD23	1:B:102:LEU:HA	1.84	0.41
2:C:96:LEU:HD12	2:C:96:LEU:HA	1.77	0.41
2:C:310:ILE:HG21	2:C:325:LEU:HB3	2.03	0.41
2:C:603:ILE:H	2:C:603:ILE:HG12	1.65	0.41
2:C:661:VAL:HB	2:C:665:ALA:HB3	2.01	0.41
2:C:693:LEU:C	2:C:693:LEU:HD23	2.45	0.41
2:C:700:VAL:HG21	2:C:1114:GLU:HG2	2.01	0.41
2:C:857:VAL:HG23	2:C:862:LEU:HD11	2.02	0.41
2:C:895:LEU:H	2:C:895:LEU:HG	1.54	0.41
2:C:1075:VAL:O	2:C:1075:VAL:HG12	2.20	0.41
3:D:83:VAL:O	3:D:91:GLU:HA	2.20	0.41
3:D:447:ILE:HD13	3:D:447:ILE:HG21	1.64	0.41
5:F:227:GLN:OE1	5:F:251:LYS:NZ	2.53	0.41
5:F:230:VAL:HG13	5:F:231:THR:H	1.85	0.41
1:G:172:LEU:H	1:G:172:LEU:CD1	2.33	0.41
2:I:339:ASN:HB3	2:I:343:HIS:H	1.84	0.41
2:I:672:GLU:H	2:I:672:GLU:HG3	1.54	0.41
2:I:798:GLN:OE1	2:I:828:PHE:CD1	2.73	0.41
2:I:850:ILE:HD12	2:I:850:ILE:HG23	1.77	0.41
2:I:1088:ASP:OD1	2:I:1092:THR:N	2.53	0.41
3:J:307:LEU:HA	3:J:307:LEU:HD23	1.19	0.41
3:J:434:ILE:HG21	3:J:434:ILE:HD13	1.46	0.41
3:J:473:THR:HG23	3:J:476:ALA:H	1.85	0.41
5:L:580:PHE:HD1	5:L:580:PHE:HA	1.62	0.41
1:A:78:ILE:HD12	1:A:78:ILE:HG23	1.77	0.41
1:A:154:PRO:O	1:A:158:ARG:HG3	2.20	0.41
2:C:490:GLN:O	2:C:491:ASP:C	2.62	0.41
2:C:494:ASN:HD22	2:C:497:PRO:CD	2.27	0.41
2:C:799:ASN:HA	2:C:1231:TYR:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:996:ARG:HD3	2:C:996:ARG:HA	1.60	0.41
2:C:1246:ARG:CZ	3:D:348:ASP:OD1	2.69	0.41
2:C:1278:LEU:HA	2:C:1278:LEU:HD23	1.67	0.41
3:D:440:VAL:O	3:D:442:ILE:HG12	2.21	0.41
3:D:525:MET:HB2	3:D:525:MET:HE3	1.52	0.41
3:D:872:LEU:O	3:D:877:VAL:HG12	2.20	0.41
5:F:230:VAL:HG13	5:F:231:THR:N	2.36	0.41
1:G:54:CYS:HB3	1:G:148:ARG:HG2	2.01	0.41
1:G:190:ALA:C	1:G:191:ARG:HD3	2.46	0.41
2:I:363:LEU:HA	2:I:363:LEU:HD23	1.62	0.41
2:I:395:TYR:HE2	2:I:397:LEU:CD1	2.33	0.41
2:I:593:LYS:HG3	2:I:595:THR:HG23	2.02	0.41
2:I:959:ASP:O	2:I:963:GLU:HG2	2.21	0.41
2:I:1330:ILE:HD13	2:I:1330:ILE:HG21	1.75	0.41
3:J:252:LEU:HD22	3:J:260:PHE:HD2	1.85	0.41
3:J:309:ASN:HB2	3:J:326:SER:HB3	2.02	0.41
3:J:331:ILE:HD13	3:J:331:ILE:HG21	1.67	0.41
3:J:352:ARG:HB3	3:J:467:ALA:HA	2.02	0.41
3:J:514:THR:CB	3:J:576:ARG:HG2	2.47	0.41
3:J:530:PRO:O	3:J:533:ALA:HB3	2.20	0.41
3:J:762:ASN:OD1	3:J:764:ARG:N	2.53	0.41
3:J:1144:LEU:HA	3:J:1144:LEU:HD23	1.57	0.41
3:J:1151:LYS:O	3:J:1153:PRO:HD3	2.21	0.41
3:J:1344:LEU:HD12	3:J:1344:LEU:N	2.35	0.41
5:L:130:VAL:HA	5:L:133:SER:HB2	2.01	0.41
5:L:312:SER:OG	5:L:313:ASP:N	2.51	0.41
2:C:518:ASN:O	2:C:519:ASN:CB	2.64	0.41
2:C:867:GLU:H	2:C:867:GLU:HG3	1.30	0.41
2:C:1007:LYS:O	2:C:1011:LEU:HG	2.20	0.41
2:C:1120:ALA:O	2:C:1123:GLY:N	2.53	0.41
2:C:1178:LYS:HD3	2:C:1178:LYS:HA	1.55	0.41
3:D:10:ALA:O	3:D:11:GLN:HB2	2.21	0.41
3:D:74:LYS:CD	3:D:87:LYS:HD3	2.47	0.41
3:D:117:LEU:HA	3:D:117:LEU:HD12	1.77	0.41
5:F:372:ALA:O	5:F:373:ARG:C	2.63	0.41
5:F:443:ILE:O	5:F:444:ALA:C	2.62	0.41
5:F:533:ASP:O	5:F:534:SER:C	2.63	0.41
1:G:50:SER:HB2	1:H:8:PHE:HZ	1.86	0.41
1:G:52:PRO:HG2	1:G:219:ARG:NH2	2.34	0.41
1:G:226:GLU:O	1:G:229:GLU:HB2	2.20	0.41
1:H:102:LEU:HA	1:H:102:LEU:HD23	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:540:ARG:H	2:I:540:ARG:HG3	1.50	0.41
2:I:819:SER:OG	2:I:820:GLU:N	2.50	0.41
2:I:1251:TYR:CD1	2:I:1301:ARG:NH2	2.89	0.41
3:J:270:ARG:O	3:J:273:ILE:HB	2.21	0.41
3:J:278:ARG:O	3:J:281:ARG:HB2	2.20	0.41
3:J:556:GLU:O	3:J:564:VAL:N	2.47	0.41
3:J:796:LEU:HD12	3:J:796:LEU:HA	1.61	0.41
3:J:1177:ILE:HG13	3:J:1186:TYR:O	2.21	0.41
3:J:1307:LEU:HD23	3:J:1312:ALA:HA	2.02	0.41
4:K:6:VAL:HG12	4:K:51:LEU:HD13	2.02	0.41
1:B:151:GLY:O	1:B:177:TYR:CD2	2.70	0.41
2:C:9:LYS:HG2	2:C:1171:ARG:HD3	2.02	0.41
2:C:142:GLU:CG	2:C:760:ASN:HD21	2.31	0.41
2:C:149:LEU:HG	2:C:451:ARG:HH11	1.84	0.41
2:C:1184:THR:HG22	2:C:1185:PRO:O	2.20	0.41
3:D:95:THR:O	3:D:95:THR:HG23	2.20	0.41
3:D:233:LYS:HA	3:D:234:PRO:HD3	1.87	0.41
3:D:430:HIS:ND1	3:D:430:HIS:N	2.66	0.41
3:D:501:VAL:HG22	3:D:502:PRO:O	2.20	0.41
3:D:506:VAL:H	3:D:506:VAL:HG12	1.52	0.41
3:D:536:LEU:O	3:D:539:SER:OG	2.37	0.41
3:D:821:MET:HA	3:D:881:LYS:HA	2.01	0.41
3:D:905:ARG:HH11	4:E:16:ARG:HD2	1.84	0.41
3:D:1295:ASN:O	3:D:1296:GLY:C	2.63	0.41
5:F:269:LEU:O	5:F:270:VAL:C	2.63	0.41
5:F:575:GLU:O	5:F:579:GLN:HG2	2.20	0.41
2:I:811:ASN:OD1	2:I:811:ASN:N	2.46	0.41
2:I:948:ILE:O	2:I:951:MET:HB3	2.20	0.41
2:I:1160:ASP:CG	2:I:1161:LEU:N	2.75	0.41
2:I:1281:TYR:CE2	3:J:431:ARG:HB2	2.55	0.41
2:I:1322:SER:O	2:I:1325:VAL:N	2.53	0.41
3:J:844:THR:HG21	3:J:858:VAL:CG2	2.50	0.41
3:J:1153:PRO:HA	3:J:1214:PRO:O	2.20	0.41
4:K:10:VAL:HG13	4:K:16:ARG:HB2	2.02	0.41
5:L:284:GLU:OE2	5:L:359:LYS:HD2	2.20	0.41
5:L:396:ASN:C	5:L:398:GLY:H	2.29	0.41
5:L:470:MET:HE3	5:L:470:MET:HB3	1.91	0.41
5:L:601:PRO:HB2	5:L:605:GLU:HG2	2.01	0.41
1:A:43:LEU:HA	1:A:43:LEU:HD23	1.64	0.41
1:A:77:ASP:OD2	2:C:755:LYS:NZ	2.38	0.41
2:C:194:LEU:HA	2:C:194:LEU:HD12	1.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:626:GLU:HB3	2:C:628:HIS:CE1	2.55	0.41
2:C:929:ILE:O	2:C:930:ASP:HB2	2.19	0.41
2:C:960:LEU:O	2:C:963:GLU:HB2	2.20	0.41
2:C:1131:MET:CE	2:C:1141:LEU:HA	2.49	0.41
2:C:1341:ASP:HB3	2:C:1342:GLU:H	1.35	0.41
3:D:203:GLU:O	3:D:207:GLU:HG2	2.19	0.41
3:D:334:LYS:CG	3:D:335:GLN:H	2.32	0.41
3:D:599:LYS:HA	3:D:599:LYS:HD3	1.66	0.41
3:D:884:SER:OG	3:D:886:VAL:HG12	2.21	0.41
3:D:909:ILE:HD12	3:D:909:ILE:HA	1.85	0.41
3:D:915:ILE:O	3:D:916:GLY:C	2.62	0.41
3:D:1227:HIS:HA	3:D:1230:THR:HG22	2.03	0.41
3:D:1256:ILE:HA	3:D:1256:ILE:HD13	1.74	0.41
5:F:519:LEU:C	5:F:519:LEU:HD23	2.45	0.41
1:H:17:GLU:OE1	1:H:25:LYS:HD3	2.20	0.41
1:H:195:ARG:CB	1:H:198:LEU:HD21	2.50	0.41
2:I:176:ILE:HD13	2:I:176:ILE:HG21	1.74	0.41
2:I:618:GLN:HG3	2:I:619:ALA:N	2.36	0.41
2:I:1132:LEU:O	2:I:1132:LEU:HD23	2.19	0.41
2:I:1301:ARG:HH11	2:I:1301:ARG:HD2	1.71	0.41
2:I:1331:ARG:HH11	2:I:1331:ARG:HD3	1.72	0.41
3:J:35:PHE:C	3:J:61:ILE:HG23	2.46	0.41
3:J:146:VAL:HG12	3:J:147:ILE:N	2.36	0.41
3:J:546:ALA:O	3:J:573:THR:HA	2.20	0.41
3:J:735:ALA:O	3:J:738:ARG:HB3	2.20	0.41
4:K:53:GLU:HB3	4:K:59:ILE:CG1	2.50	0.41
5:L:236:LYS:HD3	5:L:236:LYS:N	2.35	0.41
5:L:412:LEU:N	5:L:435:ILE:HG12	2.36	0.41
5:L:552:THR:H	5:L:552:THR:HG23	1.65	0.41
2:C:81:ASP:CG	2:C:82:VAL:H	2.29	0.41
2:C:639:LYS:O	2:C:641:GLU:N	2.54	0.41
2:C:818:VAL:HG22	2:C:1096:ILE:HG12	2.03	0.41
3:D:649:LYS:HD2	3:D:652:GLU:OE1	2.21	0.41
3:D:656:GLU:O	3:D:659:ALA:N	2.54	0.41
3:D:798:ARG:O	3:D:799:ARG:C	2.64	0.41
3:D:891:ASP:O	3:D:892:PHE:HB2	2.20	0.41
4:E:32:VAL:O	4:E:34:GLY:N	2.52	0.41
5:F:223:GLU:O	5:F:226:ALA:HB3	2.21	0.41
5:F:559:LEU:HD12	5:F:559:LEU:HA	1.63	0.41
1:H:45:ARG:HH11	1:H:45:ARG:HD3	1.69	0.41
2:I:538:LEU:H	2:I:538:LEU:HG	1.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:696:ASP:HB3	2:I:697:LYS:H	1.62	0.41
2:I:888:THR:CG2	2:I:916:SER:OG	2.68	0.41
2:I:1198:LEU:HD22	2:I:1198:LEU:HA	1.78	0.41
3:J:72:CYS:SG	3:J:73:GLY:N	2.94	0.41
3:J:370:LYS:HG3	3:J:442:ILE:C	2.45	0.41
3:J:863:LEU:HD11	3:J:901:ARG:HB3	2.02	0.41
3:J:1175:LEU:O	3:J:1187:GLU:HA	2.21	0.41
5:L:559:LEU:HA	5:L:559:LEU:HD12	1.31	0.41
2:C:289:VAL:HG13	2:C:319:LEU:HD11	2.03	0.41
2:C:513:GLN:NE2	2:C:526:TYR:CE2	2.89	0.41
2:C:530:ILE:HG23	2:C:530:ILE:HD12	1.63	0.41
2:C:704:MET:O	2:C:705:GLU:C	2.64	0.41
2:C:802:VAL:HG12	2:C:1228:GLY:O	2.20	0.41
2:C:807:TRP:O	2:C:808:ASN:C	2.63	0.41
3:D:83:VAL:H	3:D:83:VAL:HG12	1.56	0.41
3:D:394:ILE:O	3:D:395:LYS:C	2.61	0.41
3:D:500:ILE:HD12	3:D:500:ILE:HG23	1.78	0.41
3:D:678:ARG:O	3:D:679:TYR:C	2.64	0.41
3:D:860:ARG:HH12	3:D:861:ASN:CG	2.28	0.41
3:D:1158:GLU:HA	3:D:1223:LEU:HD11	2.02	0.41
3:D:1158:GLU:HG3	3:D:1186:TYR:CZ	2.56	0.41
1:G:61:ILE:HG22	1:G:62:ASP:N	2.35	0.41
1:G:66:HIS:NE2	2:I:929:ILE:HG22	2.36	0.41
1:G:86:LYS:NZ	1:G:174:ASP:HB2	2.36	0.41
1:H:93:GLN:HB2	1:H:120:ASP:HB3	2.02	0.41
2:I:658:GLN:CD	2:I:1186:VAL:HG23	2.45	0.41
2:I:688:GLN:HB2	2:I:1235:LEU:HD22	2.01	0.41
2:I:807:TRP:HE3	2:I:808:ASN:HB2	1.85	0.41
3:J:294:ASN:HD21	5:L:402:LEU:HD23	1.85	0.41
3:J:495:ASN:C	3:J:497:GLU:H	2.27	0.41
3:J:1160:SER:HA	3:J:1204:VAL:O	2.21	0.41
5:L:100:MET:HE2	5:L:100:MET:HB3	1.88	0.41
5:L:396:ASN:C	5:L:398:GLY:N	2.78	0.41
1:A:112:ALA:O	1:A:115:ILE:HG13	2.20	0.41
1:A:228:LEU:HD11	1:B:224:LEU:HD23	2.03	0.41
1:A:273:GLU:OE2	1:A:293:PRO:HD2	2.21	0.41
2:C:24:VAL:HG12	2:C:25:PRO:O	2.21	0.41
2:C:37:LYS:HA	2:C:37:LYS:HD3	1.83	0.41
2:C:138:ILE:HD11	2:C:506:PHE:HB3	2.02	0.41
2:C:548:ARG:HB3	2:C:569:ILE:O	2.21	0.41
2:C:719:LYS:O	2:C:779:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1043:ALA:HB1	2:C:1044:PRO:HD2	2.02	0.41
2:C:1172:LEU:C	2:C:1172:LEU:HD13	2.46	0.41
2:C:1172:LEU:HD22	2:C:1172:LEU:O	2.21	0.41
3:D:13:LYS:HD3	3:D:13:LYS:HA	1.91	0.41
3:D:31:ARG:CZ	3:D:106:GLU:OE2	2.69	0.41
3:D:103:GLY:C	3:D:244:VAL:HG22	2.46	0.41
3:D:112:ALA:O	3:D:300:GLN:NE2	2.46	0.41
3:D:390:LEU:N	3:D:390:LEU:HD12	2.36	0.41
3:D:442:ILE:HD12	3:D:442:ILE:HG23	1.72	0.41
3:D:519:ASN:CG	3:D:709:ARG:HH11	2.28	0.41
3:D:733:SER:O	3:D:735:ALA:N	2.54	0.41
4:E:62:GLN:O	4:E:66:VAL:HG23	2.21	0.41
5:F:137:TYR:HA	5:F:138:PRO:HD3	1.95	0.41
5:F:442:SER:O	5:F:445:ASP:N	2.54	0.41
5:F:557:LYS:O	5:F:561:MET:N	2.52	0.41
1:G:118:ASP:HB3	1:G:121:VAL:HG21	2.02	0.41
1:H:16:ILE:HA	1:H:26:VAL:HG13	2.03	0.41
1:H:44:ARG:HG3	1:H:183:ILE:HB	2.03	0.41
2:I:29:SER:O	2:I:30:ILE:C	2.62	0.41
2:I:37:LYS:HD3	2:I:37:LYS:HA	1.94	0.41
2:I:171:LEU:HD23	2:I:171:LEU:HA	1.86	0.41
2:I:195:PHE:CB	2:I:203:LYS:HD3	2.50	0.41
2:I:212:ALA:HA	2:I:359:ARG:HG3	2.03	0.41
2:I:344:GLY:O	2:I:346:TYR:CD2	2.74	0.41
2:I:521:LEU:HA	2:I:521:LEU:HD12	1.82	0.41
2:I:523:GLU:HG2	2:I:527:LYS:CE	2.36	0.41
2:I:617:ALA:HB3	2:I:653:MET:HB2	2.02	0.41
2:I:756:TYR:CD1	2:I:756:TYR:N	2.83	0.41
2:I:761:GLN:HA	2:I:762:ASN:HA	1.84	0.41
2:I:794:LEU:HD21	2:I:796:LEU:HD21	2.01	0.41
2:I:807:TRP:HE1	2:I:1086:PRO:HG3	1.85	0.41
2:I:829:THR:HG23	2:I:1059:ARG:HG2	2.03	0.41
3:J:269:TYR:O	3:J:270:ARG:C	2.62	0.41
3:J:277:ASN:O	3:J:278:ARG:C	2.64	0.41
3:J:425:ARG:HH11	3:J:425:ARG:HD2	1.60	0.41
3:J:849:LEU:HD22	3:J:849:LEU:H	1.86	0.41
3:J:908:ILE:HD13	3:J:909:ILE:N	2.35	0.41
3:J:1223:LEU:HD13	3:J:1223:LEU:HA	1.73	0.41
5:L:118:ASP:O	5:L:122:ARG:HG3	2.20	0.41
5:L:124:GLU:O	5:L:128:ASN:HB2	2.19	0.41
5:L:127:ILE:H	5:L:127:ILE:HG13	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:262:VAL:HG12	5:L:264:LYS:HG3	2.02	0.41
1:B:214:GLU:O	1:B:218:ARG:HG3	2.21	0.41
2:C:210:LEU:O	2:C:215:TYR:HB2	2.21	0.41
2:C:311:CYS:SG	2:C:311:CYS:O	2.79	0.41
2:C:384:LEU:O	2:C:387:ASN:N	2.54	0.41
2:C:619:ALA:HB1	2:C:657:THR:HA	2.03	0.41
2:C:667:LEU:HD23	2:C:667:LEU:HA	1.84	0.41
2:C:831:ILE:HG21	2:C:831:ILE:HD13	1.85	0.41
2:C:1049:ILE:HD13	2:C:1049:ILE:HG21	1.75	0.41
2:C:1143:GLU:OE1	2:C:1147:ARG:HD3	2.21	0.41
3:D:20:ILE:HG21	3:D:20:ILE:HD13	1.85	0.41
3:D:113:HIS:ND1	3:D:113:HIS:C	2.77	0.41
3:D:120:LEU:HB3	3:D:121:PRO:HD3	2.02	0.41
3:D:126:LEU:C	3:D:126:LEU:HD12	2.46	0.41
3:D:450:HIS:CE1	3:D:452:LEU:HB2	2.56	0.41
3:D:556:GLU:HG2	3:D:558:ASP:HB2	2.02	0.41
3:D:697:MET:O	3:D:701:LEU:HB2	2.21	0.41
3:D:1364:ALA:O	3:D:1367:GLN:HB3	2.20	0.41
2:I:65:ASN:O	2:I:105:TYR:HD2	2.03	0.41
2:I:229:ILE:HG21	2:I:240:GLU:OE2	2.20	0.41
2:I:865:LEU:HD23	2:I:865:LEU:HA	1.77	0.41
2:I:1341:ASP:HB3	2:I:1342:GLU:H	1.57	0.41
2:I:1342:GLU:O	3:J:1369:ARG:NH2	2.54	0.41
3:J:601:ILE:HG21	3:J:601:ILE:HD13	1.61	0.41
3:J:795:TYR:HE2	3:J:799:ARG:NE	2.17	0.41
3:J:813:ASP:OD1	3:J:883:ARG:NH2	2.52	0.41
5:L:561:MET:HA	5:L:567:MET:CE	2.50	0.41
1:A:12:ARG:HG2	1:A:13:LEU:H	1.85	0.40
1:B:197:ASP:O	1:B:197:ASP:CG	2.64	0.40
2:C:145:ILE:N	2:C:145:ILE:HD12	2.37	0.40
2:C:328:SER:OG	2:C:330:HIS:CD2	2.73	0.40
2:C:624:ASP:OD1	2:C:625:GLU:N	2.52	0.40
2:C:929:ILE:HD13	2:C:929:ILE:HG21	1.73	0.40
2:C:1211:ARG:O	2:C:1211:ARG:HG3	2.21	0.40
3:D:54:ASP:N	3:D:54:ASP:OD1	2.54	0.40
3:D:770:LEU:O	3:D:774:ILE:HG13	2.21	0.40
3:D:920:ALA:O	3:D:921:GLN:C	2.61	0.40
3:D:1264:ALA:O	3:D:1278:GLU:N	2.34	0.40
4:E:24:ALA:O	4:E:25:ARG:C	2.63	0.40
5:F:99:ARG:HA	5:F:99:ARG:HD3	1.80	0.40
1:G:50:SER:HG	1:H:35:PHE:HZ	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:75:GLN:HG2	1:G:76:GLU:OE2	2.20	0.40
1:G:108:GLY:HA2	1:G:109:PRO:HD3	1.90	0.40
1:G:170:ARG:O	1:G:171:LEU:HD13	2.20	0.40
1:H:19:VAL:O	1:H:23:HIS:HB3	2.21	0.40
2:I:327:GLN:C	2:I:327:GLN:CD	2.89	0.40
2:I:606:LEU:HD12	2:I:606:LEU:N	2.37	0.40
2:I:663:VAL:HG23	2:I:664:GLY:N	2.36	0.40
2:I:896:THR:OG1	2:I:899:GLU:HG3	2.21	0.40
3:J:470:VAL:CG1	3:J:472:LEU:HD23	2.49	0.40
3:J:648:GLU:OE2	3:J:649:LYS:HE2	2.21	0.40
3:J:847:ASP:HA	3:J:860:ARG:H	1.86	0.40
5:L:278:ASP:OD1	5:L:281:ARG:NH1	2.48	0.40
2:C:77:GLU:HA	2:C:78:PRO:HD3	1.84	0.40
2:C:131:THR:HG22	2:C:135:THR:N	2.11	0.40
2:C:183:TRP:HB2	2:C:199:ASP:HA	2.03	0.40
2:C:660:VAL:HG13	2:C:661:VAL:N	2.36	0.40
2:C:670:PHE:CD2	2:C:1113:LEU:HB3	2.56	0.40
2:C:836:LEU:O	2:C:1052:VAL:N	2.44	0.40
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.86	0.40
2:C:1243:MET:HA	3:D:353:SER:CB	2.51	0.40
3:D:242:LEU:HD23	3:D:243:PRO:O	2.21	0.40
3:D:1237:VAL:HG13	3:D:1238:GLN:N	2.36	0.40
3:D:1307:LEU:HD12	3:D:1307:LEU:N	2.36	0.40
3:D:1321:SER:HB2	3:D:1349:GLU:OE2	2.21	0.40
5:F:269:LEU:O	5:F:272:SER:N	2.54	0.40
1:G:45:ARG:HH12	1:H:37:HIS:HB2	1.86	0.40
2:I:370:MET:HE3	2:I:370:MET:HB3	1.88	0.40
2:I:1274:GLU:N	2:I:1274:GLU:CD	2.79	0.40
2:I:1332:SER:OG	3:J:327:LEU:HD13	2.21	0.40
3:J:184:ALA:O	3:J:187:ALA:HB3	2.21	0.40
3:J:279:LEU:C	3:J:279:LEU:HD23	2.46	0.40
3:J:495:ASN:C	3:J:497:GLU:N	2.79	0.40
5:L:540:LEU:C	5:L:540:LEU:HD23	2.47	0.40
1:A:182:ARG:O	1:A:183:ILE:HD12	2.21	0.40
2:C:47:TYR:HD2	2:C:47:TYR:HA	1.72	0.40
2:C:109:ALA:HB1	2:C:111:GLU:HA	2.02	0.40
2:C:142:GLU:N	2:C:760:ASN:OD1	2.54	0.40
2:C:817:LEU:HD23	2:C:1078:LYS:HB3	2.04	0.40
2:C:836:LEU:N	2:C:836:LEU:CD1	2.82	0.40
2:C:896:THR:O	2:C:897:PRO:C	2.65	0.40
2:C:1115:THR:HG22	2:C:1228:GLY:HA3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1120:ALA:HB1	2:C:1198:LEU:CD1	2.51	0.40
2:C:1239:VAL:C	2:C:1241:ASP:H	2.28	0.40
3:D:205:LEU:HD13	3:D:205:LEU:O	2.22	0.40
3:D:259:ARG:HD2	5:F:505:ILE:HD13	2.03	0.40
5:F:144:LEU:HA	5:F:144:LEU:HD12	1.78	0.40
5:F:379:MET:HG2	5:F:416:VAL:HG22	2.03	0.40
1:G:73:GLY:O	1:G:134:THR:HG22	2.22	0.40
2:I:27:LEU:HD23	2:I:27:LEU:HA	1.78	0.40
2:I:74:ARG:C	2:I:75:LEU:HD22	2.46	0.40
2:I:163:LYS:HE3	2:I:163:LYS:HB3	1.73	0.40
2:I:643:SER:OG	2:I:645:PHE:HE1	2.05	0.40
2:I:1046:VAL:H	2:I:1046:VAL:HG12	1.59	0.40
3:J:97:VAL:O	3:J:101:ARG:HG3	2.21	0.40
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.72	0.40
3:J:422:LEU:HA	3:J:422:LEU:HD12	1.83	0.40
3:J:836:ARG:HG3	3:J:869:CYS:HB3	2.03	0.40
3:J:847:ASP:HB3	3:J:856:ILE:CG2	2.51	0.40
3:J:909:ILE:O	3:J:909:ILE:HG23	2.19	0.40
5:L:587:ILE:HA	5:L:590:ILE:CD1	2.51	0.40
1:A:145:LYS:HE3	1:A:145:LYS:HB3	1.91	0.40
1:A:316:MET:HB2	5:F:600:HIS:CE1	2.57	0.40
1:B:88:LEU:HA	1:B:88:LEU:HD12	1.74	0.40
2:C:208:ILE:HD13	2:C:208:ILE:HG21	1.79	0.40
2:C:617:ALA:HB3	2:C:653:MET:CG	2.51	0.40
2:C:842:ASP:HB2	2:C:1045:GLY:O	2.21	0.40
2:C:930:ASP:HB3	2:C:1053:TYR:HB2	2.03	0.40
2:C:1061:GLN:O	2:C:1062:PRO:C	2.63	0.40
2:C:1062:PRO:HA	2:C:1076:ILE:O	2.21	0.40
3:D:515:ARG:NH2	3:D:717:VAL:HG23	2.37	0.40
3:D:592:VAL:H	3:D:592:VAL:HG22	1.69	0.40
3:D:1347:LEU:HG	3:D:1357:ILE:CG2	2.50	0.40
5:F:107:THR:OG1	5:F:108:VAL:N	2.53	0.40
5:F:110:LEU:HD23	5:F:110:LEU:HA	1.73	0.40
5:F:387:VAL:O	5:F:388:ILE:C	2.63	0.40
1:G:38:THR:N	1:H:45:ARG:NH1	2.70	0.40
2:I:41:GLN:NE2	2:I:73:TYR:CZ	2.89	0.40
2:I:518:ASN:CG	2:I:519:ASN:H	2.30	0.40
2:I:757:THR:C	2:I:833:ILE:HD12	2.46	0.40
2:I:791:LEU:HA	2:I:791:LEU:HD23	1.73	0.40
2:I:801:ARG:HA	2:I:1228:GLY:O	2.22	0.40
2:I:861:ALA:HB1	2:I:882:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:976:ARG:HH12	2:I:990:ASP:HB3	1.86	0.40
2:I:1101:LEU:HD23	3:J:725:MET:SD	2.61	0.40
2:I:1106:ARG:HE	3:J:731:ARG:HH21	1.70	0.40
3:J:47:ARG:HD2	3:J:47:ARG:HA	1.85	0.40
3:J:872:LEU:CD2	3:J:877:VAL:HG11	2.43	0.40
3:J:1261:LEU:O	3:J:1262:ARG:C	2.65	0.40
3:J:1328:THR:O	3:J:1329:THR:C	2.61	0.40
5:L:112:THR:OG1	5:L:115:GLY:N	2.51	0.40
5:L:230:VAL:HG13	5:L:231:THR:N	2.36	0.40
5:L:277:MET:HG3	5:L:362:ASN:HD21	1.86	0.40
5:L:565:ILE:HG22	5:L:566:ASP:OD2	2.21	0.40
1:A:31:LEU:CD1	1:A:201:LEU:HB2	2.51	0.40
1:A:76:GLU:HB3	1:A:81:ILE:HG12	2.03	0.40
1:A:201:LEU:HD12	1:A:201:LEU:HA	1.67	0.40
1:B:40:GLY:HA3	1:B:185:TYR:CD1	2.56	0.40
1:B:103:ASN:HA	1:B:141:SER:HB2	2.03	0.40
1:B:112:ALA:HA	1:B:115:ILE:HD11	2.03	0.40
1:B:215:GLU:HA	1:B:218:ARG:CD	2.51	0.40
2:C:495:ALA:O	2:C:496:LYS:C	2.64	0.40
2:C:556:GLY:HA2	2:C:659:GLN:O	2.21	0.40
2:C:615:VAL:HG21	2:C:645:PHE:CD2	2.57	0.40
2:C:746:ALA:HA	2:C:974:ARG:NH2	2.34	0.40
2:C:811:ASN:OD1	2:C:811:ASN:N	2.48	0.40
2:C:1251:TYR:CE1	2:C:1301:ARG:CZ	3.04	0.40
2:C:1313:HIS:HD2	3:D:477:GLN:NE2	2.19	0.40
3:D:721:SER:HA	3:D:724:MET:CE	2.45	0.40
3:D:853:THR:C	3:D:855:ASP:N	2.80	0.40
4:E:39:VAL:HG13	4:E:52:ARG:HH21	1.86	0.40
5:F:148:TYR:OH	5:F:218:ARG:HA	2.21	0.40
5:F:476:ARG:HG3	5:F:477:GLU:N	2.35	0.40
5:F:606:VAL:O	5:F:609:SER:OG	2.40	0.40
1:G:14:VAL:HG13	1:G:27:THR:HB	2.03	0.40
1:H:31:LEU:HB2	1:H:199:ASP:HB2	2.04	0.40
1:H:98:VAL:HG22	1:H:99:ILE:H	1.87	0.40
2:I:109:ALA:HB1	2:I:111:GLU:HA	2.03	0.40
2:I:239:MET:HG2	2:I:240:GLU:O	2.21	0.40
2:I:729:ALA:O	2:I:755:LYS:HD3	2.22	0.40
3:J:201:LEU:HD22	3:J:217:LEU:HD13	2.02	0.40
3:J:215:LYS:HD2	3:J:216:LYS:N	2.36	0.40
3:J:268:LEU:HD13	3:J:306:LEU:HD23	2.04	0.40
3:J:392:THR:HG21	5:L:609:SER:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:419:HIS:CD2	3:J:419:HIS:C	3.00	0.40
5:L:245:ALA:O	5:L:246:GLN:C	2.64	0.40
5:L:343:LYS:O	5:L:347:ILE:HG13	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:33:ASP:OD1	5:F:554:ARG:NH2[4_455]	1.99	0.21
2:C:44:GLU:OE1	5:F:596:ARG:NH1[4_455]	2.05	0.15
2:C:940:GLU:OE1	1:H:139:SER:OG[4_455]	2.05	0.15

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	305/329 (93%)	271 (89%)	25 (8%)	9 (3%)	3	25
1	B	213/329 (65%)	191 (90%)	20 (9%)	2 (1%)	14	46
1	G	222/329 (68%)	182 (82%)	28 (13%)	12 (5%)	1	14
1	H	213/329 (65%)	193 (91%)	20 (9%)	0	100	100
2	C	1338/1342 (100%)	1225 (92%)	103 (8%)	10 (1%)	18	51
2	I	1338/1342 (100%)	1226 (92%)	100 (8%)	12 (1%)	14	46
3	D	1162/1407 (83%)	1074 (92%)	79 (7%)	9 (1%)	16	49
3	J	1151/1407 (82%)	1064 (92%)	82 (7%)	5 (0%)	30	61
4	E	87/91 (96%)	79 (91%)	8 (9%)	0	100	100
4	K	77/91 (85%)	74 (96%)	3 (4%)	0	100	100
5	F	461/613 (75%)	422 (92%)	37 (8%)	2 (0%)	30	61
5	L	463/613 (76%)	423 (91%)	39 (8%)	1 (0%)	43	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	7030/8222 (86%)	6424 (91%)	544 (8%)	62 (1%)	14	46

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	30	PRO
1	A	324	ALA
1	B	232	VAL
2	C	345	PRO
2	C	516	ASP
2	C	519	ASN
2	C	1159	VAL
3	D	10	ALA
1	G	13	LEU
1	G	14	VAL
1	G	62	ASP
1	G	162	GLU
2	I	516	ASP
2	I	1159	VAL
1	B	13	LEU
2	C	170	VAL
1	G	172	LEU
2	I	170	VAL
2	I	519	ASN
2	I	761	GLN
3	J	108	ALA
1	A	294	ASN
2	C	697	LYS
2	C	761	GLN
3	D	110	PRO
3	D	586	GLY
1	G	19	VAL
2	I	345	PRO
1	A	14	VAL
1	A	167	PRO
2	C	1158	LYS
3	D	806	ASP
1	G	136	GLU
1	G	164	ASP
2	I	697	LYS
3	J	710	ASP

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Mol	Chain	Res	Type
1	A	62	ASP
2	C	63	SER
2	C	760	ASN
3	D	710	ASP
5	F	477	GLU
1	G	49	SER
1	G	167	PRO
1	G	230	ALA
2	I	63	SER
2	I	484	LEU
2	I	514	PHE
2	I	1158	LYS
1	A	196	THR
3	D	108	ALA
5	F	513	ASP
1	G	134	THR
3	J	831	VAL
3	D	826	ILE
3	D	831	VAL
3	J	1180	VAL
5	L	477	GLU
2	I	1186	VAL
3	J	826	ILE
3	D	1180	VAL
1	A	178	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	268/286 (94%)	247 (92%)	21 (8%)	11	38
1	B	184/286 (64%)	163 (89%)	21 (11%)	5	26
1	G	191/286 (67%)	176 (92%)	15 (8%)	11	37
1	H	183/286 (64%)	162 (88%)	21 (12%)	5	25
2	C	1155/1157 (100%)	1036 (90%)	119 (10%)	7	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	1154/1157 (100%)	1037 (90%)	117 (10%)	7	30
3	D	975/1168 (84%)	863 (88%)	112 (12%)	5	25
3	J	967/1168 (83%)	859 (89%)	108 (11%)	6	27
4	E	72/75 (96%)	64 (89%)	8 (11%)	6	27
4	K	67/75 (89%)	62 (92%)	5 (8%)	12	39
5	F	416/540 (77%)	374 (90%)	42 (10%)	7	30
5	L	418/540 (77%)	374 (90%)	44 (10%)	6	29
All	All	6050/7024 (86%)	5417 (90%)	633 (10%)	6	29

All (633) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	19	VAL
1	A	26	VAL
1	A	29	GLU
1	A	50	SER
1	A	61	ILE
1	A	64	VAL
1	A	74	VAL
1	A	115	ILE
1	A	129	VAL
1	A	133	LEU
1	A	165	GLU
1	A	215	GLU
1	A	219	ARG
1	A	231	PHE
1	A	233	ASP
1	A	234	LEU
1	A	245	GLU
1	A	246	LYS
1	A	287	VAL
1	A	305	ASP
1	B	6	THR
1	B	7	GLU
1	B	8	PHE
1	B	18	GLN
1	B	27	THR
1	B	29	GLU
1	B	50	SER

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Mol	Chain	Res	Type
1	B	58	GLU
1	B	60	GLU
1	B	64	VAL
1	B	65	LEU
1	B	75	GLN
1	B	80	GLU
1	B	97	GLU
1	B	107	ILE
1	B	110	VAL
1	B	124	VAL
1	B	133	LEU
1	B	134	THR
1	B	183	ILE
1	B	193	GLU
2	C	4	SER
2	C	11	ILE
2	C	21	VAL
2	C	22	LEU
2	C	39	ILE
2	C	42	ASP
2	C	60	GLN
2	C	82	VAL
2	C	85	CYS
2	C	90	VAL
2	C	91	THR
2	C	115	LYS
2	C	116	ASP
2	C	117	ILE
2	C	118	LYS
2	C	119	GLU
2	C	120	GLN
2	C	121	GLU
2	C	132	ASP
2	C	167	SER
2	C	170	VAL
2	C	237	LEU
2	C	285	ILE
2	C	292	ILE
2	C	299	LYS
2	C	302	ILE
2	C	306	THR
2	C	320	ASP

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Mol	Chain	Res	Type
2	C	321	LEU
2	C	353	VAL
2	C	360	LEU
2	C	377	THR
2	C	379	GLU
2	C	394	ARG
2	C	400	VAL
2	C	419	ILE
2	C	423	ASP
2	C	434	ASP
2	C	445	ILE
2	C	453	ILE
2	C	484	LEU
2	C	486	THR
2	C	490	GLN
2	C	493	ILE
2	C	503	LYS
2	C	538	LEU
2	C	539	THR
2	C	542	ARG
2	C	550	VAL
2	C	558	VAL
2	C	565	GLU
2	C	589	THR
2	C	600	THR
2	C	604	HIS
2	C	607	SER
2	C	609	ILE
2	C	615	VAL
2	C	620	ASN
2	C	623	LEU
2	C	633	LEU
2	C	639	LYS
2	C	657	THR
2	C	672	GLU
2	C	680	LEU
2	C	692	THR
2	C	697	LYS
2	C	705	GLU
2	C	714	VAL
2	C	748	ILE
2	C	765	ILE

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Mol	Chain	Res	Type
2	C	773	LEU
2	C	781	ASP
2	C	788	SER
2	C	800	MET
2	C	817	LEU
2	C	819	SER
2	C	826	ASP
2	C	840	SER
2	C	859	GLU
2	C	878	THR
2	C	890	LYS
2	C	892	GLU
2	C	946	LEU
2	C	951	MET
2	C	974	ARG
2	C	979	LEU
2	C	984	VAL
2	C	1002	LEU
2	C	1040	ASP
2	C	1046	VAL
2	C	1073	LYS
2	C	1076	ILE
2	C	1082	ILE
2	C	1083	GLU
2	C	1108	ASN
2	C	1109	ILE
2	C	1114	GLU
2	C	1134	GLN
2	C	1146	GLN
2	C	1151	LEU
2	C	1156	ARG
2	C	1159	VAL
2	C	1161	LEU
2	C	1174	GLU
2	C	1180	MET
2	C	1198	LEU
2	C	1204	LEU
2	C	1210	ILE
2	C	1238	LEU
2	C	1253	LEU
2	C	1254	VAL
2	C	1264	GLN

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Mol	Chain	Res	Type
2	C	1293	VAL
2	C	1310	ASP
2	C	1327	LEU
2	C	1331	ARG
2	C	1340	GLU
2	C	1341	ASP
2	C	1342	GLU
3	D	8	LEU
3	D	9	LYS
3	D	18	ASP
3	D	20	ILE
3	D	26	SER
3	D	46	TYR
3	D	79	LYS
3	D	83	VAL
3	D	84	ILE
3	D	92	VAL
3	D	94	GLN
3	D	95	THR
3	D	97	VAL
3	D	106	GLU
3	D	159	ILE
3	D	169	LEU
3	D	172	PHE
3	D	175	GLU
3	D	217	LEU
3	D	244	VAL
3	D	252	LEU
3	D	255	LEU
3	D	312	ARG
3	D	324	LEU
3	D	330	MET
3	D	334	LYS
3	D	363	LEU
3	D	374	LEU
3	D	394	ILE
3	D	401	VAL
3	D	416	ILE
3	D	425	ARG
3	D	429	LEU
3	D	454	CYS
3	D	490	ILE

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Mol	Chain	Res	Type
3	D	501	VAL
3	D	506	VAL
3	D	507	VAL
3	D	513	MET
3	D	514	THR
3	D	536	LEU
3	D	545	HIS
3	D	547	ARG
3	D	567	THR
3	D	568	SER
3	D	573	THR
3	D	587	LEU
3	D	594	GLN
3	D	641	ILE
3	D	646	ILE
3	D	660	GLU
3	D	661	VAL
3	D	678	ARG
3	D	680	ASN
3	D	683	ILE
3	D	685	ILE
3	D	697	MET
3	D	698	MET
3	D	701	LEU
3	D	702	GLN
3	D	707	ILE
3	D	708	ASN
3	D	710	ASP
3	D	712	GLN
3	D	717	VAL
3	D	720	ASN
3	D	740	LEU
3	D	746	LEU
3	D	754	ILE
3	D	769	VAL
3	D	770	LEU
3	D	788	LEU
3	D	798	ARG
3	D	803	VAL
3	D	810	THR
3	D	826	ILE
3	D	844	THR

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Mol	Chain	Res	Type
3	D	847	ASP
3	D	848	VAL
3	D	849	LEU
3	D	853	THR
3	D	857	LEU
3	D	858	VAL
3	D	860	ARG
3	D	881	LYS
3	D	897	HIS
3	D	908	ILE
3	D	918	ILE
3	D	1135	THR
3	D	1155	ILE
3	D	1163	VAL
3	D	1170	LYS
3	D	1177	ILE
3	D	1186	TYR
3	D	1194	ARG
3	D	1202	GLU
3	D	1221	LEU
3	D	1255	VAL
3	D	1268	ASN
3	D	1273	ASP
3	D	1274	PHE
3	D	1275	LEU
3	D	1278	GLU
3	D	1281	GLU
3	D	1284	ARG
3	D	1285	VAL
3	D	1289	ASN
3	D	1293	GLU
3	D	1298	VAL
3	D	1310	THR
3	D	1333	THR
3	D	1343	GLU
4	E	5	THR
4	E	13	ILE
4	E	16	ARG
4	E	21	LEU
4	E	28	ARG
4	E	39	VAL
4	E	46	THR

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Mol	Chain	Res	Type
4	E	58	LEU
5	F	98	VAL
5	F	100	MET
5	F	102	MET
5	F	127	ILE
5	F	130	VAL
5	F	154	GLU
5	F	247	GLU
5	F	267	ASP
5	F	297	MET
5	F	301	ASN
5	F	305	LEU
5	F	306	PHE
5	F	310	GLU
5	F	341	LEU
5	F	395	THR
5	F	400	GLN
5	F	429	THR
5	F	437	GLN
5	F	449	THR
5	F	450	ILE
5	F	471	LEU
5	F	472	GLN
5	F	479	THR
5	F	482	GLU
5	F	485	GLU
5	F	486	ARG
5	F	488	LEU
5	F	489	MET
5	F	494	ILE
5	F	502	LYS
5	F	508	GLU
5	F	530	LEU
5	F	547	VAL
5	F	558	VAL
5	F	561	MET
5	F	566	ASP
5	F	568	ASN
5	F	572	THR
5	F	580	PHE
5	F	587	ILE
5	F	603	ARG

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Mol	Chain	Res	Type
5	F	606	VAL
1	G	18	GLN
1	G	27	THR
1	G	50	SER
1	G	58	GLU
1	G	64	VAL
1	G	65	LEU
1	G	80	GLU
1	G	124	VAL
1	G	133	LEU
1	G	136	GLU
1	G	161	SER
1	G	163	GLU
1	G	171	LEU
1	G	183	ILE
1	G	193	GLU
1	H	8	PHE
1	H	16	ILE
1	H	18	GLN
1	H	27	THR
1	H	29	GLU
1	H	50	SER
1	H	58	GLU
1	H	60	GLU
1	H	64	VAL
1	H	65	LEU
1	H	75	GLN
1	H	80	GLU
1	H	97	GLU
1	H	107	ILE
1	H	110	VAL
1	H	124	VAL
1	H	133	LEU
1	H	134	THR
1	H	171	LEU
1	H	183	ILE
1	H	193	GLU
2	I	4	SER
2	I	11	ILE
2	I	21	VAL
2	I	22	LEU
2	I	39	ILE

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Mol	Chain	Res	Type
2	I	60	GLN
2	I	82	VAL
2	I	85	CYS
2	I	90	VAL
2	I	91	THR
2	I	115	LYS
2	I	116	ASP
2	I	117	ILE
2	I	118	LYS
2	I	119	GLU
2	I	121	GLU
2	I	132	ASP
2	I	167	SER
2	I	170	VAL
2	I	237	LEU
2	I	285	ILE
2	I	292	ILE
2	I	299	LYS
2	I	302	ILE
2	I	306	THR
2	I	316	GLU
2	I	320	ASP
2	I	321	LEU
2	I	353	VAL
2	I	360	LEU
2	I	377	THR
2	I	379	GLU
2	I	394	ARG
2	I	400	VAL
2	I	419	ILE
2	I	423	ASP
2	I	434	ASP
2	I	445	ILE
2	I	453	ILE
2	I	484	LEU
2	I	486	THR
2	I	490	GLN
2	I	493	ILE
2	I	503	LYS
2	I	538	LEU
2	I	539	THR
2	I	542	ARG

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Mol	Chain	Res	Type
2	I	550	VAL
2	I	558	VAL
2	I	565	GLU
2	I	589	THR
2	I	604	HIS
2	I	607	SER
2	I	609	ILE
2	I	615	VAL
2	I	620	ASN
2	I	623	LEU
2	I	633	LEU
2	I	639	LYS
2	I	657	THR
2	I	672	GLU
2	I	680	LEU
2	I	692	THR
2	I	697	LYS
2	I	705	GLU
2	I	714	VAL
2	I	748	ILE
2	I	757	THR
2	I	765	ILE
2	I	773	LEU
2	I	781	ASP
2	I	788	SER
2	I	800	MET
2	I	817	LEU
2	I	819	SER
2	I	826	ASP
2	I	840	SER
2	I	859	GLU
2	I	878	THR
2	I	890	LYS
2	I	892	GLU
2	I	946	LEU
2	I	951	MET
2	I	974	ARG
2	I	979	LEU
2	I	984	VAL
2	I	1002	LEU
2	I	1040	ASP
2	I	1046	VAL

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Mol	Chain	Res	Type
2	I	1073	LYS
2	I	1076	ILE
2	I	1082	ILE
2	I	1083	GLU
2	I	1108	ASN
2	I	1109	ILE
2	I	1114	GLU
2	I	1134	GLN
2	I	1146	GLN
2	I	1151	LEU
2	I	1156	ARG
2	I	1159	VAL
2	I	1161	LEU
2	I	1174	GLU
2	I	1180	MET
2	I	1198	LEU
2	I	1204	LEU
2	I	1210	ILE
2	I	1238	LEU
2	I	1254	VAL
2	I	1264	GLN
2	I	1293	VAL
2	I	1310	ASP
2	I	1327	LEU
2	I	1331	ARG
2	I	1340	GLU
2	I	1341	ASP
2	I	1342	GLU
3	J	18	ASP
3	J	20	ILE
3	J	26	SER
3	J	46	TYR
3	J	79	LYS
3	J	83	VAL
3	J	84	ILE
3	J	92	VAL
3	J	94	GLN
3	J	95	THR
3	J	97	VAL
3	J	106	GLU
3	J	159	ILE
3	J	169	LEU

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Mol	Chain	Res	Type
3	J	172	PHE
3	J	175	GLU
3	J	217	LEU
3	J	244	VAL
3	J	252	LEU
3	J	256	ASP
3	J	306	LEU
3	J	312	ARG
3	J	324	LEU
3	J	330	MET
3	J	334	LYS
3	J	363	LEU
3	J	374	LEU
3	J	394	ILE
3	J	401	VAL
3	J	425	ARG
3	J	429	LEU
3	J	454	CYS
3	J	490	ILE
3	J	501	VAL
3	J	506	VAL
3	J	507	VAL
3	J	510	LEU
3	J	513	MET
3	J	514	THR
3	J	536	LEU
3	J	545	HIS
3	J	547	ARG
3	J	567	THR
3	J	568	SER
3	J	573	THR
3	J	594	GLN
3	J	641	ILE
3	J	646	ILE
3	J	660	GLU
3	J	661	VAL
3	J	678	ARG
3	J	680	ASN
3	J	683	ILE
3	J	685	ILE
3	J	697	MET
3	J	698	MET

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Mol	Chain	Res	Type
3	J	701	LEU
3	J	702	GLN
3	J	707	ILE
3	J	708	ASN
3	J	710	ASP
3	J	712	GLN
3	J	717	VAL
3	J	720	ASN
3	J	740	LEU
3	J	746	LEU
3	J	754	ILE
3	J	769	VAL
3	J	770	LEU
3	J	788	LEU
3	J	798	ARG
3	J	810	THR
3	J	826	ILE
3	J	844	THR
3	J	847	ASP
3	J	848	VAL
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	858	VAL
3	J	860	ARG
3	J	881	LYS
3	J	897	HIS
3	J	908	ILE
3	J	918	ILE
3	J	1155	ILE
3	J	1163	VAL
3	J	1170	LYS
3	J	1177	ILE
3	J	1186	TYR
3	J	1194	ARG
3	J	1202	GLU
3	J	1221	LEU
3	J	1255	VAL
3	J	1268	ASN
3	J	1273	ASP
3	J	1274	PHE
3	J	1275	LEU

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Mol	Chain	Res	Type
3	J	1278	GLU
3	J	1281	GLU
3	J	1284	ARG
3	J	1285	VAL
3	J	1289	ASN
3	J	1293	GLU
3	J	1298	VAL
3	J	1310	THR
3	J	1333	THR
3	J	1343	GLU
4	K	13	ILE
4	K	21	LEU
4	K	39	VAL
4	K	46	THR
4	K	58	LEU
5	L	98	VAL
5	L	100	MET
5	L	102	MET
5	L	127	ILE
5	L	130	VAL
5	L	154	GLU
5	L	247	GLU
5	L	267	ASP
5	L	297	MET
5	L	301	ASN
5	L	305	LEU
5	L	306	PHE
5	L	310	GLU
5	L	341	LEU
5	L	395	THR
5	L	400	GLN
5	L	429	THR
5	L	437	GLN
5	L	449	THR
5	L	450	ILE
5	L	471	LEU
5	L	472	GLN
5	L	479	THR
5	L	482	GLU
5	L	485	GLU
5	L	486	ARG
5	L	488	LEU

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Mol	Chain	Res	Type
5	L	489	MET
5	L	491	GLU
5	L	494	ILE
5	L	502	LYS
5	L	508	GLU
5	L	530	LEU
5	L	547	VAL
5	L	558	VAL
5	L	561	MET
5	L	566	ASP
5	L	568	ASN
5	L	572	THR
5	L	580	PHE
5	L	587	ILE
5	L	603	ARG
5	L	606	VAL
5	L	613	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	117	HIS
1	A	128	HIS
1	A	268	ASN
1	A	276	HIS
1	A	283	GLN
1	B	137	ASN
2	C	69	GLN
2	C	120	GLN
2	C	139	ASN
2	C	343	HIS
2	C	490	GLN
2	C	494	ASN
2	C	573	ASN
2	C	628	HIS
2	C	677	ASN
2	C	761	GLN
2	C	799	ASN
2	C	1111	GLN
2	C	1116	HIS
2	C	1136	GLN

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Mol	Chain	Res	Type
2	C	1146	GLN
2	C	1237	HIS
2	C	1288	GLN
2	C	1299	ASN
2	C	1312	ASN
2	C	1313	HIS
2	C	1314	GLN
2	C	1336	ASN
3	D	94	GLN
3	D	158	GLN
3	D	196	GLN
3	D	200	GLN
3	D	209	ASN
3	D	340	GLN
3	D	365	GLN
3	D	450	HIS
3	D	560	ASN
3	D	594	GLN
3	D	669	GLN
3	D	702	GLN
3	D	716	GLN
3	D	907	HIS
3	D	910	ASN
3	D	929	GLN
3	D	1218	HIS
3	D	1227	HIS
5	F	128	ASN
5	F	131	GLN
5	F	301	ASN
5	F	317	ASN
5	F	362	ASN
5	F	396	ASN
5	F	406	GLN
5	F	437	GLN
5	F	446	GLN
5	F	472	GLN
5	F	518	HIS
5	F	579	GLN
1	G	41	ASN
1	G	75	GLN
1	H	18	GLN
1	H	132	HIS

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Mol	Chain	Res	Type
1	H	137	ASN
2	I	139	ASN
2	I	343	HIS
2	I	494	ASN
2	I	628	HIS
2	I	658	GLN
2	I	688	GLN
2	I	760	ASN
2	I	761	GLN
2	I	1013	GLN
2	I	1116	HIS
2	I	1220	GLN
2	I	1313	HIS
2	I	1314	GLN
2	I	1336	ASN
3	J	94	GLN
3	J	200	GLN
3	J	206	ASN
3	J	294	ASN
3	J	419	HIS
3	J	489	ASN
3	J	504	GLN
3	J	667	GLN
3	J	702	GLN
3	J	716	GLN
3	J	739	GLN
3	J	817	HIS
3	J	910	ASN
3	J	929	GLN
3	J	1235	ASN
3	J	1268	ASN
3	J	1279	GLN
3	J	1366	HIS
5	L	128	ASN
5	L	129	GLN
5	L	283	GLN
5	L	294	GLN
5	L	317	ASN
5	L	323	ASN
5	L	345	GLN
5	L	362	ASN
5	L	446	GLN

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Mol	Chain	Res	Type
5	L	455	HIS
5	L	464	ASN
5	L	472	GLN
5	L	545	HIS
5	L	579	GLN
5	L	600	HIS

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 6 ligands modelled in this entry, 6 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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	309/329 (93%)	-0.57	0 100 100	99, 147, 225, 245	0
1	B	217/329 (65%)	-0.45	0 100 100	112, 194, 254, 272	0
1	G	224/329 (68%)	-0.49	0 100 100	163, 206, 241, 270	0
1	H	217/329 (65%)	-0.47	0 100 100	146, 213, 252, 285	0
2	C	1340/1342 (99%)	-0.60	0 100 100	74, 121, 234, 285	0
2	I	1340/1342 (99%)	-0.57	0 100 100	86, 159, 261, 388	0
3	D	1166/1407 (82%)	-0.62	0 100 100	72, 112, 215, 264	0
3	J	1155/1407 (82%)	-0.61	0 100 100	86, 138, 229, 274	0
4	E	89/91 (97%)	-0.52	0 100 100	147, 183, 216, 241	0
4	K	79/91 (86%)	-0.45	1 (1%) 75 48	202, 277, 319, 350	0
5	F	467/613 (76%)	-0.56	0 100 100	93, 165, 290, 340	0
5	L	469/613 (76%)	-0.63	0 100 100	116, 178, 288, 353	0
All	All	7072/8222 (86%)	-0.58	1 (0%) 100 100	72, 147, 251, 388	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	K	16	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	D	1501	1/1	0.85	0.12	87,87,87,87	0
6	MG	J	1501	1/1	0.91	0.13	94,94,94,94	0
7	ZN	D	1502	1/1	0.95	0.06	134,134,134,134	0
7	ZN	J	1503	1/1	0.96	0.04	97,97,97,97	0
7	ZN	J	1502	1/1	0.99	0.04	131,131,131,131	0
7	ZN	D	1503	1/1	1.00	0.07	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.