



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 11:24 PM GMT

PDB ID : 4XLQ
Title : Crystal structure of T.aquaticus transcription initiation complex containing upstream fork (-11 base-paired) promoter
Authors : Bae, B.; Darst, S.A.
Deposited on : 2015-01-13
Resolution : 4.60 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

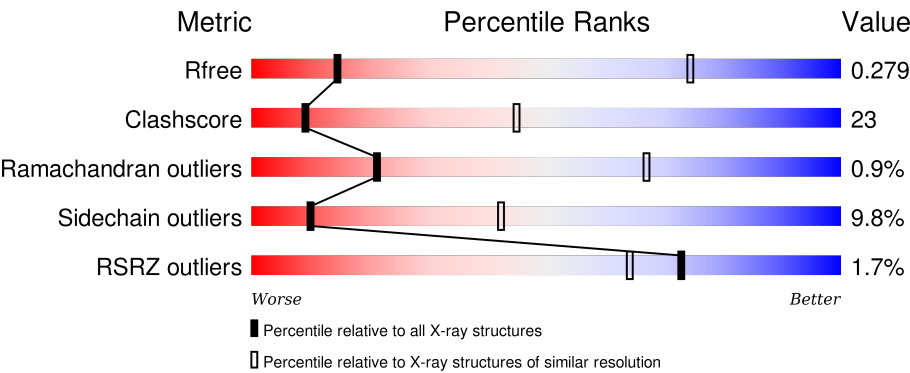
MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.60 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}	91344	1089 (5.52-3.60)
Clashscore	102246	1004 (5.52-3.64)
Ramachandran outliers	100387	1131 (5.52-3.60)
Sidechain outliers	100360	1112 (5.50-3.60)
RSRZ outliers	91569	1092 (5.52-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	314	<div><div>%</div><div><div></div><div>40%</div><div>28%</div><div>•</div><div>28%</div></div></div>
1	B	314	<div><div></div><div>33%</div><div>34%</div><div>5%</div><div>28%</div></div>
1	G	314	<div><div>5%</div><div></div><div>36%</div><div>31%</div><div>5%</div><div>28%</div></div>
1	H	314	<div><div>%</div><div></div><div>35%</div><div>32%</div><div>5%</div><div>28%</div></div>
2	C	1119	<div><div>2%</div><div></div><div>45%</div><div>48%</div><div>6%</div><div>•</div></div>

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Mol	Chain	Length	Quality of chain
2	I	1119	
3	D	1524	
3	J	1524	
4	E	99	
4	K	99	
5	F	347	
5	L	347	
6	O	30	
6	R	30	
7	P	26	
7	S	26	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 56477 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	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	B	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	G	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	H	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1112	Total	C	N	O	S	0	0	0
			8739	5531	1553	1632	23			
2	I	1112	Total	C	N	O	S	0	0	0
			8739	5531	1553	1632	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1490	Total	C	N	O	S	0	0	0
			11761	7439	2088	2196	38			
3	J	1367	Total	C	N	O	S	0	0	0
			10779	6810	1923	2010	36			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	93	Total	C	N	O	S	0	0	0
			768	490	136	138	4			
4	K	93	Total	C	N	O	S	0	0	0
			768	490	136	138	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2787	1758	502	523	4			
5	L	345	Total	C	N	O	S	0	0	0
			2787	1758	502	523	4			

- Molecule 6 is a DNA chain called DNA (30-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	O	30	Total	C	N	O	P	0	0	0
			613	296	109	179	29			
6	R	30	Total	C	N	O	P	0	0	0
			613	296	109	179	29			

- Molecule 7 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	P	25	Total	C	N	O	P	0	0	0
			510	245	91	149	25			
7	S	26	Total	C	N	O	P	0	0	0
			527	255	93	154	25			

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

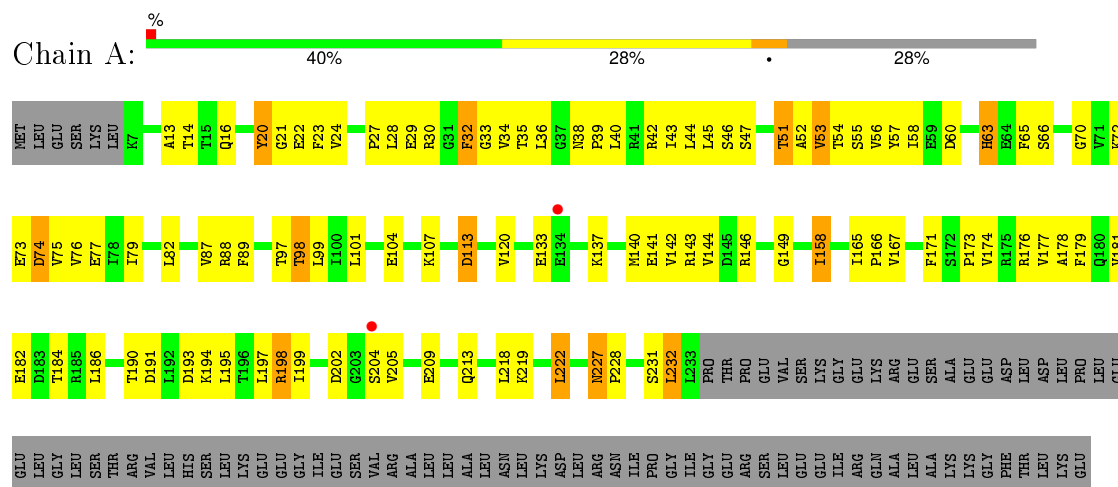
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

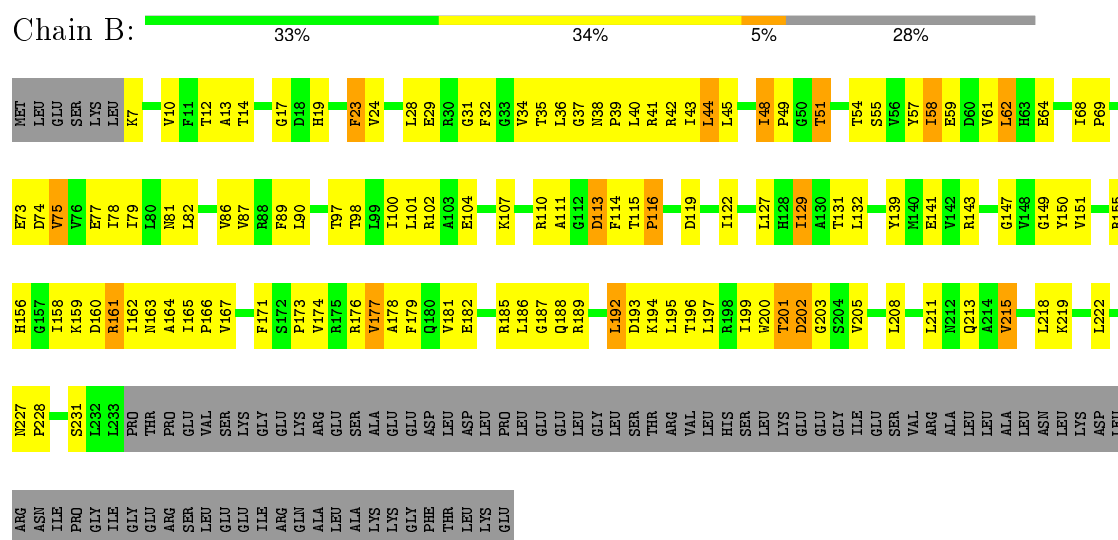
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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

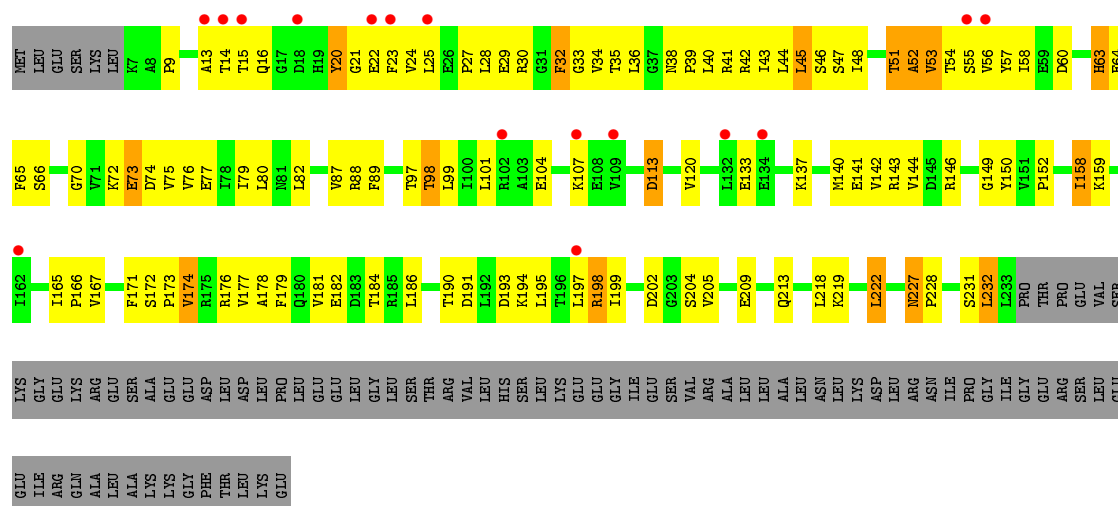


- Molecule 1: DNA-directed RNA polymerase subunit alpha

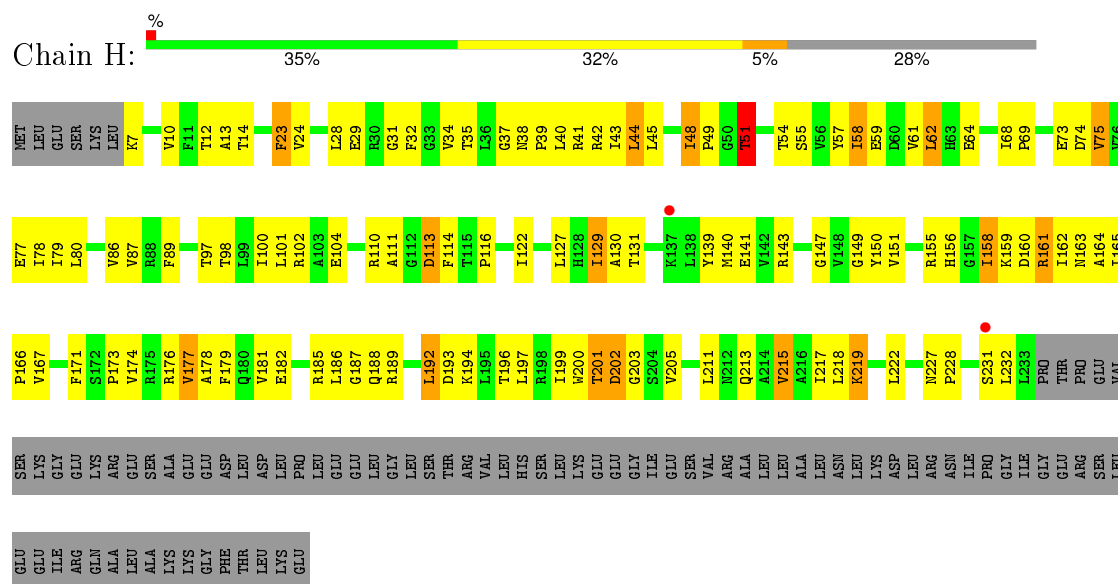


- Molecule 1: DNA-directed RNA polymerase subunit alpha

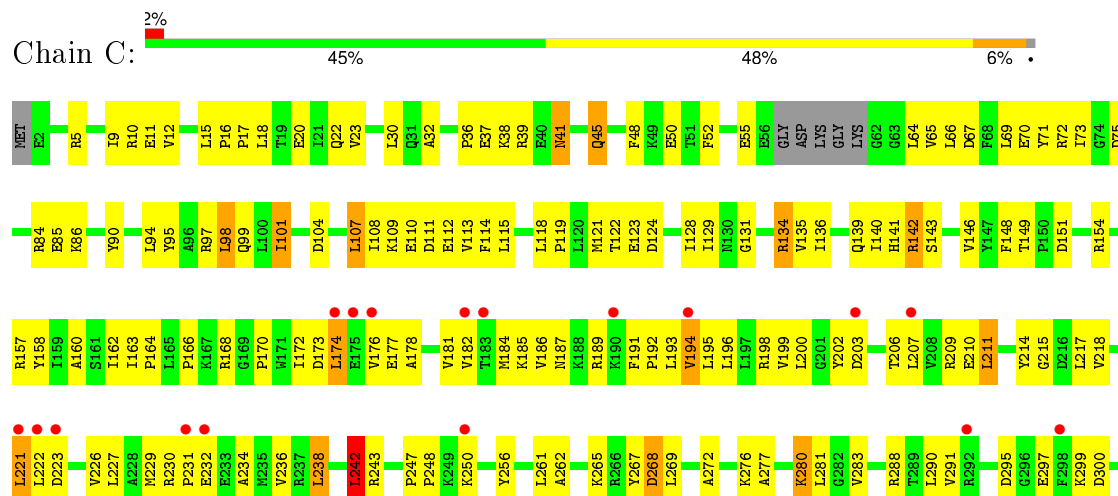




• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 2: DNA-directed RNA polymerase subunit beta

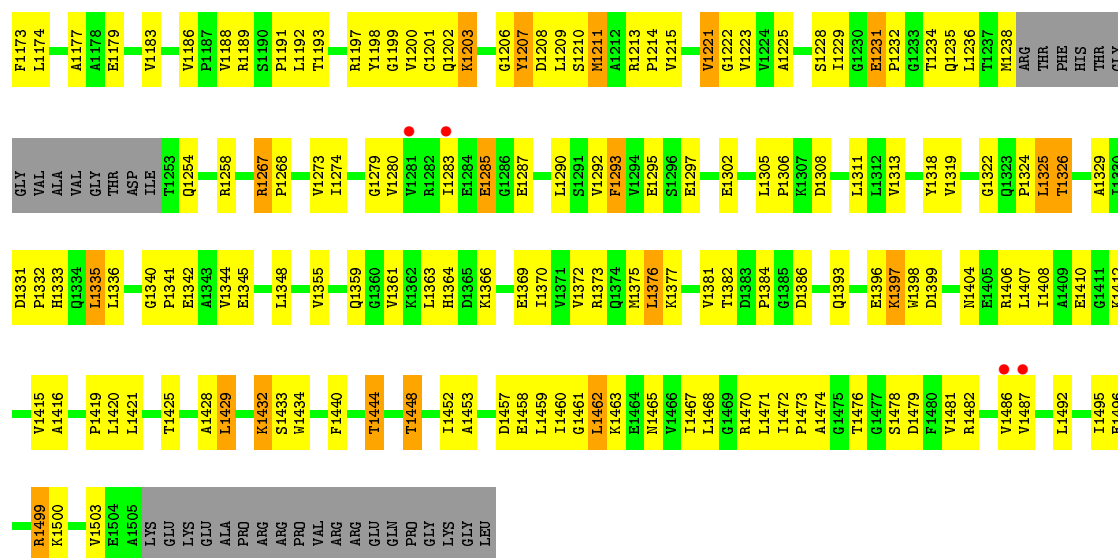




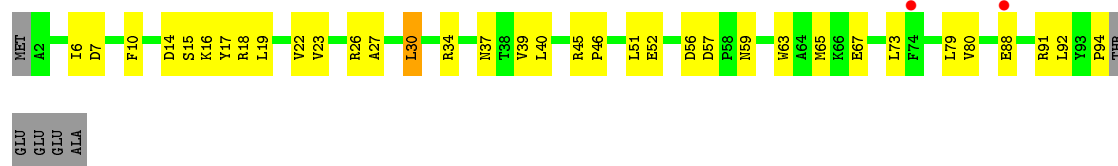




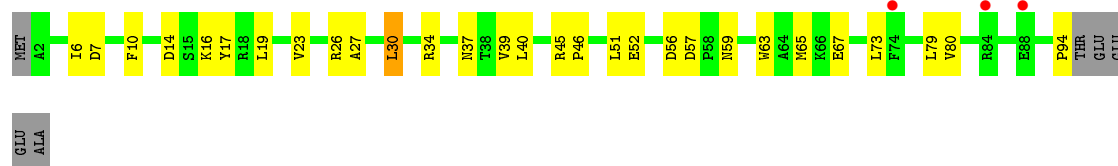
MET	K2	V5	K6	V7	V8	R9	I10	A11	L12	A13	A14	P15	S22	E25	V26	E27	E30	T31	I32	N33	Y34	L37	K38	P39	E40	R41	D42	D46	E47	R48	I49	F50	I53	K54	D55	Y56	E57	C58	K62	R65	Q66	R67	F68	K71	W72	C73	V78	E79																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
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MET	THR	PRO	LEU	VAL	GLY	GLY	GLY	ILE	VAL	GLY	GLY	GLN	PRO	LEU	ALA	GLY	LYS	GLY	LEU	ARG	LEU	PRO	ARG	GLY	ASP	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
K951	I354	V355	P356	V361	I367	I371	D372	E375	E376	E377	H388	E389	P390	I393	L394	V395	V396	K397	A398	R399	V400	Y401	P402	F403	E404	D405	D406	V407	T410	T411	G412	D413	R414	V415	V420	L421	A422	D423	K426	V427	E430	G433	R434	V435	E436	V437	D438																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
L439	V440	R442	V443	V444	R445	V446	V447	E448	S449	D450	V451	L452	D453	N454	D455	L456	R457	E458	E459	Q460	P461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	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



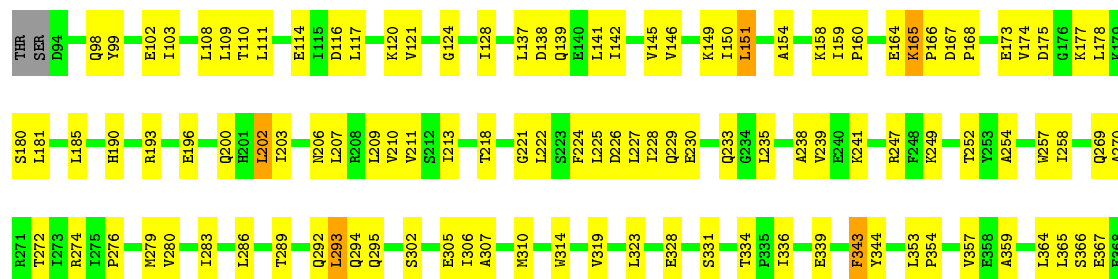
• Molecule 4: DNA-directed RNA polymerase subunit omega

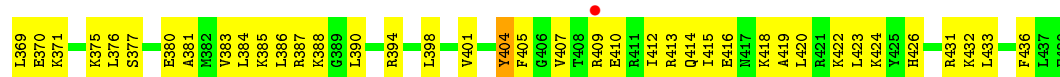


• Molecule 4: DNA-directed RNA polymerase subunit omega

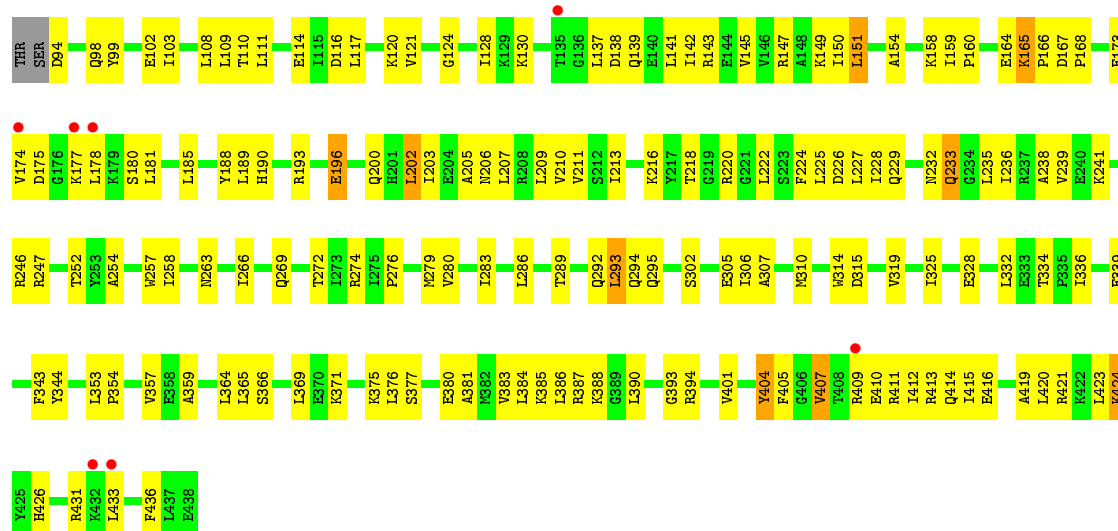


• Molecule 5: RNA polymerase sigma factor SigA





• Molecule 5: RNA polymerase sigma factor SigA



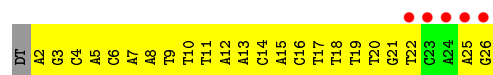
• Molecule 6: DNA (30-MER)



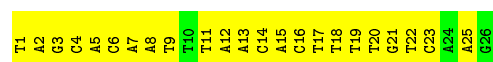
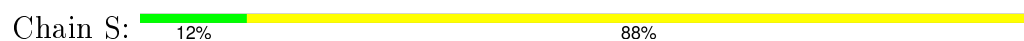
• Molecule 6: DNA (30-MER)



• Molecule 7: DNA (26-MER)



• Molecule 7: DNA (26-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	288.23Å 288.23Å 535.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.81 – 4.60 49.81 – 4.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.81-4.60) 98.6 (49.81-4.60)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 4.64Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, R_{free}	0.245 , 0.281 0.240 , 0.279	Depositor DCC
R_{free} test set	6217 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	154.6	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 174.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.17$	Xtriage
Outliers	0 of 123373 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	56477	wwPDB-VP
Average B, all atoms (Å ²)	175.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, MG

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	0.31	0/1804	0.64	1/2455 (0.0%)
1	B	0.30	0/1804	0.61	0/2455
1	G	0.31	0/1804	0.64	1/2455 (0.0%)
1	H	0.30	0/1804	0.61	0/2455
2	C	0.27	0/8905	0.55	2/12040 (0.0%)
2	I	0.27	0/8905	0.55	2/12040 (0.0%)
3	D	0.28	0/11963	0.55	3/16165 (0.0%)
3	J	0.28	0/10959	0.57	1/14802 (0.0%)
4	E	0.25	0/783	0.54	0/1054
4	K	0.25	0/783	0.53	0/1054
5	F	0.27	0/2829	0.55	1/3804 (0.0%)
5	L	0.27	0/2829	0.55	1/3804 (0.0%)
6	O	0.50	0/687	0.92	0/1059
6	R	0.50	0/687	0.91	0/1059
7	P	0.54	0/571	0.93	0/878
7	S	0.54	0/590	0.93	0/908
All	All	0.29	0/57707	0.59	12/78487 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	3
2	I	0	3
3	D	0	1
3	J	0	1
All	All	0	8

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	311	LEU	CA-CB-CG	7.45	132.43	115.30
3	D	1134	LEU	CA-CB-CG	6.98	131.36	115.30
2	I	417	GLY	N-CA-C	6.42	129.14	113.10
2	C	417	GLY	N-CA-C	6.40	129.09	113.10
3	J	1134	LEU	CA-CB-CG	5.63	128.26	115.30
1	A	52	ALA	C-N-CA	5.63	135.77	121.70
1	G	52	ALA	C-N-CA	5.47	135.38	121.70
5	F	151	LEU	CA-CB-CG	5.32	127.53	115.30
3	D	964	LEU	CA-CB-CG	5.31	127.50	115.30
2	I	242	LEU	CA-CB-CG	5.19	127.23	115.30
2	C	242	LEU	CA-CB-CG	5.16	127.17	115.30
5	L	151	LEU	CA-CB-CG	5.08	126.99	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	415	PRO	Peptide
2	C	423	ALA	Peptide
2	C	737	LEU	Peptide
3	D	1208	ASP	Peptide
2	I	415	PRO	Peptide
2	I	423	ALA	Peptide
2	I	737	LEU	Peptide
3	J	1359	GLN	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	1770	0	1799	89	0
1	B	1770	0	1799	101	0
1	G	1770	0	1799	103	0
1	H	1770	0	1799	95	0
2	C	8739	0	8841	499	0
2	I	8739	0	8841	485	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	11761	0	11976	585	0
3	J	10779	0	10993	503	0
4	E	768	0	784	37	0
4	K	768	0	784	29	0
5	F	2787	0	2866	120	0
5	L	2787	0	2866	133	0
6	O	613	0	343	28	0
6	R	613	0	343	26	0
7	P	510	0	284	27	0
7	S	527	0	297	25	0
8	D	2	0	0	0	0
8	J	2	0	0	0	0
9	D	1	0	0	0	0
9	J	1	0	0	0	0
All	All	56477	0	56414	2598	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (2598) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:707:ARG:HE	2:C:824:ARG:HE	1.17	0.90
6:R:24:DC:H42	7:S:3:DG:H1	1.18	0.90
4:E:30:LEU:HD12	4:E:37:ASN:HD21	1.39	0.88
3:D:105:VAL:HA	3:D:112:ILE:HD11	1.55	0.88
4:K:30:LEU:HD12	4:K:37:ASN:HD21	1.39	0.87
2:I:537:LYS:HZ3	2:I:905:VAL:H	1.19	0.87
1:A:158:ILE:HB	1:A:166:PRO:HG3	1.57	0.86
2:I:707:ARG:HE	2:I:824:ARG:HE	1.17	0.86
2:I:557:ARG:HG3	2:I:879:ARG:HB3	1.57	0.86
2:C:537:LYS:HZ3	2:C:905:VAL:H	1.21	0.86
3:J:105:VAL:HA	3:J:112:ILE:HD11	1.59	0.85
2:C:557:ARG:HG3	2:C:879:ARG:HB3	1.59	0.85
3:D:231:VAL:H	3:D:243:ALA:HA	1.43	0.84
1:H:48:ILE:HA	1:H:213:GLN:HE22	1.44	0.83
1:G:158:ILE:HB	1:G:166:PRO:HG3	1.58	0.83
2:C:313:LEU:HD13	2:C:321:GLU:HA	1.61	0.83
2:I:313:LEU:HD13	2:I:321:GLU:HA	1.61	0.82
2:C:857:ASP:HB3	2:C:978:ARG:HG2	1.62	0.82
1:B:48:ILE:HA	1:B:213:GLN:HE22	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:857:ASP:HB3	2:I:978:ARG:HG2	1.62	0.82
2:C:750:LYS:HD3	3:D:681:ARG:HG3	1.60	0.82
3:D:835:SER:HB3	3:D:838:ARG:HE	1.44	0.81
2:C:716:LYS:HG3	3:D:37:LEU:HD11	1.62	0.81
2:I:15:LEU:H	2:I:586:ARG:HH22	1.27	0.81
2:C:494:TYR:HB3	2:C:530:GLU:HG3	1.62	0.81
2:I:324:ASP:HB3	2:I:327:HIS:HB2	1.63	0.80
2:I:1033:GLY:HA2	3:J:620:GLY:HA3	1.64	0.80
2:I:716:LYS:HG3	3:J:37:LEU:HD11	1.63	0.80
2:C:1033:GLY:HA2	3:D:620:GLY:HA3	1.63	0.80
2:C:15:LEU:H	2:C:586:ARG:HH22	1.29	0.80
2:C:808:ARG:HH11	2:C:815:LEU:H	1.29	0.80
3:D:792:ILE:HG21	3:D:941:LEU:HD22	1.63	0.80
2:I:808:ARG:HH11	2:I:815:LEU:H	1.30	0.79
3:J:97:THR:HG21	3:J:571:LYS:HG3	1.64	0.79
1:B:151:VAL:HG13	1:B:155:ARG:HB2	1.64	0.79
3:J:1142:SER:O	3:J:1364:HIS:ND1	2.13	0.79
3:D:166:GLN:HB3	3:D:396:VAL:HG13	1.64	0.79
3:D:708:LEU:HD12	3:D:1231:GLU:HG2	1.66	0.78
5:L:164:GLU:HG3	5:L:165:LYS:HD2	1.66	0.78
2:I:1036:GLU:HA	3:J:707:THR:HG21	1.66	0.78
3:D:700:VAL:HG22	3:D:718:PRO:HG3	1.65	0.78
2:C:1008:ARG:HD3	2:C:1028:GLY:HA2	1.66	0.78
1:G:97:THR:HG23	1:G:98:THR:H	1.49	0.77
2:I:494:TYR:HB3	2:I:530:GLU:HG3	1.64	0.77
3:J:1202:GLN:NE2	3:J:1215:VAL:O	2.12	0.77
3:J:700:VAL:HG22	3:J:718:PRO:HG3	1.64	0.77
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.66	0.77
2:I:595:LEU:HD23	2:I:639:GLN:HE22	1.49	0.77
3:J:47:GLU:HG3	3:J:53:ILE:HG13	1.67	0.77
1:A:27:PRO:HD3	1:A:186:LEU:HD22	1.64	0.77
2:I:129:ILE:HD13	2:I:134:ARG:HB2	1.66	0.77
3:J:208:PRO:HA	3:J:390:PRO:HA	1.67	0.77
3:J:563:PRO:HB3	5:L:200:GLN:HB3	1.66	0.77
3:J:792:ILE:HG21	3:J:941:LEU:HD22	1.65	0.77
7:P:13:DA:H1'	7:P:14:DC:H5'	1.67	0.76
1:A:222:LEU:HD13	1:B:218:LEU:HD23	1.66	0.76
7:P:15:DA:H1'	7:P:16:DC:H5'	1.66	0.76
1:H:151:VAL:HG13	1:H:155:ARG:HB2	1.64	0.76
3:D:270:ILE:HB	3:D:282:TYR:HB2	1.67	0.76
2:C:32:ALA:HA	2:C:73:ILE:HG21	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:838:LYS:HB3	2:I:997:LEU:HB2	1.68	0.76
2:I:32:ALA:HA	2:I:73:ILE:HG21	1.68	0.76
3:D:47:GLU:HG3	3:D:53:ILE:HG13	1.68	0.76
1:A:97:THR:HG23	1:A:98:THR:H	1.48	0.76
2:I:710:ILE:HG21	2:I:756:VAL:HG21	1.66	0.76
3:D:879:ARG:HH12	3:D:905:PRO:HA	1.50	0.76
5:F:164:GLU:HG3	5:F:165:LYS:HD2	1.66	0.76
1:G:222:LEU:HD13	1:H:218:LEU:HD23	1.65	0.76
2:C:129:ILE:HD13	2:C:134:ARG:HB2	1.68	0.76
3:J:1486:VAL:HG11	4:K:26:ARG:HB2	1.68	0.75
5:L:203:ILE:HG12	5:L:239:VAL:HG21	1.68	0.75
1:A:184:THR:HB	1:A:194:LYS:HB3	1.67	0.75
5:F:203:ILE:HG12	5:F:239:VAL:HG21	1.67	0.75
3:J:1147:ARG:HB3	3:J:1188:VAL:HG11	1.66	0.75
2:I:750:LYS:HD3	3:J:681:ARG:HG3	1.67	0.75
3:D:169:TYR:HE2	3:D:395:VAL:HG12	1.50	0.75
7:S:12:DA:H1'	7:S:13:DA:H5'	1.68	0.75
1:G:27:PRO:HD3	1:G:186:LEU:HD22	1.66	0.75
1:G:184:THR:HB	1:G:194:LYS:HB3	1.69	0.75
2:C:72:ARG:HB3	2:C:95:TYR:HB2	1.69	0.75
1:G:55:SER:HB2	1:G:158:ILE:HG12	1.68	0.74
3:D:1208:ASP:O	3:D:1210:SER:N	2.20	0.74
3:J:73:CYS:HB3	3:J:78:VAL:H	1.52	0.74
3:D:73:CYS:HB3	3:D:78:VAL:H	1.51	0.74
2:C:595:LEU:HD23	2:C:639:GLN:HE22	1.50	0.74
2:C:838:LYS:HB3	2:C:997:LEU:HB2	1.69	0.74
1:A:53:VAL:HG22	1:A:54:THR:H	1.52	0.74
1:A:205:VAL:HG13	1:A:209:GLU:HB2	1.69	0.74
2:C:1036:GLU:HA	3:D:707:THR:HG21	1.70	0.74
2:C:86:LYS:HE2	2:C:813:VAL:HG23	1.70	0.74
3:D:1143:GLY:HA2	3:D:1364:HIS:CE1	2.22	0.74
2:I:370:ALA:HB1	5:L:295:GLN:HE22	1.53	0.74
2:C:419:THR:HG23	2:C:421:GLU:H	1.53	0.74
7:P:2:DA:H1'	7:P:3:DG:H5'	1.70	0.74
3:D:39:PRO:HB3	3:D:46:ASP:HA	1.70	0.73
3:D:1223:VAL:HG21	3:D:1462:LEU:HD21	1.69	0.73
2:C:724:ARG:HG3	2:C:737:LEU:HD23	1.70	0.73
4:E:30:LEU:HD12	4:E:37:ASN:ND2	2.03	0.73
1:G:53:VAL:HG22	1:G:54:THR:H	1.53	0.73
2:I:601:GLY:HA2	2:I:615:TYR:HA	1.70	0.73
3:D:1486:VAL:HG11	4:E:26:ARG:HB2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:191:LEU:HD11	3:D:197:SER:HB2	1.70	0.73
2:I:1064:ASN:HD22	5:L:359:ALA:HB2	1.53	0.73
1:H:57:TYR:CG	1:H:161:ARG:HG2	2.23	0.73
3:J:165:LYS:H	3:J:397:LYS:HE2	1.52	0.73
2:C:662:GLU:HG2	2:C:663:GLU:HG2	1.69	0.73
4:E:27:ALA:HA	4:E:30:LEU:HD22	1.71	0.73
2:C:710:ILE:HG21	2:C:756:VAL:HG21	1.69	0.73
2:C:498:GLN:HG3	3:D:1068:LEU:HD11	1.71	0.73
2:I:724:ARG:HG3	2:I:737:LEU:HD23	1.71	0.73
2:I:662:GLU:HG2	2:I:663:GLU:HG2	1.71	0.73
3:D:39:PRO:HG2	3:D:47:GLU:HB2	1.71	0.73
2:I:1008:ARG:HD3	2:I:1028:GLY:HA2	1.71	0.73
2:C:541:SER:O	2:C:545:ASN:ND2	2.22	0.72
3:J:1336:LEU:HA	3:J:1344:VAL:HG21	1.71	0.72
3:J:680:GLN:HG2	3:J:681:ARG:H	1.54	0.72
3:D:596:SER:OG	3:D:597:GLU:N	2.20	0.72
3:D:680:GLN:HG2	3:D:681:ARG:H	1.53	0.72
1:A:55:SER:HB2	1:A:158:ILE:HG12	1.70	0.72
3:J:39:PRO:HG2	3:J:47:GLU:HB2	1.71	0.72
1:B:57:TYR:CG	1:B:161:ARG:HG2	2.25	0.72
2:I:541:SER:O	2:I:545:ASN:ND2	2.23	0.72
5:L:376:LEU:HD11	5:L:423:LEU:HD11	1.72	0.72
1:G:205:VAL:HG13	1:G:209:GLU:HB2	1.72	0.72
3:D:242:LEU:H	3:D:312:ARG:HA	1.53	0.72
3:J:39:PRO:HB3	3:J:46:ASP:HA	1.72	0.72
1:B:110:ARG:H	1:B:113:ASP:HB2	1.55	0.72
2:I:146:VAL:HG12	2:I:162:ILE:HG13	1.72	0.72
3:D:97:THR:HG21	3:D:571:LYS:HG3	1.71	0.71
3:J:1211:MET:HB3	3:J:1213:ARG:HG2	1.71	0.71
3:J:410:THR:HG23	5:L:189:LEU:HD21	1.72	0.71
2:C:146:VAL:HG12	2:C:162:ILE:HG13	1.71	0.71
3:J:879:ARG:HH12	3:J:905:PRO:HA	1.55	0.71
6:O:7:DA:H61	7:P:20:DT:H3	1.38	0.71
2:C:737:LEU:HG	2:C:741:GLY:HA2	1.72	0.71
2:I:1053:LEU:HA	3:J:621:LYS:HE3	1.72	0.71
2:C:163:ILE:HD12	2:C:164:PRO:HD2	1.71	0.71
3:D:214:ASP:OD1	3:D:214:ASP:N	2.22	0.71
2:I:737:LEU:HG	2:I:741:GLY:HA2	1.72	0.71
3:D:226:PRO:HA	3:D:330:SER:HA	1.72	0.71
2:C:1053:LEU:HA	3:D:621:LYS:HE3	1.72	0.71
3:D:1003:VAL:HG21	3:D:1041:MET:HG2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:419:THR:HG23	2:I:421:GLU:H	1.55	0.71
3:D:618:LEU:HD23	3:D:1467:ILE:HG23	1.71	0.71
2:I:163:ILE:HD12	2:I:164:PRO:HD2	1.71	0.71
4:K:30:LEU:HD12	4:K:37:ASN:ND2	2.03	0.71
5:F:376:LEU:HD11	5:F:423:LEU:HD11	1.71	0.71
4:K:27:ALA:HA	4:K:30:LEU:HD22	1.72	0.70
3:J:367:ILE:HB	3:J:377:VAL:HB	1.73	0.70
1:G:219:LYS:HA	1:G:222:LEU:HD23	1.74	0.70
2:C:601:GLY:HA2	2:C:615:TYR:HA	1.72	0.70
3:J:800:LYS:HB3	3:J:822:ALA:HB2	1.72	0.70
3:J:1003:VAL:HG21	3:J:1041:MET:HG2	1.74	0.70
1:B:186:LEU:HB2	1:B:192:LEU:HD11	1.72	0.70
3:J:1267:ARG:HE	3:J:1267:ARG:H	1.39	0.70
2:C:576:ALA:HB1	2:C:580:MET:HE3	1.73	0.70
3:D:214:ASP:HA	3:D:342:PRO:HA	1.74	0.70
7:S:15:DA:H1'	7:S:16:DC:H5'	1.73	0.70
3:J:361:VAL:HG21	3:J:367:ILE:HD11	1.74	0.70
3:D:208:PRO:HA	3:D:390:PRO:HA	1.74	0.70
3:D:9:ARG:HG3	3:D:1456:LYS:HG2	1.74	0.70
2:I:576:ALA:HB1	2:I:580:MET:HE3	1.72	0.70
3:J:371:ILE:HG21	5:L:247:ARG:HH22	1.53	0.70
2:C:1101:THR:HG23	3:D:8:VAL:HG22	1.74	0.69
3:J:191:LEU:HD11	3:J:197:SER:HB2	1.73	0.69
3:D:1192:LEU:HA	3:D:1373:ARG:HG3	1.73	0.69
2:I:498:GLN:HG3	3:J:1068:LEU:HD11	1.74	0.69
6:O:17:DA:H1'	6:O:18:DA:H5'	1.73	0.69
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.73	0.69
3:J:1476:THR:HA	4:K:17:TYR:HB3	1.74	0.69
3:J:371:ILE:HG23	3:J:372:ASP:H	1.55	0.69
3:D:563:PRO:HB3	5:F:200:GLN:HB3	1.74	0.69
3:J:761:ILE:O	3:J:767:HIS:ND1	2.23	0.69
3:D:1272:ALA:HB3	3:D:1330:ILE:HD13	1.75	0.69
2:I:72:ARG:HB3	2:I:95:TYR:HB2	1.75	0.69
1:H:110:ARG:H	1:H:113:ASP:HB2	1.58	0.69
3:D:236:TYR:HB3	3:D:313:LEU:HD22	1.74	0.69
2:I:542:LEU:HD12	2:I:542:LEU:H	1.58	0.69
3:J:1105:ILE:HD12	3:J:1373:ARG:HH12	1.58	0.69
2:I:833:LEU:HD11	2:I:839:LEU:HD11	1.75	0.69
2:I:468:ARG:HB3	2:I:485:TYR:O	1.93	0.69
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.75	0.69
3:D:93:ILE:HD13	3:D:548:ILE:HG23	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:18:DA:H1'	6:R:19:DT:H5'	1.74	0.68
6:O:10:DA:H1'	6:O:11:DG:H5'	1.75	0.68
7:P:17:DT:H1'	7:P:18:DT:H5'	1.73	0.68
2:I:969:LEU:HD23	2:I:971:LYS:HE3	1.74	0.68
3:J:560:GLN:O	5:L:147:ARG:NH1	2.26	0.68
3:D:520:LEU:O	3:D:525:ARG:NH2	2.26	0.68
4:K:40:LEU:HD21	4:K:67:GLU:HA	1.75	0.68
3:D:977:ALA:HB2	3:J:831:GLY:H	1.59	0.68
2:C:568:ALA:HB1	2:C:995:MET:SD	2.34	0.68
3:D:93:ILE:HB	3:D:517:VAL:HB	1.75	0.68
1:B:59:GLU:HG3	1:B:139:TYR:HD2	1.57	0.68
2:C:200:LEU:HG	2:C:300:ASP:HB2	1.76	0.68
3:J:699:VAL:HG12	3:J:717:GLN:HG2	1.75	0.68
5:L:222:LEU:HD11	5:L:269:GLN:HG2	1.76	0.68
3:J:8:VAL:HG21	3:J:1468:LEU:HD11	1.76	0.68
3:D:1476:THR:HA	4:E:17:TYR:HB3	1.75	0.68
2:C:242:LEU:HD13	2:C:243:ARG:HB2	1.76	0.68
2:I:568:ALA:HB1	2:I:995:MET:SD	2.34	0.67
3:D:371:ILE:HG23	3:D:372:ASP:H	1.59	0.67
2:I:439:CYS:HB2	2:I:541:SER:HB3	1.75	0.67
3:D:45:PHE:HA	3:D:522:PRO:HB3	1.76	0.67
7:P:25:DA:H1'	7:P:26:DG:H5'	1.76	0.67
2:I:833:LEU:HD12	2:I:996:LYS:HE3	1.74	0.67
2:C:261:LEU:HB3	2:C:291:VAL:HG22	1.77	0.67
3:J:783:ARG:HD3	3:J:1028:ALA:O	1.94	0.67
3:J:521:PRO:HD2	3:J:524:LEU:HD12	1.76	0.67
2:C:542:LEU:HD12	2:C:542:LEU:H	1.59	0.67
2:C:995:MET:HE2	2:C:996:LYS:H	1.60	0.67
2:C:230:ARG:HB3	2:C:231:PRO:HD2	1.76	0.67
1:G:39:PRO:HG2	1:H:39:PRO:HG3	1.76	0.67
2:C:439:CYS:HB2	2:C:541:SER:HB3	1.77	0.67
3:D:1202:GLN:NE2	3:D:1215:VAL:O	2.25	0.67
3:J:1254:GLN:HB3	3:J:1258:ARG:HB2	1.77	0.67
7:P:21:DG:H1'	7:P:22:DT:H5'	1.75	0.67
2:I:211:LEU:HD13	2:I:218:VAL:HA	1.76	0.67
5:L:164:GLU:O	5:L:166:PRO:HD3	1.95	0.67
3:J:1384:PRO:HA	3:J:1415:VAL:HG13	1.76	0.67
3:D:1382:THR:HG23	3:D:1417:TRP:HA	1.77	0.67
3:J:87:ARG:HG2	3:J:523:ASP:HB3	1.77	0.67
3:J:618:LEU:HD23	3:J:1467:ILE:HG23	1.75	0.67
2:I:140:ILE:HG22	2:I:412:ALA:HA	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:397:GLU:HB2	2:I:632:ASN:HB2	1.77	0.67
2:I:229:MET:HB3	2:I:234:ALA:HB2	1.76	0.67
3:J:1140:ILE:HG23	3:J:1144:LEU:HD23	1.77	0.67
3:J:1273:VAL:HG22	3:J:1326:THR:HG22	1.77	0.67
6:O:9:DA:H1'	6:O:10:DA:H5'	1.77	0.66
2:I:207:LEU:HD21	2:I:221:LEU:HB3	1.76	0.66
5:F:164:GLU:O	5:F:166:PRO:HD3	1.95	0.66
3:J:100:ALA:HA	3:J:513:ILE:HA	1.77	0.66
2:C:229:MET:HB3	2:C:234:ALA:HB2	1.75	0.66
2:I:688:ILE:HB	2:I:849:VAL:HA	1.76	0.66
2:C:1042:ALA:HA	3:D:1224:VAL:HG22	1.75	0.66
2:I:200:LEU:HG	2:I:300:ASP:HB2	1.77	0.66
2:I:172:ILE:HA	2:I:186:VAL:HG22	1.77	0.66
3:D:783:ARG:HD3	3:D:1028:ALA:O	1.96	0.66
3:J:423:ASP:HB3	3:J:426:LYS:HB3	1.76	0.66
2:C:833:LEU:HD12	2:C:996:LYS:HE3	1.75	0.66
3:D:569:ASN:HD22	5:F:229:GLN:HE21	1.44	0.66
4:E:40:LEU:HD21	4:E:67:GLU:HA	1.76	0.66
2:I:708:TYR:CE1	2:I:827:VAL:HB	2.31	0.66
2:C:64:LEU:HD13	2:C:359:MET:HG2	1.78	0.66
2:C:777:ILE:HA	5:F:420:LEU:HD11	1.77	0.66
2:C:969:LEU:HD23	2:C:971:LYS:HE3	1.76	0.66
2:I:230:ARG:HB3	2:I:231:PRO:HD2	1.76	0.66
6:O:12:DT:H1'	6:O:13:DG:H5'	1.78	0.66
2:C:577:PRO:HA	2:C:671:ASN:HD21	1.61	0.66
3:D:354:ILE:HD11	3:D:369:ALA:HB2	1.77	0.66
2:C:468:ARG:HB3	2:C:485:TYR:O	1.95	0.66
2:I:242:LEU:HD13	2:I:243:ARG:HB2	1.76	0.66
2:I:1101:THR:HG23	3:J:8:VAL:HG22	1.78	0.66
2:I:332:ARG:HB2	2:I:465:GLY:HA3	1.77	0.66
2:I:537:LYS:HZ3	2:I:905:VAL:N	1.91	0.66
2:I:458:TYR:HB3	2:I:470:PRO:HG2	1.77	0.66
2:C:762:LYS:HB3	2:C:786:LYS:HB2	1.78	0.66
2:C:101:ILE:HG23	2:C:108:ILE:HA	1.77	0.66
6:O:24:DC:H42	7:P:3:DG:H1	1.43	0.65
2:I:101:ILE:HG23	2:I:108:ILE:HA	1.79	0.65
3:J:715:ALA:HB3	3:J:764:LEU:HA	1.78	0.65
3:D:266:GLU:HG3	3:D:286:ALA:HB2	1.77	0.65
2:C:211:LEU:HD13	2:C:218:VAL:HA	1.77	0.65
3:D:594:PRO:HB3	5:F:221:GLY:HA2	1.78	0.65
3:D:699:VAL:HG12	3:D:717:GLN:HG2	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LYS:HA	1:A:222:LEU:HD23	1.77	0.65
2:C:140:ILE:HG22	2:C:412:ALA:HA	1.77	0.65
3:J:582:ILE:HD13	3:J:603:LEU:HD12	1.79	0.65
2:I:458:TYR:HD1	2:I:538:GLN:HB3	1.61	0.65
6:R:9:DA:H1'	6:R:10:DA:H5'	1.77	0.65
3:J:100:ALA:HB2	3:J:513:ILE:HD13	1.78	0.65
2:I:710:ILE:HB	2:I:790:LEU:HD22	1.79	0.65
3:D:224:ARG:NH2	3:D:254:GLU:OE2	2.29	0.65
4:K:67:GLU:HB3	4:K:73:LEU:HD11	1.79	0.65
2:C:397:GLU:HB2	2:C:632:ASN:HB2	1.79	0.65
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	1.79	0.65
2:C:458:TYR:HB3	2:C:470:PRO:HG2	1.77	0.65
2:I:995:MET:HE2	2:I:996:LYS:H	1.60	0.65
6:R:10:DA:H1'	6:R:11:DG:H5'	1.78	0.65
3:D:8:VAL:HG21	3:D:1468:LEU:HD11	1.78	0.65
1:B:24:VAL:HG22	1:B:196:THR:HG23	1.78	0.65
3:J:1285:GLU:HB3	3:J:1290:LEU:HA	1.79	0.64
6:R:2:DT:H3	7:S:25:DA:H2	1.42	0.64
3:D:786:ILE:HD13	3:D:908:LYS:HG2	1.78	0.64
5:F:222:LEU:HD11	5:F:269:GLN:HG2	1.79	0.64
3:D:242:LEU:HD23	3:D:285:PRO:HB3	1.79	0.64
4:E:67:GLU:HB3	4:E:73:LEU:HD11	1.79	0.64
3:D:260:GLU:HB3	3:D:271:TYR:HB2	1.79	0.64
2:C:207:LEU:HD21	2:C:221:LEU:HB3	1.77	0.64
7:S:13:DA:H1'	7:S:14:DC:H5'	1.78	0.64
2:C:1051:GLU:HG2	2:C:1055:ILE:HD12	1.79	0.64
1:H:59:GLU:HB2	1:H:139:TYR:HB3	1.79	0.64
3:D:268:HIS:HB2	3:D:284:LEU:HD22	1.78	0.64
2:C:139:GLN:HB2	2:C:391:LEU:HD21	1.79	0.64
2:I:118:LEU:HD12	2:I:119:PRO:HD2	1.78	0.64
2:C:217:LEU:HD13	2:C:311:PHE:HB3	1.80	0.64
2:I:773:LEU:HB2	5:L:388:LYS:HG3	1.80	0.64
5:L:149:LYS:HD3	5:L:193:ARG:HH22	1.61	0.64
2:C:467:ILE:H	2:C:467:ILE:HD12	1.63	0.64
2:I:64:LEU:HD13	2:I:359:MET:HG2	1.80	0.64
3:D:573:MET:HA	3:D:576:GLU:HG2	1.78	0.64
2:C:710:ILE:HB	2:C:790:LEU:HD22	1.80	0.64
3:J:67:ARG:HD2	5:L:394:ARG:HB2	1.78	0.64
3:D:1048:PRO:HD3	3:D:1075:HIS:HB3	1.79	0.64
3:J:786:ILE:HD13	3:J:908:LYS:HG2	1.78	0.64
1:H:186:LEU:HB2	1:H:192:LEU:HD11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:139:GLN:HB2	2:I:391:LEU:HD21	1.80	0.64
3:D:1274:ILE:HG22	3:D:1324:PRO:HA	1.80	0.64
3:J:887:GLY:HA3	3:J:893:GLU:HA	1.79	0.64
2:I:86:LYS:HE2	2:I:813:VAL:HG23	1.79	0.64
2:I:261:LEU:HB3	2:I:291:VAL:HG22	1.80	0.63
2:C:688:ILE:HB	2:C:849:VAL:HA	1.79	0.63
1:H:24:VAL:HG22	1:H:196:THR:HG23	1.79	0.63
2:C:458:TYR:HD1	2:C:538:GLN:HB3	1.62	0.63
2:I:577:PRO:HA	2:I:671:ASN:HD21	1.63	0.63
2:I:101:ILE:HA	2:I:107:LEU:O	1.98	0.63
2:C:118:LEU:HD12	2:C:119:PRO:HD2	1.79	0.63
5:F:364:LEU:HD12	5:F:436:PHE:HZ	1.63	0.63
3:D:618:LEU:HB3	3:D:1467:ILE:HG12	1.79	0.63
6:O:18:DA:H1'	6:O:19:DT:H5'	1.78	0.63
3:J:102:ILE:HB	3:J:579:ASP:HB3	1.79	0.63
2:C:708:TYR:CE1	2:C:827:VAL:HB	2.33	0.63
2:C:1064:ASN:HD22	5:F:359:ALA:HB2	1.64	0.63
1:A:39:PRO:HG2	1:B:39:PRO:HG3	1.81	0.63
3:J:65:ARG:NH1	5:L:393:GLY:O	2.32	0.63
3:D:887:GLY:HA3	3:D:893:GLU:HA	1.80	0.63
6:O:4:DG:H1'	6:O:5:DA:H5'	1.80	0.63
2:C:833:LEU:HD11	2:C:839:LEU:HD11	1.79	0.63
2:I:217:LEU:HD13	2:I:311:PHE:HB3	1.81	0.63
2:C:723:THR:O	2:C:757:GLY:HA3	1.99	0.63
3:D:1472:ILE:HG12	3:D:1474:ALA:H	1.63	0.63
5:L:383:VAL:HA	5:L:386:LEU:HD12	1.79	0.63
2:C:1034:GLU:HG2	3:D:619:LEU:HB3	1.81	0.63
1:B:44:LEU:HD23	1:B:174:VAL:HG21	1.81	0.63
1:B:73:GLU:HB2	1:B:78:ILE:HD11	1.80	0.63
3:J:974:ILE:HG12	3:J:991:GLN:HE21	1.63	0.63
3:D:514:LEU:HD21	3:D:518:PRO:HD3	1.81	0.63
3:D:703:ASN:HB2	3:D:713:ILE:HG12	1.80	0.63
3:D:701:LEU:HD21	3:D:763:MET:HG3	1.79	0.63
2:C:172:ILE:HA	2:C:186:VAL:HG22	1.79	0.62
4:E:79:LEU:HG	4:E:80:VAL:HG13	1.80	0.62
2:I:467:ILE:HD12	2:I:467:ILE:H	1.63	0.62
3:J:835:SER:HB3	3:J:838:ARG:HE	1.63	0.62
3:D:407:VAL:HG22	3:D:409:VAL:H	1.63	0.62
3:D:761:ILE:O	3:D:767:HIS:ND1	2.26	0.62
3:D:367:ILE:HB	3:D:377:VAL:HB	1.80	0.62
2:C:773:LEU:HB2	5:F:388:LYS:HG3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:383:VAL:HA	5:F:386:LEU:HD12	1.81	0.62
2:I:607:ASP:O	2:I:609:THR:N	2.33	0.62
3:D:48:ARG:HA	3:D:78:VAL:HG22	1.81	0.62
3:J:127:LEU:HD23	3:J:461:ILE:HG13	1.81	0.62
5:L:364:LEU:HD12	5:L:436:PHE:HZ	1.63	0.62
2:C:370:ALA:HB1	5:F:295:GLN:HE22	1.64	0.62
3:J:1048:PRO:HD3	3:J:1075:HIS:HB3	1.81	0.62
3:D:1384:PRO:HA	3:D:1415:VAL:HG13	1.82	0.62
2:C:537:LYS:HZ3	2:C:905:VAL:N	1.93	0.62
3:J:1472:ILE:HG12	3:J:1474:ALA:H	1.65	0.62
2:I:123:GLU:HG2	2:I:592:LEU:HD13	1.81	0.62
3:J:701:LEU:HD21	3:J:763:MET:HG3	1.80	0.62
2:I:691:SER:HB3	2:I:868:ASP:HA	1.82	0.62
5:F:180:SER:O	5:F:181:LEU:HD12	2.00	0.62
2:I:762:LYS:HB3	2:I:786:LYS:HB2	1.80	0.62
2:I:502:PRO:HG3	2:I:510:THR:HG22	1.82	0.62
2:C:101:ILE:HA	2:C:107:LEU:O	1.99	0.62
3:J:1004:THR:HG23	3:J:1036:ARG:HB2	1.81	0.62
2:I:839:LEU:HG	2:I:996:LYS:HA	1.81	0.62
1:B:59:GLU:HB2	1:B:139:TYR:HB3	1.82	0.62
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.35	0.62
3:D:137:PRO:HA	3:D:452:ILE:HG13	1.82	0.62
1:G:46:SER:HB3	2:I:856:GLU:HG2	1.82	0.62
3:D:1202:GLN:HE21	3:D:1217:ILE:HG12	1.65	0.61
1:H:73:GLU:HB2	1:H:78:ILE:HD11	1.82	0.61
2:C:50:GLU:HA	2:C:265:LYS:HD2	1.82	0.61
1:H:44:LEU:HD23	1:H:174:VAL:HG21	1.82	0.61
6:R:10:DA:H2	7:S:17:DT:H3	1.47	0.61
2:C:107:LEU:HD12	2:C:109:LYS:HB2	1.82	0.61
3:J:772:PRO:HA	3:J:1209:LEU:HB2	1.82	0.61
3:D:974:ILE:HG12	3:D:991:GLN:HE21	1.65	0.61
3:D:168:THR:HA	3:D:394:LEU:HB2	1.81	0.61
3:D:245:LEU:HB2	3:D:309:GLY:HA2	1.81	0.61
2:C:579:VAL:HG13	2:C:842:ARG:HH22	1.64	0.61
2:C:607:ASP:O	2:C:609:THR:N	2.32	0.61
3:J:112:ILE:HG23	3:J:512:MET:HG2	1.81	0.61
2:I:36:PRO:HA	2:I:39:ARG:HD2	1.83	0.61
2:C:1090:LYS:NZ	2:C:1093:GLN:OE1	2.28	0.61
5:F:222:LEU:HB3	5:F:226:ASP:HB2	1.82	0.61
2:I:723:THR:O	2:I:757:GLY:HA3	2.00	0.61
3:D:192:ALA:HB1	3:D:193:PRO:HD2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:174:LEU:HD13	2:C:310:LEU:HD22	1.81	0.61
3:J:1313:VAL:HG21	3:J:1325:LEU:HD12	1.81	0.61
6:R:11:DG:N2	7:S:16:DC:O2	2.34	0.61
3:D:1143:GLY:HA2	3:D:1364:HIS:HE1	1.65	0.61
2:I:1016:ILE:O	3:J:87:ARG:NH2	2.34	0.61
2:C:332:ARG:HB2	2:C:465:GLY:HA3	1.82	0.61
2:C:571:LEU:HB2	2:C:574:ALA:HB2	1.81	0.61
1:G:35:THR:HG21	1:H:43:ILE:HG13	1.81	0.61
1:H:59:GLU:HG3	1:H:139:TYR:HD2	1.66	0.61
2:I:1102:LEU:HB2	3:J:7:LYS:HB2	1.83	0.61
3:J:192:ALA:HB1	3:J:193:PRO:HD2	1.81	0.61
3:D:1100:ASP:HA	3:D:1463:LYS:HE2	1.82	0.61
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.83	0.61
2:C:36:PRO:HB2	2:C:70:GLU:HG2	1.83	0.61
1:H:58:ILE:HD13	1:H:61:VAL:HB	1.82	0.61
1:G:51:THR:HG23	1:G:146:ARG:HG2	1.83	0.61
2:I:262:ALA:HB2	2:I:291:VAL:HG23	1.83	0.61
2:I:1037:VAL:HG13	2:I:1049:LEU:HD11	1.82	0.61
3:J:557:LEU:HD21	5:L:233:GLN:HG2	1.83	0.61
2:C:191:PHE:HB2	2:C:195:LEU:HD22	1.82	0.61
2:I:1034:GLU:HG2	3:J:619:LEU:HB3	1.82	0.61
3:D:1208:ASP:HB2	3:D:1215:VAL:HA	1.81	0.60
3:J:703:ASN:HB2	3:J:713:ILE:HG12	1.82	0.60
2:I:777:ILE:HA	5:L:420:LEU:HD11	1.83	0.60
4:K:79:LEU:HG	4:K:80:VAL:HG13	1.83	0.60
2:I:107:LEU:HD12	2:I:109:LYS:HB2	1.83	0.60
3:D:1111:ASP:OD1	3:D:1203:LYS:NZ	2.35	0.60
2:I:50:GLU:HA	2:I:265:LYS:HD2	1.83	0.60
2:I:36:PRO:HB2	2:I:70:GLU:HG2	1.83	0.60
2:I:1089:VAL:HG21	2:I:1111:ILE:HG21	1.83	0.60
3:D:270:ILE:HG12	3:D:284:LEU:HD11	1.82	0.60
2:C:1018:GLN:HB3	2:C:1063:ARG:NH1	2.15	0.60
3:J:7:LYS:NZ	3:J:1458:GLU:OE1	2.33	0.60
5:L:180:SER:O	5:L:181:LEU:HD12	2.00	0.60
2:I:174:LEU:HD13	2:I:310:LEU:HD22	1.82	0.60
3:J:704:ARG:HB2	3:J:745:MET:HG2	1.83	0.60
5:F:149:LYS:HD3	5:F:193:ARG:HH22	1.65	0.60
3:J:407:VAL:HG23	3:J:422:ALA:HB2	1.84	0.60
2:C:1016:ILE:HG13	2:C:1017:THR:H	1.66	0.60
3:J:822:ALA:HB3	3:J:825:ALA:HB2	1.82	0.60
2:C:668:LEU:H	2:C:993:PHE:HZ	1.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:222:LEU:HB3	5:L:226:ASP:HB2	1.83	0.60
3:D:514:LEU:HG	3:D:516:ALA:O	2.01	0.60
2:I:876:VAL:HG11	2:I:885:ILE:HD11	1.82	0.60
1:G:54:THR:HB	1:G:143:ARG:O	2.02	0.60
2:C:839:LEU:HG	2:C:996:LYS:HA	1.83	0.60
2:I:118:LEU:HD13	2:I:382:LEU:HD23	1.82	0.60
1:H:51:THR:HB	1:H:87:VAL:O	2.01	0.60
3:J:1166:LEU:HD23	3:J:1174:LEU:HD11	1.81	0.60
2:C:1005:MET:HG3	3:D:629:SER:HB2	1.83	0.60
1:A:46:SER:HB3	2:C:856:GLU:HG2	1.84	0.60
2:C:876:VAL:HG11	2:C:885:ILE:HD11	1.83	0.60
2:I:668:LEU:H	2:I:993:PHE:HZ	1.50	0.60
2:I:1005:MET:HG3	3:J:629:SER:HB2	1.82	0.60
1:B:58:ILE:HD13	1:B:61:VAL:HB	1.81	0.60
2:I:1031:ARG:HG2	2:I:1033:GLY:H	1.67	0.60
3:J:759:ALA:HA	3:J:763:MET:HB3	1.83	0.60
6:R:24:DC:N4	7:S:3:DG:H1	1.95	0.59
1:G:42:ARG:NH1	2:I:978:ARG:HA	2.17	0.59
2:I:571:LEU:HD21	2:I:995:MET:HE1	1.84	0.59
3:J:1105:ILE:HB	3:J:1222:GLY:HA3	1.83	0.59
3:D:1313:VAL:HG11	3:D:1325:LEU:HD23	1.83	0.59
2:I:571:LEU:HG	2:I:700:TYR:HA	1.84	0.59
2:I:1051:GLU:HG2	2:I:1055:ILE:HD12	1.84	0.59
3:J:27:GLU:H	3:J:42:ASP:HB3	1.67	0.59
2:C:774:LEU:HG	5:F:365:LEU:HD21	1.84	0.59
3:J:101:HIS:NE2	3:J:582:ILE:HG21	2.17	0.59
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.84	0.59
3:D:919:PHE:HA	3:D:927:THR:HG21	1.85	0.59
6:O:19:DT:H1'	6:O:20:DT:H5'	1.83	0.59
3:D:1188:VAL:HG12	3:D:1189:ARG:H	1.66	0.59
1:G:13:ALA:HB3	1:H:228:PRO:HB3	1.83	0.59
3:D:1139:ASP:O	3:D:1142:SER:HB2	2.02	0.59
2:I:571:LEU:HB2	2:I:574:ALA:HB2	1.83	0.59
3:D:92:HIS:HA	3:D:517:VAL:O	2.02	0.59
3:J:978:TYR:HB2	3:J:988:ARG:HD3	1.83	0.59
3:J:1487:VAL:HG21	3:J:1492:LEU:HD23	1.84	0.59
3:J:210:ARG:HD2	3:J:388:HIS:HB2	1.85	0.59
3:J:708:LEU:HG	3:J:709:HIS:H	1.67	0.59
3:D:433:GLY:HA2	3:D:449:SER:HB2	1.85	0.59
2:I:408:ARG:NH2	2:I:456:ALA:O	2.36	0.59
2:C:408:ARG:NH2	2:C:456:ALA:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:48:ARG:HA	3:J:78:VAL:HG22	1.84	0.59
3:J:714:GLN:HB3	3:J:765:SER:HB3	1.85	0.59
3:D:129:PHE:CE1	3:D:457:GLY:HA3	2.37	0.59
3:D:9:ARG:HG2	3:D:10:ILE:H	1.66	0.59
1:B:51:THR:HB	1:B:87:VAL:O	2.02	0.59
2:C:716:LYS:HD2	3:D:37:LEU:HD21	1.85	0.59
3:D:1364:HIS:NE2	3:D:1366:LYS:HE2	2.17	0.59
1:A:54:THR:HB	1:A:143:ARG:O	2.02	0.59
2:C:911:GLU:OE1	3:D:1062:ARG:NH2	2.34	0.59
3:D:1004:THR:HG23	3:D:1036:ARG:HB2	1.85	0.59
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	1.85	0.59
5:L:307:ALA:HB1	5:L:314:TRP:HB3	1.85	0.59
7:S:18:DT:H1'	7:S:19:DT:H5'	1.85	0.59
3:D:245:LEU:HD12	3:D:311:LEU:HD21	1.84	0.59
3:D:1192:LEU:HD23	3:D:1373:ARG:HB2	1.85	0.59
3:D:758:GLU:HG2	3:D:1476:THR:HG21	1.85	0.59
2:I:798:GLY:HA3	2:I:827:VAL:HG13	1.83	0.59
3:J:698:LYS:HG3	4:K:59:ASN:HD21	1.68	0.59
1:G:53:VAL:HG22	1:G:54:THR:N	2.18	0.58
3:D:203:ALA:HA	3:D:395:VAL:HA	1.85	0.58
2:C:413:LEU:HD12	2:C:413:LEU:H	1.68	0.58
3:J:125:GLN:HB3	3:J:131:LYS:HB3	1.84	0.58
2:I:704:HIS:CD2	2:I:831:ARG:HD2	2.37	0.58
2:C:15:LEU:HD11	2:C:457:ALA:HB1	1.85	0.58
1:G:101:LEU:HB3	1:G:140:MET:HB3	1.85	0.58
3:J:1280:VAL:O	3:J:1295:GLU:N	2.35	0.58
3:J:633:VAL:HG13	3:J:635:PRO:HD3	1.84	0.58
2:C:497:ALA:HB1	2:C:501:THR:HG21	1.85	0.58
3:J:971:LEU:HA	3:J:974:ILE:HD12	1.85	0.58
3:D:714:GLN:HB3	3:D:765:SER:HB3	1.86	0.58
3:J:1111:ASP:OD1	3:J:1203:LYS:NZ	2.36	0.58
2:C:532:MET:HG2	2:C:533:ASP:H	1.68	0.58
3:D:236:TYR:HB2	3:D:319:ALA:HB3	1.84	0.58
2:I:1016:ILE:HG13	2:I:1017:THR:H	1.68	0.58
2:C:207:LEU:HD13	2:C:222:LEU:HD23	1.85	0.58
3:D:407:VAL:HG23	3:D:422:ALA:HB2	1.86	0.58
3:D:978:TYR:HB2	3:D:988:ARG:HD3	1.85	0.58
3:D:633:VAL:HG13	3:D:635:PRO:HD3	1.85	0.58
3:D:801:GLY:HA2	3:D:821:VAL:HA	1.86	0.58
3:D:125:GLN:HB3	3:D:131:LYS:HB3	1.85	0.58
3:D:907:GLU:O	3:D:911:LEU:HG	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:380:GLU:HB2	5:F:419:ALA:HB2	1.85	0.58
3:D:262:LYS:HB2	3:D:269:LEU:HB2	1.85	0.58
2:I:236:VAL:HG21	2:I:250:LYS:HG2	1.86	0.58
1:B:177:VAL:HG12	1:B:199:ILE:HG12	1.85	0.58
2:I:911:GLU:OE1	3:J:1062:ARG:NH2	2.36	0.58
3:J:461:ILE:HB	3:J:513:ILE:HD11	1.85	0.58
2:I:774:LEU:HG	5:L:365:LEU:HD21	1.84	0.58
2:C:571:LEU:HD21	2:C:995:MET:HE1	1.84	0.58
6:R:19:DT:H1'	6:R:20:DT:H5'	1.85	0.58
2:I:5:ARG:HA	2:I:902:ILE:HB	1.84	0.58
3:D:772:PRO:HG3	3:D:1210:SER:HB3	1.86	0.58
1:H:57:TYR:CD1	1:H:161:ARG:HG2	2.38	0.58
3:J:671:LYS:HG3	5:L:436:PHE:CE2	2.39	0.58
2:C:611:ILE:HG13	2:C:625:LEU:HD11	1.86	0.58
1:A:42:ARG:NH1	2:C:978:ARG:HA	2.18	0.58
2:C:571:LEU:HG	2:C:700:TYR:HA	1.85	0.58
3:J:1101:VAL:HB	3:J:1428:ALA:HB2	1.86	0.58
3:J:137:PRO:HA	3:J:452:ILE:HG13	1.85	0.58
2:C:1071:ILE:O	3:D:659:LYS:HG2	2.04	0.58
6:R:17:DA:H1'	6:R:18:DA:H5'	1.86	0.58
3:J:520:LEU:O	3:J:525:ARG:NH2	2.37	0.58
3:D:12:LEU:HD21	3:D:1452:ILE:HD13	1.86	0.58
2:I:579:VAL:HG13	2:I:842:ARG:HH22	1.69	0.58
7:S:8:DA:H2''	7:S:9:DT:H5''	1.86	0.58
5:F:203:ILE:HG23	5:F:235:LEU:HD23	1.86	0.57
3:D:822:ALA:HB3	3:D:825:ALA:HB2	1.86	0.57
3:D:803:GLY:HA2	3:D:827:ILE:HG22	1.85	0.57
3:J:9:ARG:HG2	3:J:10:ILE:H	1.68	0.57
2:C:691:SER:HB3	2:C:868:ASP:HA	1.86	0.57
3:J:770:LEU:HB2	3:J:1210:SER:HA	1.85	0.57
1:H:177:VAL:HG12	1:H:199:ILE:HG12	1.86	0.57
1:A:51:THR:HG23	1:A:146:ARG:HG2	1.84	0.57
1:A:23:PHE:HE2	1:A:199:ILE:HD12	1.68	0.57
3:D:205:TYR:HD1	3:D:393:ILE:HG12	1.68	0.57
3:D:25:GLU:HG2	3:D:93:ILE:HA	1.86	0.57
2:I:637:PHE:HA	2:I:659:PRO:HG3	1.86	0.57
2:C:236:VAL:HG21	2:C:250:LYS:HG2	1.86	0.57
5:L:225:LEU:HA	5:L:228:ILE:HD12	1.85	0.57
2:I:557:ARG:HB2	2:I:881:ASN:HD21	1.69	0.57
2:C:1089:VAL:HG21	2:C:1111:ILE:HG21	1.86	0.57
3:D:759:ALA:HA	3:D:763:MET:HB3	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:732:ALA:O	2:I:735:ARG:HG3	2.04	0.57
2:I:191:PHE:HB2	2:I:195:LEU:HD22	1.86	0.57
2:C:1031:ARG:HG2	2:C:1033:GLY:H	1.69	0.57
3:D:443:VAL:HG22	3:D:445:ARG:H	1.69	0.57
3:J:907:GLU:O	3:J:911:LEU:HG	2.05	0.57
3:D:1087:ARG:NH2	3:D:1234:THR:O	2.37	0.57
1:H:188:GLN:HA	3:J:688:TRP:HD1	1.69	0.57
2:C:502:PRO:HG3	2:C:510:THR:HG22	1.87	0.57
3:J:1042:ARG:HB3	3:J:1057:VAL:HG21	1.86	0.57
3:J:881:LEU:O	3:J:885:ILE:HG13	2.05	0.57
2:C:162:ILE:HG22	2:C:172:ILE:HD13	1.85	0.57
2:C:1085:PHE:HA	3:D:618:LEU:HD21	1.87	0.57
3:D:171:LEU:HD21	3:D:393:ILE:HD12	1.87	0.57
2:I:532:MET:HG2	2:I:533:ASP:H	1.69	0.57
2:C:975:TYR:HA	2:C:982:PRO:HA	1.87	0.57
1:A:53:VAL:HG22	1:A:54:THR:N	2.18	0.57
1:A:35:THR:HG21	1:B:43:ILE:HG13	1.85	0.57
2:I:569:VAL:HB	2:I:635:THR:HG21	1.87	0.57
3:D:843:PHE:HB2	3:D:866:VAL:HG23	1.86	0.57
1:H:218:LEU:O	1:H:222:LEU:HG	2.05	0.57
2:C:1037:VAL:O	2:C:1041:GLU:HG3	2.05	0.57
1:A:14:THR:OG1	1:B:231:SER:OG	2.21	0.57
2:C:5:ARG:HA	2:C:902:ILE:HB	1.86	0.57
3:D:1254:GLN:HB3	3:D:1258:ARG:CB	2.34	0.57
6:O:7:DA:H1'	6:O:8:DA:H5'	1.85	0.57
3:D:244:GLU:O	3:D:310:LEU:N	2.36	0.57
2:C:1016:ILE:O	3:D:87:ARG:NH2	2.37	0.57
5:F:225:LEU:HA	5:F:228:ILE:HD12	1.85	0.57
3:D:1127:GLU:HG3	3:D:1128:VAL:HG23	1.85	0.57
3:D:1042:ARG:HB3	3:D:1057:VAL:HG21	1.86	0.57
3:D:669:ASN:ND2	5:F:364:LEU:HD11	2.20	0.57
1:H:13:ALA:HB1	1:H:23:PHE:HD1	1.69	0.57
3:D:704:ARG:HB2	3:D:745:MET:HG2	1.85	0.57
2:I:858:MET:H	2:I:977:GLY:HA3	1.70	0.57
5:F:307:ALA:HB1	5:F:314:TRP:HB3	1.87	0.57
1:B:57:TYR:CD1	1:B:161:ARG:HG2	2.39	0.56
5:F:98:GLN:O	5:F:102:GLU:HG3	2.04	0.56
5:L:150:ILE:HG12	5:L:193:ARG:HH11	1.69	0.56
3:J:1100:ASP:HA	3:J:1463:LYS:HE2	1.86	0.56
3:D:95:LEU:HG	3:D:574:LEU:HD21	1.86	0.56
2:I:567:GLN:O	2:I:998:TYR:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:8:DA:H2"	7:P:9:DT:H5"	1.87	0.56
3:D:56:TYR:HA	3:D:80:VAL:HG23	1.87	0.56
2:I:1060:ILE:HG13	2:I:1061:GLU:H	1.70	0.56
2:I:716:LYS:HD2	3:J:37:LEU:HD21	1.87	0.56
2:I:639:GLN:HB3	2:I:656:ALA:HB1	1.88	0.56
5:L:203:ILE:HG23	5:L:235:LEU:HD23	1.87	0.56
3:J:758:GLU:HG2	3:J:1476:THR:HG21	1.87	0.56
2:I:207:LEU:HD13	2:I:222:LEU:HD23	1.87	0.56
1:G:23:PHE:HE2	1:G:199:ILE:HD12	1.69	0.56
2:C:732:ALA:O	2:C:735:ARG:HG3	2.04	0.56
3:D:1176:LYS:HG3	3:J:1130:ARG:HD2	1.87	0.56
3:D:900:ILE:HG12	3:D:914:LEU:HD21	1.87	0.56
3:J:14:SER:HB3	3:J:511:TRP:CE2	2.40	0.56
3:D:881:LEU:O	3:D:885:ILE:HG13	2.05	0.56
2:I:162:ILE:HG22	2:I:172:ILE:HD13	1.86	0.56
2:I:497:ALA:HB1	2:I:501:THR:HG21	1.87	0.56
2:C:262:ALA:HB2	2:C:291:VAL:HG23	1.87	0.56
3:J:803:GLY:HA2	3:J:827:ILE:HG22	1.86	0.56
2:I:926:PHE:HE2	2:I:960:GLU:HG3	1.69	0.56
3:J:919:PHE:HA	3:J:927:THR:HG21	1.86	0.56
3:D:698:LYS:HG3	4:E:59:ASN:HD21	1.69	0.56
2:C:1069:ALA:HB3	2:C:1076:VAL:HG12	1.86	0.56
3:J:699:VAL:HA	3:J:718:PRO:HD3	1.87	0.56
1:B:218:LEU:O	1:B:222:LEU:HG	2.05	0.56
3:D:770:LEU:HB2	3:D:1210:SER:HA	1.86	0.56
3:D:1209:LEU:HD11	3:D:1364:HIS:CD2	2.40	0.56
3:D:191:LEU:HD13	3:D:195:VAL:HG12	1.87	0.56
2:I:502:PRO:HB2	2:I:509:ALA:HB3	1.86	0.56
2:I:774:LEU:HA	2:I:777:ILE:HD12	1.86	0.56
6:O:2:DT:H2"	6:O:3:DT:H71	1.86	0.56
3:J:56:TYR:HA	3:J:80:VAL:HG23	1.88	0.56
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.88	0.56
7:S:17:DT:H1'	7:S:18:DT:H5'	1.87	0.56
3:D:977:ALA:HB2	3:J:831:GLY:N	2.19	0.56
1:G:40:LEU:O	1:G:44:LEU:HB2	2.05	0.56
3:D:1487:VAL:HG21	3:D:1492:LEU:HD23	1.87	0.56
3:D:773:ALA:HB2	3:D:1228:SER:HB3	1.86	0.56
3:D:1500:LYS:HA	3:D:1503:VAL:HG22	1.88	0.56
4:E:30:LEU:HD23	4:E:63:TRP:HB3	1.88	0.56
1:A:54:THR:HG22	1:A:158:ILE:HD11	1.87	0.56
2:I:146:VAL:HG21	2:I:281:LEU:HD21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:191:LEU:HD13	3:J:195:VAL:HG12	1.88	0.56
3:J:974:ILE:HG22	3:J:988:ARG:HG3	1.86	0.56
2:I:611:ILE:HG13	2:I:625:LEU:HD11	1.88	0.56
2:C:114:PHE:HB3	5:F:295:GLN:HA	1.88	0.56
2:I:413:LEU:H	2:I:413:LEU:HD12	1.69	0.56
3:D:684:LYS:HD3	3:D:685:ASP:H	1.71	0.56
1:B:188:GLN:HA	3:D:688:TRP:HD1	1.71	0.56
3:J:1088:THR:HA	3:J:1234:THR:HG22	1.87	0.56
3:D:423:ASP:HB3	3:D:426:LYS:HB3	1.86	0.56
4:K:30:LEU:HD23	4:K:63:TRP:HB3	1.86	0.56
3:D:406:ASP:OD1	3:D:407:VAL:N	2.38	0.56
6:R:5:DA:H1'	6:R:6:DC:H5'	1.87	0.56
2:I:15:LEU:HD11	2:I:457:ALA:HB1	1.87	0.56
1:A:40:LEU:O	1:A:44:LEU:HB2	2.06	0.56
1:H:197:LEU:HG	1:H:199:ILE:HG13	1.88	0.56
2:C:202:TYR:HD1	2:C:206:THR:HG21	1.70	0.56
6:O:21:DG:H1'	6:O:22:DT:H5''	1.88	0.56
3:D:699:VAL:HA	3:D:718:PRO:HD3	1.88	0.56
2:I:211:LEU:HB3	2:I:218:VAL:HG13	1.87	0.56
2:C:831:ARG:HD3	2:C:1002:GLU:HG2	1.88	0.56
3:J:529:GLN:HA	3:J:535:PHE:HA	1.87	0.56
2:C:567:GLN:O	2:C:998:TYR:N	2.39	0.56
1:A:13:ALA:HB3	1:B:228:PRO:HB3	1.87	0.56
3:D:585:GLY:HA3	3:D:590:PRO:HG3	1.88	0.56
6:O:11:DG:N2	7:P:16:DC:O2	2.39	0.55
3:D:9:ARG:HG2	3:D:10:ILE:N	2.21	0.55
3:D:671:LYS:HG3	5:F:436:PHE:CE2	2.41	0.55
2:C:36:PRO:HA	2:C:39:ARG:HD2	1.88	0.55
3:D:784:ASP:HA	3:D:787:LEU:HD23	1.88	0.55
7:S:2:DA:H1'	7:S:3:DG:H5'	1.88	0.55
1:B:68:ILE:HD12	1:B:69:PRO:HD2	1.88	0.55
2:I:975:TYR:HA	2:I:982:PRO:HA	1.88	0.55
3:D:708:LEU:HG	3:D:709:HIS:H	1.70	0.55
2:C:328:LEU:HD21	2:C:434:HIS:HA	1.89	0.55
3:J:1166:LEU:HD12	3:J:1166:LEU:H	1.70	0.55
1:B:197:LEU:HG	1:B:199:ILE:HG13	1.88	0.55
3:D:947:ILE:HG22	3:D:1019:PRO:HB3	1.88	0.55
2:C:432:ARG:HH12	2:C:518:ARG:HE	1.53	0.55
3:D:326:GLU:HB3	3:D:331:VAL:HG23	1.89	0.55
3:D:699:VAL:HG22	3:D:760:ARG:HG2	1.88	0.55
3:D:87:ARG:HG2	3:D:523:ASP:HB3	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:683:ILE:HG22	3:D:687:VAL:HG21	1.89	0.55
3:D:101:HIS:NE2	3:D:582:ILE:HG21	2.20	0.55
3:D:1216:SER:HB2	4:E:15:SER:HB2	1.87	0.55
3:D:238:PRO:HB3	3:D:315:ARG:HA	1.88	0.55
2:C:168:ARG:HD3	2:C:268:ASP:HB2	1.88	0.55
3:D:875:THR:HG21	3:D:879:ARG:HG2	1.89	0.55
3:J:780:LYS:HB2	3:J:908:LYS:HZ1	1.72	0.55
3:D:1448:THR:O	3:D:1452:ILE:HG12	2.07	0.55
1:B:182:GLU:HG3	1:B:194:LYS:HB3	1.89	0.55
1:G:54:THR:HG22	1:G:158:ILE:HD11	1.88	0.55
3:J:1331:ASP:O	3:J:1335:LEU:HD23	2.07	0.55
2:I:852:ILE:HG22	2:I:853:LEU:H	1.71	0.55
2:I:1018:GLN:HB3	2:I:1063:ARG:NH1	2.22	0.55
1:A:178:ALA:HB3	1:A:198:ARG:HG3	1.89	0.55
1:H:68:ILE:HD12	1:H:69:PRO:HD2	1.88	0.55
3:D:973:GLN:HG3	3:J:831:GLY:HA2	1.89	0.55
3:J:911:LEU:O	3:J:915:VAL:HG23	2.05	0.55
3:J:784:ASP:HA	3:J:787:LEU:HD23	1.89	0.55
3:D:27:GLU:H	3:D:42:ASP:HB3	1.72	0.55
3:J:477:LEU:HD21	3:J:495:ARG:HD3	1.87	0.55
3:D:1380:GLU:HB3	3:D:1420:LEU:HD13	1.89	0.55
3:J:843:PHE:HB2	3:J:866:VAL:HG23	1.87	0.55
3:J:400:VAL:HB	3:J:443:VAL:HG21	1.88	0.55
2:I:448:ASN:HA	2:I:451:LEU:HD22	1.89	0.55
2:C:668:LEU:HB3	2:C:995:MET:CG	2.37	0.55
3:D:260:GLU:HA	3:D:294:GLU:HG3	1.89	0.55
2:I:712:ALA:HB3	2:I:820:ARG:HB2	1.89	0.55
3:D:1386:ASP:OD1	3:D:1386:ASP:N	2.39	0.55
6:R:12:DT:H1'	6:R:13:DG:H5'	1.89	0.55
2:C:123:GLU:HG2	2:C:592:LEU:HD13	1.87	0.55
2:C:48:PHE:O	2:C:52:PHE:HB2	2.07	0.55
4:K:45:ARG:HD2	4:K:63:TRP:CH2	2.42	0.55
2:I:1037:VAL:O	2:I:1041:GLU:HG3	2.06	0.55
3:D:238:PRO:HD3	3:D:318:THR:HG22	1.88	0.55
3:J:1345:GLU:HG2	3:J:1376:LEU:HD21	1.89	0.55
1:G:178:ALA:HB3	1:G:198:ARG:HG3	1.88	0.55
2:C:1060:ILE:HG13	2:C:1061:GLU:H	1.70	0.55
3:J:630:VAL:HG22	3:J:631:ILE:H	1.72	0.55
7:S:5:DA:H1'	7:S:6:DC:H5'	1.89	0.55
2:I:408:ARG:NH1	2:I:455:LEU:O	2.39	0.55
1:H:162:ILE:HG23	1:H:163:ASN:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:504:GLU:HG2	2:I:509:ALA:HB2	1.89	0.55
3:D:31:THR:HG21	5:F:272:THR:HG22	1.89	0.55
2:C:852:ILE:HG22	2:C:853:LEU:H	1.72	0.55
3:J:31:THR:HG21	5:L:272:THR:HG22	1.89	0.55
2:C:858:MET:H	2:C:977:GLY:HA3	1.72	0.55
3:J:875:THR:HG21	3:J:879:ARG:HG2	1.89	0.54
3:J:708:LEU:HD12	3:J:1231:GLU:HG2	1.89	0.54
3:D:630:VAL:HG22	3:D:631:ILE:H	1.72	0.54
1:B:111:ALA:HB2	1:B:127:LEU:HB3	1.87	0.54
2:I:202:TYR:HD1	2:I:206:THR:HG21	1.72	0.54
3:J:900:ILE:HG12	3:J:914:LEU:HD21	1.89	0.54
6:R:4:DG:H1	7:S:23:DC:H42	1.55	0.54
2:C:537:LYS:HD2	2:C:583:LEU:HD21	1.89	0.54
3:D:1470:ARG:HG2	3:D:1471:LEU:H	1.72	0.54
3:J:371:ILE:HG21	5:L:247:ARG:NH2	2.21	0.54
3:D:371:ILE:HG21	5:F:247:ARG:NH2	2.22	0.54
2:I:1103:ASP:OD1	2:I:1103:ASP:N	2.40	0.54
1:A:101:LEU:HB3	1:A:140:MET:HB3	1.89	0.54
2:C:713:ARG:HD3	3:D:532:GLY:H	1.71	0.54
1:B:162:ILE:HG23	1:B:163:ASN:H	1.71	0.54
3:D:371:ILE:HG21	5:F:247:ARG:HH22	1.72	0.54
2:C:90:TYR:O	2:C:119:PRO:HA	2.08	0.54
2:C:798:GLY:HA2	2:C:829:GLN:HB3	1.89	0.54
3:J:684:LYS:HD3	3:J:685:ASP:H	1.72	0.54
3:J:1208:ASP:HB2	3:J:1215:VAL:HA	1.89	0.54
2:C:194:VAL:HG23	2:C:195:LEU:HD12	1.88	0.54
3:J:119:SER:HB3	3:J:122:GLU:HG2	1.90	0.54
2:I:754:ILE:HA	2:I:791:ARG:HA	1.88	0.54
2:I:168:ARG:HD3	2:I:268:ASP:HB2	1.89	0.54
2:I:537:LYS:HD2	2:I:583:LEU:HD21	1.89	0.54
2:I:149:THR:HA	2:I:322:VAL:HG13	1.88	0.54
3:D:241:VAL:HG13	3:D:312:ARG:HG2	1.89	0.54
2:I:215:GLY:O	2:I:218:VAL:HG23	2.08	0.54
3:D:569:ASN:HA	3:D:572:ARG:NH2	2.22	0.54
2:C:1103:ASP:OD1	2:C:1103:ASP:N	2.40	0.54
3:J:415:VAL:HG21	3:J:446:VAL:HG11	1.89	0.54
5:L:280:VAL:HA	5:L:283:ILE:HD12	1.90	0.54
2:C:712:ALA:HB3	2:C:820:ARG:HB2	1.90	0.54
1:H:156:HIS:NE2	1:H:167:VAL:O	2.37	0.54
5:L:380:GLU:O	5:L:384:LEU:HB2	2.08	0.54
3:D:547:LEU:HD13	3:D:578:VAL:HG22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:969:LEU:HG	3:J:952:ASP:HB2	1.90	0.54
2:C:215:GLY:O	2:C:218:VAL:HG23	2.07	0.54
2:C:141:HIS:NE2	2:C:334:ARG:HD3	2.23	0.54
1:B:13:ALA:HB1	1:B:23:PHE:HD1	1.73	0.54
2:C:754:ILE:HG22	2:C:755:LEU:H	1.72	0.54
5:L:353:LEU:HD12	5:L:354:PRO:HD2	1.90	0.54
3:J:1377:LYS:O	3:J:1397:LYS:N	2.40	0.54
3:J:1274:ILE:HG22	3:J:1324:PRO:HA	1.89	0.54
1:H:62:LEU:HB3	1:H:163:ASN:ND2	2.23	0.54
2:C:146:VAL:HG21	2:C:281:LEU:HD21	1.89	0.54
5:F:376:LEU:HB2	5:F:381:ALA:HB2	1.89	0.54
3:D:1273:VAL:HG23	3:D:1325:LEU:HD12	1.90	0.54
2:C:754:ILE:HA	2:C:791:ARG:HA	1.90	0.54
3:J:1279:GLY:O	3:J:1319:VAL:HG22	2.08	0.54
3:D:1434:TRP:CD1	3:D:1457:ASP:HB2	2.43	0.54
2:I:343:GLN:HG3	2:I:385:PHE:HB2	1.89	0.54
5:F:154:ALA:O	5:F:158:LYS:HB2	2.07	0.54
3:D:102:ILE:HD11	3:D:587:ARG:HB2	1.89	0.54
2:C:115:LEU:HB3	2:C:378:LEU:HD23	1.90	0.54
1:B:77:GLU:HB2	3:D:872:ARG:HH21	1.72	0.54
3:D:233:LYS:HE3	3:D:234:GLU:H	1.72	0.54
3:J:423:ASP:HB2	3:J:427:VAL:HG12	1.89	0.54
3:D:147:VAL:HG21	3:D:153:LEU:HD21	1.89	0.54
2:I:194:VAL:HG23	2:I:195:LEU:HD12	1.90	0.54
3:D:1144:LEU:HD21	3:D:1186:VAL:HG21	1.89	0.54
2:I:1069:ALA:HB3	2:I:1076:VAL:HG12	1.88	0.54
2:C:468:ARG:HD3	2:C:487:THR:HG22	1.90	0.54
3:D:614:PHE:O	3:D:619:LEU:HB2	2.08	0.54
1:H:78:ILE:HD12	1:H:129:ILE:O	2.07	0.54
5:F:150:ILE:HG12	5:F:193:ARG:HH11	1.72	0.54
3:J:647:ARG:HH12	3:J:683:ILE:HD11	1.73	0.54
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.90	0.54
2:C:206:THR:HG23	2:C:209:ARG:CZ	2.38	0.54
1:H:161:ARG:HG3	1:H:162:ILE:N	2.23	0.54
2:I:668:LEU:HB3	2:I:995:MET:CG	2.38	0.54
2:I:1112:PHE:HB3	3:J:88:TYR:CD2	2.43	0.54
2:C:971:LYS:HB3	2:C:986:PRO:HB2	1.90	0.54
3:D:911:LEU:O	3:D:915:VAL:HG23	2.07	0.54
5:L:413:ARG:HE	7:S:22:DT:H2'	1.72	0.54
1:G:14:THR:OG1	1:H:231:SER:OG	2.23	0.54
1:B:176:ARG:HH11	3:D:884:ARG:HH22	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:176:ARG:HH11	3:J:884:ARG:HH22	1.54	0.54
5:L:376:LEU:HB2	5:L:381:ALA:HB2	1.90	0.53
2:C:889:HIS:CE1	2:C:970:GLY:HA3	2.43	0.53
3:D:11:ALA:HA	3:D:1451:ALA:HA	1.90	0.53
3:D:154:THR:HG22	3:D:157:GLU:HG2	1.90	0.53
3:J:572:ARG:CZ	5:L:98:GLN:HG2	2.38	0.53
5:F:210:VAL:HA	5:F:213:ILE:HD12	1.89	0.53
3:J:1336:LEU:HD22	3:J:1421:LEU:HB3	1.89	0.53
2:C:146:VAL:HG21	2:C:281:LEU:HD11	1.89	0.53
2:C:668:LEU:HB3	2:C:995:MET:HG3	1.90	0.53
2:I:950:LEU:HD21	2:I:952:LEU:HD22	1.90	0.53
2:C:64:LEU:HD22	2:C:359:MET:SD	2.47	0.53
2:C:114:PHE:HE1	5:F:294:GLN:HE21	1.55	0.53
2:I:679:PHE:H	2:I:683:ASN:HD21	1.56	0.53
2:C:759:THR:HB	2:C:785:VAL:HG21	1.90	0.53
1:G:63:HIS:HA	1:G:165:ILE:HD11	1.88	0.53
2:I:1071:ILE:O	3:J:659:LYS:HG2	2.08	0.53
2:I:457:ALA:HB3	2:I:538:GLN:HA	1.89	0.53
2:I:971:LYS:HB3	2:I:986:PRO:HB2	1.90	0.53
2:I:889:HIS:CE1	2:I:970:GLY:HA3	2.44	0.53
3:J:147:VAL:HG21	3:J:153:LEU:HD21	1.90	0.53
7:S:7:DA:H1'	7:S:8:DA:H5'	1.90	0.53
3:D:750:PRO:HG2	3:D:756:GLN:NE2	2.23	0.53
2:I:1103:ASP:HA	3:J:5:VAL:HA	1.91	0.53
5:L:98:GLN:O	5:L:102:GLU:HG3	2.09	0.53
2:C:926:PHE:HE2	2:C:960:GLU:HG3	1.72	0.53
3:D:1122:LEU:HD23	3:D:1140:ILE:HD13	1.91	0.53
2:I:726:ILE:HB	2:I:729:LEU:HB2	1.90	0.53
3:D:229:ALA:HB1	3:D:245:LEU:H	1.74	0.53
3:D:764:LEU:HD23	3:D:767:HIS:CD2	2.44	0.53
1:B:59:GLU:HG3	1:B:139:TYR:CD2	2.42	0.53
3:D:523:ASP:HA	3:D:526:PRO:HG3	1.90	0.53
2:I:754:ILE:HG22	2:I:755:LEU:H	1.72	0.53
2:I:759:THR:HB	2:I:785:VAL:HG21	1.91	0.53
2:I:943:VAL:HG21	2:I:973:VAL:HG13	1.90	0.53
5:F:207:LEU:O	5:F:211:VAL:HG23	2.08	0.53
3:J:104:PHE:CD2	3:J:512:MET:HG3	2.43	0.53
2:C:408:ARG:NH1	2:C:455:LEU:O	2.41	0.53
2:C:1086:ARG:HH11	2:C:1086:ARG:HG3	1.74	0.53
2:I:1086:ARG:HH11	2:I:1086:ARG:HG3	1.73	0.53
1:H:77:GLU:HB2	3:J:872:ARG:HH21	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:432:ARG:HH12	2:I:518:ARG:HE	1.55	0.53
5:F:145:VAL:HG21	5:F:174:VAL:HG11	1.91	0.53
3:J:175:VAL:HG13	3:J:193:PRO:HD2	1.91	0.53
3:D:1114:THR:HG21	3:D:1193:THR:O	2.09	0.53
3:D:119:SER:HB3	3:D:122:GLU:HG2	1.91	0.53
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.91	0.53
3:D:1197:ARG:HE	3:D:1398:TRP:HB3	1.72	0.53
2:C:584:GLU:CD	2:C:584:GLU:H	2.11	0.53
3:J:947:ILE:HG22	3:J:1019:PRO:HB3	1.90	0.53
2:I:48:PHE:O	2:I:52:PHE:HB2	2.09	0.53
3:J:140:ALA:HB1	3:J:161:LEU:HD23	1.91	0.53
4:E:45:ARG:HD2	4:E:63:TRP:CH2	2.43	0.53
2:C:457:ALA:HB3	2:C:538:GLN:HA	1.90	0.53
1:A:23:PHE:CE2	1:A:199:ILE:HD12	2.44	0.53
2:I:90:TYR:O	2:I:119:PRO:HA	2.07	0.53
3:D:729:HIS:HB3	3:D:732:VAL:HG22	1.91	0.53
3:J:166:GLN:HB3	3:J:396:VAL:HG13	1.91	0.53
2:I:328:LEU:HD21	2:I:434:HIS:HA	1.91	0.53
3:J:99:ALA:HB2	3:J:574:LEU:HD21	1.91	0.53
2:C:149:THR:HA	2:C:322:VAL:HG13	1.91	0.53
3:J:764:LEU:HD23	3:J:767:HIS:CD2	2.43	0.53
2:I:64:LEU:HD22	2:I:359:MET:SD	2.48	0.53
1:B:78:ILE:HD12	1:B:129:ILE:O	2.09	0.53
3:J:750:PRO:HG2	3:J:756:GLN:NE2	2.24	0.53
1:G:70:GLY:HA2	1:G:133:GLU:HG2	1.91	0.53
1:B:62:LEU:HB3	1:B:163:ASN:ND2	2.24	0.53
5:F:380:GLU:O	5:F:384:LEU:HB2	2.09	0.53
3:D:1147:ARG:NH2	3:D:1369:GLU:OE1	2.42	0.53
3:J:704:ARG:NE	3:J:705:ALA:O	2.42	0.53
3:J:131:LYS:HG3	3:J:153:LEU:O	2.09	0.53
2:I:584:GLU:H	2:I:584:GLU:CD	2.12	0.53
1:G:16:GLN:HB3	1:G:20:TYR:HB3	1.91	0.53
1:G:27:PRO:HB3	1:G:186:LEU:O	2.09	0.53
3:D:1366:LYS:O	3:D:1370:ILE:HG13	2.09	0.53
3:D:205:TYR:CD1	3:D:390:PRO:HG2	2.44	0.53
2:I:577:PRO:HG2	2:I:580:MET:HG2	1.91	0.53
3:D:757:ALA:O	3:D:761:ILE:HG13	2.09	0.53
3:J:683:ILE:HG22	3:J:687:VAL:HG21	1.91	0.53
3:D:704:ARG:NE	3:D:705:ALA:O	2.42	0.53
2:C:37:GLU:HG2	2:C:38:LYS:N	2.24	0.53
5:L:154:ALA:O	5:L:158:LYS:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:668:PRO:HB2	5:F:432:LYS:HD3	1.91	0.53
2:C:448:ASN:HA	2:C:451:LEU:HD22	1.90	0.53
5:F:137:LEU:HD22	5:F:178:LEU:HD11	1.91	0.52
2:I:206:THR:HG23	2:I:209:ARG:CZ	2.39	0.52
1:A:72:LYS:HG3	2:C:641:PRO:HB2	1.91	0.52
3:J:1293:PHE:HA	3:J:1302:GLU:HA	1.89	0.52
5:L:207:LEU:O	5:L:211:VAL:HG23	2.09	0.52
1:G:53:VAL:HA	1:G:144:VAL:HG22	1.90	0.52
3:D:104:PHE:HB3	3:D:111:LYS:HB2	1.91	0.52
3:D:928:ALA:HA	3:D:931:LEU:HD12	1.92	0.52
3:J:1107:VAL:HG13	3:J:1200:VAL:HG23	1.91	0.52
2:C:162:ILE:HB	2:C:172:ILE:HB	1.92	0.52
3:D:780:LYS:HB3	3:D:912:LYS:HZ1	1.74	0.52
1:B:45:LEU:HD21	1:B:177:VAL:HG22	1.91	0.52
2:C:851:LYS:HG2	2:C:852:ILE:H	1.75	0.52
1:B:77:GLU:HB2	3:D:872:ARG:NH2	2.25	0.52
3:D:1311:LEU:HD23	3:D:1311:LEU:H	1.75	0.52
3:D:264:LEU:HG	3:D:316:HIS:CE1	2.45	0.52
3:J:928:ALA:HA	3:J:931:LEU:HD12	1.92	0.52
2:C:304:LEU:HB2	2:C:305:PRO:HD3	1.92	0.52
3:J:968:ASP:OD1	3:J:1058:ARG:NH2	2.43	0.52
3:J:801:GLY:HA2	3:J:821:VAL:HA	1.92	0.52
3:D:831:GLY:HA3	3:J:977:ALA:HB2	1.91	0.52
3:J:154:THR:HG22	3:J:157:GLU:HG2	1.91	0.52
2:I:468:ARG:HD3	2:I:487:THR:HG22	1.92	0.52
2:I:708:TYR:HE1	2:I:827:VAL:HB	1.75	0.52
3:J:1156:LEU:HD21	3:J:1177:ALA:HA	1.92	0.52
2:C:135:VAL:HG13	2:C:393:GLN:HG3	1.91	0.52
5:F:280:VAL:HA	5:F:283:ILE:HD12	1.91	0.52
1:B:161:ARG:HG3	1:B:162:ILE:N	2.24	0.52
2:I:162:ILE:HB	2:I:172:ILE:HB	1.91	0.52
3:J:1470:ARG:HG2	3:J:1471:LEU:H	1.73	0.52
3:J:657:LEU:HG	3:J:661:MET:SD	2.49	0.52
1:A:16:GLN:HB3	1:A:20:TYR:HB3	1.90	0.52
3:J:162:ARG:O	3:J:414:ARG:NH2	2.36	0.52
2:C:290:LEU:HB3	2:C:303:PHE:CE1	2.45	0.52
2:C:1044:GLY:HA3	4:E:17:TYR:CE1	2.45	0.52
2:C:798:GLY:HA3	2:C:827:VAL:HG13	1.91	0.52
2:C:502:PRO:HB2	2:C:509:ALA:HB3	1.91	0.52
2:I:304:LEU:HB2	2:I:305:PRO:HD3	1.92	0.52
1:A:56:VAL:HG22	1:A:142:VAL:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1491:THR:HG22	4:E:92:LEU:HD12	1.91	0.52
1:A:27:PRO:HB3	1:A:186:LEU:O	2.09	0.52
3:J:1344:VAL:O	3:J:1348:LEU:HG	2.10	0.52
5:L:383:VAL:HG13	5:L:401:VAL:HG11	1.91	0.52
5:F:387:ARG:HD3	5:F:401:VAL:HG21	1.90	0.52
3:D:650:LEU:HD11	3:D:688:TRP:CZ3	2.45	0.52
2:I:851:LYS:HG2	2:I:852:ILE:H	1.74	0.52
1:G:63:HIS:CE1	1:G:65:PHE:HB2	2.45	0.52
2:I:606:VAL:HG23	2:I:645:VAL:HA	1.91	0.52
2:I:115:LEU:HB3	2:I:378:LEU:HD23	1.91	0.52
3:J:791:TYR:CZ	3:J:945:SER:HB3	2.45	0.52
3:D:348:ALA:HB1	3:D:349:PRO:HD2	1.92	0.52
3:D:639:LEU:HD22	3:D:766:ALA:HA	1.92	0.52
7:P:18:DT:H1'	7:P:19:DT:H5'	1.92	0.52
2:C:577:PRO:HG2	2:C:580:MET:HG2	1.92	0.52
3:D:224:ARG:HB3	3:D:251:PHE:CE2	2.44	0.52
3:D:477:LEU:HD21	3:D:495:ARG:HD3	1.91	0.52
2:I:37:GLU:HG2	2:I:38:LYS:N	2.25	0.52
3:J:757:ALA:O	3:J:761:ILE:HG13	2.10	0.52
2:C:848:VAL:CG2	3:D:740:PHE:HB3	2.40	0.52
3:J:95:LEU:HG	3:J:574:LEU:HD11	1.91	0.52
2:C:588:VAL:HG21	2:C:664:GLY:HA2	1.91	0.52
1:H:100:ILE:HD12	1:H:141:GLU:HG2	1.91	0.52
2:C:940:GLU:HA	2:C:973:VAL:HG11	1.91	0.52
2:C:674:VAL:O	2:C:989:VAL:HA	2.10	0.52
3:J:413:ASP:O	3:J:435:VAL:HG12	2.09	0.52
1:B:156:HIS:NE2	1:B:167:VAL:O	2.38	0.52
2:I:146:VAL:HG21	2:I:281:LEU:HD11	1.92	0.52
2:I:1083:GLU:OE2	3:J:87:ARG:NH1	2.43	0.52
2:C:950:LEU:HD21	2:C:952:LEU:HD22	1.92	0.52
2:C:211:LEU:HB3	2:C:218:VAL:HG13	1.91	0.52
2:C:704:HIS:HD2	2:C:831:ARG:HD2	1.74	0.52
5:F:383:VAL:HG13	5:F:401:VAL:HG11	1.91	0.52
2:I:135:VAL:HG11	2:I:406:HIS:CE1	2.45	0.52
2:I:195:LEU:HA	2:I:198:ARG:HD3	1.92	0.52
2:C:484:VAL:HG12	2:C:486:MET:H	1.75	0.52
3:D:299:GLU:CD	3:D:300:VAL:H	2.13	0.52
2:C:976:ASP:O	2:C:980:GLY:N	2.43	0.52
3:J:542:ASP:OD1	3:J:545:ARG:NH2	2.43	0.52
2:I:756:VAL:O	2:I:789:SER:HB2	2.09	0.51
2:C:756:VAL:O	2:C:789:SER:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1273:VAL:HG22	3:D:1326:THR:HG23	1.93	0.51
1:H:111:ALA:HB2	1:H:127:LEU:HB3	1.91	0.51
3:D:1261:GLU:OE2	3:D:1268:PRO:HA	2.10	0.51
2:I:177:GLU:HG3	2:I:178:ALA:N	2.25	0.51
3:D:140:ALA:HB1	3:D:161:LEU:HD23	1.91	0.51
3:D:1225:ALA:O	3:D:1229:ILE:HG13	2.09	0.51
2:C:706:GLU:HB3	2:C:708:TYR:CE1	2.44	0.51
3:D:71:LYS:O	3:D:80:VAL:HG12	2.10	0.51
2:I:940:GLU:HA	2:I:973:VAL:HG11	1.92	0.51
3:J:421:LEU:HD13	3:J:444:VAL:HB	1.92	0.51
3:D:938:GLY:HA2	3:D:941:LEU:HD12	1.91	0.51
3:D:708:LEU:H	3:D:708:LEU:HD23	1.76	0.51
3:J:938:GLY:HA2	3:J:941:LEU:HD12	1.91	0.51
5:F:353:LEU:HD12	5:F:354:PRO:HD2	1.91	0.51
2:I:136:ILE:HA	2:I:391:LEU:O	2.10	0.51
2:C:969:LEU:HG	3:D:952:ASP:HB2	1.92	0.51
2:I:135:VAL:HG13	2:I:393:GLN:HG3	1.92	0.51
7:P:5:DA:H1'	7:P:6:DC:H5'	1.92	0.51
5:F:249:LYS:HG2	6:O:29:DC:OP2	2.10	0.51
3:D:894:LYS:HG3	3:D:895:VAL:H	1.75	0.51
2:C:881:ASN:O	2:C:883:GLY:N	2.44	0.51
1:G:87:VAL:HG11	1:G:144:VAL:HG11	1.92	0.51
3:D:572:ARG:CZ	5:F:98:GLN:HG2	2.40	0.51
2:C:1103:ASP:HA	3:D:5:VAL:HA	1.92	0.51
2:I:876:VAL:HG13	2:I:884:GLN:HE21	1.76	0.51
3:D:131:LYS:HG3	3:D:153:LEU:O	2.10	0.51
2:I:770:GLU:HG2	5:L:366:SER:HA	1.92	0.51
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.92	0.51
2:I:1044:GLY:HA3	4:K:17:TYR:CE1	2.45	0.51
3:D:1047:LYS:HG2	3:D:1048:PRO:HD2	1.93	0.51
3:J:1376:LEU:HA	3:J:1420:LEU:O	2.11	0.51
3:J:415:VAL:HG22	3:J:433:GLY:O	2.10	0.51
3:D:1318:TYR:N	3:J:1157:GLY:O	2.43	0.51
1:A:53:VAL:HA	1:A:144:VAL:HG22	1.92	0.51
2:I:484:VAL:HG12	2:I:486:MET:H	1.75	0.51
2:C:408:ARG:HD3	2:C:542:LEU:HD21	1.92	0.51
2:I:141:HIS:NE2	2:I:334:ARG:HD3	2.25	0.51
2:I:290:LEU:HB3	2:I:303:PHE:CE1	2.45	0.51
5:L:137:LEU:HD22	5:L:178:LEU:HD11	1.93	0.51
3:D:122:GLU:HB2	3:D:152:LEU:HD21	1.93	0.51
2:I:18:LEU:H	2:I:18:LEU:HD22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:729:HIS:HB3	3:J:732:VAL:HG22	1.92	0.51
5:L:110:THR:HG22	5:L:111:LEU:H	1.75	0.51
2:C:557:ARG:HB2	2:C:881:ASN:HD21	1.74	0.51
2:I:1035:MET:HB2	3:J:707:THR:HB	1.92	0.51
3:J:1110:ALA:O	3:J:1202:GLN:HB2	2.10	0.51
2:I:195:LEU:HD23	2:I:238:LEU:HG	1.91	0.51
3:D:264:LEU:HG	3:D:316:HIS:NE2	2.26	0.51
2:C:943:VAL:HG21	2:C:973:VAL:HG13	1.91	0.51
2:C:637:PHE:HA	2:C:659:PRO:HG3	1.93	0.51
5:L:145:VAL:HG21	5:L:174:VAL:HG11	1.92	0.51
2:I:114:PHE:HE1	5:L:294:GLN:HE21	1.57	0.51
4:E:34:ARG:HH21	4:E:94:PRO:HG2	1.76	0.51
1:B:181:VAL:HG12	1:B:195:LEU:HB2	1.93	0.51
3:D:1202:GLN:NE2	3:D:1217:ILE:HG12	2.26	0.51
5:L:380:GLU:HB2	5:L:419:ALA:HB2	1.93	0.51
2:C:598:GLU:HG2	2:C:615:TYR:CZ	2.46	0.51
3:D:1170:ASP:O	3:D:1174:LEU:HG	2.11	0.51
3:J:1306:PRO:HB2	3:J:1308:ASP:OD1	2.11	0.51
3:J:773:ALA:HB2	3:J:1228:SER:HB3	1.93	0.51
5:L:218:THR:HA	5:L:227:LEU:HD11	1.93	0.51
2:C:436:GLY:HA2	2:C:538:GLN:O	2.11	0.51
3:J:780:LYS:HB3	3:J:912:LYS:HZ1	1.76	0.51
2:C:708:TYR:HE1	2:C:827:VAL:HB	1.75	0.51
3:D:1108:ARG:HB2	3:D:1108:ARG:NH1	2.26	0.51
2:I:135:VAL:HG23	2:I:407:LYS:HG2	1.92	0.51
2:C:195:LEU:HD23	2:C:238:LEU:HG	1.92	0.51
2:C:198:ARG:HH22	2:C:238:LEU:HB2	1.75	0.51
2:I:831:ARG:HD3	2:I:1002:GLU:HG2	1.93	0.51
3:J:437:VAL:HG22	3:J:444:VAL:HG13	1.91	0.51
2:C:606:VAL:HG23	2:C:645:VAL:HA	1.91	0.51
5:F:110:THR:HG22	5:F:111:LEU:H	1.76	0.51
3:D:1336:LEU:HD22	3:D:1421:LEU:HB3	1.92	0.51
1:H:49:PRO:HA	1:H:147:GLY:O	2.10	0.51
2:C:9:ILE:HD12	2:C:907:ASP:HB2	1.92	0.51
5:F:412:ILE:HD13	5:F:415:ILE:HD12	1.93	0.51
3:D:1095:THR:HG22	3:D:1230:GLY:HA3	1.93	0.51
3:J:1047:LYS:HG2	3:J:1048:PRO:HD2	1.93	0.51
3:D:1135:ARG:HH21	3:D:1357:ARG:HH12	1.59	0.51
3:D:111:LYS:HD2	3:D:1452:ILE:HG13	1.93	0.51
3:D:647:ARG:HH12	3:D:683:ILE:HD11	1.76	0.51
2:I:277:ALA:HA	2:I:280:LYS:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:252:THR:HA	6:R:29:DC:H5	1.76	0.51
5:L:116:ASP:O	5:L:120:LYS:HG3	2.10	0.51
3:J:1170:ASP:N	3:J:1170:ASP:OD2	2.43	0.50
2:I:634:GLY:O	2:I:704:HIS:HA	2.11	0.50
3:D:896:ALA:O	3:D:900:ILE:HG13	2.11	0.50
5:F:254:ALA:O	5:F:258:ILE:HG12	2.11	0.50
5:F:116:ASP:O	5:F:120:LYS:HG3	2.11	0.50
2:I:408:ARG:HD3	2:I:542:LEU:HD21	1.94	0.50
2:C:408:ARG:HG2	2:C:455:LEU:HB3	1.93	0.50
3:J:1344:VAL:HG12	3:J:1348:LEU:HD11	1.93	0.50
1:A:14:THR:HG23	1:B:231:SER:O	2.11	0.50
3:D:657:LEU:HG	3:D:661:MET:SD	2.51	0.50
1:G:14:THR:HG23	1:H:231:SER:O	2.11	0.50
5:F:252:THR:OG1	6:O:28:DA:H2'	2.11	0.50
1:G:72:LYS:HG3	2:I:641:PRO:HB2	1.92	0.50
3:D:837:GLY:HA2	3:D:840:LYS:HB3	1.93	0.50
1:B:149:GLY:O	1:B:171:PHE:HB2	2.12	0.50
2:I:524:VAL:HG22	2:I:525:ALA:H	1.76	0.50
3:D:1020:LEU:HD11	3:D:1035:ILE:HD12	1.94	0.50
5:L:165:LYS:HD2	5:L:165:LYS:H	1.76	0.50
5:F:410:GLU:O	5:F:413:ARG:HB3	2.10	0.50
2:I:668:LEU:HB3	2:I:995:MET:HG3	1.92	0.50
2:I:139:GLN:HB3	2:I:334:ARG:HB2	1.93	0.50
2:C:139:GLN:HB3	2:C:334:ARG:HB2	1.94	0.50
3:J:1285:GLU:HG2	3:J:1290:LEU:HG	1.93	0.50
1:H:45:LEU:HD21	1:H:177:VAL:HG22	1.94	0.50
3:D:1253:THR:HG22	3:D:1254:GLN:H	1.76	0.50
2:I:683:ASN:HB2	2:I:872:ASN:H	1.77	0.50
1:G:20:TYR:HD2	1:G:21:GLY:H	1.59	0.50
3:J:420:VAL:HG22	3:J:421:LEU:O	2.11	0.50
2:C:18:LEU:HD22	2:C:18:LEU:H	1.76	0.50
1:A:88:ARG:HD2	1:A:204:SER:O	2.11	0.50
4:K:34:ARG:HH21	4:K:94:PRO:HG2	1.75	0.50
3:J:479:GLU:O	3:J:482:LYS:HG2	2.12	0.50
3:D:1343:ALA:HA	3:D:1346:ARG:HG3	1.94	0.50
1:G:218:LEU:HD21	1:H:222:LEU:HD22	1.94	0.50
2:I:706:GLU:HB3	2:I:708:TYR:CE1	2.46	0.50
2:I:508:ILE:HD11	2:I:529:VAL:HG11	1.93	0.50
1:B:100:ILE:HD12	1:B:141:GLU:HG2	1.94	0.50
1:H:182:GLU:HG3	1:H:194:LYS:HB3	1.93	0.50
3:J:543:LEU:HG	3:J:600:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:989:TYR:O	3:J:993:ILE:HB	2.11	0.50
7:P:3:DG:H1'	7:P:4:DC:H5'	1.92	0.50
2:I:501:THR:HG22	2:I:514:VAL:HG23	1.94	0.50
1:B:89:PHE:HE1	1:B:97:THR:HG22	1.77	0.50
3:D:791:TYR:CZ	3:D:945:SER:HB3	2.47	0.50
2:C:113:VAL:HG12	2:C:370:ALA:HA	1.94	0.50
3:J:1231:GLU:HB3	3:J:1232:PRO:HD3	1.93	0.50
3:J:650:LEU:HD11	3:J:688:TRP:CZ3	2.46	0.50
7:P:8:DA:H1'	7:P:9:DT:H5''	1.93	0.50
1:G:23:PHE:CE2	1:G:199:ILE:HD12	2.45	0.50
2:C:403:SER:O	2:C:407:LYS:HE2	2.12	0.50
3:J:644:LEU:HG	3:J:649:ALA:HB2	1.93	0.50
3:J:654:LYS:O	3:J:658:LEU:HB2	2.11	0.50
2:I:408:ARG:HG2	2:I:455:LEU:HB3	1.93	0.50
2:C:1112:PHE:HB3	3:D:88:TYR:CD2	2.46	0.50
2:C:69:LEU:HG	2:C:98:LEU:HA	1.93	0.50
2:C:195:LEU:HA	2:C:198:ARG:HD3	1.93	0.50
5:L:431:ARG:HG2	5:L:431:ARG:O	2.12	0.50
2:C:770:GLU:HG2	5:F:366:SER:HA	1.93	0.50
3:J:1425:THR:HG22	3:J:1429:LEU:HD12	1.94	0.50
3:D:112:ILE:HD12	3:D:113:GLY:N	2.27	0.50
3:D:1473:PRO:O	3:D:1478:SER:HA	2.11	0.50
3:J:631:ILE:HD11	3:J:739:ASP:O	2.12	0.50
1:B:29:GLU:HB3	1:B:32:PHE:CD1	2.47	0.50
2:C:726:ILE:HB	2:C:729:LEU:HB2	1.92	0.50
2:I:173:ASP:O	2:I:184:MET:HG3	2.11	0.50
2:I:881:ASN:O	2:I:883:GLY:N	2.45	0.50
1:B:49:PRO:HA	1:B:147:GLY:O	2.12	0.50
2:C:627:ARG:HD2	2:C:639:GLN:H	1.76	0.50
2:C:885:ILE:HG22	2:C:889:HIS:CD2	2.47	0.50
2:I:704:HIS:HD2	2:I:831:ARG:HD2	1.75	0.50
3:J:896:ALA:O	3:J:900:ILE:HG13	2.12	0.50
2:I:387:SER:HB2	2:I:388:ARG:NH1	2.27	0.50
2:C:736:ASP:HB3	2:C:744:ARG:HG3	1.93	0.50
1:H:149:GLY:O	1:H:171:PHE:HB2	2.11	0.50
3:D:527:MET:HG3	3:D:537:THR:HB	1.92	0.50
1:G:56:VAL:HG22	1:G:142:VAL:HG12	1.94	0.50
3:J:894:LYS:HG3	3:J:895:VAL:H	1.76	0.50
2:C:177:GLU:HG3	2:C:178:ALA:N	2.27	0.50
2:C:23:VAL:HA	2:C:121:MET:SD	2.52	0.50
2:I:537:LYS:HE3	2:I:583:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:7:DA:H61	7:S:20:DT:H3	1.60	0.49
2:I:1085:PHE:HA	3:J:618:LEU:HD21	1.94	0.49
3:J:1225:ALA:O	3:J:1229:ILE:HG13	2.12	0.49
3:J:402:PRO:HA	3:J:443:VAL:HA	1.93	0.49
2:I:848:VAL:HG11	3:J:630:VAL:HG21	1.94	0.49
2:I:729:LEU:HD12	2:I:734:LEU:HD13	1.94	0.49
1:H:77:GLU:HB2	3:J:872:ARG:NH2	2.26	0.49
2:C:448:ASN:O	2:C:451:LEU:HB2	2.12	0.49
1:B:97:THR:OG1	1:B:98:THR:N	2.44	0.49
1:G:56:VAL:HG21	1:G:82:LEU:HD13	1.94	0.49
3:D:274:GLN:HG3	3:D:279:VAL:HG21	1.94	0.49
3:D:1150:ALA:HB3	3:D:1187:PRO:HB2	1.93	0.49
2:C:508:ILE:HD11	2:C:529:VAL:HG11	1.94	0.49
3:D:317:MET:SD	3:D:337:LEU:HD22	2.52	0.49
3:D:112:ILE:HG23	3:D:512:MET:SD	2.52	0.49
3:D:1110:ALA:O	3:D:1202:GLN:HB2	2.12	0.49
2:C:214:TYR:HB3	2:C:217:LEU:HD12	1.94	0.49
2:C:708:TYR:OH	2:C:796:GLU:OE1	2.24	0.49
3:D:815:ALA:HA	3:D:818:ARG:HE	1.77	0.49
2:C:37:GLU:HG2	2:C:38:LYS:H	1.77	0.49
3:D:1264:GLU:OE1	3:D:1425:THR:OG1	2.29	0.49
2:C:705:ILE:HG12	2:C:828:ALA:HB2	1.94	0.49
3:D:176:ASP:HA	3:D:389:GLU:HA	1.94	0.49
1:H:159:LYS:HA	1:H:164:ALA:HB3	1.94	0.49
3:J:129:PHE:CE1	3:J:457:GLY:HA3	2.47	0.49
2:I:976:ASP:O	2:I:980:GLY:N	2.44	0.49
1:A:218:LEU:HD21	1:B:222:LEU:HD22	1.95	0.49
2:C:1083:GLU:O	2:C:1087:VAL:HG23	2.11	0.49
3:D:18:ILE:HG12	3:D:518:PRO:HG3	1.94	0.49
3:J:650:LEU:HD21	3:J:683:ILE:HG21	1.94	0.49
2:I:848:VAL:CG2	3:J:740:PHE:HB3	2.41	0.49
2:C:581:THR:OG1	2:C:584:GLU:OE2	2.30	0.49
1:A:63:HIS:HA	1:A:165:ILE:HD11	1.94	0.49
5:F:289:THR:O	5:F:293:LEU:HG	2.12	0.49
5:F:209:LEU:HB2	6:O:30:DT:C2	2.47	0.49
3:J:711:LEU:HB3	3:J:735:ALA:HB1	1.94	0.49
3:D:1231:GLU:HB3	3:D:1232:PRO:HD3	1.94	0.49
2:I:1083:GLU:O	2:I:1087:VAL:HG23	2.11	0.49
3:D:111:LYS:O	3:D:115:LEU:HB2	2.12	0.49
2:C:390:GLN:HG2	2:C:415:PRO:HD3	1.94	0.49
3:J:639:LEU:HD22	3:J:766:ALA:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:277:ALA:HA	2:C:280:LYS:HD3	1.94	0.49
2:C:707:ARG:HB2	2:C:707:ARG:HH11	1.78	0.49
2:C:501:THR:HG22	2:C:514:VAL:HG23	1.94	0.49
1:G:35:THR:HG23	1:H:42:ARG:HB2	1.94	0.49
2:C:754:ILE:HG12	2:C:791:ARG:HD3	1.94	0.49
4:E:19:LEU:O	4:E:23:VAL:HG23	2.13	0.49
3:D:644:LEU:HG	3:D:649:ALA:HB2	1.95	0.49
2:I:588:VAL:HG21	2:I:664:GLY:HA2	1.93	0.49
3:D:849:ALA:O	3:D:853:VAL:HG23	2.13	0.49
3:J:132:TYR:HA	3:J:456:MET:HB3	1.94	0.49
3:D:638:LYS:HG3	3:D:639:LEU:N	2.27	0.49
3:D:245:LEU:CB	3:D:309:GLY:HA2	2.41	0.49
2:I:64:LEU:HD21	2:I:66:LEU:HB2	1.95	0.49
2:C:607:ASP:C	2:C:609:THR:H	2.15	0.49
3:D:1434:TRP:NE1	3:D:1457:ASP:HB2	2.27	0.49
5:L:252:THR:HA	6:R:29:DC:C5	2.48	0.49
2:C:1007:ALA:HB1	3:D:652:LEU:HD13	1.94	0.49
3:J:577:ALA:O	3:J:581:VAL:HG23	2.12	0.49
3:J:214:ASP:HA	3:J:342:PRO:HA	1.94	0.49
5:L:241:LYS:HE2	6:R:24:DC:H3'	1.95	0.49
2:I:598:GLU:HG2	2:I:615:TYR:CZ	2.47	0.49
5:F:149:LYS:HB2	5:F:193:ARG:HH12	1.78	0.49
2:C:524:VAL:HG22	2:C:525:ALA:H	1.76	0.49
5:L:254:ALA:O	5:L:258:ILE:HG12	2.13	0.49
2:C:936:VAL:HB	2:C:941:LYS:HE2	1.95	0.49
3:D:471:GLU:O	3:D:474:GLU:HB3	2.12	0.49
3:J:1361:VAL:HG12	3:J:1363:LEU:H	1.78	0.49
2:I:9:ILE:HD12	2:I:907:ASP:HB2	1.94	0.49
2:I:436:GLY:HA2	2:I:538:GLN:O	2.12	0.49
3:D:1106:VAL:HB	3:D:1108:ARG:HH12	1.78	0.49
2:C:1067:TYR:O	2:C:1071:ILE:HB	2.12	0.49
2:I:198:ARG:HH22	2:I:238:LEU:HB2	1.77	0.49
1:A:56:VAL:HG21	1:A:82:LEU:HD13	1.95	0.49
2:C:729:LEU:HD12	2:C:734:LEU:HD13	1.94	0.49
2:I:572:ILE:HD11	2:I:703:ILE:HG13	1.93	0.49
2:I:674:VAL:O	2:I:989:VAL:HA	2.12	0.49
2:I:272:ALA:O	2:I:276:LYS:N	2.39	0.49
3:D:1046:GLN:HE22	3:D:1079:LYS:HE2	1.78	0.49
1:H:151:VAL:HG12	1:H:156:HIS:HD2	1.78	0.49
2:C:65:VAL:HG12	2:C:101:ILE:HB	1.95	0.49
5:L:387:ARG:HD3	5:L:401:VAL:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:103:ILE:HD13	5:F:211:VAL:HG21	1.95	0.49
3:J:815:ALA:HA	3:J:818:ARG:HE	1.78	0.49
5:L:412:ILE:O	5:L:416:GLU:HG2	2.13	0.49
5:L:210:VAL:HA	5:L:213:ILE:HD12	1.95	0.49
2:I:193:LEU:HA	2:I:196:LEU:HD13	1.94	0.49
5:L:238:ALA:HB2	5:L:257:TRP:HB2	1.95	0.49
3:D:1131:THR:HA	3:J:1179:GLU:O	2.12	0.49
3:D:989:TYR:O	3:D:993:ILE:HB	2.12	0.49
1:A:87:VAL:HG11	1:A:144:VAL:HG11	1.95	0.49
3:J:112:ILE:HD12	3:J:113:GLY:N	2.28	0.49
5:F:165:LYS:H	5:F:165:LYS:HD2	1.78	0.49
3:D:1459:LEU:HD23	3:D:1470:ARG:HE	1.78	0.49
5:F:292:GLN:O	5:F:295:GLN:HG3	2.13	0.49
1:H:176:ARG:HG3	3:J:850:LEU:HD22	1.94	0.49
3:J:644:LEU:HD12	3:J:645:PRO:HD2	1.94	0.49
5:F:431:ARG:O	5:F:431:ARG:HG2	2.11	0.49
3:D:1280:VAL:HG22	3:D:1295:GLU:O	2.12	0.49
2:C:874:LEU:O	2:C:877:PRO:HD2	2.13	0.49
3:D:112:ILE:HD12	3:D:113:GLY:H	1.78	0.48
3:D:1377:LYS:O	3:D:1397:LYS:N	2.39	0.48
2:I:497:ALA:HB3	2:I:532:MET:HG3	1.94	0.48
2:C:952:LEU:HD23	2:C:966:LEU:HD11	1.95	0.48
2:I:65:VAL:HG12	2:I:101:ILE:HB	1.95	0.48
3:J:927:THR:HA	3:J:930:LEU:HB3	1.95	0.48
3:J:638:LYS:HG3	3:J:639:LEU:N	2.28	0.48
5:L:336:ILE:HD11	5:L:344:TYR:HA	1.95	0.48
3:J:1197:ARG:HE	3:J:1398:TRP:HB3	1.78	0.48
1:G:15:THR:O	1:H:232:LEU:HD23	2.13	0.48
5:L:220:ARG:HH22	7:S:1:DT:H3'	1.78	0.48
5:L:124:GLY:O	5:L:128:ILE:HG13	2.13	0.48
5:F:241:LYS:HE2	6:O:24:DC:H3'	1.96	0.48
2:I:22:GLN:HA	2:I:336:VAL:HG21	1.95	0.48
3:D:974:ILE:HG22	3:D:988:ARG:HG3	1.94	0.48
3:J:122:GLU:O	3:J:126:VAL:HG23	2.12	0.48
3:J:666:PHE:CE1	3:J:687:VAL:HG12	2.48	0.48
3:D:1170:ASP:OD2	3:D:1170:ASP:N	2.43	0.48
2:I:736:ASP:HB3	2:I:744:ARG:HG3	1.94	0.48
3:D:1107:VAL:HG13	3:D:1200:VAL:HG23	1.95	0.48
2:I:751:PRO:HB3	2:I:794:PRO:HA	1.94	0.48
3:J:702:LEU:HD12	3:J:746:ALA:O	2.12	0.48
2:C:11:GLU:HG3	2:C:535:SER:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:8:DA:C2'	7:P:9:DT:H5''	2.44	0.48
2:I:713:ARG:NH1	3:J:533:GLY:HA2	2.28	0.48
1:A:63:HIS:HB3	2:C:746:GLY:HA3	1.95	0.48
5:F:336:ILE:HD11	5:F:344:TYR:HA	1.94	0.48
2:C:410:ILE:O	2:C:452:ILE:HA	2.13	0.48
1:B:151:VAL:HG12	1:B:156:HIS:HD2	1.79	0.48
6:R:7:DA:H1'	6:R:8:DA:H5'	1.94	0.48
2:I:885:ILE:HG22	2:I:889:HIS:CD2	2.49	0.48
3:J:71:LYS:O	3:J:80:VAL:HG12	2.13	0.48
2:I:936:VAL:HB	2:I:941:LYS:HE2	1.94	0.48
3:D:397:LYS:HE2	3:D:448:GLU:HB3	1.94	0.48
3:D:968:ASP:OD1	3:D:1058:ARG:NH2	2.46	0.48
6:O:14:DT:H1'	6:O:15:DT:H5'	1.95	0.48
3:J:15:PRO:HG3	3:J:514:LEU:HD12	1.95	0.48
3:D:421:LEU:HD11	3:D:429:SER:HB2	1.95	0.48
3:D:806:PHE:CD1	3:D:811:GLU:HB3	2.48	0.48
1:H:156:HIS:ND1	1:H:156:HIS:O	2.46	0.48
2:C:1035:MET:HB2	3:D:707:THR:HB	1.94	0.48
2:I:69:LEU:HG	2:I:98:LEU:HA	1.94	0.48
2:I:1112:PHE:HB2	2:I:1115:LEU:HB2	1.96	0.48
1:G:36:LEU:O	1:G:39:PRO:HD2	2.14	0.48
3:D:780:LYS:HB2	3:D:908:LYS:HZ1	1.79	0.48
1:B:176:ARG:HG3	3:D:850:LEU:HD22	1.94	0.48
2:C:135:VAL:HG11	2:C:406:HIS:CE1	2.48	0.48
2:I:572:ILE:H	2:I:572:ILE:HD12	1.77	0.48
3:D:1021:TYR:CE1	3:D:1025:GLN:HG3	2.49	0.48
2:I:11:GLU:HG3	2:I:535:SER:HB2	1.94	0.48
2:C:816:LYS:HG3	2:C:817:PRO:HD2	1.94	0.48
3:J:699:VAL:HG22	3:J:760:ARG:HG2	1.96	0.48
3:J:862:ASP:O	3:J:876:SER:HA	2.13	0.48
2:I:772:ARG:HG2	5:L:388:LYS:HD2	1.96	0.48
3:J:122:GLU:HB2	3:J:152:LEU:HD21	1.95	0.48
1:B:179:PHE:HB3	1:B:197:LEU:HD13	1.96	0.48
2:C:679:PHE:H	2:C:683:ASN:HD21	1.60	0.48
2:I:37:GLU:HG2	2:I:38:LYS:H	1.78	0.48
3:D:1098:LEU:HD11	3:D:1263:PHE:CD2	2.48	0.48
3:J:1283:ILE:HA	3:J:1292:VAL:HG22	1.96	0.48
3:D:127:LEU:HD23	3:D:461:ILE:HG13	1.95	0.48
1:A:30:ARG:HG3	2:C:938:LYS:NZ	2.28	0.48
3:J:25:GLU:HG2	3:J:93:ILE:HA	1.94	0.48
3:J:716:PHE:CZ	3:J:728:LEU:HD11	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1065:LEU:HB3	3:D:1069:GLU:HB2	1.95	0.48
2:I:816:LYS:HG3	2:I:817:PRO:HD2	1.95	0.48
5:L:165:LYS:O	5:L:165:LYS:HG2	2.13	0.48
2:C:71:TYR:HD1	2:C:94:LEU:HD11	1.78	0.48
2:C:1055:ILE:HD11	2:C:1079:PRO:HD3	1.95	0.48
2:I:1089:VAL:HG11	2:I:1112:PHE:HE2	1.78	0.48
3:D:103:TRP:HE3	3:D:1448:THR:HG23	1.77	0.48
2:C:848:VAL:HG11	3:D:630:VAL:HG21	1.95	0.48
3:J:1500:LYS:HA	3:J:1503:VAL:HG22	1.95	0.48
1:A:24:VAL:HA	1:A:195:LEU:O	2.14	0.48
1:B:187:GLY:H	4:E:51:LEU:HD11	1.79	0.48
3:D:521:PRO:HD2	3:D:524:LEU:HD12	1.95	0.48
1:A:42:ARG:NH1	2:C:857:ASP:OD1	2.46	0.48
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.49	0.48
2:C:578:VAL:HG23	2:C:671:ASN:ND2	2.28	0.48
3:J:123:LEU:HG	3:J:127:LEU:HD11	1.96	0.48
2:I:448:ASN:O	2:I:451:LEU:HB2	2.14	0.48
1:G:66:SER:O	1:G:75:VAL:HG23	2.14	0.48
2:I:432:ARG:HG3	2:I:432:ARG:H	1.48	0.48
1:A:70:GLY:HA2	1:A:133:GLU:HG2	1.95	0.48
2:C:157:ARG:CZ	2:C:314:THR:HB	2.43	0.48
1:A:57:TYR:HB3	1:A:141:GLU:HG3	1.95	0.48
2:I:627:ARG:HD2	2:I:639:GLN:H	1.79	0.48
2:I:113:VAL:HG12	2:I:370:ALA:HA	1.96	0.48
3:J:876:SER:O	3:J:879:ARG:HB3	2.14	0.48
2:I:1055:ILE:HD11	2:I:1079:PRO:HD3	1.96	0.48
2:C:135:VAL:HG23	2:C:407:LYS:HG2	1.95	0.48
1:A:63:HIS:CE1	1:A:65:PHE:HB2	2.48	0.48
2:I:941:LYS:HZ2	2:I:959:PRO:HG2	1.78	0.48
2:C:660:ALA:O	2:C:667:ALA:N	2.41	0.48
3:J:1473:PRO:O	3:J:1478:SER:HA	2.13	0.48
3:J:1127:GLU:HG3	3:J:1128:VAL:HG23	1.96	0.48
4:E:26:ARG:O	4:E:30:LEU:HD13	2.14	0.48
1:G:42:ARG:NH2	1:H:31:GLY:O	2.36	0.48
1:G:42:ARG:NH1	2:I:857:ASP:OD1	2.47	0.48
3:D:862:ASP:O	3:D:876:SER:HA	2.14	0.48
5:F:165:LYS:O	5:F:165:LYS:HG2	2.14	0.48
2:I:1047:HIS:HA	2:I:1050:GLN:HG2	1.94	0.48
2:I:798:GLY:HA3	2:I:827:VAL:CG1	2.43	0.48
2:C:886:LEU:HD21	3:D:951:ILE:HD13	1.95	0.48
7:P:10:DT:H1'	7:P:11:DT:H5'	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:387:SER:HB2	2:C:388:ARG:NH1	2.29	0.48
2:C:399:ASN:HD21	2:C:566:THR:HA	1.79	0.48
2:C:714:ASP:HA	2:C:719:PRO:HA	1.95	0.48
2:C:173:ASP:O	2:C:184:MET:HG3	2.14	0.48
3:D:638:LYS:HG2	3:D:640:HIS:CE1	2.49	0.47
3:J:760:ARG:HH21	4:K:65:MET:HG3	1.79	0.47
3:D:46:ASP:O	3:D:50:PHE:HB2	2.14	0.47
3:J:1335:LEU:HD12	3:J:1344:VAL:HG22	1.96	0.47
1:A:36:LEU:O	1:A:39:PRO:HD2	2.14	0.47
5:L:178:LEU:HA	5:L:181:LEU:HD13	1.96	0.47
3:D:661:MET:HG2	3:D:666:PHE:CZ	2.49	0.47
2:C:572:ILE:HD12	2:C:572:ILE:H	1.79	0.47
5:L:412:ILE:HD13	5:L:415:ILE:HD12	1.96	0.47
2:I:886:LEU:HD21	3:J:951:ILE:HD13	1.95	0.47
1:G:88:ARG:HD2	1:G:204:SER:O	2.13	0.47
1:H:64:GLU:HG3	1:H:165:ILE:HG21	1.96	0.47
3:J:560:GLN:HE22	5:L:236:ILE:HD13	1.79	0.47
2:I:1047:HIS:HA	2:I:1050:GLN:CG	2.43	0.47
2:I:769:PRO:HG3	3:J:65:ARG:HH12	1.78	0.47
2:I:607:ASP:C	2:I:609:THR:H	2.18	0.47
2:I:22:GLN:HG3	2:I:407:LYS:HB3	1.96	0.47
2:C:209:ARG:HG3	2:C:210:GLU:N	2.29	0.47
6:O:28:DA:H1'	6:O:29:DC:H5'	1.96	0.47
3:D:475:ARG:HA	3:D:478:LEU:HD12	1.96	0.47
2:I:705:ILE:HG12	2:I:828:ALA:HB2	1.96	0.47
2:C:569:VAL:HB	2:C:635:THR:HG21	1.96	0.47
1:B:64:GLU:HG3	1:B:165:ILE:HG21	1.96	0.47
3:J:544:TYR:O	3:J:548:ILE:HG13	2.13	0.47
4:K:26:ARG:O	4:K:30:LEU:HD13	2.15	0.47
3:D:1225:ALA:HB1	3:D:1367:HIS:HB3	1.96	0.47
1:G:209:GLU:O	1:G:213:GLN:HG2	2.15	0.47
2:I:1085:PHE:HE2	3:J:1468:LEU:HD22	1.80	0.47
2:I:403:SER:O	2:I:407:LYS:HE2	2.13	0.47
2:C:876:VAL:HG13	2:C:884:GLN:HE21	1.79	0.47
1:G:177:VAL:HG13	1:G:199:ILE:HG12	1.95	0.47
1:G:44:LEU:HD13	1:G:177:VAL:HG21	1.97	0.47
3:D:650:LEU:HD21	3:D:683:ILE:HG21	1.95	0.47
3:J:977:ALA:HB3	3:J:983:LEU:HD12	1.96	0.47
1:A:20:TYR:HD2	1:A:21:GLY:H	1.62	0.47
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.97	0.47
2:I:157:ARG:CZ	2:I:314:THR:HB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:VAL:O	1:A:182:GLU:HG3	2.14	0.47
2:I:410:ILE:O	2:I:452:ILE:HA	2.14	0.47
2:C:700:TYR:HB3	2:C:833:LEU:HD13	1.96	0.47
3:D:517:VAL:O	3:D:519:VAL:HG23	2.15	0.47
3:D:1188:VAL:HG12	3:D:1189:ARG:N	2.30	0.47
3:J:708:LEU:H	3:J:708:LEU:HD23	1.79	0.47
3:J:131:LYS:HE2	3:J:152:LEU:HB3	1.96	0.47
2:I:209:ARG:HG3	2:I:210:GLU:N	2.29	0.47
2:C:374:ASN:OD1	2:C:375:SER:N	2.47	0.47
1:G:41:ARG:HD3	1:G:45:LEU:HD11	1.96	0.47
5:L:117:LEU:O	5:L:121:VAL:HG23	2.15	0.47
3:D:1153:VAL:O	3:D:1159:ARG:HB2	2.14	0.47
3:D:250:LEU:HD23	3:D:306:GLU:HG3	1.96	0.47
2:I:707:ARG:HB2	2:I:707:ARG:HH11	1.79	0.47
3:J:1366:LYS:O	3:J:1370:ILE:HG13	2.14	0.47
2:C:578:VAL:HG13	2:C:900:ARG:HG2	1.97	0.47
3:D:977:ALA:HB3	3:D:983:LEU:HD12	1.97	0.47
5:L:383:VAL:HG22	5:L:404:TYR:HE2	1.77	0.47
3:D:971:LEU:HA	3:D:974:ILE:HD12	1.95	0.47
3:J:1495:ILE:HD13	4:K:80:VAL:HB	1.95	0.47
3:J:9:ARG:HG2	3:J:10:ILE:N	2.28	0.47
2:I:570:PRO:HD2	2:I:635:THR:HG21	1.97	0.47
3:D:1302:GLU:OE2	3:D:1304:LYS:HE3	2.14	0.47
3:D:918:ALA:O	3:D:922:LEU:HB2	2.15	0.47
3:J:1114:THR:HG21	3:J:1193:THR:O	2.15	0.47
3:D:841:PHE:CE2	3:D:858:LEU:HD13	2.50	0.47
1:H:150:TYR:HD2	3:J:857:LEU:HD12	1.80	0.47
2:I:45:GLN:HA	2:I:45:GLN:HE21	1.79	0.47
3:J:1151:ARG:HA	3:J:1162:GLU:HG3	1.96	0.47
5:L:286:LEU:HD23	5:L:310:MET:HG3	1.95	0.47
4:E:45:ARG:HD2	4:E:63:TRP:HH2	1.80	0.47
1:B:156:HIS:O	1:B:156:HIS:ND1	2.48	0.47
2:I:214:TYR:HB3	2:I:217:LEU:HD12	1.97	0.47
2:C:64:LEU:HD21	2:C:66:LEU:HB2	1.95	0.47
2:C:136:ILE:HA	2:C:391:LEU:O	2.14	0.47
2:C:772:ARG:HG2	5:F:388:LYS:HD2	1.96	0.47
3:J:1444:THR:O	3:J:1448:THR:OG1	2.33	0.47
3:D:1464:GLU:CD	3:D:1464:GLU:H	2.15	0.47
5:F:238:ALA:HB2	5:F:257:TRP:HB2	1.96	0.47
1:H:54:THR:OG1	1:H:55:SER:N	2.47	0.47
3:J:849:ALA:O	3:J:853:VAL:HG23	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:874:LEU:O	2:I:877:PRO:HD2	2.14	0.47
1:G:57:TYR:HB3	1:G:141:GLU:HG3	1.95	0.47
1:H:40:LEU:O	1:H:44:LEU:HB2	2.15	0.47
1:H:34:VAL:HG11	2:I:978:ARG:HB3	1.97	0.47
3:D:930:LEU:O	3:D:934:LEU:HD12	2.15	0.47
3:J:46:ASP:O	3:J:50:PHE:HB2	2.13	0.47
6:O:5:DA:H1'	6:O:6:DC:H5'	1.96	0.47
2:C:497:ALA:HB3	2:C:532:MET:HG3	1.97	0.47
3:D:226:PRO:HD2	3:D:245:LEU:HD21	1.97	0.47
2:I:71:TYR:HD1	2:I:94:LEU:HD11	1.79	0.47
3:J:1102:ALA:HB1	3:J:1222:GLY:C	2.35	0.47
3:D:517:VAL:HG11	3:D:547:LEU:HD21	1.96	0.47
3:D:25:GLU:HA	3:D:92:HIS:O	2.14	0.47
3:D:548:ILE:HG13	3:D:548:ILE:H	1.54	0.47
2:I:952:LEU:HD23	2:I:966:LEU:HD11	1.96	0.47
3:J:1459:LEU:HB3	3:J:1465:ASN:ND2	2.30	0.47
3:D:557:LEU:HD11	5:F:229:GLN:OE1	2.14	0.47
3:D:1117:TYR:HB2	3:D:1188:VAL:O	2.14	0.47
3:J:698:LYS:HG3	4:K:59:ASN:ND2	2.29	0.47
3:D:122:GLU:O	3:D:126:VAL:HG23	2.15	0.47
3:D:635:PRO:O	3:D:935:LYS:HE2	2.15	0.47
2:I:754:ILE:HG12	2:I:791:ARG:HD3	1.95	0.47
7:S:21:DG:H1'	7:S:22:DT:H5'	1.97	0.47
2:C:888:THR:HG22	2:C:989:VAL:O	2.15	0.47
2:C:1048:THR:O	2:C:1052:MET:HG2	2.15	0.47
1:H:187:GLY:H	4:K:51:LEU:HD11	1.79	0.47
3:J:135:LEU:O	3:J:453:ASP:HB3	2.14	0.47
3:D:711:LEU:HB3	3:D:735:ALA:HB1	1.95	0.47
3:D:1211:MET:HB3	3:D:1213:ARG:HG2	1.96	0.47
1:G:30:ARG:HG3	2:I:938:LYS:NZ	2.30	0.47
3:D:810:GLU:O	3:D:813:LEU:HB3	2.14	0.47
2:I:1088:LEU:O	2:I:1092:LEU:HG	2.15	0.47
5:F:124:GLY:O	5:F:128:ILE:HG13	2.13	0.47
3:D:233:LYS:HB3	3:D:236:TYR:CE1	2.49	0.47
2:I:952:LEU:HD21	2:I:971:LYS:HZ2	1.80	0.47
2:C:430:VAL:HG12	2:C:434:HIS:CD2	2.50	0.47
2:I:609:THR:O	2:I:625:LEU:HG	2.15	0.47
3:D:1135:ARG:NH2	3:D:1357:ARG:HH22	2.13	0.47
6:R:28:DA:H1'	6:R:29:DC:H5'	1.97	0.47
3:J:486:ARG:HA	3:J:489:ARG:HG2	1.95	0.47
3:J:1021:TYR:CE1	3:J:1025:GLN:HG3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:LYS:HA	1:B:164:ALA:HB3	1.97	0.47
2:I:15:LEU:O	2:I:586:ARG:NH1	2.47	0.47
2:C:456:ALA:HB1	2:C:538:GLN:O	2.15	0.47
2:I:1035:MET:HA	2:I:1038:TRP:CE3	2.50	0.47
6:O:7:DA:N6	7:P:20:DT:H3	2.10	0.47
1:A:177:VAL:HG13	1:A:199:ILE:HG12	1.96	0.47
3:J:1341:PRO:O	3:J:1344:VAL:HB	2.15	0.47
3:J:1340:GLY:O	3:J:1344:VAL:HG23	2.15	0.47
1:G:35:THR:CG2	1:H:39:PRO:HA	2.45	0.47
2:I:299:LYS:HG3	2:I:300:ASP:H	1.80	0.47
3:J:1209:LEU:H	3:J:1209:LEU:HD12	1.80	0.47
3:D:1087:ARG:NH1	3:D:1236:LEU:O	2.48	0.47
2:C:202:TYR:CD1	2:C:206:THR:HG21	2.50	0.47
2:C:751:PRO:HB3	2:C:794:PRO:HA	1.96	0.47
2:C:1019:GLN:OE1	2:C:1057:SER:OG	2.32	0.47
3:J:918:ALA:O	3:J:922:LEU:HB2	2.14	0.47
3:D:1006:ALA:O	3:D:1010:ASN:HB2	2.15	0.47
2:I:714:ASP:HA	2:I:719:PRO:HA	1.96	0.47
2:I:1007:ALA:HB1	3:J:652:LEU:HD13	1.97	0.47
2:C:111:ASP:HB3	2:C:369:PRO:HG2	1.97	0.47
2:I:456:ALA:HB1	2:I:538:GLN:O	2.15	0.47
2:I:1038:TRP:CE2	3:J:1099:VAL:HG11	2.50	0.47
2:C:1047:HIS:HA	2:C:1050:GLN:CG	2.45	0.47
3:D:1459:LEU:HB3	3:D:1465:ASN:ND2	2.30	0.47
3:D:1373:ARG:O	3:D:1377:LYS:HB3	2.14	0.47
2:I:72:ARG:O	2:I:94:LEU:HD12	2.15	0.47
3:D:767:HIS:CE1	4:E:6:ILE:HD13	2.50	0.47
3:J:560:GLN:NE2	5:L:236:ILE:HG21	2.30	0.47
2:I:1047:HIS:O	2:I:1051:GLU:HG3	2.15	0.47
2:C:118:LEU:HD13	2:C:382:LEU:HD23	1.96	0.47
2:C:829:GLN:OE1	2:C:831:ARG:NH2	2.43	0.47
5:L:103:ILE:HD13	5:L:211:VAL:HG21	1.96	0.47
3:D:123:LEU:HG	3:D:127:LEU:HD11	1.96	0.47
3:D:632:VAL:O	3:D:727:GLN:HA	2.15	0.47
1:B:54:THR:HG22	1:B:143:ARG:O	2.15	0.47
2:I:1048:THR:O	2:I:1052:MET:HG2	2.15	0.47
2:C:676:ILE:HA	2:C:871:LEU:O	2.14	0.47
1:A:55:SER:CB	1:A:158:ILE:HG12	2.44	0.46
2:C:537:LYS:HE3	2:C:583:LEU:HD11	1.97	0.46
1:B:44:LEU:HA	1:B:48:ILE:HD13	1.96	0.46
2:C:1083:GLU:HA	2:C:1086:ARG:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1083:GLU:HA	2:I:1086:ARG:HG3	1.96	0.46
3:J:930:LEU:O	3:J:934:LEU:HD12	2.15	0.46
2:C:720:GLU:HB2	2:C:759:THR:O	2.15	0.46
3:D:1197:ARG:HG3	3:D:1398:TRP:CG	2.50	0.46
3:J:514:LEU:HD21	3:J:518:PRO:HD3	1.96	0.46
1:G:24:VAL:HA	1:G:195:LEU:O	2.14	0.46
3:J:996:TRP:CE2	3:J:1056:PRO:HD3	2.49	0.46
7:S:3:DG:H1'	7:S:4:DC:H5'	1.97	0.46
3:J:1188:VAL:HG12	3:J:1189:ARG:H	1.80	0.46
3:D:1465:ASN:HA	3:D:1468:LEU:HB2	1.96	0.46
2:C:1102:LEU:HA	2:C:1107:ASN:O	2.15	0.46
1:A:63:HIS:CD2	1:A:66:SER:HB2	2.50	0.46
2:C:941:LYS:HZ2	2:C:959:PRO:HG2	1.81	0.46
1:H:97:THR:OG1	1:H:98:THR:N	2.46	0.46
2:I:23:VAL:HA	2:I:121:MET:SD	2.54	0.46
4:K:46:PRO:HB2	4:K:57:ASP:HB3	1.98	0.46
2:C:890:LEU:HD21	2:C:914:ILE:HG12	1.97	0.46
2:C:537:LYS:NZ	2:C:905:VAL:H	2.02	0.46
3:D:876:SER:O	3:D:879:ARG:HB3	2.15	0.46
2:C:532:MET:HG2	2:C:533:ASP:N	2.29	0.46
2:C:1047:HIS:HA	2:C:1050:GLN:HG2	1.97	0.46
2:I:578:VAL:HG23	2:I:671:ASN:ND2	2.29	0.46
2:I:971:LYS:HG2	2:I:988:VAL:HG12	1.98	0.46
1:G:35:THR:HG22	1:H:39:PRO:HA	1.97	0.46
2:C:397:GLU:HG3	2:C:632:ASN:HD22	1.80	0.46
1:H:59:GLU:HG3	1:H:139:TYR:CD2	2.47	0.46
3:D:1106:VAL:HG21	3:D:1474:ALA:HB2	1.96	0.46
3:D:698:LYS:HG3	4:E:59:ASN:ND2	2.29	0.46
3:D:1331:ASP:HA	3:D:1332:PRO:HD3	1.82	0.46
3:J:1020:LEU:HD11	3:J:1035:ILE:HD12	1.95	0.46
2:C:880:MET:CE	3:D:1037:GLN:HB2	2.46	0.46
1:A:190:THR:OG1	1:A:191:ASP:N	2.47	0.46
3:J:1364:HIS:NE2	3:J:1366:LYS:HE3	2.31	0.46
3:J:82:ARG:HB2	3:J:84:ILE:HG22	1.98	0.46
2:C:886:LEU:HA	2:C:889:HIS:HB2	1.97	0.46
7:P:9:DT:H1'	7:P:10:DT:H5'	1.98	0.46
3:D:716:PHE:CZ	3:D:728:LEU:HD11	2.51	0.46
4:E:46:PRO:HB2	4:E:57:ASP:HB3	1.97	0.46
5:F:413:ARG:NH1	5:F:414:GLN:HG2	2.31	0.46
3:D:646:LYS:HA	3:D:720:LEU:HD22	1.96	0.46
3:D:264:LEU:HG	3:D:316:HIS:HE2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ARG:NH2	1:B:187:GLY:O	2.49	0.46
3:D:1166:LEU:H	3:D:1166:LEU:HD12	1.80	0.46
6:R:14:DT:H1'	6:R:15:DT:H5'	1.97	0.46
3:J:592:THR:HB	3:J:598:ARG:O	2.14	0.46
2:C:446:GLY:O	2:C:449:ILE:HG13	2.16	0.46
5:F:413:ARG:HD2	7:P:22:DT:H72	1.98	0.46
5:F:235:LEU:O	5:F:239:VAL:HG23	2.16	0.46
2:C:1035:MET:HA	2:C:1038:TRP:CE3	2.50	0.46
1:B:89:PHE:CE1	1:B:97:THR:HG22	2.51	0.46
2:C:718:GLY:HA2	2:C:719:PRO:HD3	1.78	0.46
2:C:549:PHE:HB3	2:C:552:HIS:HD2	1.80	0.46
3:D:493:ARG:HH11	3:D:494:LYS:HE3	1.81	0.46
2:I:247:PRO:HA	2:I:248:PRO:HD3	1.84	0.46
2:C:151:ASP:HB2	2:C:154:ARG:O	2.14	0.46
3:D:253:ALA:HB2	3:D:304:LEU:HG	1.96	0.46
2:C:85:GLU:HA	2:C:824:ARG:HH22	1.79	0.46
3:D:927:THR:HA	3:D:930:LEU:HB3	1.97	0.46
3:D:1205:TYR:O	3:D:1366:LYS:HD3	2.16	0.46
2:C:1085:PHE:HE2	3:D:1468:LEU:HD22	1.81	0.46
3:J:350:HIS:HB3	5:L:247:ARG:HH12	1.81	0.46
1:G:29:GLU:O	1:G:32:PHE:HB2	2.15	0.46
3:J:87:ARG:HG2	3:J:523:ASP:CB	2.45	0.46
2:C:798:GLY:HA3	2:C:827:VAL:CG1	2.45	0.46
5:F:178:LEU:HA	5:F:181:LEU:HD13	1.98	0.46
3:J:1397:LYS:HA	3:J:1397:LYS:NZ	2.30	0.46
1:H:54:THR:HG22	1:H:143:ARG:O	2.16	0.46
3:J:646:LYS:HA	3:J:720:LEU:HD22	1.98	0.46
2:I:1056:LYS:O	3:J:624:ASP:N	2.35	0.46
1:H:10:VAL:HG12	1:H:12:THR:HG23	1.98	0.46
2:C:423:ALA:O	2:C:428:ARG:HG3	2.16	0.46
3:J:1154:GLU:HG2	3:J:1159:ARG:HB3	1.98	0.46
2:I:436:GLY:O	2:I:459:ALA:HB2	2.16	0.46
2:C:15:LEU:O	2:C:586:ARG:NH1	2.48	0.46
3:D:169:TYR:CE2	3:D:395:VAL:HG12	2.40	0.46
3:J:397:LYS:HE3	3:J:448:GLU:O	2.16	0.46
2:I:532:MET:HG2	2:I:533:ASP:N	2.30	0.46
5:F:383:VAL:HG22	5:F:404:TYR:HE2	1.81	0.46
2:C:609:THR:O	2:C:625:LEU:HG	2.15	0.46
2:C:45:GLN:HE21	2:C:45:GLN:HA	1.80	0.46
5:L:410:GLU:O	5:L:413:ARG:HB3	2.15	0.46
3:D:474:GLU:O	3:D:478:LEU:HG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:527:MET:HG3	3:J:537:THR:HB	1.97	0.46
3:J:1119:SER:HA	3:J:1186:VAL:O	2.16	0.46
2:I:660:ALA:O	2:I:667:ALA:N	2.41	0.46
2:I:405:ARG:O	2:I:409:ARG:HG3	2.16	0.46
5:F:319:VAL:O	5:F:323:LEU:HB2	2.15	0.46
2:C:897:LEU:HD23	2:C:899:GLN:H	1.80	0.46
5:L:302:SER:O	5:L:306:ILE:HG22	2.16	0.46
3:J:104:PHE:HB3	3:J:111:LYS:HB2	1.98	0.46
3:J:1095:THR:O	3:J:1099:VAL:HG23	2.16	0.46
5:L:235:LEU:O	5:L:239:VAL:HG23	2.16	0.46
5:F:376:LEU:HG	5:F:423:LEU:HD21	1.98	0.46
3:J:1254:GLN:HB3	3:J:1258:ARG:CB	2.45	0.46
1:A:66:SER:O	1:A:75:VAL:HG23	2.16	0.46
3:J:93:ILE:HB	3:J:517:VAL:HB	1.98	0.46
2:C:436:GLY:O	2:C:459:ALA:HB2	2.16	0.46
5:F:412:ILE:O	5:F:416:GLU:HG2	2.16	0.46
1:A:29:GLU:O	1:A:32:PHE:HB2	2.16	0.46
1:G:63:HIS:HB2	2:I:799:ILE:HD12	1.97	0.46
2:I:1067:TYR:CE2	5:L:357:VAL:HA	2.52	0.46
2:I:744:ARG:NE	2:I:747:ALA:HB2	2.30	0.46
3:D:414:ARG:HA	3:D:414:ARG:HD2	1.68	0.46
3:D:584:ASN:OD1	3:D:591:VAL:HG12	2.16	0.46
1:B:150:TYR:HD2	3:D:857:LEU:HD12	1.80	0.46
3:D:702:LEU:HD12	3:D:746:ALA:O	2.16	0.46
5:F:202:LEU:HD21	5:F:239:VAL:HG22	1.98	0.45
3:J:522:PRO:HA	3:J:525:ARG:NH1	2.31	0.45
2:C:988:VAL:HG22	3:D:948:THR:OG1	2.16	0.45
3:D:175:VAL:HG13	3:D:193:PRO:HD2	1.99	0.45
2:I:1102:LEU:HA	2:I:1107:ASN:O	2.16	0.45
1:A:178:ALA:HB2	2:C:864:GLY:HA3	1.98	0.45
2:I:430:VAL:HG12	2:I:434:HIS:CD2	2.51	0.45
3:D:892:ASP:HB2	3:D:894:LYS:HG2	1.99	0.45
3:J:565:ILE:H	3:J:565:ILE:HD12	1.80	0.45
2:C:922:PHE:HB2	2:C:967:PHE:CD2	2.52	0.45
3:J:483:HIS:CG	3:J:484:PRO:HD2	2.50	0.45
1:H:29:GLU:HB3	1:H:32:PHE:CD1	2.51	0.45
3:J:634:GLY:O	3:J:637:LEU:N	2.30	0.45
2:C:711:GLU:HA	2:C:822:VAL:HG12	1.98	0.45
5:F:218:THR:HA	5:F:227:LEU:HD11	1.98	0.45
3:J:112:ILE:HD12	3:J:113:GLY:H	1.79	0.45
3:J:633:VAL:C	3:J:635:PRO:HD3	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:102:ILE:HB	3:D:579:ASP:HB3	1.98	0.45
1:B:176:ARG:HB3	1:B:200:TRP:CE3	2.51	0.45
3:J:1293:PHE:H	3:J:1293:PHE:HD1	1.63	0.45
3:D:264:LEU:O	3:D:267:GLY:N	2.47	0.45
3:D:990:ASP:O	3:D:993:ILE:HG22	2.17	0.45
2:I:816:LYS:HA	2:I:817:PRO:HD3	1.83	0.45
2:C:570:PRO:HD2	2:C:635:THR:HG21	1.99	0.45
1:G:76:VAL:HA	1:G:79:ILE:HD12	1.98	0.45
3:D:1277:ILE:HG12	3:D:1278:ASP:H	1.81	0.45
2:C:640:ARG:HG2	2:C:642:ARG:HH12	1.81	0.45
2:C:1009:SER:HB3	3:D:651:GLU:O	2.17	0.45
3:D:293:VAL:HB	3:D:296:GLU:HB2	1.98	0.45
2:I:122:THR:HG23	2:I:128:ILE:HD11	1.98	0.45
2:I:880:MET:CE	3:J:1037:GLN:HB2	2.46	0.45
7:S:4:DC:H2"	7:S:5:DA:C8	2.51	0.45
2:I:456:ALA:HB3	2:I:459:ALA:HB2	1.98	0.45
5:L:292:GLN:O	5:L:295:GLN:HG3	2.17	0.45
5:L:376:LEU:HB3	5:L:380:GLU:HG3	1.98	0.45
3:D:44:LEU:HG	3:D:525:ARG:HH12	1.81	0.45
3:D:350:HIS:HB2	3:D:371:ILE:HG22	1.98	0.45
3:J:102:ILE:HD11	3:J:587:ARG:HB2	1.97	0.45
3:D:1135:ARG:HB3	3:D:1139:ASP:HB3	1.98	0.45
1:H:179:PHE:HB3	1:H:197:LEU:HD13	1.99	0.45
3:D:698:LYS:HB3	3:D:756:GLN:NE2	2.31	0.45
2:I:726:ILE:HD12	2:I:729:LEU:HG	1.99	0.45
5:F:252:THR:HG1	6:O:28:DA:H8	1.64	0.45
5:L:412:ILE:HA	5:L:415:ILE:HD12	1.97	0.45
2:I:640:ARG:HG2	2:I:642:ARG:HH12	1.82	0.45
3:J:1223:VAL:HG21	3:J:1462:LEU:HD21	1.98	0.45
2:I:374:ASN:OD1	2:I:375:SER:N	2.47	0.45
2:C:193:LEU:HA	2:C:196:LEU:HD13	1.97	0.45
5:F:385:LYS:HA	5:F:390:LEU:HD12	1.98	0.45
3:J:1046:GLN:HE22	3:J:1079:LYS:HE2	1.81	0.45
2:C:272:ALA:O	2:C:276:LYS:N	2.39	0.45
1:A:44:LEU:HD13	1:A:177:VAL:HG21	1.99	0.45
2:C:242:LEU:HD11	2:C:256:TYR:CE2	2.52	0.45
3:D:974:ILE:HG12	3:D:991:GLN:HG2	1.97	0.45
3:D:1088:THR:HA	3:D:1234:THR:HG22	1.99	0.45
3:J:990:ASP:O	3:J:993:ILE:HG22	2.16	0.45
2:C:185:LYS:HA	2:C:189:ARG:O	2.16	0.45
3:D:654:LYS:O	3:D:658:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1482:ARG:HE	3:D:1483:PHE:HE1	1.65	0.45
2:C:16:PRO:HB2	2:C:460:ARG:NH2	2.31	0.45
2:C:99:GLN:HB3	2:C:110:GLU:HG3	1.99	0.45
2:C:1056:LYS:NZ	3:D:748:HIS:HB3	2.32	0.45
2:I:897:LEU:HD21	2:I:899:GLN:HG2	1.97	0.45
1:G:181:VAL:O	1:G:182:GLU:HG3	2.16	0.45
2:I:357:GLU:HG2	5:L:216:LYS:HE2	1.99	0.45
1:H:44:LEU:HA	1:H:48:ILE:HD13	1.98	0.45
3:D:1221:VAL:HG23	3:D:1222:GLY:H	1.82	0.45
2:C:639:GLN:HB3	2:C:656:ALA:HB1	1.99	0.45
3:D:1095:THR:O	3:D:1099:VAL:HG23	2.16	0.45
3:J:1135:ARG:HB2	3:J:1140:ILE:HD11	1.98	0.45
2:I:242:LEU:HD11	2:I:256:TYR:CE2	2.52	0.45
6:R:2:DT:H2"	6:R:3:DT:OP2	2.16	0.45
1:B:41:ARG:HG3	1:B:177:VAL:HG21	1.99	0.45
3:J:684:LYS:O	3:J:687:VAL:HG22	2.17	0.45
2:I:937:ASP:HB3	2:I:940:GLU:HG3	1.97	0.45
5:F:141:LEU:O	5:F:145:VAL:HG23	2.17	0.45
2:I:897:LEU:HD23	2:I:899:GLN:H	1.80	0.45
3:J:356:PRO:HB3	3:J:441:ARG:HA	1.97	0.45
4:E:18:ARG:O	4:E:22:VAL:HG23	2.17	0.45
1:B:211:LEU:O	1:B:215:VAL:HG13	2.15	0.45
3:J:1381:VAL:HG21	3:J:1393:GLN:HB3	1.98	0.45
2:C:644:ARG:HD2	2:C:647:GLN:HB3	1.98	0.45
3:D:187:LYS:N	3:D:200:ASP:OD2	2.49	0.45
2:C:405:ARG:O	2:C:409:ARG:HG3	2.16	0.45
1:G:104:GLU:HG3	1:G:137:LYS:HG2	1.97	0.45
4:K:45:ARG:HD2	4:K:63:TRP:HH2	1.82	0.45
1:B:48:ILE:HG22	1:B:173:PRO:HD2	1.99	0.45
3:D:638:LYS:HG2	3:D:640:HIS:NE2	2.32	0.45
2:I:1044:GLY:HA3	4:K:17:TYR:HE1	1.81	0.45
3:D:522:PRO:HA	3:D:525:ARG:NH1	2.32	0.45
2:I:140:ILE:HD12	2:I:332:ARG:O	2.17	0.45
2:C:774:LEU:HA	2:C:777:ILE:HD12	1.97	0.45
1:B:23:PHE:HE2	1:B:199:ILE:HB	1.81	0.45
3:D:225:ILE:O	3:D:331:VAL:HG12	2.17	0.45
5:L:413:ARG:NH1	5:L:414:GLN:HG2	2.31	0.45
3:J:638:LYS:HG2	3:J:640:HIS:CE1	2.51	0.45
2:I:890:LEU:HD21	2:I:914:ILE:HG12	1.99	0.45
1:B:202:ASP:OD1	1:B:203:GLY:N	2.49	0.45
3:D:593:ASN:ND2	5:F:331:SER:OG	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:111:ASP:HB3	2:I:369:PRO:HG2	1.98	0.45
2:I:1012:PRO:HB2	2:I:1021:LEU:HD11	1.98	0.45
2:I:878:SER:O	3:J:1034:GLN:NE2	2.49	0.45
2:I:151:ASP:HB2	2:I:154:ARG:O	2.15	0.45
1:G:190:THR:OG1	1:G:191:ASP:N	2.48	0.45
3:J:1434:TRP:CD1	3:J:1457:ASP:HB2	2.52	0.45
3:D:1161:GLU:OE2	3:D:1164:ARG:HB2	2.16	0.45
5:F:286:LEU:HD23	5:F:310:MET:HG3	1.98	0.45
1:B:48:ILE:HA	1:B:49:PRO:HD2	1.79	0.45
3:J:767:HIS:CE1	4:K:6:ILE:HD13	2.52	0.45
3:D:525:ARG:HG2	3:D:540:LEU:HD23	1.98	0.45
2:C:291:VAL:HG13	2:C:303:PHE:CE1	2.52	0.45
1:A:35:THR:HG23	1:B:42:ARG:HB2	1.99	0.45
3:J:65:ARG:HG2	5:L:393:GLY:O	2.16	0.45
3:D:815:ALA:HB1	3:D:821:VAL:HG23	1.99	0.45
7:S:8:DA:C2'	7:S:9:DT:H5"	2.46	0.45
3:D:300:VAL:HG12	3:D:301:GLY:H	1.82	0.45
1:H:211:LEU:O	1:H:215:VAL:HG13	2.16	0.45
2:I:1019:GLN:OE1	2:I:1057:SER:OG	2.34	0.45
2:I:440:PRO:O	3:J:1078:ARG:HG3	2.17	0.45
5:F:302:SER:O	5:F:306:ILE:HG22	2.16	0.45
2:C:440:PRO:O	3:D:1078:ARG:HG3	2.17	0.45
2:I:710:ILE:HD13	2:I:790:LEU:HD13	1.98	0.45
1:B:62:LEU:HD12	1:B:62:LEU:H	1.82	0.45
3:D:22:SER:HB2	3:D:92:HIS:HB3	1.98	0.45
3:J:618:LEU:HB3	3:J:1467:ILE:HG12	1.98	0.45
2:C:199:VAL:HA	2:C:231:PRO:HB3	1.99	0.45
2:I:207:LEU:HD13	2:I:227:LEU:HD11	1.97	0.45
1:B:87:VAL:HG12	1:B:122:ILE:HG12	1.97	0.45
2:C:1067:TYR:CE2	5:F:357:VAL:HA	2.52	0.45
3:D:684:LYS:O	3:D:687:VAL:HG22	2.17	0.45
2:C:584:GLU:HB3	2:C:666:LEU:HB3	1.99	0.45
1:H:185:ARG:NH2	1:H:187:GLY:O	2.50	0.45
1:B:81:ASN:OD1	3:D:867:ARG:NH2	2.49	0.45
3:J:597:GLU:O	3:J:599:PRO:HD3	2.17	0.45
3:D:14:SER:HB3	3:D:511:TRP:CD2	2.51	0.45
3:J:160:GLU:CD	3:J:165:LYS:HD3	2.38	0.45
3:D:129:PHE:CE1	3:D:571:LYS:HG2	2.52	0.45
3:D:701:LEU:HD21	3:D:763:MET:CG	2.46	0.45
2:C:937:ASP:HB3	2:C:940:GLU:HG3	1.99	0.45
2:C:751:PRO:HA	2:C:792:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:565:ILE:H	3:D:565:ILE:HD12	1.81	0.45
7:P:19:DT:H1'	7:P:20:DT:H5'	1.99	0.45
5:F:159:ILE:N	5:F:160:PRO:HD3	2.32	0.45
5:L:202:LEU:HD21	5:L:239:VAL:HG22	1.98	0.45
1:A:209:GLU:O	1:A:213:GLN:HG2	2.17	0.45
5:L:149:LYS:HB2	5:L:193:ARG:HH12	1.82	0.45
2:C:634:GLY:O	2:C:704:HIS:HA	2.17	0.45
3:D:701:LEU:HD22	3:D:713:ILE:HG22	1.98	0.45
4:K:79:LEU:HD23	4:K:80:VAL:HG22	1.99	0.45
3:D:633:VAL:C	3:D:635:PRO:HD3	2.37	0.45
2:I:429:ASP:OD1	2:I:430:VAL:N	2.43	0.45
3:J:841:PHE:CE2	3:J:858:LEU:HD13	2.52	0.45
2:I:1058:ASP:OD1	2:I:1058:ASP:N	2.49	0.45
2:C:673:LEU:HA	2:C:990:GLY:O	2.16	0.45
2:C:771:GLU:O	2:C:775:ARG:HG3	2.17	0.45
5:L:289:THR:O	5:L:293:LEU:HG	2.17	0.45
1:G:231:SER:H	1:H:14:THR:HG22	1.81	0.45
3:J:632:VAL:O	3:J:727:GLN:HA	2.17	0.45
3:D:794:GLN:HG3	3:D:795:VAL:N	2.32	0.45
2:I:446:GLY:O	2:I:449:ILE:HG13	2.16	0.45
2:C:1088:LEU:O	2:C:1092:LEU:HG	2.17	0.45
3:D:1364:HIS:CD2	3:D:1366:LYS:HE2	2.52	0.44
2:I:737:LEU:HA	2:I:737:LEU:HD12	1.61	0.44
2:C:299:LYS:HG3	2:C:300:ASP:H	1.82	0.44
1:G:28:LEU:HD11	1:G:36:LEU:HD12	1.98	0.44
5:F:181:LEU:HD23	5:F:185:LEU:HD13	1.98	0.44
2:I:682:TYR:HA	3:J:633:VAL:HG11	1.98	0.44
2:I:770:GLU:HB3	5:L:369:LEU:HD12	1.99	0.44
2:I:549:PHE:HB3	2:I:552:HIS:HD2	1.82	0.44
3:J:1479:ASP:HA	3:J:1482:ARG:HG2	1.99	0.44
3:J:1006:ALA:O	3:J:1010:ASN:HB2	2.16	0.44
2:I:1030:GLN:O	3:J:622:ARG:HA	2.17	0.44
3:D:1179:GLU:HG2	3:J:1131:THR:HG22	1.99	0.44
2:C:807:ARG:HB3	2:C:810:ASP:OD1	2.17	0.44
3:D:259:VAL:HG13	3:D:298:VAL:HG21	2.00	0.44
2:I:142:ARG:HA	2:I:331:ARG:HA	2.00	0.44
3:J:1191:PRO:O	3:J:1373:ARG:HD2	2.17	0.44
2:C:370:ALA:O	5:F:295:GLN:NE2	2.50	0.44
3:D:1312:LEU:HG	3:D:1325:LEU:O	2.17	0.44
2:I:564:MET:HG2	2:I:567:GLN:NE2	2.32	0.44
2:C:432:ARG:HH12	2:C:518:ARG:NE	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1144:LEU:HA	3:D:1144:LEU:HD12	1.53	0.44
1:G:89:PHE:CE1	1:G:120:VAL:HG12	2.52	0.44
4:K:19:LEU:O	4:K:23:VAL:HG23	2.17	0.44
3:J:810:GLU:O	3:J:813:LEU:HB3	2.17	0.44
3:J:806:PHE:CD1	3:J:811:GLU:HB3	2.52	0.44
1:B:10:VAL:HG12	1:B:12:THR:HG23	1.99	0.44
2:I:423:ALA:O	2:I:428:ARG:HG3	2.16	0.44
3:J:1406:ARG:O	3:J:1410:GLU:HG3	2.16	0.44
2:I:1009:SER:HB3	3:J:651:GLU:O	2.18	0.44
5:L:159:ILE:N	5:L:160:PRO:HD3	2.33	0.44
3:D:638:LYS:HG3	3:D:640:HIS:H	1.81	0.44
2:I:69:LEU:C	2:I:70:GLU:HG3	2.37	0.44
2:C:971:LYS:HG2	2:C:988:VAL:HG12	1.99	0.44
5:L:411:ARG:HD3	6:R:1:DC:C6	2.52	0.44
1:A:28:LEU:HD22	1:A:32:PHE:HD2	1.82	0.44
1:H:87:VAL:HG12	1:H:122:ILE:HG12	1.99	0.44
2:I:690:ILE:HG13	2:I:852:ILE:HG23	1.99	0.44
2:C:41:ASN:HA	2:C:45:GLN:HB3	1.99	0.44
1:H:176:ARG:NH1	3:J:884:ARG:HH12	2.16	0.44
2:C:744:ARG:NE	2:C:747:ALA:HB2	2.33	0.44
2:C:1030:GLN:O	3:D:622:ARG:HA	2.17	0.44
1:G:73:GLU:HB3	1:G:77:GLU:HG3	1.99	0.44
2:C:670:GLN:O	2:C:672:VAL:HG23	2.17	0.44
2:I:16:PRO:HB2	2:I:460:ARG:NH2	2.32	0.44
2:C:577:PRO:HB3	2:C:993:PHE:CG	2.52	0.44
3:J:701:LEU:HD22	3:J:713:ILE:HG22	1.98	0.44
3:D:1127:GLU:C	3:D:1129:THR:H	2.21	0.44
6:O:2:DT:H2"	6:O:3:DT:OP2	2.18	0.44
3:D:631:ILE:HD11	3:D:739:ASP:O	2.18	0.44
1:G:63:HIS:CD2	1:G:66:SER:HB2	2.53	0.44
3:J:1293:PHE:CD1	3:J:1293:PHE:N	2.85	0.44
3:D:1288:ASP:OD2	3:D:1288:ASP:N	2.50	0.44
3:D:1078:ARG:HH11	3:D:1078:ARG:HB3	1.82	0.44
2:I:550:LEU:HD11	2:I:558:ALA:HB1	1.98	0.44
1:A:79:ILE:HD13	1:A:167:VAL:HG12	2.00	0.44
2:C:333:ILE:HB	2:C:461:VAL:HG11	2.00	0.44
3:D:213:VAL:HB	3:D:345:TYR:HE1	1.82	0.44
1:A:22:GLU:HA	1:A:197:LEU:O	2.17	0.44
3:D:634:GLY:O	3:D:637:LEU:N	2.28	0.44
4:E:6:ILE:HG23	4:E:7:ASP:H	1.83	0.44
3:J:1144:LEU:HD13	3:J:1144:LEU:HA	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:682:TYR:HA	3:D:633:VAL:HG11	2.00	0.44
2:I:194:VAL:O	2:I:198:ARG:HG3	2.17	0.44
3:J:661:MET:HG2	3:J:666:PHE:CZ	2.52	0.44
2:I:526:PRO:O	2:I:529:VAL:HG12	2.17	0.44
3:J:90:MET:HE1	3:J:518:PRO:HB3	1.98	0.44
3:J:1078:ARG:HB3	3:J:1078:ARG:HH11	1.83	0.44
3:J:22:SER:HB2	3:J:92:HIS:HB3	1.97	0.44
2:I:644:ARG:HD2	2:I:647:GLN:HB3	2.00	0.44
2:C:97:ARG:HB2	2:C:112:GLU:HG3	1.99	0.44
1:A:231:SER:H	1:B:14:THR:HG22	1.82	0.44
2:I:922:PHE:HB2	2:I:967:PHE:CD2	2.53	0.44
2:I:670:GLN:O	2:I:672:VAL:HG23	2.17	0.44
2:I:994:ILE:HG22	2:I:995:MET:H	1.82	0.44
3:J:84:ILE:HD11	3:J:88:TYR:HE1	1.83	0.44
2:I:1086:ARG:NH1	2:I:1086:ARG:HG3	2.32	0.44
1:B:23:PHE:HE1	1:B:208:LEU:HD12	1.82	0.44
2:I:761:PHE:HA	2:I:785:VAL:HA	1.99	0.44
5:L:99:TYR:O	5:L:103:ILE:HG12	2.17	0.44
2:C:22:GLN:HG3	2:C:407:LYS:HB3	1.99	0.44
1:A:232:LEU:H	1:A:232:LEU:HD12	1.82	0.44
3:D:155:ASP:N	3:D:155:ASP:OD2	2.49	0.44
1:H:202:ASP:OD1	1:H:203:GLY:N	2.51	0.44
3:J:558:LEU:CD2	3:J:567:ILE:HG23	2.48	0.44
2:C:878:SER:HB2	3:D:1029:ARG:HG3	1.99	0.44
2:I:1090:LYS:NZ	2:I:1093:GLN:OE1	2.35	0.44
1:H:34:VAL:HG22	1:H:181:VAL:HG21	2.00	0.44
3:D:638:LYS:HB3	3:D:641:GLN:HE21	1.83	0.44
3:J:1202:GLN:O	3:J:1206:GLY:N	2.51	0.44
5:F:398:LEU:HB3	7:P:21:DG:OP2	2.18	0.44
1:H:41:ARG:HG3	1:H:177:VAL:HG21	2.00	0.44
3:D:117:ASP:HB2	3:D:495:ARG:CZ	2.47	0.44
3:J:1499:ARG:HH21	3:J:1500:LYS:HG3	1.83	0.44
1:A:58:ILE:HG22	1:A:60:ASP:H	1.81	0.44
2:I:714:ASP:HB2	2:I:818:GLY:O	2.18	0.44
1:G:182:GLU:O	1:G:193:ASP:HA	2.18	0.44
1:A:227:ASN:HA	1:A:228:PRO:HD2	1.75	0.44
3:J:496:LEU:HD12	3:J:499:VAL:HB	1.99	0.44
1:G:22:GLU:HA	1:G:197:LEU:O	2.18	0.44
3:D:1141:GLU:OE1	3:D:1168:LEU:HD11	2.18	0.44
2:I:834:GLN:HG2	2:I:835:VAL:H	1.82	0.44
1:B:40:LEU:O	1:B:44:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:568:ARG:HA	3:J:571:LYS:HE2	1.98	0.44
2:C:1112:PHE:HB2	2:C:1115:LEU:HB2	1.99	0.44
3:D:1199:GLY:O	3:D:1373:ARG:NH1	2.51	0.44
2:I:1089:VAL:HG13	2:I:1099:VAL:HG11	2.00	0.44
2:I:1115:LEU:HD21	3:J:84:ILE:HG23	2.00	0.44
3:J:523:ASP:HA	3:J:526:PRO:HG3	2.00	0.44
1:B:78:ILE:O	1:B:82:LEU:HG	2.18	0.44
2:C:588:VAL:HG23	2:C:596:TYR:OH	2.17	0.44
1:A:182:GLU:O	1:A:193:ASP:HA	2.18	0.44
3:J:537:THR:O	5:L:332:LEU:HG	2.18	0.44
2:C:834:GLN:HG2	2:C:835:VAL:H	1.82	0.44
5:F:173:GLU:O	5:F:177:LYS:HB2	2.18	0.44
2:I:399:ASN:HD21	2:I:566:THR:HA	1.83	0.44
3:D:209:ARG:HE	3:D:391:ALA:HB2	1.83	0.44
2:I:269:LEU:HB2	2:I:288:ARG:O	2.18	0.44
2:I:537:LYS:NZ	2:I:905:VAL:H	2.01	0.44
2:C:458:TYR:CD1	2:C:538:GLN:HB3	2.49	0.44
3:D:1370:ILE:H	3:D:1370:ILE:HG13	1.66	0.44
3:D:1068:LEU:HD12	3:D:1068:LEU:H	1.83	0.44
2:I:700:TYR:HB3	2:I:833:LEU:HD13	2.00	0.44
2:I:988:VAL:HG22	3:J:948:THR:OG1	2.18	0.44
3:D:1189:ARG:HE	3:D:1203:LYS:HB2	1.82	0.44
2:C:5:ARG:HB2	2:C:5:ARG:HE	1.70	0.44
3:D:1258:ARG:HG3	3:D:1258:ARG:O	2.18	0.44
2:I:581:THR:OG1	2:I:584:GLU:OE2	2.36	0.44
3:J:1033:GLN:O	3:J:1037:GLN:HG3	2.18	0.44
3:D:529:GLN:HA	3:D:535:PHE:HA	1.99	0.44
3:J:439:LEU:HD21	5:L:190:HIS:HB3	2.00	0.44
3:J:1038:LEU:O	3:J:1060:SER:OG	2.22	0.44
2:C:321:GLU:HG2	2:C:322:VAL:H	1.83	0.43
3:J:792:ILE:HD13	3:J:881:LEU:HD23	1.99	0.43
1:A:44:LEU:HD11	1:A:199:ILE:HD13	1.99	0.43
3:D:181:ASP:HB2	3:D:205:TYR:CD2	2.53	0.43
2:I:332:ARG:HH11	2:I:334:ARG:HD2	1.82	0.43
1:A:35:THR:CG2	1:B:39:PRO:HA	2.47	0.43
3:D:701:LEU:HD11	3:D:763:MET:HG2	2.00	0.43
3:J:635:PRO:O	3:J:935:LYS:HE2	2.18	0.43
1:G:44:LEU:HD11	1:G:199:ILE:HD13	1.99	0.43
3:J:638:LYS:HG2	3:J:640:HIS:NE2	2.33	0.43
2:I:588:VAL:HG23	2:I:596:TYR:OH	2.18	0.43
2:C:714:ASP:HB2	2:C:818:GLY:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:775:ARG:CZ	2:C:782:ALA:HB2	2.48	0.43
1:A:76:VAL:HA	1:A:79:ILE:HD12	1.99	0.43
2:I:709:GLU:HA	2:I:823:VAL:O	2.18	0.43
3:D:1368:ILE:HG13	3:D:1368:ILE:H	1.67	0.43
2:C:1012:PRO:HB2	2:C:1021:LEU:HD11	2.00	0.43
2:I:376:ARG:HB2	2:I:377:PRO:HD3	2.00	0.43
2:C:675:ALA:O	2:C:870:ILE:HA	2.18	0.43
2:I:807:ARG:HB3	2:I:810:ASP:OD1	2.18	0.43
3:J:560:GLN:HE22	5:L:236:ILE:HG21	1.82	0.43
1:G:28:LEU:HD22	1:G:32:PHE:HD2	1.83	0.43
2:C:140:ILE:HD12	2:C:332:ARG:O	2.17	0.43
5:L:407:VAL:HG12	6:R:1:DC:H3'	2.00	0.43
1:G:46:SER:OG	1:G:47:SER:N	2.51	0.43
1:G:178:ALA:HB2	2:I:864:GLY:HA3	2.01	0.43
2:C:713:ARG:O	2:C:720:GLU:HG2	2.18	0.43
3:D:154:THR:HG23	3:D:156:GLU:H	1.83	0.43
3:J:1200:VAL:HG22	3:J:1221:VAL:HG21	1.99	0.43
3:D:1033:GLN:O	3:D:1037:GLN:HG3	2.18	0.43
3:J:637:LEU:HG	3:J:641:GLN:HB3	2.01	0.43
2:I:269:LEU:H	2:I:288:ARG:HB3	1.82	0.43
5:L:246:ARG:HD3	6:R:26:DA:C6	2.54	0.43
3:D:1180:ALA:O	3:J:1132:LEU:HD12	2.18	0.43
3:J:505:SER:HB3	3:J:1453:ALA:HA	1.99	0.43
4:K:30:LEU:HA	4:K:37:ASN:HD21	1.83	0.43
3:J:1333:HIS:O	3:J:1336:LEU:HB3	2.18	0.43
2:C:1050:GLN:HE22	3:D:1470:ARG:C	2.21	0.43
2:C:1047:HIS:O	2:C:1051:GLU:HG3	2.18	0.43
2:C:1089:VAL:HG11	2:C:1112:PHE:HE2	1.82	0.43
5:F:377:SER:HB3	5:F:380:GLU:HG2	2.00	0.43
2:C:332:ARG:HH11	2:C:334:ARG:HD2	1.83	0.43
2:C:69:LEU:C	2:C:70:GLU:HG3	2.38	0.43
1:B:51:THR:HG21	1:B:86:VAL:HG23	2.00	0.43
5:F:252:THR:HA	6:O:29:DC:H5	1.83	0.43
5:L:141:LEU:O	5:L:145:VAL:HG23	2.18	0.43
2:C:897:LEU:HD21	2:C:899:GLN:HG2	1.99	0.43
3:D:1269:LYS:HG3	3:D:1270:ALA:H	1.82	0.43
3:J:34:TYR:HB2	5:L:325:ILE:HG23	2.00	0.43
2:I:390:GLN:HG2	2:I:415:PRO:HD3	1.99	0.43
1:B:107:LYS:O	1:B:132:LEU:HB2	2.17	0.43
2:I:327:HIS:O	2:I:331:ARG:HG3	2.18	0.43
6:O:5:DA:H2	7:P:22:DT:H3	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:11:DT:H1'	7:S:12:DA:H5'	2.01	0.43
5:L:376:LEU:HG	5:L:423:LEU:HD21	1.99	0.43
2:C:994:ILE:HG22	2:C:995:MET:H	1.83	0.43
3:J:1068:LEU:HD12	3:J:1068:LEU:H	1.83	0.43
2:C:65:VAL:CG1	2:C:101:ILE:HB	2.48	0.43
3:D:790:TYR:CD1	3:D:907:GLU:HB3	2.54	0.43
1:H:37:GLY:HA3	1:H:179:PHE:CE1	2.53	0.43
3:J:1042:ARG:HB3	3:J:1057:VAL:CG2	2.48	0.43
3:D:589:SER:HA	3:D:590:PRO:HD3	1.86	0.43
2:I:202:TYR:CD1	2:I:206:THR:HG21	2.53	0.43
2:I:713:ARG:O	2:I:720:GLU:HG2	2.18	0.43
3:J:892:ASP:HB2	3:J:894:LYS:HG2	2.01	0.43
1:A:57:TYR:C	1:A:58:ILE:HD12	2.39	0.43
3:D:858:LEU:HD12	3:D:859:ASP:H	1.83	0.43
1:B:55:SER:HB2	1:B:166:PRO:HA	1.99	0.43
3:J:592:THR:OG1	3:J:596:SER:O	2.29	0.43
3:J:1108:ARG:NH2	3:J:1198:TYR:O	2.50	0.43
3:J:32:ILE:HA	3:J:40:GLU:HG2	2.00	0.43
2:C:122:THR:HG23	2:C:128:ILE:HD11	1.99	0.43
3:D:67:ARG:HD2	5:F:394:ARG:HB2	1.99	0.43
5:F:276:PRO:HB2	5:F:279:MET:HG2	1.99	0.43
2:C:84:ARG:HA	2:C:131:GLY:HA2	2.00	0.43
2:I:333:ILE:HB	2:I:461:VAL:HG11	2.00	0.43
5:L:109:LEU:HD22	5:L:205:ALA:HB1	2.00	0.43
3:J:1065:LEU:HB3	3:J:1069:GLU:HB2	1.99	0.43
2:I:170:PRO:HD2	2:I:267:TYR:HD1	1.83	0.43
3:D:996:TRP:CE2	3:D:1056:PRO:HD3	2.53	0.43
1:H:213:GLN:HE21	1:H:217:ILE:HD11	1.83	0.43
1:A:42:ARG:NH2	1:B:31:GLY:O	2.41	0.43
2:C:495:THR:H	2:C:530:GLU:CG	2.31	0.43
2:C:710:ILE:HD13	2:C:790:LEU:HD13	2.00	0.43
1:B:160:ASP:O	1:B:161:ARG:HB2	2.18	0.43
3:D:242:LEU:HB3	3:D:311:LEU:O	2.19	0.43
2:C:1018:GLN:HG2	2:C:1083:GLU:HG2	2.00	0.43
3:D:970:LYS:O	3:D:973:GLN:HB3	2.18	0.43
4:E:79:LEU:HD23	4:E:80:VAL:HG22	2.00	0.43
3:D:1142:SER:HB3	3:D:1353:GLN:NE2	2.33	0.43
3:J:698:LYS:HB3	3:J:756:GLN:NE2	2.34	0.43
1:H:176:ARG:HB3	1:H:200:TRP:CE3	2.53	0.43
2:C:124:ASP:HB2	2:C:407:LYS:NZ	2.34	0.43
1:A:65:PHE:CD2	2:C:799:ILE:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:41:ASN:HA	2:I:45:GLN:HB3	2.01	0.43
2:I:1056:LYS:NZ	3:J:748:HIS:HB3	2.34	0.43
1:G:232:LEU:HD12	1:G:232:LEU:H	1.83	0.43
1:G:150:TYR:CZ	1:G:152:PRO:HG3	2.54	0.43
3:D:30:GLU:HB3	5:F:274:ARG:HB2	2.00	0.43
3:J:121:THR:O	3:J:124:GLU:HB3	2.18	0.43
2:C:269:LEU:HB2	2:C:288:ARG:O	2.18	0.43
1:G:55:SER:CB	1:G:158:ILE:HG12	2.43	0.43
2:I:321:GLU:HG2	2:I:322:VAL:H	1.84	0.43
3:J:1336:LEU:HD11	3:J:1419:PRO:HB2	1.99	0.43
2:C:1085:PHE:O	2:C:1089:VAL:HG23	2.18	0.43
3:J:354:ILE:HG23	3:J:355:VAL:HG13	2.01	0.43
2:I:577:PRO:HB3	2:I:993:PHE:CG	2.53	0.43
2:I:160:ALA:HB3	2:I:174:LEU:HD11	2.01	0.43
3:J:1149:LEU:HG	3:J:1160:LEU:HD12	2.01	0.43
2:I:343:GLN:HG3	2:I:385:PHE:CB	2.48	0.43
1:G:64:GLU:HA	1:G:75:VAL:HG11	1.99	0.43
2:C:390:GLN:CG	2:C:415:PRO:HD3	2.48	0.43
3:D:1288:ASP:CG	3:D:1289:ARG:H	2.22	0.43
3:J:1434:TRP:NE1	3:J:1457:ASP:HB2	2.33	0.43
3:D:1361:VAL:HG12	3:D:1363:LEU:H	1.84	0.43
3:D:132:TYR:HB3	3:D:454:ALA:HB1	1.99	0.43
3:J:1059:SER:HB3	3:J:1063:GLU:HB2	1.99	0.43
3:J:209:ARG:HA	3:J:347:VAL:HB	1.99	0.43
2:I:181:VAL:HG22	2:I:182:VAL:H	1.84	0.43
3:D:1110:ALA:HB2	3:D:1217:ILE:HD13	2.01	0.43
3:D:82:ARG:HB2	3:D:84:ILE:HG22	2.01	0.43
2:I:768:SER:O	2:I:772:ARG:N	2.50	0.43
1:A:28:LEU:HD11	1:A:36:LEU:HD12	2.00	0.43
5:L:181:LEU:HD23	5:L:185:LEU:HD13	1.99	0.43
3:J:56:TYR:CA	3:J:80:VAL:HG23	2.49	0.43
2:C:690:ILE:HG13	2:C:852:ILE:HG23	2.00	0.43
2:I:1067:TYR:O	2:I:1071:ILE:HB	2.19	0.43
1:H:89:PHE:HE1	1:H:97:THR:HG22	1.83	0.43
1:A:89:PHE:CE1	1:A:120:VAL:HG12	2.54	0.43
5:L:263:ASN:HA	5:L:266:ILE:CD1	2.49	0.43
2:I:676:ILE:O	2:I:987:ILE:HG23	2.18	0.43
2:C:424:GLY:O	2:C:425:PHE:HD1	2.00	0.43
5:F:117:LEU:O	5:F:121:VAL:HG23	2.18	0.43
2:C:537:LYS:CE	2:C:583:LEU:HD11	2.49	0.43
5:L:377:SER:HB3	5:L:380:GLU:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:6:ILE:HG23	4:K:7:ASP:H	1.82	0.43
3:J:406:ASP:CG	3:J:407:VAL:H	2.21	0.43
3:J:1170:ASP:O	3:J:1174:LEU:HG	2.18	0.43
1:H:23:PHE:HE2	1:H:199:ILE:HB	1.83	0.43
3:D:56:TYR:CA	3:D:80:VAL:HG23	2.49	0.43
2:I:549:PHE:HB3	2:I:552:HIS:CD2	2.54	0.43
5:L:109:LEU:HD12	5:L:114:GLU:HA	2.01	0.43
5:L:167:ASP:HB2	5:L:168:PRO:HD3	2.01	0.43
3:J:187:LYS:N	3:J:200:ASP:OD2	2.49	0.43
3:J:585:GLY:CA	3:J:590:PRO:HG3	2.48	0.43
3:J:569:ASN:ND2	5:L:229:GLN:HE21	2.16	0.43
1:G:53:VAL:CG2	1:G:54:THR:H	2.28	0.43
2:I:495:THR:H	2:I:530:GLU:CG	2.32	0.43
2:C:1086:ARG:NH1	2:C:1086:ARG:HG3	2.33	0.43
3:J:354:ILE:HG22	3:J:367:ILE:O	2.19	0.43
3:J:1192:LEU:HD23	3:J:1373:ARG:HB2	2.00	0.43
2:C:64:LEU:HD21	2:C:66:LEU:CB	2.49	0.43
3:D:1472:ILE:HA	3:D:1473:PRO:HD3	1.76	0.43
2:I:124:ASP:HA	2:I:592:LEU:HD12	2.01	0.43
2:C:160:ALA:HB3	2:C:174:LEU:HD11	2.01	0.43
3:D:1238:MET:C	3:D:1253:THR:HB	2.38	0.43
3:D:1042:ARG:HB3	3:D:1057:VAL:CG2	2.49	0.43
2:C:683:ASN:HB2	2:C:872:ASN:H	1.84	0.43
2:I:584:GLU:HB3	2:I:666:LEU:HB3	2.00	0.43
2:C:343:GLN:HG3	2:C:385:PHE:CB	2.49	0.43
3:J:349:PRO:HB2	5:L:111:LEU:HD23	2.01	0.43
3:D:210:ARG:HD2	3:D:388:HIS:HB2	2.00	0.43
3:J:155:ASP:N	3:J:155:ASP:OD2	2.52	0.43
1:H:101:LEU:HD22	1:H:102:ARG:H	1.84	0.43
2:I:99:GLN:HB3	2:I:110:GLU:HG3	2.00	0.43
3:D:553:ARG:HH11	5:F:230:GLU:HG2	1.83	0.43
2:I:536:PRO:HB3	3:J:1067:VAL:HG11	2.01	0.43
4:E:26:ARG:NH2	4:E:37:ASN:HD22	2.17	0.43
3:D:792:ILE:HD13	3:D:881:LEU:HD23	2.00	0.43
1:H:160:ASP:O	1:H:161:ARG:HB2	2.19	0.43
3:D:245:LEU:HA	3:D:245:LEU:HD23	1.75	0.43
3:D:84:ILE:HD11	3:D:88:TYR:HE1	1.84	0.43
2:C:182:VAL:O	2:C:192:PRO:HA	2.19	0.43
3:J:1149:LEU:HD22	3:J:1166:LEU:HD11	2.00	0.43
2:C:892:LEU:HD13	2:C:970:GLY:HA2	2.01	0.43
7:P:11:DT:H1'	7:P:12:DA:H5'	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:564:MET:SD	2:C:846:LYS:HG2	2.59	0.43
2:I:679:PHE:CE2	2:I:853:LEU:HD21	2.54	0.43
2:C:858:MET:SD	2:C:859:PRO:HD2	2.59	0.43
3:J:791:TYR:CE2	3:J:945:SER:HB3	2.54	0.43
3:D:218:LYS:HA	3:D:337:LEU:O	2.19	0.43
3:D:1289:ARG:HD3	3:D:1304:LYS:HD2	2.01	0.43
3:D:1293:PHE:HA	3:D:1302:GLU:HA	2.01	0.43
1:H:201:THR:HG21	1:H:205:VAL:HG23	2.01	0.43
6:R:21:DG:H1'	6:R:22:DT:H5''	2.00	0.43
5:L:143:ARG:NH1	5:L:196:GLU:OE2	2.52	0.43
3:D:439:LEU:HD21	5:F:190:HIS:HB3	2.01	0.43
2:C:543:ASN:HA	2:C:546:LEU:HD12	2.01	0.43
2:I:185:LYS:HA	2:I:189:ARG:O	2.19	0.43
1:B:34:VAL:HG11	2:C:978:ARG:HB3	2.01	0.42
2:C:456:ALA:HB3	2:C:459:ALA:HB2	2.01	0.42
3:D:789:LEU:HD13	3:D:934:LEU:HD23	2.01	0.42
1:G:97:THR:HG23	1:G:98:THR:N	2.27	0.42
1:H:62:LEU:HD12	1:H:62:LEU:H	1.83	0.42
3:J:1384:PRO:O	3:J:1415:VAL:HG22	2.19	0.42
2:I:397:GLU:HG3	2:I:632:ASN:HD22	1.84	0.42
3:D:369:ALA:HA	3:D:376:GLU:HG2	2.01	0.42
3:J:701:LEU:HD11	3:J:763:MET:HG2	2.01	0.42
2:C:181:VAL:HG22	2:C:182:VAL:H	1.83	0.42
2:I:720:GLU:HB2	2:I:759:THR:O	2.19	0.42
3:D:397:LYS:O	3:D:447:VAL:HG23	2.19	0.42
1:B:159:LYS:HG3	1:B:164:ALA:HB3	2.01	0.42
2:I:878:SER:HB2	3:J:1029:ARG:HG3	2.00	0.42
2:I:711:GLU:HA	2:I:822:VAL:HG12	2.01	0.42
5:F:167:ASP:HB2	5:F:168:PRO:HD3	2.01	0.42
3:J:837:GLY:HA2	3:J:840:LYS:HB3	2.00	0.42
1:G:48:ILE:HG22	1:G:173:PRO:HD2	2.00	0.42
2:I:424:GLY:O	2:I:425:PHE:HD1	2.01	0.42
2:C:737:LEU:HA	2:C:737:LEU:HD12	1.60	0.42
2:C:437:ARG:HD3	2:C:467:ILE:O	2.19	0.42
3:D:576:GLU:HG3	3:D:577:ALA:N	2.35	0.42
2:C:607:ASP:HB3	2:C:610:ARG:O	2.19	0.42
1:B:23:PHE:CE2	1:B:199:ILE:HB	2.54	0.42
5:F:142:ILE:HA	5:F:145:VAL:HB	2.02	0.42
3:D:1167:SER:H	3:D:1170:ASP:CG	2.22	0.42
5:L:209:LEU:HB2	6:R:30:DT:C2	2.54	0.42
2:I:941:LYS:NZ	2:I:959:PRO:HG2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:55:SER:HB2	1:H:166:PRO:HA	2.00	0.42
2:I:1019:GLN:HA	2:I:1020:PRO:HD3	1.87	0.42
5:F:302:SER:H	5:F:305:GLU:CG	2.32	0.42
3:J:1161:GLU:H	3:J:1161:GLU:HG2	1.58	0.42
3:J:30:GLU:HB3	5:L:274:ARG:HB2	2.00	0.42
1:G:43:ILE:HG13	1:H:35:THR:HG21	2.01	0.42
2:C:547:ILE:HG21	2:C:550:LEU:HD13	2.02	0.42
2:I:537:LYS:CE	2:I:583:LEU:HD11	2.49	0.42
2:I:458:TYR:CD1	2:I:538:GLN:HB3	2.48	0.42
3:J:58:CYS:HB2	3:J:78:VAL:HB	2.01	0.42
3:J:1267:ARG:NE	3:J:1267:ARG:H	2.14	0.42
3:J:1481:VAL:HG21	4:K:17:TYR:HB2	2.00	0.42
3:D:313:LEU:HD12	3:D:314:PRO:HD2	2.01	0.42
3:J:603:LEU:O	3:J:606:ILE:HG22	2.19	0.42
2:C:67:ASP:O	2:C:98:LEU:HB2	2.19	0.42
3:D:698:LYS:HG2	3:D:756:GLN:HG2	2.01	0.42
2:C:564:MET:HG2	2:C:567:GLN:NE2	2.34	0.42
3:D:1122:LEU:HD12	3:D:1184:ARG:O	2.19	0.42
2:I:328:LEU:HD23	2:I:437:ARG:HD2	2.01	0.42
1:A:34:VAL:HG22	1:A:181:VAL:HG21	2.02	0.42
3:J:853:VAL:HG22	3:J:858:LEU:HD23	2.00	0.42
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.54	0.42
3:J:103:TRP:O	3:J:107:ASP:HB2	2.19	0.42
3:J:177:ALA:HB2	3:J:393:ILE:HD11	2.01	0.42
1:B:28:LEU:O	1:B:193:ASP:N	2.51	0.42
3:D:100:ALA:HA	3:D:513:ILE:HA	2.02	0.42
3:D:1229:ILE:O	3:D:1232:PRO:HD2	2.19	0.42
2:C:639:GLN:HA	2:C:657:ASP:O	2.20	0.42
2:C:839:LEU:HA	2:C:995:MET:O	2.19	0.42
3:D:544:TYR:O	3:D:548:ILE:HG13	2.20	0.42
3:D:577:ALA:O	3:D:581:VAL:HG23	2.18	0.42
3:J:1229:ILE:O	3:J:1232:PRO:HD2	2.19	0.42
5:F:99:TYR:O	5:F:103:ILE:HG12	2.20	0.42
1:G:20:TYR:HD2	1:G:21:GLY:N	2.17	0.42
2:C:770:GLU:HB3	5:F:369:LEU:HD12	2.01	0.42
2:C:726:ILE:HD12	2:C:729:LEU:HG	2.01	0.42
2:I:751:PRO:HA	2:I:792:VAL:HG13	2.01	0.42
3:D:1021:TYR:O	3:D:1025:GLN:HB2	2.19	0.42
3:D:643:GLY:O	3:D:726:ILE:HG23	2.19	0.42
2:C:806:LEU:HB2	2:C:822:VAL:HG22	2.01	0.42
3:J:677:LEU:HD23	3:J:677:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1311:LEU:H	3:J:1311:LEU:HD23	1.83	0.42
5:L:421:ARG:HA	5:L:424:LYS:HG3	2.02	0.42
3:D:1460:ILE:HG13	3:D:1461:GLY:N	2.33	0.42
2:I:775:ARG:CZ	2:I:782:ALA:HB2	2.49	0.42
3:D:1404:ASN:O	3:D:1408:ILE:HG12	2.20	0.42
3:J:12:LEU:HD21	3:J:1452:ILE:HD13	2.01	0.42
1:H:28:LEU:HB3	1:H:193:ASP:HB2	2.01	0.42
1:A:173:PRO:HB3	1:A:202:ASP:OD1	2.20	0.42
2:C:143:SER:H	2:C:331:ARG:HA	1.85	0.42
2:C:142:ARG:HA	2:C:331:ARG:HG2	2.01	0.42
5:F:412:ILE:HA	5:F:415:ILE:HD12	2.00	0.42
2:I:971:LYS:HA	2:I:988:VAL:HA	2.00	0.42
2:I:200:LEU:HD12	2:I:200:LEU:HA	1.69	0.42
3:D:909:ASN:O	3:D:912:LYS:HB3	2.20	0.42
3:D:1047:LYS:CG	3:D:1048:PRO:HD2	2.49	0.42
2:C:194:VAL:O	2:C:198:ARG:HG3	2.19	0.42
6:O:3:DT:H2'	6:O:3:DT:H6	1.65	0.42
2:C:572:ILE:HD11	2:C:703:ILE:HG13	2.00	0.42
3:D:471:GLU:O	3:D:475:ARG:HG2	2.19	0.42
3:J:1021:TYR:O	3:J:1025:GLN:HB2	2.19	0.42
3:D:211:VAL:O	3:D:345:TYR:HD1	2.02	0.42
2:I:390:GLN:CG	2:I:415:PRO:HD3	2.49	0.42
3:D:220:ARG:O	3:D:281:ARG:HD3	2.20	0.42
1:B:101:LEU:HD22	1:B:102:ARG:H	1.85	0.42
2:C:418:LEU:HD21	2:C:427:VAL:HG11	2.01	0.42
2:C:709:GLU:HA	2:C:823:VAL:O	2.19	0.42
5:F:109:LEU:HD12	5:F:114:GLU:HA	2.02	0.42
4:E:30:LEU:HA	4:E:37:ASN:HD21	1.85	0.42
2:I:470:PRO:HA	2:I:484:VAL:O	2.20	0.42
3:D:695:ILE:HG23	3:D:718:PRO:HB2	2.02	0.42
1:H:156:HIS:CG	1:H:156:HIS:O	2.72	0.42
5:L:385:LYS:HA	5:L:390:LEU:HD12	2.02	0.42
5:F:376:LEU:HB3	5:F:380:GLU:HG3	2.01	0.42
3:D:44:LEU:HG	3:D:525:ARG:NH1	2.35	0.42
2:I:135:VAL:CG2	2:I:407:LYS:HG2	2.49	0.42
2:I:892:LEU:HD13	2:I:970:GLY:HA2	2.02	0.42
1:B:37:GLY:HA3	1:B:179:PHE:CE1	2.54	0.42
2:I:437:ARG:HH22	2:I:491:GLU:CD	2.21	0.42
3:J:95:LEU:HA	3:J:95:LEU:HD12	1.91	0.42
5:L:142:ILE:HA	5:L:145:VAL:HB	2.02	0.42
2:I:888:THR:HG22	2:I:989:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:58:ILE:HG22	1:G:60:ASP:H	1.84	0.42
2:C:549:PHE:HB3	2:C:552:HIS:CD2	2.53	0.42
2:I:399:ASN:HB2	2:I:400:PRO:HD2	2.00	0.42
2:C:550:LEU:HD11	2:C:558:ALA:HB1	2.00	0.42
1:B:115:THR:HA	1:B:116:PRO:HD3	1.85	0.42
2:C:1010:THR:HG23	2:C:1013:TYR:OH	2.20	0.42
1:G:38:ASN:HB2	1:G:179:PHE:CZ	2.54	0.42
3:D:160:GLU:CD	3:D:165:LYS:HD3	2.40	0.42
1:B:156:HIS:O	1:B:156:HIS:CG	2.72	0.42
3:D:637:LEU:HG	3:D:641:GLN:HB3	2.01	0.42
3:J:1188:VAL:HG12	3:J:1189:ARG:N	2.35	0.42
2:C:498:GLN:H	2:C:501:THR:HG23	1.85	0.42
3:D:1481:VAL:HG21	4:E:17:TYR:HB2	2.00	0.42
2:C:971:LYS:HA	2:C:988:VAL:HA	2.00	0.42
3:D:607:LEU:HB3	3:D:614:PHE:HE2	1.83	0.42
2:I:889:HIS:HA	2:I:892:LEU:HD12	2.01	0.42
2:I:858:MET:SD	2:I:859:PRO:HD2	2.60	0.42
2:C:926:PHE:CE2	2:C:960:GLU:HG3	2.55	0.42
3:J:95:LEU:HD21	3:J:578:VAL:HG21	2.01	0.42
2:C:22:GLN:HA	2:C:336:VAL:HG21	2.01	0.42
3:D:218:LYS:NZ	3:D:338:GLU:HB3	2.35	0.42
5:L:302:SER:H	5:L:305:GLU:CG	2.33	0.42
3:D:1479:ASP:HA	3:D:1482:ARG:HG2	2.01	0.42
3:J:116:LEU:HD23	3:J:468:LEU:HD22	2.00	0.42
5:F:375:LYS:HD3	5:F:426:HIS:CG	2.55	0.42
3:J:789:LEU:O	3:J:792:ILE:HG13	2.19	0.42
1:G:219:LYS:HE3	1:H:219:LYS:HD3	2.02	0.42
3:J:100:ALA:N	3:J:575:GLN:HE22	2.17	0.42
2:C:207:LEU:HD13	2:C:227:LEU:HD11	2.00	0.42
1:G:44:LEU:HD11	1:G:199:ILE:CD1	2.49	0.42
3:D:646:LYS:HE3	3:D:688:TRP:CZ2	2.55	0.42
2:C:720:GLU:CD	2:C:760:SER:HB3	2.40	0.42
2:C:713:ARG:NH1	3:D:533:GLY:HA2	2.34	0.42
3:D:1333:HIS:O	3:D:1336:LEU:HB3	2.19	0.42
2:C:526:PRO:O	2:C:529:VAL:HG12	2.19	0.42
5:L:334:THR:O	5:L:344:TYR:HB2	2.19	0.42
2:C:816:LYS:HG3	2:C:817:PRO:CD	2.50	0.42
1:G:88:ARG:HB2	1:G:204:SER:HA	2.02	0.42
3:D:508:ARG:HB2	3:D:511:TRP:NE1	2.35	0.42
5:L:173:GLU:O	5:L:177:LYS:HB2	2.20	0.42
3:J:1011:PHE:HZ	3:J:1039:CYS:HG	1.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:603:VAL:O	2:I:646:GLY:HA2	2.19	0.42
3:D:1059:SER:HB3	3:D:1063:GLU:HB2	2.00	0.42
3:D:217:ARG:HG3	3:D:341:GLU:OE1	2.20	0.42
2:C:499:ALA:N	2:C:533:ASP:HB3	2.35	0.42
2:I:1050:GLN:HE22	3:J:1470:ARG:C	2.23	0.42
2:C:1102:LEU:HD12	2:C:1107:ASN:N	2.34	0.42
2:C:437:ARG:HH22	2:C:491:GLU:CD	2.21	0.42
3:D:1254:GLN:HG3	3:D:1258:ARG:HD3	2.01	0.42
1:G:44:LEU:O	1:G:174:VAL:HG11	2.20	0.42
2:I:926:PHE:O	2:I:930:GLN:HG2	2.19	0.42
3:D:750:PRO:HG2	3:D:756:GLN:HE22	1.85	0.42
1:B:188:GLN:HA	3:D:688:TRP:CD1	2.54	0.42
2:I:432:ARG:HH22	2:I:518:ARG:NH2	2.18	0.42
3:D:895:VAL:O	3:D:899:LEU:HG	2.19	0.42
5:L:206:ASN:O	5:L:209:LEU:HB3	2.20	0.42
3:D:643:GLY:HA3	3:D:727:GLN:HB2	2.02	0.42
1:B:54:THR:OG1	1:B:55:SER:N	2.50	0.42
2:C:1056:LYS:O	3:D:624:ASP:N	2.35	0.42
1:G:89:PHE:HE1	1:G:120:VAL:HG12	1.85	0.42
2:C:269:LEU:H	2:C:288:ARG:HB3	1.84	0.42
1:A:104:GLU:HG3	1:A:137:LYS:HG2	2.00	0.42
3:J:178:LEU:HD11	3:J:190:GLU:O	2.20	0.42
2:C:376:ARG:HB2	2:C:377:PRO:HD3	2.01	0.42
2:C:603:VAL:O	2:C:646:GLY:HA2	2.19	0.42
4:E:88:GLU:HG2	4:E:91:ARG:NH2	2.35	0.42
3:D:1255:GLY:O	3:D:1259:VAL:HG23	2.20	0.42
1:H:48:ILE:HG22	1:H:173:PRO:HD2	2.02	0.42
5:F:160:PRO:HG2	5:F:164:GLU:HG2	2.01	0.42
3:D:205:TYR:CD1	3:D:393:ILE:HG12	2.53	0.42
3:J:790:TYR:CD1	3:J:907:GLU:HB3	2.55	0.42
2:C:679:PHE:CE2	2:C:853:LEU:HD21	2.55	0.42
2:C:761:PHE:HA	2:C:785:VAL:HA	2.01	0.42
3:J:815:ALA:HB1	3:J:821:VAL:HG23	2.02	0.42
2:C:525:ALA:HB1	2:C:527:GLU:OE2	2.20	0.42
2:C:399:ASN:HB2	2:C:400:PRO:HD2	2.01	0.42
2:I:549:PHE:HB3	2:I:886:LEU:HD12	2.01	0.42
3:J:12:LEU:HD12	3:J:507:ASN:HB3	2.02	0.42
2:I:648:ARG:HG2	2:I:648:ARG:H	1.69	0.42
2:C:380:ALA:O	2:C:383:ARG:HG2	2.20	0.42
3:J:1206:GLY:HA2	3:J:1215:VAL:HG12	2.02	0.41
1:A:44:LEU:HD11	1:A:199:ILE:CD1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1215:VAL:HG21	3:D:1221:VAL:CG1	2.50	0.41
2:I:98:LEU:HD22	2:I:113:VAL:HG22	2.02	0.41
2:I:950:LEU:HD11	2:I:952:LEU:HD13	2.02	0.41
3:J:521:PRO:HA	3:J:522:PRO:HD3	1.95	0.41
1:B:75:VAL:O	1:B:79:ILE:HG13	2.21	0.41
3:D:15:PRO:HG3	3:D:514:LEU:HD12	2.02	0.41
3:J:1047:LYS:CG	3:J:1048:PRO:HD2	2.50	0.41
3:J:771:SER:HA	3:J:772:PRO:HD3	1.93	0.41
3:D:646:LYS:HE3	3:D:688:TRP:HZ2	1.84	0.41
3:D:1216:SER:HB2	4:E:16:LYS:H	1.85	0.41
3:J:1274:ILE:HD12	3:J:1322:GLY:HA2	2.02	0.41
3:J:643:GLY:HA3	3:J:727:GLN:HB2	2.02	0.41
3:J:643:GLY:O	3:J:726:ILE:HG23	2.20	0.41
5:F:343:PHE:HD2	5:F:343:PHE:HA	1.75	0.41
2:C:339:LEU:O	2:C:342:ASP:HB2	2.19	0.41
4:K:10:PHE:CE1	4:K:16:LYS:HG2	2.55	0.41
2:C:170:PRO:HD2	2:C:267:TYR:HD1	1.85	0.41
2:C:535:SER:O	2:C:538:GLN:HG2	2.20	0.41
3:D:638:LYS:HB3	3:D:641:GLN:NE2	2.35	0.41
2:I:838:LYS:HG2	2:I:997:LEU:HD12	2.02	0.41
2:C:72:ARG:O	2:C:94:LEU:HD12	2.20	0.41
2:I:1064:ASN:ND2	5:L:359:ALA:HB2	2.27	0.41
3:J:1207:TYR:H	3:J:1214:PRO:HA	1.84	0.41
3:J:1465:ASN:OD1	3:J:1470:ARG:HB3	2.20	0.41
3:D:1475:GLY:HA2	4:E:17:TYR:CZ	2.55	0.41
2:I:291:VAL:HG13	2:I:303:PHE:CE1	2.56	0.41
2:C:952:LEU:HD21	2:C:971:LYS:HZ2	1.84	0.41
5:F:181:LEU:HB3	5:F:185:LEU:HB2	2.03	0.41
2:C:191:PHE:HA	2:C:192:PRO:HD3	1.89	0.41
2:I:5:ARG:HE	2:I:5:ARG:HB2	1.72	0.41
3:D:698:LYS:HG3	4:E:59:ASN:OD1	2.20	0.41
3:D:666:PHE:CE1	3:D:687:VAL:HG12	2.55	0.41
2:C:124:ASP:HB2	2:C:407:LYS:HZ2	1.85	0.41
3:D:216:LEU:HB3	3:D:218:LYS:HE2	2.01	0.41
2:C:399:ASN:O	2:C:402:SER:HB2	2.20	0.41
1:G:227:ASN:HA	1:G:228:PRO:HD2	1.75	0.41
3:D:1307:LYS:HB3	3:D:1307:LYS:HE3	1.76	0.41
5:L:315:ASP:O	5:L:319:VAL:HG12	2.20	0.41
2:I:537:LYS:NZ	2:I:905:VAL:HG22	2.35	0.41
1:A:99:LEU:HD13	1:A:144:VAL:HG23	2.02	0.41
1:A:53:VAL:CG2	1:A:54:THR:H	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:530:GLU:HG2	2:C:530:GLU:H	1.60	0.41
5:F:398:LEU:HD12	5:F:412:ILE:HB	2.02	0.41
3:D:58:CYS:HB2	3:D:78:VAL:HB	2.01	0.41
3:J:1105:ILE:HG23	3:J:1199:GLY:HA2	2.02	0.41
2:I:1085:PHE:CE2	3:J:1468:LEU:HD22	2.56	0.41
2:I:1095:LEU:HD11	3:J:603:LEU:HB3	2.02	0.41
2:I:344:PHE:HA	2:I:382:LEU:HD11	2.01	0.41
3:D:869:LEU:HD21	3:D:893:GLU:HG3	2.02	0.41
2:I:1034:GLU:HG3	2:I:1034:GLU:H	1.69	0.41
5:F:146:VAL:HG12	5:F:150:ILE:HG13	2.02	0.41
2:C:941:LYS:NZ	2:C:959:PRO:HG2	2.35	0.41
3:J:569:ASN:HD22	5:L:229:GLN:HE21	1.66	0.41
1:H:80:LEU:HD23	3:J:867:ARG:HB2	2.02	0.41
3:J:203:ALA:HA	3:J:395:VAL:HA	2.02	0.41
3:J:1236:LEU:HD22	3:J:1355:VAL:HG12	2.02	0.41
3:D:502:PHE:CE1	3:D:509:PRO:HB3	2.55	0.41
1:B:49:PRO:HD2	1:B:213:GLN:HE22	1.86	0.41
3:D:789:LEU:O	3:D:792:ILE:HG13	2.21	0.41
2:I:839:LEU:HA	2:I:995:MET:O	2.20	0.41
2:C:1044:GLY:HA3	4:E:17:TYR:HE1	1.84	0.41
3:D:1147:ARG:HB3	3:D:1188:VAL:CG1	2.51	0.41
2:I:198:ARG:HB2	2:I:198:ARG:HE	1.50	0.41
1:B:176:ARG:NH1	3:D:884:ARG:HH12	2.18	0.41
5:L:94:ASP:O	5:L:98:GLN:HB2	2.21	0.41
1:G:57:TYR:C	1:G:58:ILE:HD12	2.41	0.41
4:E:52:GLU:H	4:E:52:GLU:HG3	1.59	0.41
2:I:89:THR:HB	2:I:91:GLN:NE2	2.35	0.41
5:F:367:GLU:O	5:F:370:GLU:N	2.51	0.41
3:J:1386:ASP:HB2	3:J:1412:LYS:HB3	2.02	0.41
2:I:673:LEU:HA	2:I:990:GLY:O	2.20	0.41
3:D:231:VAL:N	3:D:243:ALA:HA	2.23	0.41
2:I:530:GLU:HG2	2:I:530:GLU:H	1.59	0.41
3:D:371:ILE:HG23	3:D:372:ASP:N	2.32	0.41
3:J:525:ARG:HB2	3:J:541:ASN:OD1	2.20	0.41
2:C:429:ASP:OD1	2:C:430:VAL:N	2.43	0.41
1:H:51:THR:HG21	1:H:86:VAL:HG23	2.02	0.41
3:J:401:TYR:HE1	3:J:446:VAL:HB	1.85	0.41
3:D:1263:PHE:CE2	3:D:1371:VAL:HG11	2.55	0.41
2:I:676:ILE:HA	2:I:871:LEU:O	2.20	0.41
3:D:1460:ILE:HG13	3:D:1461:GLY:H	1.85	0.41
5:L:276:PRO:HB2	5:L:279:MET:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ASN:HB2	1:A:179:PHE:CZ	2.56	0.41
3:D:1442:ASN:O	3:D:1446:VAL:HG23	2.20	0.41
2:C:520:GLU:HA	2:C:521:PRO:HD3	1.92	0.41
3:D:886:VAL:O	3:D:890:VAL:HG23	2.20	0.41
2:C:1095:LEU:HD11	3:D:603:LEU:HB3	2.02	0.41
3:D:775:GLY:HA2	3:D:1209:LEU:HB3	2.03	0.41
2:C:1090:LYS:HE3	3:D:88:TYR:O	2.19	0.41
2:C:215:GLY:O	2:C:217:LEU:N	2.54	0.41
2:I:64:LEU:HD21	2:I:66:LEU:CB	2.50	0.41
3:J:786:ILE:CD1	3:J:908:LYS:HG2	2.48	0.41
2:C:307:LEU:HD12	2:C:310:LEU:HD23	2.03	0.41
1:G:63:HIS:HD2	1:G:66:SER:HB2	1.86	0.41
2:C:508:ILE:HG21	2:C:526:PRO:HB3	2.02	0.41
2:I:718:GLY:HA2	2:I:719:PRO:HD3	1.78	0.41
3:J:1031:ASN:O	3:J:1034:GLN:HB3	2.20	0.41
1:G:48:ILE:HD13	1:G:48:ILE:HA	1.90	0.41
5:L:421:ARG:O	5:L:424:LYS:HB2	2.21	0.41
4:K:52:GLU:H	4:K:52:GLU:HG3	1.60	0.41
2:C:1070:ILE:H	2:C:1070:ILE:HG13	1.55	0.41
1:B:201:THR:HG21	1:B:205:VAL:HG23	2.03	0.41
1:G:149:GLY:O	1:G:171:PHE:HB2	2.21	0.41
3:J:1382:THR:O	3:J:1416:ALA:HB3	2.20	0.41
1:A:74:ASP:O	1:A:77:GLU:HB3	2.20	0.41
2:I:418:LEU:HD21	2:I:427:VAL:HG11	2.01	0.41
3:D:1310:ARG:HH21	3:D:1327:ARG:NH1	2.18	0.41
2:C:557:ARG:CG	2:C:879:ARG:HB3	2.40	0.41
3:D:691:LEU:O	3:D:695:ILE:HG13	2.20	0.41
7:P:14:DC:H2"	7:P:15:DA:OP2	2.21	0.41
5:F:210:VAL:HG21	5:F:235:LEU:HD22	2.03	0.41
2:I:574:ALA:HA	2:I:670:GLN:CG	2.51	0.41
2:I:995:MET:HE3	2:I:995:MET:HA	2.02	0.41
2:I:952:LEU:HD21	2:I:971:LYS:NZ	2.34	0.41
5:L:232:ASN:O	5:L:236:ILE:HG13	2.20	0.41
3:J:1465:ASN:HA	3:J:1468:LEU:HB2	2.02	0.41
2:I:291:VAL:HB	2:I:299:LYS:O	2.20	0.41
3:D:354:ILE:HG13	3:D:369:ALA:H	1.85	0.41
3:J:67:ARG:HD2	5:L:394:ARG:CB	2.48	0.41
3:J:669:ASN:HD22	5:L:364:LEU:HD11	1.86	0.41
2:C:98:LEU:HD22	2:C:113:VAL:HG22	2.01	0.41
3:D:1117:TYR:HA	3:D:1193:THR:HG21	2.02	0.41
3:J:650:LEU:HD21	3:J:688:TRP:HZ3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:750:PRO:HB2	3:D:756:GLN:HA	2.03	0.41
1:B:32:PHE:O	1:B:36:LEU:HG	2.20	0.41
1:A:65:PHE:CE1	2:C:703:ILE:HD13	2.55	0.41
2:I:744:ARG:NH1	2:I:746:GLY:O	2.54	0.41
3:J:1125:MET:HA	3:J:1132:LEU:HA	2.03	0.41
3:D:184:GLU:HG2	3:D:184:GLU:H	1.66	0.41
2:I:167:LYS:HB3	2:I:167:LYS:HE3	1.93	0.41
2:I:237:ARG:HH22	2:I:241:LEU:HD21	1.86	0.41
3:D:1011:PHE:HZ	3:D:1039:CYS:HG	1.62	0.41
3:J:970:LYS:O	3:J:973:GLN:HB3	2.21	0.41
1:G:99:LEU:HD13	1:G:144:VAL:HG23	2.02	0.41
3:J:1366:LYS:O	3:J:1369:GLU:HB2	2.21	0.41
3:D:760:ARG:HH21	4:E:65:MET:HG3	1.86	0.41
7:S:14:DC:H2''	7:S:15:DA:OP2	2.20	0.41
5:L:381:ALA:O	5:L:385:LYS:HG3	2.21	0.41
2:C:889:HIS:HA	2:C:892:LEU:HD12	2.02	0.41
3:J:573:MET:HE3	5:L:225:LEU:HB3	2.01	0.41
3:J:664:LYS:HE2	3:J:666:PHE:HE2	1.86	0.41
5:F:207:LEU:HD23	5:F:207:LEU:HA	1.87	0.41
2:I:525:ALA:HA	2:I:526:PRO:HD3	1.91	0.41
3:J:638:LYS:HG3	3:J:640:HIS:H	1.86	0.41
2:I:585:GLU:O	2:I:588:VAL:HG22	2.20	0.41
1:H:55:SER:HB2	1:H:158:ILE:HG23	2.03	0.41
3:J:858:LEU:HD12	3:J:859:ASP:H	1.86	0.41
3:D:213:VAL:HG13	3:D:384:VAL:O	2.21	0.41
2:C:97:ARG:NH2	2:C:112:GLU:HB2	2.36	0.41
3:J:589:SER:HA	3:J:590:PRO:HD3	1.95	0.41
2:C:696:LYS:NZ	2:C:855:VAL:HG11	2.36	0.41
1:A:149:GLY:O	1:A:171:PHE:HB2	2.21	0.41
3:D:121:THR:O	3:D:124:GLU:HB3	2.20	0.41
3:J:1396:GLU:HB3	3:J:1399:ASP:OD1	2.21	0.41
2:C:537:LYS:NZ	2:C:905:VAL:HG22	2.36	0.41
1:G:52:ALA:O	1:G:53:VAL:HG12	2.21	0.41
2:C:857:ASP:N	2:C:857:ASP:OD1	2.54	0.41
5:L:160:PRO:HG2	5:L:164:GLU:HG2	2.03	0.41
7:P:16:DC:H2''	7:P:17:DT:OP2	2.21	0.41
5:F:206:ASN:O	5:F:210:VAL:HG23	2.20	0.41
6:O:24:DC:H1'	6:O:25:DT:H5'	2.01	0.41
3:D:229:ALA:HB1	3:D:245:LEU:N	2.36	0.41
2:C:1089:VAL:HG13	2:C:1099:VAL:HG11	2.03	0.41
2:C:1086:ARG:HB3	3:D:88:TYR:HE2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:571:LEU:CD2	2:I:995:MET:HE1	2.51	0.41
2:I:215:GLY:O	2:I:217:LEU:N	2.54	0.41
2:C:229:MET:CB	2:C:234:ALA:HB2	2.46	0.41
2:C:328:LEU:HD23	2:C:437:ARG:HD2	2.03	0.41
2:I:55:GLU:HA	2:I:64:LEU:O	2.20	0.41
2:I:1102:LEU:HD12	2:I:1107:ASN:N	2.35	0.41
5:L:181:LEU:HB3	5:L:185:LEU:HB2	2.03	0.41
3:J:137:PRO:HG3	3:J:148:GLU:HA	2.02	0.41
1:H:13:ALA:CB	1:H:23:PHE:HD1	2.34	0.41
3:J:657:LEU:HD22	3:J:691:LEU:HD13	2.03	0.41
1:A:14:THR:O	1:A:14:THR:HG22	2.21	0.41
3:J:1084:THR:O	3:J:1088:THR:HG23	2.21	0.41
4:E:10:PHE:CE1	4:E:16:LYS:HG2	2.56	0.41
2:I:683:ASN:OD1	2:I:872:ASN:HB2	2.21	0.41
2:I:872:ASN:ND2	3:J:784:ASP:OD2	2.54	0.41
2:C:45:GLN:HE21	2:C:48:PHE:HD2	1.69	0.41
1:G:14:THR:O	1:G:14:THR:HG22	2.21	0.41
3:J:542:ASP:O	3:J:545:ARG:HB3	2.20	0.41
3:J:654:LYS:HB3	3:J:655:PRO:HD3	2.03	0.41
3:J:1429:LEU:HG	3:J:1440:PHE:HD1	1.85	0.41
3:J:895:VAL:O	3:J:899:LEU:HG	2.20	0.41
2:C:525:ALA:HA	2:C:526:PRO:HD3	1.92	0.41
5:F:334:THR:O	5:F:344:TYR:HB2	2.21	0.41
2:I:944:LEU:HD13	2:I:959:PRO:HB3	2.02	0.41
3:D:1271:LYS:HG3	3:D:1331:ASP:HB2	2.03	0.41
2:C:670:GLN:HE22	2:C:699:PHE:HA	1.85	0.41
1:G:171:PHE:O	1:G:172:SER:OG	2.37	0.41
2:C:474:VAL:HG23	2:C:478:VAL:O	2.21	0.41
2:I:93:PRO:HG3	2:I:117:HIS:NE2	2.36	0.41
3:D:1038:LEU:O	3:D:1060:SER:OG	2.23	0.41
2:C:648:ARG:H	2:C:648:ARG:HG2	1.67	0.41
5:L:375:LYS:HD3	5:L:426:HIS:CG	2.56	0.41
3:J:1372:VAL:HA	3:J:1375:MET:SD	2.61	0.41
2:I:97:ARG:NH2	2:I:112:GLU:HB2	2.36	0.41
3:J:182:GLY:H	3:J:204:LEU:HD23	1.86	0.41
1:G:158:ILE:HG22	1:G:159:LYS:N	2.36	0.41
2:I:639:GLN:HA	2:I:657:ASP:O	2.21	0.41
6:O:6:DC:H2"	6:O:7:DA:OP2	2.21	0.41
2:C:291:VAL:HB	2:C:299:LYS:O	2.21	0.41
2:I:1085:PHE:O	2:I:1089:VAL:HG23	2.21	0.41
2:C:988:VAL:H	3:D:948:THR:HG21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:SER:OG	1:A:47:SER:N	2.54	0.41
3:J:691:LEU:O	3:J:695:ILE:HG13	2.20	0.41
3:D:900:ILE:HG12	3:D:914:LEU:CD2	2.51	0.41
5:F:154:ALA:HB1	5:F:158:LYS:HE2	2.02	0.41
1:A:33:GLY:O	1:A:195:LEU:HD21	2.21	0.41
2:C:603:VAL:HA	2:C:613:VAL:HG12	2.03	0.41
3:J:1460:ILE:HG13	3:J:1461:GLY:N	2.36	0.41
1:A:43:ILE:HG13	1:B:35:THR:HG21	2.02	0.41
3:J:886:VAL:O	3:J:890:VAL:HG23	2.21	0.41
2:C:536:PRO:HB3	3:D:1067:VAL:HG11	2.02	0.41
1:A:97:THR:HG23	1:A:98:THR:N	2.27	0.40
7:S:19:DT:H1'	7:S:20:DT:H5'	2.02	0.40
3:J:1331:ASP:HA	3:J:1332:PRO:HD3	1.83	0.40
2:C:1063:ARG:HH21	5:F:353:LEU:HD23	1.86	0.40
2:I:670:GLN:HE22	2:I:699:PHE:HA	1.86	0.40
3:D:786:ILE:CD1	3:D:908:LYS:HG2	2.49	0.40
3:J:974:ILE:HG12	3:J:991:GLN:HG2	2.03	0.40
2:I:124:ASP:HB2	2:I:407:LYS:NZ	2.36	0.40
3:J:698:LYS:HG2	3:J:756:GLN:HG2	2.03	0.40
1:H:188:GLN:HA	3:J:688:TRP:CD1	2.52	0.40
7:P:7:DA:H1'	7:P:8:DA:H5'	2.02	0.40
3:D:698:LYS:H	4:E:59:ASN:ND2	2.19	0.40
5:F:99:TYR:HE2	5:F:211:VAL:HG22	1.86	0.40
3:J:547:LEU:HD13	3:J:578:VAL:HG22	2.03	0.40
2:C:585:GLU:O	2:C:588:VAL:HG22	2.22	0.40
2:C:529:VAL:HG13	2:C:529:VAL:O	2.21	0.40
1:H:159:LYS:HG3	1:H:164:ALA:HB3	2.03	0.40
5:L:206:ASN:O	5:L:210:VAL:HG23	2.22	0.40
3:D:1290:LEU:HB2	3:D:1307:LYS:HA	2.03	0.40
1:A:107:LYS:HE2	1:A:113:ASP:OD2	2.21	0.40
2:C:512:ARG:H	2:C:512:ARG:HG2	1.54	0.40
2:I:6:PHE:HE1	2:I:901:TYR:HB3	1.86	0.40
2:I:1010:THR:HG23	2:I:1013:TYR:OH	2.21	0.40
1:B:90:LEU:HB2	1:B:119:ASP:HB3	2.03	0.40
2:C:865:THR:HA	2:C:866:PRO:HD2	1.94	0.40
2:C:223:ASP:OD1	2:C:226:VAL:HG23	2.21	0.40
2:C:317:VAL:HA	2:C:318:PRO:HD3	1.97	0.40
2:I:352:ALA:O	2:I:356:ARG:HG3	2.20	0.40
1:A:40:LEU:HG	1:A:218:LEU:HD22	2.03	0.40
3:D:285:PRO:HD2	3:D:288:MET:SD	2.61	0.40
2:C:577:PRO:HD3	2:C:993:PHE:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:498:GLN:H	2:I:501:THR:HG23	1.87	0.40
2:C:1103:ASP:OD1	2:C:1107:ASN:HB2	2.21	0.40
1:B:79:ILE:HA	1:B:82:LEU:HD12	2.03	0.40
3:D:1273:VAL:HG23	3:D:1325:LEU:HB2	2.03	0.40
3:D:684:LYS:HB3	3:D:686:GLU:HG3	2.04	0.40
3:D:101:HIS:HE2	3:D:582:ILE:HG21	1.84	0.40
2:C:166:PRO:C	2:C:168:ARG:H	2.25	0.40
2:I:246:ASP:HA	2:I:247:PRO:HD3	1.94	0.40
2:I:360:VAL:HG21	5:L:216:LYS:NZ	2.37	0.40
3:J:1129:THR:C	3:J:1131:THR:H	2.25	0.40
2:I:399:ASN:O	2:I:402:SER:HB2	2.21	0.40
3:J:1268:PRO:HB3	3:J:1329:ALA:HB3	2.04	0.40
2:I:1070:ILE:H	2:I:1070:ILE:HG13	1.58	0.40
2:C:561:GLY:O	2:C:565:GLN:HG2	2.21	0.40
3:D:178:LEU:HD11	3:D:190:GLU:O	2.21	0.40
1:B:17:GLY:HA3	1:B:19:HIS:CE1	2.56	0.40
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.84	0.40
3:D:640:HIS:O	3:D:717:GLN:HB2	2.21	0.40
3:D:229:ALA:O	3:D:244:GLU:HB2	2.21	0.40
3:J:1207:TYR:HA	3:J:1213:ARG:O	2.21	0.40
2:I:65:VAL:CG1	2:I:101:ILE:HB	2.50	0.40
3:D:545:ARG:NH1	5:F:269:GLN:O	2.54	0.40
3:J:869:LEU:HD21	3:J:893:GLU:HG3	2.03	0.40
2:I:607:ASP:HB3	2:I:610:ARG:O	2.21	0.40
3:J:669:ASN:ND2	5:L:364:LEU:HD11	2.36	0.40
3:J:704:ARG:HB3	3:J:736:PHE:CD2	2.57	0.40
3:D:131:LYS:HE2	3:D:152:LEU:HB3	2.04	0.40
1:H:23:PHE:CE2	1:H:199:ILE:HB	2.55	0.40
3:J:692:GLU:HA	3:J:695:ILE:HD12	2.04	0.40
1:B:182:GLU:CG	1:B:194:LYS:HB3	2.52	0.40
3:D:256:SER:HB3	3:D:300:VAL:HG23	2.03	0.40
3:D:388:HIS:C	3:D:389:GLU:HG3	2.41	0.40
3:D:1107:VAL:HA	3:D:1200:VAL:O	2.21	0.40
1:G:34:VAL:HG22	1:G:181:VAL:HG21	2.03	0.40
3:J:1396:GLU:OE2	3:J:1432:LYS:HD3	2.21	0.40
3:J:348:ALA:HB3	3:J:351:MET:HG3	2.03	0.40
3:D:551:ASN:O	3:D:555:LYS:HG3	2.22	0.40
5:F:418:LYS:O	5:F:422:LYS:HB2	2.21	0.40
7:P:15:DA:H2'	7:P:15:DA:OP2	2.22	0.40
2:I:299:LYS:HG3	2:I:300:ASP:N	2.36	0.40
2:I:199:VAL:HA	2:I:231:PRO:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:192:LEU:N	1:H:192:LEU:HD23	2.36	0.40
3:J:65:ARG:HA	3:J:65:ARG:HD3	1.93	0.40
2:I:609:THR:O	2:I:625:LEU:N	2.54	0.40
3:J:701:LEU:HD21	3:J:763:MET:CG	2.48	0.40
3:J:1153:VAL:HB	3:J:1160:LEU:HB3	2.04	0.40
2:I:725:ASP:O	2:I:759:THR:HG21	2.21	0.40
2:C:158:TYR:HD1	2:C:314:THR:HA	1.86	0.40
3:J:853:VAL:HA	3:J:858:LEU:HB3	2.04	0.40
1:G:195:LEU:HA	1:G:195:LEU:HD23	1.88	0.40
1:G:33:GLY:O	1:G:195:LEU:HD21	2.21	0.40
1:G:79:ILE:HD13	1:G:167:VAL:HG12	2.02	0.40
3:D:654:LYS:HB3	3:D:655:PRO:HD3	2.03	0.40
1:G:173:PRO:HB3	1:G:202:ASP:OD1	2.21	0.40
2:C:464:LEU:HD23	2:C:464:LEU:HA	1.95	0.40
5:L:130:LYS:HG2	5:L:188:TYR:CZ	2.56	0.40
3:D:1125:MET:N	3:D:1132:LEU:HD23	2.36	0.40
2:I:341:ALA:O	2:I:345:ARG:HG2	2.21	0.40
2:I:17:PRO:O	2:I:19:THR:N	2.55	0.40
1:G:9:PRO:HB2	1:G:25:LEU:HD11	2.03	0.40
2:C:327:HIS:O	2:C:331:ARG:HG3	2.22	0.40
2:C:627:ARG:HD3	2:C:639:GLN:O	2.21	0.40
1:B:192:LEU:N	1:B:192:LEU:HD23	2.36	0.40
3:J:1134:LEU:HD22	3:J:1135:ARG:N	2.37	0.40
1:A:35:THR:HG22	1:B:39:PRO:HA	2.02	0.40
1:H:129:ILE:HG22	1:H:130:ALA:N	2.37	0.40
3:D:1267:ARG:HA	3:D:1268:PRO:HD3	1.93	0.40
5:L:145:VAL:HG21	5:L:174:VAL:CG1	2.52	0.40
2:I:585:GLU:HG2	2:I:665:PHE:CD1	2.56	0.40
3:D:711:LEU:HD13	3:D:711:LEU:HA	1.95	0.40
2:C:878:SER:O	3:D:1034:GLN:NE2	2.51	0.40
3:D:553:ARG:HB3	3:D:570:GLU:OE1	2.20	0.40
2:I:554:ASP:OD2	2:I:556:ASN:HB2	2.22	0.40
3:D:364:GLY:HA2	3:D:379:ALA:O	2.21	0.40
1:H:75:VAL:O	1:H:79:ILE:HG13	2.21	0.40
3:D:598:ARG:HA	3:D:599:PRO:HD3	1.77	0.40
3:J:1404:ASN:O	3:J:1408:ILE:HG12	2.21	0.40
1:G:107:LYS:HE2	1:G:113:ASP:OD2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	225/314 (72%)	200 (89%)	23 (10%)	2 (1%)	21	67
1	B	225/314 (72%)	200 (89%)	20 (9%)	5 (2%)	8	51
1	G	225/314 (72%)	200 (89%)	23 (10%)	2 (1%)	21	67
1	H	225/314 (72%)	201 (89%)	18 (8%)	6 (3%)	6	47
2	C	1108/1119 (99%)	958 (86%)	139 (12%)	11 (1%)	19	65
2	I	1108/1119 (99%)	956 (86%)	140 (13%)	12 (1%)	17	64
3	D	1486/1524 (98%)	1315 (88%)	162 (11%)	9 (1%)	30	74
3	J	1361/1524 (89%)	1201 (88%)	150 (11%)	10 (1%)	26	71
4	E	91/99 (92%)	75 (82%)	16 (18%)	0	100	100
4	K	91/99 (92%)	75 (82%)	16 (18%)	0	100	100
5	F	343/347 (99%)	299 (87%)	42 (12%)	2 (1%)	30	74
5	L	343/347 (99%)	302 (88%)	40 (12%)	1 (0%)	46	83
All	All	6831/7434 (92%)	5982 (88%)	789 (12%)	60 (1%)	21	67

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
3	D	1128	VAL
3	D	1209	LEU
1	G	53	VAL
3	J	1128	VAL
2	C	608	GLY
2	C	972	VAL
3	D	666	PHE
2	I	608	GLY
2	I	972	VAL
3	J	1287	GLU
1	B	161	ARG

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Mol	Chain	Res	Type
2	C	882	LEU
1	H	161	ARG
2	I	882	LEU
3	J	422	ALA
1	A	98	THR
3	J	1130	ARG
1	B	178	ALA
2	C	295	ASP
2	C	365	ASP
2	C	607	ASP
3	D	1075	HIS
1	G	98	THR
1	H	178	ALA
2	I	295	ASP
2	I	365	ASP
2	I	607	ASP
3	J	1075	HIS
3	J	1207	TYR
1	B	202	ASP
3	D	667	ALA
5	F	270	ALA
1	H	51	THR
1	H	202	ASP
2	C	870	ILE
2	C	1016	ILE
3	D	1221	VAL
2	I	870	ILE
2	I	1016	ILE
3	J	667	ALA
3	J	1221	VAL
2	C	989	VAL
3	D	670	VAL
3	D	947	ILE
5	F	407	VAL
3	J	947	ILE
1	H	116	PRO
2	I	989	VAL
3	J	670	VAL
5	L	407	VAL
1	B	48	ILE
1	B	116	PRO
2	C	17	PRO

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Mol	Chain	Res	Type
2	C	852	ILE
3	D	259	VAL
1	H	48	ILE
2	I	17	PRO
2	I	852	ILE
2	I	1060	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/270 (72%)	179 (92%)	15 (8%)	16	55
1	B	194/270 (72%)	172 (89%)	22 (11%)	7	36
1	G	194/270 (72%)	178 (92%)	16 (8%)	14	51
1	H	194/270 (72%)	171 (88%)	23 (12%)	6	34
2	C	931/936 (100%)	840 (90%)	91 (10%)	10	42
2	I	931/936 (100%)	840 (90%)	91 (10%)	10	42
3	D	1252/1281 (98%)	1114 (89%)	138 (11%)	8	37
3	J	1150/1281 (90%)	1028 (89%)	122 (11%)	8	39
4	E	83/88 (94%)	79 (95%)	4 (5%)	31	69
4	K	83/88 (94%)	79 (95%)	4 (5%)	31	69
5	F	296/299 (99%)	276 (93%)	20 (7%)	20	59
5	L	296/299 (99%)	276 (93%)	20 (7%)	20	59
All	All	5798/6288 (92%)	5232 (90%)	566 (10%)	10	42

All (566) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	TYR
1	A	32	PHE
1	A	45	LEU
1	A	51	THR

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Mol	Chain	Res	Type
1	A	63	HIS
1	A	73	GLU
1	A	74	ASP
1	A	113	ASP
1	A	158	ILE
1	A	174	VAL
1	A	176	ARG
1	A	198	ARG
1	A	222	LEU
1	A	227	ASN
1	A	232	LEU
1	B	7	LYS
1	B	23	PHE
1	B	38	ASN
1	B	44	LEU
1	B	51	THR
1	B	58	ILE
1	B	62	LEU
1	B	74	ASP
1	B	75	VAL
1	B	104	GLU
1	B	113	ASP
1	B	114	PHE
1	B	129	ILE
1	B	131	THR
1	B	158	ILE
1	B	177	VAL
1	B	189	ARG
1	B	192	LEU
1	B	201	THR
1	B	215	VAL
1	B	219	LYS
1	B	227	ASN
2	C	10	ARG
2	C	12	VAL
2	C	20	GLU
2	C	30	LEU
2	C	41	ASN
2	C	45	GLN
2	C	55	GLU
2	C	75	ASP
2	C	98	LEU

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Mol	Chain	Res	Type
2	C	101	ILE
2	C	104	ASP
2	C	107	LEU
2	C	134	ARG
2	C	142	ARG
2	C	148	PHE
2	C	174	LEU
2	C	176	VAL
2	C	187	ASN
2	C	194	VAL
2	C	203	ASP
2	C	211	LEU
2	C	221	LEU
2	C	232	GLU
2	C	238	LEU
2	C	242	LEU
2	C	268	ASP
2	C	280	LYS
2	C	283	VAL
2	C	297	GLU
2	C	308	ARG
2	C	323	ASP
2	C	336	VAL
2	C	361	MET
2	C	365	ASP
2	C	383	ARG
2	C	413	LEU
2	C	421	GLU
2	C	425	PHE
2	C	430	VAL
2	C	434	HIS
2	C	438	ILE
2	C	485	TYR
2	C	503	LEU
2	C	506	ASP
2	C	512	ARG
2	C	514	VAL
2	C	516	ARG
2	C	523	ILE
2	C	527	GLU
2	C	530	GLU
2	C	542	LEU

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Mol	Chain	Res	Type
2	C	543	ASN
2	C	571	LEU
2	C	579	VAL
2	C	604	VAL
2	C	653	ASP
2	C	673	LEU
2	C	685	GLU
2	C	707	ARG
2	C	729	LEU
2	C	754	ILE
2	C	761	PHE
2	C	784	ASP
2	C	788	THR
2	C	808	ARG
2	C	823	VAL
2	C	839	LEU
2	C	848	VAL
2	C	857	ASP
2	C	868	ASP
2	C	869	VAL
2	C	892	LEU
2	C	896	PHE
2	C	897	LEU
2	C	899	GLN
2	C	920	GLU
2	C	926	PHE
2	C	934	PHE
2	C	936	VAL
2	C	950	LEU
2	C	952	LEU
2	C	968	ASP
2	C	969	LEU
2	C	972	VAL
2	C	994	ILE
2	C	995	MET
2	C	1001	VAL
2	C	1035	MET
2	C	1061	GLU
2	C	1075	ASP
2	C	1112	PHE
3	D	5	VAL
3	D	26	VAL

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Mol	Chain	Res	Type
3	D	37	LEU
3	D	54	LYS
3	D	62	LYS
3	D	66	GLN
3	D	68	PHE
3	D	80	VAL
3	D	92	HIS
3	D	121	THR
3	D	135	LEU
3	D	152	LEU
3	D	154	THR
3	D	155	ASP
3	D	166	GLN
3	D	168	THR
3	D	171	LEU
3	D	178	LEU
3	D	180	LYS
3	D	214	ASP
3	D	233	LYS
3	D	247	GLU
3	D	251	PHE
3	D	259	VAL
3	D	266	GLU
3	D	277	GLU
3	D	281	ARG
3	D	297	ILE
3	D	306	GLU
3	D	315	ARG
3	D	327	GLU
3	D	332	HIS
3	D	334	THR
3	D	335	LEU
3	D	347	VAL
3	D	350	HIS
3	D	389	GLU
3	D	408	GLU
3	D	414	ARG
3	D	423	ASP
3	D	442	ASN
3	D	450	TYR
3	D	461	ILE
3	D	464	LEU

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Mol	Chain	Res	Type
3	D	475	ARG
3	D	525	ARG
3	D	538	SER
3	D	546	ARG
3	D	548	ILE
3	D	576	GLU
3	D	596	SER
3	D	598	ARG
3	D	619	LEU
3	D	636	GLN
3	D	639	LEU
3	D	658	LEU
3	D	683	ILE
3	D	685	ASP
3	D	688	TRP
3	D	694	VAL
3	D	707	THR
3	D	708	LEU
3	D	709	HIS
3	D	717	GLN
3	D	747	VAL
3	D	748	HIS
3	D	762	GLN
3	D	776	GLU
3	D	787	LEU
3	D	810	GLU
3	D	811	GLU
3	D	832	ARG
3	D	835	SER
3	D	838	ARG
3	D	850	LEU
3	D	861	GLN
3	D	865	THR
3	D	875	THR
3	D	897	GLN
3	D	899	LEU
3	D	903	ASP
3	D	908	LYS
3	D	909	ASN
3	D	930	LEU
3	D	932	ASP
3	D	945	SER

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Mol	Chain	Res	Type
3	D	964	LEU
3	D	976	GLN
3	D	1004	THR
3	D	1015	TYR
3	D	1029	ARG
3	D	1066	THR
3	D	1078	ARG
3	D	1094	LEU
3	D	1100	ASP
3	D	1107	VAL
3	D	1108	ARG
3	D	1112	CYS
3	D	1120	VAL
3	D	1123	PHE
3	D	1130	ARG
3	D	1134	LEU
3	D	1137	ARG
3	D	1139	ASP
3	D	1144	LEU
3	D	1156	LEU
3	D	1160	LEU
3	D	1161	GLU
3	D	1162	GLU
3	D	1170	ASP
3	D	1179	GLU
3	D	1201	CYS
3	D	1203	LYS
3	D	1213	ARG
3	D	1231	GLU
3	D	1256	LEU
3	D	1258	ARG
3	D	1267	ARG
3	D	1278	ASP
3	D	1285	GLU
3	D	1295	GLU
3	D	1297	GLU
3	D	1302	GLU
3	D	1305	LEU
3	D	1310	ARG
3	D	1312	LEU
3	D	1342	GLU
3	D	1380	GLU

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Mol	Chain	Res	Type
3	D	1382	THR
3	D	1386	ASP
3	D	1395	LEU
3	D	1407	LEU
3	D	1413	VAL
3	D	1444	THR
3	D	1448	THR
3	D	1459	LEU
3	D	1462	LEU
3	D	1499	ARG
4	E	14	ASP
4	E	30	LEU
4	E	39	VAL
4	E	56	ASP
5	F	108	LEU
5	F	138	ASP
5	F	139	GLN
5	F	151	LEU
5	F	165	LYS
5	F	175	ASP
5	F	196	GLU
5	F	202	LEU
5	F	224	PHE
5	F	233	GLN
5	F	293	LEU
5	F	328	GLU
5	F	339	GLU
5	F	343	PHE
5	F	371	LYS
5	F	404	TYR
5	F	405	PHE
5	F	409	ARG
5	F	424	LYS
5	F	433	LEU
1	G	20	TYR
1	G	32	PHE
1	G	45	LEU
1	G	51	THR
1	G	63	HIS
1	G	73	GLU
1	G	74	ASP
1	G	80	LEU

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Mol	Chain	Res	Type
1	G	113	ASP
1	G	158	ILE
1	G	174	VAL
1	G	176	ARG
1	G	198	ARG
1	G	222	LEU
1	G	227	ASN
1	G	232	LEU
1	H	7	LYS
1	H	23	PHE
1	H	38	ASN
1	H	44	LEU
1	H	51	THR
1	H	58	ILE
1	H	62	LEU
1	H	74	ASP
1	H	75	VAL
1	H	104	GLU
1	H	113	ASP
1	H	114	PHE
1	H	129	ILE
1	H	131	THR
1	H	140	MET
1	H	158	ILE
1	H	177	VAL
1	H	189	ARG
1	H	192	LEU
1	H	201	THR
1	H	215	VAL
1	H	219	LYS
1	H	227	ASN
2	I	10	ARG
2	I	12	VAL
2	I	20	GLU
2	I	30	LEU
2	I	41	ASN
2	I	45	GLN
2	I	55	GLU
2	I	75	ASP
2	I	98	LEU
2	I	101	ILE
2	I	104	ASP

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Mol	Chain	Res	Type
2	I	107	LEU
2	I	134	ARG
2	I	142	ARG
2	I	148	PHE
2	I	174	LEU
2	I	176	VAL
2	I	187	ASN
2	I	194	VAL
2	I	203	ASP
2	I	211	LEU
2	I	221	LEU
2	I	232	GLU
2	I	238	LEU
2	I	242	LEU
2	I	268	ASP
2	I	280	LYS
2	I	283	VAL
2	I	297	GLU
2	I	308	ARG
2	I	323	ASP
2	I	336	VAL
2	I	361	MET
2	I	365	ASP
2	I	383	ARG
2	I	413	LEU
2	I	421	GLU
2	I	425	PHE
2	I	430	VAL
2	I	434	HIS
2	I	438	ILE
2	I	485	TYR
2	I	487	THR
2	I	503	LEU
2	I	506	ASP
2	I	512	ARG
2	I	514	VAL
2	I	523	ILE
2	I	527	GLU
2	I	530	GLU
2	I	542	LEU
2	I	543	ASN
2	I	571	LEU

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Mol	Chain	Res	Type
2	I	579	VAL
2	I	604	VAL
2	I	653	ASP
2	I	673	LEU
2	I	685	GLU
2	I	707	ARG
2	I	729	LEU
2	I	754	ILE
2	I	761	PHE
2	I	784	ASP
2	I	788	THR
2	I	808	ARG
2	I	823	VAL
2	I	839	LEU
2	I	848	VAL
2	I	857	ASP
2	I	868	ASP
2	I	869	VAL
2	I	892	LEU
2	I	896	PHE
2	I	897	LEU
2	I	899	GLN
2	I	920	GLU
2	I	926	PHE
2	I	934	PHE
2	I	936	VAL
2	I	950	LEU
2	I	952	LEU
2	I	968	ASP
2	I	969	LEU
2	I	972	VAL
2	I	994	ILE
2	I	995	MET
2	I	1001	VAL
2	I	1035	MET
2	I	1061	GLU
2	I	1075	ASP
2	I	1112	PHE
3	J	26	VAL
3	J	37	LEU
3	J	54	LYS
3	J	62	LYS

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Mol	Chain	Res	Type
3	J	66	GLN
3	J	68	PHE
3	J	80	VAL
3	J	121	THR
3	J	135	LEU
3	J	154	THR
3	J	155	ASP
3	J	166	GLN
3	J	168	THR
3	J	171	LEU
3	J	178	LEU
3	J	180	LYS
3	J	210	ARG
3	J	211	VAL
3	J	350	HIS
3	J	375	GLU
3	J	399	ARG
3	J	404	GLU
3	J	410	THR
3	J	411	THR
3	J	414	ARG
3	J	423	ASP
3	J	430	GLU
3	J	450	TYR
3	J	462	GLN
3	J	512	MET
3	J	513	ILE
3	J	523	ASP
3	J	525	ARG
3	J	548	ILE
3	J	574	LEU
3	J	576	GLU
3	J	598	ARG
3	J	600	LEU
3	J	619	LEU
3	J	636	GLN
3	J	639	LEU
3	J	658	LEU
3	J	683	ILE
3	J	685	ASP
3	J	688	TRP
3	J	694	VAL

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Mol	Chain	Res	Type
3	J	707	THR
3	J	708	LEU
3	J	709	HIS
3	J	717	GLN
3	J	747	VAL
3	J	748	HIS
3	J	762	GLN
3	J	776	GLU
3	J	787	LEU
3	J	810	GLU
3	J	811	GLU
3	J	832	ARG
3	J	835	SER
3	J	838	ARG
3	J	850	LEU
3	J	861	GLN
3	J	865	THR
3	J	875	THR
3	J	897	GLN
3	J	899	LEU
3	J	903	ASP
3	J	908	LYS
3	J	909	ASN
3	J	930	LEU
3	J	932	ASP
3	J	945	SER
3	J	958	GLU
3	J	964	LEU
3	J	976	GLN
3	J	1004	THR
3	J	1015	TYR
3	J	1029	ARG
3	J	1066	THR
3	J	1078	ARG
3	J	1094	LEU
3	J	1100	ASP
3	J	1107	VAL
3	J	1112	CYS
3	J	1132	LEU
3	J	1134	LEU
3	J	1137	ARG
3	J	1149	LEU

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Mol	Chain	Res	Type
3	J	1159	ARG
3	J	1160	LEU
3	J	1161	GLU
3	J	1162	GLU
3	J	1170	ASP
3	J	1173	PHE
3	J	1183	VAL
3	J	1201	CYS
3	J	1203	LYS
3	J	1211	MET
3	J	1231	GLU
3	J	1235	GLN
3	J	1238	MET
3	J	1267	ARG
3	J	1285	GLU
3	J	1293	PHE
3	J	1297	GLU
3	J	1305	LEU
3	J	1318	TYR
3	J	1325	LEU
3	J	1326	THR
3	J	1335	LEU
3	J	1342	GLU
3	J	1376	LEU
3	J	1397	LYS
3	J	1407	LEU
3	J	1429	LEU
3	J	1432	LYS
3	J	1433	SER
3	J	1444	THR
3	J	1448	THR
3	J	1462	LEU
3	J	1496	GLU
3	J	1499	ARG
4	K	14	ASP
4	K	30	LEU
4	K	39	VAL
4	K	56	ASP
5	L	108	LEU
5	L	138	ASP
5	L	139	GLN
5	L	151	LEU

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Mol	Chain	Res	Type
5	L	165	LYS
5	L	175	ASP
5	L	196	GLU
5	L	202	LEU
5	L	224	PHE
5	L	233	GLN
5	L	293	LEU
5	L	328	GLU
5	L	339	GLU
5	L	343	PHE
5	L	371	LYS
5	L	404	TYR
5	L	405	PHE
5	L	409	ARG
5	L	424	LYS
5	L	433	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	HIS
1	A	212	ASN
1	B	128	HIS
1	B	163	ASN
1	B	213	GLN
2	C	41	ASN
2	C	45	GLN
2	C	393	GLN
2	C	498	GLN
2	C	538	GLN
2	C	567	GLN
2	C	639	GLN
2	C	671	ASN
2	C	765	GLN
2	C	845	ASN
2	C	881	ASN
2	C	962	GLN
2	C	1050	GLN
2	C	1100	GLN
3	D	130	ASN
3	D	274	GLN
3	D	350	HIS

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Mol	Chain	Res	Type
3	D	362	GLN
3	D	549	ASN
3	D	552	ASN
3	D	560	GLN
3	D	569	ASN
3	D	593	ASN
3	D	680	GLN
3	D	703	ASN
3	D	756	GLN
3	D	762	GLN
3	D	768	ASN
3	D	794	GLN
3	D	897	GLN
3	D	991	GLN
3	D	1046	GLN
3	D	1116	ASN
3	D	1235	GLN
3	D	1359	GLN
4	E	37	ASN
4	E	59	ASN
5	F	233	GLN
5	F	294	GLN
5	F	295	GLN
5	F	417	ASN
5	F	426	HIS
1	G	63	HIS
1	G	81	ASN
1	G	212	ASN
1	H	128	HIS
1	H	163	ASN
1	H	213	GLN
2	I	22	GLN
2	I	41	ASN
2	I	45	GLN
2	I	393	GLN
2	I	498	GLN
2	I	538	GLN
2	I	567	GLN
2	I	639	GLN
2	I	671	ASN
2	I	765	GLN
2	I	845	ASN

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Mol	Chain	Res	Type
2	I	881	ASN
2	I	962	GLN
2	I	1050	GLN
2	I	1100	GLN
3	J	130	ASN
3	J	549	ASN
3	J	560	GLN
3	J	703	ASN
3	J	756	GLN
3	J	762	GLN
3	J	794	GLN
3	J	897	GLN
3	J	991	GLN
3	J	1046	GLN
4	K	37	ASN
4	K	59	ASN
5	L	229	GLN
5	L	294	GLN
5	L	295	GLN
5	L	417	ASN
5	L	426	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	227/314 (72%)	0.08	2 (0%) 85 80	107, 189, 236, 264	0
1	B	227/314 (72%)	-0.23	0 100 100	94, 161, 214, 264	0
1	G	227/314 (72%)	0.39	16 (7%) 19 15	116, 199, 240, 276	0
1	H	227/314 (72%)	-0.13	2 (0%) 85 80	116, 173, 216, 267	0
2	C	1112/1119 (99%)	-0.03	21 (1%) 70 61	90, 179, 243, 314	0
2	I	1112/1119 (99%)	0.01	25 (2%) 65 56	94, 185, 244, 315	0
3	D	1490/1524 (97%)	-0.13	13 (0%) 85 80	64, 149, 204, 259	0
3	J	1367/1524 (89%)	-0.08	18 (1%) 79 71	79, 159, 217, 264	0
4	E	93/99 (93%)	0.05	2 (2%) 65 56	100, 159, 205, 238	0
4	K	93/99 (93%)	0.03	3 (3%) 51 41	112, 168, 216, 253	0
5	F	345/347 (99%)	-0.10	1 (0%) 94 92	115, 185, 255, 300	0
5	L	345/347 (99%)	-0.11	7 (2%) 68 59	121, 188, 252, 300	0
6	O	30/30 (100%)	0.70	4 (13%) 4 6	154, 221, 293, 311	0
6	R	30/30 (100%)	0.22	0 100 100	164, 221, 257, 267	0
7	P	25/26 (96%)	0.81	5 (20%) 1 3	172, 235, 306, 326	0
7	S	26/26 (100%)	0.07	0 100 100	184, 224, 263, 283	0
All	All	6976/7546 (92%)	-0.05	119 (1%) 73 64	64, 171, 235, 326	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	176	VAL	5.1
2	I	175	GLU	4.6
2	C	221	LEU	4.4
1	G	13	ALA	4.1
2	C	175	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
2	I	176	VAL	3.6
5	L	432	LYS	3.6
3	D	666	PHE	3.5
7	P	22	DT	3.5
3	J	406	ASP	3.5
2	C	190	LYS	3.5
2	I	207	LEU	3.5
2	I	181	VAL	3.4
2	I	221	LEU	3.4
2	I	232	GLU	3.3
3	J	407	VAL	3.2
2	I	182	VAL	3.2
1	G	14	THR	3.2
2	C	174	LEU	3.2
2	C	222	LEU	3.1
3	J	1487	VAL	3.1
2	I	217	LEU	3.0
3	D	444	VAL	3.0
2	C	207	LEU	3.0
2	C	720	GLU	2.9
2	I	649	VAL	2.9
2	C	182	VAL	2.9
7	P	23	DC	2.9
1	G	56	VAL	2.9
2	C	194	VAL	2.9
3	D	256	SER	2.8
2	I	222	LEU	2.8
3	D	1486	VAL	2.8
6	O	3	DT	2.8
1	G	107	LYS	2.8
2	C	232	GLU	2.8
2	C	203	ASP	2.7
2	I	190	LYS	2.7
7	P	26	DG	2.7
3	D	446	VAL	2.6
6	O	2	DT	2.6
1	G	55	SER	2.6
2	I	183	THR	2.6
3	J	421	LEU	2.6
6	O	1	DC	2.6
2	C	231	PRO	2.6
3	J	437	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	I	250	LYS	2.5
2	I	174	LEU	2.5
2	I	416	GLY	2.5
4	K	74	PHE	2.5
1	G	22	GLU	2.5
1	G	132	LEU	2.5
4	K	84	ARG	2.5
1	G	23	PHE	2.5
3	D	1487	VAL	2.5
1	G	134	GLU	2.4
3	D	324	ALA	2.4
3	J	436	GLU	2.4
3	D	1279	GLY	2.4
1	G	25	LEU	2.4
4	E	88	GLU	2.4
7	P	25	DA	2.4
2	C	292	ARG	2.4
2	I	298	PHE	2.3
2	C	641	PRO	2.3
1	A	134	GLU	2.3
6	O	5	DA	2.3
3	J	1281	VAL	2.3
2	C	183	THR	2.3
3	J	367	ILE	2.3
3	J	1041	MET	2.3
1	G	18	ASP	2.3
3	D	1238	MET	2.3
2	I	296	GLY	2.3
3	J	1283	ILE	2.3
2	C	722	ILE	2.3
1	G	109	VAL	2.2
2	C	250	LYS	2.2
5	L	177	LYS	2.2
5	F	409	ARG	2.2
3	J	216	LEU	2.2
3	J	1486	VAL	2.2
3	D	445	ARG	2.2
2	I	219	GLN	2.2
5	L	135	THR	2.2
5	L	174	VAL	2.2
3	D	255	GLU	2.2
3	J	341	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	I	101	ILE	2.2
7	P	24	DA	2.2
1	G	15	THR	2.2
2	C	298	PHE	2.2
3	D	257	GLY	2.2
1	H	137	LYS	2.2
2	I	934	PHE	2.1
3	J	444	VAL	2.1
3	J	1040	GLY	2.1
4	K	88	GLU	2.1
1	A	204	SER	2.1
5	L	433	LEU	2.1
2	I	178	ALA	2.1
3	J	427	VAL	2.1
2	C	223	ASP	2.1
2	C	721	ARG	2.1
2	I	310	LEU	2.1
2	I	214	TYR	2.1
1	H	231	SER	2.1
1	G	162	ILE	2.1
3	J	68	PHE	2.1
1	G	102	ARG	2.1
1	G	197	LEU	2.1
5	L	178	LEU	2.1
2	I	508	ILE	2.0
2	I	648	ARG	2.0
4	E	74	PHE	2.0
5	L	409	ARG	2.0
3	D	1313	VAL	2.0
3	J	215	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
8	ZN	D	2001	1/1	0.99	0.13	-0.59	107,107,107,107	0
8	ZN	J	2001	1/1	0.97	0.12	-1.01	166,166,166,166	0
8	ZN	D	2002	1/1	0.96	0.16	-1.20	182,182,182,182	0
8	ZN	J	2002	1/1	0.93	0.07	-1.44	147,147,147,147	0
9	MG	D	2003	1/1	0.82	0.45	-	286,286,286,286	0
9	MG	J	2003	1/1	0.84	0.41	-	331,331,331,331	0

6.5 Other polymers [i](#)

There are no such residues in this entry.