



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:46 AM GMT

PDB ID : 3PRX
Title : Structure of Complement C5 in Complex with CVF and SSL7
Authors : Laursen, N.S.; Andersen, G.R.; Sottrup-Jensen, L.; Andersen, K.R.; Spillner, E.; Braren, I.
Deposited on : 2010-11-30
Resolution : 4.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

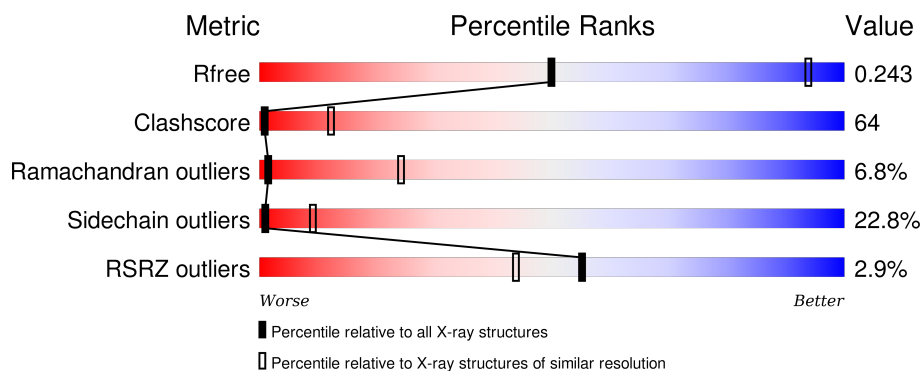
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1059 (5.00-3.60)
Clashscore	102246	1166 (5.00-3.60)
Ramachandran outliers	100387	1106 (5.00-3.60)
Sidechain outliers	100360	1089 (5.00-3.60)
RSRZ outliers	91569	1062 (5.00-3.60)

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	1676	<div> <div>24%</div> <div>50%</div> <div>21%</div> <div>• •</div> </div>
1	C	1676	<div> <div>3%</div> <div>23%</div> <div>51%</div> <div>21%</div> <div>• •</div> </div>
2	B	1642	<div> <div>23%</div> <div>38%</div> <div>13%</div> <div>26%</div> </div>
2	D	1642	<div> <div>2%</div> <div>22%</div> <div>39%</div> <div>12%</div> <div>26%</div> </div>
3	X	231	<div> <div>13%</div> <div>26%</div> <div>44%</div> <div>11%</div> <div>•</div> <div>17%</div> </div>

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Mol	Chain	Length	Quality of chain
3	Y	231	<div><div></div><div>7%</div><div>24%</div><div>45%</div><div>13%</div><div>•</div><div>17%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 48236 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 Complement C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1626	Total	C	N	O	S	0	0	0
			12874	8242	2113	2467	52			
1	C	1626	Total	C	N	O	S	0	0	0
			12874	8242	2113	2467	52			

- Molecule 2 is a protein called Cobra venom factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1215	Total	C	N	O	S	0	0	0
			9635	6143	1617	1836	39			
2	D	1215	Total	C	N	O	S	0	0	0
			9635	6143	1617	1836	39			

- Molecule 3 is a protein called Superantigen-like protein 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	191	Total	C	N	O	S	0	0	0
			1539	965	267	306	1			
3	Y	191	Total	C	N	O	S	0	0	0
			1539	965	267	306	1			

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

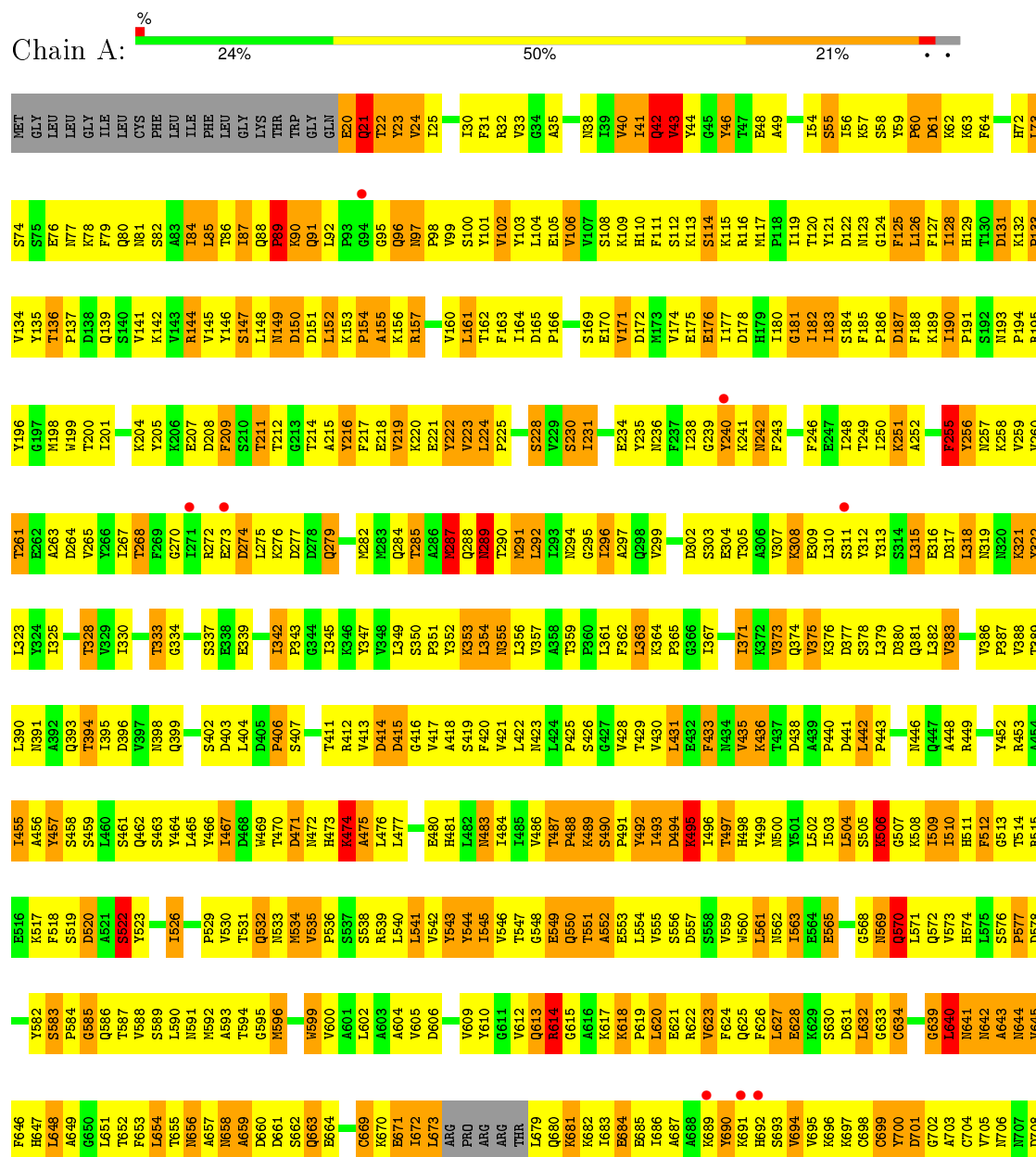
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	D	2	Total	C	N	O	0	0
			28	16	2	10		
5	D	2	Total	C	N	O	0	0
			28	16	2	10		

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: Complement C5



L1611	S1489	V1359	I1294	M1231	I1164	G1101	F1034	T971	L907	T844	V780	E709
V1612	P1490	H1360	E1296	L1232	D1166	G1102	H1035	E972	H908	V845	F781	I710
K1613	A1491	T1361	G1296	G1233	T1166	M1103	S1036	E972	H908	Y846	R782	C711
R1614	T1492	V1362	L1297	H1234	A1167	S1103	D1037	K974	I910	M847	R783	E712
R1615	P1493	T1363	T1298	L1235	L1168	L1105	P1038	K975	I911	Y848	K784	Q713
Q1616	F1494	V1364	E1299	D1236	A1171	L1106	E1041	K976	F912	R849	Q785	
V1617	V1495	V1365	Y1300	S1237	A1172	W1107	E1042	L977	S913	T850	L786	I718
L1618	I1432	H1366	S1301	S1238	D1172	L1108	K1043	S978	L914	S851	Q787	S719
L1619	S1433	K1367	L1302	V1239	L1175	V1107	Q1043	S979	E915	G852	F788	L720
M1620	S1434	T1368	L1303	E1109	M1110	Q1043	K1044	K980	F916	M853	A789	
G1621	M1435	S1369	P1240	N1241	L1111	K1047	F917	G981	T916	Q854	L790	C724
K1622	E1436	T1370	K1305	T1242	L1112	L1048	Y911	F918	L917	F855	F791	I725
E1623		S1371	G1306	G1243	Q1113	L1049	L983	L982	G919	C856	D792	L726
		E1372	L1307	T1244	L1114	L1050	L984	L983	G920	V857	S793	A727
		E1373	L1309	A1246	D1114	E1051	G985	G985	L923	K858	L794	F728
				Q1183	Q1183	E1051	E986	T795	L729	M859	T795	
		S1376		M1247	S1117	G1052	L988	T987	K925	V862	T796	
		L1379	I1313	V1248	F1184	M1053	L988	T987	T926	E863	I799	C731
		K1380	D1314	E1249	F1186	L1054	S989	T987	L927	G864	Q800	C732
		D1382	V1315	T1250	L1187	S1055	L990		R928	I865	G801	V734
		T1383	S1316	T1251	L1188	M1057		S993	V929	C866	V802	
		Q1384	Y1317	Y1253	L1189	L1056		S993	V930	T867	G803	Q737
		L1385	K1318	Y1253	Q1123	M1061		K994	P931	S868	I804	L738
		Q1386	K1319	A1254	S1191	Y1064		K995		E869	S805	R739
		T1386	K1320	L1255	A1192	S1065		K996		S870	N806	
			G1321	L1256	Y1193	S1066		T997		P871	T807	I742
			A1322	T1257	A1194	S1067		N998		V872	G808	S743
			L1323	S1258	L1195	L1066		R936		I873	I809	HIS
			K1324	L1259	S1196	S1067		S938		D874	C810	LVS
			N1325	N1260	L1197	Q1068		T1001		H875	V811	ASP
			Y1326	L1261	G1198	M1069		H1002		Q876	A812	NET
			K1327	K1262	D1199	K1070		L1003		G877	D813	GLN
			M1328	T1263	K1200	G1071		L1004		T878	V815	LEU
			T1329	I1264	T1201	S1072		S1007		K879	I816	G1Y
			D1330	Y1135	Y1135	S1073		A1008		C883	A817	L752
			K1331	Q1203	M1140	A1074		E1011		V884	K818	H753
			N1332	Q1204	S1141	T1076		L1012		R885	V819	K754
			F1333	S1207	L1142	L1077		M1013		Q886	F820	L755
			G1334	I1208	Y1143	L1078		S1014		K887	K821	T756
			R1336		L1144	T1079		V888		D822	V823	L757
			V1340	A1211	T1145	F1081		G951		G890	G890	L758
			L1341	L1212	A1146	A1082		P1017		F824	L825	P759
			L1342	K1213	F1147	L1083		Y1018		S891	L826	V760
			S1343	R1214	T1148	L1083		F1019		S892	B826	
			N1344	E1215	Y1149	R1084		Y1020		S893	M827	I765
			D1344	A1216	G1151	L1086		V1021		E894	L828	S767
			Q1278	L1217	L1152	Q1087		F1022		L895	I829	S767
			R1279	V1218	K1219	Q1088		H1023		V896	P830	V768
			Y1280	K1219	R1153	V1089		Y1024		T897		F769
			V1348	G1220	K1154	N1089		L1025		F898	V833	F770
			S1349	N1221	A1155	N1090		E1026		T899	V834	E771
			T1350	P1222	F1156	K1091		Y1027		V900	E837	S772
			G1351	P1223	D1157	Y1092		G1028		L901	I837	W773
			F1352	Y1285	L1158	Y1093		N1029		P302	I838	L774
			S1355	T1287	C1159	E1094		H1030		E904	I839	
			L1356	Q1288	P1160	Q1095		L1037		E904	Q840	
			A1357	D1289	L1161	N1096		M1032		I905		H777
			G1358	A1293	K1163	N1098		T1033		G906		L779

• Molecule 1: Complement C5

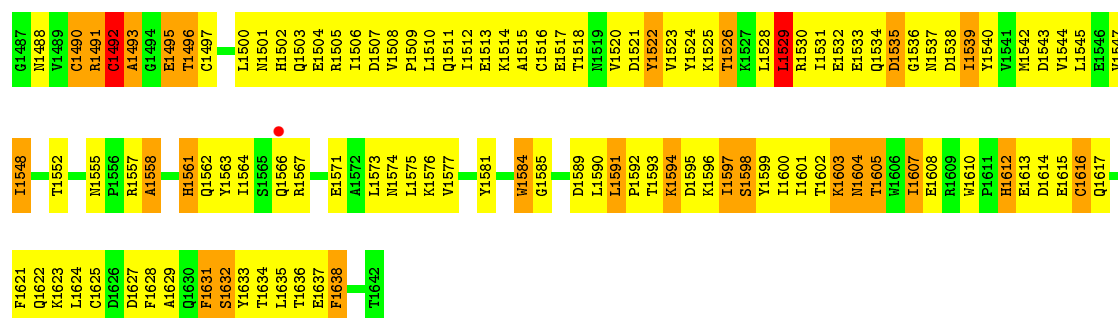




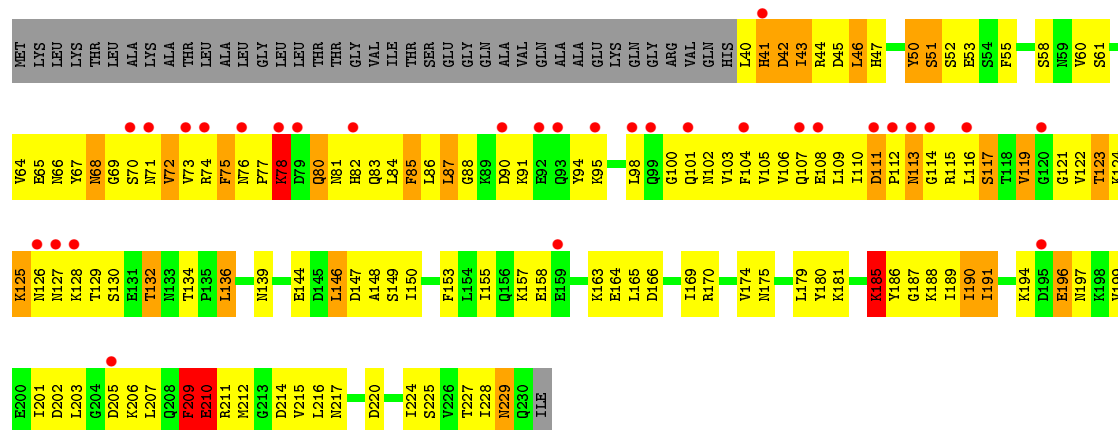




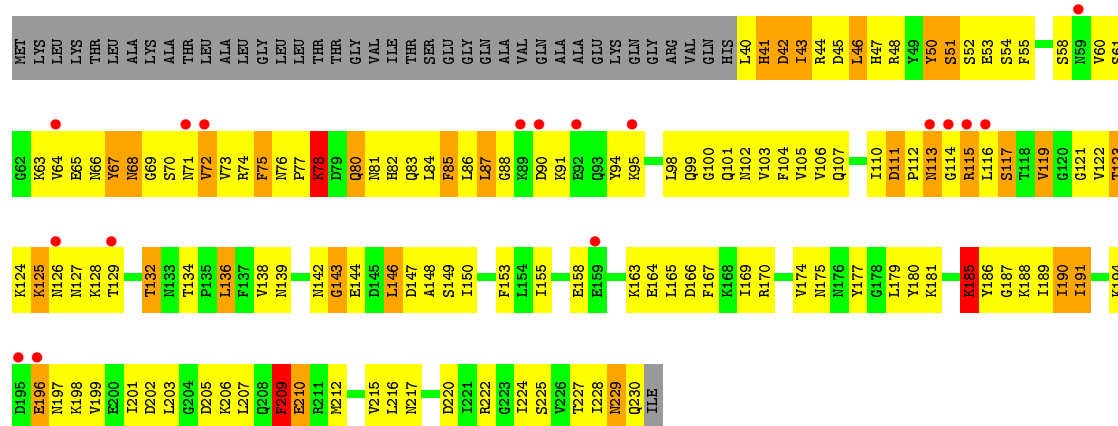
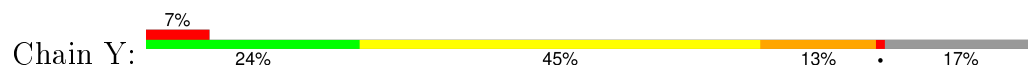
V1421	V1348	E1285	LYS	ASN	ALA	ALA	HIS	S923	S860	ARG	GLN	V538	V1471
A1422	V1349	V1286	LYS	ALA	ASP	ASP	LEU	I924	T861	ASP	ASP	V539	S472
V1423	E1350	P1287	PHE	PRO	HIS	HIS	ILE	V925	R862	ASN	LEU	K541	Q475
I1424	N1351	I1288	ASP	VAL	SER	SER	ILE	T926	R863	ASN	ARG	D542	I476
I1425	I1352	R1289	THR	LEU	TYR	TYR	THR	I927	Q864	T736	LYS	T543	K477
I1426	H1353	Y1290	GLN	SER	ALA	ALA	PRO	R928	R865	D737	CYS	C544	Y478
Y1426	R1291	R1291	GLY	GLY	ALA	ALA	SER	K929	R866	G738	CYS	R545	Y479
L1427	I1292	I1292	PRO	THR	PHE	PHE	GLY	L930	R867	T739	GLU	G546	F479
N1428	ALA	ALA	ILE	MET	THR	THR	CYS	D931	Q868	I740	ASP	T547	T480
V1430	E1294	Y1294	VAL	GLN	ASN	ASN	GLY	P932	R869	D741	VAL	L548	Y481
V1430	E1295	GLY	ARG	GLY	ARG	ARG	GLY	R933	R870	R742	MET	V549	L482
H1432	N1296	N1296	TRP	GLY	ALA	ALA	GLN	V937	R871	D743	HIS	V550	L483
H1432	A1297	A1297	LYS	ILE	SER	SER	ASN	V937	T872	T744	GLU	K551	L484
S1433	L1298	L1298	THR	GLN	SER	SER	MET	G938	R873	I745	ASN	G552	
E1434	L1299	L1299	ASP	GLY	SER	SER	ILE	G939	R874	I746	PRO	D553	K488
D1435	A1300	A1300	ALA	ALA	TRP	TRP	ARG	T940	L875	I747	PRO	N554	F490
E1436	R1301	R1301	ASN	GLU	LEU	LEU	MET	Q941	S876	R748	GLY	L555	
C1437	K1366	T1302	PHE	GLU	THR	THR	ALA	Q942	S877	T749	TYR	I556	K491
L1438	I1367	V1303	TYR	GLU	ALA	ALA	ALA	E943	R878	D750	THR	Q557	Y492
H1439	C1368	E1304	GLY	VAL	TYR	TYR	PRO	T944	R879	F751	CYS	M558	G493
	T1369	T1305	GLU	VAL	VAL	VAL	VAL	I945	R880	P752	GLU	P559	R494
I1442	R1370	THR	TYR	LEU	VAL	VAL	ILE	K946	P881	T753	LYS	G560	
K1444	Y1371	THR	THR	ASP	LYS	LYS	ALA	A947	R882		ARG	A561	R497
L1372	L1372	GLY	GLN	ASP	VAL	VAL	THR	R948	V883	L756	ALA	A562	R498
				PHE	PHE	PHE	TYR	K949	T884	L757	LYS	M563	
D1376	D1376	THR	THR	ILE	ALA	ALA	TYR	L950	V885	L758	TYR	K564	
S1377	S1377	GLN	GLN	LEU	MET	MET	LEU	D951	P886	T759	ILE	I565	Q501
T1378	T1378	ALA	ALA	VAL	ALA	ALA	ASP	R952	K826	K760	GLN	K566	I502
M1379	T1314	THR	VAL	VAL	ALA	ALA	THR	R953	R888	D761	GLU	S640	I503
V1450	T1380	ALA	ALA	ALA	LEU	LEU	THR	R954	Q889	L762	GLY	E568	V504
I1451	I1381	MET	MET	SER	MET	MET	GLU	P955	Q890	T763	ASP	G569	T505
	I1382	ALA	ALA	GLU	VAL	VAL	GLN	D956	R891	E764	ALA	D570	I507
G1454	D1383	G1319	PHE	SER	ALA	ALA	TRP	T957	E895	E765	CYS	L508	L508
S1455	I1384	T1322	GLN	LYS	GLY	GLY	GLU	E958	R896	Q769	LYS	A573	H509
V1456	S1385	M1323	ALA	THR	ILE	ILE	THR	I959	K937		ALA	R574	T511
K1457	M1386	T1324	LEU	ILE	SER	SER	LEU	E960	K937	S772	PHE	V575	P512
V1458	L1387	L1325	ALA	CYS	HIS	HIS	GLY	T961	A898	S773	LEU	V580	D513
Y1459			GLU	ASN	GLY	GLY	ILE	K962		T774	LEU	D581	L514
	F1390	L1326	TYR	ASP	ILE	ILE	ASN	I963	Q901	T775	GLU	K582	T511
	L1391	T1327	GLU	TYR	ILE	ILE	ARG	I964	E902	K776	CYS	R583	D513
	P1392	T1328	ILE	ASN	VAL	VAL	ARG	I965	A903	T777	LYS	V584	L515
D1465	D1393	Y1329	GLN	ALA	ASN	GLN	THR	Q966	L904	S778	ARG	V584	F518
E1466	A1394	M1330	MET	HIS	SER	GLY	THR	Q967	Q905	T779	ASP	Y585	R519
	E1395	A1331	PRO	THR	LEU	VAL	GLU	P968	S906	R780	ILE	Y585	F520
		Q1332	THR	ASP	ARG	ARG	VAL	P969	D907	L780	LYS	M588	V521
		L1333	HIS	HIS	TRP	TRP	ASN	VAL	G908	R781	VAL	A522	A522
		GLN	GLN	SER	ASN	ASN	GLN	ALA	V909	T782	GLY	I593	V523
		LYS	LYS	ILE	LEU	LEU	ILE	GLN	R910	S783	ARG	S594	V524
		ALA	ALA	ILE	LEU	LEU	VAL	ILE	K911	I784	ASP	Q595	Q525
		ASN	LYS	LYS	ASN	ASN	THR	ILE	K912	T785	GLU	V526	V526
		ASN	ALA	ALA	ARG	ARG	GLY	GLU	L913	T786	ASN	I598	G527
			TYR	THR	GLN	GLN	TYR	ASN	R914	K787	ALA	M599	N528
			ALA	ASN	GLN	GLN	ALA	SER	V915	V788	ARG	D600	N529
			LEU	TYR	PRO	GLN	ILE	ILE	V916	V789	GLU	T601	E530
			LEU	GLN	ASP	GLN	GLN	GLY	P917	P854	SER	I602	V531
			ALA	LYS	GLY	GLY	MET	GLY	E918	A855	ALA	E603	V532
			LEU	LYS	ALA	ALA	VAL	SER	G919	R856	LEU	K604	A533
			LYS	LYS	PHE	PHE	TYR	LYS	V920	C857	PHE	S605	L481
			TYR	TYR	LYS	LYS	LYS	LEU	Q921	S858	LEU	D606	G535
			MET	GLU	GLU	GLU	LYS	ASN	K922	P796	ALA	F607	



• Molecule 3: Superantigen-like protein 7



• Molecule 3: Superantigen-like protein 7



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	163.65Å 181.96Å 392.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.21 – 4.30 49.21 – 4.30	Depositor EDS
% Data completeness (in resolution range)	96.9 (49.21-4.30) 96.9 (49.21-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.83 (at 4.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.208 , 0.261 0.191 , 0.243	Depositor DCC
R_{free} test set	1815 reflections (2.33%)	DCC
Wilson B-factor (Å ²)	116.2	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 160.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 77966 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	48236	wwPDB-VP
Average B, all atoms (Å ²)	167.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.60	1/13151 (0.0%)	0.80	3/17841 (0.0%)
1	C	0.60	0/13151	0.80	5/17841 (0.0%)
2	B	0.53	1/9833 (0.0%)	0.73	2/13345 (0.0%)
2	D	0.54	0/9833	0.74	3/13345 (0.0%)
3	X	0.47	1/1560 (0.1%)	0.67	1/2096 (0.0%)
3	Y	0.49	0/1560	0.69	1/2096 (0.0%)
All	All	0.57	3/49088 (0.0%)	0.77	15/66564 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	210	GLU	C-N	5.35	1.46	1.34
2	B	347	PHE	CB-CG	-5.29	1.42	1.51
1	A	42	GLN	CB-CG	5.16	1.66	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	347	PHE	CB-CA-C	-7.26	95.88	110.40
2	D	347	PHE	CB-CA-C	-6.90	96.60	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	640	LEU	CA-CB-CG	6.49	130.23	115.30
1	C	640	LEU	CA-CB-CG	6.30	129.80	115.30
1	A	871	PRO	CA-N-CD	-6.16	102.87	111.50
2	D	347	PHE	CB-CG-CD2	-6.11	116.52	120.80
1	C	166	PRO	CA-N-CD	-5.83	103.33	111.50
2	D	1326	LEU	CA-CB-CG	5.60	128.18	115.30
1	C	1195	LEU	CA-CB-CG	-5.40	102.89	115.30
1	C	1256	LEU	CA-CB-CG	-5.26	103.20	115.30
2	B	1326	LEU	CA-CB-CG	5.23	127.33	115.30
3	Y	209	PHE	N-CA-C	5.17	124.97	111.00
3	X	209	PHE	N-CA-C	5.16	124.92	111.00
1	C	673	LEU	CA-CB-CG	5.12	127.07	115.30
1	A	673	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1504	GLN	Peptide
1	A	98	PRO	Peptide
1	C	1504	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	12874	0	12814	1855	0
1	C	12874	0	12814	1901	0
2	B	9635	0	9630	1082	0
2	D	9635	0	9630	1079	0
3	X	1539	0	1530	166	0
3	Y	1539	0	1530	194	0
4	A	14	0	13	1	0
4	C	14	0	13	2	0
5	B	56	0	50	6	0
5	D	56	0	50	7	0
All	All	48236	0	48074	6152	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 64.

All (6152) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1525:CYS:O	1:A:1528:VAL:HG22	1.34	1.25
3:X:207:LEU:O	3:X:207:LEU:HD12	1.32	1.24
3:Y:207:LEU:HD12	3:Y:207:LEU:O	1.32	1.23
1:C:386:VAL:H	1:C:411:THR:HG22	1.03	1.17
1:A:500:ASN:HB2	1:A:543:TYR:CE1	1.79	1.17
2:B:518:PHE:HE2	2:B:538:VAL:HB	1.12	1.15
2:D:1607:ILE:H	2:D:1607:ILE:HD12	1.10	1.15
1:C:500:ASN:HB2	1:C:543:TYR:CE1	1.80	1.14
1:C:1562:LYS:HD3	1:C:1664:LEU:HD21	1.19	1.14
1:C:535:VAL:HG23	1:C:536:PRO:HD3	1.27	1.14
2:D:261:ALA:HB2	2:D:320:VAL:HG23	1.30	1.13
1:C:1228:TRP:H	1:C:1251:THR:HG22	1.13	1.13
2:D:518:PHE:CE2	2:D:538:VAL:HB	1.83	1.13
1:A:386:VAL:H	1:A:411:THR:HG22	1.03	1.12
1:A:535:VAL:HG23	1:A:536:PRO:HD3	1.28	1.12
1:C:1525:CYS:O	1:C:1528:VAL:HG22	1.49	1.12
2:B:518:PHE:CE2	2:B:538:VAL:HB	1.84	1.11
1:A:1012:LEU:HD22	1:A:1085:VAL:HG21	1.33	1.10
1:A:25:ILE:H	1:A:655:THR:CG2	1.64	1.10
1:C:979:VAL:HG21	1:C:1326:TYR:CE1	1.86	1.10
2:D:1473:HIS:HD2	2:D:1474:PRO:HD2	1.10	1.10
2:B:1613:GLU:O	2:B:1616:CYS:HB2	1.49	1.09
2:D:829:GLN:HG3	2:D:1480:LEU:HD13	1.12	1.09
1:A:182:ILE:HG12	1:A:804:ILE:HD11	1.10	1.09
1:C:120:THR:HG22	1:C:122:ASP:H	1.17	1.09
2:D:1594:LYS:HE2	2:D:1594:LYS:HA	1.30	1.09
1:C:421:VAL:HG11	2:D:505:THR:HG22	1.35	1.08
1:A:936:ARG:HG3	1:A:936:ARG:HH11	1.15	1.08
1:A:25:ILE:H	1:A:655:THR:HG23	1.18	1.08
1:A:1228:TRP:H	1:A:1251:THR:HG22	1.13	1.08
1:A:979:VAL:HG21	1:A:1326:TYR:CE1	1.86	1.08
1:A:944:LEU:HD11	1:A:1313:ILE:HD11	1.35	1.08
1:A:353:LYS:HE3	1:A:378:SER:HA	1.19	1.07
2:D:518:PHE:HE2	2:D:538:VAL:HB	1.13	1.07
2:B:263:VAL:HG22	2:B:318:VAL:HG23	1.37	1.07
1:C:353:LYS:HE3	1:C:378:SER:HA	1.21	1.07
2:D:380:VAL:HG12	2:D:387:MET:HB3	1.29	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1068:VAL:HA	1:C:1078:LEU:HD12	1.35	1.06
2:B:261:ALA:HB2	2:B:320:VAL:HG23	1.31	1.05
1:C:591:ASN:HB3	1:C:785:GLN:HE21	1.16	1.05
1:C:936:ARG:HG3	1:C:936:ARG:HH11	1.13	1.05
2:D:954:VAL:HB	2:D:957:THR:HG21	1.38	1.05
1:A:120:THR:HG22	1:A:122:ASP:H	1.11	1.05
1:C:1560:ALA:HB2	1:C:1620:MET:HG3	1.38	1.05
1:C:127:PHE:HE2	1:C:623:VAL:HG13	1.21	1.05
2:B:1594:LYS:HA	2:B:1594:LYS:HE2	1.30	1.04
1:A:955:ARG:HG2	1:A:1350:THR:HG23	1.37	1.04
1:C:128:ILE:HG22	1:C:145:VAL:HG22	1.40	1.04
1:A:222:TYR:CE1	1:A:768:TYR:HB2	1.94	1.03
1:A:830:PRO:HG3	1:A:1483:PHE:CZ	1.94	1.03
2:D:1473:HIS:CD2	2:D:1474:PRO:HD2	1.92	1.02
1:A:1068:VAL:HA	1:A:1078:LEU:HD12	1.36	1.02
1:C:1133:LEU:H	1:C:1133:LEU:HD12	1.20	1.02
2:B:1473:HIS:HD2	2:B:1474:PRO:HD2	1.22	1.02
1:C:1623:GLU:HB2	1:C:1638:PRO:HG3	1.38	1.02
1:C:944:LEU:HD11	1:C:1313:ILE:HD11	1.36	1.02
1:A:1102:ASN:ND2	1:C:1162:VAL:HG22	1.74	1.02
2:B:965:ILE:HG13	2:B:1301:ARG:HB2	1.42	1.02
2:D:563:MET:HG3	2:D:780:LEU:HD23	1.42	1.02
1:C:830:PRO:HG3	1:C:1483:PHE:CZ	1.93	1.01
1:A:470:THR:HG22	2:B:450:THR:HG22	1.42	1.01
1:C:1620:MET:HB2	1:C:1644:TRP:HB3	1.42	1.01
2:B:954:VAL:HB	2:B:957:THR:HG21	1.40	1.01
1:C:869:GLU:O	1:C:871:PRO:HD3	1.58	1.01
2:B:829:GLN:HG3	2:B:1480:LEU:HD13	1.40	1.01
1:A:1133:LEU:H	1:A:1133:LEU:HD12	1.21	1.01
2:D:263:VAL:HG22	2:D:318:VAL:HG23	1.42	1.00
2:B:1505:ARG:HG3	2:B:1505:ARG:HH11	1.24	1.00
1:A:1562:LYS:HD2	1:A:1648:TRP:HZ2	1.26	1.00
1:A:1556:GLU:HB3	1:A:1622:LYS:HE2	1.43	1.00
2:B:469:ASN:HD22	2:B:469:ASN:C	1.65	1.00
1:C:60:PRO:HD2	1:C:61:ASP:H	1.27	1.00
1:C:182:ILE:HG12	1:C:804:ILE:HD11	1.40	1.00
2:B:380:VAL:HG12	2:B:387:MET:HB3	1.40	1.00
2:D:829:GLN:CG	2:D:1480:LEU:HD13	1.91	1.00
1:A:591:ASN:HB3	1:A:785:GLN:HE21	1.22	1.00
1:A:1623:GLU:HB2	1:A:1638:PRO:HG3	1.44	1.00
2:D:840:VAL:HG12	2:D:841:ASN:H	1.27	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1012:LEU:HD22	1:C:1085:VAL:HG21	1.41	0.99
1:A:656:ASN:OD1	1:A:658:ASN:HB3	1.62	0.99
1:A:869:GLU:O	1:A:871:PRO:HD3	1.62	0.99
1:A:373:VAL:HG11	1:A:435:VAL:HG11	1.41	0.99
2:D:482:LEU:HB3	2:D:492:VAL:HG23	1.45	0.99
1:C:1493:PHE:HD1	1:C:1494:THR:N	1.60	0.99
1:A:222:TYR:HE1	1:A:768:TYR:HB2	1.24	0.99
1:A:838:GLN:HA	1:A:901:LEU:HB2	1.45	0.99
3:X:194:LYS:HZ2	3:X:197:ASN:HB2	1.28	0.98
1:C:1585:TYR:HD1	1:C:1671:ILE:HG21	1.28	0.98
1:C:1219:LYS:NZ	1:C:1239:VAL:HG11	1.76	0.98
2:B:851:LEU:HD23	2:B:852:TYR:H	1.28	0.98
1:A:371:ILE:HG22	1:A:420:PHE:HB2	1.46	0.98
1:A:128:ILE:HG22	1:A:145:VAL:HG22	1.40	0.98
2:D:469:ASN:C	2:D:469:ASN:HD22	1.66	0.98
1:A:292:LEU:HA	1:A:297:ALA:HB2	1.44	0.98
2:D:384:PHE:CD1	2:D:400:LEU:HG	1.97	0.98
1:C:373:VAL:HG11	1:C:435:VAL:HG11	1.42	0.98
2:D:965:ILE:HG13	2:D:1301:ARG:HB2	1.46	0.98
2:B:526:VAL:HG23	2:B:530:GLU:HB3	1.46	0.97
2:B:384:PHE:CD1	2:B:400:LEU:HG	1.99	0.97
1:A:60:PRO:HD2	1:A:61:ASP:H	1.25	0.97
1:A:1525:CYS:O	1:A:1528:VAL:CG2	2.13	0.97
2:D:435:TYR:HD1	2:D:436:GLN:H	1.10	0.97
1:A:1526:LYS:O	1:A:1529:GLU:HG3	1.63	0.97
1:A:1008:ALA:HB3	1:A:1078:LEU:HD11	1.46	0.97
1:C:955:ARG:HG2	1:C:1350:THR:HG23	1.45	0.97
1:A:1365:VAL:HG22	1:A:1366:HIS:H	1.29	0.97
1:A:884:VAL:O	1:A:885:ARG:HB2	1.65	0.97
1:A:576:SER:HB3	1:A:577:PRO:HD3	1.45	0.97
1:C:1612:VAL:HB	1:C:1615:ARG:HB3	1.46	0.96
1:C:33:VAL:HG21	1:C:121:TYR:CD1	1.99	0.96
1:C:576:SER:HB3	1:C:577:PRO:HD3	1.47	0.96
1:A:1560:ALA:HB2	1:A:1620:MET:HG3	1.42	0.96
2:D:526:VAL:HG23	2:D:530:GLU:HB3	1.47	0.96
2:D:244:HIS:HB3	2:D:291:LYS:HD2	1.46	0.96
1:A:234:GLU:HG3	1:A:235:TYR:CD2	2.00	0.96
1:C:656:ASN:OD1	1:C:658:ASN:HB3	1.64	0.96
1:C:234:GLU:HG3	1:C:235:TYR:CD2	2.01	0.96
1:C:702:GLY:HA2	1:C:728:PHE:CE1	2.01	0.96
1:C:292:LEU:HA	1:C:297:ALA:HB2	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1612:VAL:HB	1:A:1615:ARG:HB3	1.46	0.96
1:C:706:ASN:ND2	1:C:709:GLU:H	1.64	0.96
1:A:500:ASN:CB	1:A:543:TYR:HE1	1.79	0.95
1:A:706:ASN:ND2	1:A:709:GLU:H	1.64	0.95
1:A:1493:PHE:HD1	1:A:1494:THR:N	1.64	0.95
1:C:500:ASN:HB2	1:C:543:TYR:HE1	1.20	0.95
2:B:237:ILE:HD11	2:B:309:LEU:HB2	1.46	0.95
1:C:838:GLN:HA	1:C:901:LEU:HB2	1.43	0.95
2:B:563:MET:HG3	2:B:780:LEU:HD23	1.47	0.95
1:A:868:SER:HA	1:A:1527:CYS:HB2	1.47	0.95
1:C:569:ASN:O	1:C:570:GLN:HB2	1.66	0.95
3:Y:194:LYS:HZ2	3:Y:197:ASN:HB2	1.29	0.94
1:A:33:VAL:HG21	1:A:121:TYR:CD1	2.02	0.94
1:A:500:ASN:HB2	1:A:543:TYR:HE1	1.17	0.94
2:D:380:VAL:HG12	2:D:387:MET:CB	1.96	0.94
1:C:706:ASN:HD22	1:C:709:GLU:H	1.02	0.94
1:C:230:SER:HB3	1:C:251:LYS:HG3	1.49	0.94
1:A:1559:TYR:OH	1:A:1591:VAL:HA	1.67	0.94
1:A:702:GLY:HA2	1:A:728:PHE:CE1	2.03	0.94
1:A:419:SER:HB2	2:B:459:ASN:HD22	1.30	0.94
1:A:706:ASN:HD22	1:A:709:GLU:H	1.01	0.94
2:D:829:GLN:HE22	2:D:883:VAL:HG13	1.33	0.94
2:D:851:LEU:HD23	2:D:852:TYR:H	1.31	0.94
3:X:81:ASN:O	3:X:115:ARG:HB2	1.68	0.94
1:C:1124:TYR:HA	1:C:1465:ASN:OD1	1.66	0.94
1:A:430:VAL:HG11	1:A:453:ARG:HH21	1.33	0.94
1:A:24:VAL:HA	1:A:655:THR:OG1	1.66	0.94
1:C:1061:ASN:HB2	1:C:1065:SER:O	1.68	0.94
2:B:840:VAL:HG12	2:B:841:ASN:H	1.30	0.94
2:B:1528:LEU:HD23	2:B:1576:LYS:O	1.68	0.93
1:A:1219:LYS:NZ	1:A:1239:VAL:HG11	1.83	0.93
3:Y:81:ASN:O	3:Y:115:ARG:HB2	1.68	0.93
1:C:596:MET:H	1:C:782:ARG:HH11	1.03	0.93
1:A:1490:PRO:HB3	1:A:1510:SER:HB2	1.50	0.93
1:C:830:PRO:HG3	1:C:1483:PHE:HZ	1.33	0.93
1:A:606:ASP:O	1:A:609:VAL:HG23	1.68	0.93
1:C:884:VAL:O	1:C:885:ARG:HB2	1.65	0.93
1:A:596:MET:H	1:A:782:ARG:HH11	1.09	0.93
1:C:357:VAL:HA	1:C:672:ILE:HG21	1.50	0.92
1:A:569:ASN:O	1:A:570:GLN:HB2	1.65	0.92
1:A:87:ILE:HD13	1:A:87:ILE:N	1.84	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:HIS:HB3	2:B:291:LYS:HD2	1.48	0.92
2:B:1473:HIS:CD2	2:B:1474:PRO:HD2	2.03	0.92
2:D:521:VAL:HG13	2:D:535:SER:HB3	1.52	0.92
1:C:135:TYR:HE1	1:C:141:VAL:HA	1.35	0.92
2:B:482:LEU:HB3	2:B:492:VAL:HG23	1.48	0.92
1:A:1012:LEU:CD2	1:A:1085:VAL:HG21	2.00	0.92
1:C:1556:GLU:HB3	1:C:1622:LYS:HE2	1.51	0.91
1:A:944:LEU:CD1	1:A:1313:ILE:HD11	2.00	0.91
1:A:353:LYS:CE	1:A:378:SER:HA	2.01	0.91
2:B:563:MET:HE2	2:B:564:LYS:H	1.35	0.91
1:A:849:ARG:HG2	1:A:849:ARG:HH11	1.36	0.91
3:Y:166:ASP:CG	3:Y:207:LEU:CD2	2.38	0.91
1:A:753:HIS:O	1:A:754:MET:HB3	1.68	0.91
3:X:50:TYR:CE2	3:X:170:ARG:HD2	2.06	0.91
1:A:1562:LYS:HD2	1:A:1648:TRP:CZ2	2.05	0.91
1:C:1008:ALA:HB3	1:C:1078:LEU:HD11	1.52	0.91
1:A:135:TYR:HE1	1:A:141:VAL:HA	1.34	0.91
1:C:553:GLU:HA	1:C:658:ASN:HB2	1.53	0.91
2:D:469:ASN:CG	2:D:472:SER:HB2	1.92	0.91
2:D:1528:LEU:HD23	2:D:1576:LYS:O	1.70	0.91
1:C:1490:PRO:HB3	1:C:1510:SER:HB2	1.53	0.91
2:B:1341:ASN:ND2	2:B:1342:LYS:HG2	1.86	0.90
1:C:849:ARG:HH11	1:C:849:ARG:HG2	1.35	0.90
3:Y:170:ARG:HH22	3:Y:206:LYS:HA	1.37	0.90
1:C:1559:TYR:OH	1:C:1591:VAL:HA	1.71	0.90
1:A:33:VAL:HG21	1:A:121:TYR:CE1	2.06	0.90
1:A:230:SER:HB3	1:A:251:LYS:HG3	1.50	0.90
2:D:1590:LEU:HD23	2:D:1591:LEU:H	1.36	0.90
1:C:430:VAL:HG11	1:C:453:ARG:HH21	1.36	0.90
2:B:435:TYR:HD1	2:B:436:GLN:H	1.11	0.90
2:B:221:LEU:HD11	2:B:753:LYS:HG2	1.52	0.90
1:C:25:ILE:H	1:C:655:THR:HG23	1.35	0.90
1:A:1232:LEU:HD11	1:A:1233:GLN:HE21	1.36	0.90
1:A:315:LEU:HD13	1:A:317:ASP:HB2	1.53	0.90
1:A:481:HIS:CE1	1:A:529:PRO:HB3	2.06	0.90
1:C:315:LEU:HD13	1:C:317:ASP:HB2	1.54	0.90
2:D:221:LEU:HD11	2:D:753:LYS:HG2	1.53	0.90
2:B:120:LEU:HD12	2:B:121:LEU:H	1.37	0.90
3:Y:50:TYR:CE2	3:Y:170:ARG:HD2	2.06	0.89
1:A:502:LEU:HB2	1:A:541:LEU:CD2	2.01	0.89
1:A:1068:VAL:HG21	1:A:1124:TYR:CD1	2.06	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:584:PRO:HB3	1:C:792:ASP:HA	1.54	0.89
1:C:1232:LEU:HD11	1:C:1233:GLN:HE21	1.35	0.89
2:D:1273:LEU:HB2	2:D:1319:GLY:HA3	1.52	0.89
2:B:469:ASN:CG	2:B:472:SER:HB2	1.92	0.89
2:B:1273:LEU:HB2	2:B:1319:GLY:HA3	1.53	0.89
1:A:1404:ALA:HB1	1:A:1493:PHE:CE2	2.08	0.89
1:C:753:HIS:O	1:C:754:MET:HB3	1.72	0.89
1:C:500:ASN:CB	1:C:543:TYR:HE1	1.83	0.89
1:C:60:PRO:CD	1:C:61:ASP:H	1.86	0.89
1:C:576:SER:HB2	1:C:589:SER:HB2	1.52	0.89
1:A:576:SER:HB2	1:A:589:SER:HB2	1.54	0.89
1:C:481:HIS:CE1	1:C:529:PRO:HB3	2.06	0.89
1:A:60:PRO:CD	1:A:61:ASP:H	1.85	0.89
2:D:237:ILE:HD11	2:D:309:LEU:HB2	1.55	0.89
2:B:416:ASN:HA	2:B:425:GLN:HE22	1.37	0.89
1:C:59:TYR:CG	1:C:60:PRO:HD3	2.07	0.89
1:A:31:PHE:HB2	1:A:119:ILE:HG22	1.53	0.88
1:A:618:LYS:H	1:A:619:PRO:HD3	1.38	0.88
1:C:23:TYR:CD1	1:C:655:THR:HB	2.09	0.88
1:A:1576:LYS:HG2	1:A:1601:ILE:HG22	1.53	0.88
1:A:59:TYR:CG	1:A:60:PRO:HD3	2.08	0.88
1:A:980:LYS:HD3	1:A:986:GLU:HA	1.55	0.88
1:A:830:PRO:HG3	1:A:1483:PHE:HZ	1.36	0.88
1:C:511:HIS:CE1	3:Y:149:SER:OG	2.26	0.88
3:X:77:PRO:HD2	3:X:80:GLN:O	1.74	0.88
2:D:519:ARG:NH1	2:D:608:GLY:HA3	1.89	0.88
2:B:829:GLN:HE22	2:B:883:VAL:HG13	1.36	0.88
2:B:455:LYS:O	2:B:458:ASP:HB2	1.72	0.88
3:Y:77:PRO:HD2	3:Y:80:GLN:O	1.73	0.88
1:C:386:VAL:N	1:C:411:THR:HG22	1.88	0.88
1:C:532:GLN:HE21	1:C:568:GLY:HA2	1.38	0.88
2:D:750:ASP:OD1	2:D:752:PRO:HD3	1.73	0.87
2:D:120:LEU:HD12	2:D:121:LEU:H	1.38	0.87
1:A:386:VAL:N	1:A:411:THR:HG22	1.88	0.87
1:A:1124:TYR:HA	1:A:1465:ASN:OD1	1.74	0.87
1:C:31:PHE:HB2	1:C:119:ILE:HG22	1.54	0.87
1:C:606:ASP:O	1:C:609:VAL:HG23	1.72	0.87
1:A:467:ILE:HG22	1:A:486:VAL:HG22	1.55	0.87
1:C:78:LYS:NZ	3:Y:144:GLU:HA	1.88	0.87
2:B:1590:LEU:HD23	2:B:1591:LEU:H	1.36	0.87
2:D:1607:ILE:H	2:D:1607:ILE:CD1	1.81	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1473:HIS:HB3	2:D:1476:LYS:HB2	1.55	0.87
1:A:120:THR:HG22	1:A:122:ASP:N	1.88	0.87
1:C:944:LEU:CD1	1:C:1313:ILE:HD11	2.05	0.87
1:A:584:PRO:HB3	1:A:792:ASP:HA	1.57	0.87
3:Y:58:SER:HB3	3:Y:102:ASN:ND2	1.90	0.87
2:B:494:ARG:HG3	2:B:494:ARG:HH11	1.39	0.87
3:Y:166:ASP:CG	3:Y:207:LEU:HD21	1.95	0.87
1:A:1068:VAL:HG13	1:A:1069:TRP:H	1.39	0.87
1:C:33:VAL:HG21	1:C:121:TYR:CE1	2.09	0.87
1:C:502:LEU:HB2	1:C:541:LEU:CD2	2.05	0.87
2:B:347:PHE:O	2:B:350:THR:HG22	1.75	0.87
1:A:1365:VAL:HG22	1:A:1366:HIS:N	1.84	0.87
1:C:353:LYS:CE	1:C:378:SER:HA	2.03	0.86
2:D:455:LYS:O	2:D:458:ASP:HB2	1.74	0.86
1:C:1585:TYR:CD1	1:C:1671:ILE:HG21	2.10	0.86
1:C:934:VAL:HG22	1:C:1366:HIS:CD2	2.10	0.86
1:A:182:ILE:HG12	1:A:804:ILE:CD1	2.02	0.86
1:C:1068:VAL:HG13	1:C:1069:TRP:H	1.40	0.86
1:A:1560:ALA:CB	1:A:1620:MET:HG3	2.05	0.86
1:C:572:GLN:HB2	1:C:593:ALA:HB3	1.56	0.86
2:B:750:ASP:OD1	2:B:752:PRO:HD3	1.75	0.86
1:C:618:LYS:H	1:C:619:PRO:HD3	1.38	0.86
1:A:855:PHE:HA	2:B:904:LEU:HD11	1.57	0.86
3:X:166:ASP:CG	3:X:207:LEU:CD2	2.42	0.86
2:D:416:ASN:HA	2:D:425:GLN:HE22	1.40	0.86
1:C:599:TRP:O	1:C:803:GLY:HA2	1.74	0.86
1:C:1562:LYS:HD2	1:C:1648:TRP:CZ2	2.11	0.86
1:A:936:ARG:HG3	1:A:936:ARG:NH1	1.89	0.86
1:C:127:PHE:CE2	1:C:623:VAL:HG13	2.08	0.86
1:A:1546:GLU:O	1:A:1667:PHE:HZ	1.57	0.86
1:A:618:LYS:N	1:A:619:PRO:CD	2.38	0.86
1:C:463:SER:HB3	1:C:491:PRO:HA	1.57	0.86
1:C:1560:ALA:CB	1:C:1620:MET:HG3	2.04	0.86
1:C:618:LYS:N	1:C:619:PRO:CD	2.38	0.86
1:C:120:THR:HG22	1:C:122:ASP:N	1.90	0.86
1:C:1315:VAL:HG12	1:C:1324:HIS:O	1.76	0.86
1:A:23:TYR:CD1	1:A:23:TYR:N	2.40	0.86
1:C:504:LEU:CD1	1:C:509:ILE:HG23	2.06	0.86
1:C:1404:ALA:HB1	1:C:1493:PHE:CE2	2.10	0.86
2:D:1341:ASN:ND2	2:D:1342:LYS:HG2	1.91	0.86
1:A:24:VAL:HG21	1:A:554:LEU:HD11	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:ILE:HD12	1:C:201:ILE:HG22	1.57	0.86
2:B:1444:LYS:HE2	2:B:1447:GLU:HA	1.58	0.86
2:B:850:LEU:HB2	2:B:882:PHE:HE1	1.41	0.86
2:B:151:ASP:HB2	2:B:794:PHE:HZ	1.38	0.86
2:B:519:ARG:NH1	2:B:608:GLY:HA3	1.91	0.86
1:C:1219:LYS:HZ1	1:C:1239:VAL:HG11	1.40	0.85
1:C:1068:VAL:HG21	1:C:1124:TYR:CD1	2.10	0.85
1:C:696:LYS:HZ3	1:C:759:PRO:HD2	1.38	0.85
3:X:58:SER:HB3	3:X:102:ASN:ND2	1.91	0.85
3:Y:207:LEU:CD1	3:Y:207:LEU:O	2.22	0.85
1:C:936:ARG:HH11	1:C:936:ARG:CG	1.89	0.85
2:D:850:LEU:HB2	2:D:882:PHE:CE1	2.11	0.85
2:B:1590:LEU:HD23	2:B:1591:LEU:N	1.91	0.85
2:D:151:ASP:HB2	2:D:794:PHE:HZ	1.39	0.85
1:C:1531:ASP:OD2	1:C:1531:ASP:C	2.14	0.85
3:X:170:ARG:HD3	3:X:203:LEU:HD23	1.59	0.85
2:D:518:PHE:HE2	2:D:538:VAL:CB	1.88	0.85
1:C:1576:LYS:HG2	1:C:1601:ILE:HG22	1.59	0.85
1:A:1333:PHE:O	1:A:1334:LEU:HB2	1.77	0.85
1:A:641:ASN:ND2	1:A:643:ALA:HB3	1.90	0.85
2:B:850:LEU:HB2	2:B:882:PHE:CE1	2.12	0.85
1:C:371:ILE:HG22	1:C:420:PHE:HB2	1.56	0.85
1:A:1003:LEU:HD11	1:A:1286:SER:HA	1.59	0.85
1:A:1315:VAL:HG12	1:A:1324:HIS:O	1.76	0.85
1:A:127:PHE:HE2	1:A:623:VAL:HG13	1.40	0.85
1:A:315:LEU:HD12	1:A:318:LEU:HG	1.59	0.85
1:C:467:ILE:HG22	1:C:486:VAL:HG22	1.59	0.85
1:C:222:TYR:CE1	1:C:768:TYR:HB2	2.12	0.85
2:D:161:VAL:HG21	2:D:180:LEU:HD21	1.58	0.85
1:C:1365:VAL:HG22	1:C:1366:HIS:H	1.40	0.85
1:C:1278:GLN:OE1	1:C:1283:GLY:HA2	1.76	0.85
2:D:326:SER:HB2	2:D:819:GLN:HG3	1.59	0.85
2:B:518:PHE:HE2	2:B:538:VAL:CB	1.89	0.84
2:B:380:VAL:HG12	2:B:387:MET:CB	2.06	0.84
1:A:145:VAL:HB	1:A:183:ILE:HG13	1.58	0.84
1:C:315:LEU:HD12	1:C:318:LEU:HG	1.59	0.84
2:B:1512:ILE:O	2:B:1516:CYS:HB2	1.77	0.84
1:A:391:ASN:HD21	1:A:406:PRO:HG3	1.41	0.84
1:C:641:ASN:ND2	1:C:643:ALA:HB3	1.93	0.84
1:A:284:GLN:HG2	1:A:310:LEU:HD21	1.59	0.84
1:C:614:ARG:HD2	1:C:615:GLY:N	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:ARG:HD2	1:A:615:GLY:N	1.92	0.84
1:A:696:LYS:HZ3	1:A:759:PRO:HD2	1.42	0.84
2:B:481:TYR:O	2:B:481:TYR:HD2	1.61	0.84
2:B:175:SER:H	2:B:1300:ALA:HB2	1.42	0.84
1:C:133:PRO:HD2	1:C:609:VAL:HG11	1.60	0.84
1:A:1123:GLN:HA	1:A:1123:GLN:HE21	1.42	0.84
2:D:933:ARG:HG3	2:D:933:ARG:HH11	1.40	0.84
2:D:1444:LYS:HE2	2:D:1447:GLU:HA	1.59	0.84
1:C:1575:VAL:HB	1:C:1602:LYS:O	1.76	0.83
1:A:191:PRO:HD2	1:A:194:PRO:HB3	1.60	0.83
1:A:1278:GLN:OE1	1:A:1283:GLY:HA2	1.78	0.83
1:C:145:VAL:HB	1:C:183:ILE:HG13	1.60	0.83
2:B:925:VAL:HG22	2:B:1326:LEU:HD23	1.60	0.83
3:X:207:LEU:CD1	3:X:207:LEU:O	2.22	0.83
1:C:1526:LYS:O	1:C:1529:GLU:HB2	1.78	0.83
2:D:1590:LEU:HD23	2:D:1591:LEU:N	1.91	0.83
2:D:925:VAL:HG22	2:D:1326:LEU:HD23	1.59	0.83
1:C:980:LYS:HD3	1:C:986:GLU:HA	1.60	0.83
2:D:563:MET:HE2	2:D:564:LYS:H	1.39	0.83
2:D:824:VAL:HG21	2:D:830:VAL:HG11	1.60	0.83
1:A:1061:ASN:HB2	1:A:1065:SER:O	1.77	0.83
1:A:1571:GLU:HB2	1:A:1574:PHE:CZ	2.13	0.83
2:D:847:ARG:HG3	2:D:869:GLN:HG2	1.60	0.83
2:D:175:SER:H	2:D:1300:ALA:HB2	1.41	0.83
2:B:494:ARG:NH1	2:B:494:ARG:HG3	1.91	0.83
2:D:347:PHE:O	2:D:350:THR:HG22	1.78	0.83
1:C:284:GLN:HG2	1:C:310:LEU:HD21	1.61	0.83
2:D:494:ARG:HG3	2:D:494:ARG:HH11	1.43	0.83
2:D:481:TYR:HE1	2:D:506:MET:SD	2.02	0.83
1:C:618:LYS:N	1:C:619:PRO:HD3	1.93	0.83
1:A:1056:ILE:HD11	1:A:1066:TYR:CE2	2.14	0.83
1:A:1228:TRP:N	1:A:1251:THR:HG22	1.94	0.83
1:C:1623:GLU:HB2	1:C:1638:PRO:CG	2.07	0.83
1:A:895:LEU:HD12	1:A:896:VAL:H	1.42	0.83
2:D:1500:LEU:HD12	2:D:1501:ASN:H	1.44	0.83
1:A:572:GLN:HB2	1:A:593:ALA:HB3	1.60	0.83
2:D:44:GLU:HG2	2:D:82:LEU:HB2	1.61	0.83
2:D:563:MET:HG3	2:D:780:LEU:CD2	2.09	0.82
2:B:1331:ALA:O	2:B:1332:GLN:HB3	1.79	0.82
1:A:1066:TYR:H	1:A:1079:THR:HG23	1.44	0.82
3:Y:86:LEU:HG	3:Y:91:LYS:HB2	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:ASN:HD21	1:C:406:PRO:HG3	1.42	0.82
1:C:493:ILE:HG23	1:C:495:LYS:H	1.43	0.82
1:C:1573:VAL:HB	1:C:1603:LYS:HD3	1.60	0.82
1:A:1153:ARG:HD2	1:A:1197:LEU:HB3	1.58	0.82
1:A:936:ARG:HH11	1:A:936:ARG:CG	1.92	0.82
1:C:824:PHE:HD2	1:C:824:PHE:H	1.27	0.82
1:C:250:ILE:HD11	1:C:265:VAL:HG11	1.61	0.82
3:X:70:SER:HB3	3:X:91:LYS:HE3	1.61	0.82
1:A:1219:LYS:HZ1	1:A:1239:VAL:HG11	1.44	0.82
1:A:1546:GLU:HG2	1:A:1663:ASN:ND2	1.95	0.82
2:B:521:VAL:HG13	2:B:535:SER:HB3	1.60	0.82
1:C:1123:GLN:HE21	1:C:1123:GLN:HA	1.45	0.82
2:D:481:TYR:O	2:D:481:TYR:HD2	1.62	0.82
3:X:86:LEU:HG	3:X:91:LYS:HB2	1.59	0.82
2:B:326:SER:HB2	2:B:819:GLN:HG3	1.60	0.82
1:C:500:ASN:HB2	1:C:543:TYR:CD1	2.14	0.82
2:D:168:PRO:HG3	2:D:196:THR:C	2.00	0.82
1:A:1585:TYR:CE2	1:A:1586:LYS:HB3	2.15	0.82
1:A:1570:VAL:HA	1:A:1574:PHE:O	1.80	0.82
1:A:1590:ALA:HB1	1:A:1635:TYR:CE1	2.14	0.82
2:D:850:LEU:HB2	2:D:882:PHE:HE1	1.41	0.82
1:A:546:VAL:O	1:A:553:GLU:HB3	1.78	0.82
1:A:171:VAL:HG12	1:A:172:ASP:N	1.93	0.81
2:D:250:ARG:HG2	2:D:256:GLU:HA	1.61	0.81
1:C:1582:LEU:HD21	1:C:1616:GLN:HG2	1.62	0.81
1:C:1228:TRP:N	1:C:1251:THR:HG22	1.94	0.81
2:B:200:VAL:HG12	2:B:211:THR:OG1	1.80	0.81
1:A:1575:VAL:HB	1:A:1602:LYS:O	1.79	0.81
1:A:1488:LEU:O	1:A:1488:LEU:HD12	1.80	0.81
1:A:25:ILE:N	1:A:655:THR:CG2	2.44	0.81
1:A:1582:LEU:HD21	1:A:1616:GLN:HG2	1.62	0.81
2:B:435:TYR:HD1	2:B:436:GLN:N	1.78	0.81
1:C:696:LYS:HZ3	1:C:759:PRO:CD	1.93	0.81
2:B:933:ARG:HH11	2:B:933:ARG:HG3	1.44	0.81
1:C:1218:VAL:HG12	1:C:1219:LYS:H	1.46	0.81
1:C:1049:LEU:HD11	1:C:1089:VAL:HG13	1.63	0.81
1:C:1020:TYR:HE1	1:C:1295:GLU:HG3	1.45	0.81
2:B:168:PRO:HG3	2:B:196:THR:C	2.01	0.81
1:A:500:ASN:HB2	1:A:543:TYR:CD1	2.16	0.81
2:D:1607:ILE:N	2:D:1607:ILE:HD12	1.94	0.81
1:A:1576:LYS:HG2	1:A:1601:ILE:CG2	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:435:TYR:HD1	2:D:436:GLN:N	1.78	0.81
2:B:795:THR:HG22	2:B:796:PRO:HD2	1.61	0.81
1:A:618:LYS:N	1:A:619:PRO:HD3	1.94	0.81
2:B:322:THR:HG22	2:B:327:ASP:O	1.80	0.81
2:D:961:THR:HG22	2:D:1327:THR:HG23	1.63	0.81
1:A:123:ASN:HB3	1:A:209:PHE:CD1	2.16	0.81
1:A:23:TYR:CD1	1:A:655:THR:HB	2.16	0.81
1:C:1531:ASP:O	1:C:1531:ASP:OD2	1.97	0.81
2:D:954:VAL:HG12	2:D:955:PRO:HD2	1.63	0.81
1:C:1067:SER:HA	1:C:1074:ALA:HA	1.63	0.81
1:A:267:ILE:CD1	1:A:299:VAL:HG11	2.11	0.81
1:C:87:ILE:N	1:C:87:ILE:HD13	1.96	0.81
2:D:795:THR:HG22	2:D:796:PRO:HD2	1.63	0.81
1:C:1199:ASP:OD1	1:C:1201:THR:HG23	1.81	0.81
1:C:1620:MET:HB2	1:C:1644:TRP:CB	2.10	0.80
1:C:1623:GLU:CB	1:C:1638:PRO:HG3	2.11	0.80
2:B:469:ASN:HD22	2:B:470:ALA:N	1.79	0.80
1:C:523:TYR:CE1	2:D:359:PRO:HG2	2.16	0.80
1:C:149:ASN:HD22	1:C:149:ASN:H	1.26	0.80
1:A:22:THR:HG21	1:A:657:ALA:HB2	1.62	0.80
1:A:504:LEU:CD1	1:A:509:ILE:HG23	2.11	0.80
1:C:617:LYS:HD2	1:C:622:ARG:HH21	1.46	0.80
3:Y:70:SER:HB3	3:Y:91:LYS:HE3	1.61	0.80
3:X:166:ASP:CG	3:X:207:LEU:HD21	2.01	0.80
1:A:584:PRO:HD3	1:A:820:PHE:HB2	1.63	0.80
1:C:584:PRO:HD3	1:C:820:PHE:HB2	1.63	0.80
1:A:1190:ILE:HG12	1:A:1253:TYR:CD1	2.17	0.80
2:D:69:PHE:CE2	2:D:71:THR:HB	2.16	0.80
2:B:824:VAL:HG21	2:B:830:VAL:HG11	1.62	0.80
1:A:1573:VAL:HB	1:A:1603:LYS:HD3	1.63	0.80
1:A:1232:LEU:HG	1:A:1233:GLN:HG3	1.63	0.80
1:A:1213:LYS:HG2	1:A:1266:TYR:HE2	1.45	0.80
1:C:1333:PHE:O	1:C:1334:LEU:HB2	1.79	0.80
1:C:1152:ILE:CG2	1:C:1168:LEU:HD21	2.10	0.80
2:B:161:VAL:HG21	2:B:180:LEU:HD21	1.62	0.80
2:D:344:GLN:HE21	2:D:344:GLN:HA	1.46	0.80
1:C:1571:GLU:HB2	1:C:1574:PHE:CZ	2.16	0.80
2:B:1341:ASN:HD22	2:B:1342:LYS:HG2	1.44	0.80
1:C:371:ILE:HD11	1:C:433:PHE:CE2	2.16	0.80
1:C:492:TYR:CD2	1:C:493:ILE:N	2.50	0.80
2:B:69:PHE:CE2	2:B:71:THR:HB	2.17	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1067:SER:HB3	1:C:1072:GLY:O	1.81	0.80
2:B:1562:GLN:HE22	2:B:1596:LYS:NZ	1.78	0.80
2:B:44:GLU:HG2	2:B:82:LEU:HB2	1.63	0.80
1:A:243:PHE:CE1	1:A:316:GLU:HB3	2.17	0.80
1:C:243:PHE:CE1	1:C:316:GLU:HB3	2.16	0.80
1:A:599:TRP:O	1:A:803:GLY:HA2	1.81	0.80
1:A:796:THR:HG23	1:A:818:LYS:HB3	1.64	0.80
1:A:706:ASN:HD22	1:A:709:GLU:N	1.79	0.80
3:Y:165:LEU:O	3:Y:169:ILE:HG12	1.82	0.80
3:Y:188:LYS:HD3	3:Y:202:ASP:HA	1.64	0.80
1:C:1570:VAL:HA	1:C:1574:PHE:O	1.82	0.79
1:C:1066:TYR:H	1:C:1079:THR:HG23	1.46	0.79
2:D:344:GLN:NE2	2:D:344:GLN:HA	1.96	0.79
2:D:1383:ASP:HB3	2:D:1457:LYS:HB2	1.63	0.79
2:D:818:LEU:HB3	2:D:911:LYS:HD2	1.63	0.79
1:A:1546:GLU:O	1:A:1667:PHE:CZ	2.35	0.79
2:B:151:ASP:HB2	2:B:794:PHE:CZ	2.18	0.79
3:X:125:LYS:HA	3:X:127:ASN:N	1.98	0.79
1:A:442:LEU:HD23	1:A:443:PRO:HD2	1.64	0.79
1:C:1341:LEU:HB2	1:C:1342:LEU:HD23	1.63	0.79
2:B:1284:ARG:HD2	2:B:1285:GLU:H	1.45	0.79
2:D:557:GLN:HA	2:D:557:GLN:OE1	1.82	0.79
1:C:1232:LEU:HG	1:C:1233:GLN:HG3	1.62	0.79
2:D:1341:ASN:HD22	2:D:1342:LYS:HG2	1.48	0.79
2:B:137:TYR:CZ	2:B:143:VAL:HG22	2.17	0.79
1:C:799:ILE:HG22	1:C:815:VAL:O	1.82	0.79
1:C:1562:LYS:HD3	1:C:1664:LEU:CD2	2.10	0.79
1:A:696:LYS:NZ	1:A:759:PRO:HD2	1.98	0.79
2:B:218:LYS:HB3	2:B:822:TYR:CD2	2.17	0.79
1:C:135:TYR:CE1	1:C:141:VAL:HA	2.17	0.79
2:B:481:TYR:HE1	2:B:506:MET:SD	2.05	0.79
3:X:170:ARG:HH22	3:X:206:LYS:HA	1.47	0.79
1:A:78:LYS:NZ	3:X:144:GLU:HA	1.98	0.79
1:C:1153:ARG:HD2	1:C:1197:LEU:HB3	1.64	0.79
1:C:1012:LEU:CD2	1:C:1085:VAL:HG21	2.12	0.79
1:C:706:ASN:HD22	1:C:709:GLU:N	1.79	0.79
2:D:165:PHE:CZ	2:D:199:ILE:HD11	2.18	0.79
1:C:191:PRO:HD2	1:C:194:PRO:HB3	1.64	0.79
1:A:532:GLN:HA	1:A:532:GLN:OE1	1.83	0.79
1:A:830:PRO:CG	1:A:1483:PHE:HZ	1.95	0.79
2:D:872:ILE:HG22	2:D:878:ARG:HG3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:934:VAL:HG22	1:A:1366:HIS:CD2	2.17	0.79
2:D:1284:ARG:HD2	2:D:1285:GLU:H	1.46	0.79
1:C:470:THR:HB	2:D:450:THR:O	1.81	0.79
2:B:872:ILE:HG22	2:B:878:ARG:HG3	1.65	0.79
1:C:765:ILE:O	1:C:765:ILE:HD12	1.82	0.79
2:B:961:THR:HG22	2:B:1327:THR:HG23	1.64	0.79
1:A:371:ILE:HD11	1:A:433:PHE:CE2	2.18	0.78
1:C:1031:TRP:CZ2	1:C:1042:LYS:HG3	2.17	0.78
2:D:1505:ARG:CZ	2:D:1623:LYS:HZ1	1.95	0.78
1:A:824:PHE:HD2	1:A:824:PHE:H	1.30	0.78
1:A:1497:GLU:OE1	1:A:1500:ARG:HD3	1.83	0.78
1:A:1133:LEU:CD1	1:A:1133:LEU:H	1.96	0.78
1:C:696:LYS:NZ	1:C:759:PRO:HD2	1.97	0.78
1:A:1573:VAL:CG1	1:A:1603:LYS:HD3	2.13	0.78
2:B:847:ARG:HG3	2:B:869:GLN:HG2	1.64	0.78
1:C:20:GLU:C	1:C:21:GLN:HG3	2.03	0.78
2:D:1349:VAL:HA	2:D:1364:MET:O	1.83	0.78
1:C:111:PHE:CE2	1:C:113:LYS:HB2	2.18	0.78
1:C:1622:LYS:NZ	1:C:1642:LEU:HD23	1.98	0.78
1:A:830:PRO:HG3	1:A:1483:PHE:CE2	2.18	0.78
1:A:492:TYR:CD2	1:A:493:ILE:N	2.50	0.78
2:D:494:ARG:HG3	2:D:494:ARG:NH1	1.97	0.78
1:A:1573:VAL:O	1:A:1603:LYS:HG2	1.84	0.78
2:B:265:PHE:CD2	2:B:294:LEU:HB2	2.18	0.78
1:A:471:ASP:OD2	1:A:474:LYS:HB3	1.83	0.78
1:A:1623:GLU:HB2	1:A:1638:PRO:CG	2.12	0.78
1:A:617:LYS:HD2	1:A:622:ARG:HH21	1.49	0.78
1:C:1108:VAL:HG21	1:C:1167:ALA:HB2	1.65	0.78
1:C:23:TYR:HD1	1:C:23:TYR:N	1.81	0.78
1:A:1049:LEU:HD11	1:A:1089:VAL:HG13	1.65	0.78
1:A:804:ILE:HG22	1:A:809:ILE:HG13	1.65	0.78
2:B:563:MET:HG3	2:B:780:LEU:CD2	2.13	0.78
1:A:1190:ILE:HG12	1:A:1253:TYR:CE1	2.18	0.78
3:Y:166:ASP:OD1	3:Y:207:LEU:HD23	1.82	0.78
2:D:385:HIS:CE1	3:Y:142:ASN:HD21	2.01	0.78
1:A:391:ASN:ND2	1:A:406:PRO:HG3	1.99	0.78
3:Y:132:THR:HG23	3:Y:155:ILE:HB	1.65	0.78
1:A:284:GLN:HG2	1:A:310:LEU:CD2	2.13	0.78
2:D:69:PHE:HE2	2:D:71:THR:HB	1.47	0.78
2:B:598:ILE:CD1	2:B:800:ILE:HG21	2.14	0.78
1:C:442:LEU:HD23	1:C:443:PRO:HD2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:TYR:N	1:C:23:TYR:CD1	2.42	0.78
1:A:1160:PRO:HG2	1:C:1098:ASN:OD1	1.83	0.78
1:A:250:ILE:HD11	1:A:265:VAL:HG11	1.64	0.78
1:A:1199:ASP:OD1	1:A:1201:THR:HG23	1.84	0.78
2:D:261:ALA:HB2	2:D:320:VAL:CG2	2.13	0.78
2:D:151:ASP:HB2	2:D:794:PHE:CZ	2.18	0.78
2:B:1383:ASP:HB3	2:B:1457:LYS:HB2	1.66	0.78
2:D:1331:ALA:O	2:D:1332:GLN:HB3	1.82	0.78
1:A:1535:MET:H	1:A:1608:ASN:HB3	1.49	0.78
1:A:1056:ILE:HD11	1:A:1066:TYR:CD2	2.18	0.78
1:C:1593:GLU:HB2	1:C:1596:SER:OG	1.83	0.78
1:A:42:GLN:HA	1:A:80:GLN:HG3	1.65	0.77
2:D:285:ILE:N	2:D:285:ILE:HD12	1.97	0.77
2:B:69:PHE:HE2	2:B:71:THR:HB	1.47	0.77
1:C:391:ASN:ND2	1:C:406:PRO:HG3	1.98	0.77
2:D:137:TYR:CZ	2:D:143:VAL:HG22	2.19	0.77
2:D:218:LYS:HB3	2:D:822:TYR:CD2	2.18	0.77
2:D:422:ARG:HH12	3:Y:44:ARG:HA	1.49	0.77
1:A:22:THR:CG2	1:A:657:ALA:HB2	2.15	0.77
1:C:463:SER:CB	1:C:491:PRO:HA	2.13	0.77
1:C:532:GLN:NE2	1:C:568:GLY:HA2	1.98	0.77
2:B:557:GLN:HA	2:B:557:GLN:OE1	1.82	0.77
1:C:1213:LYS:HG2	1:C:1266:TYR:HE2	1.48	0.77
1:C:1190:ILE:HG12	1:C:1253:TYR:CD1	2.19	0.77
1:A:20:GLU:C	1:A:21:GLN:HG3	2.04	0.77
1:C:968:VAL:HG23	1:C:971:THR:HG21	1.67	0.77
1:C:535:VAL:CG2	1:C:536:PRO:HD3	2.13	0.77
1:C:830:PRO:CG	1:C:1483:PHE:HZ	1.96	0.77
1:A:1162:VAL:H	1:C:1102:ASN:ND2	1.82	0.77
1:C:1585:TYR:HD1	1:C:1671:ILE:CG2	1.97	0.77
1:A:576:SER:CB	1:A:577:PRO:HD3	2.15	0.77
1:C:1573:VAL:HG12	1:C:1603:LYS:HB3	1.66	0.77
1:C:55:SER:O	1:C:56:ILE:HD13	1.85	0.77
2:D:1446:PHE:HD2	2:D:1448:VAL:HG22	1.49	0.77
1:A:1179:THR:CG2	1:A:1208:ILE:HD13	2.15	0.77
1:C:471:ASP:OD2	1:C:474:LYS:HB3	1.84	0.77
1:A:1213:LYS:HG2	1:A:1266:TYR:CE2	2.20	0.77
1:C:42:GLN:HB2	1:C:80:GLN:NE2	1.99	0.77
1:A:979:VAL:HG21	1:A:1326:TYR:HE1	1.50	0.77
2:B:285:ILE:HD12	2:B:285:ILE:N	2.00	0.77
1:C:284:GLN:HG2	1:C:310:LEU:CD2	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:765:ILE:O	1:A:765:ILE:HD12	1.84	0.77
1:A:23:TYR:HD1	1:A:23:TYR:N	1.79	0.77
1:C:576:SER:CB	1:C:577:PRO:HD3	2.15	0.77
1:C:613:GLN:O	1:C:613:GLN:HG3	1.85	0.77
2:D:598:ILE:CD1	2:D:800:ILE:HG21	2.13	0.77
1:A:906:GLY:H	1:A:929:VAL:HB	1.50	0.77
1:C:532:GLN:OE1	1:C:532:GLN:HA	1.83	0.77
2:B:224:PHE:CZ	2:B:329:VAL:HG22	2.20	0.77
1:A:135:TYR:CE1	1:A:141:VAL:HA	2.17	0.77
1:A:1161:LEU:HD12	1:C:1105:LEU:HD13	1.67	0.77
2:D:1613:GLU:O	2:D:1616:CYS:HB2	1.85	0.77
2:B:954:VAL:HG12	2:B:955:PRO:HD2	1.67	0.76
3:Y:87:LEU:HA	3:Y:91:LYS:HD3	1.67	0.76
1:C:25:ILE:H	1:C:655:THR:CG2	1.98	0.76
1:A:1218:VAL:HG12	1:A:1219:LYS:H	1.50	0.76
1:C:128:ILE:HG13	1:C:215:ALA:HB2	1.66	0.76
1:C:1576:LYS:HG2	1:C:1601:ILE:CG2	2.16	0.76
1:A:1161:LEU:HA	1:C:1102:ASN:HD21	1.49	0.76
3:Y:170:ARG:HD3	3:Y:203:LEU:HD23	1.65	0.76
1:A:23:TYR:H	1:A:23:TYR:HD1	1.29	0.76
1:C:1560:ALA:HB3	1:C:1585:TYR:HE2	1.50	0.76
2:B:469:ASN:ND2	2:B:469:ASN:C	2.37	0.76
1:C:1573:VAL:CG1	1:C:1603:LYS:HD3	2.15	0.76
1:C:1003:LEU:HD11	1:C:1286:SER:HA	1.65	0.76
1:C:267:ILE:CD1	1:C:299:VAL:HG11	2.15	0.76
2:D:478:TYR:HD1	2:D:478:TYR:O	1.68	0.76
1:C:78:LYS:HZ2	3:Y:144:GLU:HA	1.50	0.76
2:D:1496:THR:HG23	2:D:1603:LYS:HD2	1.66	0.76
2:B:478:TYR:O	2:B:478:TYR:HD1	1.67	0.76
3:X:150:ILE:HD12	3:X:150:ILE:O	1.86	0.76
1:C:43:VAL:HG13	1:C:79:PHE:HB3	1.68	0.76
1:C:1562:LYS:HD2	1:C:1648:TRP:HZ2	1.49	0.76
1:A:696:LYS:HZ3	1:A:759:PRO:CD	1.98	0.76
2:D:1280:GLU:HG2	2:D:1287:PRO:HB3	1.66	0.76
1:C:1320:LYS:CD	1:C:1321:GLY:H	1.99	0.76
1:C:171:VAL:HG12	1:C:172:ASP:N	1.97	0.76
1:C:1494:THR:HB	1:C:1506:THR:HG23	1.68	0.76
1:C:849:ARG:HG2	1:C:849:ARG:NH1	1.95	0.76
1:C:315:LEU:CD1	1:C:318:LEU:HG	2.15	0.76
3:Y:125:LYS:HA	3:Y:127:ASN:N	2.00	0.76
2:B:250:ARG:HG2	2:B:256:GLU:HA	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:422:ARG:HD3	2:B:422:ARG:H	1.49	0.76
1:A:25:ILE:N	1:A:655:THR:HG23	1.99	0.76
1:C:830:PRO:HG3	1:C:1483:PHE:CE2	2.21	0.76
1:A:1213:LYS:HE2	1:A:1266:TYR:CD2	2.21	0.76
1:A:641:ASN:HD21	1:A:643:ALA:HB3	1.50	0.76
1:C:351:PRO:HG2	1:C:352:TYR:CD2	2.20	0.76
3:Y:136:LEU:O	3:Y:136:LEU:HG	1.84	0.76
1:C:1304:VAL:HG12	1:C:1305:LYS:N	2.01	0.76
2:D:415:THR:OG1	2:D:425:GLN:HB2	1.85	0.76
1:A:386:VAL:H	1:A:411:THR:CG2	1.92	0.76
1:C:1497:GLU:OE1	1:C:1500:ARG:HD3	1.86	0.76
1:C:144:ARG:HD2	1:C:146:TYR:CE1	2.20	0.76
1:C:804:ILE:HG22	1:C:809:ILE:HG13	1.67	0.76
2:D:322:THR:HG22	2:D:327:ASP:O	1.84	0.76
1:A:111:PHE:CE2	1:A:113:LYS:HB2	2.21	0.75
2:D:954:VAL:HB	2:D:957:THR:CG2	2.15	0.75
1:C:1179:THR:CG2	1:C:1208:ILE:HD13	2.16	0.75
1:C:1488:LEU:HD12	1:C:1488:LEU:O	1.85	0.75
2:B:261:ALA:HB2	2:B:320:VAL:CG2	2.13	0.75
1:A:315:LEU:CD1	1:A:318:LEU:HG	2.15	0.75
2:D:200:VAL:HG12	2:D:211:THR:OG1	1.87	0.75
1:A:463:SER:HB3	1:A:491:PRO:HA	1.68	0.75
1:C:796:THR:HG23	1:C:818:LYS:HB3	1.67	0.75
1:C:1585:TYR:CE2	1:C:1586:LYS:HB3	2.22	0.75
1:A:1379:LEU:HD11	1:A:1505:CYS:O	1.86	0.75
1:C:596:MET:N	1:C:782:ARG:HD3	2.01	0.75
2:B:825:VAL:O	2:B:828:GLU:HG3	1.87	0.75
2:B:1583:ILE:HG12	2:B:1607:ILE:HG23	1.66	0.75
1:A:1067:SER:HB3	1:A:1072:GLY:O	1.85	0.75
2:B:344:GLN:HA	2:B:344:GLN:NE2	2.02	0.75
1:A:1560:ALA:HB3	1:A:1585:TYR:HE2	1.52	0.75
2:B:42:LEU:HD11	2:B:82:LEU:HD12	1.67	0.75
1:A:1108:VAL:HG21	1:A:1167:ALA:HB2	1.69	0.75
1:A:1162:VAL:H	1:C:1102:ASN:HD21	1.34	0.75
2:D:148:PHE:CE2	2:D:792:VAL:HG11	2.21	0.75
1:C:1068:VAL:HA	1:C:1078:LEU:CD1	2.15	0.75
1:C:180:ILE:HB	1:C:599:TRP:CZ3	2.22	0.75
2:D:422:ARG:HD3	2:D:422:ARG:H	1.50	0.75
2:D:1424:ILE:HG12	2:D:1426:TYR:CE2	2.22	0.75
1:C:539:ARG:NH2	1:C:634:CYS:H	1.84	0.75
1:A:1244:THR:HG23	1:A:1502:ASP:OD2	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:PHE:CE1	1:A:452:TYR:HB2	2.21	0.75
2:D:469:ASN:C	2:D:469:ASN:ND2	2.39	0.75
2:B:1284:ARG:CD	2:B:1285:GLU:H	2.00	0.75
1:C:1104:LEU:O	1:C:1108:VAL:HG12	1.87	0.75
1:A:539:ARG:NH2	1:A:634:CYS:H	1.85	0.75
2:B:948:ARG:HH21	2:B:948:ARG:HB2	1.51	0.75
1:A:535:VAL:CG2	1:A:536:PRO:HD3	2.13	0.75
1:A:1638:PRO:O	1:A:1639:LEU:HB2	1.87	0.75
1:C:1504:GLN:HG3	1:C:1505:CYS:HA	1.69	0.75
1:A:128:ILE:HD12	1:A:201:ILE:HG22	1.67	0.75
2:D:1347:VAL:HG22	2:D:1367:ILE:HG23	1.69	0.75
1:C:38:ASN:HA	1:C:84:ILE:HG22	1.68	0.75
2:B:818:LEU:HB3	2:B:911:LYS:HD2	1.69	0.75
1:C:260:VAL:HG12	1:C:261:THR:H	1.50	0.75
2:D:265:PHE:CD2	2:D:294:LEU:HB2	2.21	0.75
1:C:44:TYR:HB2	1:C:545:ILE:HD12	1.69	0.75
2:B:829:GLN:CG	2:B:1480:LEU:HD13	2.17	0.75
1:A:255:PHE:HE1	1:A:258:LYS:CB	1.98	0.75
1:C:1320:LYS:HD2	1:C:1321:GLY:H	1.51	0.75
1:C:549:GLU:CD	1:C:550:GLN:H	1.89	0.75
1:A:111:PHE:HE2	1:A:113:LYS:HB2	1.52	0.74
1:C:1218:VAL:HG12	1:C:1219:LYS:N	2.02	0.74
2:B:508:LEU:HD12	2:B:509:HIS:H	1.52	0.74
1:C:1314:ASP:HA	1:C:1325:ASN:HB2	1.68	0.74
1:A:1402:ILE:HG13	1:A:1479:ILE:HD11	1.69	0.74
2:D:261:ALA:CB	2:D:320:VAL:HG23	2.15	0.74
1:C:1244:THR:HG23	1:C:1502:ASP:OD2	1.87	0.74
2:D:42:LEU:HD11	2:D:82:LEU:HD12	1.68	0.74
1:A:849:ARG:NH1	1:A:849:ARG:HG2	1.94	0.74
1:C:415:ASP:HB2	1:C:417:VAL:HB	1.69	0.74
1:C:224:LEU:HD23	1:C:225:PRO:HD2	1.70	0.74
1:C:33:VAL:HG21	1:C:121:TYR:HD1	1.51	0.74
2:B:1473:HIS:HB3	2:B:1476:LYS:HB2	1.68	0.74
2:D:615:GLN:HB2	2:D:616:ASN:ND2	2.03	0.74
1:A:613:GLN:HG3	1:A:613:GLN:O	1.85	0.74
3:X:87:LEU:HA	3:X:91:LYS:HD3	1.69	0.74
1:C:961:TYR:HE2	1:C:1343:ASN:HA	1.53	0.74
1:C:640:LEU:H	1:C:644:ASN:HB3	1.53	0.74
1:A:1562:LYS:HD3	1:A:1664:LEU:HD21	1.70	0.74
1:A:1067:SER:HA	1:A:1074:ALA:HA	1.68	0.74
1:A:1314:ASP:HA	1:A:1325:ASN:HB2	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:895:LEU:HD12	1:C:896:VAL:H	1.52	0.74
1:C:285:THR:HG22	1:C:285:THR:O	1.86	0.74
1:C:1056:ILE:HD11	1:C:1066:TYR:CE2	2.23	0.74
2:D:469:ASN:HD22	2:D:470:ALA:N	1.86	0.74
1:A:1047:LYS:HE2	1:A:1051:GLU:OE2	1.86	0.74
2:D:34:ARG:HD3	2:D:124:GLN:HG2	1.69	0.74
1:A:258:LYS:HD3	1:A:893:SER:OG	1.85	0.74
1:A:1402:ILE:HG13	1:A:1479:ILE:CD1	2.17	0.74
1:C:538:SER:O	1:C:561:LEU:HB2	1.88	0.74
2:D:758:LEU:HD13	2:D:760:LYS:HE2	1.69	0.74
1:C:1024:TYR:HA	1:C:1302:LEU:HD21	1.69	0.74
1:A:620:LEU:O	1:A:623:VAL:HG23	1.88	0.74
1:C:123:ASN:HB3	1:C:209:PHE:CD1	2.23	0.74
1:C:695:VAL:HG13	1:C:724:CYS:HA	1.70	0.74
1:A:42:GLN:HB2	1:A:80:GLN:NE2	2.02	0.74
2:D:620:VAL:HG12	2:D:621:PHE:HD2	1.53	0.74
1:A:128:ILE:HG13	1:A:215:ALA:HB2	1.69	0.74
1:A:1152:ILE:CG2	1:A:1168:LEU:HD21	2.17	0.74
1:C:993:SER:C	1:C:995:GLU:H	1.91	0.74
1:A:1031:TRP:CZ2	1:A:1042:LYS:HG3	2.22	0.74
2:D:1525:LYS:HD2	2:D:1610:TRP:CZ2	2.22	0.74
1:A:538:SER:O	1:A:561:LEU:HB2	1.86	0.73
1:C:1622:LYS:HZ3	1:C:1642:LEU:HD23	1.52	0.73
1:C:1013:MET:SD	1:C:1016:VAL:HG21	2.28	0.73
2:B:344:GLN:HA	2:B:344:GLN:HE21	1.52	0.73
1:A:144:ARG:HD2	1:A:146:TYR:CE1	2.22	0.73
1:C:1186:PHE:HA	1:C:1250:THR:HG22	1.70	0.73
3:X:132:THR:HG23	3:X:155:ILE:HB	1.70	0.73
1:A:503:ILE:HB	1:A:511:HIS:HB2	1.69	0.73
1:C:1627:ILE:HD12	1:C:1629:TYR:HB3	1.69	0.73
1:C:127:PHE:CD2	1:C:623:VAL:HG22	2.23	0.73
1:C:133:PRO:HD2	1:C:609:VAL:CG1	2.17	0.73
1:A:1020:TYR:HE1	1:A:1295:GLU:HG3	1.52	0.73
2:B:1435:ASP:OD1	5:B:2003:NAG:H81	1.88	0.73
1:C:1133:LEU:H	1:C:1133:LEU:CD1	1.95	0.73
1:A:1370:THR:HG23	1:A:1373:GLU:OE1	1.88	0.73
1:C:222:TYR:HE1	1:C:768:TYR:HB2	1.51	0.73
1:A:1341:LEU:HB2	1:A:1342:LEU:HD23	1.69	0.73
3:X:111:ASP:OD1	3:X:112:PRO:HD2	1.89	0.73
1:A:1593:GLU:HB2	1:A:1596:SER:OG	1.88	0.73
2:D:948:ARG:HB2	2:D:948:ARG:HH21	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1365:VAL:HG22	1:C:1366:HIS:N	2.01	0.73
1:C:433:PHE:CE1	1:C:452:TYR:HB2	2.23	0.73
1:C:1190:ILE:HG12	1:C:1253:TYR:CE1	2.23	0.73
2:B:1349:VAL:HA	2:B:1364:MET:O	1.88	0.73
1:C:42:GLN:NE2	1:C:44:TYR:N	2.37	0.73
1:C:936:ARG:NH1	1:C:936:ARG:HG3	1.87	0.73
1:A:1068:VAL:HA	1:A:1078:LEU:CD1	2.17	0.73
1:C:1056:ILE:HD11	1:C:1066:TYR:CD2	2.23	0.73
2:B:484:LEU:HB2	2:B:519:ARG:HG3	1.70	0.73
1:A:160:VAL:HG22	1:A:175:GLU:HB3	1.71	0.73
1:C:1493:PHE:CD1	1:C:1494:THR:N	2.52	0.73
2:B:1607:ILE:H	2:B:1607:ILE:HD12	1.53	0.73
2:B:620:VAL:HG12	2:B:621:PHE:HD2	1.52	0.73
2:D:1508:VAL:HB	2:D:1509:PRO:HD3	1.70	0.73
3:X:165:LEU:O	3:X:169:ILE:HG12	1.89	0.73
1:C:906:GLY:H	1:C:929:VAL:HB	1.53	0.73
1:C:111:PHE:HE2	1:C:113:LYS:HB2	1.50	0.73
1:C:489:LYS:CG	1:C:490:SER:N	2.50	0.73
1:A:182:ILE:CG1	1:A:804:ILE:HD11	2.06	0.73
1:A:968:VAL:HG23	1:A:971:THR:OG1	1.88	0.73
2:B:415:THR:OG1	2:B:425:GLN:HB2	1.89	0.73
1:A:470:THR:HB	2:B:450:THR:O	1.89	0.73
1:C:1573:VAL:O	1:C:1603:LYS:HG2	1.89	0.73
1:C:255:PHE:HE1	1:C:258:LYS:CB	2.02	0.73
1:C:1626:GLN:HB2	1:C:1635:TYR:HD1	1.53	0.73
1:C:1527:CYS:C	1:C:1529:GLU:N	2.34	0.73
1:A:700:TYR:C	1:A:700:TYR:HD2	1.92	0.73
2:D:825:VAL:O	2:D:828:GLU:HG3	1.88	0.73
1:C:220:LYS:HD3	1:C:765:ILE:HG23	1.69	0.73
2:B:548:LEU:HD22	2:B:793:SER:HB3	1.70	0.73
1:C:160:VAL:HG22	1:C:175:GLU:HB3	1.71	0.73
1:C:494:ASP:O	1:C:496:ILE:N	2.22	0.72
2:B:844:ILE:HG13	2:B:872:ILE:HG12	1.71	0.72
1:A:415:ASP:HB2	1:A:417:VAL:HB	1.69	0.72
1:A:993:SER:C	1:A:995:GLU:H	1.93	0.72
2:D:1482:ASN:HB2	2:D:1495:GLU:HG2	1.69	0.72
1:A:514:THR:O	1:A:515:ARG:HD3	1.89	0.72
1:C:963:ILE:HG23	1:C:967:LEU:HD23	1.72	0.72
1:C:1213:LYS:HG2	1:C:1266:TYR:CE2	2.24	0.72
1:C:1152:ILE:HG21	1:C:1168:LEU:HD21	1.70	0.72
2:B:148:PHE:CE2	2:B:792:VAL:HG11	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:LYS:HG2	1:A:518:PHE:N	2.04	0.72
1:C:700:TYR:C	1:C:700:TYR:HD2	1.92	0.72
2:D:850:LEU:HD12	2:D:851:LEU:H	1.53	0.72
1:A:493:ILE:HG23	1:A:495:LYS:H	1.55	0.72
1:A:1573:VAL:HG12	1:A:1603:LYS:HB3	1.70	0.72
2:B:1347:VAL:HG22	2:B:1367:ILE:HG23	1.70	0.72
1:A:695:VAL:HG13	1:A:724:CYS:HA	1.70	0.72
2:D:834:ALA:O	2:D:835:ILE:HD13	1.89	0.72
1:A:149:ASN:HD22	1:A:149:ASN:H	1.36	0.72
1:C:365:PRO:HD2	1:C:464:TYR:CD2	2.25	0.72
1:C:1358:THR:HB	1:C:1360:HIS:CE1	2.24	0.72
2:D:844:ILE:HG13	2:D:872:ILE:HG12	1.72	0.72
2:B:34:ARG:HD3	2:B:124:GLN:HG2	1.71	0.72
1:A:799:ILE:HG22	1:A:815:VAL:O	1.90	0.72
1:C:238:ILE:HD12	1:C:347:TYR:HE1	1.53	0.72
1:C:330:ILE:HG22	1:C:337:SER:CB	2.20	0.72
2:B:1279:ILE:HG22	2:B:1288:ILE:HB	1.71	0.72
1:A:483:ASN:ND2	2:B:399:ILE:HB	2.04	0.72
1:C:1255:LEU:O	1:C:1255:LEU:HD12	1.90	0.72
1:C:374:GLN:HA	1:C:416:GLY:O	1.88	0.72
1:A:148:LEU:HD23	1:A:152:LEU:CD1	2.19	0.72
3:X:68:ASN:CG	3:X:69:GLY:H	1.92	0.72
1:C:24:VAL:N	1:C:655:THR:HG21	2.04	0.72
1:C:495:LYS:CE	1:C:495:LYS:HA	2.19	0.72
1:C:1278:GLN:OE1	1:C:1283:GLY:CA	2.37	0.72
1:A:1228:TRP:H	1:A:1251:THR:CG2	1.98	0.72
1:A:830:PRO:CG	1:A:1483:PHE:CZ	2.72	0.72
1:A:1623:GLU:CB	1:A:1638:PRO:HG3	2.18	0.72
1:C:1573:VAL:CB	1:C:1603:LYS:HD3	2.19	0.72
1:A:38:ASN:HA	1:A:84:ILE:HG22	1.71	0.72
1:A:43:VAL:HG13	1:A:79:PHE:HB3	1.69	0.72
2:B:261:ALA:CB	2:B:320:VAL:HG23	2.16	0.72
1:C:234:GLU:HG3	1:C:235:TYR:HD2	1.51	0.72
1:C:365:PRO:HD2	1:C:464:TYR:CE2	2.24	0.72
1:A:260:VAL:HG12	1:A:261:THR:H	1.54	0.72
1:A:1560:ALA:HB3	1:A:1585:TYR:CE2	2.25	0.72
1:C:1329:THR:OG1	1:C:1331:LYS:HG2	1.90	0.72
1:C:1108:VAL:HG11	1:C:1164:ILE:HG22	1.70	0.72
2:D:1506:ILE:HD11	2:D:1628:PHE:HE1	1.53	0.72
1:C:1560:ALA:HB3	1:C:1585:TYR:CE2	2.24	0.72
1:A:373:VAL:HG23	1:A:418:ALA:HB3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:64:VAL:HG11	3:X:95:LYS:O	1.90	0.72
2:B:1313:VAL:HG11	2:B:1323:MET:SD	2.29	0.72
1:A:1347:ILE:O	1:A:1347:ILE:HG22	1.89	0.72
1:A:225:PRO:HG3	1:A:766:ARG:HB2	1.71	0.72
1:A:1076:THR:CG2	1:A:1120:GLU:HA	2.18	0.72
1:A:1493:PHE:CD1	1:A:1494:THR:N	2.55	0.72
1:C:596:MET:HA	1:C:782:ARG:HG2	1.70	0.72
1:A:1304:VAL:HG12	1:A:1305:LYS:N	2.03	0.72
2:B:162:ILE:CG2	2:B:202:LYS:HG2	2.20	0.72
1:C:489:LYS:HG3	1:C:490:SER:H	1.55	0.71
1:C:491:PRO:HB2	1:C:493:ILE:O	1.89	0.71
1:C:620:LEU:O	1:C:623:VAL:HG23	1.88	0.71
1:C:1163:LYS:O	1:C:1166:THR:HG22	1.90	0.71
2:D:481:TYR:HB2	2:D:520:PHE:CE1	2.25	0.71
1:C:386:VAL:H	1:C:411:THR:CG2	1.92	0.71
1:C:1068:VAL:HG13	1:C:1069:TRP:N	2.06	0.71
2:B:563:MET:HB3	2:B:778:PHE:CE2	2.25	0.71
1:C:1567:SER:HB3	1:C:1578:LYS:HB2	1.70	0.71
3:Y:166:ASP:OD2	3:Y:207:LEU:HG	1.89	0.71
2:D:23:ALA:HB3	2:D:528:ASN:HD22	1.55	0.71
2:B:618:LEU:HD11	2:B:635:ASN:O	1.90	0.71
1:A:351:PRO:HG2	1:A:352:TYR:CD2	2.25	0.71
1:A:1104:LEU:O	1:A:1108:VAL:HG12	1.91	0.71
1:C:1423:VAL:HG13	1:C:1496:TYR:CD2	2.24	0.71
3:Y:68:ASN:CG	3:Y:69:GLY:H	1.93	0.71
1:C:979:VAL:HG21	1:C:1326:TYR:HE1	1.52	0.71
1:A:1069:TRP:CZ3	1:A:1451:THR:HG21	2.25	0.71
1:C:61:ASP:O	1:C:62:LYS:HB2	1.90	0.71
2:D:1523:VAL:HG22	2:D:1584:TRP:HB2	1.72	0.71
1:A:42:GLN:NE2	1:A:44:TYR:N	2.38	0.71
1:A:552:ALA:HB2	1:A:657:ALA:HB3	1.73	0.71
1:C:42:GLN:HA	1:C:80:GLN:HG3	1.72	0.71
2:B:435:TYR:CD1	2:B:436:GLN:N	2.59	0.71
1:A:491:PRO:O	1:A:492:TYR:C	2.28	0.71
1:A:981:GLY:CA	1:A:1333:PHE:HB2	2.21	0.71
1:C:222:TYR:HD2	1:C:223:VAL:N	1.88	0.71
1:C:1381:ILE:HG12	1:C:1382:ASP:N	2.05	0.71
1:C:1450:PHE:CZ	1:C:1475:VAL:HB	2.24	0.71
2:D:1371:TYR:CG	2:D:1377:SER:HB3	2.25	0.71
1:C:530:VAL:HG23	1:C:534:MET:HE2	1.71	0.71
2:D:1562:GLN:HE22	2:D:1596:LYS:NZ	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:HD23	1:A:225:PRO:HD2	1.71	0.71
2:D:1284:ARG:CD	2:D:1285:GLU:H	2.02	0.71
1:A:44:TYR:HB2	1:A:545:ILE:HD12	1.71	0.71
1:A:961:TYR:HE2	1:A:1343:ASN:HA	1.55	0.71
1:A:489:LYS:CG	1:A:490:SER:N	2.53	0.71
1:A:491:PRO:HB2	1:A:493:ILE:O	1.89	0.71
1:A:374:GLN:HA	1:A:416:GLY:O	1.91	0.71
2:B:1280:GLU:HG2	2:B:1287:PRO:HB3	1.73	0.71
1:C:906:GLY:O	1:C:908:HIS:CE1	2.44	0.71
1:C:961:TYR:CE2	1:C:1343:ASN:HA	2.25	0.71
1:C:1219:LYS:HZ3	1:C:1239:VAL:HG11	1.55	0.71
1:A:774:LEU:HD12	1:A:799:ILE:HD11	1.71	0.71
1:C:967:LEU:HD12	1:C:968:VAL:N	2.04	0.71
1:A:1024:TYR:HA	1:A:1302:LEU:HD21	1.73	0.71
1:A:423:ASN:OD1	2:B:504:VAL:HG22	1.91	0.71
1:A:1268:ASN:HD22	1:A:1268:ASN:H	1.38	0.71
3:X:64:VAL:HG23	3:X:71:ASN:OD1	1.91	0.71
2:B:1446:PHE:HD2	2:B:1448:VAL:HG22	1.54	0.71
1:A:40:VAL:HG21	1:A:512:PHE:HD1	1.55	0.71
2:B:1593:THR:HG22	2:B:1594:LYS:N	2.06	0.71
1:C:1638:PRO:O	1:C:1639:LEU:HB2	1.89	0.71
1:A:99:VAL:O	1:A:119:ILE:HD11	1.90	0.71
2:B:481:TYR:HB2	2:B:520:PHE:CE1	2.25	0.71
1:A:640:LEU:H	1:A:644:ASN:HB3	1.56	0.71
1:A:1573:VAL:CB	1:A:1603:LYS:HD3	2.21	0.71
1:A:1179:THR:HG21	1:A:1208:ILE:HD13	1.72	0.71
2:B:165:PHE:CZ	2:B:199:ILE:HD11	2.26	0.71
1:A:1076:THR:HG22	1:A:1120:GLU:OE2	1.91	0.70
2:B:850:LEU:HD12	2:B:851:LEU:H	1.55	0.70
1:A:234:GLU:HG3	1:A:235:TYR:HD2	1.50	0.70
1:A:255:PHE:CE1	1:A:258:LYS:HB3	2.25	0.70
1:A:906:GLY:O	1:A:908:HIS:CE1	2.43	0.70
2:D:162:ILE:CG2	2:D:202:LYS:HG2	2.20	0.70
1:A:365:PRO:HD2	1:A:464:TYR:CD2	2.25	0.70
2:D:508:LEU:HD12	2:D:509:HIS:H	1.55	0.70
1:A:398:ASN:O	1:A:399:GLN:HB2	1.90	0.70
2:B:758:LEU:HD13	2:B:760:LYS:HE2	1.72	0.70
1:C:1543:ILE:O	1:C:1547:THR:HG23	1.90	0.70
1:A:963:ILE:HG23	1:A:967:LEU:HD23	1.72	0.70
1:A:765:ILE:HD13	1:A:767:SER:O	1.91	0.70
1:C:109:LYS:HD3	1:C:110:HIS:CE1	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1186:PHE:HA	1:A:1250:THR:HG22	1.73	0.70
1:A:1525:CYS:C	1:A:1528:VAL:HG22	2.12	0.70
3:X:166:ASP:OD1	3:X:207:LEU:HD23	1.91	0.70
1:A:238:ILE:HD12	1:A:347:TYR:HE1	1.55	0.70
1:A:1013:MET:SD	1:A:1016:VAL:HG21	2.31	0.70
2:B:1482:ASN:HB2	2:B:1495:GLU:HG2	1.72	0.70
1:A:1127:ILE:HD11	1:A:1143:TYR:CD2	2.27	0.70
1:A:504:LEU:HD21	1:A:651:LEU:HG	1.74	0.70
1:C:491:PRO:O	1:C:492:TYR:C	2.26	0.70
1:C:968:VAL:HG12	1:C:1368:THR:HG22	1.73	0.70
1:C:503:ILE:HB	1:C:511:HIS:HB2	1.72	0.70
3:Y:80:GLN:HG3	3:Y:114:GLY:C	2.12	0.70
1:C:152:LEU:HD11	1:C:627:LEU:HD11	1.73	0.70
1:A:131:ASP:HB3	1:A:142:LYS:HB2	1.74	0.70
2:D:1381:ILE:HG21	2:D:1459:TYR:HE1	1.56	0.70
1:C:131:ASP:O	1:C:132:LYS:HG2	1.91	0.70
1:C:1127:ILE:H	1:C:1127:ILE:HD12	1.56	0.70
2:B:615:GLN:HB2	2:B:616:ASN:ND2	2.06	0.70
3:Y:146:LEU:HD22	3:Y:147:ASP:N	2.06	0.70
1:A:1076:THR:HG21	1:A:1120:GLU:HA	1.72	0.70
2:B:950:LEU:HD22	2:B:1329:TYR:CZ	2.26	0.70
1:C:869:GLU:C	1:C:871:PRO:HD3	2.11	0.70
2:B:1615:GLU:HB3	2:B:1621:PHE:CD1	2.26	0.70
2:D:618:LEU:HD11	2:D:635:ASN:O	1.92	0.70
1:A:961:TYR:CE2	1:A:1343:ASN:HA	2.27	0.70
2:B:28:ILE:HD12	2:B:42:LEU:HD23	1.73	0.70
2:D:1445:HIS:CG	2:D:1446:PHE:N	2.59	0.70
1:C:1112:GLN:HE21	1:C:1171:ALA:HB2	1.54	0.70
1:A:685:GLU:HA	1:A:685:GLU:OE1	1.92	0.70
1:C:255:PHE:CE1	1:C:258:LYS:HB3	2.27	0.70
3:Y:47:HIS:HE1	3:Y:181:LYS:HE2	1.56	0.70
2:D:262:PHE:HE1	2:D:282:ARG:HG3	1.56	0.70
1:A:1504:GLN:HG3	1:A:1505:CYS:HA	1.72	0.70
1:C:690:TYR:O	1:C:690:TYR:CG	2.43	0.70
2:B:1424:ILE:H	2:B:1424:ILE:HD13	1.56	0.70
1:C:975:ARG:NH2	1:C:1346:LEU:HD22	2.06	0.70
1:C:517:LYS:HG2	1:C:518:PHE:N	2.05	0.70
1:C:968:VAL:CG2	1:C:971:THR:HG21	2.22	0.70
2:B:954:VAL:HB	2:B:957:THR:CG2	2.19	0.70
1:C:419:SER:HB2	2:D:459:ASN:HD22	1.56	0.70
1:C:1047:LYS:HE2	1:C:1051:GLU:OE2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:THR:HG22	1:A:285:THR:O	1.91	0.70
1:C:639:GLY:HA2	1:C:648:LEU:HD13	1.74	0.70
1:C:1625:LEU:O	1:C:1627:ILE:HG23	1.91	0.70
1:C:938:SER:O	1:C:940:SER:N	2.25	0.70
1:A:1616:GLN:OE1	1:A:1650:ARG:HD3	1.92	0.70
1:C:99:VAL:O	1:C:119:ILE:HD11	1.91	0.70
2:D:237:ILE:O	2:D:306:LEU:HD11	1.92	0.70
1:A:330:ILE:HG22	1:A:337:SER:CB	2.21	0.70
3:Y:111:ASP:OD1	3:Y:112:PRO:HD2	1.91	0.70
3:X:136:LEU:HG	3:X:136:LEU:O	1.91	0.70
1:C:476:LEU:HB3	1:C:563:ILE:HA	1.73	0.69
2:D:1480:LEU:HD12	2:D:1481:LEU:N	2.06	0.69
3:Y:170:ARG:NH2	3:Y:206:LYS:HA	2.06	0.69
1:C:1370:THR:HG23	1:C:1373:GLU:OE1	1.91	0.69
1:C:1219:LYS:CE	1:C:1239:VAL:HG21	2.22	0.69
1:A:1278:GLN:OE1	1:A:1283:GLY:CA	2.40	0.69
2:D:484:LEU:HB2	2:D:519:ARG:HG3	1.73	0.69
1:A:148:LEU:HD23	1:A:152:LEU:HD12	1.74	0.69
1:A:587:THR:HG22	1:A:789:ALA:HB2	1.72	0.69
1:A:1567:SER:HB3	1:A:1578:LYS:HB2	1.74	0.69
3:X:73:VAL:HG23	3:X:74:ARG:N	2.07	0.69
1:C:1646:GLU:OE2	1:C:1660:PHE:HZ	1.75	0.69
1:A:1646:GLU:OE2	1:A:1660:PHE:HZ	1.75	0.69
1:A:596:MET:HA	1:A:782:ARG:HG2	1.74	0.69
1:A:495:LYS:HA	1:A:495:LYS:CE	2.17	0.69
1:A:849:ARG:NH2	2:B:555:LEU:HB2	2.07	0.69
2:D:825:VAL:N	2:D:828:GLU:OE1	2.25	0.69
2:D:148:PHE:HB3	2:D:800:ILE:HD11	1.75	0.69
1:A:1543:ILE:O	1:A:1547:THR:HG23	1.91	0.69
1:C:1429:PRO:HB2	1:C:1432:ILE:CG1	2.22	0.69
2:B:834:ALA:O	2:B:835:ILE:HD13	1.92	0.69
1:C:1585:TYR:CE1	1:C:1671:ILE:HG12	2.28	0.69
1:A:33:VAL:HG21	1:A:121:TYR:HD1	1.57	0.69
1:C:1404:ALA:HB1	1:C:1493:PHE:HE2	1.57	0.69
2:D:435:TYR:CD1	2:D:436:GLN:N	2.58	0.69
1:C:1019:PHE:C	1:C:1019:PHE:CD2	2.65	0.69
3:Y:73:VAL:HG23	3:Y:74:ARG:N	2.07	0.69
1:C:658:ASN:O	1:C:659:ALA:HB3	1.91	0.69
1:A:1494:THR:HB	1:A:1506:THR:HG23	1.74	0.69
1:A:463:SER:CB	1:A:491:PRO:HA	2.23	0.69
1:A:1329:THR:OG1	1:A:1331:LYS:HG2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:422:ARG:NH1	3:Y:44:ARG:HA	2.07	0.69
1:C:238:ILE:HB	1:C:347:TYR:CD1	2.28	0.69
2:B:1445:HIS:CG	2:B:1446:PHE:N	2.59	0.69
1:C:131:ASP:HB3	1:C:142:LYS:HB2	1.72	0.69
2:B:236:TYR:CZ	2:B:424:ARG:HD2	2.27	0.69
2:D:859:ALA:HB1	2:D:866:TYR:CD1	2.27	0.69
3:Y:50:TYR:HE2	3:Y:170:ARG:NH1	1.90	0.69
1:C:1366:HIS:N	1:C:1366:HIS:ND1	2.40	0.69
1:C:1627:ILE:O	1:C:1627:ILE:HD12	1.92	0.69
1:C:1228:TRP:H	1:C:1251:THR:CG2	1.98	0.69
1:A:234:GLU:HG3	1:A:235:TYR:CE2	2.28	0.69
1:A:1404:ALA:HB1	1:A:1493:PHE:HE2	1.57	0.69
1:A:1108:VAL:HG11	1:A:1164:ILE:HG22	1.73	0.69
1:C:24:VAL:HA	1:C:655:THR:OG1	1.93	0.69
2:D:262:PHE:CE1	2:D:282:ARG:HG3	2.27	0.69
2:D:224:PHE:CZ	2:D:329:VAL:HG22	2.27	0.69
1:C:144:ARG:HD2	1:C:146:TYR:HE1	1.58	0.69
2:D:824:VAL:HG22	2:D:825:VAL:H	1.58	0.69
1:C:257:ASN:HD21	1:C:892:SER:HA	1.58	0.69
1:A:1423:VAL:HG13	1:A:1496:TYR:CD2	2.27	0.69
2:B:230:PRO:HG3	2:B:333:GLN:HG2	1.73	0.69
2:D:127:PHE:HE2	2:D:602:ILE:HG23	1.57	0.69
2:B:1371:TYR:CG	2:B:1377:SER:HB3	2.27	0.69
1:C:77:ASN:HD21	1:C:81:ASN:HB2	1.57	0.69
1:C:1549:LYS:NZ	1:C:1667:PHE:HB3	2.07	0.69
1:C:115:LYS:HB2	1:C:654:LEU:HD21	1.74	0.69
1:C:1525:CYS:O	1:C:1529:GLU:HG3	1.93	0.69
1:C:837:GLU:HG2	1:C:1488:LEU:HA	1.75	0.69
2:D:840:VAL:HG12	2:D:841:ASN:N	2.06	0.69
1:A:700:TYR:CD2	1:A:700:TYR:C	2.64	0.69
1:A:127:PHE:CE2	1:A:623:VAL:HG13	2.27	0.69
1:C:148:LEU:HD23	1:C:152:LEU:CD1	2.22	0.69
2:D:950:LEU:HD22	2:D:1329:TYR:CZ	2.28	0.69
1:C:1423:VAL:HG13	1:C:1496:TYR:CE2	2.27	0.69
2:D:1382:ILE:HB	2:D:1425:ILE:HB	1.74	0.69
1:C:1347:ILE:O	1:C:1347:ILE:HG22	1.93	0.69
2:B:859:ALA:HB1	2:B:866:TYR:CD1	2.28	0.69
1:A:1429:PRO:HB2	1:A:1432:ILE:CG1	2.23	0.69
1:C:587:THR:HG22	1:C:789:ALA:HB2	1.74	0.69
3:X:188:LYS:HD3	3:X:202:ASP:HA	1.75	0.69
1:C:307:VAL:CG1	1:C:313:TYR:HB2	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1086:LEU:HD12	1:A:1095:GLN:HG3	1.75	0.69
2:D:1593:THR:HG22	2:D:1594:LYS:N	2.07	0.69
1:C:1069:TRP:CZ3	1:C:1451:THR:HG21	2.28	0.69
2:D:148:PHE:CB	2:D:800:ILE:HD11	2.22	0.69
1:A:549:GLU:CD	1:A:549:GLU:H	1.96	0.69
1:A:1218:VAL:HG12	1:A:1219:LYS:N	2.07	0.69
2:D:813:VAL:HG12	2:D:840:VAL:HG22	1.75	0.69
1:C:596:MET:N	1:C:782:ARG:HH11	1.85	0.69
2:B:136:ILE:HA	2:B:215:ASP:O	1.92	0.69
1:A:123:ASN:HB3	1:A:209:PHE:HD1	1.56	0.69
1:C:166:PRO:HD3	1:C:199:TRP:HA	1.75	0.69
2:D:1610:TRP:CD2	2:D:1628:PHE:CD2	2.81	0.69
1:A:92:LEU:HD12	1:C:1029:ASN:ND2	2.07	0.69
2:D:114:ARG:O	2:D:115:LEU:HD23	1.93	0.69
2:D:1435:ASP:OD1	5:D:2003:NAG:H81	1.92	0.69
2:B:1381:ILE:HG21	2:B:1459:TYR:HE1	1.57	0.69
1:A:467:ILE:CG2	1:A:486:VAL:HG22	2.23	0.68
1:A:222:TYR:HD2	1:A:223:VAL:N	1.90	0.68
2:B:950:LEU:HD22	2:B:1329:TYR:CE1	2.27	0.68
3:X:98:LEU:HD22	3:X:101:GLN:OE1	1.93	0.68
2:D:1446:PHE:CD2	2:D:1448:VAL:HG22	2.27	0.68
1:A:1180:LEU:O	1:A:1182:ALA:N	2.26	0.68
1:A:1320:LYS:CD	1:A:1321:GLY:H	2.06	0.68
1:A:1525:CYS:N	1:A:1528:VAL:HG13	2.07	0.68
1:A:494:ASP:O	1:A:496:ILE:N	2.27	0.68
2:D:1279:ILE:HG22	2:D:1288:ILE:HB	1.74	0.68
2:D:548:LEU:HD22	2:D:793:SER:HB3	1.75	0.68
1:A:25:ILE:H	1:A:655:THR:HG21	1.56	0.68
1:C:1504:GLN:HG3	1:C:1505:CYS:N	2.09	0.68
1:A:61:ASP:O	1:A:62:LYS:HB2	1.92	0.68
1:A:639:GLY:HA2	1:A:648:LEU:HD13	1.74	0.68
2:D:197:TRP:HB2	2:D:214:PHE:CE1	2.28	0.68
1:C:1268:ASN:H	1:C:1268:ASN:HD22	1.42	0.68
1:A:255:PHE:HE1	1:A:258:LYS:HB2	1.56	0.68
2:D:1424:ILE:HD13	2:D:1424:ILE:H	1.59	0.68
1:C:91:GLN:O	1:C:92:LEU:HG	1.92	0.68
2:B:1424:ILE:HG12	2:B:1426:TYR:CE2	2.28	0.68
2:D:913:LEU:HD23	2:D:914:LYS:N	2.09	0.68
1:C:705:VAL:N	1:C:739:ARG:HH22	1.92	0.68
1:A:543:TYR:O	1:A:543:TYR:HD1	1.77	0.68
1:C:1671:ILE:HA	1:C:1675:GLY:H	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1366:HIS:ND1	1:A:1366:HIS:N	2.41	0.68
1:A:690:TYR:CG	1:A:690:TYR:O	2.46	0.68
3:Y:64:VAL:HG11	3:Y:95:LYS:O	1.93	0.68
1:A:228:SER:O	1:A:252:ALA:HA	1.93	0.68
2:B:114:ARG:O	2:B:115:LEU:HD23	1.93	0.68
1:A:938:SER:O	1:A:940:SER:N	2.27	0.68
1:A:1608:ASN:O	1:A:1610:GLU:N	2.27	0.68
1:C:1226:ARG:CZ	1:C:1266:TYR:HE1	2.07	0.68
2:B:1345:LEU:HA	2:B:1368:CYS:O	1.93	0.68
1:C:307:VAL:HG13	1:C:313:TYR:HB2	1.76	0.68
1:C:104:LEU:HD12	1:C:105:GLU:H	1.59	0.68
2:B:464:PHE:HB2	2:B:504:VAL:O	1.94	0.68
1:C:774:LEU:HD12	1:C:799:ILE:HD11	1.76	0.68
1:A:174:VAL:HG22	1:A:175:GLU:N	2.09	0.68
2:D:1313:VAL:HG11	2:D:1323:MET:SD	2.34	0.68
1:A:1386:ILE:HG13	1:A:1387:GLU:H	1.59	0.68
1:A:1673:LEU:O	1:A:1674:ASN:HB2	1.94	0.68
1:C:25:ILE:HD13	1:C:41:ILE:HB	1.76	0.68
1:C:641:ASN:HD21	1:C:643:ALA:HB3	1.58	0.68
1:A:1068:VAL:HG13	1:A:1069:TRP:N	2.08	0.68
1:C:742:ILE:HG13	1:C:752:LEU:O	1.94	0.68
1:C:1323:LEU:HD12	1:C:1324:HIS:H	1.59	0.68
1:C:148:LEU:HD23	1:C:152:LEU:HD12	1.76	0.68
1:A:255:PHE:CE1	1:A:258:LYS:CB	2.77	0.68
1:A:1127:ILE:H	1:A:1127:ILE:HD12	1.59	0.68
1:C:1673:LEU:O	1:C:1674:ASN:HB2	1.94	0.68
1:A:1585:TYR:CD2	1:A:1586:LYS:N	2.61	0.68
1:A:698:CYS:C	1:A:700:TYR:H	1.97	0.68
3:Y:86:LEU:HG	3:Y:91:LYS:CB	2.24	0.68
1:A:101:TYR:CE2	1:C:1305:LYS:HE3	2.28	0.68
1:C:1179:THR:HG21	1:C:1208:ILE:HD13	1.76	0.68
3:X:134:THR:HG22	3:X:153:PHE:O	1.94	0.68
1:A:77:ASN:HD21	1:A:81:ASN:HB2	1.59	0.68
1:C:1034:PHE:CE2	1:C:1041:GLU:HG2	2.29	0.68
1:A:829:ILE:HG12	1:A:925:LYS:HG2	1.74	0.68
3:X:228:ILE:O	3:X:228:ILE:HG22	1.94	0.68
3:X:166:ASP:OD2	3:X:207:LEU:HG	1.94	0.68
1:C:1631:PHE:N	1:C:1631:PHE:CD2	2.60	0.68
1:C:784:LYS:HG2	1:C:785:GLN:N	2.07	0.68
2:D:28:ILE:HD12	2:D:42:LEU:HD23	1.74	0.68
1:C:700:TYR:C	1:C:700:TYR:CD2	2.63	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1123:GLN:NE2	1:A:1123:GLN:HA	2.08	0.68
1:C:382:LEU:HD13	1:C:415:ASP:C	2.14	0.68
1:C:938:SER:C	1:C:940:SER:H	1.96	0.68
1:C:373:VAL:HG23	1:C:418:ALA:HB3	1.74	0.68
1:A:706:ASN:ND2	1:A:709:GLU:N	2.38	0.68
1:C:222:TYR:C	1:C:222:TYR:HD2	1.97	0.68
1:C:1266:TYR:O	1:C:1266:TYR:CD1	2.45	0.68
2:B:218:LYS:HB3	2:B:822:TYR:HD2	1.59	0.68
1:C:330:ILE:HG22	1:C:337:SER:HB2	1.76	0.68
2:B:133:ASP:HA	2:B:757:TRP:HZ3	1.59	0.68
1:A:161:LEU:HD11	1:A:185:PHE:CD1	2.29	0.68
1:A:40:VAL:CG2	1:A:512:PHE:HD1	2.06	0.67
3:Y:150:ILE:HD12	3:Y:150:ILE:O	1.93	0.67
1:A:1309:LEU:HD13	1:A:1328:MET:HG3	1.75	0.67
1:C:1341:LEU:HB2	1:C:1342:LEU:CD2	2.24	0.67
1:A:365:PRO:HD2	1:A:464:TYR:CE2	2.28	0.67
1:C:517:LYS:HG2	1:C:518:PHE:H	1.59	0.67
1:A:1320:LYS:HD2	1:A:1321:GLY:H	1.58	0.67
2:B:243:PHE:HD1	2:B:314:LEU:HD23	1.58	0.67
1:A:1450:PHE:CZ	1:A:1475:VAL:HB	2.28	0.67
2:D:28:ILE:HG12	2:D:628:LEU:HD13	1.75	0.67
1:C:471:ASP:OD2	1:C:474:LYS:HD2	1.94	0.67
1:C:1159:CYS:O	1:C:1161:LEU:N	2.27	0.67
1:A:517:LYS:HG2	1:A:518:PHE:H	1.58	0.67
1:C:1202:HIS:CD2	1:C:1203:PRO:HD2	2.28	0.67
3:X:179:LEU:HD12	3:X:180:TYR:N	2.10	0.67
1:A:612:VAL:HG21	1:A:769:PHE:CZ	2.29	0.67
1:A:1358:THR:HB	1:A:1360:HIS:CE1	2.29	0.67
2:B:261:ALA:CB	2:B:285:ILE:HD11	2.24	0.67
1:A:470:THR:HG22	2:B:450:THR:CG2	2.22	0.67
1:C:576:SER:HB2	1:C:589:SER:CB	2.24	0.67
1:A:267:ILE:HD11	1:A:299:VAL:HG11	1.74	0.67
1:A:357:VAL:HA	1:A:672:ILE:HG21	1.76	0.67
3:Y:166:ASP:CG	3:Y:207:LEU:HD23	2.14	0.67
3:X:80:GLN:HG3	3:X:114:GLY:C	2.15	0.67
1:C:1142:LEU:HD11	1:C:1179:THR:HA	1.77	0.67
1:A:1423:VAL:HG13	1:A:1496:TYR:CE2	2.30	0.67
1:A:88:GLN:O	1:A:90:LYS:HD3	1.94	0.67
1:A:704:CYS:C	1:A:739:ARG:HH22	1.98	0.67
1:A:1112:GLN:HE21	1:A:1171:ALA:HB2	1.59	0.67
1:A:1244:THR:HG22	1:A:1246:ARG:N	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:596:MET:H	1:C:782:ARG:NH1	1.87	0.67
2:B:149:SER:O	2:B:794:PHE:HE1	1.78	0.67
1:A:1266:TYR:CD1	1:A:1266:TYR:O	2.48	0.67
1:A:640:LEU:O	1:A:640:LEU:HD12	1.93	0.67
1:A:207:GLU:O	1:A:209:PHE:N	2.28	0.67
1:A:1034:PHE:CE2	1:A:1041:GLU:HG2	2.29	0.67
2:D:1539:ILE:HD12	2:D:1539:ILE:H	1.59	0.67
2:D:556:ILE:H	2:D:556:ILE:HD12	1.58	0.67
1:A:222:TYR:C	1:A:222:TYR:HD2	1.98	0.67
2:B:1480:LEU:HD12	2:B:1481:LEU:N	2.10	0.67
1:C:1049:LEU:HD11	1:C:1089:VAL:CG1	2.24	0.67
2:D:531:ILE:HD11	2:D:634:LEU:HD23	1.76	0.67
1:C:1493:PHE:CD1	1:C:1493:PHE:C	2.67	0.67
2:B:299:PHE:HE1	2:B:303:PHE:HD2	1.43	0.67
1:A:1019:PHE:CD2	1:A:1019:PHE:C	2.67	0.67
1:C:765:ILE:HD13	1:C:767:SER:O	1.94	0.67
1:A:1163:LYS:O	1:A:1166:THR:HG22	1.94	0.67
1:A:1341:LEU:H	1:A:1341:LEU:HD22	1.60	0.67
2:B:1602:THR:C	2:B:1604:ASN:H	1.97	0.67
1:A:104:LEU:HD12	1:A:105:GLU:H	1.59	0.67
2:B:262:PHE:HE1	2:B:282:ARG:HG3	1.60	0.67
1:A:586:GLN:O	1:A:586:GLN:HG3	1.95	0.67
1:C:180:ILE:HB	1:C:599:TRP:CE3	2.30	0.67
1:A:596:MET:N	1:A:782:ARG:HD3	2.10	0.67
1:A:742:ILE:HG13	1:A:752:LEU:O	1.94	0.67
1:C:690:TYR:C	1:C:692:HIS:H	1.98	0.67
2:D:1444:LYS:CE	2:D:1447:GLU:HA	2.25	0.67
1:A:190:ILE:HG22	1:A:191:PRO:N	2.09	0.67
1:A:1142:LEU:HD11	1:A:1179:THR:HA	1.77	0.67
3:Y:47:HIS:CE1	3:Y:181:LYS:HE2	2.30	0.67
1:A:865:ILE:O	1:A:866:CYS:O	2.11	0.67
1:A:109:LYS:HD3	1:A:110:HIS:CE1	2.30	0.67
1:C:1535:MET:H	1:C:1608:ASN:HB3	1.60	0.67
1:C:1077:TRP:NE1	1:C:1147:PHE:CE1	2.62	0.67
2:B:1562:GLN:HE22	2:B:1596:LYS:HZ2	1.42	0.67
2:B:1505:ARG:NH1	2:B:1505:ARG:HG3	1.93	0.67
1:C:474:LYS:HD3	1:C:474:LYS:H	1.60	0.67
3:Y:41:HIS:O	3:Y:42:ASP:HB2	1.95	0.67
1:C:493:ILE:HG23	1:C:495:LYS:N	2.10	0.67
2:D:1594:LYS:HA	2:D:1594:LYS:CE	2.15	0.67
1:C:1504:GLN:HG3	1:C:1505:CYS:CA	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:783:SER:HB2	2:B:787:TRP:HZ2	1.60	0.67
1:C:473:HIS:O	1:C:473:HIS:CD2	2.47	0.67
2:B:824:VAL:HG22	2:B:825:VAL:H	1.60	0.67
1:C:1341:LEU:H	1:C:1341:LEU:HD22	1.60	0.67
2:B:30:PRO:HG3	2:B:489:ILE:HG13	1.77	0.67
2:D:603:GLU:O	2:D:605:SER:N	2.27	0.67
2:D:829:GLN:HG3	2:D:1480:LEU:CD1	2.07	0.67
1:C:944:LEU:HD23	1:C:944:LEU:N	2.10	0.67
1:A:459:SER:OG	1:A:461:SER:HB3	1.94	0.67
3:X:86:LEU:HG	3:X:91:LYS:CB	2.23	0.67
1:A:796:THR:HG23	1:A:818:LYS:CB	2.25	0.67
2:D:144:LEU:H	2:D:144:LEU:HD23	1.59	0.67
2:D:243:PHE:HD1	2:D:314:LEU:HD23	1.58	0.67
1:A:530:VAL:HG23	1:A:534:MET:HE2	1.75	0.66
1:A:1219:LYS:CE	1:A:1239:VAL:HG21	2.25	0.66
2:D:481:TYR:HB2	2:D:520:PHE:HE1	1.58	0.66
1:C:698:CYS:C	1:C:700:TYR:H	1.97	0.66
3:Y:128:LYS:HB2	3:Y:158:GLU:HB2	1.77	0.66
1:C:1323:LEU:HD12	1:C:1324:HIS:N	2.10	0.66
1:A:947:ARG:O	1:A:949:ILE:HG12	1.95	0.66
1:C:222:TYR:C	1:C:222:TYR:CD2	2.68	0.66
2:B:196:THR:HG23	2:B:215:ASP:OD1	1.95	0.66
2:B:422:ARG:H	2:B:422:ARG:CD	2.08	0.66
2:B:1382:ILE:HB	2:B:1425:ILE:HB	1.77	0.66
1:C:583:SER:O	1:C:586:GLN:HG2	1.94	0.66
3:X:166:ASP:CG	3:X:207:LEU:HD23	2.14	0.66
1:A:1643:THR:HG22	1:A:1644:TRP:N	2.09	0.66
2:B:1444:LYS:CE	2:B:1447:GLU:HA	2.25	0.66
1:C:1226:ARG:HB3	1:C:1269:PRO:HB2	1.75	0.66
1:A:474:LYS:H	1:A:474:LYS:HD3	1.59	0.66
2:B:599:TRP:HA	2:B:599:TRP:CE3	2.29	0.66
2:B:1450:PHE:CD1	2:B:1451:ILE:N	2.64	0.66
1:A:115:LYS:CB	1:A:654:LEU:HD21	2.25	0.66
1:C:1643:THR:HG22	1:C:1644:TRP:N	2.11	0.66
1:C:480:GLU:O	1:C:530:VAL:HG12	1.95	0.66
1:A:473:HIS:CD2	1:A:473:HIS:O	2.49	0.66
1:C:1113:LEU:CD2	1:C:1114:ASP:H	2.07	0.66
1:C:525:SER:H	2:D:401:ASN:HD21	1.40	0.66
2:D:131:GLN:OE1	2:D:146:ARG:NH1	2.28	0.66
3:Y:205:ASP:O	3:Y:206:LYS:C	2.33	0.66
1:A:25:ILE:HD13	1:A:41:ILE:HB	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:640:LEU:HD12	1:C:640:LEU:O	1.95	0.66
1:C:1076:THR:CG2	1:C:1120:GLU:HA	2.24	0.66
1:C:1309:LEU:HD13	1:C:1328:MET:HG3	1.77	0.66
2:D:1602:THR:C	2:D:1604:ASN:H	1.99	0.66
2:B:1606:TRP:CD1	2:B:1606:TRP:C	2.69	0.66
1:C:467:ILE:CG2	1:C:486:VAL:HG22	2.25	0.66
1:C:1219:LYS:HD3	1:C:1239:VAL:HG21	1.77	0.66
1:C:706:ASN:ND2	1:C:709:GLU:N	2.38	0.66
2:D:241:GLU:O	2:D:296:ARG:HD3	1.95	0.66
1:A:1226:ARG:HB3	1:A:1269:PRO:HB2	1.78	0.66
1:A:471:ASP:OD2	1:A:474:LYS:HD2	1.96	0.66
1:A:307:VAL:HG13	1:A:313:TYR:HB2	1.78	0.66
2:D:1450:PHE:CD1	2:D:1451:ILE:N	2.64	0.66
3:Y:228:ILE:HG22	3:Y:228:ILE:O	1.93	0.66
1:C:685:GLU:HA	1:C:685:GLU:OE1	1.94	0.66
1:A:484:ILE:CD1	1:A:540:LEU:HD21	2.26	0.66
1:C:931:PRO:HB2	1:C:1366:HIS:CD2	2.30	0.66
1:C:1562:LYS:CD	1:C:1664:LEU:HD21	2.12	0.66
1:C:127:PHE:HD2	1:C:623:VAL:HG22	1.60	0.66
1:C:1024:TYR:HA	1:C:1302:LEU:CD2	2.26	0.66
2:D:964:ILE:HG13	2:D:1302:THR:HG23	1.77	0.66
1:C:1352:PHE:CD2	1:C:1352:PHE:N	2.62	0.66
1:A:238:ILE:HB	1:A:347:TYR:CD1	2.31	0.66
1:C:234:GLU:HG3	1:C:235:TYR:CE2	2.29	0.66
1:A:702:GLY:CA	1:A:728:PHE:CE1	2.78	0.66
1:A:690:TYR:CD2	1:A:690:TYR:O	2.49	0.66
1:C:190:ILE:HG22	1:C:191:PRO:N	2.11	0.66
2:B:961:THR:CG2	2:B:1327:THR:HG23	2.25	0.66
2:D:1445:HIS:CG	2:D:1446:PHE:H	2.14	0.66
2:B:147:VAL:HG12	2:B:183:PHE:HE1	1.60	0.66
2:B:476:ILE:HD11	2:B:524:TYR:CG	2.30	0.66
1:A:632:LEU:N	1:A:632:LEU:HD23	2.11	0.66
1:C:639:GLY:H	1:C:645:VAL:HA	1.60	0.66
1:C:935:LYS:HD3	1:C:1373:GLU:OE2	1.94	0.66
1:A:869:GLU:C	1:A:871:PRO:HD3	2.15	0.66
1:C:670:LYS:HD2	1:C:671:GLU:HG2	1.78	0.66
3:Y:98:LEU:HD22	3:Y:101:GLN:OE1	1.96	0.66
1:C:255:PHE:HE1	1:C:258:LYS:HB2	1.61	0.66
2:D:961:THR:CG2	2:D:1327:THR:HG23	2.25	0.66
2:B:1417:MET:HG2	2:B:1443:LEU:HD23	1.76	0.66
1:C:228:SER:O	1:C:252:ALA:HA	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:ILE:CG2	1:A:420:PHE:HB2	2.23	0.66
1:A:968:VAL:HG12	1:A:1368:THR:HG22	1.78	0.66
2:B:523:TYR:CD1	2:B:523:TYR:C	2.68	0.66
2:D:69:PHE:CG	2:D:87:ILE:HG22	2.31	0.66
1:C:1213:LYS:HE2	1:C:1266:TYR:CD2	2.31	0.66
2:D:1345:LEU:HA	2:D:1368:CYS:O	1.96	0.66
1:C:436:LYS:HB2	1:C:449:ARG:HG2	1.77	0.66
1:C:1127:ILE:HD11	1:C:1143:TYR:CD2	2.31	0.66
1:A:1566:THR:O	1:A:1613:LYS:HE3	1.95	0.66
2:B:131:GLN:OE1	2:B:146:ARG:NH1	2.29	0.66
1:A:1618:LEU:HD22	1:A:1619:ILE:H	1.60	0.66
2:D:236:TYR:CZ	2:D:424:ARG:HD2	2.31	0.66
1:C:1379:LEU:HD11	1:C:1505:CYS:O	1.95	0.66
1:C:671:GLU:O	1:C:672:ILE:HB	1.96	0.66
1:C:981:GLY:CA	1:C:1333:PHE:HB2	2.25	0.66
1:C:1034:PHE:CD2	1:C:1041:GLU:HG2	2.30	0.66
2:D:57:PHE:HD1	2:D:59:HIS:HE2	1.44	0.66
2:D:230:PRO:HG3	2:D:333:GLN:HG2	1.77	0.66
1:A:1202:HIS:CD2	1:A:1203:PRO:HD2	2.31	0.66
1:C:495:LYS:HE2	1:C:495:LYS:HA	1.76	0.65
1:A:955:ARG:NH1	1:A:1352:PHE:HA	2.11	0.65
2:D:563:MET:HB3	2:D:778:PHE:CE2	2.31	0.65
1:A:62:LYS:HE2	1:A:103:TYR:CE2	2.31	0.65
1:A:1163:LYS:HZ1	1:C:1109:GLU:CD	1.99	0.65
1:C:705:VAL:HA	1:C:739:ARG:NH1	2.11	0.65
2:B:194:LEU:HD12	2:B:217:ARG:HA	1.78	0.65
1:A:25:ILE:HB	1:A:654:LEU:HB2	1.78	0.65
1:C:511:HIS:CE1	3:Y:149:SER:HG	2.14	0.65
1:A:87:ILE:HD13	1:A:87:ILE:H	1.61	0.65
1:A:489:LYS:HG3	1:A:490:SER:H	1.60	0.65
1:A:436:LYS:HB2	1:A:449:ARG:HG2	1.78	0.65
1:A:641:ASN:O	1:A:643:ALA:N	2.29	0.65
1:A:895:LEU:HD12	1:A:896:VAL:N	2.11	0.65
1:A:633:GLY:O	1:A:634:CYS:HB2	1.96	0.65
1:C:704:CYS:C	1:C:739:ARG:HH22	2.00	0.65
1:C:934:VAL:CG2	1:C:1366:HIS:CD2	2.79	0.65
1:C:505:SER:OG	1:C:506:LYS:HD3	1.97	0.65
1:A:935:LYS:HD3	1:A:1373:GLU:OE2	1.95	0.65
1:A:884:VAL:CG1	1:A:886:GLN:HG2	2.26	0.65
1:C:123:ASN:HB3	1:C:209:PHE:HD1	1.61	0.65
1:A:1585:TYR:CG	1:A:1586:LYS:N	2.64	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:481:TYR:CE2	2:D:493:GLY:CA	2.79	0.65
1:C:884:VAL:O	1:C:885:ARG:CB	2.42	0.65
1:C:443:PRO:HD2	1:C:446:ASN:HB2	1.78	0.65
2:D:128:LEU:O	2:D:129:PHE:CD1	2.49	0.65
2:B:1491:ARG:HG3	2:B:1492:CYS:H	1.62	0.65
1:C:1145:THR:O	1:C:1149:VAL:HG23	1.97	0.65
3:X:47:HIS:HE1	3:X:181:LYS:HE2	1.62	0.65
3:Y:207:LEU:HD12	3:Y:207:LEU:C	2.14	0.65
1:C:1667:PHE:O	1:C:1671:ILE:HG22	1.97	0.65
1:C:535:VAL:HG23	1:C:536:PRO:CD	2.15	0.65
2:B:69:PHE:CG	2:B:87:ILE:HG22	2.32	0.65
3:X:41:HIS:O	3:X:42:ASP:HB2	1.96	0.65
2:D:133:ASP:HA	2:D:757:TRP:HZ3	1.60	0.65
1:A:875:HIS:HB3	2:B:901:GLN:NE2	2.11	0.65
1:A:505:SER:OG	1:A:506:LYS:HD3	1.97	0.65
1:C:504:LEU:HD12	1:C:509:ILE:HG23	1.77	0.65
1:C:40:VAL:HG21	1:C:512:PHE:HD1	1.62	0.65
1:C:514:THR:O	1:C:515:ARG:HD3	1.95	0.65
1:C:1564:SER:HB2	1:C:1616:GLN:HG3	1.78	0.65
2:D:282:ARG:C	2:D:283:ILE:HD12	2.17	0.65
1:A:884:VAL:O	1:A:885:ARG:CB	2.41	0.65
2:D:239:GLY:H	2:D:296:ARG:NH2	1.95	0.65
1:C:1123:GLN:NE2	1:C:1123:GLN:HA	2.11	0.65
2:D:422:ARG:CD	2:D:422:ARG:H	2.08	0.65
3:Y:43:ILE:HG23	3:Y:44:ARG:H	1.60	0.65
1:C:1180:LEU:O	1:C:1182:ALA:N	2.29	0.65
1:A:1034:PHE:CD2	1:A:1041:GLU:HG2	2.32	0.65
2:D:127:PHE:CE2	2:D:602:ILE:HG23	2.32	0.65
3:Y:179:LEU:HD12	3:Y:180:TYR:N	2.11	0.65
2:D:421:PRO:HB2	2:D:423:GLU:OE2	1.96	0.65
1:C:24:VAL:HG11	1:C:543:TYR:CE2	2.31	0.65
1:C:1075:SER:HB2	1:C:1120:GLU:OE1	1.96	0.65
1:C:1076:THR:HG21	1:C:1120:GLU:HA	1.79	0.65
1:C:936:ARG:NH2	1:C:1284:PHE:CE1	2.64	0.65
1:A:222:TYR:CD2	1:A:222:TYR:C	2.70	0.65
1:A:60:PRO:CD	1:A:61:ASP:N	2.56	0.65
2:B:783:SER:HB2	2:B:787:TRP:CZ2	2.32	0.65
1:A:705:VAL:N	1:A:739:ARG:HH22	1.94	0.65
1:A:1381:ILE:HG12	1:A:1382:ASP:N	2.12	0.65
2:D:557:GLN:HE21	2:D:563:MET:CE	2.10	0.65
2:B:23:ALA:HB3	2:B:528:ASN:HD22	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:237:ILE:HD11	2:B:309:LEU:CB	2.24	0.65
1:C:1231:ASN:HB2	1:C:1235:LYS:HG3	1.77	0.65
2:B:460:LEU:HD23	2:B:460:LEU:O	1.97	0.65
1:A:131:ASP:O	1:A:132:LYS:HG2	1.97	0.65
1:A:865:ILE:O	1:A:866:CYS:C	2.35	0.65
1:C:863:GLU:H	1:C:863:GLU:CD	2.00	0.65
2:B:144:LEU:H	2:B:144:LEU:HD23	1.62	0.65
3:Y:53:GLU:HB3	3:Y:55:PHE:CE2	2.32	0.65
1:C:492:TYR:HD2	1:C:493:ILE:H	1.44	0.65
1:C:690:TYR:O	1:C:690:TYR:CD2	2.49	0.65
2:B:825:VAL:N	2:B:828:GLU:OE1	2.29	0.65
2:D:1515:ALA:HB1	2:D:1523:VAL:HG21	1.79	0.65
2:B:1445:HIS:CG	2:B:1446:PHE:H	2.15	0.65
1:C:1429:PRO:HB2	1:C:1432:ILE:HG13	1.78	0.65
2:B:1371:TYR:O	2:B:1432:HIS:HA	1.97	0.65
2:B:262:PHE:CE1	2:B:282:ARG:HG3	2.30	0.65
2:B:887:LEU:CD2	2:B:1490:CYS:HB3	2.27	0.65
2:D:167:THR:HG23	2:D:171:ILE:H	1.61	0.65
3:X:50:TYR:HE2	3:X:170:ARG:NH1	1.94	0.65
1:C:24:VAL:CG1	1:C:24:VAL:O	2.45	0.65
1:A:931:PRO:HB2	1:A:1366:HIS:CD2	2.32	0.65
1:C:884:VAL:CG1	1:C:886:GLN:HG2	2.27	0.65
2:B:481:TYR:HB2	2:B:520:PHE:HE1	1.59	0.65
1:A:1259:LEU:HD11	1:A:1300:TYR:HB2	1.78	0.65
1:A:690:TYR:C	1:A:692:HIS:H	2.00	0.65
2:D:1387:LEU:HB2	2:D:1390:PHE:CD2	2.32	0.65
1:C:1304:VAL:CG1	1:C:1305:LYS:N	2.60	0.65
2:B:603:GLU:O	2:B:605:SER:N	2.28	0.65
1:A:1244:THR:H	1:A:1247:MET:HE3	1.62	0.64
1:A:492:TYR:HD2	1:A:493:ILE:H	1.45	0.64
2:D:299:PHE:HE1	2:D:303:PHE:HD2	1.45	0.64
1:A:705:VAL:HA	1:A:739:ARG:NH1	2.12	0.64
1:A:307:VAL:CG1	1:A:313:TYR:HB2	2.27	0.64
2:D:433:ILE:HG22	2:D:434:ALA:O	1.96	0.64
2:B:364:VAL:HG21	2:B:379:VAL:HG21	1.79	0.64
1:A:554:LEU:H	1:A:658:ASN:HD22	1.43	0.64
1:C:1244:THR:HG22	1:C:1246:ARG:N	2.13	0.64
1:A:1352:PHE:N	1:A:1352:PHE:CD2	2.62	0.64
2:B:838:ASN:OD1	2:B:840:VAL:HG23	1.97	0.64
1:A:423:ASN:HB3	2:B:501:GLN:NE2	2.13	0.64
3:X:70:SER:CB	3:X:91:LYS:HE3	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:814:PHE:HZ	2:B:846:VAL:HG21	1.62	0.64
2:B:913:LEU:HD23	2:B:914:LYS:N	2.12	0.64
3:X:170:ARG:O	3:X:174:VAL:HG23	1.97	0.64
1:A:494:ASP:OD1	1:A:495:LYS:HE2	1.97	0.64
1:C:207:GLU:O	1:C:209:PHE:N	2.29	0.64
2:D:1506:ILE:CD1	2:D:1628:PHE:HE1	2.09	0.64
3:X:179:LEU:HD12	3:X:180:TYR:H	1.62	0.64
2:B:524:TYR:O	2:B:524:TYR:HD1	1.79	0.64
1:C:1427:SER:HB3	1:C:1492:THR:HG23	1.79	0.64
1:A:1627:ILE:HG13	1:A:1627:ILE:O	1.98	0.64
1:A:656:ASN:HB3	1:A:659:ALA:H	1.63	0.64
1:C:24:VAL:HG11	1:C:543:TYR:OH	1.97	0.64
1:C:829:ILE:HG12	1:C:925:LYS:HG2	1.80	0.64
1:C:119:ILE:O	1:C:119:ILE:HD12	1.97	0.64
1:C:1086:LEU:HD12	1:C:1095:GLN:HG3	1.79	0.64
2:D:26:THR:OG1	2:D:44:GLU:HB2	1.98	0.64
1:A:837:GLU:HG2	1:A:1488:LEU:HA	1.78	0.64
1:A:947:ARG:O	1:A:949:ILE:N	2.30	0.64
1:C:1566:THR:O	1:C:1613:LYS:HE3	1.98	0.64
1:C:1423:VAL:CG1	1:C:1496:TYR:CE2	2.80	0.64
1:A:917:TRP:HB3	2:B:558:MET:SD	2.38	0.64
3:X:205:ASP:O	3:X:206:LYS:C	2.33	0.64
1:C:429:THR:HA	1:C:456:ALA:HB2	1.80	0.64
3:X:170:ARG:HD3	3:X:203:LEU:CD2	2.27	0.64
1:A:1077:TRP:NE1	1:A:1147:PHE:CE1	2.66	0.64
2:D:523:TYR:C	2:D:523:TYR:CD1	2.70	0.64
1:A:1504:GLN:HG3	1:A:1505:CYS:N	2.11	0.64
1:A:820:PHE:O	1:A:821:LYS:HG3	1.98	0.64
3:Y:64:VAL:HG23	3:Y:71:ASN:OD1	1.97	0.64
1:C:255:PHE:CE1	1:C:258:LYS:CB	2.80	0.64
2:D:1446:PHE:HB3	2:D:1448:VAL:HG22	1.79	0.64
1:C:1548:ARG:HD3	1:C:1548:ARG:H	1.63	0.64
2:D:1547:VAL:HG23	2:D:1557:ARG:NH1	2.12	0.64
2:B:1623:LYS:HA	2:B:1623:LYS:HZ3	1.63	0.64
1:C:362:PHE:CE1	1:C:640:LEU:HB2	2.33	0.64
1:C:60:PRO:HD2	1:C:61:ASP:N	2.09	0.64
2:D:149:SER:O	2:D:794:PHE:HE1	1.80	0.64
1:A:583:SER:O	1:A:586:GLN:HG2	1.96	0.64
2:B:421:PRO:HB2	2:B:423:GLU:OE2	1.98	0.64
1:C:161:LEU:H	1:C:161:LEU:HD12	1.62	0.64
1:A:24:VAL:CG1	1:A:24:VAL:O	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:VAL:HG23	1:A:536:PRO:CD	2.16	0.64
1:A:1024:TYR:HA	1:A:1302:LEU:CD2	2.28	0.64
2:B:1615:GLU:HB3	2:B:1621:PHE:HD1	1.63	0.64
1:A:1365:VAL:CG2	1:A:1366:HIS:H	2.08	0.64
2:D:136:ILE:HA	2:D:215:ASP:O	1.97	0.64
2:D:130:ILE:HD13	2:D:199:ILE:HG22	1.80	0.64
2:D:1505:ARG:CZ	2:D:1623:LYS:NZ	2.61	0.64
1:C:260:VAL:HG12	1:C:261:THR:N	2.12	0.64
2:D:599:TRP:CE3	2:D:599:TRP:HA	2.31	0.64
2:D:464:PHE:HB2	2:D:504:VAL:O	1.98	0.64
1:A:480:GLU:O	1:A:530:VAL:HG12	1.98	0.64
1:A:24:VAL:CG2	1:A:554:LEU:HD11	2.27	0.64
1:C:1525:CYS:N	1:C:1528:VAL:HG13	2.13	0.64
1:C:883:CYS:O	1:C:884:VAL:O	2.16	0.64
1:A:1232:LEU:CD1	1:A:1233:GLN:HE21	2.11	0.64
1:A:1323:LEU:HD12	1:A:1324:HIS:H	1.63	0.64
1:C:436:LYS:HA	1:C:448:ALA:O	1.97	0.64
3:X:194:LYS:NZ	3:X:197:ASN:HB2	2.10	0.64
2:D:964:ILE:CG2	2:D:964:ILE:O	2.46	0.64
3:X:128:LYS:HB2	3:X:158:GLU:HB2	1.78	0.64
1:A:1304:VAL:CG1	1:A:1305:LYS:N	2.61	0.64
3:Y:70:SER:CB	3:Y:91:LYS:HE3	2.28	0.64
2:D:218:LYS:HB3	2:D:822:TYR:HD2	1.59	0.64
1:A:144:ARG:HD2	1:A:146:TYR:HE1	1.62	0.64
3:X:73:VAL:HG22	3:X:84:LEU:HB3	1.80	0.64
1:C:1402:ILE:HG13	1:C:1479:ILE:CD1	2.28	0.64
1:C:612:VAL:HG21	1:C:769:PHE:CZ	2.32	0.64
1:C:632:LEU:HD23	1:C:632:LEU:N	2.13	0.64
2:B:534:ASP:HA	2:B:620:VAL:HG21	1.80	0.63
2:D:1591:LEU:C	2:D:1591:LEU:HD23	2.19	0.63
2:D:1417:MET:HG2	2:D:1443:LEU:HD23	1.80	0.63
1:C:693:SER:C	1:C:695:VAL:H	2.01	0.63
2:B:1446:PHE:CD2	2:B:1448:VAL:HG22	2.33	0.63
2:D:543:THR:OG1	2:D:544:CYS:N	2.30	0.63
2:D:355:LYS:O	2:D:358:MET:HB3	1.97	0.63
1:A:1101:CYS:HB3	1:C:1161:LEU:HD11	1.81	0.63
1:C:483:ASN:ND2	2:D:399:ILE:HB	2.14	0.63
1:A:653:PHE:CD1	1:A:660:ASP:HB3	2.33	0.63
3:X:50:TYR:CE2	3:X:170:ARG:CD	2.80	0.63
1:C:459:SER:OG	1:C:461:SER:HB3	1.97	0.63
2:B:221:LEU:CD1	2:B:753:LYS:HG2	2.25	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1286:SER:HB2	1:C:1499:HIS:HA	1.80	0.63
2:D:58:VAL:HG12	2:D:104:VAL:HG22	1.80	0.63
3:Y:134:THR:HG22	3:Y:153:PHE:O	1.97	0.63
1:C:633:GLY:O	1:C:634:CYS:HB2	1.98	0.63
2:D:1371:TYR:O	2:D:1432:HIS:HA	1.97	0.63
1:A:671:GLU:O	1:A:672:ILE:HB	1.97	0.63
3:Y:179:LEU:HD12	3:Y:180:TYR:H	1.62	0.63
1:C:393:GLN:HG2	1:C:403:ASP:OD1	1.99	0.63
1:C:982:LEU:C	1:C:984:VAL:H	2.01	0.63
3:X:207:LEU:HD12	3:X:207:LEU:C	2.14	0.63
1:A:1219:LYS:HD3	1:A:1239:VAL:HG21	1.80	0.63
2:B:829:GLN:HG2	2:B:885:VAL:CG1	2.28	0.63
2:B:58:VAL:HG12	2:B:104:VAL:HG22	1.80	0.63
1:A:91:GLN:O	1:A:92:LEU:HG	1.96	0.63
1:C:423:ASN:CG	2:D:504:VAL:HG22	2.18	0.63
3:X:43:ILE:HG23	3:X:44:ARG:H	1.62	0.63
2:D:194:LEU:HD12	2:D:217:ARG:HA	1.80	0.63
1:A:1459:HIS:CD2	1:A:1459:HIS:N	2.66	0.63
1:A:531:THR:O	1:A:534:MET:HG3	1.98	0.63
1:A:476:LEU:HB3	1:A:563:ILE:HA	1.80	0.63
1:C:512:PHE:CD2	1:C:512:PHE:O	2.51	0.63
1:A:60:PRO:HD2	1:A:61:ASP:N	2.08	0.63
1:C:473:HIS:ND1	2:D:455:LYS:HE3	2.13	0.63
1:A:1286:SER:HB2	1:A:1499:HIS:HA	1.80	0.63
1:C:947:ARG:O	1:C:949:ILE:N	2.31	0.63
1:A:443:PRO:HD2	1:A:446:ASN:HB2	1.80	0.63
2:B:127:PHE:HE2	2:B:602:ILE:HG23	1.62	0.63
1:A:153:LYS:HB3	1:A:154:PRO:HD2	1.80	0.63
1:C:238:ILE:HB	1:C:347:TYR:HD1	1.62	0.63
1:A:330:ILE:HG22	1:A:337:SER:HB2	1.79	0.63
1:A:1618:LEU:HD22	1:A:1619:ILE:N	2.12	0.63
2:B:1539:ILE:HD12	2:B:1539:ILE:H	1.62	0.63
1:C:104:LEU:HD12	1:C:105:GLU:N	2.13	0.63
1:C:512:PHE:HE2	3:Y:148:ALA:HB3	1.63	0.63
2:B:965:ILE:CG1	2:B:1301:ARG:HB2	2.25	0.63
1:C:830:PRO:CG	1:C:1483:PHE:CZ	2.74	0.63
1:A:199:TRP:HB2	1:A:217:PHE:CE1	2.34	0.63
1:C:238:ILE:HD12	1:C:347:TYR:CE1	2.33	0.63
1:A:977:LEU:HD22	1:A:978:SER:H	1.63	0.63
1:C:1629:TYR:CE1	1:C:1631:PHE:CD1	2.86	0.63
2:B:261:ALA:HB3	2:B:285:ILE:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:965:ILE:CG1	2:D:1301:ARG:HB2	2.26	0.63
1:C:702:GLY:CA	1:C:728:PHE:CE1	2.77	0.63
1:A:1013:MET:CE	1:A:1287:THR:HB	2.28	0.63
1:C:614:ARG:HD2	1:C:615:GLY:H	1.63	0.63
2:D:1447:GLU:HG3	2:D:1447:GLU:O	1.98	0.63
1:C:949:ILE:HG22	1:C:950:TYR:CE1	2.33	0.63
1:A:1236:ASP:O	1:A:1238:SER:N	2.29	0.63
2:D:963:ILE:HD11	2:D:1311:ILE:HG21	1.81	0.63
1:C:1459:HIS:CD2	1:C:1459:HIS:N	2.66	0.63
1:C:24:VAL:CA	1:C:655:THR:HG21	2.28	0.63
2:D:296:ARG:HG3	2:D:296:ARG:HH11	1.63	0.63
2:B:1591:LEU:C	2:B:1591:LEU:HD23	2.19	0.63
2:D:142:PRO:HB3	2:D:187:ASN:ND2	2.14	0.63
2:D:1431:SER:HB3	2:D:1433:SER:H	1.64	0.63
1:C:653:PHE:CD1	1:C:660:ASP:HB3	2.33	0.63
1:C:491:PRO:C	1:C:493:ILE:N	2.49	0.63
1:C:543:TYR:HD1	1:C:543:TYR:O	1.82	0.63
1:C:1229:LYS:NZ	1:C:1240:PRO:HD2	2.14	0.63
1:A:938:SER:C	1:A:940:SER:H	2.01	0.63
2:B:620:VAL:HG12	2:B:621:PHE:CD2	2.32	0.63
1:C:824:PHE:CE2	1:C:846:TYR:HB2	2.34	0.63
2:B:1500:LEU:HD11	2:B:1608:GLU:HA	1.80	0.63
2:B:1500:LEU:HD13	2:B:1607:ILE:O	1.99	0.63
1:C:88:GLN:O	1:C:90:LYS:HD3	1.99	0.63
1:C:195:ARG:HD3	1:C:1058:SER:HA	1.80	0.63
3:Y:170:ARG:O	3:Y:174:VAL:HG23	1.98	0.62
1:A:502:LEU:HB2	1:A:541:LEU:HD23	1.79	0.62
1:C:656:ASN:HB3	1:C:659:ALA:H	1.64	0.62
1:C:1641:SER:C	1:C:1643:THR:H	2.03	0.62
1:C:752:LEU:O	1:C:752:LEU:HG	1.99	0.62
1:A:1152:ILE:HG21	1:A:1168:LEU:HD21	1.81	0.62
1:A:152:LEU:HD11	1:A:627:LEU:HD11	1.81	0.62
2:D:364:VAL:HG21	2:D:379:VAL:HG21	1.81	0.62
1:A:1626:GLN:HG2	1:A:1626:GLN:O	1.98	0.62
1:C:1493:PHE:HD1	1:C:1493:PHE:C	2.00	0.62
1:A:967:LEU:HD12	1:A:968:VAL:N	2.14	0.62
1:C:101:TYR:CE1	1:C:116:ARG:NH2	2.67	0.62
1:A:614:ARG:HD2	1:A:615:GLY:H	1.63	0.62
2:D:1505:ARG:NE	2:D:1623:LYS:NZ	2.47	0.62
2:D:950:LEU:HD22	2:D:1329:TYR:CE1	2.33	0.62
2:B:1607:ILE:HD12	2:B:1607:ILE:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:HD12	1:C:1029:ASN:HD21	1.64	0.62
1:C:1622:LYS:HD2	1:C:1642:LEU:HB3	1.81	0.62
1:C:1527:CYS:O	1:C:1528:VAL:C	2.36	0.62
1:A:1556:GLU:CB	1:A:1622:LYS:HE2	2.24	0.62
1:C:59:TYR:CD1	1:C:60:PRO:HD3	2.34	0.62
1:A:123:ASN:O	1:A:211:THR:HG21	1.98	0.62
2:B:57:PHE:HD1	2:B:59:HIS:HE2	1.47	0.62
2:D:30:PRO:HG3	2:D:489:ILE:HG13	1.81	0.62
2:B:964:ILE:HG13	2:B:1302:THR:HG23	1.82	0.62
1:A:506:LYS:HE2	1:A:533:ASN:O	1.98	0.62
1:A:543:TYR:O	1:A:543:TYR:CD1	2.51	0.62
1:A:551:THR:O	1:A:552:ALA:CB	2.47	0.62
1:C:1627:ILE:O	1:C:1627:ILE:CG1	2.46	0.62
1:C:506:LYS:HE2	1:C:533:ASN:O	1.99	0.62
1:C:1219:LYS:HE2	1:C:1239:VAL:HG21	1.81	0.62
1:C:834:VAL:O	1:C:837:GLU:HB2	2.00	0.62
2:D:524:TYR:HD1	2:D:524:TYR:O	1.83	0.62
2:D:384:PHE:O	2:D:385:HIS:C	2.38	0.62
2:D:850:LEU:HD12	2:D:851:LEU:N	2.14	0.62
2:B:265:PHE:CE2	2:B:294:LEU:HB2	2.34	0.62
1:C:267:ILE:HD11	1:C:299:VAL:HG11	1.81	0.62
2:D:294:LEU:HD12	2:D:295:LYS:N	2.14	0.62
2:B:1387:LEU:HB2	2:B:1390:PHE:CD2	2.34	0.62
2:B:1623:LYS:HD2	2:B:1623:LYS:N	2.11	0.62
2:B:76:ASN:HB2	2:B:77:PRO:HD2	1.82	0.62
1:C:270:GLY:HA3	1:C:282:MET:HG2	1.80	0.62
2:B:355:LYS:HD2	2:B:355:LYS:N	2.15	0.62
1:A:20:GLU:O	1:A:20:GLU:CD	2.37	0.62
3:X:146:LEU:HD22	3:X:147:ASP:N	2.14	0.62
1:A:938:SER:OG	1:A:1284:PHE:CZ	2.53	0.62
1:C:623:VAL:O	1:C:624:PHE:C	2.38	0.62
1:A:837:GLU:O	1:A:901:LEU:HD12	2.00	0.62
2:D:61:PHE:CG	2:D:62:PRO:HA	2.35	0.62
1:C:222:TYR:CD2	1:C:223:VAL:N	2.66	0.62
1:C:824:PHE:N	1:C:824:PHE:HD2	1.97	0.62
1:C:199:TRP:HB2	1:C:217:PHE:CE1	2.34	0.62
1:A:1423:VAL:CG1	1:A:1496:TYR:CE2	2.81	0.62
1:C:1386:ILE:HG13	1:C:1387:GLU:H	1.63	0.62
2:B:1547:VAL:HG23	2:B:1557:ARG:NH1	2.14	0.62
1:A:682:LYS:HZ3	1:A:686:ILE:HD11	1.64	0.62
1:A:511:HIS:CE1	3:X:149:SER:OG	2.52	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1616:GLN:OE1	1:C:1650:ARG:HB3	1.98	0.62
2:D:147:VAL:HG12	2:D:183:PHE:HE1	1.64	0.62
1:C:968:VAL:HG23	1:C:971:THR:CG2	2.30	0.62
2:D:563:MET:CG	2:D:780:LEU:HD23	2.25	0.62
1:A:884:VAL:HG12	1:A:885:ARG:N	2.15	0.62
1:C:412:ARG:HD2	2:D:458:ASP:OD1	2.00	0.62
1:A:1056:ILE:CD1	1:A:1066:TYR:CE2	2.82	0.62
1:C:1271:ILE:O	1:C:1275:SER:HB3	2.00	0.62
1:A:1429:PRO:HB2	1:A:1432:ILE:HG13	1.80	0.62
2:D:510:ILE:HG23	2:D:514:LEU:HD12	1.81	0.62
1:C:512:PHE:CE2	3:Y:148:ALA:HB3	2.35	0.62
1:C:1585:TYR:CD2	1:C:1586:LYS:N	2.67	0.62
2:D:221:LEU:CD1	2:D:753:LYS:HG2	2.29	0.62
2:D:355:LYS:N	2:D:355:LYS:HD2	2.14	0.62
1:A:238:ILE:HD12	1:A:347:TYR:CE1	2.33	0.62
1:A:495:LYS:HA	1:A:495:LYS:HE2	1.80	0.62
2:D:69:PHE:CD2	2:D:70:GLN:N	2.68	0.62
1:C:1142:LEU:HD13	1:C:1187:THR:HG21	1.82	0.62
2:B:1446:PHE:HB3	2:B:1448:VAL:HG22	1.81	0.62
2:D:162:ILE:HG21	2:D:202:LYS:HG2	1.82	0.62
2:D:1532:GLU:O	2:D:1539:ILE:HD12	1.99	0.62
3:Y:179:LEU:HG	3:Y:180:TYR:CD2	2.35	0.62
2:D:923:SER:O	2:D:924:ILE:HD12	2.00	0.62
1:C:936:ARG:NH2	1:C:1284:PHE:HE1	1.98	0.62
2:B:1562:GLN:NE2	2:B:1596:LYS:NZ	2.48	0.62
2:B:922:LYS:HE3	2:B:1329:TYR:CZ	2.34	0.62
2:D:534:ASP:HA	2:D:620:VAL:HG21	1.82	0.62
1:A:1226:ARG:CZ	1:A:1266:TYR:HE1	2.13	0.62
1:C:125:PHE:CE1	1:C:627:LEU:HD21	2.34	0.62
1:C:1333:PHE:CD1	1:C:1334:LEU:HD13	2.34	0.62
2:B:148:PHE:CB	2:B:800:ILE:HD11	2.30	0.62
1:C:442:LEU:HD23	1:C:443:PRO:CD	2.29	0.62
1:A:161:LEU:HD11	1:A:185:PHE:CE1	2.35	0.62
1:A:104:LEU:HD12	1:A:105:GLU:N	2.15	0.62
1:C:976:ILE:HB	1:C:1362:THR:HG22	1.82	0.62
2:B:829:GLN:HA	2:B:885:VAL:HG12	1.81	0.62
1:A:1646:GLU:OE2	1:A:1660:PHE:CZ	2.53	0.62
1:A:1493:PHE:CD1	1:A:1493:PHE:C	2.73	0.62
1:A:317:ASP:C	1:A:319:ASN:H	2.03	0.62
1:A:382:LEU:HD13	1:A:415:ASP:C	2.19	0.62
1:C:690:TYR:CE1	1:C:692:HIS:HA	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:344:GLN:HB2	2:B:367:THR:O	2.00	0.62
2:D:928:VAL:HG23	2:D:1323:MET:HB3	1.82	0.62
3:X:47:HIS:CE1	3:X:181:LYS:HE2	2.35	0.62
1:A:488:PRO:HG3	1:A:499:TYR:OH	2.00	0.62
2:B:1523:VAL:HG22	2:B:1584:TRP:HB2	1.81	0.62
2:B:1431:SER:HB3	2:B:1433:SER:H	1.64	0.62
2:D:873:LYS:HD2	2:D:873:LYS:N	2.15	0.62
2:D:380:VAL:CG1	2:D:387:MET:HB3	2.17	0.61
2:B:1562:GLN:HB2	2:B:1598:SER:HB3	1.82	0.61
1:A:1102:ASN:HD21	1:C:1162:VAL:H	1.44	0.61
1:A:1648:TRP:NE1	1:A:1664:LEU:HD21	2.15	0.61
1:C:849:ARG:CG	1:C:849:ARG:HH11	2.11	0.61
2:D:34:ARG:HD2	2:D:488:LYS:NZ	2.15	0.61
1:A:779:LEU:HD12	1:A:780:VAL:N	2.15	0.61
1:A:442:LEU:HD23	1:A:443:PRO:CD	2.30	0.61
1:A:585:GLY:O	1:A:789:ALA:HB1	2.00	0.61
1:C:705:VAL:HA	1:C:739:ARG:CZ	2.30	0.61
1:C:161:LEU:HD11	1:C:185:PHE:CD1	2.35	0.61
3:X:53:GLU:HB3	3:X:55:PHE:CE2	2.35	0.61
1:C:513:GLY:HA2	3:Y:146:LEU:HD13	1.82	0.61
2:D:219:TYR:CD1	2:D:220:VAL:N	2.69	0.61
1:A:1076:THR:HG22	1:A:1120:GLU:CD	2.20	0.61
2:D:620:VAL:HG12	2:D:621:PHE:CD2	2.34	0.61
1:A:596:MET:N	1:A:782:ARG:HH11	1.90	0.61
2:B:416:ASN:HA	2:B:425:GLN:NE2	2.14	0.61
3:X:58:SER:HB2	3:X:125:LYS:HE3	1.82	0.61
2:D:161:VAL:HG21	2:D:180:LEU:CD2	2.28	0.61
1:C:796:THR:HG23	1:C:818:LYS:CB	2.30	0.61
2:D:1610:TRP:CE3	2:D:1628:PHE:CD2	2.87	0.61
1:C:1381:ILE:O	1:C:1382:ASP:HB3	2.00	0.61
2:D:1380:THR:HG22	2:D:1381:ILE:H	1.64	0.61
1:C:1211:ALA:HA	1:C:1214:ARG:HH11	1.65	0.61
2:B:543:THR:OG1	2:B:544:CYS:N	2.31	0.61
3:Y:166:ASP:CB	3:Y:207:LEU:HD21	2.30	0.61
1:C:641:ASN:O	1:C:643:ALA:N	2.33	0.61
1:C:23:TYR:CE1	1:C:655:THR:HB	2.35	0.61
1:A:1219:LYS:HZ3	1:A:1239:VAL:HG11	1.61	0.61
1:C:1053:MET:SD	1:C:1089:VAL:HG21	2.40	0.61
1:A:576:SER:HB2	1:A:589:SER:CB	2.27	0.61
1:A:1504:GLN:HG3	1:A:1505:CYS:CA	2.30	0.61
2:B:120:LEU:HD12	2:B:121:LEU:N	2.11	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:69:PHE:CD1	2:D:87:ILE:HG22	2.36	0.61
2:D:1347:VAL:HG21	2:D:1456:VAL:HG11	1.81	0.61
2:B:137:TYR:CE2	2:B:143:VAL:HG22	2.35	0.61
2:B:162:ILE:HG21	2:B:202:LYS:HG2	1.81	0.61
1:C:586:GLN:O	1:C:586:GLN:HG3	2.00	0.61
1:A:653:PHE:CE1	1:A:660:ASP:HB3	2.35	0.61
1:A:393:GLN:HG2	1:A:403:ASP:OD1	2.00	0.61
2:D:1511:GLN:HG2	2:D:1631:PHE:CE1	2.35	0.61
1:A:44:TYR:CE1	1:A:497:THR:HG21	2.35	0.61
1:C:955:ARG:NH1	1:C:1352:PHE:HA	2.15	0.61
1:A:1365:VAL:CG2	1:A:1366:HIS:N	2.60	0.61
1:A:855:PHE:HA	2:B:904:LEU:CD1	2.28	0.61
1:A:824:PHE:CE2	1:A:846:TYR:HD1	2.19	0.61
2:B:242:ASN:OD1	2:B:295:LYS:HD2	1.99	0.61
2:B:1623:LYS:HA	2:B:1623:LYS:CE	2.30	0.61
2:B:1623:LYS:HA	2:B:1623:LYS:NZ	2.15	0.61
1:A:270:GLY:HA3	1:A:282:MET:HG2	1.83	0.61
2:D:410:PRO:HA	2:D:431:THR:HG22	1.83	0.61
2:D:342:PRO:HG2	2:D:420:LEU:HD13	1.81	0.61
1:C:927:LEU:HD23	1:C:928:ARG:N	2.16	0.61
1:A:868:SER:CA	1:A:1527:CYS:HB2	2.28	0.61
3:Y:139:ASN:HD22	3:Y:148:ALA:CB	2.12	0.61
3:Y:139:ASN:HD22	3:Y:148:ALA:HB1	1.66	0.61
1:A:1641:SER:C	1:A:1643:THR:H	2.02	0.61
2:D:964:ILE:O	2:D:964:ILE:HG22	2.00	0.61
2:B:237:ILE:O	2:B:306:LEU:HD11	1.99	0.61
1:C:317:ASP:C	1:C:319:ASN:H	2.03	0.61
1:C:149:ASN:H	1:C:149:ASN:ND2	1.97	0.61
2:B:128:LEU:O	2:B:129:PHE:CD1	2.53	0.61
2:B:1344:HIS:O	2:B:1369:THR:HA	2.01	0.61
3:Y:73:VAL:HG22	3:Y:84:LEU:HB3	1.80	0.61
2:D:1344:HIS:O	2:D:1369:THR:HA	2.01	0.61
1:C:177:ILE:HG22	1:C:178:ASP:H	1.66	0.61
1:C:837:GLU:O	1:C:901:LEU:HD12	2.00	0.61
1:A:1147:PHE:O	1:A:1150:ILE:HB	2.01	0.61
1:A:871:PRO:HD2	1:A:872:VAL:N	2.15	0.61
1:C:742:ILE:HG21	1:C:753:HIS:HA	1.83	0.61
1:C:481:HIS:HE1	1:C:529:PRO:HB3	1.64	0.61
1:C:20:GLU:O	1:C:20:GLU:CD	2.39	0.61
1:A:1163:LYS:NZ	1:C:1109:GLU:CD	2.54	0.61
1:C:1188:LEU:HD23	1:C:1212:LEU:HD13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:581:ASP:O	2:D:582:LYS:C	2.39	0.61
1:C:44:TYR:CE1	1:C:497:THR:HG21	2.35	0.61
2:D:384:PHE:HD1	2:D:400:LEU:HG	1.60	0.61
2:B:384:PHE:O	2:B:385:HIS:C	2.38	0.61
1:A:493:ILE:HG23	1:A:495:LYS:HB2	1.82	0.61
2:B:103:TYR:CD2	2:B:120:LEU:HD13	2.35	0.61
2:B:484:LEU:HD11	2:B:626:LEU:HD11	1.83	0.61
1:A:267:ILE:HD12	1:A:299:VAL:HG11	1.83	0.61
2:B:1583:ILE:HG12	2:B:1607:ILE:CG2	2.30	0.61
1:A:1033:ILE:HG23	1:A:1034:PHE:N	2.14	0.61
2:D:1506:ILE:O	2:D:1508:VAL:N	2.34	0.61
1:A:260:VAL:HG12	1:A:261:THR:N	2.15	0.61
1:A:161:LEU:HD11	1:A:185:PHE:CG	2.36	0.61
1:C:653:PHE:CE1	1:C:660:ASP:HB3	2.35	0.61
3:X:191:ILE:HD12	3:X:199:VAL:HB	1.82	0.61
3:Y:50:TYR:CE2	3:Y:170:ARG:CD	2.81	0.61
1:A:24:VAL:HG11	1:A:543:TYR:CE2	2.35	0.61
1:C:489:LYS:CG	1:C:490:SER:H	2.13	0.61
1:C:1582:LEU:HD11	1:C:1648:TRP:HZ2	1.66	0.61
1:A:1049:LEU:HD11	1:A:1089:VAL:CG1	2.30	0.61
1:C:60:PRO:CD	1:C:61:ASP:N	2.56	0.61
2:B:219:TYR:CD1	2:B:220:VAL:N	2.69	0.61
1:C:153:LYS:HB3	1:C:154:PRO:HD2	1.83	0.61
2:D:34:ARG:HD2	2:D:488:LYS:HZ3	1.66	0.61
1:C:1612:VAL:HB	1:C:1615:ARG:CB	2.26	0.61
2:D:416:ASN:HA	2:D:425:GLN:NE2	2.15	0.61
2:B:1610:TRP:CD2	2:B:1628:PHE:HD2	2.19	0.61
1:A:59:TYR:CD1	1:A:60:PRO:HD3	2.36	0.61
2:B:599:TRP:CZ3	2:B:602:ILE:HD12	2.36	0.61
1:A:428:VAL:HG22	1:A:429:THR:H	1.65	0.61
3:Y:191:ILE:HD12	3:Y:199:VAL:HB	1.83	0.61
1:C:40:VAL:CG2	1:C:512:PHE:HD1	2.14	0.61
1:C:1147:PHE:O	1:C:1150:ILE:HB	2.00	0.61
1:A:1620:MET:HB2	1:A:1644:TRP:HB3	1.83	0.61
1:A:1667:PHE:O	1:A:1671:ILE:HG22	2.01	0.61
2:D:841:ASN:O	2:D:842:GLU:C	2.40	0.61
2:B:244:HIS:HB3	2:B:291:LYS:CD	2.29	0.61
2:B:1447:GLU:HG3	2:B:1447:GLU:O	2.00	0.61
2:D:1500:LEU:HD11	2:D:1608:GLU:O	2.01	0.61
1:A:824:PHE:CE2	1:A:846:TYR:HB2	2.36	0.61
2:B:1544:VAL:HB	2:B:1557:ARG:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:433:ILE:HG22	2:B:434:ALA:O	2.01	0.61
1:A:658:ASN:OD1	1:A:658:ASN:C	2.40	0.60
2:D:829:GLN:NE2	2:D:883:VAL:HG13	2.10	0.60
2:B:1561:HIS:CE1	2:B:1597:ILE:HD13	2.35	0.60
1:A:1535:MET:HA	1:A:1645:ILE:HB	1.83	0.60
1:A:119:ILE:O	1:A:119:ILE:HD12	2.01	0.60
1:C:822:ASP:HA	1:C:849:ARG:HD2	1.83	0.60
1:C:502:LEU:HB2	1:C:541:LEU:HD23	1.83	0.60
1:C:824:PHE:CE2	1:C:846:TYR:HD1	2.19	0.60
1:C:1268:ASN:H	1:C:1268:ASN:ND2	1.98	0.60
2:D:1391:LEU:HB2	2:D:1417:MET:HE2	1.83	0.60
2:B:342:PRO:HG2	2:B:420:LEU:HD13	1.83	0.60
3:X:170:ARG:NH2	3:X:206:LYS:HA	2.16	0.60
1:A:532:GLN:NE2	1:A:568:GLY:HA2	2.16	0.60
1:C:873:ILE:O	1:C:873:ILE:HD12	2.01	0.60
2:D:814:PHE:HZ	2:D:846:VAL:HG21	1.66	0.60
1:C:1232:LEU:CD1	1:C:1233:GLN:HE21	2.09	0.60
1:A:1268:ASN:H	1:A:1268:ASN:ND2	1.99	0.60
1:A:1003:LEU:N	1:A:1003:LEU:HD23	2.16	0.60
1:C:256:TYR:HD2	1:C:846:TYR:CE1	2.19	0.60
1:C:1054:LEU:HD23	1:C:1057:MET:HE2	1.83	0.60
2:D:1610:TRP:CD2	2:D:1628:PHE:HD2	2.18	0.60
2:D:133:ASP:OD2	2:D:134:LYS:HG2	2.01	0.60
1:A:1627:ILE:O	1:A:1629:TYR:N	2.34	0.60
2:D:581:ASP:O	2:D:583:ALA:N	2.34	0.60
1:A:177:ILE:HG22	1:A:178:ASP:H	1.65	0.60
2:B:167:THR:HG23	2:B:171:ILE:H	1.65	0.60
1:C:43:VAL:HG11	1:C:73:LEU:CD1	2.31	0.60
1:C:457:TYR:HE1	1:C:556:SER:O	1.85	0.60
1:A:987:ILE:CD1	1:A:1294:ILE:HG23	2.31	0.60
2:B:841:ASN:O	2:B:842:GLU:C	2.38	0.60
2:B:844:ILE:CD1	2:B:872:ILE:HD11	2.32	0.60
1:C:243:PHE:HE2	1:C:304:GLU:HA	1.66	0.60
1:A:1323:LEU:HD12	1:A:1324:HIS:N	2.16	0.60
1:C:171:VAL:HG11	1:C:1054:LEU:HD11	1.82	0.60
2:D:242:ASN:OD1	2:D:295:LYS:HD2	2.00	0.60
1:A:1211:ALA:HA	1:A:1214:ARG:HH11	1.66	0.60
1:C:322:TYR:N	1:C:322:TYR:CD2	2.68	0.60
1:A:1427:SER:HB3	1:A:1492:THR:HG23	1.81	0.60
1:A:500:ASN:CB	1:A:543:TYR:CE1	2.61	0.60
1:C:1549:LYS:HZ2	1:C:1667:PHE:HB3	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1487:PHE:O	1:C:1488:LEU:C	2.40	0.60
2:B:756:LEU:HD12	2:B:758:LEU:HG	1.84	0.60
2:D:916:VAL:HG22	2:D:917:PRO:O	2.02	0.60
3:X:88:GLY:HA2	3:X:210:GLU:O	2.01	0.60
2:D:196:THR:HG23	2:D:215:ASP:OD1	2.01	0.60
1:A:443:PRO:HG2	1:A:446:ASN:OD1	2.01	0.60
1:C:196:TYR:CE1	1:C:221:GLU:HB2	2.37	0.60
1:C:351:PRO:HG2	1:C:352:TYR:CE2	2.35	0.60
1:A:1042:LYS:NZ	1:C:92:LEU:HD13	2.17	0.60
1:A:693:SER:C	1:A:695:VAL:H	2.05	0.60
2:B:269:ILE:HA	2:B:312:HIS:CD2	2.36	0.60
1:C:1646:GLU:OE2	1:C:1660:PHE:CZ	2.54	0.60
1:C:531:THR:O	1:C:534:MET:HG3	2.01	0.60
2:B:1473:HIS:CD2	2:B:1474:PRO:CD	2.84	0.60
1:A:1585:TYR:HE1	1:A:1671:ILE:HG12	1.66	0.60
2:B:435:TYR:OH	2:B:532:VAL:HG22	2.00	0.60
2:D:484:LEU:HD11	2:D:626:LEU:HD11	1.84	0.60
2:D:933:ARG:HG3	2:D:933:ARG:NH1	2.14	0.60
1:C:209:PHE:H	1:C:209:PHE:HD2	1.48	0.60
2:B:1381:ILE:HG21	2:B:1459:TYR:CE1	2.35	0.60
1:A:161:LEU:H	1:A:161:LEU:HD12	1.65	0.60
2:B:738:GLY:O	2:B:901:GLN:HA	2.02	0.60
1:A:503:ILE:HD11	1:A:540:LEU:HD13	1.83	0.60
1:A:1564:SER:HB2	1:A:1616:GLN:HG3	1.82	0.60
1:A:238:ILE:HB	1:A:347:TYR:HD1	1.67	0.60
1:C:702:GLY:CA	1:C:728:PHE:CD1	2.84	0.60
2:B:556:ILE:H	2:B:556:ILE:HD12	1.65	0.60
2:D:120:LEU:HD12	2:D:121:LEU:N	2.13	0.60
1:A:1213:LYS:HE2	1:A:1266:TYR:CE2	2.37	0.60
2:B:127:PHE:CE2	2:B:602:ILE:HG23	2.37	0.60
1:A:670:LYS:HD2	1:A:671:GLU:HG2	1.84	0.60
1:A:1548:ARG:HD3	1:A:1548:ARG:H	1.66	0.60
2:D:233:LYS:HG3	2:D:233:LYS:O	2.01	0.60
1:C:931:PRO:HG2	1:C:1366:HIS:NE2	2.16	0.60
2:D:1561:HIS:CE1	2:D:1597:ILE:HD13	2.37	0.60
2:B:61:PHE:HB3	2:B:103:TYR:HB2	1.83	0.60
1:A:690:TYR:CE1	1:A:692:HIS:HA	2.36	0.60
1:C:199:TRP:CD1	1:C:219:VAL:HB	2.37	0.60
2:D:137:TYR:CE2	2:D:143:VAL:HG22	2.36	0.60
1:A:101:TYR:CE1	1:A:116:ARG:NH2	2.70	0.60
1:C:209:PHE:CD2	1:C:209:PHE:N	2.68	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:963:ILE:HD11	2:B:1311:ILE:HG21	1.84	0.60
1:C:115:LYS:CB	1:C:654:LEU:HD21	2.32	0.60
1:C:25:ILE:CD1	1:C:41:ILE:HB	2.31	0.60
1:A:1053:MET:SD	1:A:1089:VAL:HG21	2.42	0.60
1:C:820:PHE:O	1:C:821:LYS:HG3	2.00	0.60
1:A:436:LYS:HA	1:A:448:ALA:O	2.01	0.60
1:C:824:PHE:HE2	1:C:846:TYR:HB2	1.65	0.60
1:C:1226:ARG:CZ	1:C:1266:TYR:CE1	2.85	0.60
1:C:1259:LEU:HD11	1:C:1300:TYR:HB2	1.84	0.60
2:B:294:LEU:HD12	2:B:295:LYS:N	2.16	0.60
1:C:174:VAL:HG22	1:C:175:GLU:N	2.15	0.60
1:A:1128:LYS:C	1:A:1129:LEU:HD23	2.22	0.60
2:B:133:ASP:OD2	2:B:134:LYS:HG2	2.01	0.60
2:D:1510:LEU:HD21	2:D:1514:LYS:NZ	2.15	0.60
1:C:1239:VAL:O	1:C:1239:VAL:HG12	2.02	0.60
1:A:931:PRO:HG2	1:A:1366:HIS:NE2	2.17	0.60
1:A:209:PHE:N	1:A:209:PHE:CD2	2.70	0.60
1:C:154:PRO:O	1:C:155:ALA:CB	2.50	0.60
1:C:165:ASP:O	1:C:167:GLU:N	2.35	0.60
2:B:1380:THR:HG22	2:B:1381:ILE:H	1.67	0.60
2:B:96:THR:HG21	2:B:102:GLN:OE1	2.02	0.60
1:C:1608:ASN:O	1:C:1610:GLU:N	2.35	0.60
1:C:1150:ILE:CD1	1:C:1193:TYR:CD2	2.85	0.60
1:A:1671:ILE:HA	1:A:1675:GLY:H	1.66	0.60
2:B:557:GLN:HE21	2:B:563:MET:CE	2.14	0.60
1:C:569:ASN:ND2	1:C:570:GLN:H	2.00	0.60
1:A:1231:ASN:HB2	1:A:1235:LYS:HG3	1.83	0.60
2:B:197:TRP:HB2	2:B:214:PHE:CE1	2.36	0.60
1:A:474:LYS:H	1:A:474:LYS:CD	2.15	0.60
1:C:443:PRO:HG2	1:C:446:ASN:OD1	2.02	0.60
1:A:1341:LEU:HB2	1:A:1342:LEU:CD2	2.31	0.60
1:A:705:VAL:HA	1:A:739:ARG:CZ	2.31	0.60
2:B:510:ILE:HG23	2:B:514:LEU:HD12	1.84	0.60
1:A:55:SER:O	1:A:56:ILE:HD13	2.01	0.60
2:B:296:ARG:HH11	2:B:296:ARG:HG3	1.66	0.60
1:A:25:ILE:HB	1:A:655:THR:HG23	1.84	0.59
1:A:551:THR:O	1:A:552:ALA:HB2	2.00	0.59
1:A:457:TYR:OH	1:A:555:VAL:HG22	2.02	0.59
1:C:1560:ALA:HB2	1:C:1620:MET:CG	2.25	0.59
1:C:1585:TYR:CG	1:C:1586:LYS:N	2.69	0.59
2:D:476:ILE:CG2	2:D:476:ILE:O	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:476:ILE:HD11	2:D:524:TYR:CG	2.36	0.59
2:B:523:TYR:HB3	2:B:533:ALA:HB2	1.83	0.59
1:A:362:PHE:HE1	1:A:640:LEU:HB2	1.67	0.59
1:C:1329:THR:H	1:C:1332:ASN:HB2	1.67	0.59
1:A:443:PRO:HG2	1:A:446:ASN:HB2	1.84	0.59
1:A:824:PHE:HD2	1:A:824:PHE:N	1.99	0.59
1:A:429:THR:HA	1:A:456:ALA:HB2	1.84	0.59
1:C:342:ILE:HD12	1:C:345:ILE:HD11	1.84	0.59
1:A:504:LEU:HD12	1:A:509:ILE:HG23	1.85	0.59
1:A:25:ILE:N	1:A:655:THR:HG21	2.12	0.59
1:C:967:LEU:HD12	1:C:968:VAL:H	1.66	0.59
2:D:261:ALA:CB	2:D:285:ILE:HD11	2.32	0.59
2:B:531:ILE:HD11	2:B:634:LEU:HD23	1.84	0.59
2:D:1486:ILE:HD11	2:D:1591:LEU:HD22	1.85	0.59
3:Y:101:GLN:HA	3:Y:125:LYS:HB3	1.84	0.59
1:A:1056:ILE:CD1	1:A:1066:TYR:HE2	2.15	0.59
1:C:1152:ILE:HG22	1:C:1168:LEU:HD21	1.82	0.59
2:B:508:LEU:HD12	2:B:509:HIS:N	2.16	0.59
3:X:68:ASN:CG	3:X:69:GLY:N	2.55	0.59
3:Y:68:ASN:CG	3:Y:69:GLY:N	2.55	0.59
3:X:179:LEU:HG	3:X:180:TYR:CD2	2.36	0.59
1:A:612:VAL:HG12	1:A:612:VAL:O	2.01	0.59
1:C:493:ILE:HG23	1:C:495:LYS:HB2	1.85	0.59
1:A:222:TYR:CD2	1:A:223:VAL:N	2.69	0.59
2:B:829:GLN:NE2	2:B:883:VAL:HG13	2.13	0.59
1:A:1559:TYR:HH	1:A:1591:VAL:HA	1.66	0.59
1:A:838:GLN:HA	1:A:901:LEU:CB	2.29	0.59
1:A:1612:VAL:HB	1:A:1615:ARG:CB	2.26	0.59
2:B:69:PHE:CD1	2:B:87:ILE:HG22	2.37	0.59
1:A:949:ILE:HG22	1:A:950:TYR:CE1	2.37	0.59
1:A:199:TRP:CD1	1:A:219:VAL:HB	2.37	0.59
1:A:209:PHE:H	1:A:209:PHE:HD2	1.50	0.59
1:C:1320:LYS:CE	1:C:1321:GLY:H	2.15	0.59
1:A:1381:ILE:O	1:A:1382:ASP:HB3	2.02	0.59
1:A:1113:LEU:CD2	1:A:1114:ASP:H	2.15	0.59
1:C:1618:LEU:HD22	1:C:1619:ILE:N	2.16	0.59
1:C:979:VAL:HG21	1:C:1326:TYR:CZ	2.35	0.59
2:D:783:SER:HB2	2:D:787:TRP:HZ2	1.67	0.59
2:B:309:LEU:HB3	2:B:338:ILE:HD12	1.84	0.59
1:A:623:VAL:HG12	1:A:624:PHE:N	2.18	0.59
2:B:1424:ILE:H	2:B:1424:ILE:CD1	2.14	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LYS:HB2	1:A:654:LEU:HD21	1.85	0.59
1:C:515:ARG:NH1	1:C:526:ILE:HG22	2.16	0.59
1:C:1615:ARG:NH1	1:C:1647:TYR:CE1	2.70	0.59
1:A:1487:PHE:N	1:A:1487:PHE:CD2	2.68	0.59
1:A:1493:PHE:HD1	1:A:1493:PHE:C	2.06	0.59
2:B:813:VAL:HG12	2:B:840:VAL:HG22	1.85	0.59
1:C:1152:ILE:HG21	1:C:1168:LEU:CD2	2.31	0.59
1:A:874:ASP:HA	1:A:878:THR:O	2.03	0.59
1:A:1011:GLU:O	1:A:1014:SER:HB3	2.02	0.59
1:A:503:ILE:CB	1:A:511:HIS:HB2	2.33	0.59
1:C:1487:PHE:CD2	1:C:1487:PHE:N	2.70	0.59
1:C:987:ILE:CD1	1:C:1294:ILE:HG23	2.33	0.59
2:D:1473:HIS:CD2	2:D:1474:PRO:CD	2.79	0.59
2:D:738:GLY:O	2:D:901:GLN:HA	2.03	0.59
1:A:356:LEU:HG	1:A:452:TYR:CZ	2.38	0.59
2:B:525:GLN:HA	2:B:530:GLU:O	2.03	0.59
2:D:61:PHE:HB3	2:D:103:TYR:HB2	1.83	0.59
1:A:1329:THR:H	1:A:1332:ASN:HB2	1.68	0.59
2:B:148:PHE:HB3	2:B:800:ILE:HD11	1.83	0.59
2:D:243:PHE:HE1	2:D:336:ILE:HG21	1.67	0.59
2:B:241:GLU:O	2:B:296:ARG:HD3	2.02	0.59
1:A:936:ARG:NH2	1:A:1284:PHE:CE1	2.71	0.59
1:A:1219:LYS:HE2	1:A:1239:VAL:HG21	1.85	0.59
2:B:1609:ARG:HG2	2:B:1609:ARG:HH11	1.68	0.59
1:A:361:LEU:N	1:A:361:LEU:HD12	2.16	0.59
1:C:569:ASN:CG	1:C:570:GLN:H	2.06	0.59
2:B:26:THR:OG1	2:B:44:GLU:HB2	2.02	0.59
2:B:71:THR:HG23	2:B:72:ARG:N	2.18	0.59
1:A:1066:TYR:N	1:A:1079:THR:HG23	2.16	0.59
2:B:130:ILE:HD13	2:B:199:ILE:HG22	1.83	0.59
2:D:745:ILE:HD11	2:D:907:ASP:H	1.66	0.59
1:C:680:GLN:HG3	1:C:681:LYS:N	2.17	0.59
3:X:106:VAL:HG22	3:X:163:LYS:CE	2.32	0.59
1:A:24:VAL:HG11	1:A:543:TYR:OH	2.01	0.59
1:A:702:GLY:CA	1:A:728:PHE:CD1	2.85	0.59
1:A:491:PRO:C	1:A:493:ILE:N	2.51	0.59
1:A:752:LEU:HG	1:A:752:LEU:O	2.02	0.59
1:C:474:LYS:CD	1:C:474:LYS:H	2.15	0.59
1:C:617:LYS:HD2	1:C:622:ARG:NH2	2.17	0.59
1:C:1013:MET:CE	1:C:1287:THR:HB	2.32	0.59
2:D:1505:ARG:NE	2:D:1623:LYS:HZ2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:922:LYS:HE3	2:D:1329:TYR:CZ	2.38	0.59
1:A:774:LEU:HG	1:A:788:PHE:CE1	2.38	0.59
1:A:813:ASP:O	1:A:815:VAL:HG23	2.03	0.59
1:C:1450:PHE:HZ	1:C:1475:VAL:HB	1.66	0.59
2:B:316:ALA:HB3	2:B:333:GLN:HB3	1.85	0.59
1:A:790:LEU:HB3	1:A:791:PRO:CD	2.32	0.59
1:C:355:ASN:HD22	1:C:355:ASN:N	2.01	0.59
2:B:746:ILE:H	2:B:746:ILE:HD13	1.68	0.59
1:A:505:SER:HB3	1:A:510:ILE:CD1	2.32	0.59
1:A:78:LYS:HZ1	3:X:144:GLU:HA	1.65	0.59
1:A:855:PHE:CA	2:B:904:LEU:HD11	2.31	0.59
2:B:961:THR:HG22	2:B:1327:THR:CG2	2.32	0.59
1:A:720:LEU:HD13	1:A:724:CYS:HB3	1.83	0.59
1:A:1352:PHE:HD2	1:A:1352:PHE:N	2.01	0.59
1:C:182:ILE:HG12	1:C:804:ILE:CD1	2.25	0.59
2:D:476:ILE:CG2	2:D:497:ARG:HD3	2.33	0.59
1:A:1493:PHE:HE1	1:A:1495:VAL:HG12	1.67	0.59
2:D:309:LEU:HB3	2:D:338:ILE:HD12	1.85	0.59
2:D:103:TYR:CD2	2:D:120:LEU:HD13	2.37	0.59
1:A:257:ASN:HB2	1:A:848:TYR:CE2	2.37	0.59
1:A:1159:CYS:N	1:A:1160:PRO:CD	2.66	0.59
1:C:1402:ILE:HG13	1:C:1479:ILE:HD11	1.84	0.59
1:A:825:LEU:HG	1:A:826:GLU:N	2.18	0.59
1:A:84:ILE:HD12	1:A:84:ILE:H	1.68	0.58
1:A:944:LEU:N	1:A:944:LEU:HD23	2.18	0.58
1:C:1076:THR:HG22	1:C:1120:GLU:CD	2.23	0.58
1:C:1451:THR:O	1:C:1452:ASP:HB3	2.03	0.58
1:A:955:ARG:HH12	1:A:1352:PHE:HA	1.66	0.58
1:A:883:CYS:O	1:A:884:VAL:O	2.21	0.58
1:A:644:ASN:CG	1:A:648:LEU:HD12	2.23	0.58
1:C:154:PRO:O	1:C:155:ALA:HB3	2.03	0.58
2:D:69:PHE:CD2	2:D:69:PHE:C	2.76	0.58
1:C:267:ILE:HG22	1:C:268:THR:N	2.18	0.58
1:C:975:ARG:NH1	1:C:1340:VAL:HG11	2.18	0.58
2:D:546:GLY:HA3	2:D:570:ASP:OD1	2.02	0.58
1:A:865:ILE:C	1:A:866:CYS:O	2.41	0.58
1:A:322:TYR:CD2	1:A:322:TYR:N	2.70	0.58
5:B:2001:NAG:C3	5:B:2002:NAG:O5	2.51	0.58
2:B:820:MET:HG3	2:B:821:PRO:HD2	1.85	0.58
1:A:544:TYR:CD2	1:A:544:TYR:C	2.76	0.58
1:C:1562:LYS:HD3	1:C:1648:TRP:HE1	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1229:LYS:NZ	1:C:1238:SER:OG	2.34	0.58
1:C:838:GLN:HA	1:C:901:LEU:CB	2.28	0.58
1:C:1451:THR:O	1:C:1452:ASP:CB	2.51	0.58
1:C:1110:ASN:N	1:C:1110:ASN:OD1	2.36	0.58
2:B:481:TYR:CE2	2:B:493:GLY:CA	2.86	0.58
1:A:1065:SER:HB3	1:A:1106:TRP:CD2	2.38	0.58
1:C:172:ASP:OD2	1:C:1050:LYS:HD3	2.02	0.58
1:A:863:GLU:H	1:A:863:GLU:CD	2.07	0.58
2:B:476:ILE:HD11	2:B:524:TYR:CD2	2.37	0.58
3:X:166:ASP:CB	3:X:207:LEU:HD21	2.32	0.58
1:A:512:PHE:CD2	1:A:512:PHE:O	2.56	0.58
1:C:1219:LYS:CD	1:C:1239:VAL:HG21	2.33	0.58
1:C:1076:THR:HG22	1:C:1120:GLU:OE2	2.02	0.58
1:C:623:VAL:HG12	1:C:624:PHE:N	2.18	0.58
1:A:702:GLY:O	1:A:732:CYS:HB2	2.03	0.58
2:D:606:ASP:O	2:D:606:ASP:OD1	2.21	0.58
1:C:356:LEU:HG	1:C:452:TYR:CZ	2.38	0.58
1:A:171:VAL:CG1	1:A:172:ASP:N	2.67	0.58
1:A:824:PHE:N	1:A:824:PHE:CD2	2.70	0.58
2:D:137:TYR:CE1	2:D:143:VAL:HG22	2.37	0.58
2:D:265:PHE:CE2	2:D:294:LEU:HB2	2.38	0.58
2:B:243:PHE:HE1	2:B:336:ILE:HG21	1.67	0.58
2:B:1532:GLU:O	2:B:1539:ILE:HD12	2.04	0.58
1:A:680:GLN:HG3	1:A:681:LYS:N	2.19	0.58
1:A:126:LEU:HD11	1:A:205:TYR:CE2	2.39	0.58
1:A:25:ILE:CD1	1:A:41:ILE:HB	2.33	0.58
1:C:362:PHE:HE1	1:C:640:LEU:HB2	1.66	0.58
2:D:829:GLN:HG2	2:D:885:VAL:CG1	2.34	0.58
2:B:1593:THR:CG2	2:B:1594:LYS:N	2.67	0.58
1:A:950:TYR:CE2	1:A:1356:LEU:HD11	2.38	0.58
1:A:1572:ASN:O	1:A:1573:VAL:HG23	2.04	0.58
2:D:344:GLN:HB2	2:D:367:THR:O	2.03	0.58
1:C:813:ASP:O	1:C:815:VAL:HG23	2.02	0.58
2:B:183:PHE:CD2	2:B:183:PHE:N	2.70	0.58
2:B:1563:TYR:HB3	2:B:1601:ILE:HD11	1.86	0.58
2:B:45:ALA:HB3	2:B:81:MET:HE3	1.85	0.58
1:A:504:LEU:HD23	1:A:649:ALA:O	2.03	0.58
1:C:1240:PRO:HB2	1:C:1242:THR:HG23	1.84	0.58
1:C:938:SER:OG	1:C:1284:PHE:CZ	2.57	0.58
1:A:134:VAL:C	1:A:135:TYR:HD2	2.07	0.58
1:A:412:ARG:HD2	2:B:458:ASP:OD1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1391:LEU:HD12	2:B:1417:MET:HE1	1.84	0.58
1:A:1011:GLU:HG3	1:A:1055:SER:OG	2.03	0.58
2:D:887:LEU:CD2	2:D:1490:CYS:HB3	2.34	0.58
1:A:1549:LYS:HD3	1:A:1667:PHE:HB3	1.85	0.58
1:A:784:LYS:HG2	1:A:785:GLN:N	2.18	0.58
2:D:615:GLN:HB2	2:D:616:ASN:HD22	1.68	0.58
2:B:851:LEU:HD23	2:B:852:TYR:N	2.10	0.58
2:D:24:LEU:HB3	2:D:46:HIS:HB2	1.84	0.58
2:B:28:ILE:HG12	2:B:628:LEU:HD13	1.84	0.58
2:B:61:PHE:CG	2:B:62:PRO:HA	2.38	0.58
2:B:795:THR:HG22	2:B:796:PRO:CD	2.32	0.58
1:C:309:GLU:HG2	1:C:310:LEU:HD12	1.86	0.58
1:A:1152:ILE:HG22	1:A:1168:LEU:HD21	1.83	0.58
2:D:1623:LYS:HB3	2:D:1623:LYS:NZ	2.18	0.58
2:D:218:LYS:HD3	2:D:822:TYR:CE2	2.39	0.58
1:A:907:LEU:HG	1:A:908:HIS:N	2.17	0.58
3:X:119:VAL:HG21	3:X:209:PHE:HB3	1.85	0.58
2:D:1491:ARG:HG3	2:D:1492:CYS:H	1.67	0.58
1:A:902:PRO:O	1:A:903:LEU:HD13	2.02	0.58
1:A:421:VAL:HG11	2:B:505:THR:HG22	1.86	0.58
1:A:1527:CYS:O	1:A:1529:GLU:N	2.36	0.58
1:A:534:MET:HB3	1:A:538:SER:OG	2.04	0.58
1:C:553:GLU:HA	1:C:658:ASN:CB	2.31	0.58
1:C:81:ASN:CG	1:C:82:SER:H	2.07	0.58
1:C:1618:LEU:HD22	1:C:1619:ILE:H	1.67	0.58
2:B:1624:LEU:HG	2:B:1628:PHE:CE1	2.38	0.58
1:C:1065:SER:HB3	1:C:1106:TRP:CD2	2.39	0.58
2:B:1528:LEU:HD13	2:B:1542:MET:HE2	1.84	0.58
1:C:1019:PHE:HD2	1:C:1020:TYR:N	2.01	0.58
2:B:1500:LEU:CD1	2:B:1500:LEU:C	2.72	0.58
2:B:348:THR:HA	2:B:352:LYS:NZ	2.19	0.58
1:C:163:PHE:CD2	1:C:188:PHE:CD1	2.91	0.58
1:C:854:GLN:NE2	1:C:854:GLN:H	2.02	0.58
1:C:364:LYS:HE3	1:C:457:TYR:HD1	1.68	0.58
1:C:967:LEU:HD13	1:C:1365:VAL:CG2	2.34	0.58
1:C:484:ILE:CD1	1:C:540:LEU:HD21	2.33	0.58
1:C:368:PRO:HG3	2:D:505:THR:HB	1.85	0.58
1:C:936:ARG:HH12	1:C:1284:PHE:HZ	1.50	0.58
2:B:844:ILE:HG13	2:B:872:ILE:CG1	2.34	0.58
1:A:1333:PHE:CD1	1:A:1334:LEU:HD13	2.39	0.58
1:A:639:GLY:H	1:A:645:VAL:HA	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:LEU:N	1:C:361:LEU:HD12	2.18	0.58
2:D:71:THR:HG23	2:D:72:ARG:N	2.18	0.58
2:B:599:TRP:HE3	2:B:599:TRP:HA	1.68	0.58
1:C:350:SER:OG	1:C:352:TYR:O	2.20	0.58
1:A:788:PHE:HD2	1:A:788:PHE:N	2.02	0.58
1:A:132:LYS:NZ	1:A:139:GLN:HE22	2.01	0.58
1:C:1411:SER:N	1:C:1414:GLU:HG3	2.19	0.58
2:B:1450:PHE:HD1	2:B:1451:ILE:H	1.51	0.58
2:B:1534:GLN:HG3	2:B:1535:ASP:OD2	2.04	0.58
2:B:746:ILE:HD13	2:B:746:ILE:N	2.18	0.58
2:B:1278:THR:HB	2:B:1314:THR:HB	1.84	0.58
2:B:581:ASP:O	2:B:582:LYS:C	2.42	0.58
3:Y:106:VAL:HG22	3:Y:163:LYS:CE	2.33	0.58
2:D:283:ILE:HD12	2:D:283:ILE:N	2.18	0.58
2:B:1628:PHE:O	2:B:1629:ALA:C	2.41	0.58
2:B:850:LEU:HD12	2:B:851:LEU:N	2.19	0.58
1:A:1493:PHE:HD1	1:A:1494:THR:H	1.48	0.58
2:D:1528:LEU:HD13	2:D:1542:MET:HE2	1.86	0.58
1:A:1255:LEU:HD12	1:A:1255:LEU:O	2.03	0.58
1:C:1003:LEU:N	1:C:1003:LEU:HD23	2.19	0.58
1:A:350:SER:OG	1:A:352:TYR:O	2.20	0.58
1:A:1411:SER:N	1:A:1414:GLU:HG3	2.19	0.58
1:A:1496:TYR:CD2	1:A:1496:TYR:N	2.71	0.58
1:A:1496:TYR:HD2	1:A:1496:TYR:N	2.02	0.58
1:C:161:LEU:HD11	1:C:185:PHE:CG	2.39	0.58
1:A:342:ILE:HG22	1:A:343:PRO:HD2	1.86	0.58
1:C:655:THR:O	1:C:656:ASN:C	2.42	0.58
1:A:1431:GLY:HA2	1:A:1483:PHE:CE1	2.39	0.58
2:D:844:ILE:HG13	2:D:872:ILE:CG1	2.34	0.58
2:B:481:TYR:O	2:B:481:TYR:CD2	2.51	0.58
2:B:69:PHE:CD2	2:B:70:GLN:N	2.72	0.58
2:D:825:VAL:HG22	2:D:916:VAL:HG13	1.85	0.58
1:C:1271:ILE:HD13	1:C:1300:TYR:CZ	2.39	0.58
1:A:824:PHE:HE2	1:A:846:TYR:HB2	1.69	0.58
1:A:1159:CYS:SG	1:A:1161:LEU:HD23	2.44	0.58
1:C:720:LEU:HD13	1:C:724:CYS:HB3	1.84	0.58
1:C:1113:LEU:HD22	1:C:1114:ASP:H	1.68	0.58
2:B:239:GLY:H	2:B:296:ARG:NH2	2.02	0.58
2:D:36:ASP:OD1	2:D:90:PRO:HA	2.04	0.58
1:A:1408:TYR:CE2	1:A:1410:PRO:HA	2.39	0.58
1:A:927:LEU:HD23	1:A:928:ARG:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1035:HIS:ND1	1:A:1035:HIS:N	2.52	0.58
2:D:460:LEU:O	2:D:460:LEU:HD23	2.04	0.58
1:C:1536:GLN:HG3	1:C:1536:GLN:O	2.04	0.58
1:C:23:TYR:C	1:C:655:THR:HG21	2.24	0.57
1:A:1053:MET:CE	1:A:1086:LEU:HD13	2.33	0.57
1:A:1560:ALA:HB2	1:A:1620:MET:CG	2.27	0.57
1:A:599:TRP:CD1	1:A:779:LEU:HA	2.39	0.57
1:A:1159:CYS:O	1:A:1161:LEU:N	2.37	0.57
1:A:265:VAL:O	1:A:289:ASN:HA	2.04	0.57
2:D:508:LEU:HD12	2:D:509:HIS:N	2.18	0.57
3:Y:110:ILE:HG22	3:Y:111:ASP:O	2.04	0.57
1:A:1541:LEU:HD21	1:A:1543:ILE:HD12	1.86	0.57
1:C:585:GLY:O	1:C:789:ALA:HB1	2.04	0.57
2:B:964:ILE:CG2	2:B:964:ILE:O	2.51	0.57
2:B:167:THR:HG22	2:B:171:ILE:O	2.03	0.57
1:C:680:GLN:O	1:C:684:GLU:HG3	2.04	0.57
2:B:36:ASP:OD1	2:B:90:PRO:HA	2.04	0.57
1:A:1468:PRO:HD3	1:A:1473:LEU:HD13	1.85	0.57
5:D:2001:NAG:C3	5:D:2002:NAG:O5	2.51	0.57
2:D:362:LEU:HD13	2:D:411:ILE:HD12	1.86	0.57
1:A:512:PHE:CE2	3:X:148:ALA:HB3	2.39	0.57
1:A:1093:VAL:O	1:A:1093:VAL:HG12	2.03	0.57
1:C:1011:GLU:HG3	1:C:1055:SER:OG	2.04	0.57
2:D:783:SER:HB2	2:D:787:TRP:CZ2	2.39	0.57
2:D:481:TYR:HE2	2:D:493:GLY:CA	2.17	0.57
2:D:523:TYR:HB3	2:D:533:ALA:HB2	1.86	0.57
3:Y:194:LYS:NZ	3:Y:197:ASN:HB2	2.10	0.57
1:A:489:LYS:CG	1:A:490:SER:H	2.15	0.57
2:B:449:ILE:HD13	2:B:462:VAL:HG23	1.85	0.57
2:D:916:VAL:HG23	2:D:917:PRO:HD2	1.86	0.57
1:C:55:SER:C	1:C:56:ILE:HD13	2.23	0.57
2:D:913:LEU:C	2:D:913:LEU:HD23	2.24	0.57
3:Y:185:LYS:HG2	3:Y:186:TYR:CE2	2.38	0.57
2:B:1536:GLY:O	2:B:1567:ARG:HG2	2.04	0.57
1:C:1560:ALA:O	1:C:1561:TYR:HD2	1.86	0.57
1:C:1053:MET:CE	1:C:1086:LEU:HD22	2.34	0.57
3:Y:78:LYS:C	3:Y:78:LYS:HD2	2.25	0.57
1:C:687:ALA:O	1:C:690:TYR:HB3	2.04	0.57
1:A:623:VAL:O	1:A:624:PHE:C	2.38	0.57
1:A:190:ILE:HG22	1:A:191:PRO:CD	2.34	0.57
1:A:1145:THR:O	1:A:1149:VAL:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1346:ASN:HB2	2:D:1368:CYS:HB2	1.86	0.57
2:B:137:TYR:CE1	2:B:143:VAL:HG22	2.40	0.57
1:C:1159:CYS:SG	1:C:1161:LEU:HD23	2.45	0.57
2:D:1279:ILE:CG2	2:D:1288:ILE:HB	2.35	0.57
1:C:488:PRO:HG3	1:C:499:TYR:OH	2.03	0.57
2:B:873:LYS:HD2	2:B:873:LYS:N	2.18	0.57
1:C:1468:PRO:HD3	1:C:1473:LEU:HD13	1.86	0.57
1:C:503:ILE:CB	1:C:511:HIS:HB2	2.34	0.57
2:B:383:ALA:C	2:B:384:PHE:CD2	2.78	0.57
2:D:519:ARG:CZ	2:D:608:GLY:HA3	2.34	0.57
2:B:161:VAL:HG21	2:B:180:LEU:CD2	2.33	0.57
2:B:266:GLY:HA2	2:B:276:ILE:HG13	1.84	0.57
1:A:1162:VAL:N	1:C:1102:ASN:HD21	2.02	0.57
3:X:111:ASP:CG	3:X:112:PRO:HD2	2.24	0.57
2:B:963:ILE:CG1	2:B:1325:ILE:HG12	2.35	0.57
1:A:532:GLN:HE21	1:A:568:GLY:HA2	1.69	0.57
2:D:789:VAL:HG23	2:D:806:TYR:O	2.04	0.57
2:D:443:ASN:OD1	2:D:469:ASN:HB3	2.05	0.57
2:D:244:HIS:HB3	2:D:291:LYS:CD	2.28	0.57
1:A:133:PRO:HD2	1:A:609:VAL:HG11	1.86	0.57
1:A:822:ASP:HA	1:A:849:ARG:HD2	1.87	0.57
1:A:243:PHE:HE2	1:A:304:GLU:HA	1.70	0.57
3:X:125:LYS:HA	3:X:127:ASN:H	1.69	0.57
1:C:225:PRO:HG3	1:C:766:ARG:HB2	1.85	0.57
2:D:1443:LEU:N	2:D:1443:LEU:HD13	2.19	0.57
2:B:1498:SER:O	2:B:1573:LEU:HD23	2.04	0.57
2:B:1349:VAL:HG22	2:B:1363:LEU:HD12	1.86	0.57
1:A:455:ILE:HG22	1:A:456:ALA:N	2.20	0.57
2:B:963:ILE:HG13	2:B:1325:ILE:HG12	1.86	0.57
1:A:457:TYR:HE1	1:A:556:SER:O	1.88	0.57
1:A:512:PHE:HE2	3:X:148:ALA:HB3	1.70	0.57
1:C:489:LYS:C	1:C:491:PRO:HD3	2.24	0.57
1:A:980:LYS:HD3	1:A:986:GLU:CA	2.33	0.57
1:A:1075:SER:HB2	1:A:1120:GLU:OE1	2.04	0.57
1:A:481:HIS:HE1	1:A:529:PRO:HB3	1.64	0.57
1:C:358:ALA:H	1:C:672:ILE:CG2	2.18	0.57
1:A:742:ILE:HG21	1:A:753:HIS:HA	1.86	0.57
2:B:519:ARG:CZ	2:B:608:GLY:HA3	2.34	0.57
1:A:943:THR:OG1	1:A:1275:SER:OG	2.22	0.57
2:D:199:ILE:HG22	2:D:199:ILE:O	2.05	0.57
1:C:126:LEU:HD11	1:C:205:TYR:CE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:PHE:CG	1:A:112:SER:N	2.73	0.57
1:C:457:TYR:CE2	1:C:641:ASN:HA	2.39	0.57
1:C:1562:LYS:CD	1:C:1648:TRP:HE1	2.18	0.57
1:C:599:TRP:O	1:C:803:GLY:CA	2.49	0.57
1:A:493:ILE:HG23	1:A:495:LYS:N	2.18	0.57
1:A:1130:GLN:OE1	1:A:1232:LEU:HD22	2.03	0.57
1:C:571:LEU:HD12	1:C:593:ALA:O	2.05	0.57
2:B:168:PRO:HG3	2:B:197:TRP:N	2.20	0.57
2:D:961:THR:HG22	2:D:1327:THR:CG2	2.32	0.57
2:D:1371:TYR:CD1	2:D:1377:SER:HB3	2.40	0.57
2:D:556:ILE:CD1	2:D:556:ILE:H	2.14	0.57
1:A:274:ASP:HA	1:A:322:TYR:CD2	2.40	0.57
1:A:342:ILE:HD12	1:A:345:ILE:HD11	1.87	0.57
1:A:196:TYR:CE1	1:A:221:GLU:HB2	2.40	0.57
1:A:1526:LYS:C	1:A:1529:GLU:HG3	2.24	0.57
1:C:23:TYR:O	1:C:655:THR:HB	2.04	0.57
1:A:1552:ALA:HB2	1:A:1620:MET:CE	2.34	0.57
2:B:484:LEU:HD11	2:B:626:LEU:CD1	2.34	0.57
3:X:101:GLN:HA	3:X:125:LYS:HB3	1.86	0.57
1:A:1268:ASN:N	1:A:1269:PRO:CD	2.67	0.57
1:A:981:GLY:HA3	1:A:1333:PHE:HB2	1.85	0.57
1:C:805:SER:O	1:C:807:THR:N	2.38	0.57
2:B:825:VAL:HG22	2:B:916:VAL:HG13	1.86	0.57
1:A:779:LEU:C	1:A:779:LEU:HD12	2.25	0.57
1:C:788:PHE:HD2	1:C:788:PHE:N	2.03	0.57
1:C:443:PRO:HG2	1:C:446:ASN:HB2	1.85	0.57
2:D:218:LYS:HD3	2:D:822:TYR:HE2	1.67	0.57
2:D:1381:ILE:HG21	2:D:1459:TYR:CE1	2.37	0.57
2:D:1450:PHE:HD1	2:D:1451:ILE:H	1.53	0.57
1:A:977:LEU:HD22	1:A:978:SER:N	2.19	0.57
1:A:359:THR:HG23	1:A:359:THR:O	2.03	0.57
1:A:492:TYR:CE2	1:A:493:ILE:HB	2.39	0.57
3:X:75:PHE:O	3:X:77:PRO:HD3	2.05	0.57
3:X:78:LYS:HD2	3:X:78:LYS:C	2.25	0.57
3:X:100:GLY:O	3:X:125:LYS:HG2	2.04	0.57
1:A:571:LEU:HD23	1:A:812:ALA:HB2	1.87	0.57
1:A:544:TYR:HD2	1:A:544:TYR:C	2.08	0.57
1:A:1221:ASN:HA	1:A:1222:PRO:C	2.23	0.57
1:C:610:TYR:N	1:C:610:TYR:CD1	2.71	0.57
1:A:22:THR:HG22	1:A:23:TYR:CE1	2.40	0.57
1:A:1239:VAL:HG12	1:A:1239:VAL:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1451:THR:O	1:A:1452:ASP:CB	2.53	0.57
1:A:1569:THR:O	1:A:1570:VAL:HG23	2.05	0.57
2:D:383:ALA:C	2:D:384:PHE:CD2	2.78	0.57
1:A:1429:PRO:HB2	1:A:1432:ILE:HG12	1.86	0.57
2:D:243:PHE:CE1	2:D:336:ILE:HG21	2.40	0.57
2:D:1544:VAL:HB	2:D:1557:ARG:HA	1.87	0.57
1:C:163:PHE:CE2	1:C:188:PHE:CD1	2.93	0.57
2:D:51:PRO:O	2:D:52:LYS:HG3	2.05	0.57
3:X:129:THR:HG22	3:X:129:THR:O	2.05	0.57
1:A:512:PHE:CD2	1:A:512:PHE:C	2.77	0.56
1:C:514:THR:HG22	1:C:515:ARG:N	2.19	0.56
1:C:534:MET:HB3	1:C:538:SER:OG	2.05	0.56
1:C:1527:CYS:O	1:C:1529:GLU:N	2.38	0.56
1:A:1240:PRO:HB2	1:A:1242:THR:HG23	1.86	0.56
1:A:953:ILE:HD11	1:A:955:ARG:HH21	1.69	0.56
2:D:795:THR:HG22	2:D:796:PRO:CD	2.33	0.56
1:A:1213:LYS:HE2	1:A:1266:TYR:HD2	1.69	0.56
1:A:1226:ARG:O	1:A:1270:VAL:HG22	2.05	0.56
1:A:1333:PHE:O	1:A:1334:LEU:CB	2.51	0.56
1:A:362:PHE:CE1	1:A:640:LEU:HB2	2.40	0.56
1:C:84:ILE:H	1:C:84:ILE:HD12	1.70	0.56
2:B:476:ILE:O	2:B:476:ILE:CG2	2.52	0.56
2:D:558:MET:O	2:D:561:ALA:CB	2.53	0.56
1:C:938:SER:C	1:C:940:SER:N	2.58	0.56
2:B:1562:GLN:HE22	2:B:1596:LYS:HZ1	1.52	0.56
2:D:844:ILE:CD1	2:D:872:ILE:HD11	2.35	0.56
1:C:1056:ILE:CD1	1:C:1066:TYR:CE2	2.88	0.56
1:C:1493:PHE:HE1	1:C:1495:VAL:HG12	1.69	0.56
1:A:920:LYS:HZ3	2:B:842:GLU:CD	2.08	0.56
2:B:840:VAL:HG12	2:B:841:ASN:N	2.11	0.56
3:Y:75:PHE:O	3:Y:77:PRO:HD3	2.05	0.56
1:C:571:LEU:HD23	1:C:812:ALA:HB2	1.86	0.56
1:A:1271:ILE:O	1:A:1275:SER:HB3	2.05	0.56
1:C:153:LYS:HB3	1:C:154:PRO:CD	2.34	0.56
2:D:1424:ILE:CD1	2:D:1424:ILE:H	2.17	0.56
2:B:964:ILE:HG22	2:B:964:ILE:O	2.04	0.56
2:D:1631:PHE:CD2	2:D:1632:SER:N	2.73	0.56
1:A:982:LEU:C	1:A:984:VAL:H	2.09	0.56
3:X:185:LYS:HG2	3:X:186:TYR:CE2	2.40	0.56
1:C:543:TYR:CD1	1:C:543:TYR:O	2.57	0.56
1:C:511:HIS:CE1	3:Y:149:SER:CB	2.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:857:CYS:HB3	2:D:885:VAL:HG22	1.87	0.56
1:A:979:VAL:HG21	1:A:1326:TYR:CZ	2.36	0.56
1:C:128:ILE:HD12	1:C:201:ILE:CG2	2.32	0.56
1:A:263:ALA:HB3	1:A:292:LEU:HB3	1.86	0.56
1:A:395:ILE:HD12	1:A:395:ILE:O	2.06	0.56
2:D:1273:LEU:CB	2:D:1319:GLY:HA3	2.31	0.56
1:C:742:ILE:CG2	1:C:753:HIS:HA	2.34	0.56
1:C:473:HIS:O	1:C:473:HIS:HD2	1.88	0.56
1:A:915:GLU:HB2	2:B:905:TRP:CZ2	2.40	0.56
1:A:309:GLU:HG2	1:A:310:LEU:HD12	1.86	0.56
1:A:309:GLU:HG2	1:A:310:LEU:N	2.21	0.56
1:A:1117:SER:HA	1:A:1145:THR:OG1	2.05	0.56
2:B:916:VAL:HG23	2:B:917:PRO:HD2	1.86	0.56
1:C:981:GLY:HA3	1:C:1333:PHE:HB2	1.85	0.56
2:D:1288:ILE:CD1	2:D:1303:VAL:HG21	2.36	0.56
1:C:524:GLN:HB2	2:D:401:ASN:OD1	2.05	0.56
3:X:47:HIS:O	3:X:51:SER:HB2	2.06	0.56
2:B:173:VAL:HG11	2:B:186:TYR:OH	2.06	0.56
2:B:581:ASP:O	2:B:583:ALA:N	2.38	0.56
2:B:843:ASP:HA	2:B:873:LYS:O	2.06	0.56
1:A:550:GLN:HG2	1:A:550:GLN:O	2.04	0.56
2:D:269:ILE:HA	2:D:312:HIS:CD2	2.40	0.56
2:D:348:THR:HA	2:D:352:LYS:NZ	2.20	0.56
1:C:1000:LEU:O	1:C:1001:THR:HG23	2.06	0.56
1:C:512:PHE:HD2	1:C:512:PHE:O	1.89	0.56
1:A:1094:GLU:H	1:A:1094:GLU:CD	2.07	0.56
1:A:1227:PHE:CD1	1:A:1227:PHE:C	2.78	0.56
1:C:1352:PHE:HD2	1:C:1352:PHE:N	2.01	0.56
1:C:395:ILE:O	1:C:395:ILE:HD12	2.05	0.56
2:D:235:PHE:HB3	2:D:338:ILE:HG23	1.88	0.56
1:C:265:VAL:O	1:C:289:ASN:HA	2.05	0.56
1:A:267:ILE:HG22	1:A:268:THR:N	2.21	0.56
1:C:695:VAL:CG1	1:C:724:CYS:HA	2.35	0.56
1:A:149:ASN:HD22	1:A:149:ASN:N	1.99	0.56
1:A:587:THR:CG2	1:A:789:ALA:HB2	2.34	0.56
1:C:161:LEU:HD11	1:C:185:PHE:CE1	2.39	0.56
1:A:680:GLN:O	1:A:684:GLU:HG3	2.04	0.56
1:C:22:THR:HG22	1:C:23:TYR:CE1	2.40	0.56
1:C:641:ASN:OD1	1:C:644:ASN:HB2	2.06	0.56
2:B:1562:GLN:NE2	2:B:1596:LYS:HZ2	2.03	0.56
2:D:435:TYR:OH	2:D:532:VAL:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1217:LEU:HD13	1:C:1237:SER:HA	1.88	0.56
1:A:617:LYS:HB3	1:A:619:PRO:HD2	1.88	0.56
3:X:77:PRO:O	3:X:78:LYS:HB3	2.06	0.56
2:D:484:LEU:HD11	2:D:626:LEU:CD1	2.35	0.56
1:A:308:LYS:HG3	1:A:309:GLU:N	2.21	0.56
2:D:39:GLU:OE1	2:D:488:LYS:HB3	2.06	0.56
2:D:183:PHE:CD2	2:D:183:PHE:N	2.72	0.56
1:A:827:MET:SD	1:A:843:GLY:HA3	2.45	0.56
2:B:913:LEU:C	2:B:913:LEU:HD23	2.26	0.56
1:A:1548:ARG:C	1:A:1550:GLN:H	2.09	0.56
2:B:946:LYS:HA	2:B:1310:ASP:OD1	2.05	0.56
2:B:142:PRO:HB3	2:B:187:ASN:ND2	2.20	0.56
1:A:355:ASN:HD22	1:A:355:ASN:N	2.03	0.56
1:A:25:ILE:CB	1:A:655:THR:HG23	2.36	0.56
2:D:953:ARG:CZ	2:D:959:ILE:HD11	2.36	0.56
2:B:1509:PRO:O	2:B:1512:ILE:HG13	2.06	0.56
2:D:494:ARG:CG	2:D:494:ARG:HH11	2.15	0.56
1:C:149:ASN:HD22	1:C:149:ASN:N	1.92	0.56
2:D:1510:LEU:HD21	2:D:1514:LYS:HZ1	1.70	0.56
1:C:827:MET:SD	1:C:843:GLY:HA3	2.45	0.56
1:A:42:GLN:CA	1:A:80:GLN:HG3	2.35	0.56
1:A:655:THR:O	1:A:656:ASN:C	2.43	0.56
1:A:33:VAL:HG21	1:A:121:TYR:HE1	1.66	0.56
1:A:489:LYS:C	1:A:491:PRO:HD3	2.26	0.56
1:A:135:TYR:CD1	1:A:141:VAL:HG22	2.41	0.56
1:A:351:PRO:HG2	1:A:352:TYR:CE2	2.40	0.56
2:B:595:GLN:O	2:B:598:ILE:HB	2.05	0.56
1:C:267:ILE:HD12	1:C:299:VAL:HG11	1.88	0.56
1:A:788:PHE:CD2	1:A:788:PHE:N	2.73	0.56
1:C:874:ASP:HA	1:C:878:THR:O	2.05	0.56
1:C:1585:TYR:CD1	1:C:1671:ILE:HG12	2.41	0.56
2:D:518:PHE:CD2	2:D:538:VAL:HB	2.38	0.56
2:D:829:GLN:HA	2:D:885:VAL:HG12	1.88	0.56
1:C:135:TYR:CD1	1:C:141:VAL:HG22	2.40	0.56
1:C:1323:LEU:CD1	1:C:1324:HIS:H	2.19	0.56
1:A:1110:ASN:OD1	1:A:1110:ASN:N	2.38	0.56
3:X:110:ILE:HG22	3:X:111:ASP:O	2.05	0.56
2:D:599:TRP:HA	2:D:599:TRP:HE3	1.70	0.56
2:D:167:THR:HG23	2:D:171:ILE:N	2.20	0.56
2:D:1384:ILE:HB	2:D:1423:VAL:HG12	1.87	0.56
1:A:43:VAL:HG11	1:A:73:LEU:CD1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:VAL:HG21	1:C:554:LEU:HD11	1.88	0.56
1:C:1559:TYR:CD1	1:C:1561:TYR:HE2	2.23	0.56
1:A:59:TYR:CE1	1:A:60:PRO:HG3	2.41	0.56
1:A:59:TYR:CE2	1:A:99:VAL:HG21	2.41	0.56
2:D:525:GLN:HA	2:D:530:GLU:O	2.05	0.56
2:B:520:PHE:O	2:B:535:SER:HA	2.06	0.56
3:Y:127:ASN:OD1	3:Y:158:GLU:HB3	2.06	0.56
2:D:824:VAL:HG22	2:D:825:VAL:N	2.20	0.56
1:C:774:LEU:HG	1:C:788:PHE:CE1	2.41	0.56
2:B:1288:ILE:CD1	2:B:1303:VAL:HG21	2.36	0.56
1:C:1429:PRO:HB2	1:C:1432:ILE:HG12	1.86	0.56
2:D:599:TRP:CZ3	2:D:602:ILE:HD12	2.40	0.56
2:B:282:ARG:C	2:B:283:ILE:HD12	2.25	0.56
2:B:345:ILE:HD11	2:B:427:THR:N	2.21	0.56
1:A:115:LYS:HB2	1:A:654:LEU:CD2	2.35	0.56
1:A:78:LYS:HG3	3:X:146:LEU:HB2	1.87	0.56
1:C:1559:TYR:CD1	1:C:1561:TYR:CE2	2.94	0.56
1:A:1095:GLN:O	1:A:1097:GLN:N	2.39	0.56
2:D:829:GLN:HE22	2:D:883:VAL:CG1	2.14	0.56
2:D:885:VAL:HG23	2:D:885:VAL:O	2.06	0.56
1:A:1598:ILE:HG22	1:A:1599:THR:H	1.70	0.56
1:C:577:PRO:CD	1:C:588:VAL:HG23	2.36	0.56
2:B:789:VAL:HG23	2:B:806:TYR:O	2.05	0.56
2:B:69:PHE:C	2:B:69:PHE:CD2	2.79	0.56
2:B:916:VAL:HG22	2:B:917:PRO:O	2.05	0.56
2:D:422:ARG:HH12	3:Y:44:ARG:CA	2.18	0.56
1:C:1128:LYS:C	1:C:1129:LEU:HD23	2.27	0.56
1:A:1450:PHE:HZ	1:A:1475:VAL:HB	1.70	0.56
2:D:40:GLN:HG3	2:D:86:THR:HG23	1.88	0.56
2:D:826:LYS:NZ	2:D:1488:ASN:HB3	2.21	0.56
1:A:1132:THR:O	1:A:1134:PRO:N	2.39	0.55
2:B:1621:PHE:O	2:B:1622:GLN:C	2.43	0.55
2:B:1628:PHE:O	2:B:1630:GLN:N	2.39	0.55
1:A:1585:TYR:CE1	1:A:1671:ILE:HG12	2.40	0.55
2:D:355:LYS:O	2:D:358:MET:CB	2.54	0.55
1:A:290:THR:O	1:A:291:MET:HB2	2.05	0.55
1:A:489:LYS:HG2	1:A:490:SER:N	2.21	0.55
2:B:34:ARG:HD2	2:B:488:LYS:NZ	2.21	0.55
1:A:610:TYR:CD1	1:A:610:TYR:N	2.73	0.55
1:C:617:LYS:HB3	1:C:619:PRO:HD2	1.88	0.55
2:B:1284:ARG:CG	2:B:1285:GLU:N	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1280:GLU:HG2	2:D:1287:PRO:CB	2.33	0.55
2:D:595:GLN:O	2:D:598:ILE:HB	2.07	0.55
2:D:1612:HIS:O	2:D:1613:GLU:C	2.44	0.55
2:D:1424:ILE:HG12	2:D:1426:TYR:HE2	1.70	0.55
1:C:693:SER:C	1:C:695:VAL:N	2.60	0.55
1:A:695:VAL:CG1	1:A:724:CYS:HA	2.35	0.55
1:A:680:GLN:HB2	1:A:684:GLU:OE2	2.06	0.55
1:C:126:LEU:HD11	1:C:205:TYR:CZ	2.41	0.55
3:Y:146:LEU:HD21	3:Y:148:ALA:HB2	1.88	0.55
2:D:1593:THR:CG2	2:D:1594:LYS:N	2.68	0.55
1:A:1219:LYS:CD	1:A:1239:VAL:HG21	2.36	0.55
3:Y:100:GLY:O	3:Y:125:LYS:HG2	2.05	0.55
3:Y:58:SER:HB2	3:Y:125:LYS:HE3	1.87	0.55
1:C:1274:LEU:O	1:C:1277:GLU:N	2.37	0.55
1:C:1108:VAL:HG21	1:C:1167:ALA:CB	2.34	0.55
1:C:351:PRO:HG3	1:C:442:LEU:HD11	1.88	0.55
2:B:1371:TYR:CD1	2:B:1377:SER:HB3	2.41	0.55
1:A:1421:HIS:HD2	1:A:1422:ALA:N	2.03	0.55
1:A:1433:SER:OG	1:A:1482:LEU:HD12	2.06	0.55
1:C:644:ASN:CG	1:C:648:LEU:HD12	2.26	0.55
1:C:1562:LYS:O	1:C:1563:VAL:CG1	2.54	0.55
1:C:1627:ILE:O	1:C:1627:ILE:CD1	2.54	0.55
1:C:1527:CYS:C	1:C:1529:GLU:H	2.10	0.55
1:A:1053:MET:CE	1:A:1086:LEU:HD22	2.37	0.55
2:D:481:TYR:CE2	2:D:493:GLY:HA3	2.41	0.55
1:A:198:MET:SD	1:A:218:GLU:HG3	2.45	0.55
1:A:1190:ILE:HG22	1:A:1191:SER:N	2.20	0.55
1:C:1083:LEU:HD13	1:C:1104:LEU:HD23	1.89	0.55
1:C:549:GLU:CD	1:C:550:GLN:N	2.60	0.55
3:Y:41:HIS:O	3:Y:42:ASP:CB	2.54	0.55
2:B:355:LYS:O	2:B:358:MET:HB3	2.07	0.55
3:Y:40:LEU:HD11	3:Y:209:PHE:CZ	2.41	0.55
1:C:855:PHE:HA	2:D:904:LEU:HD11	1.87	0.55
1:A:1453:TYR:O	1:A:1453:TYR:CG	2.59	0.55
1:A:364:LYS:HE3	1:A:457:TYR:HD1	1.72	0.55
1:C:77:ASN:ND2	1:C:81:ASN:HB2	2.22	0.55
1:C:1611:LEU:HD13	1:C:1617:TYR:CD1	2.41	0.55
1:C:478:VAL:CG1	1:C:566:LYS:HD3	2.37	0.55
2:B:42:LEU:HD22	2:B:492:VAL:HG21	1.87	0.55
1:A:1232:LEU:HG	1:A:1233:GLN:N	2.21	0.55
1:C:1130:GLN:OE1	1:C:1232:LEU:HD22	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:788:PHE:CD2	1:C:788:PHE:N	2.74	0.55
2:D:456:PRO:CG	2:D:515:ILE:HD11	2.37	0.55
1:A:428:VAL:HG22	1:A:429:THR:N	2.22	0.55
1:A:532:GLN:O	1:A:535:VAL:HG13	2.07	0.55
1:C:504:LEU:HD21	1:C:651:LEU:HG	1.88	0.55
3:Y:146:LEU:HD22	3:Y:146:LEU:C	2.26	0.55
1:A:180:ILE:HG22	1:A:181:GLY:N	2.22	0.55
2:D:1562:GLN:HB2	2:D:1598:SER:HB3	1.88	0.55
1:A:934:VAL:CG2	1:A:1366:HIS:CD2	2.88	0.55
1:A:1056:ILE:O	1:A:1056:ILE:HG12	2.05	0.55
3:X:87:LEU:HA	3:X:91:LYS:CD	2.37	0.55
1:C:1287:THR:OG1	1:C:1288:GLN:N	2.39	0.55
1:C:1108:VAL:CG2	1:C:1167:ALA:HB2	2.36	0.55
1:A:1180:LEU:HG	1:A:1208:ILE:HG12	1.89	0.55
1:C:1180:LEU:HG	1:C:1208:ILE:HG12	1.88	0.55
1:A:153:LYS:HB3	1:A:154:PRO:CD	2.35	0.55
2:B:130:ILE:HG12	2:B:147:VAL:HG23	1.87	0.55
2:D:512:PRO:HA	2:D:515:ILE:HD12	1.87	0.55
2:B:1606:TRP:C	2:B:1606:TRP:HD1	2.10	0.55
2:B:558:MET:O	2:B:561:ALA:CB	2.55	0.55
2:D:343:TYR:HE1	2:D:420:LEU:HD11	1.72	0.55
2:D:826:LYS:HG3	2:D:887:LEU:O	2.05	0.55
2:B:51:PRO:O	2:B:52:LYS:HG3	2.06	0.55
2:D:76:ASN:HB2	2:D:77:PRO:HD2	1.88	0.55
1:A:923:LEU:HD23	1:A:924:VAL:N	2.22	0.55
1:C:24:VAL:HA	1:C:655:THR:HG21	1.87	0.55
1:C:1615:ARG:HD2	1:C:1647:TYR:HD1	1.71	0.55
1:A:1228:TRP:N	1:A:1228:TRP:CE3	2.75	0.55
2:D:28:ILE:HD13	2:D:621:PHE:HE1	1.70	0.55
2:D:1591:LEU:C	2:D:1591:LEU:CD2	2.75	0.55
1:C:256:TYR:HB3	1:C:848:TYR:OH	2.06	0.55
1:C:947:ARG:O	1:C:949:ILE:HG12	2.06	0.55
1:A:851:SER:O	1:A:890:GLY:HA2	2.07	0.55
1:A:1272:LYS:O	1:A:1276:GLU:HG3	2.07	0.55
1:C:1453:TYR:O	1:C:1453:TYR:CG	2.59	0.55
2:B:365:TYR:HA	2:B:394:GLY:O	2.07	0.55
2:B:233:LYS:HG3	2:B:233:LYS:O	2.05	0.55
1:A:811:VAL:O	1:A:811:VAL:HG12	2.05	0.55
2:D:261:ALA:HB3	2:D:285:ILE:HD11	1.88	0.55
2:B:1594:LYS:CE	2:B:1594:LYS:HA	2.18	0.55
1:C:1132:THR:O	1:C:1134:PRO:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:838:ASN:OD1	2:D:840:VAL:HG23	2.07	0.55
2:D:481:TYR:HE2	2:D:493:GLY:HA3	1.71	0.55
2:D:476:ILE:HG23	2:D:476:ILE:O	2.06	0.55
1:C:1327:LYS:O	1:C:1332:ASN:ND2	2.39	0.55
2:D:130:ILE:HD13	2:D:199:ILE:CG2	2.36	0.55
2:B:276:ILE:O	2:B:277:PRO:C	2.45	0.55
1:A:1188:LEU:HD23	1:A:1212:LEU:HA	1.89	0.55
1:C:510:ILE:HA	3:Y:150:ILE:HG13	1.87	0.55
1:C:599:TRP:CD1	1:C:779:LEU:HA	2.41	0.55
1:A:1571:GLU:O	1:A:1574:PHE:CD2	2.60	0.55
2:D:42:LEU:HD22	2:D:492:VAL:HG21	1.89	0.55
1:A:834:VAL:O	1:A:837:GLU:HB2	2.07	0.55
1:A:596:MET:H	1:A:782:ARG:NH1	1.92	0.55
1:A:569:ASN:ND2	1:A:570:GLN:H	2.04	0.55
2:B:1591:LEU:C	2:B:1591:LEU:CD2	2.75	0.55
1:C:824:PHE:CD2	1:C:824:PHE:N	2.69	0.55
1:C:1019:PHE:CD2	1:C:1020:TYR:N	2.75	0.55
1:C:1333:PHE:O	1:C:1334:LEU:CB	2.53	0.55
3:Y:134:THR:CG2	3:Y:153:PHE:HB3	2.37	0.55
2:B:847:ARG:O	2:B:898:ALA:HA	2.07	0.55
2:D:1349:VAL:HG22	2:D:1363:LEU:HD12	1.88	0.55
1:A:906:GLY:O	1:A:908:HIS:NE2	2.40	0.55
1:C:539:ARG:HE	1:C:633:GLY:HA3	1.71	0.55
2:B:928:VAL:HG23	2:B:1323:MET:HB3	1.87	0.55
2:D:1602:THR:H	2:D:1605:THR:HB	1.72	0.55
1:C:612:VAL:O	1:C:612:VAL:HG12	2.06	0.55
2:B:343:TYR:HE1	2:B:420:LEU:HD11	1.71	0.55
2:B:862:LYS:HD2	2:B:1588:SER:OG	2.06	0.55
1:A:1344:ASP:OD1	1:A:1345:ASP:N	2.40	0.55
1:C:1383:THR:HG21	1:C:1511:THR:HG22	1.88	0.55
1:A:85:LEU:HD22	1:A:85:LEU:N	2.22	0.55
1:A:873:ILE:HD12	1:A:873:ILE:O	2.06	0.55
1:C:1561:TYR:CD1	1:C:1581:LEU:HD21	2.42	0.55
1:C:1556:GLU:CB	1:C:1622:LYS:HE2	2.30	0.55
1:C:1218:VAL:CG1	1:C:1219:LYS:H	2.17	0.55
2:B:285:ILE:CD1	2:B:285:ILE:N	2.70	0.55
1:C:145:VAL:HB	1:C:183:ILE:CG1	2.34	0.55
2:B:443:ASN:OD1	2:B:469:ASN:HB3	2.06	0.55
1:C:697:LYS:O	1:C:700:TYR:HB3	2.06	0.55
1:C:290:THR:O	1:C:291:MET:HB2	2.07	0.55
1:A:1013:MET:HA	1:A:1016:VAL:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:ARG:C	1:A:614:ARG:HD2	2.24	0.55
1:C:199:TRP:CB	1:C:217:PHE:CE1	2.90	0.55
2:D:1381:ILE:HB	2:D:1459:TYR:CD1	2.42	0.55
3:Y:107:GLN:OE1	3:Y:110:ILE:HD11	2.07	0.55
2:B:243:PHE:CE1	2:B:336:ILE:HG21	2.42	0.55
2:D:184:TRP:HB2	2:D:185:PRO:CD	2.37	0.55
2:B:923:SER:O	2:B:924:ILE:HD12	2.07	0.55
2:B:447:VAL:O	2:B:447:VAL:HG13	2.06	0.55
3:Y:50:TYR:HE2	3:Y:170:ARG:CZ	2.19	0.55
1:A:44:TYR:CZ	1:A:497:THR:HG21	2.41	0.55
1:C:503:ILE:HD11	1:C:540:LEU:HD13	1.89	0.55
1:C:1227:PHE:HB2	1:C:1251:THR:HG21	1.89	0.55
1:A:936:ARG:HH12	1:A:1284:PHE:HZ	1.53	0.55
2:B:965:ILE:HG13	2:B:1301:ARG:CB	2.26	0.55
1:C:1095:GLN:O	1:C:1097:GLN:N	2.41	0.55
1:C:134:VAL:C	1:C:135:TYR:HD2	2.10	0.55
2:B:26:THR:HG22	2:B:630:THR:HG22	1.88	0.55
2:B:523:TYR:HD2	2:B:621:PHE:HZ	1.55	0.55
1:C:308:LYS:HG3	1:C:309:GLU:N	2.21	0.55
3:Y:87:LEU:HA	3:Y:91:LYS:CD	2.36	0.55
1:C:171:VAL:CG1	1:C:172:ASP:N	2.70	0.55
1:A:773:TRP:HZ3	1:A:788:PHE:CE1	2.25	0.55
1:A:1474:CYS:HB3	1:A:1476:ARG:NH1	2.22	0.55
1:C:342:ILE:HG22	1:C:343:PRO:HD2	1.88	0.55
2:D:1530:ARG:HG3	2:D:1530:ARG:HH11	1.72	0.55
1:A:42:GLN:HE21	1:A:43:VAL:C	2.11	0.54
1:C:505:SER:HB3	1:C:510:ILE:CD1	2.37	0.54
1:C:127:PHE:HE2	1:C:623:VAL:CG1	2.09	0.54
1:C:1601:ILE:O	1:C:1638:PRO:O	2.25	0.54
2:B:126:SER:O	2:B:208:GLU:HG3	2.07	0.54
2:B:380:VAL:CG1	2:B:387:MET:HB3	2.27	0.54
2:B:39:GLU:OE1	2:B:488:LYS:HB3	2.07	0.54
2:D:1506:ILE:CD1	2:D:1628:PHE:CE1	2.89	0.54
3:Y:47:HIS:O	3:Y:51:SER:HB2	2.07	0.54
3:Y:111:ASP:CG	3:Y:112:PRO:HD2	2.27	0.54
1:C:587:THR:CG2	1:C:789:ALA:HB2	2.37	0.54
1:C:705:VAL:HA	1:C:739:ARG:NH2	2.21	0.54
2:B:1522:TYR:N	2:B:1522:TYR:CD2	2.73	0.54
2:B:167:THR:HG23	2:B:171:ILE:N	2.23	0.54
2:D:1536:GLY:O	2:D:1567:ARG:HG2	2.07	0.54
2:D:96:THR:HG21	2:D:102:GLN:OE1	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1221:ASN:HA	1:C:1222:PRO:C	2.26	0.54
1:A:1554:LYS:HG3	1:A:1555:PRO:HD2	1.88	0.54
2:B:1633:TYR:CE1	2:B:1637:GLU:OE1	2.59	0.54
1:A:662:SER:O	1:A:663:GLN:HG2	2.07	0.54
1:C:231:ILE:O	1:C:231:ILE:HG23	2.06	0.54
1:C:967:LEU:HD13	1:C:1365:VAL:HG22	1.89	0.54
1:C:1562:LYS:O	1:C:1563:VAL:HG13	2.06	0.54
2:B:953:ARG:CZ	2:B:959:ILE:HD11	2.37	0.54
1:A:871:PRO:CD	1:A:872:VAL:N	2.68	0.54
1:A:694:VAL:O	1:A:697:LYS:HE2	2.06	0.54
1:A:494:ASP:CG	1:A:495:LYS:HE2	2.28	0.54
1:A:316:GLU:HG2	1:A:349:LEU:HD23	1.88	0.54
1:A:1013:MET:HE2	1:A:1287:THR:HB	1.88	0.54
1:C:222:TYR:CD1	1:C:768:TYR:HB2	2.42	0.54
1:A:824:PHE:CZ	1:A:846:TYR:HD1	2.26	0.54
1:C:549:GLU:CG	1:C:550:GLN:H	2.19	0.54
1:C:428:VAL:HG22	1:C:429:THR:H	1.72	0.54
1:A:1421:HIS:CD2	1:A:1421:HIS:C	2.78	0.54
1:A:1421:HIS:CE1	1:A:1498:TYR:CD1	2.95	0.54
1:A:854:GLN:H	1:A:854:GLN:NE2	2.05	0.54
2:B:410:PRO:HA	2:B:431:THR:HG22	1.89	0.54
1:C:359:THR:HG23	1:C:359:THR:O	2.08	0.54
3:Y:166:ASP:HB2	3:Y:207:LEU:HD21	1.89	0.54
1:A:656:ASN:CG	1:A:658:ASN:HB3	2.27	0.54
1:C:1236:ASP:O	1:C:1238:SER:N	2.35	0.54
1:C:1011:GLU:O	1:C:1014:SER:HB3	2.08	0.54
2:B:1593:THR:CG2	2:B:1594:LYS:H	2.20	0.54
1:A:1562:LYS:CD	1:A:1648:TRP:CZ2	2.86	0.54
1:A:1611:LEU:HD13	1:A:1617:TYR:CD1	2.43	0.54
2:D:1486:ILE:HD11	2:D:1591:LEU:CD2	2.37	0.54
1:C:472:ASN:O	1:C:473:HIS:HB3	2.06	0.54
1:C:696:LYS:NZ	1:C:759:PRO:CD	2.64	0.54
3:X:125:LYS:HA	3:X:126:ASN:C	2.25	0.54
1:C:1013:MET:HA	1:C:1016:VAL:HG23	1.90	0.54
2:B:218:LYS:HD3	2:B:822:TYR:HE2	1.72	0.54
2:D:1387:LEU:HD21	2:D:1472:TYR:CE1	2.42	0.54
1:A:472:ASN:O	1:A:473:HIS:HB3	2.07	0.54
3:X:46:LEU:HD12	3:X:180:TYR:CE1	2.43	0.54
1:C:1117:SER:HA	1:C:1145:THR:OG1	2.07	0.54
1:C:455:ILE:HG22	1:C:456:ALA:N	2.22	0.54
2:D:559:PRO:HG2	2:D:812:LYS:HD2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ILE:HD13	1:A:41:ILE:CB	2.37	0.54
1:A:44:TYR:CB	1:A:545:ILE:HD12	2.38	0.54
1:C:42:GLN:HE21	1:C:43:VAL:C	2.10	0.54
1:C:658:ASN:O	1:C:659:ALA:CB	2.55	0.54
1:C:1582:LEU:HD11	1:C:1648:TRP:CZ2	2.43	0.54
1:C:1562:LYS:HD2	1:C:1648:TRP:CE2	2.42	0.54
1:C:1569:THR:O	1:C:1570:VAL:HG23	2.07	0.54
2:D:775:THR:HG22	2:D:776:MET:H	1.71	0.54
2:B:954:VAL:HG23	2:B:1330:ASN:O	2.07	0.54
1:C:779:LEU:HD12	1:C:780:VAL:N	2.22	0.54
2:B:775:THR:HG22	2:B:776:MET:H	1.72	0.54
1:A:490:SER:N	1:A:491:PRO:CD	2.70	0.54
1:A:1020:TYR:CE1	1:A:1295:GLU:HG3	2.39	0.54
2:B:1443:LEU:N	2:B:1443:LEU:HD13	2.23	0.54
1:C:680:GLN:HG3	1:C:681:LYS:H	1.72	0.54
1:A:126:LEU:HD11	1:A:205:TYR:CZ	2.43	0.54
2:D:1278:THR:HB	2:D:1314:THR:HB	1.90	0.54
1:A:1279:ARG:HD3	1:A:1280:TYR:N	2.22	0.54
2:D:503:LEU:C	2:D:503:LEU:HD23	2.28	0.54
1:C:234:GLU:HB3	1:C:246:PHE:HE1	1.72	0.54
1:A:594:THR:O	1:A:782:ARG:HD2	2.07	0.54
1:A:1402:ILE:HG13	1:A:1479:ILE:HD13	1.89	0.54
1:C:895:LEU:HD12	1:C:896:VAL:N	2.22	0.54
1:A:989:SER:O	1:A:993:SER:CB	2.56	0.54
2:D:1636:THR:HG22	2:D:1637:GLU:HG3	1.89	0.54
1:A:705:VAL:HA	1:A:739:ARG:NH2	2.22	0.54
3:X:119:VAL:HG21	3:X:209:PHE:CB	2.38	0.54
1:A:1188:LEU:HD23	1:A:1212:LEU:HD13	1.88	0.54
1:C:662:SER:O	1:C:663:GLN:HG2	2.07	0.54
1:A:1084:ARG:HD2	1:A:1154:LYS:HG3	1.90	0.54
2:B:1274:ASN:OD1	2:B:1291:ARG:NH2	2.41	0.54
1:C:515:ARG:HG3	1:C:526:ILE:CG2	2.38	0.54
1:C:987:ILE:HD11	1:C:1294:ILE:HG23	1.90	0.54
1:A:1133:LEU:HD12	1:A:1133:LEU:N	2.06	0.54
1:A:145:VAL:HB	1:A:183:ILE:CG1	2.33	0.54
2:D:126:SER:O	2:D:208:GLU:HG3	2.08	0.54
1:C:594:THR:O	1:C:782:ARG:HD2	2.08	0.54
1:C:309:GLU:HG2	1:C:310:LEU:N	2.22	0.54
1:C:155:ALA:O	1:C:157:ARG:N	2.40	0.54
1:A:100:SER:O	1:A:101:TYR:HB2	2.06	0.54
2:B:1288:ILE:HD13	2:B:1303:VAL:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:LYS:HD3	1:C:110:HIS:HE1	1.73	0.54
1:C:1112:GLN:NE2	1:C:1171:ALA:HB2	2.21	0.54
1:C:1188:LEU:HD23	1:C:1212:LEU:CD1	2.37	0.54
1:C:680:GLN:HB2	1:C:684:GLU:OE2	2.07	0.54
1:A:903:LEU:N	1:A:903:LEU:HD22	2.23	0.54
2:B:1638:PHE:O	2:B:1639:GLY:O	2.26	0.54
1:A:1440:LYS:O	1:A:1444:GLU:HG3	2.08	0.54
1:C:1084:ARG:HD2	1:C:1154:LYS:HG3	1.88	0.54
3:X:50:TYR:HE2	3:X:170:ARG:CZ	2.21	0.54
1:C:23:TYR:HE2	1:C:111:PHE:CD2	2.26	0.54
1:C:489:LYS:HG2	1:C:490:SER:N	2.22	0.54
1:C:1278:GLN:NE2	1:C:1293:ALA:HB1	2.22	0.54
1:A:1102:ASN:HD21	1:C:1162:VAL:HG22	1.67	0.54
1:A:1549:LYS:HD3	1:A:1667:PHE:CB	2.38	0.54
1:C:1082:ALA:O	1:C:1086:LEU:HD23	2.07	0.54
2:D:46:HIS:ND1	2:D:525:GLN:HG2	2.22	0.54
1:A:316:GLU:HG2	1:A:349:LEU:CD2	2.37	0.54
1:C:614:ARG:HD2	1:C:614:ARG:C	2.24	0.54
1:A:199:TRP:CB	1:A:217:PHE:CE1	2.91	0.54
3:Y:86:LEU:HG	3:Y:91:LYS:HG3	1.88	0.54
1:C:1020:TYR:CE1	1:C:1295:GLU:HG3	2.35	0.54
2:D:69:PHE:CE1	2:D:87:ILE:HA	2.43	0.54
1:A:154:PRO:O	1:A:155:ALA:CB	2.55	0.54
2:B:1279:ILE:CG2	2:B:1288:ILE:HB	2.35	0.54
1:A:398:ASN:O	1:A:399:GLN:CB	2.56	0.54
1:C:1112:GLN:HB2	1:C:1118:PHE:CE1	2.43	0.54
2:B:184:TRP:HB2	2:B:185:PRO:CD	2.37	0.54
1:A:917:TRP:HA	1:A:917:TRP:CE3	2.43	0.54
1:C:612:VAL:HG21	1:C:769:PHE:HZ	1.72	0.54
2:B:861:THR:O	2:B:863:GLY:N	2.41	0.54
1:A:847:ASN:ND2	1:A:853:MET:HB3	2.23	0.54
2:D:861:THR:O	2:D:863:GLY:N	2.41	0.54
3:X:139:ASN:HD22	3:X:148:ALA:HB1	1.72	0.54
1:C:512:PHE:C	1:C:512:PHE:CD2	2.75	0.54
1:C:656:ASN:CG	1:C:658:ASN:HB3	2.26	0.54
2:D:1562:GLN:HE22	2:D:1596:LYS:HZ2	1.53	0.54
2:B:1611:PRO:HD3	2:B:1624:LEU:HD23	1.90	0.54
1:C:1094:GLU:CD	1:C:1094:GLU:H	2.11	0.54
2:B:28:ILE:HD13	2:B:621:PHE:HE1	1.72	0.54
1:A:641:ASN:OD1	1:A:644:ASN:HB2	2.08	0.54
2:D:168:PRO:HG3	2:D:197:TRP:N	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:ILE:HD12	1:C:219:VAL:HG21	1.90	0.54
1:A:1108:VAL:CG2	1:A:1167:ALA:HB2	2.38	0.54
2:D:595:GLN:OE1	2:D:595:GLN:HA	2.07	0.54
2:D:1509:PRO:O	2:D:1512:ILE:HG13	2.08	0.54
3:Y:163:LYS:HG3	3:Y:212:MET:SD	2.48	0.54
2:B:941:GLN:HE21	2:B:943:GLU:HG2	1.71	0.54
1:A:771:GLU:HG3	1:A:772:SER:O	2.08	0.54
1:A:74:SER:HA	1:A:79:PHE:HE1	1.73	0.54
1:C:497:THR:OG1	1:C:498:HIS:N	2.38	0.54
1:C:1133:LEU:HB2	1:C:1134:PRO:HD3	1.90	0.54
2:B:175:SER:N	2:B:1300:ALA:HB2	2.20	0.54
1:C:753:HIS:O	1:C:754:MET:CB	2.52	0.54
3:Y:125:LYS:HA	3:Y:127:ASN:H	1.72	0.54
1:C:1286:SER:OG	1:C:1287:THR:N	2.40	0.54
1:C:950:TYR:C	1:C:952:THR:H	2.11	0.54
2:B:595:GLN:OE1	2:B:595:GLN:HA	2.06	0.54
1:C:907:LEU:HG	1:C:908:HIS:N	2.23	0.54
2:D:57:PHE:HD1	2:D:59:HIS:NE2	2.05	0.54
1:C:1548:ARG:C	1:C:1550:GLN:H	2.11	0.54
1:A:484:ILE:HG23	1:A:526:ILE:HG13	1.88	0.54
1:C:490:SER:N	1:C:491:PRO:CD	2.71	0.54
1:C:44:TYR:CB	1:C:545:ILE:HD12	2.36	0.54
2:D:528:ASN:OD1	2:D:528:ASN:N	2.41	0.54
1:A:134:VAL:C	1:A:135:TYR:CD2	2.81	0.54
1:C:430:VAL:HG11	1:C:453:ARG:NH2	2.17	0.54
1:C:87:ILE:N	1:C:87:ILE:CD1	2.66	0.54
2:D:820:MET:HG3	2:D:821:PRO:HD2	1.90	0.54
1:C:773:TRP:HZ3	1:C:788:PHE:CE1	2.25	0.54
2:B:736:GLU:CD	2:B:737:ASP:H	2.11	0.54
2:D:1415:ASN:O	2:D:1417:MET:HG3	2.08	0.54
2:D:952:ASP:O	2:D:1331:ALA:HA	2.08	0.54
1:C:796:THR:HA	1:C:818:LYS:HA	1.89	0.54
2:B:826:LYS:HG3	2:B:887:LEU:O	2.08	0.54
1:A:1629:TYR:CE1	1:A:1634:ARG:NH2	2.76	0.54
2:D:585:TYR:CD2	2:D:788:VAL:HG11	2.42	0.54
1:C:24:VAL:HG11	1:C:543:TYR:CZ	2.43	0.53
2:D:1593:THR:CG2	2:D:1594:LYS:H	2.21	0.53
1:C:625:GLN:O	1:C:628:GLU:HB3	2.08	0.53
1:A:1150:ILE:CD1	1:A:1193:TYR:CD2	2.91	0.53
1:A:1623:GLU:HB2	1:A:1638:PRO:CD	2.38	0.53
2:D:476:ILE:HD11	2:D:524:TYR:CD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:ILE:H	2:B:87:ILE:HD12	1.73	0.53
1:A:287:MET:HG2	1:A:299:VAL:HG21	1.89	0.53
1:C:1199:ASP:C	1:C:1201:THR:H	2.10	0.53
1:C:1268:ASN:N	1:C:1269:PRO:CD	2.71	0.53
2:D:130:ILE:HG12	2:D:147:VAL:HG23	1.89	0.53
1:C:1190:ILE:HG22	1:C:1191:SER:N	2.22	0.53
2:D:1344:HIS:ND1	5:D:2003:NAG:H82	2.23	0.53
2:B:243:PHE:CD1	2:B:314:LEU:HD23	2.41	0.53
5:B:2001:NAG:H3	5:B:2002:NAG:O5	2.07	0.53
1:C:1421:HIS:CE1	1:C:1498:TYR:CD1	2.95	0.53
1:C:25:ILE:HD13	1:C:41:ILE:CB	2.36	0.53
1:C:40:VAL:HG23	1:C:41:ILE:H	1.73	0.53
1:C:980:LYS:HD3	1:C:986:GLU:CA	2.37	0.53
1:C:33:VAL:CG2	1:C:121:TYR:HD1	2.20	0.53
2:D:437:THR:HG23	2:D:444:TYR:CD1	2.43	0.53
2:B:384:PHE:HD1	2:B:400:LEU:HG	1.67	0.53
1:C:263:ALA:HB3	1:C:292:LEU:HB3	1.90	0.53
2:B:606:ASP:OD1	2:B:606:ASP:O	2.26	0.53
1:C:222:TYR:HE2	1:C:224:LEU:CA	2.21	0.53
1:A:250:ILE:HD11	1:A:265:VAL:CG1	2.37	0.53
2:B:1345:LEU:HD21	2:B:1456:VAL:HG12	1.90	0.53
1:C:1304:VAL:CG1	1:C:1305:LYS:H	2.21	0.53
3:X:107:GLN:HB3	3:X:116:LEU:HD22	1.90	0.53
1:A:149:ASN:O	1:A:151:ASP:N	2.40	0.53
1:C:1548:ARG:HE	1:C:1550:GLN:NE2	2.07	0.53
1:C:982:LEU:C	1:C:984:VAL:N	2.61	0.53
2:D:963:ILE:HG13	2:D:1325:ILE:HG12	1.90	0.53
2:B:546:GLY:HA3	2:B:570:ASP:OD1	2.08	0.53
1:A:1631:PHE:CD2	1:A:1631:PHE:N	2.74	0.53
2:D:365:TYR:HA	2:D:394:GLY:O	2.08	0.53
1:A:24:VAL:O	1:A:24:VAL:HG12	2.08	0.53
1:C:1213:LYS:HE2	1:C:1266:TYR:CE2	2.43	0.53
2:B:218:LYS:HD3	2:B:822:TYR:CE2	2.43	0.53
2:D:1548:ILE:HG23	2:D:1635:LEU:CB	2.39	0.53
1:A:77:ASN:ND2	1:A:81:ASN:HB2	2.23	0.53
1:A:81:ASN:CG	1:A:82:SER:H	2.12	0.53
2:B:1522:TYR:N	2:B:1522:TYR:HD2	2.07	0.53
2:B:1384:ILE:HB	2:B:1423:VAL:HG12	1.90	0.53
2:D:1386:MET:CE	2:D:1386:MET:HA	2.38	0.53
1:C:1370:THR:O	1:C:1371:SER:C	2.47	0.53
1:C:1581:LEU:HD12	1:C:1592:ALA:HB1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1218:VAL:CG1	1:A:1219:LYS:H	2.20	0.53
2:B:952:ASP:N	2:B:952:ASP:OD1	2.33	0.53
2:B:885:VAL:HG23	2:B:885:VAL:O	2.08	0.53
1:C:600:VAL:HA	1:C:802:VAL:O	2.08	0.53
1:C:953:ILE:HD11	1:C:955:ARG:HH21	1.73	0.53
2:B:563:MET:HE3	2:B:563:MET:HA	1.89	0.53
1:C:884:VAL:HG12	1:C:885:ARG:N	2.23	0.53
2:B:481:TYR:C	2:B:481:TYR:CD2	2.82	0.53
1:C:149:ASN:O	1:C:150:ASP:C	2.46	0.53
3:Y:43:ILE:O	3:Y:44:ARG:C	2.45	0.53
1:C:382:LEU:HD13	1:C:415:ASP:O	2.09	0.53
3:X:134:THR:CG2	3:X:153:PHE:HB3	2.38	0.53
2:B:236:TYR:CE1	2:B:424:ARG:HD2	2.43	0.53
1:A:1320:LYS:CE	1:A:1321:GLY:H	2.21	0.53
1:C:917:TRP:CE3	1:C:917:TRP:HA	2.43	0.53
1:A:24:VAL:N	1:A:655:THR:HG21	2.23	0.53
1:C:493:ILE:HG22	1:C:493:ILE:O	2.08	0.53
1:C:554:LEU:H	1:C:658:ASN:ND2	2.06	0.53
1:C:1620:MET:CB	1:C:1644:TRP:CB	2.85	0.53
1:A:804:ILE:CG2	1:A:809:ILE:HG13	2.36	0.53
2:D:1561:HIS:CD2	2:D:1597:ILE:HD13	2.43	0.53
2:D:851:LEU:HD23	2:D:852:TYR:N	2.13	0.53
1:C:523:TYR:CD1	2:D:359:PRO:HG2	2.43	0.53
1:A:1180:LEU:CD2	1:A:1208:ILE:HG12	2.38	0.53
2:D:1615:GLU:HB3	2:D:1621:PHE:CD1	2.43	0.53
1:C:1204:GLN:HA	1:C:1204:GLN:OE1	2.09	0.53
1:C:790:LEU:HB3	1:C:791:PRO:CD	2.38	0.53
1:C:363:LEU:HD12	1:C:456:ALA:HA	1.90	0.53
1:C:916:THR:C	1:C:918:PHE:H	2.11	0.53
2:B:585:TYR:CD2	2:B:788:VAL:HG11	2.44	0.53
2:D:1400:LEU:HD22	2:D:1406:ARG:HH12	1.73	0.53
3:X:217:ASN:HB2	3:X:220:ASP:OD2	2.08	0.53
1:C:655:THR:OG1	1:C:656:ASN:N	2.41	0.53
1:C:1619:ILE:HG12	1:C:1645:ILE:CD1	2.38	0.53
2:B:1504:GLU:CD	2:B:1504:GLU:H	2.11	0.53
1:A:1569:THR:O	1:A:1570:VAL:CG2	2.57	0.53
1:A:128:ILE:CG2	1:A:145:VAL:HG22	2.28	0.53
2:D:175:SER:N	2:D:1300:ALA:HB2	2.19	0.53
2:B:24:LEU:HB3	2:B:46:HIS:HB2	1.91	0.53
1:C:250:ILE:HD11	1:C:265:VAL:CG1	2.37	0.53
1:A:1572:ASN:C	1:A:1573:VAL:HG23	2.28	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:VAL:HA	1:A:802:VAL:O	2.07	0.53
1:C:1320:LYS:HD2	1:C:1321:GLY:N	2.21	0.53
1:C:123:ASN:O	1:C:211:THR:HG21	2.07	0.53
1:C:720:LEU:HD11	1:C:724:CYS:SG	2.48	0.53
3:Y:107:GLN:HB3	3:Y:116:LEU:HD22	1.90	0.53
2:D:345:ILE:HD11	2:D:427:THR:N	2.23	0.53
1:A:1274:LEU:O	1:A:1277:GLU:N	2.42	0.53
3:Y:170:ARG:HD3	3:Y:203:LEU:CD2	2.38	0.53
1:A:115:LYS:HB3	1:A:654:LEU:HD21	1.91	0.53
1:C:1598:ILE:HG22	1:C:1599:THR:H	1.73	0.53
1:C:532:GLN:HE21	1:C:568:GLY:CA	2.14	0.53
2:D:1593:THR:HB	2:D:1596:LYS:O	2.09	0.53
2:D:954:VAL:HG23	2:D:1330:ASN:O	2.08	0.53
1:C:1056:ILE:CD1	1:C:1066:TYR:HE2	2.22	0.53
1:C:955:ARG:HH12	1:C:1352:PHE:HA	1.74	0.53
1:C:1159:CYS:C	1:C:1161:LEU:H	2.11	0.53
2:D:129:PHE:CE2	2:D:598:ILE:HG23	2.44	0.53
1:C:1142:LEU:HD13	1:C:1187:THR:CG2	2.38	0.53
2:D:266:GLY:HA2	2:D:276:ILE:HG13	1.90	0.53
1:C:1496:TYR:N	1:C:1496:TYR:HD2	2.06	0.53
1:C:1381:ILE:O	1:C:1382:ASP:CB	2.55	0.53
2:D:745:ILE:CG2	2:D:897:LYS:HD3	2.39	0.53
2:D:204:GLU:O	2:D:205:HIS:HB2	2.08	0.53
1:C:461:SER:C	1:C:463:SER:H	2.12	0.53
1:C:23:TYR:O	1:C:655:THR:CB	2.56	0.53
1:C:1228:TRP:N	1:C:1228:TRP:CE3	2.77	0.53
1:A:1451:THR:O	1:A:1452:ASP:HB3	2.07	0.53
2:B:469:ASN:ND2	2:B:472:SER:H	2.06	0.53
2:D:523:TYR:HD2	2:D:621:PHE:HZ	1.54	0.53
2:B:46:HIS:ND1	2:B:525:GLN:HG2	2.24	0.53
1:A:1615:ARG:NH1	1:A:1647:TYR:CE1	2.77	0.53
3:Y:194:LYS:NZ	3:Y:197:ASN:HD22	2.06	0.53
1:A:702:GLY:HA3	1:A:728:PHE:CD1	2.44	0.53
1:A:758:LEU:HB3	1:A:759:PRO:HD2	1.91	0.53
2:B:824:VAL:HG22	2:B:825:VAL:N	2.24	0.53
1:C:949:ILE:HG22	1:C:950:TYR:CZ	2.44	0.53
1:C:1159:CYS:N	1:C:1160:PRO:CD	2.72	0.53
1:A:906:GLY:N	1:A:929:VAL:HB	2.21	0.53
2:B:1466:GLU:HA	2:B:1466:GLU:OE1	2.08	0.53
2:D:353:TYR:HA	2:D:433:ILE:O	2.09	0.53
2:D:745:ILE:HG13	2:D:906:SER:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:573:VAL:O	1:C:574:HIS:ND1	2.42	0.53
2:D:622:GLU:OE2	2:D:637:LYS:HD3	2.09	0.53
2:D:285:ILE:CD1	2:D:285:ILE:N	2.67	0.53
2:D:1480:LEU:HD12	2:D:1480:LEU:C	2.28	0.53
1:A:979:VAL:HG11	1:A:1326:TYR:HE1	1.73	0.53
1:A:968:VAL:HG22	1:A:1366:HIS:O	2.08	0.53
1:C:694:VAL:O	1:C:697:LYS:HE2	2.09	0.53
1:C:569:ASN:CG	1:C:570:GLN:N	2.62	0.53
1:A:702:GLY:HA2	1:A:728:PHE:HE1	1.70	0.53
2:B:618:LEU:HD22	2:B:636:THR:HA	1.89	0.53
3:X:127:ASN:OD1	3:X:158:GLU:HB3	2.07	0.53
3:Y:88:GLY:HA2	3:Y:210:GLU:O	2.08	0.53
1:C:824:PHE:CZ	1:C:846:TYR:HD1	2.27	0.53
1:C:771:GLU:HG3	1:C:772:SER:O	2.09	0.53
1:A:1204:GLN:OE1	1:A:1204:GLN:HA	2.09	0.53
1:C:1626:GLN:HB2	1:C:1635:TYR:CD1	2.40	0.53
1:A:149:ASN:O	1:A:150:ASP:C	2.47	0.53
2:B:1313:VAL:HG21	2:B:1323:MET:HE2	1.90	0.53
1:A:425:PRO:HG3	2:B:498:ARG:NH1	2.24	0.53
1:A:1454:GLN:HG3	1:A:1461:ILE:HB	1.90	0.53
2:B:622:GLU:OE2	2:B:637:LYS:HD3	2.09	0.53
3:X:166:ASP:HB2	3:X:207:LEU:HD21	1.90	0.53
1:A:655:THR:OG1	1:A:656:ASN:N	2.41	0.53
1:C:111:PHE:HE2	1:C:113:LYS:CB	2.20	0.53
1:C:1549:LYS:HD3	1:C:1667:PHE:CD2	2.44	0.53
1:C:1627:ILE:O	1:C:1629:TYR:N	2.42	0.53
1:A:1242:THR:OG1	1:A:1243:GLY:N	2.42	0.53
2:B:175:SER:O	2:B:1299:LEU:HD12	2.09	0.53
1:A:1559:TYR:CD1	1:A:1561:TYR:HE2	2.27	0.53
2:B:231:SER:HB3	2:B:244:HIS:HB2	1.90	0.53
2:B:481:TYR:C	2:B:481:TYR:HD2	2.10	0.53
2:B:482:LEU:CD1	2:B:521:VAL:HB	2.39	0.53
1:A:1066:TYR:H	1:A:1079:THR:CG2	2.19	0.53
1:A:599:TRP:NE1	1:A:779:LEU:HA	2.24	0.53
2:B:512:PRO:HA	2:B:515:ILE:HD12	1.90	0.53
1:C:691:LYS:C	1:C:693:SER:H	2.11	0.53
1:C:689:LYS:O	1:C:691:LYS:N	2.42	0.53
2:D:456:PRO:HG3	2:D:515:ILE:HD11	1.91	0.53
1:A:612:VAL:HG21	1:A:769:PHE:HZ	1.71	0.53
1:A:363:LEU:HD12	1:A:456:ALA:HA	1.90	0.53
2:B:1281:LEU:HB2	2:B:1283:ASP:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1534:GLN:HG3	2:D:1535:ASP:OD2	2.09	0.53
1:C:1035:HIS:N	1:C:1035:HIS:ND1	2.56	0.53
1:C:24:VAL:HA	1:C:655:THR:CG2	2.39	0.52
1:C:658:ASN:OD1	1:C:658:ASN:C	2.47	0.52
1:C:1552:ALA:HB1	1:C:1585:TYR:OH	2.09	0.52
1:C:1644:TRP:O	1:C:1645:ILE:HD13	2.08	0.52
1:C:530:VAL:HG23	1:C:534:MET:CE	2.40	0.52
1:A:1097:GLN:HG3	1:A:1158:ILE:HG22	1.90	0.52
1:A:804:ILE:HG22	1:A:809:ILE:CG1	2.37	0.52
2:B:1593:THR:HB	2:B:1596:LYS:O	2.09	0.52
2:D:736:GLU:CD	2:D:737:ASP:H	2.13	0.52
1:C:1097:GLN:HG3	1:C:1158:ILE:HG22	1.90	0.52
1:A:967:LEU:HD13	1:A:1365:VAL:CG2	2.39	0.52
1:C:576:SER:CB	1:C:589:SER:H	2.22	0.52
2:B:780:LEU:HD11	2:B:787:TRP:CD1	2.43	0.52
2:B:39:GLU:O	2:B:87:ILE:HD12	2.08	0.52
1:A:1226:ARG:CZ	1:A:1266:TYR:CE1	2.92	0.52
1:A:687:ALA:O	1:A:690:TYR:HB3	2.08	0.52
1:C:906:GLY:O	1:C:908:HIS:NE2	2.42	0.52
1:A:689:LYS:HG2	1:A:699:CYS:SG	2.48	0.52
1:A:720:LEU:HD11	1:A:724:CYS:SG	2.49	0.52
2:D:941:GLN:HE21	2:D:943:GLU:HG2	1.74	0.52
1:A:1112:GLN:NE2	1:A:1171:ALA:HB2	2.24	0.52
2:B:1602:THR:C	2:B:1604:ASN:N	2.63	0.52
3:Y:129:THR:HG22	3:Y:129:THR:O	2.09	0.52
2:B:357:GLY:HA3	2:B:404:LEU:HD12	1.91	0.52
2:B:229:GLN:OE1	2:B:229:GLN:HA	2.09	0.52
2:B:1530:ARG:HH11	2:B:1530:ARG:HG3	1.74	0.52
1:A:938:SER:C	1:A:940:SER:N	2.62	0.52
1:C:1066:TYR:CD1	1:C:1066:TYR:N	2.77	0.52
2:D:481:TYR:CD2	2:D:481:TYR:O	2.52	0.52
2:D:469:ASN:ND2	2:D:472:SER:H	2.07	0.52
1:C:702:GLY:HA2	1:C:728:PHE:HE1	1.67	0.52
1:A:920:LYS:NZ	2:B:842:GLU:CD	2.63	0.52
1:C:1232:LEU:HG	1:C:1233:GLN:N	2.24	0.52
3:Y:61:SER:O	3:Y:75:PHE:CZ	2.61	0.52
1:C:541:LEU:HD23	1:C:541:LEU:O	2.09	0.52
1:A:1152:ILE:HG21	1:A:1168:LEU:CD2	2.39	0.52
2:D:139:PRO:HG2	2:D:218:LYS:HE2	1.91	0.52
2:D:1548:ILE:HG23	2:D:1635:LEU:HB2	1.92	0.52
2:D:234:PHE:CE1	2:D:236:TYR:CE1	2.98	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:GLU:HB2	1:C:185:PHE:CE1	2.43	0.52
1:A:680:GLN:HG3	1:A:681:LYS:H	1.75	0.52
1:C:610:TYR:N	1:C:610:TYR:HD1	2.06	0.52
3:Y:217:ASN:HB2	3:Y:220:ASP:OD2	2.10	0.52
1:C:24:VAL:HG12	1:C:24:VAL:O	2.09	0.52
1:C:44:TYR:CZ	1:C:497:THR:HG21	2.45	0.52
1:A:1082:ALA:O	1:A:1086:LEU:HD23	2.09	0.52
1:C:979:VAL:C	1:C:980:LYS:HG2	2.28	0.52
1:C:986:GLU:HG2	1:C:987:ILE:N	2.25	0.52
1:A:1076:THR:HG22	1:A:1120:GLU:HA	1.90	0.52
1:C:59:TYR:CE2	1:C:99:VAL:HG21	2.44	0.52
1:C:779:LEU:C	1:C:779:LEU:HD12	2.30	0.52
1:C:1093:VAL:O	1:C:1093:VAL:HG12	2.08	0.52
1:A:461:SER:C	1:A:463:SER:H	2.13	0.52
1:A:742:ILE:CG2	1:A:753:HIS:HA	2.38	0.52
1:A:696:LYS:NZ	1:A:759:PRO:CD	2.65	0.52
1:C:989:SER:O	1:C:993:SER:CB	2.57	0.52
2:B:476:ILE:O	2:B:476:ILE:HG23	2.08	0.52
1:A:1381:ILE:O	1:A:1382:ASP:CB	2.57	0.52
2:D:1522:TYR:CD2	2:D:1522:TYR:N	2.76	0.52
3:X:43:ILE:HG23	3:X:44:ARG:N	2.25	0.52
2:D:1529:LEU:O	2:D:1577:VAL:HG13	2.10	0.52
2:B:929:LYS:NZ	2:B:1322:THR:OG1	2.43	0.52
1:C:645:VAL:HG12	1:C:646:PHE:N	2.22	0.52
1:C:1641:SER:O	1:C:1642:LEU:HB2	2.10	0.52
1:A:1559:TYR:CD1	1:A:1561:TYR:CE2	2.97	0.52
1:C:59:TYR:CE1	1:C:60:PRO:HG3	2.44	0.52
1:A:577:PRO:CD	1:A:588:VAL:HG23	2.39	0.52
1:C:577:PRO:HD2	1:C:588:VAL:HG23	1.92	0.52
1:A:753:HIS:O	1:A:754:MET:CB	2.49	0.52
1:C:1130:GLN:NE2	1:C:1230:ASP:HB3	2.25	0.52
1:A:641:ASN:O	1:A:642:ASN:C	2.47	0.52
3:X:87:LEU:HD12	3:X:210:GLU:HA	1.91	0.52
1:C:1013:MET:HE3	1:C:1287:THR:HB	1.89	0.52
1:C:190:ILE:HG22	1:C:191:PRO:CD	2.39	0.52
2:D:1284:ARG:CG	2:D:1285:GLU:N	2.72	0.52
2:D:598:ILE:HD12	2:D:800:ILE:HG21	1.92	0.52
1:C:238:ILE:HG23	1:C:242:ASN:HD22	1.75	0.52
2:D:316:ALA:HB3	2:D:333:GLN:HB3	1.90	0.52
2:D:963:ILE:CG1	2:D:1325:ILE:HG12	2.40	0.52
2:B:1595:ASP:OD1	2:B:1595:ASP:N	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:PHE:HD2	1:A:512:PHE:O	1.93	0.52
3:X:139:ASN:HD22	3:X:148:ALA:CB	2.22	0.52
1:C:25:ILE:HB	1:C:654:LEU:HB2	1.90	0.52
1:C:979:VAL:HG11	1:C:1326:TYR:HE1	1.74	0.52
1:C:421:VAL:HG23	2:D:507:ASN:ND2	2.24	0.52
1:A:222:TYR:HE2	1:A:224:LEU:CA	2.22	0.52
1:C:599:TRP:NE1	1:C:779:LEU:HA	2.25	0.52
1:A:837:GLU:O	1:A:901:LEU:HB2	2.10	0.52
2:D:1292:ILE:HD12	2:D:1296:ASN:OD1	2.10	0.52
2:B:528:ASN:N	2:B:528:ASN:OD1	2.41	0.52
1:C:702:GLY:HA3	1:C:728:PHE:CD1	2.45	0.52
2:B:870:PHE:CD1	2:B:878:ARG:NH2	2.78	0.52
1:A:1287:THR:OG1	1:A:1288:GLN:N	2.40	0.52
1:A:239:GLY:O	1:A:241:LYS:N	2.43	0.52
1:C:993:SER:C	1:C:995:GLU:N	2.59	0.52
2:D:144:LEU:HD23	2:D:144:LEU:N	2.25	0.52
2:B:57:PHE:HD1	2:B:59:HIS:NE2	2.07	0.52
2:D:343:TYR:CE1	2:D:420:LEU:HD11	2.45	0.52
1:C:396:ASP:HB3	1:C:398:ASN:H	1.74	0.52
2:D:966:GLN:HG3	2:D:966:GLN:O	2.09	0.52
1:C:1279:ARG:HD3	1:C:1280:TYR:N	2.25	0.52
1:C:500:ASN:O	1:C:542:VAL:HG13	2.09	0.52
1:C:934:VAL:CG1	1:C:935:LYS:N	2.73	0.52
2:B:1622:GLN:O	2:B:1625:CYS:HB2	2.10	0.52
1:A:1532:CYS:O	1:A:1641:SER:N	2.43	0.52
2:B:437:THR:HG23	2:B:444:TYR:CD1	2.45	0.52
2:D:481:TYR:C	2:D:481:TYR:HD2	2.12	0.52
2:D:175:SER:O	2:D:1299:LEU:HD12	2.09	0.52
1:A:610:TYR:HD1	1:A:610:TYR:N	2.08	0.52
2:D:484:LEU:HD11	2:D:626:LEU:HG	1.92	0.52
1:C:125:PHE:CD1	1:C:627:LEU:HD21	2.45	0.52
1:C:1226:ARG:O	1:C:1270:VAL:HG22	2.09	0.52
2:B:1280:GLU:HB2	2:B:1312:THR:HB	1.91	0.52
1:A:161:LEU:HD11	1:A:185:PHE:CZ	2.45	0.52
1:C:544:TYR:C	1:C:544:TYR:CD2	2.83	0.52
2:D:351:PRO:N	2:D:611:ALA:HB3	2.24	0.52
1:A:1527:CYS:O	1:A:1528:VAL:C	2.48	0.52
1:A:111:PHE:HE2	1:A:113:LYS:CB	2.23	0.52
1:A:543:TYR:CD1	1:A:543:TYR:C	2.81	0.52
1:A:24:VAL:CA	1:A:655:THR:HG21	2.40	0.52
3:X:150:ILE:C	3:X:150:ILE:HD12	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1247:MET:O	1:A:1251:THR:HG23	2.10	0.52
2:D:520:PHE:O	2:D:535:SER:HA	2.10	0.52
2:D:531:ILE:HD11	2:D:634:LEU:CD2	2.38	0.52
2:D:929:LYS:NZ	2:D:1322:THR:OG1	2.42	0.52
1:A:934:VAL:CG1	1:A:935:LYS:N	2.73	0.52
1:A:1019:PHE:HD2	1:A:1020:TYR:N	2.07	0.52
2:B:1280:GLU:HG2	2:B:1287:PRO:CB	2.38	0.52
1:C:165:ASP:C	1:C:167:GLU:H	2.12	0.52
1:C:1496:TYR:N	1:C:1496:TYR:CD2	2.75	0.52
1:A:396:ASP:HB3	1:A:398:ASN:HB2	1.92	0.52
1:A:161:LEU:HD11	1:A:185:PHE:CD2	2.44	0.52
3:X:119:VAL:O	3:X:163:LYS:HD2	2.10	0.52
2:D:965:ILE:HG13	2:D:1301:ARG:CB	2.31	0.52
1:C:135:TYR:CE1	1:C:141:VAL:HG22	2.45	0.52
2:B:523:TYR:HD1	2:B:523:TYR:C	2.12	0.52
1:A:135:TYR:CE1	1:A:141:VAL:HG22	2.44	0.52
1:A:1265:ASN:C	1:A:1267:VAL:H	2.12	0.52
1:A:190:ILE:HD12	1:A:219:VAL:HG21	1.92	0.52
2:B:216:VAL:O	2:B:216:VAL:CG1	2.57	0.52
1:A:1161:LEU:HA	1:C:1102:ASN:ND2	2.21	0.52
1:A:1163:LYS:HE3	1:C:1109:GLU:HG2	1.92	0.52
1:C:171:VAL:CG1	1:C:1054:LEU:HD11	2.40	0.52
1:C:1033:ILE:HG23	1:C:1034:PHE:N	2.24	0.52
2:D:1602:THR:C	2:D:1604:ASN:N	2.63	0.52
1:C:274:ASP:HA	1:C:322:TYR:CD2	2.45	0.52
2:B:941:GLN:HE21	2:B:943:GLU:CG	2.22	0.52
1:A:377:ASP:OD2	1:A:379:LEU:HB2	2.10	0.52
1:A:32:ARG:O	1:A:35:ALA:HB3	2.09	0.52
3:Y:103:VAL:HG22	3:Y:122:VAL:HG22	1.91	0.52
2:B:452:THR:O	2:B:453:GLU:O	2.28	0.52
1:C:968:VAL:HG22	1:C:1366:HIS:O	2.10	0.52
3:Y:61:SER:O	3:Y:75:PHE:HZ	1.92	0.52
2:D:1500:LEU:HD12	2:D:1501:ASN:N	2.20	0.52
2:D:800:ILE:HG23	2:D:801:CYS:N	2.24	0.52
2:D:1539:ILE:HG23	2:D:1564:ILE:HG12	1.91	0.52
2:B:1450:PHE:HD1	2:B:1451:ILE:N	2.08	0.52
2:B:476:ILE:CG2	2:B:497:ARG:HD3	2.39	0.52
2:D:433:ILE:CG2	2:D:434:ALA:N	2.72	0.52
2:D:887:LEU:HD23	2:D:1490:CYS:HB3	1.91	0.52
3:Y:119:VAL:O	3:Y:163:LYS:HD2	2.10	0.52
1:C:825:LEU:HG	1:C:826:GLU:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:103:VAL:HG22	3:X:122:VAL:HG22	1.91	0.52
1:A:113:LYS:HE2	1:A:654:LEU:O	2.10	0.52
1:C:120:THR:HG22	1:C:121:TYR:N	2.24	0.52
2:B:1593:THR:HG22	2:B:1594:LYS:H	1.73	0.52
1:A:222:TYR:CD1	1:A:768:TYR:HB2	2.42	0.52
1:C:1431:GLY:HA2	1:C:1483:PHE:CE1	2.45	0.52
2:B:1503:GLN:NE2	2:B:1506:ILE:HG12	2.25	0.52
2:B:437:THR:HG21	2:B:443:ASN:N	2.25	0.52
1:C:180:ILE:CB	1:C:599:TRP:CE3	2.93	0.52
1:A:645:VAL:HG12	1:A:646:PHE:N	2.24	0.52
3:X:86:LEU:HG	3:X:91:LYS:HG3	1.92	0.52
1:C:1098:ASN:O	1:C:1101:CYS:HB2	2.10	0.52
2:B:283:ILE:N	2:B:283:ILE:HD12	2.25	0.52
2:D:558:MET:O	2:D:561:ALA:HB3	2.10	0.52
2:D:1530:ARG:NH1	2:D:1530:ARG:HG3	2.25	0.52
1:C:1408:TYR:CE2	1:C:1410:PRO:HA	2.44	0.52
1:C:40:VAL:CG2	1:C:41:ILE:N	2.73	0.51
1:C:78:LYS:HZ1	3:Y:144:GLU:HA	1.70	0.51
1:C:1559:TYR:HH	1:C:1591:VAL:HA	1.74	0.51
1:A:1021:VAL:HG12	1:A:1022:PHE:N	2.26	0.51
1:A:1298:THR:O	1:A:1299:GLU:C	2.49	0.51
2:D:756:LEU:HD12	2:D:758:LEU:HG	1.92	0.51
1:A:1581:LEU:HD12	1:A:1592:ALA:HB1	1.90	0.51
1:A:1640:ASP:O	1:A:1643:THR:HB	2.11	0.51
2:D:437:THR:HG21	2:D:443:ASN:N	2.25	0.51
2:D:469:ASN:CB	2:D:472:SER:HB2	2.40	0.51
1:A:234:GLU:HB3	1:A:246:PHE:HE1	1.74	0.51
1:A:1612:VAL:HG23	1:A:1617:TYR:OH	2.10	0.51
2:D:519:ARG:NH1	2:D:606:ASP:OD2	2.44	0.51
1:A:1013:MET:HE3	1:A:1287:THR:HB	1.91	0.51
1:C:1226:ARG:NE	1:C:1266:TYR:HE1	2.08	0.51
1:C:950:TYR:CE2	1:C:1356:LEU:HD11	2.46	0.51
1:C:219:VAL:O	1:C:219:VAL:HG12	2.10	0.51
1:A:1199:ASP:C	1:A:1201:THR:H	2.13	0.51
2:D:216:VAL:CG1	2:D:216:VAL:O	2.58	0.51
3:Y:43:ILE:HG23	3:Y:44:ARG:N	2.23	0.51
1:C:436:LYS:HB2	1:C:449:ARG:CG	2.41	0.51
2:B:1381:ILE:HB	2:B:1459:TYR:CD1	2.44	0.51
1:A:1385:ASP:O	1:A:1386:ILE:HB	2.09	0.51
1:C:1385:ASP:O	1:C:1386:ILE:HB	2.09	0.51
1:C:914:LEU:HD11	1:C:916:THR:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1351:ASN:O	2:B:1352:ILE:HG12	2.09	0.51
2:D:1595:ASP:OD1	2:D:1595:ASP:N	2.40	0.51
3:Y:187:GLY:C	3:Y:203:LEU:HD12	2.31	0.51
1:C:1227:PHE:CD1	1:C:1227:PHE:C	2.84	0.51
1:A:1093:VAL:HG12	1:A:1095:GLN:HE21	1.74	0.51
1:A:120:THR:HG22	1:A:121:TYR:N	2.24	0.51
1:A:1534:GLN:HA	1:A:1608:ASN:HD22	1.75	0.51
1:A:1540:ASP:N	1:A:1660:PHE:CD1	2.78	0.51
2:D:481:TYR:C	2:D:481:TYR:CD2	2.84	0.51
2:D:523:TYR:C	2:D:523:TYR:HD1	2.14	0.51
2:B:1275:LEU:HD21	2:B:1319:GLY:O	2.10	0.51
3:Y:77:PRO:O	3:Y:78:LYS:HB3	2.10	0.51
1:C:472:ASN:O	1:C:473:HIS:CB	2.57	0.51
1:A:949:ILE:HG22	1:A:949:ILE:O	2.09	0.51
2:D:87:ILE:HD12	2:D:87:ILE:H	1.75	0.51
1:C:287:MET:HG2	1:C:299:VAL:HG21	1.92	0.51
2:B:948:ARG:NH2	2:B:948:ARG:HB2	2.23	0.51
2:D:1466:GLU:HA	2:D:1466:GLU:OE1	2.10	0.51
1:C:525:SER:H	2:D:401:ASN:ND2	2.06	0.51
1:A:976:ILE:HB	1:A:1362:THR:HG22	1.92	0.51
3:X:146:LEU:C	3:X:146:LEU:HD22	2.31	0.51
1:C:465:LEU:HD11	1:C:486:VAL:HG13	1.93	0.51
1:A:985:GLY:O	1:A:986:GLU:C	2.49	0.51
1:A:1560:ALA:O	1:A:1561:TYR:HD2	1.92	0.51
1:A:698:CYS:HB3	1:A:728:PHE:HB2	1.92	0.51
2:D:239:GLY:N	2:D:296:ARG:NH2	2.59	0.51
2:D:1581:TYR:HD1	2:D:1608:GLU:O	1.93	0.51
1:C:1017:PRO:O	1:C:1018:VAL:C	2.48	0.51
1:A:351:PRO:HG3	1:A:442:LEU:HD11	1.92	0.51
2:B:188:LEU:HD13	2:B:216:VAL:HG21	1.93	0.51
2:D:276:ILE:O	2:D:277:PRO:C	2.47	0.51
1:C:689:LYS:HG2	1:C:699:CYS:SG	2.51	0.51
2:B:1390:PHE:CD1	2:B:1442:ILE:HG13	2.44	0.51
1:A:693:SER:C	1:A:695:VAL:N	2.63	0.51
1:A:148:LEU:HG	1:A:153:LYS:O	2.10	0.51
1:A:365:PRO:HG2	1:A:464:TYR:CE2	2.46	0.51
1:C:161:LEU:HD11	1:C:185:PHE:CD2	2.45	0.51
3:Y:119:VAL:HG21	3:Y:209:PHE:HB3	1.92	0.51
1:C:1279:ARG:NH1	1:C:1280:TYR:CD2	2.78	0.51
2:D:946:LYS:HA	2:D:1310:ASP:OD1	2.10	0.51
2:B:745:ILE:CG2	2:B:897:LYS:HD3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:745:ILE:HG13	2:B:906:SER:HB2	1.91	0.51
1:C:72:HIS:C	1:C:72:HIS:CD2	2.83	0.51
1:C:1229:LYS:HZ3	1:C:1240:PRO:HD2	1.74	0.51
1:A:936:ARG:NH2	1:A:1284:PHE:HE1	2.08	0.51
2:B:952:ASP:O	2:B:1331:ALA:HA	2.10	0.51
1:C:698:CYS:C	1:C:700:TYR:N	2.62	0.51
2:B:565:ILE:O	2:B:776:MET:HB3	2.11	0.51
2:B:563:MET:CG	2:B:780:LEU:HD23	2.30	0.51
3:X:113:ASN:ND2	3:X:115:ARG:NH1	2.58	0.51
2:B:58:VAL:HG12	2:B:104:VAL:CG2	2.40	0.51
2:D:89:ILE:HD11	2:D:104:VAL:HG11	1.92	0.51
2:D:1438:LEU:O	2:D:1438:LEU:HD13	2.11	0.51
1:A:154:PRO:O	1:A:155:ALA:HB3	2.10	0.51
2:D:1381:ILE:CG2	2:D:1459:TYR:CE1	2.93	0.51
2:B:1343:PHE:CD1	2:B:1458:VAL:HG11	2.46	0.51
2:D:342:PRO:HG2	2:D:420:LEU:CD1	2.41	0.51
1:A:274:ASP:CG	1:A:275:LEU:H	2.14	0.51
1:A:1188:LEU:HD23	1:A:1212:LEU:CD1	2.41	0.51
2:B:1514:LYS:O	2:B:1517:GLU:HB2	2.09	0.51
2:D:746:ILE:N	2:D:746:ILE:HD13	2.25	0.51
2:D:1274:ASN:OD1	2:D:1291:ARG:NH2	2.42	0.51
1:A:656:ASN:CB	1:A:659:ALA:H	2.23	0.51
1:C:511:HIS:HE1	3:Y:149:SER:OG	1.92	0.51
1:A:180:ILE:O	1:A:182:ILE:N	2.44	0.51
1:C:1124:TYR:CA	1:C:1465:ASN:OD1	2.50	0.51
2:B:1561:HIS:CD2	2:B:1597:ILE:HD13	2.46	0.51
2:B:1330:ASN:N	2:B:1330:ASN:ND2	2.58	0.51
3:X:194:LYS:NZ	3:X:197:ASN:HD22	2.08	0.51
2:D:231:SER:HB3	2:D:244:HIS:HB2	1.91	0.51
1:A:584:PRO:CB	1:A:792:ASP:HA	2.37	0.51
2:B:1273:LEU:CB	2:B:1319:GLY:HA3	2.35	0.51
2:D:122:SER:OG	2:D:124:GLN:HB3	2.11	0.51
2:D:69:PHE:HD2	2:D:69:PHE:C	2.14	0.51
1:C:1327:LYS:HG3	1:C:1328:MET:H	1.75	0.51
1:A:472:ASN:O	1:A:473:HIS:CB	2.58	0.51
2:B:1391:LEU:HB2	2:B:1417:MET:HE2	1.93	0.51
2:B:1381:ILE:CG2	2:B:1459:TYR:CE1	2.94	0.51
1:C:1188:LEU:HD23	1:C:1212:LEU:HA	1.92	0.51
2:B:204:GLU:O	2:B:205:HIS:HB2	2.10	0.51
1:A:165:ASP:HB2	1:A:166:PRO:CD	2.40	0.51
1:A:40:VAL:CG2	1:A:512:PHE:CD1	2.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:ALA:CB	1:A:657:ALA:HB3	2.39	0.51
1:C:111:PHE:CG	1:C:112:SER:N	2.78	0.51
1:C:492:TYR:CE2	1:C:493:ILE:HB	2.46	0.51
1:C:59:TYR:CD2	1:C:99:VAL:HG21	2.46	0.51
2:D:847:ARG:O	2:D:898:ALA:HA	2.10	0.51
2:B:46:HIS:CG	2:B:525:GLN:HG2	2.45	0.51
1:A:1234:HIS:O	1:A:1235:LYS:HB2	2.10	0.51
1:A:1217:LEU:HD13	1:A:1237:SER:HA	1.93	0.51
1:A:914:LEU:HD11	1:A:916:THR:HG22	1.93	0.51
2:D:795:THR:CG2	2:D:796:PRO:HD2	2.39	0.51
1:A:625:GLN:O	1:A:628:GLU:HB3	2.11	0.51
3:X:88:GLY:O	3:X:91:LYS:N	2.38	0.51
1:C:1031:TRP:CH2	1:C:1042:LYS:HG3	2.45	0.51
1:C:20:GLU:C	1:C:21:GLN:CG	2.77	0.51
1:C:1544:SER:HA	1:C:1547:THR:OG1	2.11	0.51
1:A:875:HIS:HB3	2:B:901:GLN:HE22	1.74	0.51
2:B:573:ALA:HB3	2:B:762:LEU:HD13	1.93	0.51
2:B:353:TYR:HA	2:B:433:ILE:O	2.11	0.51
1:A:193:ASN:OD1	1:A:1070:LYS:HE2	2.11	0.51
1:C:827:MET:HE2	1:C:912:PHE:CE2	2.46	0.51
1:A:1084:ARG:HG2	1:A:1084:ARG:HH11	1.75	0.51
2:B:1530:ARG:NH1	2:B:1530:ARG:HG3	2.26	0.51
2:D:189:PRO:C	2:D:191:LEU:H	2.12	0.51
2:D:1351:ASN:O	2:D:1352:ILE:HG12	2.10	0.51
1:C:1440:LYS:O	1:C:1444:GLU:HG3	2.11	0.51
1:A:33:VAL:CG2	1:A:121:TYR:HD1	2.23	0.51
1:C:1571:GLU:O	1:C:1574:PHE:CD2	2.64	0.51
1:A:1133:LEU:CD1	1:A:1133:LEU:N	2.71	0.51
1:A:1552:ALA:HB2	1:A:1620:MET:HE1	1.93	0.51
1:A:1601:ILE:O	1:A:1638:PRO:O	2.29	0.51
1:A:361:LEU:HD21	1:A:452:TYR:HB3	1.92	0.51
2:B:870:PHE:HB2	2:B:871:PRO:CD	2.41	0.51
1:A:459:SER:HG	1:A:461:SER:HB3	1.74	0.51
1:C:199:TRP:HB2	1:C:217:PHE:CD1	2.46	0.51
1:A:257:ASN:ND2	1:A:892:SER:O	2.43	0.51
2:D:1482:ASN:H	2:D:1495:GLU:HG2	1.76	0.51
1:A:689:LYS:HD3	1:A:730:GLU:OE2	2.11	0.51
2:D:1548:ILE:CG2	2:D:1635:LEU:HB3	2.40	0.51
1:C:958:GLU:HA	1:C:1346:LEU:O	2.10	0.51
2:D:603:GLU:C	2:D:605:SER:H	2.14	0.51
2:B:343:TYR:CE1	2:B:420:LEU:HD11	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1554:LYS:HG3	1:C:1555:PRO:HD2	1.93	0.51
2:D:902:GLU:HG3	2:D:902:GLU:O	2.11	0.51
1:C:974:LYS:O	1:C:1364:VAL:HG12	2.11	0.51
1:A:1527:CYS:C	1:A:1529:GLU:N	2.64	0.51
1:C:513:GLY:CA	3:Y:146:LEU:HD13	2.41	0.51
1:C:1564:SER:CB	1:C:1616:GLN:HG3	2.41	0.51
1:C:1615:ARG:HD2	1:C:1647:TYR:CD1	2.45	0.51
1:A:1085:VAL:O	1:A:1089:VAL:HG23	2.10	0.51
1:C:804:ILE:CG2	1:C:809:ILE:HG13	2.38	0.51
1:A:59:TYR:CD2	1:A:99:VAL:HG21	2.46	0.51
1:A:849:ARG:HH21	2:B:556:ILE:HD12	1.76	0.51
1:C:847:ASN:ND2	1:C:853:MET:HB3	2.26	0.51
2:B:89:ILE:HD11	2:B:104:VAL:HG11	1.93	0.51
1:C:1323:LEU:CG	1:C:1324:HIS:H	2.24	0.51
1:A:1304:VAL:CG1	1:A:1305:LYS:H	2.23	0.51
3:X:88:GLY:C	3:X:90:ASP:H	2.14	0.51
1:A:473:HIS:O	1:A:473:HIS:HD2	1.90	0.51
1:C:123:ASN:OD1	1:C:123:ASN:C	2.49	0.51
2:B:862:LYS:HZ2	2:B:1519:ASN:HB3	1.75	0.51
1:C:396:ASP:HB3	1:C:398:ASN:HB2	1.92	0.51
2:B:745:ILE:HD11	2:B:907:ASP:H	1.75	0.51
2:B:1386:MET:HA	2:B:1386:MET:CE	2.40	0.51
1:A:974:LYS:O	1:A:1364:VAL:HG12	2.11	0.51
1:A:1536:GLN:HG3	1:A:1536:GLN:O	2.10	0.51
3:Y:166:ASP:OD2	3:Y:207:LEU:CD2	2.59	0.51
1:C:1619:ILE:HG12	1:C:1645:ILE:HD13	1.93	0.51
1:C:961:TYR:C	1:C:961:TYR:CD1	2.83	0.51
1:C:477:LEU:N	1:C:477:LEU:HD22	2.25	0.51
2:D:1562:GLN:HE22	2:D:1596:LYS:HZ1	1.57	0.51
2:D:1562:GLN:NE2	2:D:1596:LYS:NZ	2.56	0.51
1:A:1240:PRO:O	1:A:1242:THR:N	2.43	0.51
1:C:62:LYS:HE2	1:C:103:TYR:CE2	2.45	0.51
1:A:1430:THR:O	1:A:1485:VAL:HG11	2.10	0.51
1:A:238:ILE:HG23	1:A:242:ASN:HD22	1.75	0.51
1:A:569:ASN:CG	1:A:570:GLN:H	2.15	0.51
2:B:1457:LYS:HG2	2:B:1469:THR:OG1	2.10	0.51
2:B:1387:LEU:HD21	2:B:1472:TYR:CE1	2.46	0.51
2:D:243:PHE:CD1	2:D:314:LEU:HD23	2.43	0.51
3:X:106:VAL:HG22	3:X:163:LYS:HE3	1.93	0.51
2:D:1538:ASP:OD2	2:D:1567:ARG:HD2	2.11	0.51
2:D:746:ILE:HD13	2:D:746:ILE:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLY:O	1:A:96:GLN:O	2.29	0.51
2:B:280:LEU:HD11	2:B:1379:MET:HG3	1.93	0.51
1:A:573:VAL:O	1:A:574:HIS:ND1	2.44	0.51
1:A:945:ASP:C	1:A:945:ASP:OD1	2.47	0.51
3:X:166:ASP:OD2	3:X:207:LEU:CD2	2.57	0.51
1:C:459:SER:HG	1:C:461:SER:HB3	1.75	0.51
1:C:530:VAL:CG2	1:C:563:ILE:HD12	2.40	0.51
1:C:1240:PRO:O	1:C:1242:THR:N	2.44	0.51
1:C:1242:THR:OG1	1:C:1243:GLY:N	2.43	0.51
1:C:1569:THR:O	1:C:1570:VAL:CG2	2.59	0.51
1:C:1093:VAL:HG12	1:C:1095:GLN:HE21	1.76	0.51
2:B:902:GLU:HG3	2:B:902:GLU:O	2.11	0.51
1:C:698:CYS:HB3	1:C:728:PHE:HB2	1.93	0.51
1:A:697:LYS:O	1:A:700:TYR:HB3	2.10	0.51
3:Y:113:ASN:ND2	3:Y:115:ARG:NH1	2.59	0.51
1:A:1232:LEU:CG	1:A:1233:GLN:HG3	2.37	0.51
1:C:1031:TRP:CZ3	1:C:1042:LYS:HA	2.46	0.51
1:A:1033:ILE:HG23	1:A:1034:PHE:H	1.75	0.51
3:X:107:GLN:OE1	3:X:110:ILE:HD11	2.10	0.51
1:A:977:LEU:HD23	1:A:1361:VAL:HG22	1.93	0.51
2:B:962:LYS:HD2	2:B:1302:THR:HG21	1.91	0.51
2:B:1526:THR:HA	2:B:1545:LEU:HD13	1.92	0.51
1:C:1421:HIS:C	1:C:1421:HIS:CD2	2.83	0.51
2:B:204:GLU:O	2:B:204:GLU:HG3	2.10	0.51
2:B:54:LEU:HD23	2:B:54:LEU:N	2.26	0.51
1:C:23:TYR:CD1	1:C:655:THR:CB	2.89	0.50
1:C:1648:TRP:NE1	1:C:1664:LEU:HD21	2.25	0.50
1:A:614:ARG:N	1:A:614:ARG:HD2	2.26	0.50
2:B:1284:ARG:HG3	2:B:1285:GLU:N	2.26	0.50
2:B:265:PHE:O	2:B:276:ILE:HG13	2.11	0.50
1:A:220:LYS:HD3	1:A:765:ILE:HG23	1.93	0.50
2:D:1343:PHE:CG	2:D:1458:VAL:HG11	2.46	0.50
2:B:134:LYS:HD2	2:B:584:VAL:HG11	1.93	0.50
2:D:1600:ILE:O	2:D:1600:ILE:HG13	2.11	0.50
2:D:1600:ILE:O	2:D:1602:THR:HG23	2.11	0.50
2:D:410:PRO:CA	2:D:431:THR:HG22	2.41	0.50
2:B:923:SER:HB3	2:B:1328:PHE:CE1	2.47	0.50
2:B:351:PRO:N	2:B:611:ALA:HB3	2.26	0.50
1:C:1099:SER:O	1:C:1100:ILE:C	2.47	0.50
1:A:25:ILE:HG13	1:A:106:VAL:HG21	1.92	0.50
1:A:541:LEU:HD23	1:A:541:LEU:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LYS:HZ2	3:X:144:GLU:HA	1.71	0.50
1:C:1622:LYS:CD	1:C:1642:LEU:HB3	2.40	0.50
1:A:375:VAL:O	1:A:383:VAL:HG13	2.11	0.50
1:A:1245:ALA:HB2	1:A:1285:TYR:HB3	1.93	0.50
2:B:285:ILE:HD12	2:B:285:ILE:H	1.74	0.50
2:B:1330:ASN:HD22	2:B:1330:ASN:N	2.09	0.50
2:D:44:GLU:OE1	2:D:480:THR:HG21	2.11	0.50
2:D:208:GLU:OE1	2:D:210:TYR:HB2	2.11	0.50
1:A:698:CYS:C	1:A:700:TYR:N	2.63	0.50
1:A:496:ILE:HG22	1:A:496:ILE:O	2.10	0.50
1:A:415:ASP:OD1	1:A:415:ASP:N	2.44	0.50
1:A:1327:LYS:HG3	1:A:1328:MET:H	1.75	0.50
2:D:1624:LEU:O	2:D:1625:CYS:C	2.50	0.50
1:A:689:LYS:O	1:A:691:LYS:N	2.43	0.50
1:C:365:PRO:HG2	1:C:464:TYR:CE2	2.47	0.50
2:D:1343:PHE:CD1	2:D:1458:VAL:HG11	2.46	0.50
2:D:236:TYR:CE1	2:D:424:ARG:HD2	2.45	0.50
3:X:41:HIS:O	3:X:42:ASP:CB	2.58	0.50
1:C:1565:ILE:HB	1:C:1614:GLY:H	1.76	0.50
3:X:85:PHE:N	3:X:85:PHE:CD1	2.78	0.50
1:C:54:ILE:HG12	1:C:106:VAL:HG13	1.92	0.50
1:C:1640:ASP:O	1:C:1643:THR:HB	2.12	0.50
1:A:1227:PHE:HB2	1:A:1251:THR:HG21	1.92	0.50
1:C:784:LYS:HG2	1:C:785:GLN:H	1.75	0.50
1:C:1602:LYS:HE3	1:C:1609:ALA:O	2.11	0.50
1:A:1064:TYR:HD2	1:A:1102:ASN:CB	2.25	0.50
2:B:164:GLU:HA	2:B:174:SER:O	2.10	0.50
1:A:470:THR:CG2	2:B:450:THR:HG22	2.29	0.50
1:A:1643:THR:CG2	1:A:1644:TRP:N	2.73	0.50
1:C:180:ILE:O	1:C:182:ILE:N	2.45	0.50
1:C:804:ILE:HG22	1:C:809:ILE:CG1	2.39	0.50
2:D:620:VAL:HG12	2:D:621:PHE:N	2.26	0.50
2:D:962:LYS:HD2	2:D:1302:THR:HG21	1.92	0.50
1:A:395:ILE:CG1	1:A:430:VAL:HB	2.42	0.50
3:Y:58:SER:HB3	3:Y:102:ASN:HD22	1.72	0.50
1:A:1226:ARG:NE	1:A:1266:TYR:HE1	2.08	0.50
1:C:149:ASN:O	1:C:151:ASP:N	2.44	0.50
1:C:1226:ARG:NE	1:C:1266:TYR:CE1	2.80	0.50
1:C:1153:ARG:CZ	1:C:1168:LEU:HD12	2.42	0.50
2:D:1438:LEU:HD22	2:D:1439:HIS:N	2.26	0.50
1:C:1064:TYR:HD2	1:C:1102:ASN:CB	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:864:GLY:HA3	1:C:907:LEU:HD22	1.92	0.50
1:C:1474:CYS:HB3	1:C:1476:ARG:NH1	2.26	0.50
2:D:1288:ILE:HD13	2:D:1303:VAL:HG21	1.92	0.50
3:X:43:ILE:O	3:X:44:ARG:C	2.48	0.50
2:D:45:ALA:HB3	2:D:81:MET:HE3	1.93	0.50
1:A:987:ILE:HD11	1:A:1294:ILE:HG23	1.91	0.50
2:D:565:ILE:HG22	2:D:806:TYR:HE2	1.77	0.50
1:C:923:LEU:HD23	1:C:924:VAL:N	2.26	0.50
1:A:481:HIS:ND1	1:A:529:PRO:HB3	2.26	0.50
1:C:670:LYS:HD2	1:C:671:GLU:H	1.76	0.50
1:C:134:VAL:C	1:C:135:TYR:CD2	2.85	0.50
2:B:503:LEU:HD23	2:B:503:LEU:C	2.32	0.50
1:A:1130:GLN:NE2	1:A:1230:ASP:HB3	2.26	0.50
3:X:61:SER:N	3:X:75:PHE:HZ	2.09	0.50
1:C:239:GLY:O	1:C:241:LYS:N	2.44	0.50
1:C:1320:LYS:CD	1:C:1321:GLY:N	2.72	0.50
2:D:1427:LEU:N	2:D:1427:LEU:HD13	2.26	0.50
2:B:575:VAL:O	2:B:759:THR:HA	2.12	0.50
1:C:274:ASP:CG	1:C:275:LEU:H	2.15	0.50
2:B:942:LEU:HD13	2:B:1314:THR:HG23	1.92	0.50
1:C:396:ASP:HB2	1:C:400:GLU:H	1.75	0.50
1:C:1408:TYR:O	1:C:1410:PRO:HD3	2.11	0.50
2:B:40:GLN:HG3	2:B:86:THR:HG23	1.93	0.50
1:A:124:GLY:C	1:A:125:PHE:CG	2.84	0.50
1:C:1549:LYS:HD3	1:C:1667:PHE:CG	2.47	0.50
1:C:902:PRO:O	1:C:903:LEU:HD13	2.10	0.50
1:A:1540:ASP:HA	1:A:1660:PHE:HD1	1.76	0.50
1:A:577:PRO:HD2	1:A:588:VAL:HG23	1.93	0.50
1:C:243:PHE:CE2	1:C:304:GLU:HA	2.45	0.50
2:B:484:LEU:HD11	2:B:626:LEU:HG	1.93	0.50
1:A:796:THR:HA	1:A:818:LYS:HA	1.93	0.50
2:B:1438:LEU:HD22	2:B:1439:HIS:N	2.26	0.50
1:A:1179:THR:HG22	1:A:1180:LEU:HD23	1.94	0.50
1:A:958:GLU:HA	1:A:1346:LEU:O	2.12	0.50
1:A:396:ASP:HB3	1:A:398:ASN:H	1.76	0.50
2:B:1589:ASP:HB3	2:B:1600:ILE:HG13	1.94	0.50
2:B:1600:ILE:O	2:B:1602:THR:HG23	2.11	0.50
2:D:745:ILE:HD11	2:D:907:ASP:N	2.26	0.50
2:D:204:GLU:HG3	2:D:204:GLU:O	2.12	0.50
3:X:85:PHE:N	3:X:85:PHE:HD1	2.10	0.50
1:C:851:SER:O	1:C:890:GLY:HA2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1456:LYS:HG3	1:C:1457:ASP:OD2	2.11	0.50
2:D:54:LEU:N	2:D:54:LEU:HD23	2.25	0.50
2:D:415:THR:O	2:D:425:GLN:CD	2.50	0.50
1:C:837:GLU:O	1:C:901:LEU:HB2	2.11	0.50
1:A:1576:LYS:CG	1:A:1601:ILE:HG22	2.33	0.50
2:D:846:VAL:HG22	2:D:847:ARG:N	2.26	0.50
1:C:1056:ILE:HG12	1:C:1056:ILE:O	2.10	0.50
1:A:492:TYR:CD2	1:A:493:ILE:HB	2.46	0.50
1:C:316:GLU:HG2	1:C:349:LEU:HD23	1.94	0.50
1:A:1066:TYR:CD1	1:A:1066:TYR:N	2.80	0.50
1:C:539:ARG:NE	1:C:633:GLY:HA3	2.27	0.50
1:C:691:LYS:C	1:C:693:SER:N	2.64	0.50
2:D:1610:TRP:CE3	2:D:1628:PHE:CE2	3.00	0.50
1:A:691:LYS:C	1:A:693:SER:N	2.65	0.50
1:A:691:LYS:C	1:A:693:SER:H	2.12	0.50
2:B:1343:PHE:CG	2:B:1458:VAL:HG11	2.46	0.50
2:B:887:LEU:HD23	2:B:1490:CYS:HB3	1.92	0.50
2:B:558:MET:O	2:B:561:ALA:HB3	2.11	0.50
1:A:1548:ARG:HE	1:A:1550:GLN:NE2	2.09	0.50
2:B:946:LYS:H	2:B:946:LYS:CD	2.23	0.50
1:C:856:CYS:HB3	1:C:915:GLU:HG2	1.94	0.50
2:D:357:GLY:HA3	2:D:404:LEU:HD12	1.94	0.50
1:C:95:GLY:O	1:C:96:GLN:O	2.30	0.50
1:A:163:PHE:CE2	1:A:188:PHE:CD1	2.99	0.50
1:C:1433:SER:OG	1:C:1482:LEU:HD12	2.11	0.50
1:A:1383:THR:HG21	1:A:1511:THR:HG22	1.93	0.50
1:C:1365:VAL:CG2	1:C:1366:HIS:H	2.18	0.50
1:C:1430:THR:O	1:C:1485:VAL:HG11	2.11	0.50
1:C:985:GLY:O	1:C:986:GLU:C	2.50	0.50
2:D:1593:THR:HG22	2:D:1594:LYS:H	1.72	0.50
2:D:565:ILE:O	2:D:776:MET:HB3	2.11	0.50
1:C:911:ASN:OD1	1:C:924:VAL:HG22	2.12	0.50
1:C:1021:VAL:HG12	1:C:1022:PHE:N	2.27	0.50
2:D:476:ILE:HG12	2:D:524:TYR:CD2	2.47	0.50
2:D:1290:TYR:CD2	2:D:1301:ARG:HB3	2.46	0.50
2:B:338:ILE:C	2:B:339:VAL:HG13	2.32	0.50
1:C:614:ARG:N	1:C:614:ARG:HD2	2.26	0.50
2:D:1623:LYS:HB3	2:D:1623:LYS:HZ2	1.77	0.50
2:B:1346:ASN:HB2	2:B:1368:CYS:HB2	1.93	0.50
1:A:1408:TYR:O	1:A:1410:PRO:HD3	2.12	0.50
1:C:661:ASP:OD2	1:C:663:GLN:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1084:ARG:HA	1:C:1151:GLY:HA2	1.94	0.50
1:C:544:TYR:C	1:C:544:TYR:HD2	2.15	0.50
2:B:362:LEU:HD13	2:B:411:ILE:HD12	1.94	0.50
3:X:229:ASN:N	3:X:229:ASN:OD1	2.45	0.50
3:Y:166:ASP:OD2	3:Y:207:LEU:CG	2.58	0.50
1:A:23:TYR:O	1:A:655:THR:HB	2.12	0.50
1:A:530:VAL:HG23	1:A:534:MET:CE	2.39	0.50
1:C:78:LYS:HG3	3:Y:146:LEU:HB2	1.92	0.50
1:C:1245:ALA:HB2	1:C:1285:TYR:HB3	1.94	0.50
1:C:33:VAL:HG23	1:C:120:THR:O	2.11	0.50
1:A:1147:PHE:C	1:A:1147:PHE:CD2	2.85	0.50
2:B:1292:ILE:CD1	2:B:1301:ARG:HE	2.24	0.50
2:B:206:SER:O	2:B:208:GLU:N	2.45	0.50
2:B:208:GLU:OE1	2:B:210:TYR:HB2	2.12	0.50
2:D:780:LEU:HD11	2:D:787:TRP:CD1	2.47	0.50
2:B:857:CYS:HB3	2:B:885:VAL:HG22	1.93	0.50
2:D:46:HIS:CG	2:D:525:GLN:HG2	2.46	0.50
1:A:234:GLU:HB3	1:A:246:PHE:CE1	2.47	0.50
1:A:950:TYR:HD1	1:A:1268:ASN:OD1	1.94	0.50
1:A:199:TRP:HB2	1:A:217:PHE:CD1	2.47	0.50
1:C:523:TYR:CE1	2:D:359:PRO:CG	2.93	0.50
2:D:952:ASP:N	2:D:952:ASP:OD1	2.31	0.50
1:A:1347:ILE:CG2	1:A:1347:ILE:O	2.60	0.50
3:Y:107:GLN:CD	3:Y:110:ILE:HD11	2.32	0.50
1:C:1033:ILE:HD13	1:C:1034:PHE:CE1	2.47	0.50
1:C:32:ARG:O	1:C:35:ALA:HB3	2.12	0.50
1:A:24:VAL:HA	1:A:655:THR:CB	2.42	0.50
1:C:74:SER:HA	1:C:79:PHE:HE1	1.77	0.50
1:C:1582:LEU:O	1:C:1583:ASP:C	2.50	0.50
1:C:1240:PRO:C	1:C:1242:THR:N	2.65	0.50
1:A:1012:LEU:HD22	1:A:1085:VAL:CG2	2.25	0.50
2:B:1609:ARG:NH1	2:B:1609:ARG:HG2	2.25	0.50
1:A:1563:VAL:HA	1:A:1582:LEU:H	1.77	0.50
1:A:1582:LEU:O	1:A:1583:ASP:C	2.50	0.50
1:A:1616:GLN:OE1	1:A:1650:ARG:HB3	2.12	0.50
1:A:1540:ASP:CA	1:A:1660:PHE:HD1	2.25	0.50
2:B:881:PRO:O	2:B:882:PHE:CD2	2.65	0.50
1:A:1370:THR:O	1:A:1371:SER:C	2.49	0.50
3:X:61:SER:O	3:X:75:PHE:CZ	2.65	0.50
1:A:916:THR:C	1:A:918:PHE:H	2.15	0.50
1:C:1263:ASP:O	1:C:1265:ASN:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ALA:O	1:A:157:ARG:N	2.45	0.50
2:D:1381:ILE:HB	2:D:1459:TYR:HD1	1.77	0.50
2:B:1427:LEU:N	2:B:1427:LEU:HD13	2.27	0.50
1:A:612:VAL:HG21	1:A:769:PHE:CE2	2.46	0.50
2:B:1601:ILE:HD12	2:B:1601:ILE:H	1.76	0.50
1:A:236:ASN:HD22	1:A:379:LEU:HD21	1.76	0.50
3:Y:103:VAL:HG22	3:Y:122:VAL:HG13	1.94	0.50
3:Y:104:PHE:CE1	3:Y:164:GLU:HG3	2.47	0.50
1:C:1365:VAL:CG2	1:C:1366:HIS:N	2.73	0.49
1:C:1147:PHE:CD2	1:C:1147:PHE:C	2.86	0.49
1:C:820:PHE:CG	1:C:821:LYS:N	2.80	0.49
1:C:690:TYR:C	1:C:692:HIS:N	2.66	0.49
1:C:689:LYS:HD3	1:C:730:GLU:OE2	2.12	0.49
1:A:149:ASN:H	1:A:149:ASN:ND2	2.05	0.49
2:B:243:PHE:CD2	2:B:243:PHE:C	2.85	0.49
2:B:559:PRO:HG2	2:B:812:LYS:HD2	1.93	0.49
1:C:161:LEU:HD11	1:C:185:PHE:CZ	2.47	0.49
2:B:1539:ILE:HG23	2:B:1564:ILE:HG12	1.94	0.49
2:D:1529:LEU:HD11	2:D:1543:ASP:HB2	1.94	0.49
1:A:805:SER:O	1:A:807:THR:N	2.45	0.49
1:A:560:TRP:HH2	1:A:673:LEU:HD22	1.77	0.49
3:Y:215:VAL:C	3:Y:216:LEU:HD22	2.32	0.49
1:A:484:ILE:HD12	1:A:540:LEU:CD2	2.42	0.49
3:X:146:LEU:HD21	3:X:148:ALA:HB2	1.94	0.49
1:C:42:GLN:HE21	1:C:44:TYR:N	2.10	0.49
1:A:1053:MET:HE2	1:A:1086:LEU:CD1	2.42	0.49
1:C:1162:VAL:HG23	1:C:1163:LYS:N	2.27	0.49
2:B:1480:LEU:C	2:B:1480:LEU:HD12	2.33	0.49
1:A:1598:ILE:HG22	1:A:1599:THR:N	2.27	0.49
1:A:1215:GLU:O	1:A:1217:LEU:HD23	2.12	0.49
1:A:571:LEU:CD2	1:A:812:ALA:HB2	2.41	0.49
2:D:1391:LEU:HD12	2:D:1417:MET:HE1	1.92	0.49
2:B:147:VAL:HG12	2:B:183:PHE:CE1	2.45	0.49
2:B:199:ILE:O	2:B:199:ILE:HG22	2.11	0.49
1:A:1544:SER:HA	1:A:1547:THR:OG1	2.12	0.49
3:Y:41:HIS:N	3:Y:41:HIS:ND1	2.60	0.49
2:D:923:SER:HB3	2:D:1328:PHE:CE1	2.47	0.49
1:A:55:SER:C	1:A:56:ILE:HD13	2.32	0.49
1:C:998:ASN:HB3	1:C:1000:LEU:HG	1.94	0.49
1:C:663:GLN:CG	1:C:664:GLU:N	2.74	0.49
1:C:734:VAL:HA	1:C:737:GLN:HG2	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:ASN:O	1:A:659:ALA:HB3	2.11	0.49
2:D:563:MET:HA	2:D:563:MET:HE3	1.94	0.49
2:D:756:LEU:HD22	2:D:778:PHE:CD1	2.48	0.49
2:B:1611:PRO:HG3	2:B:1624:LEU:HB3	1.94	0.49
3:X:61:SER:N	3:X:75:PHE:CZ	2.80	0.49
1:C:757:LEU:O	1:C:758:LEU:HD23	2.12	0.49
1:A:983:LEU:HD21	1:A:1271:ILE:HD12	1.94	0.49
1:A:1323:LEU:CD1	1:A:1324:HIS:H	2.24	0.49
3:Y:71:ASN:O	3:Y:72:VAL:HG23	2.13	0.49
2:B:218:LYS:HB3	2:B:822:TYR:CE2	2.46	0.49
1:C:1180:LEU:CD2	1:C:1208:ILE:HG12	2.43	0.49
2:D:167:THR:HG22	2:D:171:ILE:O	2.12	0.49
2:D:1522:TYR:N	2:D:1522:TYR:HD2	2.10	0.49
2:D:963:ILE:CD1	2:D:1311:ILE:HG21	2.41	0.49
1:A:680:GLN:O	1:A:682:LYS:N	2.45	0.49
1:C:398:ASN:O	1:C:399:GLN:HB2	2.13	0.49
1:C:1537:GLU:O	1:C:1539:LEU:N	2.44	0.49
1:A:23:TYR:HA	1:A:43:VAL:HA	1.94	0.49
1:C:515:ARG:CZ	1:C:526:ILE:HG22	2.42	0.49
1:C:1643:THR:CG2	1:C:1644:TRP:N	2.74	0.49
1:C:903:LEU:HD22	1:C:903:LEU:N	2.27	0.49
1:A:987:ILE:HD13	1:A:1294:ILE:HG23	1.94	0.49
1:A:1068:VAL:CG1	1:A:1069:TRP:H	2.17	0.49
1:A:1077:TRP:NE1	1:A:1147:PHE:CD1	2.80	0.49
2:D:564:LYS:HA	2:D:776:MET:O	2.12	0.49
2:B:1506:ILE:CD1	2:B:1628:PHE:CE1	2.95	0.49
1:A:1487:PHE:O	1:A:1488:LEU:C	2.50	0.49
1:C:296:ILE:CG2	1:C:297:ALA:N	2.76	0.49
2:B:481:TYR:HE2	2:B:493:GLY:CA	2.24	0.49
1:C:243:PHE:HE2	1:C:304:GLU:CA	2.25	0.49
1:C:541:LEU:HB2	1:C:558:SER:HB3	1.95	0.49
1:A:1327:LYS:O	1:A:1332:ASN:ND2	2.46	0.49
1:A:1019:PHE:CD2	1:A:1020:TYR:N	2.80	0.49
2:D:322:THR:HG21	2:D:327:ASP:H	1.78	0.49
1:C:613:GLN:O	1:C:615:GLY:N	2.46	0.49
2:D:916:VAL:CG2	2:D:917:PRO:N	2.76	0.49
1:C:255:PHE:HB2	1:C:846:TYR:OH	2.12	0.49
1:C:87:ILE:H	1:C:87:ILE:HD13	1.73	0.49
2:B:1415:ASN:O	2:B:1417:MET:HG3	2.12	0.49
2:D:1371:TYR:CD1	2:D:1377:SER:CB	2.95	0.49
1:C:1541:LEU:HD21	1:C:1543:ILE:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1522:TYR:CD2	2:B:1522:TYR:O	2.65	0.49
2:B:963:ILE:CD1	2:B:1311:ILE:HG21	2.42	0.49
3:Y:119:VAL:HG13	3:Y:212:MET:SD	2.52	0.49
3:Y:106:VAL:HG22	3:Y:163:LYS:HE3	1.93	0.49
1:A:196:TYR:HE2	1:A:1070:LYS:NZ	2.10	0.49
1:C:916:THR:O	1:C:918:PHE:N	2.46	0.49
3:X:104:PHE:CE1	3:X:164:GLU:HG3	2.47	0.49
2:D:643:LYS:HG3	2:D:644:CYS:N	2.27	0.49
3:Y:85:PHE:CE1	3:Y:117:SER:HB3	2.47	0.49
1:A:1537:GLU:O	1:A:1539:LEU:N	2.45	0.49
1:A:998:ASN:HB3	1:A:1000:LEU:HG	1.93	0.49
2:B:643:LYS:HG3	2:B:644:CYS:N	2.27	0.49
1:A:23:TYR:HE2	1:A:111:PHE:CD2	2.30	0.49
2:B:1619:GLU:C	2:B:1621:PHE:H	2.15	0.49
1:C:234:GLU:HB3	1:C:246:PHE:CE1	2.47	0.49
2:B:565:ILE:HG22	2:B:806:TYR:HE2	1.77	0.49
2:D:235:PHE:HB3	2:D:338:ILE:CG2	2.43	0.49
1:C:758:LEU:HB3	1:C:759:PRO:HD2	1.93	0.49
2:D:825:VAL:HB	2:D:828:GLU:CD	2.33	0.49
3:X:71:ASN:O	3:X:72:VAL:HG23	2.12	0.49
2:B:168:PRO:HD3	2:B:197:TRP:CD1	2.47	0.49
1:C:1226:ARG:CB	1:C:1269:PRO:HB2	2.42	0.49
1:A:1423:VAL:HG11	1:A:1496:TYR:CZ	2.47	0.49
2:D:511:THR:O	2:D:513:ASP:N	2.46	0.49
2:B:59:HIS:HB3	2:B:64:LYS:HA	1.95	0.49
2:D:408:SER:HB3	2:D:410:PRO:HD3	1.95	0.49
2:D:942:LEU:HD13	2:D:1314:THR:HG23	1.95	0.49
1:C:377:ASP:OD2	1:C:379:LEU:HB2	2.12	0.49
1:C:85:LEU:HD22	1:C:85:LEU:N	2.27	0.49
1:A:74:SER:HA	1:A:79:PHE:CE1	2.47	0.49
1:C:1557:ILE:HD13	1:C:1622:LYS:HG3	1.93	0.49
1:A:1564:SER:CB	1:A:1616:GLN:HG3	2.43	0.49
2:D:26:THR:HG22	2:D:630:THR:HG22	1.94	0.49
2:B:564:LYS:HA	2:B:776:MET:O	2.13	0.49
2:B:560:GLY:HA2	2:B:780:LEU:O	2.13	0.49
1:A:820:PHE:CG	1:A:821:LYS:N	2.81	0.49
1:C:100:SER:O	1:C:101:TYR:HB2	2.11	0.49
1:A:1286:SER:OG	1:A:1287:THR:N	2.46	0.49
1:A:719:SER:OG	1:A:1123:GLN:HG3	2.12	0.49
1:A:1249:GLU:O	1:A:1253:TYR:HD2	1.96	0.49
1:C:719:SER:OG	1:C:1123:GLN:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ASN:N	1:A:211:THR:HG23	2.27	0.49
2:B:916:VAL:CG2	2:B:917:PRO:N	2.74	0.49
2:B:1347:VAL:HG21	2:B:1456:VAL:HG11	1.94	0.49
2:D:1526:THR:HA	2:D:1545:LEU:HD13	1.95	0.49
1:C:423:ASN:HB3	2:D:501:GLN:NE2	2.27	0.49
1:C:682:LYS:HZ2	1:C:686:ILE:CD1	2.26	0.49
1:A:1318:LYS:HB2	1:A:1345:ASP:HB2	1.94	0.49
2:D:1533:GLU:OE1	2:D:1533:GLU:HA	2.13	0.49
2:D:280:LEU:HD22	2:D:1462:TYR:HE2	1.76	0.49
2:B:1400:LEU:HD22	2:B:1406:ARG:HH12	1.77	0.49
1:A:514:THR:HG22	1:A:515:ARG:N	2.27	0.49
1:C:1620:MET:CB	1:C:1644:TRP:HB3	2.27	0.49
1:A:766:ARG:H	1:A:766:ARG:HD3	1.78	0.49
2:B:620:VAL:HG12	2:B:621:PHE:N	2.28	0.49
2:B:494:ARG:CG	2:B:494:ARG:HH11	2.12	0.49
3:Y:86:LEU:HG	3:Y:91:LYS:CG	2.43	0.49
1:C:257:ASN:HD21	1:C:892:SER:CA	2.23	0.49
3:X:88:GLY:C	3:X:90:ASP:N	2.66	0.49
1:A:600:VAL:CG2	1:A:780:VAL:HG21	2.42	0.49
2:B:1285:GLU:O	2:B:1287:PRO:HD3	2.13	0.49
1:A:1098:ASN:O	1:A:1101:CYS:HB2	2.13	0.49
1:A:1162:VAL:HG23	1:A:1163:LYS:N	2.27	0.49
2:D:218:LYS:HB3	2:D:822:TYR:CE2	2.47	0.49
1:A:100:SER:C	1:A:101:TYR:HD2	2.16	0.49
2:D:948:ARG:HB2	2:D:948:ARG:NH2	2.25	0.49
1:C:1475:VAL:CG2	1:C:1476:ARG:N	2.75	0.49
2:D:243:PHE:CD2	2:D:243:PHE:C	2.86	0.49
2:D:361:GLU:HB3	2:D:399:ILE:HD13	1.95	0.49
1:C:1454:GLN:HG3	1:C:1461:ILE:HB	1.94	0.49
2:D:63:ARG:HB3	2:D:65:GLN:HG3	1.95	0.49
2:B:1529:LEU:HD11	2:B:1543:ASP:HB2	1.93	0.49
2:D:1502:HIS:ND1	2:D:1503:GLN:N	2.51	0.49
2:D:463:ASN:OD1	2:D:505:THR:OG1	2.31	0.49
2:B:469:ASN:CB	2:B:472:SER:HB2	2.42	0.49
2:D:847:ARG:HG3	2:D:869:GLN:CG	2.36	0.49
1:C:296:ILE:HG23	1:C:297:ALA:N	2.26	0.49
1:C:571:LEU:CD2	1:C:812:ALA:HB2	2.43	0.49
2:B:519:ARG:NH1	2:B:606:ASP:OD2	2.45	0.49
2:D:322:THR:CG2	2:D:327:ASP:H	2.25	0.49
1:A:191:PRO:O	1:A:194:PRO:HD3	2.13	0.49
1:A:571:LEU:HD12	1:A:593:ALA:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:933:ARG:NH1	2:B:933:ARG:HG3	2.18	0.49
2:B:825:VAL:HB	2:B:828:GLU:CD	2.32	0.49
1:C:1265:ASN:C	1:C:1267:VAL:H	2.15	0.49
2:D:1443:LEU:CD1	2:D:1443:LEU:N	2.76	0.49
1:A:1204:GLN:O	1:A:1208:ILE:HG13	2.13	0.49
2:D:1621:PHE:O	2:D:1622:GLN:C	2.50	0.49
1:A:174:VAL:HG22	1:A:175:GLU:H	1.77	0.49
1:C:1140:ASN:O	1:C:1143:TYR:HB3	2.13	0.49
1:C:1411:SER:H	1:C:1414:GLU:HG3	1.78	0.49
1:C:518:PHE:O	1:C:520:ASP:N	2.42	0.49
2:D:573:ALA:HB3	2:D:762:LEU:HD13	1.93	0.49
2:D:1602:THR:O	2:D:1604:ASN:N	2.41	0.49
1:C:862:VAL:O	1:C:863:GLU:C	2.51	0.49
1:C:682:LYS:NZ	1:C:686:ILE:CD1	2.75	0.49
2:D:189:PRO:C	2:D:191:LEU:N	2.66	0.49
1:C:272:ARG:HG3	1:C:279:GLN:O	2.13	0.49
1:C:945:ASP:OD1	1:C:945:ASP:C	2.48	0.49
1:C:1562:LYS:HD3	1:C:1648:TRP:NE1	2.27	0.49
2:B:1299:LEU:HB3	2:B:1301:ARG:HD3	1.94	0.49
2:D:462:VAL:HG21	2:D:520:PHE:CE2	2.48	0.49
2:B:531:ILE:O	2:B:617:ASN:ND2	2.39	0.49
1:A:849:ARG:HH11	1:A:849:ARG:CG	2.12	0.49
1:C:395:ILE:CG1	1:C:430:VAL:HB	2.43	0.49
1:A:757:LEU:O	1:A:758:LEU:HD23	2.12	0.49
3:Y:87:LEU:HD12	3:Y:210:GLU:HA	1.95	0.49
1:C:148:LEU:HA	1:C:154:PRO:O	2.12	0.49
2:D:58:VAL:HG12	2:D:104:VAL:CG2	2.41	0.49
1:C:165:ASP:C	1:C:167:GLU:N	2.66	0.49
2:D:1390:PHE:CD1	2:D:1442:ILE:HG13	2.47	0.49
1:C:1423:VAL:HG11	1:C:1496:TYR:CZ	2.48	0.49
1:C:1450:PHE:HB3	1:C:1463:GLN:O	2.12	0.49
2:D:548:LEU:HD23	2:D:803:ALA:HB2	1.94	0.49
1:A:1386:ILE:HG13	1:A:1387:GLU:N	2.27	0.49
2:B:144:LEU:N	2:B:144:LEU:HD23	2.28	0.49
2:B:946:LYS:N	2:B:946:LYS:HD3	2.27	0.49
2:D:1281:LEU:HB2	2:D:1283:ASP:HB2	1.95	0.49
1:A:1456:LYS:HG3	1:A:1457:ASP:OD2	2.13	0.49
3:X:50:TYR:HE2	3:X:170:ARG:HD2	1.72	0.49
3:Y:50:TYR:CE2	3:Y:170:ARG:CZ	2.95	0.49
1:A:515:ARG:NH1	1:A:526:ILE:HG22	2.27	0.49
1:C:115:LYS:HB2	1:C:654:LEU:CD2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1559:TYR:O	1:C:1621:GLY:N	2.46	0.49
1:C:1629:TYR:O	1:C:1630:ASN:HB2	2.13	0.49
1:A:1069:TRP:HH2	1:A:1465:ASN:ND2	2.10	0.49
1:C:1085:VAL:O	1:C:1089:VAL:HG23	2.13	0.49
2:D:481:TYR:CE1	2:D:506:MET:SD	2.93	0.49
1:C:1493:PHE:HD1	1:C:1494:THR:H	1.50	0.49
1:A:423:ASN:CG	2:B:504:VAL:HG22	2.33	0.49
1:A:189:LYS:HG3	1:A:190:ILE:O	2.13	0.49
1:A:1190:ILE:CG1	1:A:1253:TYR:CE1	2.94	0.49
1:A:123:ASN:C	1:A:211:THR:HG21	2.32	0.49
1:C:1255:LEU:C	1:C:1255:LEU:HD12	2.31	0.49
2:D:1280:GLU:HB2	2:D:1312:THR:HB	1.95	0.49
2:D:188:LEU:HD13	2:D:216:VAL:HG21	1.95	0.49
1:C:1128:LYS:HD3	1:C:1414:GLU:OE1	2.13	0.49
1:A:1566:THR:HG23	1:A:1578:LYS:O	2.13	0.49
2:B:1382:ILE:CD1	2:B:1458:VAL:HG22	2.43	0.49
2:B:1381:ILE:HB	2:B:1459:TYR:HD1	1.78	0.49
1:A:1475:VAL:CG2	1:A:1476:ARG:N	2.76	0.49
1:A:682:LYS:NZ	1:A:686:ILE:CD1	2.76	0.49
2:B:239:GLY:N	2:B:296:ARG:NH2	2.61	0.49
2:D:1567:ARG:NH1	2:D:1567:ARG:HG3	2.28	0.49
1:C:96:GLN:O	1:C:97:ASN:O	2.31	0.49
2:D:889:GLN:HA	2:D:915:VAL:HB	1.95	0.49
1:C:1318:LYS:HB2	1:C:1345:ASP:HB2	1.95	0.49
1:C:1559:TYR:CE1	1:C:1587:THR:HA	2.47	0.48
1:A:1022:PHE:CE2	1:A:1092:TYR:CD1	3.01	0.48
1:A:1278:GLN:NE2	1:A:1293:ALA:HB1	2.28	0.48
2:B:1610:TRP:CD2	2:B:1628:PHE:CD2	2.99	0.48
1:A:963:ILE:CG2	1:A:967:LEU:HD23	2.41	0.48
1:C:596:MET:SD	1:C:782:ARG:HG2	2.53	0.48
1:C:1234:HIS:O	1:C:1235:LYS:HB2	2.12	0.48
1:A:354:LEU:HB2	1:A:374:GLN:O	2.13	0.48
3:Y:61:SER:N	3:Y:75:PHE:CZ	2.81	0.48
3:Y:61:SER:N	3:Y:75:PHE:HZ	2.11	0.48
1:C:371:ILE:CG2	1:C:420:PHE:HB2	2.34	0.48
1:C:523:TYR:CZ	2:D:359:PRO:HD2	2.48	0.48
2:B:830:VAL:CG2	2:B:831:GLU:N	2.74	0.48
2:B:1344:HIS:ND1	5:B:2003:NAG:H82	2.27	0.48
1:A:1565:ILE:HB	1:A:1614:GLY:H	1.78	0.48
2:D:1601:ILE:HD12	2:D:1601:ILE:H	1.78	0.48
2:D:945:ILE:N	2:D:945:ILE:HD12	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ILE:HG12	1:A:106:VAL:HG13	1.94	0.48
1:A:24:VAL:HG11	1:A:543:TYR:CZ	2.48	0.48
1:A:477:LEU:HD23	1:A:480:GLU:OE1	2.14	0.48
1:C:496:ILE:HG22	1:C:496:ILE:O	2.12	0.48
1:C:1562:LYS:CD	1:C:1648:TRP:NE1	2.76	0.48
1:C:1622:LYS:HZ2	1:C:1642:LEU:HB3	1.78	0.48
2:B:1614:ASP:O	2:B:1616:CYS:N	2.46	0.48
1:A:1641:SER:O	1:A:1642:LEU:HB2	2.14	0.48
1:C:1377:PHE:CD2	1:C:1495:VAL:HG22	2.48	0.48
3:X:81:ASN:O	3:X:115:ARG:CB	2.53	0.48
1:A:1231:ASN:O	1:A:1233:GLN:N	2.46	0.48
3:Y:125:LYS:HA	3:Y:126:ASN:C	2.27	0.48
1:A:1017:PRO:O	1:A:1018:VAL:C	2.51	0.48
1:A:613:GLN:O	1:A:615:GLY:N	2.46	0.48
2:B:925:VAL:HG22	2:B:1326:LEU:CD2	2.39	0.48
1:C:124:GLY:C	1:C:125:PHE:CG	2.86	0.48
1:C:1271:ILE:CD1	1:C:1300:TYR:CZ	2.96	0.48
2:B:216:VAL:O	2:B:216:VAL:HG13	2.13	0.48
2:B:598:ILE:HD12	2:B:800:ILE:HG21	1.92	0.48
1:C:248:ILE:HB	1:C:299:VAL:HG13	1.93	0.48
1:A:689:LYS:CG	1:A:699:CYS:SG	3.01	0.48
1:C:136:THR:O	1:C:139:GLN:HG3	2.12	0.48
2:B:615:GLN:HB2	2:B:616:ASN:HD22	1.75	0.48
2:B:580:VAL:CG1	2:B:584:VAL:HG23	2.43	0.48
1:A:853:MET:O	1:A:888:VAL:HG12	2.13	0.48
3:X:103:VAL:HG22	3:X:122:VAL:HG13	1.94	0.48
1:A:163:PHE:CD2	1:A:188:PHE:CD1	3.00	0.48
1:A:560:TRP:CH2	1:A:673:LEU:CD2	2.96	0.48
2:D:853:ASN:C	2:D:853:ASN:OD1	2.52	0.48
1:A:272:ARG:HG3	1:A:279:GLN:O	2.13	0.48
1:A:734:VAL:HA	1:A:737:GLN:HG2	1.94	0.48
1:A:1376:SER:OG	1:A:1503:LYS:HG3	2.13	0.48
2:B:1533:GLU:OE1	2:B:1533:GLU:HA	2.12	0.48
3:X:187:GLY:C	3:X:203:LEU:HD12	2.33	0.48
1:C:43:VAL:HG12	1:C:79:PHE:O	2.13	0.48
1:C:514:THR:CG2	1:C:515:ARG:N	2.77	0.48
1:A:1240:PRO:C	1:A:1242:THR:N	2.67	0.48
1:C:1077:TRP:NE1	1:C:1147:PHE:CD1	2.79	0.48
1:A:1671:ILE:CD1	1:A:1676:CYS:SG	3.01	0.48
2:D:628:LEU:HB3	2:D:636:THR:HG23	1.96	0.48
2:D:850:LEU:HB2	2:D:882:PHE:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:TYR:HE2	1:C:224:LEU:HA	1.79	0.48
1:A:284:GLN:H	1:A:310:LEU:HD22	1.78	0.48
2:B:322:THR:HG21	2:B:327:ASP:H	1.79	0.48
1:C:443:PRO:CD	1:C:446:ASN:HB2	2.42	0.48
1:C:1142:LEU:HD21	1:C:1179:THR:OG1	2.14	0.48
1:C:695:VAL:HG12	1:C:727:ALA:CB	2.44	0.48
2:D:580:VAL:CG1	2:D:584:VAL:HG23	2.43	0.48
3:Y:85:PHE:CD1	3:Y:85:PHE:N	2.81	0.48
1:A:1000:LEU:O	1:A:1001:THR:HG23	2.13	0.48
1:A:997:ILE:O	1:A:997:ILE:HG13	2.13	0.48
1:C:977:LEU:HD23	1:C:1361:VAL:HG22	1.96	0.48
1:A:500:ASN:ND2	1:A:543:TYR:CE1	2.77	0.48
1:C:494:ASP:OD1	1:C:495:LYS:HE2	2.13	0.48
1:C:964:PRO:HG2	1:C:1365:VAL:HG11	1.95	0.48
1:C:1563:VAL:HA	1:C:1582:LEU:H	1.78	0.48
1:A:1431:GLY:HA2	1:A:1483:PHE:HE1	1.78	0.48
2:B:1611:PRO:CD	2:B:1624:LEU:HD23	2.44	0.48
2:D:210:TYR:CG	2:D:211:THR:N	2.81	0.48
1:A:576:SER:CB	1:A:589:SER:H	2.27	0.48
1:A:493:ILE:O	1:A:493:ILE:HG22	2.12	0.48
2:B:628:LEU:HB3	2:B:636:THR:HG23	1.95	0.48
1:C:1231:ASN:O	1:C:1233:GLN:N	2.47	0.48
1:C:481:HIS:ND1	1:C:529:PRO:HB3	2.27	0.48
1:A:1226:ARG:NE	1:A:1266:TYR:CE1	2.82	0.48
1:A:1286:SER:CB	1:A:1499:HIS:HA	2.44	0.48
1:C:950:TYR:HD1	1:C:1268:ASN:OD1	1.96	0.48
2:D:1285:GLU:O	2:D:1287:PRO:HD3	2.13	0.48
2:D:1525:LYS:HD2	2:D:1610:TRP:CH2	2.48	0.48
1:C:132:LYS:NZ	1:C:139:GLN:HE22	2.11	0.48
2:D:860:SER:OG	2:D:866:TYR:N	2.39	0.48
1:A:1320:LYS:HD2	1:A:1321:GLY:N	2.27	0.48
2:D:941:GLN:HE21	2:D:943:GLU:CG	2.26	0.48
1:C:322:TYR:N	1:C:322:TYR:HD2	2.10	0.48
1:A:1057:MET:HB3	1:A:1057:MET:HE2	1.77	0.48
1:A:825:LEU:HB2	1:A:845:VAL:HG23	1.96	0.48
1:C:236:ASN:HD22	1:C:379:LEU:HD21	1.78	0.48
2:D:853:ASN:HA	2:D:854:PRO:HD3	1.58	0.48
2:D:32:VAL:HB	2:D:607:PHE:CZ	2.48	0.48
3:X:50:TYR:CE2	3:X:170:ARG:CZ	2.96	0.48
1:A:465:LEU:HG	1:A:466:TYR:N	2.28	0.48
1:A:515:ARG:CZ	1:A:526:ILE:HG22	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:545:ILE:HG23	1:C:554:LEU:HD21	1.95	0.48
1:C:554:LEU:H	1:C:658:ASN:HD22	1.61	0.48
1:A:1563:VAL:HG12	1:A:1581:LEU:HA	1.96	0.48
1:A:430:VAL:HG11	1:A:453:ARG:NH2	2.14	0.48
1:C:883:CYS:O	1:C:884:VAL:C	2.51	0.48
1:A:690:TYR:C	1:A:692:HIS:N	2.67	0.48
1:C:1031:TRP:CE2	1:C:1042:LYS:HG3	2.47	0.48
1:C:1204:GLN:O	1:C:1208:ILE:HG13	2.13	0.48
1:A:1042:LYS:HZ1	1:C:92:LEU:HD13	1.77	0.48
1:A:174:VAL:CG2	1:A:175:GLU:N	2.74	0.48
2:B:548:LEU:HD23	2:B:803:ALA:HB2	1.96	0.48
1:A:1411:SER:H	1:A:1414:GLU:HG3	1.78	0.48
1:A:92:LEU:HD13	1:C:1026:GLU:OE2	2.13	0.48
2:D:1344:HIS:ND1	5:D:2003:NAG:C8	2.77	0.48
1:C:682:LYS:NZ	1:C:686:ILE:HD11	2.28	0.48
1:C:856:CYS:HB2	2:D:904:LEU:HD21	1.95	0.48
1:A:911:ASN:OD1	1:A:924:VAL:HG22	2.14	0.48
1:A:663:GLN:CG	1:A:664:GLU:N	2.76	0.48
1:A:1084:ARG:HA	1:A:1151:GLY:HA2	1.94	0.48
2:B:32:VAL:HB	2:B:607:PHE:CZ	2.48	0.48
1:A:25:ILE:CD1	1:A:41:ILE:HG13	2.43	0.48
1:A:541:LEU:HB2	1:A:557:ASP:O	2.13	0.48
1:C:367:ILE:HD13	1:C:466:TYR:CD2	2.48	0.48
1:C:971:THR:O	1:C:971:THR:OG1	2.23	0.48
2:B:1624:LEU:O	2:B:1625:CYS:C	2.52	0.48
1:C:119:ILE:C	1:C:119:ILE:HD12	2.34	0.48
2:D:870:PHE:HB2	2:D:871:PRO:CD	2.42	0.48
2:B:384:PHE:CD2	2:B:384:PHE:N	2.81	0.48
1:A:461:SER:CB	1:A:553:GLU:OE2	2.61	0.48
2:B:378:PRO:HB2	2:B:416:ASN:O	2.14	0.48
2:B:795:THR:CG2	2:B:796:PRO:HD2	2.36	0.48
1:A:981:GLY:HA3	1:A:1333:PHE:CD1	2.49	0.48
1:C:1255:LEU:HD13	1:C:1267:VAL:HG13	1.95	0.48
1:A:1142:LEU:HD13	1:A:1187:THR:HG21	1.95	0.48
1:C:539:ARG:NH2	1:C:634:CYS:N	2.60	0.48
3:X:41:HIS:ND1	3:X:41:HIS:N	2.62	0.48
1:C:1421:HIS:HD2	1:C:1422:ALA:N	2.11	0.48
1:A:859:MET:HB3	1:A:898:PHE:CE1	2.49	0.48
1:A:973:ILE:O	1:A:973:ILE:HG22	2.12	0.48
1:A:20:GLU:C	1:A:21:GLN:CG	2.77	0.48
1:C:23:TYR:CE2	1:C:111:PHE:CD2	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1622:LYS:NZ	1:C:1642:LEU:HB3	2.29	0.48
1:C:1068:VAL:CG1	1:C:1069:TRP:H	2.18	0.48
2:B:224:PHE:CE1	2:B:320:VAL:CG1	2.96	0.48
1:C:871:PRO:CD	1:C:872:VAL:N	2.75	0.48
1:C:1066:TYR:N	1:C:1079:THR:HG23	2.21	0.48
2:D:27:LEU:O	2:D:628:LEU:HD12	2.14	0.48
2:D:524:TYR:CE1	2:D:532:VAL:HG12	2.49	0.48
1:C:243:PHE:CE2	1:C:304:GLU:CA	2.96	0.48
3:X:77:PRO:O	3:X:78:LYS:CB	2.61	0.48
2:D:61:PHE:CD1	2:D:62:PRO:HA	2.48	0.48
1:C:361:LEU:HD21	1:C:452:TYR:HB3	1.94	0.48
1:C:627:LEU:HA	1:C:627:LEU:HD23	1.69	0.48
1:A:1161:LEU:CD1	1:C:1105:LEU:HD13	2.41	0.48
2:D:216:VAL:HG13	2:D:216:VAL:O	2.13	0.48
1:C:161:LEU:HD21	1:C:185:PHE:CD2	2.49	0.48
2:B:570:ASP:O	2:B:573:ALA:HB2	2.14	0.48
2:D:1631:PHE:HD2	2:D:1632:SER:N	2.11	0.48
2:D:345:ILE:HG13	2:D:428:LYS:HB3	1.96	0.48
2:D:229:GLN:HA	2:D:229:GLN:OE1	2.14	0.48
1:C:1560:ALA:O	1:C:1561:TYR:CD2	2.66	0.48
1:C:1583:ASP:N	1:C:1594:LYS:HZ1	2.11	0.48
1:C:532:GLN:O	1:C:535:VAL:HG13	2.14	0.48
1:A:1090:ASN:ND2	1:A:1158:ILE:HG12	2.29	0.48
2:B:441:SER:HB2	2:B:443:ASN:ND2	2.29	0.48
1:C:30:ILE:HG22	1:C:31:PHE:N	2.28	0.48
1:C:1066:TYR:H	1:C:1079:THR:CG2	2.23	0.48
1:A:30:ILE:HG22	1:A:31:PHE:N	2.29	0.48
1:A:59:TYR:CD2	1:A:60:PRO:HD3	2.49	0.48
1:A:964:PRO:HG2	1:A:1365:VAL:HG11	1.95	0.48
1:A:494:ASP:OD2	1:A:495:LYS:HE2	2.14	0.48
2:B:462:VAL:HG21	2:B:520:PHE:CE2	2.48	0.48
1:A:1234:HIS:CG	1:A:1235:LYS:H	2.31	0.48
1:C:1573:VAL:HG12	1:C:1603:LYS:HD3	1.94	0.48
2:D:1442:ILE:C	2:D:1443:LEU:HD13	2.34	0.48
1:C:354:LEU:HB2	1:C:374:GLN:O	2.14	0.48
2:B:130:ILE:HD13	2:B:199:ILE:CG2	2.44	0.48
2:B:866:TYR:HE2	2:B:868:GLN:OE1	1.96	0.48
2:D:59:HIS:HB3	2:D:64:LYS:HA	1.96	0.48
2:B:575:VAL:HG23	2:B:762:LEU:CD1	2.44	0.48
2:B:25:TYR:CE2	2:B:113:VAL:HG22	2.48	0.48
2:B:853:ASN:C	2:B:853:ASN:OD1	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:LEU:HD11	1:A:486:VAL:HG13	1.95	0.48
1:C:500:ASN:O	1:C:542:VAL:HA	2.14	0.48
2:D:285:ILE:HD12	2:D:285:ILE:H	1.71	0.48
2:B:224:PHE:HE1	2:B:320:VAL:HG11	1.79	0.48
2:B:1504:GLU:CD	2:B:1505:ARG:H	2.15	0.48
2:B:1610:TRP:HA	2:B:1628:PHE:CE2	2.49	0.48
2:B:235:PHE:HB3	2:B:338:ILE:HG23	1.96	0.48
3:Y:88:GLY:C	3:Y:90:ASP:N	2.66	0.48
1:C:153:LYS:HG2	1:C:806:ASN:O	2.13	0.48
2:D:1345:LEU:HD21	2:D:1456:VAL:HG12	1.96	0.48
2:D:1628:PHE:O	2:D:1629:ALA:C	2.51	0.48
2:B:603:GLU:C	2:B:605:SER:H	2.16	0.48
2:B:1534:GLN:HA	2:B:1534:GLN:OE1	2.13	0.48
1:A:548:GLY:HA3	1:A:550:GLN:OE1	2.14	0.48
1:C:999:ILE:HD12	1:C:1001:THR:O	2.14	0.48
2:D:1535:ASP:C	2:D:1537:ASN:H	2.17	0.48
1:C:543:TYR:CD1	1:C:543:TYR:C	2.86	0.48
1:C:504:LEU:HD23	1:C:649:ALA:O	2.14	0.48
1:A:1022:PHE:O	1:A:1024:TYR:N	2.47	0.48
1:A:1244:THR:HG22	1:A:1246:ARG:H	1.75	0.48
2:D:760:LYS:HE3	2:D:776:MET:SD	2.54	0.48
1:A:1534:GLN:HG3	1:A:1534:GLN:O	2.14	0.48
1:A:1559:TYR:CE2	1:A:1590:ALA:O	2.67	0.48
2:D:618:LEU:HD22	2:D:636:THR:HA	1.95	0.48
1:A:965:LEU:C	1:A:967:LEU:H	2.17	0.48
1:C:576:SER:HB2	1:C:589:SER:H	1.79	0.48
1:C:198:MET:SD	1:C:218:GLU:HG3	2.54	0.48
1:A:243:PHE:CE2	1:A:304:GLU:HA	2.48	0.48
1:A:436:LYS:HB2	1:A:449:ARG:CG	2.43	0.48
1:C:371:ILE:CD1	1:C:433:PHE:CE2	2.93	0.48
1:A:1323:LEU:CG	1:A:1324:HIS:H	2.27	0.48
2:D:56:ILE:O	2:D:70:GLN:HA	2.14	0.48
3:Y:132:THR:CG2	3:Y:155:ILE:HB	2.41	0.48
2:B:478:TYR:CD1	2:B:478:TYR:O	2.58	0.48
1:A:1140:ASN:O	1:A:1143:TYR:HB3	2.14	0.48
2:D:1381:ILE:CG2	2:D:1459:TYR:HE1	2.25	0.48
1:C:525:SER:CB	2:D:399:ILE:HG21	2.44	0.48
2:B:541:LYS:O	2:B:543:THR:CG2	2.62	0.48
1:C:680:GLN:O	1:C:684:GLU:CG	2.62	0.48
1:A:274:ASP:HA	1:A:322:TYR:CE2	2.49	0.48
5:D:2001:NAG:H3	5:D:2002:NAG:O5	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:VAL:O	1:C:399:GLN:NE2	2.46	0.48
1:C:733:VAL:O	1:C:737:GLN:HG2	2.14	0.48
1:C:859:MET:HB3	1:C:898:PHE:CE1	2.49	0.48
1:C:1376:SER:OG	1:C:1503:LYS:HG3	2.14	0.48
2:B:370:ASP:N	2:B:370:ASP:OD1	2.46	0.48
1:A:43:VAL:HG12	1:A:79:PHE:O	2.13	0.47
1:C:1612:VAL:HG23	1:C:1617:TYR:OH	2.14	0.47
1:C:534:MET:CB	1:C:538:SER:OG	2.62	0.47
1:C:1247:MET:O	1:C:1251:THR:HG23	2.14	0.47
1:A:986:GLU:HG2	1:A:987:ILE:N	2.29	0.47
1:C:1076:THR:HG22	1:C:1120:GLU:HA	1.94	0.47
1:A:1583:ASP:N	1:A:1594:LYS:HZ1	2.12	0.47
2:D:482:LEU:CD1	2:D:521:VAL:HB	2.44	0.47
1:A:883:CYS:N	2:B:902:GLU:OE2	2.46	0.47
1:A:1379:LEU:HD21	1:A:1495:VAL:HG13	1.95	0.47
2:B:69:PHE:CE1	2:B:87:ILE:HA	2.49	0.47
1:A:614:ARG:CD	1:A:614:ARG:N	2.76	0.47
2:D:69:PHE:HD2	2:D:70:GLN:N	2.12	0.47
2:D:165:PHE:CZ	2:D:199:ILE:CD1	2.96	0.47
1:A:1108:VAL:HG21	1:A:1167:ALA:CB	2.40	0.47
1:C:1186:PHE:HA	1:C:1250:THR:CG2	2.41	0.47
1:A:1113:LEU:HD22	1:A:1114:ASP:H	1.77	0.47
1:C:682:LYS:HZ3	1:C:686:ILE:HD11	1.79	0.47
2:D:52:LYS:HE3	2:D:111:PRO:O	2.13	0.47
1:C:977:LEU:HD22	1:C:978:SER:H	1.78	0.47
2:B:1393:ASP:OD1	2:B:1395:GLU:HB3	2.14	0.47
2:B:63:ARG:HB3	2:B:65:GLN:HG3	1.95	0.47
1:A:38:ASN:ND2	3:X:150:ILE:HG12	2.28	0.47
1:C:1534:GLN:HG3	1:C:1534:GLN:O	2.13	0.47
1:C:1598:ILE:HG22	1:C:1599:THR:N	2.29	0.47
1:A:1053:MET:HE1	1:A:1086:LEU:HD13	1.95	0.47
1:C:944:LEU:HD23	1:C:944:LEU:H	1.78	0.47
1:C:871:PRO:HD2	1:C:872:VAL:N	2.29	0.47
2:B:1506:ILE:HB	2:B:1627:ASP:HB3	1.97	0.47
1:A:837:GLU:OE2	1:A:1430:THR:HB	2.14	0.47
2:B:220:VAL:O	2:B:222:PRO:N	2.47	0.47
2:B:56:ILE:O	2:B:70:GLN:HA	2.14	0.47
2:D:237:ILE:HD11	2:D:309:LEU:CB	2.36	0.47
2:B:322:THR:CG2	2:B:327:ASP:H	2.27	0.47
1:A:123:ASN:C	1:A:123:ASN:OD1	2.53	0.47
1:C:285:THR:O	1:C:285:THR:CG2	2.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:575:VAL:O	2:D:759:THR:HA	2.14	0.47
2:B:1371:TYR:CD1	2:B:1377:SER:CB	2.98	0.47
1:A:682:LYS:NZ	1:A:686:ILE:HD11	2.29	0.47
2:B:544:CYS:HB3	2:B:546:GLY:O	2.13	0.47
2:B:862:LYS:HZ2	2:B:1519:ASN:CB	2.27	0.47
1:C:394:THR:HG23	1:C:402:SER:O	2.14	0.47
1:A:42:GLN:HE22	1:A:44:TYR:HB2	1.78	0.47
1:C:489:LYS:HG2	1:C:490:SER:OG	2.14	0.47
1:C:1583:ASP:N	1:C:1594:LYS:NZ	2.63	0.47
1:C:216:TYR:CD2	1:C:216:TYR:N	2.82	0.47
2:B:955:PRO:O	2:B:957:THR:HG23	2.14	0.47
1:A:1562:LYS:HD3	1:A:1648:TRP:HE1	1.80	0.47
1:A:1562:LYS:O	1:A:1563:VAL:CG1	2.62	0.47
1:C:1506:THR:HG22	1:C:1507:MET:N	2.29	0.47
1:A:569:ASN:CG	1:A:570:GLN:N	2.68	0.47
3:Y:88:GLY:C	3:Y:90:ASP:H	2.15	0.47
1:C:1003:LEU:HA	1:C:1004:PRO:HD2	1.51	0.47
2:D:148:PHE:CZ	2:D:792:VAL:HG11	2.48	0.47
2:B:1279:ILE:HG22	2:B:1288:ILE:CB	2.43	0.47
3:X:42:ASP:HB3	3:X:45:ASP:HB2	1.95	0.47
2:D:1370:ARG:NH1	2:D:1372:LEU:HG	2.29	0.47
2:D:25:TYR:CE2	2:D:113:VAL:HG22	2.49	0.47
2:B:41:ILE:O	2:B:85:PRO:HD2	2.14	0.47
2:D:386:SER:O	2:D:398:LEU:HD11	2.14	0.47
1:C:641:ASN:O	1:C:642:ASN:C	2.53	0.47
1:C:1069:TRP:HH2	1:C:1465:ASN:ND2	2.12	0.47
2:D:1330:ASN:ND2	2:D:1330:ASN:N	2.62	0.47
1:C:1637:TYR:N	1:C:1637:TYR:CD2	2.83	0.47
2:B:1506:ILE:CD1	2:B:1628:PHE:HE1	2.27	0.47
1:A:1559:TYR:O	1:A:1621:GLY:N	2.47	0.47
1:C:592:MET:O	1:C:783:ARG:HA	2.15	0.47
2:D:531:ILE:O	2:D:617:ASN:ND2	2.41	0.47
1:A:87:ILE:CD1	1:A:87:ILE:N	2.55	0.47
1:C:316:GLU:HG2	1:C:349:LEU:CD2	2.43	0.47
1:A:1018:VAL:HG11	1:A:1048:LYS:HB3	1.95	0.47
2:D:161:VAL:CG2	2:D:180:LEU:HD21	2.38	0.47
2:D:1638:PHE:N	2:D:1638:PHE:CD2	2.82	0.47
2:B:1482:ASN:H	2:B:1495:GLU:HG2	1.79	0.47
2:B:575:VAL:CG2	2:B:762:LEU:HD11	2.44	0.47
2:B:1567:ARG:HD2	2:B:1567:ARG:HA	1.63	0.47
3:X:103:VAL:HA	3:X:121:GLY:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1386:MET:HE2	2:B:1386:MET:HA	1.96	0.47
1:C:560:TRP:CH2	1:C:673:LEU:CD2	2.98	0.47
1:C:1663:ASN:O	1:C:1666:GLU:HB3	2.14	0.47
1:A:72:HIS:CD2	1:A:72:HIS:C	2.87	0.47
2:D:1399:ARG:HG2	2:D:1399:ARG:HH11	1.79	0.47
1:C:968:VAL:HG23	1:C:971:THR:OG1	2.14	0.47
2:B:1614:ASP:C	2:B:1616:CYS:N	2.67	0.47
2:D:778:PHE:N	2:D:778:PHE:CD2	2.83	0.47
2:B:120:LEU:HA	2:B:120:LEU:HD13	1.76	0.47
1:A:617:LYS:HD2	1:A:622:ARG:NH2	2.22	0.47
1:A:1271:ILE:HD13	1:A:1300:TYR:CZ	2.50	0.47
1:C:284:GLN:H	1:C:310:LEU:HD22	1.79	0.47
1:C:1572:ASN:O	1:C:1573:VAL:HG23	2.14	0.47
2:B:148:PHE:CZ	2:B:792:VAL:HG11	2.50	0.47
2:B:1575:LEU:HD13	2:B:1581:TYR:CZ	2.49	0.47
2:B:1575:LEU:N	2:B:1575:LEU:CD2	2.77	0.47
2:D:1482:ASN:HB2	2:D:1495:GLU:HA	1.96	0.47
1:A:695:VAL:HG12	1:A:727:ALA:CB	2.44	0.47
2:B:1446:PHE:C	2:B:1448:VAL:H	2.18	0.47
2:B:173:VAL:HA	2:B:964:ILE:CD1	2.44	0.47
2:D:843:ASP:HA	2:D:873:LYS:O	2.14	0.47
2:D:96:THR:HG22	2:D:97:ASP:N	2.30	0.47
1:A:510:ILE:O	1:A:511:HIS:ND1	2.48	0.47
1:A:20:GLU:HB2	1:A:551:THR:CB	2.44	0.47
1:C:963:ILE:HA	1:C:973:ILE:HD11	1.97	0.47
1:C:840:GLN:HE21	1:C:897:THR:HG21	1.80	0.47
2:D:870:PHE:CD1	2:D:878:ARG:NH2	2.83	0.47
1:C:1079:THR:HB	1:C:1107:LEU:HD11	1.96	0.47
1:A:419:SER:CB	2:B:459:ASN:HD22	2.15	0.47
1:A:243:PHE:HE2	1:A:304:GLU:CA	2.28	0.47
2:D:484:LEU:HD11	2:D:626:LEU:CG	2.45	0.47
2:D:794:PHE:C	2:D:794:PHE:CD2	2.88	0.47
1:A:1328:MET:HE2	1:A:1328:MET:HA	1.97	0.47
1:C:224:LEU:CD2	1:C:225:PRO:HD2	2.43	0.47
1:C:614:ARG:N	1:C:614:ARG:CD	2.76	0.47
2:D:1438:LEU:C	2:D:1438:LEU:HD13	2.34	0.47
1:A:443:PRO:CD	1:A:446:ASN:HB2	2.44	0.47
1:A:892:SER:HB3	1:A:893:SER:H	1.41	0.47
3:Y:136:LEU:HA	3:Y:224:ILE:O	2.14	0.47
2:D:1523:VAL:O	2:D:1548:ILE:HB	2.14	0.47
2:D:543:THR:O	2:D:599:TRP:NE1	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:433:ILE:HG22	2:D:434:ALA:N	2.28	0.47
1:C:1427:SER:CB	1:C:1492:THR:HG23	2.44	0.47
1:C:680:GLN:O	1:C:682:LYS:N	2.48	0.47
3:X:119:VAL:HG13	3:X:212:MET:SD	2.55	0.47
1:C:1468:PRO:CD	1:C:1473:LEU:HD13	2.44	0.47
2:D:280:LEU:HD11	2:D:1379:MET:HG3	1.97	0.47
2:B:35:THR:HB	2:B:91:ALA:HB2	1.97	0.47
2:D:1517:GLU:O	2:D:1518:THR:C	2.53	0.47
1:A:231:ILE:HG23	1:A:231:ILE:O	2.14	0.47
3:X:166:ASP:OD2	3:X:207:LEU:CG	2.62	0.47
1:C:383:VAL:O	1:C:383:VAL:CG2	2.62	0.47
1:A:20:GLU:CB	1:A:551:THR:HG22	2.44	0.47
1:A:506:LYS:HD2	1:A:536:PRO:HG2	1.96	0.47
1:A:656:ASN:OD1	1:A:658:ASN:CB	2.51	0.47
1:C:42:GLN:HE22	1:C:44:TYR:HB2	1.80	0.47
1:C:1552:ALA:HB2	1:C:1620:MET:CE	2.45	0.47
1:A:1293:ALA:O	1:A:1294:ILE:C	2.51	0.47
1:C:923:LEU:C	1:C:923:LEU:HD23	2.34	0.47
1:C:1504:GLN:OE1	1:C:1506:THR:OG1	2.28	0.47
2:D:206:SER:O	2:D:208:GLU:N	2.47	0.47
2:D:173:VAL:HG11	2:D:186:TYR:OH	2.13	0.47
1:A:59:TYR:CD1	1:A:60:PRO:HG3	2.49	0.47
1:C:576:SER:CB	1:C:577:PRO:CD	2.91	0.47
2:B:563:MET:HB3	2:B:778:PHE:HE2	1.78	0.47
1:C:595:GLY:O	1:C:596:MET:C	2.52	0.47
1:C:670:LYS:HD2	1:C:671:GLU:N	2.29	0.47
2:B:34:ARG:HD2	2:B:488:LYS:HZ3	1.79	0.47
1:C:1215:GLU:OE1	1:C:1235:LYS:HD3	2.15	0.47
2:B:794:PHE:C	2:B:794:PHE:CD2	2.88	0.47
1:A:1307:LEU:H	1:A:1307:LEU:HD22	1.79	0.47
1:A:1309:LEU:CD1	1:A:1328:MET:HG3	2.44	0.47
2:D:168:PRO:HD3	2:D:197:TRP:CD1	2.49	0.47
1:C:1268:ASN:HB2	1:C:1269:PRO:HD3	1.97	0.47
1:C:1309:LEU:O	1:C:1329:THR:HA	2.15	0.47
2:D:1623:LYS:NZ	2:D:1623:LYS:CB	2.78	0.47
2:B:846:VAL:HG22	2:B:847:ARG:N	2.28	0.47
2:D:1387:LEU:O	2:D:1390:PHE:HB2	2.14	0.47
2:B:511:THR:O	2:B:513:ASP:N	2.48	0.47
1:C:240:TYR:CD2	1:C:241:LYS:N	2.82	0.47
1:A:1159:CYS:O	1:A:1161:LEU:HD23	2.14	0.47
2:D:143:VAL:O	2:D:143:VAL:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1249:GLU:O	1:C:1253:TYR:HD2	1.98	0.47
2:D:478:TYR:CD1	2:D:478:TYR:O	2.58	0.47
1:C:1179:THR:HG22	1:C:1180:LEU:HD23	1.97	0.47
1:A:1031:TRP:CZ3	1:A:1042:LYS:HA	2.50	0.47
2:D:1506:ILE:HD12	2:D:1628:PHE:CE1	2.49	0.47
1:A:518:PHE:O	1:A:520:ASP:N	2.43	0.47
1:A:1186:PHE:HA	1:A:1250:THR:CG2	2.43	0.47
2:D:108:VAL:O	2:D:114:ARG:HA	2.15	0.47
2:B:108:VAL:O	2:B:114:ARG:HA	2.14	0.47
2:D:314:LEU:HD12	2:D:314:LEU:HA	1.71	0.47
1:A:1279:ARG:NH1	1:A:1280:TYR:CD2	2.83	0.47
2:B:280:LEU:HD22	2:B:1462:TYR:HE2	1.78	0.47
2:B:642:ALA:O	2:B:643:LYS:HB3	2.15	0.47
2:B:83:VAL:C	2:B:85:PRO:HD3	2.35	0.47
2:B:189:PRO:C	2:B:191:LEU:H	2.17	0.47
2:D:249:ALA:O	2:D:257:VAL:HB	2.15	0.47
1:A:394:THR:HG23	1:A:402:SER:O	2.14	0.47
2:D:566:LYS:O	2:D:567:LEU:HD23	2.15	0.47
1:C:532:GLN:O	1:C:534:MET:N	2.47	0.47
3:Y:150:ILE:HD12	3:Y:150:ILE:C	2.34	0.47
1:C:1240:PRO:HB2	1:C:1242:THR:CG2	2.45	0.47
1:C:1076:THR:HG23	1:C:1077:TRP:N	2.29	0.47
1:A:1585:TYR:CZ	1:A:1586:LYS:HB3	2.49	0.47
2:D:813:VAL:CG1	2:D:840:VAL:HG22	2.43	0.47
2:D:482:LEU:HD11	2:D:521:VAL:HB	1.97	0.47
2:D:173:VAL:HG13	2:D:964:ILE:HD11	1.95	0.47
1:A:576:SER:CB	1:A:577:PRO:CD	2.91	0.47
2:B:482:LEU:HD11	2:B:521:VAL:HB	1.96	0.47
1:C:473:HIS:CE1	2:D:455:LYS:NZ	2.83	0.47
1:A:1047:LYS:O	1:A:1048:LYS:C	2.53	0.47
1:A:802:VAL:HG12	1:A:803:GLY:N	2.29	0.47
1:C:993:SER:O	1:C:995:GLU:N	2.48	0.47
2:B:230:PRO:HG3	2:B:333:GLN:CG	2.44	0.47
1:C:1402:ILE:HG13	1:C:1479:ILE:HD13	1.95	0.47
1:A:680:GLN:O	1:A:684:GLU:CG	2.62	0.47
2:B:79:GLY:O	2:B:81:MET:N	2.47	0.47
2:B:1567:ARG:NH1	2:B:1567:ARG:HG3	2.29	0.47
3:Y:85:PHE:N	3:Y:85:PHE:HD1	2.13	0.47
1:A:25:ILE:HG12	1:A:655:THR:CG2	2.45	0.47
1:A:530:VAL:CG2	1:A:563:ILE:HD12	2.45	0.47
1:C:25:ILE:HG13	1:C:106:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1593:THR:HG21	2:D:1596:LYS:HE3	1.97	0.47
1:C:263:ALA:O	1:C:291:MET:HE3	2.14	0.47
3:Y:194:LYS:HZ2	3:Y:197:ASN:HD22	1.63	0.47
1:C:1215:GLU:HA	1:C:1215:GLU:OE1	2.15	0.47
3:Y:128:LYS:HD3	3:Y:158:GLU:CD	2.35	0.47
1:C:407:SER:O	1:C:420:PHE:HE1	1.98	0.47
1:C:148:LEU:HG	1:C:153:LYS:O	2.14	0.47
1:A:239:GLY:O	1:A:240:TYR:C	2.52	0.47
1:A:975:ARG:NH1	1:A:1340:VAL:HG11	2.30	0.47
1:A:161:LEU:HD11	1:A:185:PHE:CE2	2.49	0.47
2:B:466:VAL:HG12	2:B:524:TYR:HE2	1.79	0.47
2:B:341:SER:HA	2:B:342:PRO:HD3	1.72	0.47
2:B:463:ASN:OD1	2:B:505:THR:OG1	2.33	0.47
1:C:997:ILE:HG13	1:C:997:ILE:O	2.15	0.47
2:B:1517:GLU:O	2:B:1518:THR:C	2.53	0.47
1:A:1084:ARG:CA	1:A:1151:GLY:HA2	2.45	0.47
3:Y:229:ASN:OD1	3:Y:229:ASN:N	2.46	0.47
1:A:111:PHE:CE2	1:A:113:LYS:CB	2.96	0.47
1:A:543:TYR:HB3	1:A:556:SER:HB3	1.97	0.47
1:C:510:ILE:O	1:C:511:HIS:ND1	2.48	0.47
2:D:1561:HIS:NE2	2:D:1597:ILE:CD1	2.78	0.47
2:B:829:GLN:HE22	2:B:883:VAL:CG1	2.19	0.47
1:A:1133:LEU:HB2	1:A:1134:PRO:HD3	1.97	0.47
1:A:1637:TYR:N	1:A:1637:TYR:CD2	2.83	0.47
2:B:787:TRP:HB2	2:B:808:ILE:HG22	1.97	0.47
3:X:86:LEU:HG	3:X:91:LYS:CG	2.45	0.47
2:D:1367:ILE:HB	2:D:1438:LEU:CD1	2.45	0.47
1:A:186:PRO:O	1:A:187:ASP:C	2.53	0.47
1:C:525:SER:HB2	2:D:399:ILE:HG21	1.96	0.47
3:Y:46:LEU:HD12	3:Y:180:TYR:CE1	2.50	0.47
2:D:1522:TYR:CD2	2:D:1522:TYR:O	2.68	0.47
3:X:52:SER:OG	3:X:53:GLU:N	2.48	0.47
2:B:433:ILE:CG2	2:B:434:ALA:N	2.78	0.47
3:X:85:PHE:CE1	3:X:117:SER:HB3	2.50	0.47
1:C:323:LEU:HD22	1:C:324:TYR:N	2.30	0.47
3:X:166:ASP:O	3:X:170:ARG:HG3	2.15	0.46
1:A:24:VAL:HG11	1:A:543:TYR:HE2	1.79	0.46
1:A:497:THR:OG1	1:A:498:HIS:N	2.48	0.46
1:A:515:ARG:HG3	1:A:526:ILE:CG2	2.45	0.46
1:C:23:TYR:HA	1:C:43:VAL:HA	1.96	0.46
1:C:461:SER:HB2	1:C:553:GLU:CD	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:263:VAL:HG21	2:D:292:ALA:CB	2.45	0.46
1:A:1583:ASP:N	1:A:1594:LYS:NZ	2.64	0.46
2:B:338:ILE:O	2:B:339:VAL:CG1	2.64	0.46
2:B:563:MET:CE	2:B:563:MET:HA	2.45	0.46
1:C:481:HIS:HB2	2:D:388:GLY:HA2	1.96	0.46
2:D:750:ASP:OD1	2:D:750:ASP:C	2.53	0.46
2:B:1486:ILE:HD11	2:B:1591:LEU:CD2	2.45	0.46
2:D:1457:LYS:HG2	2:D:1469:THR:OG1	2.15	0.46
1:C:219:VAL:CG1	1:C:219:VAL:O	2.63	0.46
1:C:1083:LEU:HD22	1:C:1104:LEU:HD21	1.96	0.46
1:C:239:GLY:O	1:C:240:TYR:C	2.53	0.46
1:C:689:LYS:CG	1:C:699:CYS:SG	3.03	0.46
2:D:1371:TYR:HB2	2:D:1377:SER:HB3	1.97	0.46
2:B:236:TYR:C	2:B:238:ASP:H	2.18	0.46
2:D:866:TYR:HE2	2:D:868:GLN:OE1	1.99	0.46
2:B:1602:THR:O	2:B:1604:ASN:N	2.43	0.46
2:B:342:PRO:HG2	2:B:420:LEU:CD1	2.44	0.46
1:C:1453:TYR:O	1:C:1453:TYR:CD1	2.67	0.46
1:C:302:ASP:HB3	1:C:305:THR:HB	1.97	0.46
2:D:319:THR:HG23	2:D:330:VAL:CG1	2.45	0.46
2:D:447:VAL:HG13	2:D:447:VAL:O	2.15	0.46
1:C:23:TYR:HE2	1:C:111:PHE:HD2	1.62	0.46
1:C:656:ASN:CB	1:C:659:ALA:H	2.27	0.46
1:C:1616:GLN:OE1	1:C:1650:ARG:HD3	2.15	0.46
1:C:963:ILE:CG2	1:C:967:LEU:HD23	2.42	0.46
2:D:481:TYR:CE2	2:D:493:GLY:N	2.83	0.46
2:D:1299:LEU:HB3	2:D:1301:ARG:HD3	1.96	0.46
1:A:1506:THR:HG22	1:A:1507:MET:N	2.31	0.46
2:B:613:SER:HA	2:B:620:VAL:HG23	1.96	0.46
1:C:1232:LEU:CG	1:C:1233:GLN:HG3	2.38	0.46
1:A:287:MET:SD	1:A:299:VAL:HG23	2.55	0.46
2:D:39:GLU:O	2:D:87:ILE:HD12	2.15	0.46
2:B:143:VAL:O	2:B:143:VAL:HG12	2.15	0.46
1:C:189:LYS:HG3	1:C:190:ILE:O	2.15	0.46
2:B:961:THR:HG22	2:B:1327:THR:CB	2.45	0.46
1:A:1031:TRP:CH2	1:A:1042:LYS:HG3	2.51	0.46
1:C:906:GLY:N	1:C:929:VAL:HB	2.24	0.46
1:A:152:LEU:HD13	1:A:152:LEU:HA	1.49	0.46
1:A:975:ARG:NH2	1:A:1346:LEU:HD22	2.30	0.46
2:B:541:LYS:O	2:B:543:THR:HG23	2.15	0.46
2:B:45:ALA:HB3	2:B:81:MET:CE	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1453:TYR:CD1	1:A:1453:TYR:O	2.69	0.46
2:B:52:LYS:HE3	2:B:111:PRO:O	2.14	0.46
2:B:929:LYS:HD3	2:B:929:LYS:HA	1.74	0.46
1:C:1080:ALA:CB	1:C:1148:THR:HG22	2.44	0.46
2:D:452:THR:O	2:D:453:GLU:O	2.34	0.46
1:A:20:GLU:OE2	1:A:20:GLU:O	2.33	0.46
1:A:74:SER:C	1:A:79:PHE:CE1	2.89	0.46
1:C:500:ASN:CB	1:C:543:TYR:CE1	2.64	0.46
1:C:554:LEU:N	1:C:658:ASN:HD22	2.13	0.46
1:C:1622:LYS:HD2	1:C:1642:LEU:CB	2.44	0.46
1:A:1068:VAL:CG1	1:A:1069:TRP:N	2.78	0.46
2:B:953:ARG:CG	2:B:954:VAL:N	2.78	0.46
2:B:1504:GLU:O	2:B:1624:LEU:HD13	2.14	0.46
2:D:449:ILE:HD13	2:D:462:VAL:HG23	1.97	0.46
2:B:44:GLU:OE1	2:B:480:THR:HG21	2.15	0.46
3:X:61:SER:O	3:X:75:PHE:HZ	1.97	0.46
3:Y:58:SER:HB3	3:Y:102:ASN:HD21	1.77	0.46
1:A:1304:VAL:HG12	1:A:1305:LYS:H	1.80	0.46
1:A:127:PHE:CE1	1:A:626:PHE:CD2	3.04	0.46
1:C:949:ILE:O	1:C:949:ILE:HG22	2.14	0.46
1:C:365:PRO:HG2	1:C:464:TYR:HE2	1.79	0.46
1:A:773:TRP:CE3	1:A:774:LEU:HB2	2.51	0.46
2:D:575:VAL:CG2	2:D:762:LEU:HD11	2.46	0.46
2:D:1589:ASP:HB3	2:D:1600:ILE:HG13	1.97	0.46
2:B:1535:ASP:C	2:B:1537:ASN:H	2.18	0.46
1:A:923:LEU:HD23	1:A:923:LEU:C	2.35	0.46
2:D:810:VAL:CG1	2:D:811:MET:N	2.79	0.46
2:D:1294:TYR:O	2:D:1294:TYR:CD2	2.67	0.46
1:A:500:ASN:O	1:A:542:VAL:HG13	2.16	0.46
1:C:489:LYS:NZ	2:D:502:ASN:H	2.13	0.46
2:D:920:VAL:O	2:D:1330:ASN:HA	2.15	0.46
2:D:787:TRP:HB2	2:D:808:ILE:HG22	1.96	0.46
1:C:829:ILE:HA	1:C:830:PRO:HD3	1.78	0.46
2:B:850:LEU:HB2	2:B:882:PHE:CD1	2.50	0.46
2:D:466:VAL:HG12	2:D:524:TYR:HE2	1.80	0.46
2:D:929:LYS:HD3	2:D:929:LYS:HA	1.70	0.46
2:B:778:PHE:CD2	2:B:778:PHE:N	2.82	0.46
2:B:69:PHE:C	2:B:69:PHE:HD2	2.19	0.46
2:D:296:ARG:HG3	2:D:296:ARG:NH1	2.29	0.46
3:Y:77:PRO:O	3:Y:78:LYS:CB	2.63	0.46
2:B:137:TYR:HB2	2:B:216:VAL:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:GLU:HG3	1:C:547:THR:CB	2.45	0.46
2:B:129:PHE:CE2	2:B:598:ILE:HG23	2.50	0.46
1:C:241:LYS:NZ	1:C:351:PRO:HB3	2.30	0.46
2:B:1367:ILE:HD13	2:B:1456:VAL:HG21	1.96	0.46
1:C:174:VAL:HG22	1:C:175:GLU:H	1.80	0.46
1:A:993:SER:O	1:A:995:GLU:N	2.49	0.46
2:B:130:ILE:HG21	2:B:199:ILE:HG21	1.98	0.46
1:C:428:VAL:HG22	1:C:429:THR:N	2.29	0.46
1:A:680:GLN:O	1:A:681:LYS:C	2.53	0.46
1:C:680:GLN:O	1:C:681:LYS:C	2.54	0.46
3:Y:119:VAL:HG21	3:Y:209:PHE:CB	2.44	0.46
3:Y:185:LYS:HG2	3:Y:186:TYR:CD2	2.51	0.46
1:C:1080:ALA:HB1	1:C:1148:THR:HA	1.97	0.46
2:B:1496:THR:HG23	2:B:1603:LYS:HD2	1.98	0.46
2:B:1499:SER:HA	2:B:1572:ALA:O	2.16	0.46
2:B:1399:ARG:HG2	2:B:1399:ARG:HH11	1.79	0.46
2:B:940:THR:HG22	2:B:940:THR:O	2.15	0.46
1:C:811:VAL:HG12	1:C:811:VAL:O	2.16	0.46
1:A:504:LEU:HD21	1:A:651:LEU:CG	2.44	0.46
1:A:534:MET:CB	1:A:538:SER:OG	2.63	0.46
1:C:42:GLN:CA	1:C:80:GLN:HG3	2.42	0.46
1:C:1535:MET:HA	1:C:1645:ILE:HB	1.98	0.46
2:D:1561:HIS:NE2	2:D:1597:ILE:HD13	2.29	0.46
1:C:1022:PHE:CE2	1:C:1092:TYR:CD1	3.04	0.46
2:B:481:TYR:HE2	2:B:493:GLY:HA3	1.81	0.46
2:B:750:ASP:C	2:B:750:ASP:OD1	2.53	0.46
1:A:1255:LEU:HD13	1:A:1267:VAL:HG13	1.97	0.46
2:D:825:VAL:HG11	2:D:918:GLU:HB3	1.97	0.46
2:B:599:TRP:CE3	2:B:602:ILE:HD12	2.51	0.46
1:A:1159:CYS:C	1:A:1161:LEU:H	2.18	0.46
2:B:1573:LEU:HB3	2:B:1575:LEU:HD23	1.97	0.46
2:B:1363:LEU:HD23	2:B:1442:ILE:HG12	1.98	0.46
1:A:787:GLN:O	1:A:788:PHE:HB3	2.15	0.46
2:B:361:GLU:HB3	2:B:399:ILE:HD13	1.98	0.46
3:X:136:LEU:HA	3:X:224:ILE:O	2.14	0.46
1:A:161:LEU:HD21	1:A:185:PHE:CD2	2.51	0.46
3:X:179:LEU:HD11	3:X:180:TYR:CE1	2.50	0.46
1:A:274:ASP:CG	1:A:275:LEU:N	2.69	0.46
2:B:352:LYS:HG3	2:B:430:MET:HE1	1.98	0.46
2:D:1567:ARG:HG3	2:D:1567:ARG:HH11	1.80	0.46
2:D:1534:GLN:OE1	2:D:1534:GLN:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1563:TYR:HB3	2:D:1601:ILE:HD11	1.96	0.46
1:A:42:GLN:OE1	1:A:500:ASN:ND2	2.48	0.46
1:C:78:LYS:O	1:C:80:GLN:N	2.49	0.46
1:A:1244:THR:O	1:A:1245:ALA:C	2.54	0.46
1:A:1671:ILE:HD13	1:A:1676:CYS:SG	2.56	0.46
1:C:1093:VAL:HG12	1:C:1095:GLN:NE2	2.30	0.46
1:A:371:ILE:CD1	1:A:433:PHE:CE2	2.96	0.46
1:A:128:ILE:HD12	1:A:201:ILE:CG2	2.41	0.46
1:A:216:TYR:CD2	1:A:216:TYR:N	2.82	0.46
2:B:525:GLN:NE2	2:B:528:ASN:H	2.13	0.46
1:A:119:ILE:HD12	1:A:119:ILE:C	2.36	0.46
1:A:86:THR:C	1:A:87:ILE:HD13	2.35	0.46
1:C:853:MET:O	1:C:888:VAL:HG12	2.15	0.46
1:A:374:GLN:HG2	1:A:382:LEU:CD2	2.45	0.46
1:A:644:ASN:O	1:A:645:VAL:C	2.54	0.46
2:D:933:ARG:HH11	2:D:933:ARG:CG	2.18	0.46
2:D:1573:LEU:HB3	2:D:1575:LEU:HD23	1.98	0.46
1:C:1572:ASN:C	1:C:1573:VAL:HG23	2.35	0.46
2:B:1500:LEU:HD22	2:B:1607:ILE:HB	1.98	0.46
2:B:1424:ILE:HD13	2:B:1424:ILE:N	2.27	0.46
1:C:705:VAL:HA	1:C:739:ARG:HH12	1.80	0.46
3:Y:42:ASP:HB3	3:Y:45:ASP:HB2	1.98	0.46
2:B:476:ILE:HG12	2:B:524:TYR:CD2	2.50	0.46
1:A:982:LEU:C	1:A:984:VAL:N	2.68	0.46
2:D:1351:ASN:N	2:D:1351:ASN:OD1	2.44	0.46
1:A:125:PHE:CD1	1:A:125:PHE:N	2.83	0.46
2:D:398:LEU:HA	2:D:398:LEU:HD23	1.53	0.46
1:C:909:ASN:HD21	4:C:2003:NAG:H83	1.81	0.46
2:B:398:LEU:HA	2:B:398:LEU:HD23	1.50	0.46
1:C:1426:ILE:O	1:C:1426:ILE:HG22	2.16	0.46
1:A:25:ILE:CG2	1:A:654:LEU:HB2	2.45	0.46
1:A:554:LEU:H	1:A:658:ASN:ND2	2.11	0.46
1:C:25:ILE:CD1	1:C:41:ILE:HG13	2.46	0.46
1:C:1622:LYS:HZ2	1:C:1642:LEU:HD23	1.80	0.46
1:C:1246:ARG:HB2	1:C:1246:ARG:CZ	2.46	0.46
1:A:383:VAL:HG23	1:A:386:VAL:HG23	1.98	0.46
1:A:938:SER:OG	1:A:1284:PHE:CE2	2.68	0.46
1:A:1227:PHE:HA	1:A:1228:TRP:CE3	2.51	0.46
1:C:1133:LEU:N	1:C:1133:LEU:CD1	2.71	0.46
1:A:1561:TYR:CD1	1:A:1581:LEU:HD21	2.50	0.46
1:A:296:ILE:CG2	1:A:297:ALA:N	2.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:384:PHE:CD2	2:D:384:PHE:N	2.84	0.46
2:B:338:ILE:O	2:B:339:VAL:HG13	2.16	0.46
2:B:557:GLN:OE1	2:B:557:GLN:CA	2.58	0.46
1:A:219:VAL:HG12	1:A:219:VAL:O	2.15	0.46
1:A:248:ILE:HB	1:A:299:VAL:HG13	1.97	0.46
1:C:1309:LEU:CD1	1:C:1328:MET:HG3	2.45	0.46
2:D:275:SER:O	2:D:277:PRO:HD3	2.16	0.46
1:A:1025:LEU:HD13	1:A:1031:TRP:CZ3	2.51	0.46
1:A:827:MET:HE2	1:A:912:PHE:CE2	2.51	0.46
2:B:267:VAL:HG22	2:B:314:LEU:CD1	2.46	0.46
2:B:345:ILE:HG13	2:B:428:LYS:HB3	1.98	0.46
2:B:582:LYS:O	2:B:583:ALA:C	2.53	0.46
5:D:2001:NAG:HO3	5:D:2002:NAG:C5	2.29	0.46
1:C:560:TRP:HH2	1:C:673:LEU:HD22	1.80	0.46
1:C:1406:ALA:O	1:C:1472:PHE:HA	2.16	0.46
2:B:1508:VAL:HG13	2:B:1631:PHE:HB2	1.97	0.46
3:Y:174:VAL:O	3:Y:174:VAL:HG12	2.15	0.46
1:C:1582:LEU:C	1:C:1594:LYS:HZ2	2.19	0.46
2:D:806:TYR:CD1	2:D:806:TYR:C	2.89	0.46
2:B:953:ARG:CG	2:B:954:VAL:H	2.29	0.46
1:A:1641:SER:C	1:A:1643:THR:N	2.69	0.46
2:D:164:GLU:HA	2:D:174:SER:O	2.16	0.46
1:C:291:MET:HE2	1:C:291:MET:HB3	1.79	0.46
2:B:122:SER:OG	2:B:124:GLN:HB3	2.15	0.46
1:A:374:GLN:HG2	1:A:382:LEU:HD21	1.96	0.46
2:B:484:LEU:HD11	2:B:626:LEU:CG	2.45	0.46
1:C:766:ARG:H	1:C:766:ARG:HD3	1.80	0.46
2:D:830:VAL:CG2	2:D:831:GLU:N	2.75	0.46
2:D:1284:ARG:HG3	2:D:1285:GLU:N	2.30	0.46
2:B:148:PHE:CZ	2:B:792:VAL:CG1	2.99	0.46
1:C:351:PRO:CG	1:C:442:LEU:HD11	2.45	0.46
1:C:1305:LYS:O	1:C:1307:LEU:HD13	2.16	0.46
2:D:1506:ILE:HD11	2:D:1628:PHE:CE1	2.43	0.46
1:A:993:SER:C	1:A:995:GLU:N	2.60	0.46
1:A:1127:ILE:HD11	1:A:1143:TYR:CE2	2.50	0.46
1:A:1128:LYS:O	1:A:1129:LEU:HD23	2.15	0.46
2:D:511:THR:O	2:D:512:PRO:C	2.54	0.46
2:B:96:THR:HG22	2:B:97:ASP:O	2.16	0.46
1:C:1081:PHE:O	1:C:1084:ARG:HB3	2.15	0.46
2:D:191:LEU:HD12	2:D:958:GLU:HG2	1.98	0.46
2:B:1510:LEU:O	2:B:1513:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:493:ILE:CG2	1:C:495:LYS:HB2	2.46	0.46
1:C:477:LEU:HD23	1:C:480:GLU:OE1	2.15	0.46
2:B:954:VAL:O	2:B:957:THR:HG23	2.16	0.46
2:B:1505:ARG:CG	2:B:1505:ARG:HH11	2.07	0.46
1:A:1637:TYR:N	1:A:1637:TYR:HD2	2.14	0.46
1:C:1379:LEU:HD21	1:C:1495:VAL:HG13	1.97	0.46
1:A:296:ILE:HG23	1:A:297:ALA:N	2.30	0.46
2:B:87:ILE:H	2:B:87:ILE:CD1	2.26	0.46
3:X:58:SER:HB3	3:X:102:ASN:HD22	1.75	0.46
2:D:1446:PHE:C	2:D:1448:VAL:H	2.19	0.46
2:D:148:PHE:HB2	2:D:800:ILE:HD11	1.95	0.46
1:A:100:SER:C	1:A:101:TYR:CD2	2.89	0.46
1:C:382:LEU:HA	1:C:382:LEU:HD23	1.80	0.46
1:C:307:VAL:O	1:C:311:SER:HB2	2.16	0.46
1:A:186:PRO:O	1:A:187:ASP:O	2.33	0.46
2:B:184:TRP:N	2:B:184:TRP:CE3	2.81	0.46
2:B:355:LYS:O	2:B:358:MET:CB	2.63	0.46
1:C:1436:GLU:HG2	1:C:1453:TYR:HE2	1.81	0.46
1:A:164:ILE:HG22	1:A:165:ASP:O	2.16	0.46
2:B:1529:LEU:CD1	2:B:1529:LEU:N	2.79	0.46
1:A:909:ASN:HD21	4:A:2003:NAG:C8	2.29	0.46
1:A:592:MET:O	1:A:783:ARG:HA	2.15	0.46
2:B:566:LYS:O	2:B:567:LEU:HD23	2.16	0.46
1:A:22:THR:HG21	1:A:657:ALA:CB	2.39	0.46
1:A:20:GLU:HB2	1:A:551:THR:HG22	1.98	0.46
1:C:545:ILE:HG12	1:C:545:ILE:H	1.41	0.46
1:C:553:GLU:HA	1:C:658:ASN:HD22	1.81	0.46
1:C:1582:LEU:C	1:C:1594:LYS:NZ	2.70	0.46
1:C:1627:ILE:O	1:C:1627:ILE:HG13	2.16	0.46
2:D:857:CYS:HB3	2:D:885:VAL:CG2	2.45	0.46
1:C:1068:VAL:CG1	1:C:1069:TRP:N	2.76	0.46
2:D:954:VAL:CG1	2:D:955:PRO:HD2	2.38	0.46
2:B:210:TYR:CG	2:B:211:THR:N	2.84	0.46
1:C:1298:THR:O	1:C:1299:GLU:C	2.53	0.46
2:B:525:GLN:CD	2:B:525:GLN:O	2.54	0.46
1:C:569:ASN:H	1:C:569:ASN:HD22	1.64	0.46
1:A:382:LEU:HD22	1:A:416:GLY:HA3	1.97	0.46
3:X:128:LYS:HD3	3:X:158:GLU:CD	2.36	0.46
1:A:690:TYR:CZ	1:A:692:HIS:CB	2.99	0.46
1:A:1079:THR:HB	1:A:1107:LEU:HD11	1.98	0.46
2:B:916:VAL:HG22	2:B:917:PRO:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1332:ASN:O	1:C:1333:PHE:O	2.34	0.46
2:D:1347:VAL:CG2	2:D:1456:VAL:HG11	2.43	0.46
2:B:139:PRO:HG2	2:B:218:LYS:HE2	1.96	0.46
1:C:165:ASP:HA	1:C:166:PRO:HD2	1.76	0.46
1:C:1156:PHE:O	1:C:1160:PRO:HD3	2.16	0.46
2:D:1525:LYS:HE3	2:D:1610:TRP:CE2	2.51	0.46
1:C:1346:LEU:HA	1:C:1346:LEU:HD12	1.48	0.46
1:A:285:THR:CG2	1:A:285:THR:O	2.63	0.46
1:A:862:VAL:O	1:A:863:GLU:C	2.53	0.46
2:B:524:TYR:CD1	2:B:524:TYR:C	2.89	0.46
1:C:161:LEU:HD11	1:C:185:PHE:CE2	2.50	0.46
2:D:873:LYS:CD	2:D:873:LYS:N	2.79	0.46
2:B:96:THR:HG22	2:B:97:ASP:N	2.31	0.46
1:A:322:TYR:N	1:A:322:TYR:HD2	2.13	0.46
3:Y:215:VAL:O	3:Y:216:LEU:HD13	2.15	0.46
2:B:1631:PHE:CD2	2:B:1632:SER:N	2.84	0.46
2:B:105:VAL:HG12	2:B:118:VAL:HA	1.97	0.46
2:B:640:SER:O	2:B:641:ALA:HB2	2.16	0.46
3:X:190:ILE:HG12	3:X:190:ILE:O	2.16	0.46
2:B:1429:LYS:H	2:B:1429:LYS:HE3	1.80	0.46
1:A:364:LYS:N	1:A:364:LYS:HD2	2.32	0.45
1:A:25:ILE:CB	1:A:654:LEU:HB2	2.46	0.45
2:B:518:PHE:H	2:B:518:PHE:HD2	1.64	0.45
1:C:108:SER:OG	1:C:111:PHE:N	2.49	0.45
1:C:114:SER:O	1:C:115:LYS:HE2	2.16	0.45
1:C:965:LEU:HD23	1:C:1629:TYR:CD1	2.51	0.45
1:C:1641:SER:C	1:C:1643:THR:N	2.69	0.45
1:C:1162:VAL:CG2	1:C:1163:LYS:N	2.79	0.45
2:B:1290:TYR:CD2	2:B:1301:ARG:HB3	2.51	0.45
2:D:758:LEU:HD23	2:D:758:LEU:HA	1.70	0.45
2:D:851:LEU:HD21	2:D:865:ARG:HH21	1.81	0.45
1:C:1234:HIS:CG	1:C:1235:LYS:H	2.34	0.45
2:B:416:ASN:CA	2:B:425:GLN:HE22	2.20	0.45
1:C:1317:TYR:CE1	1:C:1342:LEU:HD12	2.51	0.45
1:A:148:LEU:HA	1:A:154:PRO:O	2.15	0.45
3:Y:68:ASN:OD1	3:Y:69:GLY:N	2.40	0.45
2:D:575:VAL:HG23	2:D:762:LEU:CD1	2.46	0.45
2:B:1382:ILE:HG12	2:B:1427:LEU:HD11	1.98	0.45
2:B:144:LEU:HB3	2:B:185:PRO:HB3	1.97	0.45
1:A:560:TRP:CH2	1:A:562:ASN:HB2	2.51	0.45
1:A:999:ILE:HD12	1:A:1001:THR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1393:ASP:OD1	2:D:1395:GLU:HB3	2.15	0.45
1:C:328:THR:HG22	1:C:328:THR:O	2.16	0.45
1:A:376:LYS:HA	1:A:381:GLN:O	2.15	0.45
1:C:465:LEU:HD23	1:C:556:SER:HA	1.98	0.45
1:C:535:VAL:HA	1:C:563:ILE:CD1	2.46	0.45
1:C:1525:CYS:C	1:C:1528:VAL:HG22	2.28	0.45
1:A:1022:PHE:HE2	1:A:1092:TYR:CD1	2.34	0.45
1:A:1562:LYS:O	1:A:1563:VAL:HG13	2.16	0.45
1:A:871:PRO:HD2	1:A:872:VAL:H	1.78	0.45
2:D:618:LEU:HG	2:D:634:LEU:HD11	1.98	0.45
1:A:263:ALA:O	1:A:291:MET:HE3	2.16	0.45
2:D:208:GLU:O	2:D:209:ASN:C	2.55	0.45
1:A:883:CYS:O	1:A:884:VAL:C	2.54	0.45
2:B:756:LEU:HD22	2:B:778:PHE:CD1	2.51	0.45
1:A:718:ILE:HD11	1:A:728:PHE:CD2	2.51	0.45
1:C:690:TYR:CZ	1:C:692:HIS:CB	2.98	0.45
1:A:1213:LYS:CG	1:A:1266:TYR:HE2	2.22	0.45
1:C:590:LEU:HD21	1:C:774:LEU:HD11	1.99	0.45
1:C:20:GLU:HG3	1:C:547:THR:HB	1.98	0.45
3:X:107:GLN:CD	3:X:110:ILE:HD11	2.36	0.45
2:B:1482:ASN:HB2	2:B:1495:GLU:HA	1.97	0.45
2:B:132:THR:O	2:B:133:ASP:C	2.55	0.45
1:A:705:VAL:HA	1:A:739:ARG:HH12	1.81	0.45
1:C:185:PHE:HD1	1:C:186:PRO:HD2	1.82	0.45
2:B:570:ASP:O	2:B:573:ALA:CB	2.64	0.45
1:A:455:ILE:HG22	1:A:456:ALA:H	1.79	0.45
3:X:119:VAL:HG22	3:X:212:MET:HB2	1.99	0.45
2:D:79:GLY:O	2:D:81:MET:N	2.50	0.45
1:A:733:VAL:O	1:A:737:GLN:HG2	2.15	0.45
2:D:107:GLN:HG3	2:D:116:GLU:HG3	1.98	0.45
1:A:57:LYS:O	1:A:102:VAL:HG22	2.16	0.45
1:A:76:GLU:O	1:A:76:GLU:CD	2.55	0.45
1:A:532:GLN:O	1:A:533:ASN:C	2.55	0.45
1:A:506:LYS:HD2	1:A:536:PRO:HD2	1.97	0.45
1:C:1278:GLN:NE2	1:C:1293:ALA:CB	2.79	0.45
1:C:979:VAL:CG2	1:C:1326:TYR:CE1	2.79	0.45
2:D:954:VAL:O	2:D:957:THR:HG23	2.15	0.45
1:A:1646:GLU:HG2	1:A:1660:PHE:CZ	2.51	0.45
1:A:961:TYR:CD1	1:A:961:TYR:C	2.89	0.45
2:B:760:LYS:HE3	2:B:776:MET:SD	2.55	0.45
1:A:436:LYS:CB	1:A:449:ARG:HG2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:103:TYR:N	2:D:103:TYR:CD2	2.85	0.45
1:A:1300:TYR:CD2	1:A:1300:TYR:C	2.89	0.45
1:A:1249:GLU:HG3	1:A:1289:ASP:CA	2.46	0.45
1:C:150:ASP:CG	1:C:151:ASP:N	2.70	0.45
1:A:240:TYR:CD2	1:A:241:LYS:N	2.85	0.45
2:D:130:ILE:HG21	2:D:199:ILE:HG21	1.98	0.45
2:D:1446:PHE:CD2	2:D:1448:VAL:HG13	2.51	0.45
2:D:1508:VAL:HB	2:D:1509:PRO:CD	2.44	0.45
1:A:365:PRO:HG2	1:A:464:TYR:HE2	1.80	0.45
1:A:1128:LYS:HD3	1:A:1414:GLU:OE1	2.16	0.45
2:D:1380:THR:HG22	2:D:1381:ILE:N	2.31	0.45
2:B:1371:TYR:HB2	2:B:1377:SER:HB3	1.99	0.45
1:C:96:GLN:HG3	1:C:97:ASN:N	2.31	0.45
2:D:63:ARG:CB	2:D:65:GLN:HG3	2.46	0.45
2:B:853:ASN:HA	2:B:854:PRO:HD3	1.56	0.45
1:A:710:THR:OG1	1:A:713:GLN:HG3	2.16	0.45
1:C:578:ASP:O	1:C:578:ASP:CG	2.55	0.45
1:C:760:VAL:O	1:C:760:VAL:HG22	2.16	0.45
1:C:484:ILE:HD13	1:C:540:LEU:HD21	1.96	0.45
2:D:953:ARG:CG	2:D:954:VAL:H	2.29	0.45
1:A:224:LEU:CD2	1:A:225:PRO:HD2	2.44	0.45
2:D:778:PHE:N	2:D:778:PHE:HD2	2.14	0.45
1:C:600:VAL:CG2	1:C:780:VAL:HG21	2.46	0.45
2:D:1296:ASN:O	2:D:1297:ALA:C	2.54	0.45
1:A:61:ASP:O	1:A:62:LYS:CB	2.64	0.45
2:B:778:PHE:N	2:B:778:PHE:HD2	2.13	0.45
2:B:531:ILE:HD11	2:B:634:LEU:CD2	2.45	0.45
1:A:1215:GLU:HA	1:A:1215:GLU:OE1	2.16	0.45
1:A:855:PHE:HB2	1:A:914:LEU:HD11	1.98	0.45
1:C:690:TYR:CE1	1:C:696:LYS:HD2	2.52	0.45
1:A:1268:ASN:ND2	1:A:1268:ASN:N	2.64	0.45
1:A:1305:LYS:O	1:A:1307:LEU:HD13	2.17	0.45
1:C:773:TRP:CE3	1:C:774:LEU:HB2	2.52	0.45
1:A:989:SER:O	1:A:993:SER:HB3	2.16	0.45
2:D:1633:TYR:CE1	2:D:1637:GLU:OE1	2.69	0.45
2:B:178:VAL:HG21	2:B:183:PHE:CD1	2.52	0.45
2:D:1313:VAL:HG21	2:D:1323:MET:HE2	1.98	0.45
2:B:962:LYS:HD2	2:B:1302:THR:CG2	2.46	0.45
1:A:661:ASP:OD2	1:A:663:GLN:N	2.50	0.45
1:A:909:ASN:HA	1:A:926:THR:HA	1.98	0.45
3:X:60:VAL:O	3:X:60:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:139:ASN:HB2	3:X:227:THR:HG23	1.98	0.45
1:C:640:LEU:H	1:C:644:ASN:CB	2.27	0.45
1:C:74:SER:HA	1:C:79:PHE:CE1	2.51	0.45
1:C:1561:TYR:HE1	1:C:1581:LEU:HG	1.82	0.45
1:C:970:LYS:C	1:C:971:THR:CG2	2.85	0.45
2:B:922:LYS:NZ	2:B:952:ASP:OD2	2.50	0.45
1:A:1557:ILE:HD13	1:A:1622:LYS:HG3	1.99	0.45
1:A:481:HIS:CD2	2:B:387:MET:HG3	2.51	0.45
2:D:44:GLU:OE2	2:D:523:TYR:OH	2.33	0.45
1:A:407:SER:O	1:A:420:PHE:HE1	1.99	0.45
2:B:842:GLU:O	2:B:844:ILE:HG23	2.17	0.45
2:B:103:TYR:CD2	2:B:103:TYR:N	2.83	0.45
1:C:473:HIS:CE1	2:D:455:LYS:HE3	2.51	0.45
1:A:1328:MET:HB2	1:A:1328:MET:HE3	1.85	0.45
1:C:420:PHE:CD2	1:C:420:PHE:N	2.84	0.45
1:A:248:ILE:HD13	1:A:325:ILE:HD13	1.99	0.45
2:B:188:LEU:HD13	2:B:216:VAL:CG2	2.47	0.45
2:B:456:PRO:CG	2:B:515:ILE:HD11	2.46	0.45
2:B:1344:HIS:ND1	5:B:2003:NAG:C8	2.79	0.45
2:B:162:ILE:HG22	2:B:202:LYS:O	2.16	0.45
1:A:136:THR:O	1:A:139:GLN:HG3	2.17	0.45
2:D:570:ASP:O	2:D:573:ALA:CB	2.65	0.45
1:A:1468:PRO:CD	1:A:1473:LEU:HD13	2.45	0.45
2:D:1529:LEU:N	2:D:1529:LEU:CD1	2.80	0.45
2:D:105:VAL:HG12	2:D:118:VAL:HA	1.99	0.45
1:A:1023:HIS:O	1:A:1027:THR:HB	2.15	0.45
2:D:315:TYR:CD1	2:D:315:TYR:C	2.89	0.45
1:A:40:VAL:CG2	1:A:41:ILE:N	2.79	0.45
1:A:554:LEU:N	1:A:658:ASN:HD22	2.13	0.45
2:B:518:PHE:CD2	2:B:518:PHE:O	2.70	0.45
2:D:378:PRO:HA	2:D:389:THR:HA	1.99	0.45
1:A:222:TYR:HE2	1:A:224:LEU:HA	1.81	0.45
1:A:1648:TRP:NE1	1:A:1664:LEU:CD2	2.79	0.45
1:A:1570:VAL:HG22	1:A:1575:VAL:HA	1.99	0.45
1:A:1488:LEU:HD12	1:A:1488:LEU:C	2.37	0.45
2:B:780:LEU:HD11	2:B:787:TRP:HD1	1.82	0.45
1:A:419:SER:HB2	2:B:459:ASN:ND2	2.14	0.45
2:B:613:SER:HA	2:B:620:VAL:CG2	2.46	0.45
1:C:224:LEU:HD23	1:C:225:PRO:CD	2.44	0.45
1:A:690:TYR:CE1	1:A:696:LYS:HD2	2.52	0.45
1:C:892:SER:HB3	1:C:893:SER:H	1.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:LYS:HE2	2:B:180:LEU:HD12	1.99	0.45
1:C:20:GLU:O	1:C:20:GLU:OE2	2.34	0.45
1:A:288:GLN:O	1:A:289:ASN:C	2.55	0.45
1:A:1180:LEU:HD21	1:A:1208:ILE:HA	1.98	0.45
2:B:1391:LEU:HB2	2:B:1417:MET:CE	2.47	0.45
1:A:774:LEU:HG	1:A:788:PHE:HE1	1.80	0.45
2:B:1343:PHE:CZ	2:B:1371:TYR:HD1	2.35	0.45
2:D:184:TRP:CE3	2:D:184:TRP:N	2.81	0.45
1:C:1113:LEU:HD23	1:C:1114:ASP:H	1.81	0.45
2:B:862:LYS:NZ	2:B:1519:ASN:HB3	2.32	0.45
2:B:410:PRO:CA	2:B:431:THR:HG22	2.46	0.45
3:Y:222:ARG:HB2	3:Y:222:ARG:HE	1.60	0.45
1:A:532:GLN:O	1:A:534:MET:N	2.49	0.45
1:A:532:GLN:HA	1:A:535:VAL:HG13	1.98	0.45
1:C:465:LEU:HG	1:C:466:TYR:N	2.30	0.45
1:C:503:ILE:O	1:C:510:ILE:HG12	2.17	0.45
2:D:378:PRO:HB2	2:D:416:ASN:O	2.17	0.45
2:B:208:GLU:O	2:B:209:ASN:C	2.55	0.45
1:C:1106:TRP:CZ2	1:C:1111:TYR:HE2	2.34	0.45
2:B:481:TYR:CE1	2:B:506:MET:SD	2.97	0.45
1:A:916:THR:O	1:A:918:PHE:N	2.50	0.45
1:A:1226:ARG:CD	1:A:1266:TYR:HE1	2.29	0.45
1:A:1332:ASN:O	1:A:1333:PHE:O	2.35	0.45
1:C:284:GLN:HG2	1:C:310:LEU:CD1	2.47	0.45
1:A:256:TYR:HB3	1:A:848:TYR:OH	2.17	0.45
1:C:374:GLN:HG2	1:C:382:LEU:CD2	2.47	0.45
1:C:382:LEU:HD22	1:C:416:GLY:HA3	1.97	0.45
2:D:1382:ILE:CD1	2:D:1458:VAL:HG22	2.47	0.45
1:A:1186:PHE:HD1	1:A:1250:THR:HG22	1.82	0.45
2:B:267:VAL:HG22	2:B:314:LEU:HD12	1.99	0.45
2:D:1524:TYR:HB3	2:D:1544:VAL:HG13	1.98	0.45
1:C:612:VAL:HG21	1:C:769:PHE:CE2	2.52	0.45
1:C:274:ASP:OD1	1:C:277:ASP:CG	2.55	0.45
2:B:1567:ARG:HH11	2:B:1567:ARG:HG3	1.82	0.45
1:C:376:LYS:HA	1:C:381:GLN:O	2.16	0.45
2:B:855:ALA:O	2:B:856:PHE:CD1	2.70	0.45
2:D:83:VAL:C	2:D:85:PRO:HD3	2.36	0.45
1:A:505:SER:O	1:A:506:LYS:C	2.55	0.45
1:C:111:PHE:CE2	1:C:113:LYS:CB	2.94	0.45
1:C:1244:THR:H	1:C:1247:MET:HE3	1.81	0.45
2:D:953:ARG:CG	2:D:954:VAL:N	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:THR:CG2	1:A:121:TYR:N	2.80	0.45
2:D:615:GLN:CB	2:D:616:ASN:HD22	2.29	0.45
1:A:839:ILE:HA	1:A:839:ILE:HD12	1.71	0.45
1:A:961:TYR:HE1	1:A:963:ILE:HG12	1.82	0.45
2:B:44:GLU:OE2	2:B:523:TYR:OH	2.31	0.45
1:C:847:ASN:OD1	1:C:847:ASN:C	2.55	0.45
2:B:415:THR:O	2:B:425:GLN:CD	2.55	0.45
1:C:356:LEU:HG	1:C:452:TYR:CE2	2.51	0.45
1:A:1142:LEU:HD13	1:A:1187:THR:CG2	2.47	0.45
1:C:1304:VAL:HG12	1:C:1305:LYS:H	1.77	0.45
1:C:174:VAL:CG2	1:C:175:GLU:N	2.80	0.45
2:B:173:VAL:HG13	2:B:964:ILE:HD11	1.98	0.45
1:A:274:ASP:OD1	1:A:277:ASP:CG	2.55	0.45
1:A:560:TRP:CH2	1:A:673:LEU:HD22	2.51	0.45
1:C:977:LEU:HD22	1:C:978:SER:N	2.32	0.45
2:B:107:GLN:HG3	2:B:116:GLU:HG3	1.98	0.45
1:C:1272:LYS:O	1:C:1276:GLU:HG3	2.16	0.45
2:B:891:LEU:H	2:B:891:LEU:HG	1.21	0.45
1:A:1636:ILE:HG22	1:A:1636:ILE:O	2.16	0.45
1:A:23:TYR:CE2	1:A:111:PHE:CD2	3.05	0.45
1:A:477:LEU:HD22	1:A:477:LEU:N	2.31	0.45
1:C:491:PRO:O	1:C:493:ILE:N	2.48	0.45
1:C:1629:TYR:HD2	1:C:1629:TYR:H	1.65	0.45
1:A:1053:MET:HE2	1:A:1086:LEU:HD13	1.98	0.45
1:A:1093:VAL:HG12	1:A:1095:GLN:NE2	2.31	0.45
2:B:1561:HIS:NE2	2:B:1597:ILE:CD1	2.80	0.45
2:B:1561:HIS:NE2	2:B:1597:ILE:HD13	2.30	0.45
1:A:481:HIS:CE1	2:B:387:MET:CE	3.00	0.45
2:D:524:TYR:CD1	2:D:524:TYR:C	2.90	0.45
1:A:491:PRO:O	1:A:491:PRO:HG2	2.17	0.45
2:B:481:TYR:CE2	2:B:493:GLY:HA3	2.51	0.45
1:C:606:ASP:OD2	1:C:795:THR:HG21	2.17	0.45
2:D:824:VAL:CG2	2:D:828:GLU:OE1	2.64	0.45
1:C:1013:MET:HE2	1:C:1287:THR:HB	1.97	0.45
2:D:1623:LYS:HA	2:D:1623:LYS:HD2	1.68	0.45
2:B:598:ILE:HD13	2:B:800:ILE:HG21	1.95	0.45
1:A:1127:ILE:HB	1:A:1129:LEU:HD21	1.98	0.45
1:A:1474:CYS:HB3	1:A:1476:ARG:HH12	1.82	0.45
3:Y:191:ILE:O	3:Y:198:LYS:HA	2.17	0.45
2:D:96:THR:HG22	2:D:97:ASP:O	2.16	0.45
2:D:1386:MET:HE2	2:D:1386:MET:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:GLN:O	1:A:97:ASN:O	2.35	0.45
1:A:760:VAL:HG22	1:A:760:VAL:O	2.17	0.45
2:B:297:ASP:N	2:B:297:ASP:OD2	2.49	0.45
1:A:1080:ALA:CB	1:A:1148:THR:HG22	2.47	0.45
1:A:506:LYS:O	1:A:508:LYS:N	2.49	0.45
1:C:24:VAL:HG11	1:C:543:TYR:HE2	1.75	0.45
1:C:1646:GLU:HG2	1:C:1660:PHE:CZ	2.52	0.45
2:D:224:PHE:CE1	2:D:320:VAL:CG1	3.01	0.45
1:C:923:LEU:HD21	1:C:925:LYS:HD3	1.99	0.45
1:A:1560:ALA:O	1:A:1561:TYR:HB3	2.17	0.45
1:A:1638:PRO:HG2	1:A:1639:LEU:H	1.81	0.45
2:D:436:GLN:O	2:D:437:THR:C	2.54	0.45
2:D:965:ILE:HD13	2:D:1277:ILE:HD13	1.99	0.45
2:D:173:VAL:HA	2:D:964:ILE:CD1	2.47	0.45
1:C:577:PRO:HD2	1:C:588:VAL:CG2	2.47	0.45
2:D:525:GLN:CD	2:D:525:GLN:O	2.55	0.45
1:A:596:MET:SD	1:A:782:ARG:HG2	2.57	0.45
1:A:489:LYS:NZ	2:B:502:ASN:H	2.14	0.45
2:B:628:LEU:HD12	2:B:629:THR:H	1.81	0.45
1:C:473:HIS:CE1	2:D:455:LYS:CE	3.00	0.45
1:A:950:TYR:C	1:A:952:THR:H	2.20	0.45
1:A:190:ILE:CG2	1:A:191:PRO:CD	2.95	0.45
1:C:1013:MET:O	1:C:1015:VAL:N	2.50	0.45
1:C:190:ILE:CG2	1:C:191:PRO:N	2.80	0.45
2:B:1347:VAL:CG2	2:B:1367:ILE:HG23	2.43	0.45
2:B:1500:LEU:HD13	2:B:1501:ASN:N	2.32	0.45
1:C:1250:THR:O	1:C:1252:ALA:N	2.50	0.45
2:B:133:ASP:CA	2:B:757:TRP:HZ3	2.28	0.45
1:A:862:VAL:HG12	1:A:863:GLU:OE1	2.16	0.45
2:D:176:ASN:HB3	2:D:184:TRP:HZ2	1.82	0.45
1:A:1054:LEU:HD23	1:A:1057:MET:HE1	1.98	0.45
2:D:810:VAL:HG12	2:D:811:MET:N	2.31	0.45
1:A:96:GLN:HG3	1:A:97:ASN:N	2.32	0.45
2:B:63:ARG:CB	2:B:65:GLN:HG3	2.47	0.45
2:B:1631:PHE:CD2	2:B:1631:PHE:C	2.90	0.45
1:C:259:VAL:HB	1:C:295:GLY:CA	2.46	0.45
1:A:840:GLN:HE21	1:A:897:THR:HG21	1.81	0.45
1:A:523:TYR:CE2	2:B:465:ASN:CG	2.90	0.45
1:C:439:ALA:O	1:C:441:ASP:N	2.43	0.45
1:A:476:LEU:HA	1:A:476:LEU:HD23	1.83	0.44
1:C:554:LEU:HB2	1:C:642:ASN:OD1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:ASN:O	1:C:78:LYS:C	2.54	0.44
1:C:963:ILE:HA	1:C:964:PRO:HD3	1.72	0.44
1:C:506:LYS:O	1:C:508:LYS:N	2.51	0.44
1:A:1240:PRO:HB2	1:A:1242:THR:CG2	2.47	0.44
2:B:1609:ARG:O	2:B:1611:PRO:HD3	2.17	0.44
1:A:60:PRO:CG	1:A:61:ASP:H	2.30	0.44
2:D:525:GLN:NE2	2:D:528:ASN:H	2.15	0.44
1:A:491:PRO:HB2	1:A:493:ILE:C	2.36	0.44
2:B:523:TYR:CB	2:B:533:ALA:HB2	2.47	0.44
2:B:61:PHE:CD1	2:B:62:PRO:HA	2.52	0.44
1:A:1066:TYR:HD1	1:A:1079:THR:HG23	1.83	0.44
1:A:1156:PHE:O	1:A:1160:PRO:HD3	2.17	0.44
1:A:149:ASN:O	1:A:152:LEU:N	2.25	0.44
2:D:1343:PHE:CZ	2:D:1371:TYR:HD1	2.35	0.44
2:D:1425:ILE:HG22	2:D:1427:LEU:HD12	1.98	0.44
2:D:1382:ILE:HG12	2:D:1427:LEU:HD11	1.99	0.44
2:B:580:VAL:HG13	2:B:584:VAL:CG2	2.47	0.44
2:B:176:ASN:HB3	2:B:184:TRP:HZ2	1.82	0.44
1:C:1386:ILE:HG13	1:C:1387:GLU:N	2.29	0.44
3:X:40:LEU:HD11	3:X:209:PHE:CZ	2.52	0.44
2:B:1637:GLU:O	2:B:1638:PHE:CG	2.70	0.44
1:C:662:SER:O	1:C:663:GLN:C	2.56	0.44
2:D:946:LYS:N	2:D:946:LYS:HD3	2.32	0.44
2:B:280:LEU:HG	2:B:280:LEU:O	2.16	0.44
2:B:189:PRO:C	2:B:191:LEU:N	2.69	0.44
2:D:640:SER:O	2:D:641:ALA:HB2	2.16	0.44
2:D:31:ALA:O	2:D:119:VAL:HG12	2.17	0.44
3:X:201:ILE:HD13	3:X:207:LEU:HD23	2.00	0.44
1:C:500:ASN:OD1	1:C:514:THR:HG23	2.18	0.44
1:C:639:GLY:HA2	1:C:648:LEU:CD1	2.44	0.44
1:C:624:PHE:CD1	1:C:625:GLN:N	2.85	0.44
2:B:1593:THR:HG21	2:B:1596:LYS:HE3	2.00	0.44
2:B:1597:ILE:HD11	2:B:1599:TYR:CE1	2.53	0.44
2:B:1611:PRO:HA	2:B:1615:GLU:OE1	2.17	0.44
2:D:739:PHE:CE2	2:D:847:ARG:NE	2.85	0.44
1:A:356:LEU:HG	1:A:452:TYR:CE2	2.53	0.44
1:C:700:TYR:O	1:C:703:ALA:N	2.50	0.44
1:A:694:VAL:HG12	1:A:694:VAL:O	2.16	0.44
1:A:134:VAL:HA	1:A:218:GLU:O	2.17	0.44
1:C:584:PRO:CB	1:C:792:ASP:HA	2.37	0.44
2:D:235:PHE:CE2	2:D:299:PHE:CE2	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1259:LEU:HD21	1:A:1267:VAL:HG11	1.98	0.44
2:B:1284:ARG:CG	2:B:1285:GLU:H	2.29	0.44
1:C:374:GLN:HG2	1:C:382:LEU:HD21	1.98	0.44
1:A:1033:ILE:CG2	1:A:1034:PHE:N	2.80	0.44
1:C:330:ILE:HG22	1:C:337:SER:HB3	1.99	0.44
2:D:336:ILE:HD13	2:D:336:ILE:HA	1.79	0.44
1:A:653:PHE:CE1	1:A:660:ASP:CB	3.00	0.44
2:D:111:PRO:O	2:D:113:VAL:HG23	2.18	0.44
2:B:1617:GLN:HG2	2:B:1617:GLN:H	1.66	0.44
1:A:1525:CYS:N	1:A:1528:VAL:CG1	2.79	0.44
1:A:535:VAL:O	1:A:563:ILE:HG12	2.17	0.44
1:C:1532:CYS:O	1:C:1641:SER:N	2.51	0.44
2:D:1597:ILE:HD11	2:D:1599:TYR:CE1	2.53	0.44
2:D:838:ASN:HB2	2:D:844:ILE:HD11	1.98	0.44
1:C:1022:PHE:O	1:C:1024:TYR:N	2.50	0.44
1:A:576:SER:HB2	1:A:589:SER:H	1.81	0.44
1:A:243:PHE:CE2	1:A:304:GLU:CA	3.00	0.44
1:C:502:LEU:HB2	1:C:541:LEU:HD21	1.97	0.44
1:A:1226:ARG:CD	1:A:1266:TYR:CE1	3.01	0.44
1:A:624:PHE:CD1	1:A:625:GLN:N	2.85	0.44
1:A:1153:ARG:CZ	1:A:1168:LEU:HD12	2.47	0.44
1:C:1286:SER:CB	1:C:1499:HIS:HA	2.46	0.44
2:D:344:GLN:O	2:D:366:VAL:HA	2.17	0.44
2:D:1345:LEU:HD12	2:D:1368:CYS:O	2.17	0.44
1:A:351:PRO:CG	1:A:442:LEU:HD11	2.48	0.44
2:D:148:PHE:CZ	2:D:792:VAL:CG1	3.00	0.44
2:D:1610:TRP:CE2	2:D:1628:PHE:HD2	2.35	0.44
3:Y:179:LEU:HD11	3:Y:180:TYR:CE1	2.51	0.44
2:B:345:ILE:HD11	2:B:427:THR:CA	2.47	0.44
1:A:421:VAL:HG23	2:B:507:ASN:ND2	2.32	0.44
2:B:111:PRO:O	2:B:113:VAL:HG23	2.18	0.44
1:C:667:GLU:HA	1:C:668:PRO:HD3	1.79	0.44
1:A:414:ASP:OD1	1:A:414:ASP:N	2.50	0.44
1:A:465:LEU:HD12	1:A:466:TYR:H	1.83	0.44
3:Y:139:ASN:HB2	3:Y:227:THR:HG23	2.00	0.44
1:C:532:GLN:O	1:C:533:ASN:C	2.53	0.44
1:C:1219:LYS:HE2	1:C:1239:VAL:CG2	2.45	0.44
1:A:1069:TRP:CH2	1:A:1465:ASN:ND2	2.85	0.44
1:C:1298:THR:O	1:C:1301:SER:N	2.51	0.44
1:A:493:ILE:CG2	1:A:495:LYS:HB2	2.45	0.44
1:A:981:GLY:O	1:A:1356:LEU:O	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:88:GLY:O	3:Y:91:LYS:N	2.43	0.44
1:C:257:ASN:ND2	1:C:892:SER:HA	2.27	0.44
1:A:1573:VAL:HG12	1:A:1603:LYS:HD3	1.95	0.44
1:C:1268:ASN:N	1:C:1269:PRO:HD2	2.33	0.44
2:B:739:PHE:CE2	2:B:847:ARG:NE	2.86	0.44
2:B:847:ARG:HG3	2:B:869:GLN:CG	2.42	0.44
2:B:515:ILE:HG21	2:B:599:TRP:CZ2	2.52	0.44
2:D:1371:TYR:CB	2:D:1377:SER:HB3	2.48	0.44
2:D:150:MET:HG3	2:D:602:ILE:HD11	2.00	0.44
2:D:570:ASP:O	2:D:573:ALA:HB2	2.17	0.44
1:A:632:LEU:N	1:A:632:LEU:CD2	2.68	0.44
2:D:1522:TYR:HD1	2:D:1524:TYR:CE1	2.35	0.44
2:D:1522:TYR:HD1	2:D:1524:TYR:CZ	2.35	0.44
1:A:977:LEU:CD2	1:A:1361:VAL:HG22	2.48	0.44
1:C:854:GLN:NE2	1:C:854:GLN:N	2.65	0.44
3:X:185:LYS:HG2	3:X:186:TYR:CD2	2.53	0.44
1:C:398:ASN:O	1:C:399:GLN:CB	2.64	0.44
2:D:642:ALA:O	2:D:643:LYS:HB3	2.17	0.44
1:A:532:GLN:CA	1:A:532:GLN:OE1	2.57	0.44
1:A:73:LEU:HB2	1:A:79:PHE:HA	1.98	0.44
1:C:1549:LYS:H	1:C:1549:LYS:HG2	1.41	0.44
1:C:930:VAL:HA	1:C:931:PRO:HD3	1.82	0.44
1:C:480:GLU:HG2	2:D:389:THR:HB	2.00	0.44
1:C:120:THR:CG2	1:C:121:TYR:N	2.81	0.44
1:C:1637:TYR:N	1:C:1637:TYR:HD2	2.15	0.44
1:A:1561:TYR:HE1	1:A:1598:ILE:HD11	1.83	0.44
1:A:1559:TYR:HE2	1:A:1590:ALA:O	1.98	0.44
2:D:445:LEU:HD23	2:D:533:ALA:HA	1.98	0.44
2:D:613:SER:HA	2:D:620:VAL:HG23	1.99	0.44
2:D:962:LYS:HD2	2:D:1302:THR:CG2	2.47	0.44
1:C:316:GLU:HA	1:C:319:ASN:HB2	1.99	0.44
2:D:89:ILE:CD1	2:D:104:VAL:HG11	2.48	0.44
2:B:830:VAL:HG23	2:B:831:GLU:N	2.32	0.44
3:Y:188:LYS:HD3	3:Y:202:ASP:CA	2.42	0.44
2:D:134:LYS:HD2	2:D:584:VAL:HG11	1.99	0.44
2:B:558:MET:HA	2:B:559:PRO:HD3	1.85	0.44
1:C:1459:HIS:HD2	1:C:1459:HIS:N	2.15	0.44
1:A:421:VAL:HG23	2:B:507:ASN:HD22	1.81	0.44
5:D:2001:NAG:O3	5:D:2002:NAG:O5	2.34	0.44
1:A:1421:HIS:CD2	1:A:1422:ALA:N	2.85	0.44
2:D:946:LYS:CD	2:D:946:LYS:H	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:909:ASN:HA	1:C:926:THR:HA	1.99	0.44
2:D:41:ILE:O	2:D:85:PRO:HD2	2.18	0.44
1:A:333:THR:OG1	1:A:334:GLY:N	2.50	0.44
2:B:257:VAL:CG1	2:B:258:GLU:N	2.80	0.44
2:B:47:GLY:O	2:B:48:ASP:HB2	2.17	0.44
1:C:510:ILE:HA	3:Y:150:ILE:CG1	2.48	0.44
1:C:535:VAL:HA	1:C:563:ILE:HD11	1.99	0.44
2:D:220:VAL:O	2:D:222:PRO:N	2.50	0.44
2:D:518:PHE:HE2	2:D:538:VAL:CG1	2.30	0.44
1:A:979:VAL:C	1:A:980:LYS:HG2	2.37	0.44
2:D:1330:ASN:N	2:D:1330:ASN:HD22	2.15	0.44
1:A:1663:ASN:O	1:A:1666:GLU:HB3	2.18	0.44
1:C:60:PRO:CG	1:C:61:ASP:H	2.30	0.44
1:C:779:LEU:O	1:C:781:PRO:HD3	2.18	0.44
1:A:60:PRO:CG	1:A:61:ASP:N	2.81	0.44
1:C:694:VAL:O	1:C:694:VAL:HG12	2.18	0.44
1:A:606:ASP:OD2	1:A:795:THR:HG21	2.18	0.44
1:A:569:ASN:HD22	1:A:569:ASN:H	1.64	0.44
1:A:1003:LEU:HA	1:A:1004:PRO:HD2	1.49	0.44
1:A:284:GLN:HG2	1:A:310:LEU:CD1	2.47	0.44
2:D:1444:LYS:NZ	2:D:1447:GLU:HA	2.32	0.44
2:D:824:VAL:HG21	2:D:830:VAL:CG1	2.41	0.44
1:C:152:LEU:HA	1:C:152:LEU:HD13	1.48	0.44
1:C:1268:ASN:ND2	1:C:1268:ASN:N	2.66	0.44
2:D:818:LEU:HG	2:D:820:MET:HE3	2.00	0.44
2:D:1365:LEU:HD21	2:D:1472:TYR:CE1	2.53	0.44
2:D:1454:GLY:HA3	2:D:1472:TYR:CE2	2.53	0.44
2:B:1438:LEU:HD13	2:B:1438:LEU:C	2.37	0.44
1:C:415:ASP:OD1	1:C:415:ASP:N	2.48	0.44
2:D:1525:LYS:HE3	2:D:1610:TRP:NE1	2.32	0.44
2:B:1387:LEU:O	2:B:1390:PHE:HB2	2.16	0.44
2:B:1425:ILE:HG22	2:B:1427:LEU:HD12	2.00	0.44
1:A:671:GLU:HB2	1:A:672:ILE:H	1.66	0.44
2:B:1523:VAL:O	2:B:1548:ILE:HB	2.18	0.44
2:B:296:ARG:HA	2:B:296:ARG:HD2	1.90	0.44
2:B:1282:PRO:O	2:B:1283:ASP:C	2.56	0.44
2:B:386:SER:O	2:B:398:LEU:HD11	2.18	0.44
2:B:930:LEU:HD13	2:B:1315:ALA:HB2	1.99	0.44
1:C:1428:LEU:HD11	1:C:1434:ALA:HB2	1.99	0.44
1:C:1200:LYS:HE3	1:C:1200:LYS:HB3	1.79	0.44
1:C:1636:ILE:O	1:C:1636:ILE:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLN:HE21	1:A:44:TYR:N	2.10	0.44
2:B:518:PHE:CD2	2:B:538:VAL:HB	2.42	0.44
1:C:41:ILE:HG21	1:C:41:ILE:HD13	1.63	0.44
1:C:40:VAL:HG23	1:C:41:ILE:N	2.32	0.44
1:C:491:PRO:HB2	1:C:493:ILE:C	2.37	0.44
1:C:492:TYR:CD2	1:C:493:ILE:HB	2.53	0.44
1:C:1582:LEU:CD2	1:C:1616:GLN:HG2	2.40	0.44
1:C:970:LYS:HD3	1:C:1640:ASP:OD2	2.18	0.44
1:A:383:VAL:HG23	1:A:386:VAL:CG2	2.48	0.44
1:A:1096:ASN:O	1:A:1097:GLN:C	2.55	0.44
1:A:1024:TYR:HB2	1:A:1298:THR:CG2	2.48	0.44
2:D:857:CYS:CB	2:D:885:VAL:CG2	2.95	0.44
1:A:180:ILE:CG2	1:A:181:GLY:N	2.81	0.44
1:C:33:VAL:HG21	1:C:121:TYR:HE1	1.73	0.44
2:D:1594:LYS:O	2:D:1596:LYS:HG2	2.17	0.44
1:A:955:ARG:O	1:A:1349:SER:HA	2.18	0.44
2:B:922:LYS:HE3	2:B:1329:TYR:OH	2.18	0.44
1:A:1540:ASP:HA	1:A:1660:PHE:CD1	2.53	0.44
1:C:59:TYR:CD1	1:C:60:PRO:HG3	2.53	0.44
1:C:180:ILE:HG13	1:C:599:TRP:CZ3	2.52	0.44
1:C:180:ILE:HG22	1:C:181:GLY:N	2.32	0.44
1:A:316:GLU:HA	1:A:319:ASN:HB2	1.99	0.44
2:B:1486:ILE:HG13	2:B:1486:ILE:O	2.18	0.44
1:A:1016:VAL:O	1:A:1020:TYR:HD2	2.01	0.44
1:A:1066:TYR:CD1	1:A:1079:THR:HG23	2.53	0.44
1:A:599:TRP:O	1:A:803:GLY:CA	2.58	0.44
2:D:178:VAL:HG21	2:D:183:PHE:CD1	2.53	0.44
1:C:443:PRO:CG	1:C:446:ASN:HB2	2.48	0.44
1:A:250:ILE:HG13	1:A:250:ILE:O	2.17	0.44
1:C:1180:LEU:HD21	1:C:1208:ILE:HA	2.00	0.44
1:C:436:LYS:CB	1:C:449:ARG:HG2	2.43	0.44
2:D:834:ALA:C	2:D:835:ILE:HD13	2.38	0.44
1:C:238:ILE:HB	1:C:347:TYR:CE1	2.52	0.44
1:A:483:ASN:HD21	2:B:399:ILE:HB	1.81	0.44
3:Y:73:VAL:CG2	3:Y:74:ARG:N	2.78	0.44
1:A:307:VAL:O	1:A:311:SER:HB2	2.18	0.44
1:A:1627:ILE:HD12	1:A:1629:TYR:HB3	2.00	0.44
2:B:1522:TYR:CE2	2:B:1585:GLY:N	2.79	0.44
1:A:273:GLU:O	1:A:274:ASP:HB3	2.17	0.44
2:D:1567:ARG:HA	2:D:1567:ARG:HD2	1.65	0.44
2:B:63:ARG:HD2	2:B:65:GLN:NE2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:THR:HB	2:D:91:ALA:HB2	1.99	0.44
1:C:375:VAL:O	1:C:383:VAL:HG13	2.16	0.44
1:C:839:ILE:HG23	1:C:840:GLN:N	2.31	0.44
1:C:901:LEU:HA	1:C:902:PRO:HD3	1.82	0.44
1:A:804:ILE:HG22	1:A:809:ILE:CB	2.48	0.44
2:B:263:VAL:HG21	2:B:292:ALA:CB	2.47	0.44
1:A:1561:TYR:HE1	1:A:1581:LEU:HG	1.82	0.44
1:A:1644:TRP:O	1:A:1645:ILE:HD13	2.18	0.44
1:C:1023:HIS:O	1:C:1027:THR:HB	2.17	0.44
1:A:238:ILE:HB	1:A:347:TYR:CE1	2.53	0.44
1:A:321:LYS:O	1:A:347:TYR:HB2	2.18	0.44
1:A:1234:HIS:CG	1:A:1235:LYS:N	2.85	0.44
1:A:856:CYS:HB3	1:A:915:GLU:HG2	1.99	0.44
1:A:915:GLU:CB	2:B:905:TRP:CZ2	3.00	0.44
3:X:91:LYS:NZ	3:X:95:LYS:HE3	2.33	0.44
1:C:1020:TYR:CE1	1:C:1295:GLU:HA	2.52	0.44
1:C:787:GLN:O	1:C:788:PHE:HB3	2.16	0.44
1:A:1163:LYS:CE	1:C:1109:GLU:HG2	2.48	0.44
1:A:1156:PHE:CE1	1:A:1164:ILE:HG13	2.53	0.44
2:B:1438:LEU:HD13	2:B:1438:LEU:O	2.18	0.44
1:A:1031:TRP:CE2	1:A:1042:LYS:HG3	2.52	0.44
1:A:1317:TYR:CE1	1:A:1342:LEU:HD12	2.53	0.44
2:B:1443:LEU:CD1	2:B:1443:LEU:N	2.80	0.44
1:A:132:LYS:HZ1	1:A:139:GLN:HE22	1.65	0.44
2:B:524:TYR:C	2:B:524:TYR:HD1	2.19	0.44
2:B:345:ILE:HG12	2:B:345:ILE:H	1.60	0.44
1:C:917:TRP:HB3	2:D:558:MET:SD	2.58	0.44
1:A:1023:HIS:CD2	1:A:1023:HIS:O	2.70	0.44
2:B:1404:VAL:O	2:B:1428:ASN:ND2	2.50	0.44
2:D:855:ALA:O	2:D:856:PHE:CD1	2.71	0.44
1:A:302:ASP:HB3	1:A:305:THR:HB	2.00	0.44
2:B:949:LYS:H	2:B:949:LYS:HG3	1.54	0.44
1:A:42:GLN:HG2	1:A:43:VAL:H	1.83	0.44
1:A:506:LYS:HD2	1:A:536:PRO:CD	2.48	0.44
1:A:513:GLY:HA2	3:X:146:LEU:HD13	2.00	0.44
1:C:24:VAL:CG2	1:C:554:LEU:HD11	2.48	0.44
1:C:1629:TYR:HE1	1:C:1631:PHE:CD1	2.34	0.44
1:C:532:GLN:CA	1:C:532:GLN:OE1	2.59	0.44
1:A:383:VAL:CG2	1:A:386:VAL:HG21	2.48	0.44
1:C:1069:TRP:CH2	1:C:1465:ASN:ND2	2.86	0.44
1:A:1007:SER:OG	1:A:1008:ALA:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1559:TYR:CE1	1:A:1587:THR:HA	2.53	0.44
1:A:1644:TRP:NE1	1:A:1646:GLU:OE1	2.48	0.44
1:C:60:PRO:CG	1:C:61:ASP:N	2.81	0.44
2:D:397:LYS:NZ	2:D:449:ILE:O	2.51	0.44
2:B:309:LEU:O	2:B:310:VAL:C	2.54	0.44
1:C:317:ASP:O	1:C:319:ASN:N	2.50	0.44
1:A:382:LEU:HD13	1:A:415:ASP:O	2.18	0.44
1:A:949:ILE:HG22	1:A:950:TYR:CZ	2.53	0.44
1:A:1305:LYS:HG3	1:C:101:TYR:OH	2.17	0.44
1:A:643:ALA:O	1:A:644:ASN:C	2.55	0.44
1:C:223:VAL:O	1:C:225:PRO:HD3	2.18	0.44
1:C:1019:PHE:CZ	1:C:1088:GLN:HB3	2.53	0.44
1:A:443:PRO:CG	1:A:446:ASN:HB2	2.48	0.44
2:B:275:SER:O	2:B:277:PRO:HD3	2.17	0.44
1:C:248:ILE:HD13	1:C:325:ILE:HD13	2.00	0.44
1:C:989:SER:O	1:C:993:SER:HB3	2.17	0.44
2:B:1442:ILE:C	2:B:1443:LEU:HD13	2.38	0.44
2:D:1637:GLU:C	2:D:1638:PHE:CD2	2.91	0.44
1:A:176:GLU:HB2	1:A:185:PHE:CE1	2.52	0.44
2:B:243:PHE:C	2:B:243:PHE:HD2	2.20	0.44
2:D:1539:ILE:HD12	2:D:1539:ILE:N	2.32	0.44
1:C:680:GLN:CG	1:C:681:LYS:H	2.31	0.44
2:D:966:GLN:OE1	2:D:1298:LEU:HD13	2.17	0.44
1:C:137:PRO:O	1:C:138:ASP:HB2	2.18	0.44
3:X:215:VAL:O	3:X:216:LEU:HD13	2.18	0.44
2:B:889:GLN:HA	2:B:915:VAL:HB	1.99	0.44
2:D:1521:ASP:OD1	2:D:1552:THR:OG1	2.36	0.44
1:C:1561:TYR:HE1	1:C:1598:ILE:HD11	1.82	0.43
1:C:535:VAL:O	1:C:563:ILE:HG12	2.18	0.43
2:D:285:ILE:CD1	2:D:285:ILE:H	2.30	0.43
2:D:283:ILE:O	2:D:285:ILE:HD12	2.18	0.43
1:C:1227:PHE:HA	1:C:1228:TRP:CE3	2.53	0.43
2:D:736:GLU:HA	2:D:847:ARG:NH2	2.33	0.43
1:C:1090:ASN:ND2	1:C:1158:ILE:HG12	2.33	0.43
2:B:881:PRO:C	2:B:882:PHE:CD2	2.91	0.43
2:B:783:SER:HB3	2:B:785:THR:HG22	2.00	0.43
2:D:850:LEU:CD1	2:D:851:LEU:N	2.81	0.43
1:A:856:CYS:HB2	2:B:904:LEU:HG	1.99	0.43
2:D:1575:LEU:HD13	2:D:1581:TYR:CZ	2.53	0.43
1:A:472:ASN:HA	1:A:474:LYS:HD2	1.99	0.43
2:D:137:TYR:HB2	2:D:216:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1610:TRP:CD2	2:D:1628:PHE:CE2	3.06	0.43
1:A:150:ASP:CG	1:A:151:ASP:N	2.72	0.43
2:D:1635:LEU:O	2:D:1636:THR:C	2.55	0.43
1:A:1320:LYS:HD2	1:A:1320:LYS:HA	1.90	0.43
2:D:913:LEU:C	2:D:913:LEU:CD2	2.86	0.43
2:D:243:PHE:HD2	2:D:243:PHE:C	2.22	0.43
1:A:1627:ILE:O	1:A:1627:ILE:CG1	2.63	0.43
1:C:682:LYS:HZ2	1:C:686:ILE:HD12	1.81	0.43
2:D:932:PRO:HB3	2:D:939:GLY:O	2.18	0.43
1:C:713:GLN:HG3	1:C:713:GLN:H	1.44	0.43
1:C:1257:THR:O	1:C:1261:LEU:HD23	2.17	0.43
2:D:875:LEU:HG	2:D:875:LEU:O	2.18	0.43
1:A:578:ASP:CG	1:A:578:ASP:O	2.56	0.43
1:A:23:TYR:HE2	1:A:111:PHE:HD2	1.65	0.43
1:A:108:SER:OG	1:A:111:PHE:N	2.50	0.43
1:A:475:ALA:O	1:A:476:LEU:HB2	2.18	0.43
1:A:484:ILE:HD13	1:A:540:LEU:HD21	1.98	0.43
1:A:387:PRO:HB2	1:A:438:ASP:HB3	2.00	0.43
1:C:1293:ALA:O	1:C:1294:ILE:C	2.56	0.43
1:A:1075:SER:OG	1:A:1078:LEU:HB2	2.18	0.43
1:C:1638:PRO:O	1:C:1639:LEU:CB	2.62	0.43
1:C:955:ARG:O	1:C:1349:SER:HA	2.18	0.43
1:A:577:PRO:HD2	1:A:588:VAL:CG2	2.48	0.43
1:A:317:ASP:C	1:A:319:ASN:N	2.71	0.43
1:A:855:PHE:HB2	1:A:914:LEU:CD1	2.48	0.43
1:C:419:SER:C	1:C:420:PHE:CD2	2.92	0.43
2:B:326:SER:OG	2:B:327:ASP:N	2.51	0.43
2:B:961:THR:HG22	2:B:1327:THR:OG1	2.18	0.43
2:B:361:GLU:HB3	2:B:399:ILE:CD1	2.48	0.43
1:C:131:ASP:OD2	1:C:132:LYS:HG3	2.18	0.43
2:B:234:PHE:CE1	2:B:236:TYR:CE1	3.06	0.43
2:D:943:GLU:HB2	2:D:1313:VAL:HG23	2.00	0.43
2:D:142:PRO:HB3	2:D:187:ASN:HD22	1.83	0.43
1:C:273:GLU:O	1:C:274:ASP:HB3	2.17	0.43
1:A:359:THR:CG2	1:A:359:THR:O	2.65	0.43
1:C:1084:ARG:CA	1:C:1151:GLY:HA2	2.48	0.43
1:C:1364:VAL:HG13	1:C:1364:VAL:O	2.18	0.43
2:D:930:LEU:HD13	2:D:1315:ALA:HB2	1.99	0.43
1:C:276:LYS:HA	1:C:276:LYS:HD2	1.76	0.43
1:A:40:VAL:HG12	1:A:509:ILE:HD12	2.01	0.43
1:A:465:LEU:HD12	1:A:487:THR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:504:LEU:HD21	1:C:651:LEU:CG	2.48	0.43
1:C:478:VAL:HG11	1:C:566:LYS:HD3	2.01	0.43
2:D:518:PHE:CE2	2:D:538:VAL:CB	2.71	0.43
2:B:1296:ASN:O	2:B:1297:ALA:C	2.56	0.43
2:B:951:ASP:C	2:B:953:ARG:H	2.13	0.43
2:B:1506:ILE:HD11	2:B:1628:PHE:HE1	1.84	0.43
2:D:358:MET:HE2	2:D:467:LYS:HD2	1.99	0.43
2:D:449:ILE:HG23	2:D:449:ILE:O	2.18	0.43
2:D:628:LEU:HD12	2:D:629:THR:H	1.82	0.43
3:Y:81:ASN:O	3:Y:115:ARG:CB	2.53	0.43
1:A:1215:GLU:OE1	1:A:1235:LYS:HD3	2.18	0.43
2:B:89:ILE:CD1	2:B:104:VAL:HG11	2.48	0.43
1:C:742:ILE:CG1	1:C:752:LEU:O	2.65	0.43
1:A:127:PHE:CD1	1:A:127:PHE:N	2.85	0.43
1:A:1249:GLU:O	1:A:1253:TYR:CD2	2.71	0.43
1:C:1226:ARG:HD3	1:C:1266:TYR:CE1	2.54	0.43
2:B:161:VAL:CG2	2:B:180:LEU:HD21	2.43	0.43
1:A:241:LYS:NZ	1:A:351:PRO:HB3	2.34	0.43
2:B:736:GLU:HA	2:B:847:ARG:NH2	2.33	0.43
2:B:456:PRO:HG3	2:B:515:ILE:HD11	2.01	0.43
1:A:1156:PHE:CE2	1:A:1160:PRO:HB3	2.54	0.43
2:D:265:PHE:O	2:D:276:ILE:HG13	2.18	0.43
3:X:169:ILE:HG21	3:X:189:ILE:HD13	1.99	0.43
1:A:1112:GLN:HB2	1:A:1118:PHE:CE1	2.54	0.43
2:D:361:GLU:HB3	2:D:399:ILE:CD1	2.47	0.43
2:D:580:VAL:HG13	2:D:584:VAL:HG23	2.00	0.43
1:C:862:VAL:HG12	1:C:863:GLU:OE1	2.18	0.43
1:C:990:ALA:HB1	1:C:1000:LEU:HD11	2.00	0.43
2:B:745:ILE:CG2	2:B:745:ILE:O	2.66	0.43
1:A:165:ASP:CB	1:A:166:PRO:CD	2.96	0.43
1:C:1439:LEU:O	1:C:1440:LYS:C	2.57	0.43
1:A:990:ALA:HB1	1:A:1000:LEU:HD11	2.01	0.43
1:A:231:ILE:HG12	1:A:231:ILE:O	2.18	0.43
3:Y:54:SER:HB2	3:Y:167:PHE:CE1	2.54	0.43
1:C:389:THR:OG1	1:C:408:LYS:HE2	2.18	0.43
1:A:1257:THR:O	1:A:1261:LEU:HD23	2.19	0.43
1:A:1189:ALA:O	1:A:1192:ALA:HB3	2.19	0.43
2:B:1566:GLN:H	2:B:1566:GLN:HG2	1.50	0.43
3:Y:201:ILE:HD13	3:Y:207:LEU:HD23	2.00	0.43
1:A:500:ASN:OD1	1:A:514:THR:HG23	2.17	0.43
1:A:484:ILE:HD12	1:A:540:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:PHE:HE1	2:B:320:VAL:CG1	2.31	0.43
1:A:1076:THR:HG23	1:A:1077:TRP:N	2.34	0.43
1:A:1546:GLU:HG2	1:A:1663:ASN:HD21	1.80	0.43
2:D:613:SER:HA	2:D:620:VAL:CG2	2.49	0.43
2:B:851:LEU:HD11	2:B:865:ARG:NH2	2.33	0.43
1:A:595:GLY:O	1:A:596:MET:C	2.57	0.43
1:C:671:GLU:HG2	1:C:671:GLU:H	1.62	0.43
2:D:1528:LEU:HD11	2:D:1540:TYR:HB3	1.99	0.43
1:C:847:ASN:OD1	1:C:849:ARG:N	2.51	0.43
1:A:317:ASP:O	1:A:319:ASN:N	2.51	0.43
1:C:433:PHE:N	1:C:433:PHE:CD1	2.87	0.43
2:D:124:GLN:HG3	2:D:124:GLN:O	2.18	0.43
1:A:1573:VAL:HB	1:A:1603:LYS:CD	2.43	0.43
1:C:1300:TYR:C	1:C:1300:TYR:CD2	2.91	0.43
1:C:1327:LYS:C	1:C:1332:ASN:HD22	2.22	0.43
1:C:949:ILE:HA	1:C:949:ILE:HD13	1.81	0.43
1:C:1317:TYR:CZ	1:C:1342:LEU:HG	2.53	0.43
2:B:1454:GLY:O	2:B:1471:PHE:HD1	2.00	0.43
1:C:1358:THR:HB	1:C:1360:HIS:HE1	1.77	0.43
2:D:580:VAL:HG13	2:D:584:VAL:CG2	2.49	0.43
2:B:433:ILE:HG22	2:B:434:ALA:N	2.33	0.43
1:C:274:ASP:HA	1:C:322:TYR:CE2	2.53	0.43
2:B:269:ILE:HG13	2:B:272:ALA:HB3	2.01	0.43
2:B:1378:THR:O	2:B:1379:MET:C	2.57	0.43
2:B:191:LEU:HD12	2:B:958:GLU:HG2	1.99	0.43
2:B:319:THR:HG23	2:B:330:VAL:CG1	2.48	0.43
3:Y:138:VAL:HG12	3:Y:138:VAL:O	2.18	0.43
2:D:1404:VAL:O	2:D:1428:ASN:ND2	2.51	0.43
2:D:1614:ASP:O	2:D:1617:GLN:HG2	2.18	0.43
1:A:1439:LEU:HA	1:A:1439:LEU:HD23	1.64	0.43
3:Y:196:GLU:CD	3:Y:196:GLU:N	2.72	0.43
1:C:837:GLU:OE2	1:C:1430:THR:HB	2.19	0.43
1:C:987:ILE:HD13	1:C:1294:ILE:HG23	2.00	0.43
1:A:33:VAL:CG2	1:A:121:TYR:CD1	2.88	0.43
2:B:954:VAL:CG1	2:B:955:PRO:HD2	2.42	0.43
1:A:1589:GLU:O	1:A:1591:VAL:N	2.51	0.43
1:A:1582:LEU:CD2	1:A:1616:GLN:HG2	2.42	0.43
2:D:355:LYS:HE2	2:D:445:LEU:O	2.18	0.43
2:D:1292:ILE:CD1	2:D:1301:ARG:HE	2.31	0.43
1:C:290:THR:CG2	1:C:297:ALA:HB1	2.48	0.43
2:D:881:PRO:O	2:D:882:PHE:CD2	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:SER:O	1:A:462:GLN:HB2	2.17	0.43
1:C:222:TYR:HE2	1:C:224:LEU:N	2.17	0.43
2:D:830:VAL:HG23	2:D:831:GLU:N	2.33	0.43
2:D:961:THR:HG22	2:D:1327:THR:CB	2.48	0.43
2:D:56:ILE:HD11	2:D:73:VAL:HG23	2.01	0.43
2:D:1391:LEU:HA	2:D:1392:PRO:HD3	1.85	0.43
2:B:800:ILE:HG23	2:B:801:CYS:N	2.31	0.43
1:A:1072:GLY:O	1:A:1073:SER:C	2.55	0.43
1:A:1025:LEU:HD11	1:A:1034:PHE:HZ	1.82	0.43
2:D:1408:ILE:HD13	2:D:1425:ILE:HA	2.00	0.43
2:B:1459:TYR:HB3	2:B:1466:GLU:HB3	1.99	0.43
1:A:829:ILE:CG1	1:A:925:LYS:HG2	2.47	0.43
1:A:109:LYS:HD3	1:A:110:HIS:HE1	1.77	0.43
1:A:984:VAL:HG12	1:A:988:LEU:HD12	2.01	0.43
3:X:185:LYS:CG	3:X:186:TYR:CE2	3.01	0.43
1:C:916:THR:C	1:C:918:PHE:N	2.71	0.43
1:C:1538:GLU:O	1:C:1539:LEU:C	2.57	0.43
1:C:259:VAL:HB	1:C:295:GLY:HA2	2.00	0.43
1:A:1428:LEU:HD11	1:A:1434:ALA:HB2	1.98	0.43
3:Y:166:ASP:O	3:Y:170:ARG:HG3	2.18	0.43
1:C:23:TYR:HD1	1:C:23:TYR:H	1.31	0.43
1:C:113:LYS:HE2	1:C:654:LEU:O	2.19	0.43
2:D:518:PHE:CD2	2:D:518:PHE:O	2.72	0.43
1:C:839:ILE:CD1	1:C:1485:VAL:HG12	2.49	0.43
1:C:901:LEU:HD23	1:C:1527:CYS:SG	2.59	0.43
2:D:618:LEU:CD1	2:D:635:ASN:O	2.65	0.43
2:D:476:ILE:O	2:D:497:ARG:HG2	2.18	0.43
2:D:1273:LEU:C	2:D:1273:LEU:HD12	2.39	0.43
1:C:472:ASN:HA	1:C:474:LYS:HD2	2.01	0.43
2:D:326:SER:OG	2:D:327:ASP:N	2.52	0.43
1:C:1226:ARG:CD	1:C:1266:TYR:CE1	3.01	0.43
1:C:1271:ILE:HD13	1:C:1300:TYR:CE2	2.53	0.43
1:A:1162:VAL:CG2	1:A:1163:LYS:N	2.82	0.43
1:A:1142:LEU:HD21	1:A:1179:THR:OG1	2.19	0.43
1:C:131:ASP:OD2	1:C:132:LYS:CG	2.66	0.43
1:A:680:GLN:CG	1:A:681:LYS:N	2.81	0.43
1:C:177:ILE:HD13	1:C:177:ILE:N	2.33	0.43
1:C:996:GLY:O	1:C:998:ASN:N	2.52	0.43
1:A:847:ASN:C	1:A:847:ASN:OD1	2.55	0.43
1:A:96:GLN:CG	1:A:97:ASN:H	2.31	0.43
3:Y:229:ASN:C	3:Y:230:GLN:HG3	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:ALA:O	2:B:257:VAL:HB	2.18	0.43
2:B:763:THR:C	2:B:764:GLU:HG2	2.39	0.43
2:D:47:GLY:O	2:D:48:ASP:HB2	2.19	0.43
3:X:108:GLU:O	3:X:109:LEU:HG	2.18	0.43
1:A:503:ILE:O	1:A:510:ILE:HG12	2.19	0.43
1:C:501:TYR:O	1:C:512:PHE:HA	2.19	0.43
1:C:551:THR:HB	1:C:657:ALA:HB1	2.00	0.43
1:C:532:GLN:HA	1:C:535:VAL:HG13	2.00	0.43
1:C:980:LYS:HB3	1:C:980:LYS:HE2	1.79	0.43
2:D:951:ASP:C	2:D:953:ARG:H	2.19	0.43
1:A:953:ILE:CD1	1:A:955:ARG:HH21	2.32	0.43
1:A:1646:GLU:HG2	1:A:1660:PHE:HZ	1.84	0.43
1:C:1023:HIS:O	1:C:1023:HIS:CD2	2.71	0.43
1:A:133:PRO:HD2	1:A:609:VAL:CG1	2.48	0.43
2:B:1486:ILE:HD11	2:B:1591:LEU:HD21	2.00	0.43
2:D:828:GLU:O	2:D:886:PRO:HD2	2.18	0.43
2:D:916:VAL:HG22	2:D:917:PRO:N	2.33	0.43
1:A:1106:TRP:CZ2	1:A:1111:TYR:HE2	2.37	0.43
1:C:1213:LYS:HE2	1:C:1266:TYR:HD2	1.78	0.43
2:B:1367:ILE:HB	2:B:1438:LEU:CD1	2.49	0.43
1:C:1249:GLU:O	1:C:1253:TYR:CD2	2.72	0.43
1:A:864:GLY:HA3	1:A:907:LEU:HD22	2.00	0.43
1:A:631:ASP:C	1:A:633:GLY:H	2.22	0.43
1:C:417:VAL:O	1:C:417:VAL:HG12	2.18	0.43
1:C:365:PRO:CD	1:C:464:TYR:CE2	2.98	0.43
1:A:670:LYS:HD2	1:A:671:GLU:H	1.83	0.43
1:C:274:ASP:CG	1:C:275:LEU:N	2.70	0.43
1:A:523:TYR:CE2	2:B:465:ASN:ND2	2.86	0.43
1:A:1043:GLN:O	1:A:1044:LYS:C	2.54	0.43
1:C:1665:ASP:O	1:C:1668:ALA:HB3	2.19	0.43
3:X:211:ARG:O	3:X:214:ASP:HB2	2.18	0.43
2:D:1430:VAL:HA	2:D:1436:GLU:OE2	2.19	0.43
2:B:490:PHE:C	2:B:490:PHE:CD1	2.90	0.43
2:D:551:LYS:HE2	2:D:551:LYS:HB2	1.91	0.43
1:C:383:VAL:CG2	1:C:386:VAL:HG21	2.49	0.43
1:C:505:SER:HB3	1:C:510:ILE:HD13	2.01	0.43
1:C:938:SER:OG	1:C:1284:PHE:CE2	2.71	0.43
1:A:33:VAL:HG23	1:A:120:THR:O	2.18	0.43
1:A:1571:GLU:O	1:A:1574:PHE:N	2.46	0.43
1:C:1012:LEU:HD11	1:C:1056:ILE:HG13	2.01	0.43
1:C:1053:MET:O	1:C:1056:ILE:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:384:PHE:CE1	2:D:400:LEU:HG	2.51	0.43
2:D:1528:LEU:HD21	2:D:1531:ILE:HD11	2.01	0.43
2:D:1275:LEU:HD21	2:D:1319:GLY:O	2.19	0.43
1:A:1263:ASP:O	1:A:1265:ASN:N	2.52	0.43
2:D:933:ARG:NH1	2:D:933:ARG:CG	2.79	0.43
1:C:258:LYS:HD3	1:C:893:SER:OG	2.17	0.43
1:A:539:ARG:HE	1:A:633:GLY:HA3	1.83	0.43
1:A:1317:TYR:CZ	1:A:1342:LEU:HG	2.54	0.43
1:C:1566:THR:HG23	1:C:1578:LYS:O	2.18	0.43
1:C:587:THR:HA	1:C:789:ALA:HA	2.00	0.43
1:A:1403:VAL:HG22	1:A:1476:ARG:HB3	2.01	0.43
2:D:144:LEU:HB3	2:D:185:PRO:HB3	2.01	0.43
2:D:582:LYS:O	2:D:583:ALA:C	2.56	0.43
2:B:345:ILE:HD11	2:B:426:ALA:C	2.38	0.43
3:Y:163:LYS:HG3	3:Y:212:MET:CE	2.49	0.43
1:A:996:GLY:O	1:A:998:ASN:N	2.51	0.43
2:B:1529:LEU:N	2:B:1529:LEU:HD12	2.34	0.43
1:C:64:PHE:HD2	1:C:66:TYR:CE1	2.36	0.43
1:A:1037:ASP:HA	1:A:1038:PRO:HD3	1.62	0.43
1:A:1426:ILE:HG22	1:A:1426:ILE:O	2.18	0.43
1:A:484:ILE:CD1	1:A:540:LEU:CD2	2.97	0.43
1:C:492:TYR:CE2	1:C:546:VAL:HG11	2.53	0.43
2:D:222:PRO:HG2	2:D:329:VAL:HG12	1.99	0.43
2:D:1562:GLN:NE2	2:D:1596:LYS:HZ2	2.15	0.43
2:B:247:ILE:CD1	2:B:318:VAL:HG21	2.49	0.43
2:D:780:LEU:HD11	2:D:787:TRP:HD1	1.84	0.43
1:C:802:VAL:HG12	1:C:803:GLY:N	2.34	0.43
1:A:1602:LYS:HE3	1:A:1609:ALA:O	2.18	0.43
2:D:481:TYR:HE2	2:D:493:GLY:N	2.16	0.43
1:A:390:LEU:HD23	1:A:420:PHE:CD1	2.54	0.43
1:A:433:PHE:CZ	1:A:452:TYR:HB2	2.54	0.43
1:A:931:PRO:CB	1:A:1366:HIS:CD2	3.02	0.43
2:B:794:PHE:CD2	2:B:795:THR:N	2.86	0.43
1:A:1309:LEU:O	1:A:1329:THR:HA	2.19	0.43
1:A:1016:VAL:N	1:A:1017:PRO:CD	2.81	0.43
1:C:1072:GLY:O	1:C:1073:SER:C	2.57	0.43
1:A:1208:ILE:HG22	1:A:1208:ILE:O	2.19	0.43
2:D:1424:ILE:HD13	2:D:1424:ILE:N	2.29	0.43
2:D:1482:ASN:HB3	2:D:1493:ALA:CB	2.49	0.43
2:D:1459:TYR:HB3	2:D:1466:GLU:HB3	1.99	0.43
1:C:132:LYS:HZ1	1:C:139:GLN:HE22	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:975:ARG:CZ	1:C:1340:VAL:HG11	2.49	0.43
2:B:114:ARG:O	2:B:114:ARG:NE	2.51	0.43
2:D:146:ARG:CB	2:D:146:ARG:HH11	2.32	0.43
2:B:810:VAL:O	2:B:811:MET:HB2	2.19	0.43
2:D:1544:VAL:C	2:D:1545:LEU:HD12	2.40	0.43
2:B:1564:ILE:O	2:B:1601:ILE:HD12	2.19	0.43
1:C:653:PHE:CE1	1:C:660:ASP:CB	3.00	0.43
2:D:40:GLN:O	2:D:489:ILE:HD12	2.18	0.43
2:D:341:SER:HA	2:D:342:PRO:HD3	1.72	0.43
1:C:855:PHE:HB2	1:C:914:LEU:HD11	2.00	0.43
1:A:1538:GLU:O	1:A:1539:LEU:C	2.54	0.43
1:A:701:ASP:CG	1:A:1446:VAL:HG23	2.39	0.43
1:C:701:ASP:N	1:C:701:ASP:OD1	2.52	0.43
3:X:174:VAL:HG12	3:X:174:VAL:O	2.19	0.43
1:C:1643:THR:HG22	1:C:1644:TRP:H	1.84	0.43
1:C:511:HIS:CE1	3:Y:149:SER:HB3	2.54	0.43
1:C:1244:THR:O	1:C:1245:ALA:C	2.57	0.43
1:C:837:GLU:O	1:C:901:LEU:CD1	2.65	0.43
1:A:1219:LYS:HB2	1:A:1219:LYS:HE3	1.76	0.43
1:C:628:GLU:HG3	1:C:628:GLU:O	2.18	0.43
1:C:1639:LEU:HA	1:C:1639:LEU:HD22	1.76	0.43
1:A:1556:GLU:HB3	1:A:1622:LYS:CE	2.31	0.43
1:A:373:VAL:CG2	1:A:418:ALA:HB3	2.43	0.43
2:B:851:LEU:HD21	2:B:865:ARG:HH21	1.83	0.43
2:B:840:VAL:CG1	2:B:841:ASN:N	2.77	0.43
1:C:317:ASP:C	1:C:319:ASN:N	2.70	0.43
2:D:1454:GLY:O	2:D:1471:PHE:HD1	2.01	0.43
1:A:1083:LEU:HD13	1:A:1104:LEU:HD23	2.00	0.43
2:B:1454:GLY:HA3	2:B:1472:TYR:CE2	2.54	0.43
2:D:1635:LEU:HD23	2:D:1635:LEU:HA	1.70	0.43
1:C:1127:ILE:HD11	1:C:1143:TYR:CE2	2.54	0.43
3:Y:45:ASP:OD1	3:Y:48:ARG:NH1	2.51	0.43
1:C:487:THR:HA	1:C:488:PRO:HD3	1.83	0.43
1:A:1084:ARG:HG2	1:A:1084:ARG:NH1	2.33	0.43
2:D:550:VAL:HG22	2:D:567:LEU:HD21	2.01	0.43
2:B:764:GLU:HG3	2:B:772:SER:HB3	2.01	0.43
1:A:1406:ALA:O	1:A:1472:PHE:HA	2.18	0.43
2:B:895:GLU:HA	2:B:909:VAL:O	2.19	0.43
1:A:582:TYR:O	1:A:819:VAL:HG13	2.18	0.43
2:B:315:TYR:C	2:B:315:TYR:CD1	2.91	0.43
3:X:196:GLU:N	3:X:196:GLU:CD	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1175:LEU:HD23	1:C:1175:LEU:HA	1.88	0.43
1:A:40:VAL:HG23	1:A:41:ILE:H	1.83	0.42
1:C:515:ARG:HG3	1:C:515:ARG:NH1	2.33	0.42
1:C:1562:LYS:C	1:C:1563:VAL:HG13	2.38	0.42
1:A:1093:VAL:O	1:A:1094:GLU:C	2.57	0.42
1:C:33:VAL:CG2	1:C:121:TYR:CD1	2.87	0.42
1:A:1245:ALA:O	1:A:1246:ARG:C	2.56	0.42
2:B:247:ILE:HD11	2:B:318:VAL:HG21	2.01	0.42
1:C:1075:SER:OG	1:C:1078:LEU:HB2	2.18	0.42
1:A:223:VAL:O	1:A:225:PRO:HD3	2.19	0.42
1:C:869:GLU:HB2	1:C:871:PRO:HG3	2.01	0.42
2:D:878:ARG:HE	2:D:1421:VAL:CG2	2.32	0.42
2:B:235:PHE:CE2	2:B:299:PHE:CE2	3.06	0.42
1:C:569:ASN:HD21	1:C:810:CYS:HB2	1.84	0.42
3:Y:194:LYS:HG2	3:Y:197:ASN:HB3	2.01	0.42
1:A:640:LEU:H	1:A:644:ASN:CB	2.28	0.42
1:A:824:PHE:CE2	1:A:846:TYR:CD1	3.05	0.42
2:D:1471:PHE:O	2:D:1478:THR:O	2.37	0.42
1:A:1163:LYS:NZ	1:C:1109:GLU:HG2	2.34	0.42
2:B:1469:THR:O	2:B:1470:LYS:HG2	2.19	0.42
2:D:267:VAL:HG22	2:D:314:LEU:CD1	2.49	0.42
1:C:161:LEU:N	1:C:161:LEU:HD12	2.32	0.42
1:C:1402:ILE:CG2	1:C:1403:VAL:N	2.82	0.42
2:B:1522:TYR:HD1	2:B:1524:TYR:CZ	2.36	0.42
2:B:345:ILE:HG13	2:B:428:LYS:CB	2.49	0.42
1:A:997:ILE:O	1:A:998:ASN:O	2.37	0.42
2:D:63:ARG:HD2	2:D:65:GLN:NE2	2.33	0.42
2:B:1631:PHE:HD2	2:B:1632:SER:N	2.16	0.42
1:A:710:THR:N	1:A:713:GLN:OE1	2.50	0.42
1:A:522:SER:HB2	1:A:523:TYR:H	1.54	0.42
1:C:117:MET:HE2	1:C:117:MET:HB2	1.71	0.42
2:B:875:LEU:HG	2:B:875:LEU:O	2.19	0.42
1:A:108:SER:HG	1:A:111:PHE:C	2.22	0.42
1:A:364:LYS:HE2	1:A:465:LEU:O	2.18	0.42
1:C:108:SER:HG	1:C:111:PHE:C	2.23	0.42
1:C:73:LEU:HB2	1:C:79:PHE:HA	2.01	0.42
1:C:1622:LYS:HZ3	1:C:1642:LEU:CD2	2.27	0.42
1:C:969:PRO:C	1:C:971:THR:HG23	2.40	0.42
1:C:973:ILE:HG22	1:C:973:ILE:O	2.17	0.42
1:A:1219:LYS:HE2	1:A:1239:VAL:CG2	2.49	0.42
1:C:871:PRO:O	1:C:873:ILE:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1560:ALA:O	1:A:1561:TYR:CB	2.67	0.42
1:A:291:MET:HB3	1:A:291:MET:HE2	1.75	0.42
2:D:126:SER:OG	2:D:152:HIS:HD2	2.02	0.42
1:C:1110:ASN:O	1:C:1111:TYR:CD1	2.72	0.42
1:A:461:SER:HB3	1:A:553:GLU:OE2	2.19	0.42
1:A:491:PRO:CG	1:A:491:PRO:O	2.67	0.42
2:B:449:ILE:HA	2:B:449:ILE:HD12	1.71	0.42
1:A:821:LYS:HB3	1:A:822:ASP:H	1.34	0.42
1:A:949:ILE:CG2	1:A:949:ILE:O	2.66	0.42
1:C:100:SER:C	1:C:101:TYR:HD2	2.22	0.42
1:A:639:GLY:HA2	1:A:648:LEU:CD1	2.45	0.42
3:Y:91:LYS:NZ	3:Y:95:LYS:HE3	2.34	0.42
1:A:1146:ALA:HB3	1:A:1190:ILE:CG2	2.48	0.42
2:D:820:MET:HA	2:D:821:PRO:HD3	1.73	0.42
1:C:190:ILE:CG2	1:C:191:PRO:CD	2.97	0.42
1:A:255:PHE:O	1:A:256:TYR:HB2	2.19	0.42
1:A:689:LYS:CD	1:A:730:GLU:OE2	2.67	0.42
2:D:1548:ILE:CG2	2:D:1635:LEU:CB	2.95	0.42
1:C:1673:LEU:O	1:C:1674:ASN:CB	2.65	0.42
1:A:862:VAL:O	1:A:865:ILE:HG13	2.19	0.42
2:D:1370:ARG:HG3	2:D:1431:SER:O	2.19	0.42
2:B:1544:VAL:C	2:B:1545:LEU:HD12	2.40	0.42
2:B:1538:ASP:OD2	2:B:1567:ARG:HD2	2.19	0.42
1:C:1344:ASP:OD1	1:C:1345:ASP:N	2.52	0.42
2:B:967:GLY:O	2:B:969:PRO:HD3	2.18	0.42
2:D:417:HIS:O	2:D:419:ASP:N	2.52	0.42
1:C:383:VAL:HG23	1:C:386:VAL:HG23	2.01	0.42
1:C:386:VAL:HA	1:C:387:PRO:HD3	1.83	0.42
1:C:1644:TRP:O	1:C:1645:ILE:CD1	2.66	0.42
1:A:1244:THR:N	1:A:1247:MET:HE3	2.33	0.42
1:A:946:PRO:O	1:A:953:ILE:HG13	2.19	0.42
1:A:1559:TYR:HB3	1:A:1637:TYR:HE1	1.84	0.42
2:D:482:LEU:CB	2:D:492:VAL:HG23	2.33	0.42
1:A:420:PHE:N	1:A:420:PHE:CD2	2.86	0.42
1:A:290:THR:CG2	1:A:297:ALA:HB1	2.48	0.42
2:B:878:ARG:HE	2:B:1421:VAL:CG2	2.32	0.42
1:A:489:LYS:HZ3	2:B:501:GLN:HA	1.85	0.42
1:A:1226:ARG:HD3	1:A:1266:TYR:HE1	1.85	0.42
1:A:1327:LYS:HG3	1:A:1328:MET:N	2.35	0.42
1:A:949:ILE:O	1:A:950:TYR:CD1	2.72	0.42
3:Y:71:ASN:HD22	3:Y:91:LYS:CD	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:153:PHE:CE1	3:Y:169:ILE:HD13	2.55	0.42
2:B:1583:ILE:CG1	2:B:1607:ILE:HG23	2.42	0.42
1:C:354:LEU:HD22	1:C:448:ALA:HB1	2.01	0.42
1:A:185:PHE:HD1	1:A:186:PRO:HD2	1.84	0.42
1:C:1468:PRO:HD2	1:C:1473:LEU:HB2	2.01	0.42
3:X:217:ASN:ND2	3:X:220:ASP:OD2	2.48	0.42
1:C:1080:ALA:HB2	1:C:1148:THR:HG22	2.02	0.42
2:D:451:SER:O	2:D:452:THR:HG23	2.19	0.42
1:C:909:ASN:HD21	4:C:2003:NAG:C8	2.32	0.42
1:A:1348:VAL:HG11	1:A:1359:VAL:HG21	2.01	0.42
2:D:568:GLU:HA	2:D:772:SER:O	2.19	0.42
1:A:111:PHE:O	1:A:112:SER:OG	2.30	0.42
1:A:49:ALA:CB	1:A:74:SER:HB2	2.50	0.42
1:C:969:PRO:O	1:C:971:THR:HG23	2.19	0.42
1:A:386:VAL:HA	1:A:387:PRO:HD3	1.82	0.42
2:D:247:ILE:CD1	2:D:318:VAL:HG21	2.48	0.42
2:B:1610:TRP:CE3	2:B:1628:PHE:CD2	3.08	0.42
2:B:1626:ASP:O	2:B:1627:ASP:C	2.58	0.42
1:A:1560:ALA:O	1:A:1561:TYR:CD2	2.70	0.42
1:A:1648:TRP:HE1	1:A:1664:LEU:HD21	1.82	0.42
2:D:616:ASN:OD1	2:D:618:LEU:HB2	2.20	0.42
3:X:194:LYS:HG2	3:X:197:ASN:HB3	2.00	0.42
1:A:433:PHE:N	1:A:433:PHE:CD1	2.88	0.42
1:A:216:TYR:HD2	1:A:216:TYR:N	2.16	0.42
2:D:174:SER:HA	2:D:1300:ALA:HB2	2.02	0.42
2:D:964:ILE:HG22	2:D:1324:THR:OG1	2.18	0.42
1:A:968:VAL:CG2	1:A:971:THR:HG21	2.49	0.42
2:B:563:MET:SD	2:B:808:ILE:HD11	2.60	0.42
2:B:449:ILE:HG23	2:B:449:ILE:O	2.18	0.42
1:A:243:PHE:O	1:A:303:SER:HB2	2.18	0.42
1:A:315:LEU:HD11	1:A:318:LEU:HG	1.99	0.42
1:A:683:ILE:O	1:A:687:ALA:HB3	2.19	0.42
1:C:1328:MET:HE2	1:C:1328:MET:HA	2.01	0.42
2:D:1391:LEU:HB2	2:D:1417:MET:CE	2.48	0.42
2:D:1612:HIS:N	2:D:1615:GLU:OE1	2.46	0.42
2:B:344:GLN:O	2:B:366:VAL:HA	2.18	0.42
2:B:236:TYR:O	2:B:238:ASP:N	2.52	0.42
2:D:859:ALA:CB	2:D:866:TYR:CD1	3.00	0.42
1:A:829:ILE:HD12	1:A:829:ILE:N	2.34	0.42
1:C:455:ILE:HG22	1:C:456:ALA:H	1.83	0.42
2:D:345:ILE:HD11	2:D:427:THR:CA	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1188:LEU:CD2	1:C:1212:LEU:HA	2.49	0.42
1:A:662:SER:O	1:A:663:GLN:C	2.57	0.42
3:Y:217:ASN:ND2	3:Y:220:ASP:OD2	2.51	0.42
1:C:1439:LEU:HA	1:C:1439:LEU:HD23	1.71	0.42
1:C:333:THR:OG1	1:C:334:GLY:N	2.52	0.42
1:C:1189:ALA:O	1:C:1192:ALA:HB3	2.19	0.42
2:B:74:ASP:OD1	2:B:74:ASP:N	2.45	0.42
2:D:781:ARG:HD3	2:D:781:ARG:HA	1.53	0.42
1:A:114:SER:O	1:A:115:LYS:HE2	2.20	0.42
1:C:40:VAL:CG2	1:C:512:PHE:CD1	2.99	0.42
1:C:42:GLN:OE1	1:C:500:ASN:ND2	2.52	0.42
1:C:554:LEU:HD23	1:C:554:LEU:HA	1.64	0.42
2:D:224:PHE:HE1	2:D:320:VAL:CG1	2.33	0.42
1:C:215:ALA:C	1:C:216:TYR:CD2	2.93	0.42
1:C:1637:TYR:HB3	1:C:1638:PRO:HD2	2.01	0.42
1:C:804:ILE:HG22	1:C:809:ILE:CB	2.49	0.42
1:A:837:GLU:O	1:A:901:LEU:CD1	2.65	0.42
1:C:134:VAL:HA	1:C:218:GLU:O	2.19	0.42
3:Y:125:LYS:HD2	3:Y:126:ASN:HA	2.02	0.42
2:D:455:LYS:O	2:D:458:ASP:CB	2.58	0.42
2:B:1444:LYS:NZ	2:B:1447:GLU:HA	2.34	0.42
1:A:571:LEU:HG	1:A:812:ALA:HB2	2.02	0.42
1:C:1267:VAL:O	1:C:1270:VAL:HB	2.19	0.42
1:C:981:GLY:O	1:C:1356:LEU:O	2.38	0.42
2:B:1284:ARG:HD2	2:B:1285:GLU:N	2.24	0.42
2:D:147:VAL:HG12	2:D:183:PHE:CE1	2.50	0.42
1:C:191:PRO:O	1:C:194:PRO:HD3	2.20	0.42
1:C:1161:LEU:O	1:C:1164:ILE:HG12	2.19	0.42
2:B:1383:ASP:O	2:B:1456:VAL:HA	2.18	0.42
2:D:188:LEU:HD13	2:D:216:VAL:CG2	2.50	0.42
1:C:693:SER:O	1:C:695:VAL:N	2.53	0.42
3:X:153:PHE:CZ	3:X:169:ILE:HD13	2.55	0.42
1:C:997:ILE:O	1:C:998:ASN:O	2.37	0.42
3:Y:103:VAL:HA	3:Y:121:GLY:O	2.19	0.42
2:D:280:LEU:HD22	2:D:1462:TYR:CE2	2.54	0.42
1:C:328:THR:OG1	1:C:339:GLU:HG2	2.19	0.42
2:B:781:ARG:HA	2:B:781:ARG:HD3	1.53	0.42
3:Y:190:ILE:O	3:Y:190:ILE:HG12	2.18	0.42
1:C:383:VAL:HG23	1:C:386:VAL:CG2	2.49	0.42
1:A:545:ILE:HG12	1:A:545:ILE:H	1.44	0.42
1:C:461:SER:O	1:C:462:GLN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:VAL:HG12	1:C:509:ILE:HD12	2.00	0.42
1:C:74:SER:C	1:C:79:PHE:CE1	2.93	0.42
1:C:1560:ALA:C	1:C:1561:TYR:CD2	2.93	0.42
1:C:839:ILE:HD12	1:C:1485:VAL:HG12	2.01	0.42
1:A:1298:THR:O	1:A:1301:SER:N	2.53	0.42
1:C:1283:GLY:HA3	1:C:1290:THR:HG23	2.02	0.42
1:A:1239:VAL:N	1:A:1240:PRO:CD	2.82	0.42
2:D:955:PRO:O	2:D:957:THR:HG23	2.20	0.42
1:C:216:TYR:HD2	1:C:216:TYR:N	2.17	0.42
1:C:1571:GLU:O	1:C:1574:PHE:N	2.49	0.42
2:B:164:GLU:HB2	2:B:200:VAL:HG23	2.02	0.42
2:B:965:ILE:O	2:B:1301:ARG:HG2	2.19	0.42
1:C:829:ILE:CD1	1:C:829:ILE:N	2.82	0.42
1:C:829:ILE:HD12	1:C:829:ILE:N	2.33	0.42
2:B:1610:TRP:CE3	2:B:1628:PHE:HD2	2.38	0.42
2:D:736:GLU:C	2:D:738:GLY:H	2.22	0.42
2:D:838:ASN:CG	2:D:838:ASN:O	2.58	0.42
2:D:523:TYR:CB	2:D:533:ALA:HB2	2.48	0.42
2:D:200:VAL:HG12	2:D:211:THR:HG1	1.80	0.42
1:C:718:ILE:HD11	1:C:728:PHE:CD2	2.54	0.42
2:B:785:THR:OG1	2:B:786:THR:N	2.51	0.42
2:B:968:ASP:O	2:B:1273:LEU:HD23	2.20	0.42
1:C:752:LEU:O	1:C:752:LEU:CG	2.67	0.42
1:A:622:ARG:HD3	1:A:622:ARG:HA	1.73	0.42
3:Y:101:GLN:HB3	3:Y:123:THR:O	2.20	0.42
1:A:129:HIS:CE1	1:A:620:LEU:HD21	2.54	0.42
1:C:949:ILE:O	1:C:950:TYR:CD1	2.73	0.42
2:B:599:TRP:O	2:B:600:ASP:C	2.55	0.42
2:D:952:ASP:O	2:D:1331:ALA:CA	2.67	0.42
1:C:287:MET:SD	1:C:299:VAL:HG23	2.60	0.42
1:A:160:VAL:HG11	1:A:204:LYS:HE3	2.01	0.42
2:D:504:VAL:HG12	2:D:504:VAL:O	2.19	0.42
2:B:296:ARG:NH1	2:B:296:ARG:HG3	2.32	0.42
1:C:680:GLN:CG	1:C:681:LYS:N	2.80	0.42
1:A:205:TYR:HA	1:A:205:TYR:HD2	1.73	0.42
3:Y:119:VAL:HG22	3:Y:212:MET:HB2	2.01	0.42
2:B:873:LYS:CD	2:B:873:LYS:N	2.82	0.42
3:X:83:GLN:HG2	3:X:85:PHE:HE1	1.85	0.42
2:D:80:GLY:O	2:D:81:MET:HB2	2.18	0.42
1:C:96:GLN:CG	1:C:97:ASN:H	2.29	0.42
1:C:582:TYR:O	1:C:819:VAL:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:905:ILE:O	1:A:905:ILE:HG22	2.19	0.42
1:A:115:LYS:HE2	1:A:115:LYS:HB2	1.82	0.42
1:C:506:LYS:HD2	1:C:536:PRO:HG2	2.01	0.42
1:C:1239:VAL:O	1:C:1240:PRO:C	2.58	0.42
1:A:1147:PHE:HD2	1:A:1147:PHE:C	2.23	0.42
1:A:1639:LEU:HD22	1:A:1639:LEU:HA	1.76	0.42
1:C:1022:PHE:HE2	1:C:1092:TYR:CD1	2.37	0.42
2:D:1290:TYR:HD2	2:D:1301:ARG:HB3	1.83	0.42
1:A:883:CYS:HB2	2:B:902:GLU:OE2	2.20	0.42
2:B:806:TYR:C	2:B:806:TYR:CD1	2.90	0.42
3:Y:194:LYS:HZ2	3:Y:197:ASN:CB	2.15	0.42
1:A:700:TYR:O	1:A:703:ALA:N	2.52	0.42
2:B:1528:LEU:HD21	2:B:1531:ILE:HD11	2.02	0.42
1:C:821:LYS:HB3	1:C:822:ASP:H	1.31	0.42
2:D:159:LYS:HE2	2:D:180:LEU:HD12	2.01	0.42
1:A:309:GLU:CG	1:A:310:LEU:N	2.83	0.42
2:B:933:ARG:HH11	2:B:933:ARG:CG	2.21	0.42
1:A:255:PHE:HB2	1:A:846:TYR:OH	2.20	0.42
2:B:275:SER:C	2:B:277:PRO:HD3	2.40	0.42
1:A:1083:LEU:HD22	1:A:1104:LEU:HD21	2.00	0.42
1:C:1190:ILE:CG1	1:C:1253:TYR:CE1	2.99	0.42
1:C:123:ASN:N	1:C:211:THR:HG23	2.33	0.42
2:D:1624:LEU:O	2:D:1627:ASP:N	2.53	0.42
2:D:1633:TYR:HE1	2:D:1637:GLU:OE1	2.03	0.42
2:B:1371:TYR:CB	2:B:1377:SER:HB3	2.50	0.42
2:D:114:ARG:O	2:D:114:ARG:NE	2.52	0.42
2:B:580:VAL:HG13	2:B:584:VAL:HG23	2.00	0.42
2:B:1491:ARG:HG3	2:B:1492:CYS:N	2.33	0.42
2:B:516:PRO:HG2	2:B:603:GLU:HG3	2.00	0.42
2:B:811:MET:HG3	2:B:812:LYS:N	2.35	0.42
2:B:355:LYS:N	2:B:355:LYS:CD	2.82	0.42
1:C:1386:ILE:HG22	1:C:1399:TYR:O	2.19	0.42
2:B:1423:VAL:CG1	2:B:1423:VAL:O	2.67	0.42
2:B:203:TYR:O	2:B:204:GLU:C	2.57	0.42
1:C:1440:LYS:O	1:C:1443:VAL:HG12	2.20	0.42
1:A:259:VAL:HB	1:A:295:GLY:CA	2.49	0.42
2:D:764:GLU:O	2:D:765:GLU:C	2.58	0.42
2:B:1521:ASP:OD1	2:B:1552:THR:OG1	2.35	0.42
1:C:23:TYR:CE1	1:C:655:THR:CB	3.03	0.42
1:C:367:ILE:HD13	1:C:466:TYR:HD2	1.84	0.42
2:D:1598:SER:C	2:D:1599:TYR:HD1	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1246:ARG:HG3	1:A:1246:ARG:O	2.18	0.42
2:B:1594:LYS:O	2:B:1596:LYS:HG2	2.20	0.42
1:A:1643:THR:HG22	1:A:1644:TRP:H	1.82	0.42
2:B:838:ASN:OD1	2:B:838:ASN:C	2.58	0.42
2:B:121:LEU:HA	2:B:121:LEU:HD12	1.72	0.42
1:A:1265:ASN:C	1:A:1267:VAL:N	2.73	0.42
1:A:950:TYR:HE2	1:A:1356:LEU:HD11	1.84	0.42
1:A:308:LYS:CG	1:A:309:GLU:N	2.81	0.42
2:D:1575:LEU:CD2	2:D:1575:LEU:N	2.83	0.42
1:C:1016:VAL:O	1:C:1020:TYR:HD2	2.03	0.42
1:C:1329:THR:HG1	1:C:1331:LYS:HG2	1.85	0.42
1:C:773:TRP:CZ3	1:C:788:PHE:CE1	3.08	0.42
2:B:513:ASP:OD2	2:B:513:ASP:N	2.52	0.42
1:A:1161:LEU:O	1:A:1164:ILE:HG12	2.20	0.42
2:B:234:PHE:CD1	2:B:234:PHE:C	2.93	0.42
2:D:1279:ILE:HG22	2:D:1288:ILE:CB	2.44	0.42
1:A:829:ILE:N	1:A:829:ILE:CD1	2.82	0.42
2:D:1522:TYR:HE2	2:D:1585:GLY:C	2.23	0.42
2:B:745:ILE:HD11	2:B:907:ASP:N	2.34	0.42
3:X:215:VAL:C	3:X:216:LEU:HD22	2.40	0.42
2:D:1513:GLU:O	2:D:1516:CYS:N	2.53	0.42
3:X:157:LYS:HA	3:X:157:LYS:HD3	1.83	0.42
3:Y:60:VAL:HG23	3:Y:60:VAL:O	2.19	0.42
1:A:500:ASN:O	1:A:542:VAL:HA	2.19	0.42
1:C:971:THR:O	1:C:972:GLU:C	2.58	0.42
2:D:220:VAL:O	2:D:221:LEU:C	2.57	0.42
1:C:1069:TRP:HH2	1:C:1465:ASN:CG	2.24	0.42
1:C:781:PRO:C	1:C:783:ARG:H	2.20	0.42
2:D:869:GLN:O	2:D:870:PHE:HB3	2.20	0.42
1:C:1066:TYR:HD1	1:C:1066:TYR:N	2.18	0.42
2:B:780:LEU:CD1	2:B:787:TRP:CD1	3.03	0.42
1:A:698:CYS:O	1:A:700:TYR:N	2.52	0.42
1:A:569:ASN:HD21	1:A:810:CYS:HB2	1.84	0.42
2:B:618:LEU:HG	2:B:634:LEU:HD11	2.01	0.42
2:B:56:ILE:HD11	2:B:73:VAL:HG23	2.01	0.42
1:A:354:LEU:HD22	1:A:448:ALA:HB1	2.02	0.42
1:A:644:ASN:ND2	1:A:648:LEU:HD12	2.35	0.42
1:A:1106:TRP:O	1:A:1110:ASN:OD1	2.38	0.42
1:A:1149:VAL:O	1:A:1153:ARG:HB2	2.19	0.42
2:B:736:GLU:OE1	2:B:737:ASP:N	2.51	0.42
1:C:352:TYR:HE2	1:C:442:LEU:CD1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1159:CYS:SG	1:A:1161:LEU:CD2	3.07	0.42
1:C:436:LYS:HG3	1:C:437:THR:N	2.34	0.42
1:A:590:LEU:HD21	1:A:774:LEU:HD11	2.01	0.42
2:D:1520:VAL:HG11	2:D:1584:TRP:CD1	2.55	0.42
2:B:834:ALA:C	2:B:835:ILE:HD13	2.39	0.42
2:D:1511:GLN:O	2:D:1514:LYS:HB2	2.20	0.42
1:A:825:LEU:HB2	1:A:845:VAL:CG2	2.50	0.42
2:B:141:SER:HA	2:B:142:PRO:HD3	1.85	0.42
1:A:854:GLN:N	1:A:854:GLN:NE2	2.68	0.42
1:A:604:ALA:O	1:A:772:SER:HB3	2.19	0.42
2:B:1294:TYR:O	2:B:1294:TYR:CD2	2.73	0.42
2:D:1555:ASN:O	2:D:1558:ALA:HB3	2.20	0.42
1:A:1297:LEU:CD1	1:A:1297:LEU:H	2.33	0.42
1:C:1652:THR:HG22	1:C:1653:THR:N	2.35	0.42
1:A:502:LEU:O	1:A:503:ILE:HD13	2.19	0.42
2:B:518:PHE:HE2	2:B:538:VAL:CG1	2.33	0.42
1:C:644:ASN:HA	1:C:644:ASN:HD22	1.59	0.42
1:C:651:LEU:HD23	1:C:651:LEU:HA	1.69	0.42
1:C:931:PRO:CB	1:C:1366:HIS:CD2	3.00	0.42
1:C:835:ARG:HH22	1:C:971:THR:HG22	1.84	0.42
2:D:416:ASN:CA	2:D:425:GLN:HE22	2.22	0.42
1:C:839:ILE:HA	1:C:839:ILE:HD12	1.78	0.42
1:A:1090:ASN:HD22	1:A:1158:ILE:HG12	1.85	0.42
1:A:1245:ALA:O	1:A:1247:MET:N	2.52	0.42
1:C:215:ALA:C	1:C:216:TYR:HD2	2.23	0.42
1:C:698:CYS:O	1:C:700:TYR:N	2.53	0.42
2:B:844:ILE:O	2:B:871:PRO:HA	2.20	0.42
1:A:1232:LEU:HG	1:A:1233:GLN:H	1.83	0.42
1:A:417:VAL:HG12	1:A:417:VAL:O	2.20	0.42
2:D:1349:VAL:O	2:D:1350:GLU:HB3	2.20	0.42
1:A:1156:PHE:HZ	1:A:1165:ASP:HB2	1.84	0.42
2:D:1615:GLU:HB3	2:D:1621:PHE:CE1	2.54	0.42
1:C:267:ILE:CG2	1:C:268:THR:N	2.83	0.42
1:A:117:MET:HB2	1:A:117:MET:HE2	1.68	0.42
2:B:460:LEU:CD2	2:B:508:LEU:HB3	2.50	0.42
1:C:689:LYS:CD	1:C:730:GLU:OE2	2.68	0.42
1:A:989:SER:O	1:A:993:SER:HB2	2.19	0.42
2:D:581:ASP:C	2:D:583:ALA:N	2.73	0.42
2:B:341:SER:HB2	2:B:426:ALA:HB2	2.02	0.42
1:A:177:ILE:N	1:A:177:ILE:HD13	2.35	0.42
1:A:1548:ARG:C	1:A:1550:GLN:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:946:LYS:N	2:B:946:LYS:CD	2.82	0.42
2:B:1518:THR:HG23	2:B:1519:ASN:H	1.85	0.42
2:D:1282:PRO:O	2:D:1283:ASP:C	2.57	0.42
1:C:977:LEU:CD2	1:C:1361:VAL:HG22	2.49	0.42
1:A:259:VAL:HB	1:A:295:GLY:HA2	2.01	0.42
2:B:932:PRO:HB3	2:B:939:GLY:O	2.20	0.42
1:C:27:ALA:HB1	1:C:28:PRO:CD	2.50	0.42
1:C:414:ASP:OD1	1:C:414:ASP:N	2.53	0.42
1:C:1559:TYR:HE1	1:C:1587:THR:HA	1.85	0.41
1:C:505:SER:O	1:C:506:LYS:C	2.56	0.41
1:C:510:ILE:HG22	3:Y:150:ILE:HD11	2.01	0.41
1:C:1243:GLY:O	1:C:1285:TYR:CE2	2.73	0.41
1:A:1069:TRP:HH2	1:A:1465:ASN:CG	2.23	0.41
1:C:1576:LYS:CG	1:C:1601:ILE:HG22	2.40	0.41
2:B:1331:ALA:O	2:B:1332:GLN:CB	2.55	0.41
1:C:1022:PHE:O	1:C:1023:HIS:C	2.58	0.41
2:B:438:GLN:HE22	2:B:530:GLU:HA	1.85	0.41
1:A:961:TYR:CE2	1:A:1343:ASN:CA	3.00	0.41
3:X:113:ASN:HD21	3:X:115:ARG:HG2	1.85	0.41
3:Y:100:GLY:O	3:Y:125:LYS:CG	2.67	0.41
1:C:308:LYS:CG	1:C:309:GLU:N	2.82	0.41
1:C:1573:VAL:HG12	1:C:1603:LYS:CB	2.45	0.41
1:A:123:ASN:O	1:A:211:THR:CG2	2.66	0.41
1:C:943:THR:CG2	1:C:1356:LEU:HD21	2.50	0.41
1:C:1108:VAL:CG2	1:C:1167:ALA:CB	2.97	0.41
2:D:1329:TYR:CD2	2:D:1329:TYR:N	2.88	0.41
1:C:1307:LEU:H	1:C:1307:LEU:HD22	1.85	0.41
1:C:1208:ILE:HG22	1:C:1208:ILE:O	2.19	0.41
2:D:276:ILE:HB	2:D:279:SER:OG	2.20	0.41
2:B:1349:VAL:O	2:B:1350:GLU:HB3	2.20	0.41
1:A:1113:LEU:HD23	1:A:1114:ASP:H	1.85	0.41
1:A:1011:GLU:HG3	1:A:1055:SER:CB	2.50	0.41
5:B:2001:NAG:O3	5:B:2002:NAG:O5	2.38	0.41
3:Y:209:PHE:O	3:Y:212:MET:HB2	2.20	0.41
1:A:1554:LYS:CG	1:A:1555:PRO:HD2	2.50	0.41
2:D:946:LYS:CD	2:D:946:LYS:N	2.83	0.41
2:B:632:THR:O	2:B:633:ASN:C	2.56	0.41
1:C:644:ASN:O	1:C:645:VAL:C	2.58	0.41
1:A:979:VAL:CG2	1:A:1326:TYR:HE1	2.27	0.41
2:B:126:SER:OG	2:B:152:HIS:HD2	2.02	0.41
2:D:355:LYS:HA	2:D:356:PRO:HD3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:ILE:CD1	1:A:1485:VAL:HG12	2.50	0.41
2:D:524:TYR:HD1	2:D:524:TYR:C	2.22	0.41
2:B:506:MET:O	2:B:506:MET:HG2	2.17	0.41
1:A:613:GLN:C	1:A:615:GLY:N	2.73	0.41
1:C:1016:VAL:N	1:C:1017:PRO:CD	2.83	0.41
2:D:961:THR:HG22	2:D:1327:THR:OG1	2.19	0.41
3:Y:169:ILE:HG21	3:Y:189:ILE:HD13	2.02	0.41
1:C:1342:LEU:H	1:C:1342:LEU:HG	1.50	0.41
2:B:1581:TYR:HA	2:B:1608:GLU:O	2.20	0.41
1:C:260:VAL:CG1	1:C:261:THR:N	2.82	0.41
1:A:1423:VAL:HG22	1:A:1496:TYR:HE2	1.85	0.41
1:C:1033:ILE:HG23	1:C:1034:PHE:CD1	2.55	0.41
1:C:984:VAL:HG12	1:C:988:LEU:HD12	2.01	0.41
2:B:355:LYS:HA	2:B:356:PRO:HD3	1.85	0.41
1:A:544:TYR:HD2	1:A:544:TYR:O	2.04	0.41
1:A:1084:ARG:HB2	1:A:1151:GLY:HA2	2.00	0.41
2:D:203:TYR:O	2:D:204:GLU:C	2.59	0.41
2:B:1529:LEU:O	2:B:1577:VAL:HG13	2.20	0.41
2:B:816:ILE:HD12	2:B:909:VAL:HG23	2.02	0.41
1:A:602:LEU:HA	1:A:801:GLY:HA2	2.02	0.41
2:D:874:ALA:C	2:D:876:SER:N	2.72	0.41
2:B:966:GLN:HG3	2:B:966:GLN:O	2.20	0.41
2:D:1410:ARG:HA	2:D:1410:ARG:HD2	1.81	0.41
1:C:498:HIS:ND1	1:C:516:GLU:HA	2.35	0.41
1:C:504:LEU:HD13	1:C:509:ILE:HG23	1.99	0.41
2:B:1598:SER:C	2:B:1599:TYR:HD1	2.22	0.41
1:A:222:TYR:HE2	1:A:224:LEU:N	2.18	0.41
2:B:1476:LYS:HB3	2:B:1476:LYS:HE3	1.90	0.41
1:A:1571:GLU:O	1:A:1574:PHE:CG	2.73	0.41
2:D:355:LYS:N	2:D:355:LYS:CD	2.81	0.41
3:X:194:LYS:HZ2	3:X:197:ASN:HD22	1.68	0.41
2:D:469:ASN:ND2	2:D:472:SER:N	2.69	0.41
1:A:491:PRO:O	1:A:493:ILE:N	2.52	0.41
2:B:481:TYR:CE2	2:B:493:GLY:N	2.88	0.41
2:D:235:PHE:CZ	2:D:296:ARG:NE	2.87	0.41
1:C:622:ARG:HD3	1:C:622:ARG:HA	1.73	0.41
1:A:1153:ARG:NH2	1:A:1172:ASP:OD2	2.53	0.41
1:C:149:ASN:O	1:C:152:LEU:N	2.23	0.41
1:C:1226:ARG:CD	1:C:1266:TYR:HE1	2.32	0.41
1:C:981:GLY:HA3	1:C:1333:PHE:CD1	2.55	0.41
1:C:604:ALA:O	1:C:772:SER:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:TYR:HA	1:C:219:VAL:HG12	2.02	0.41
2:D:922:LYS:NZ	2:D:952:ASP:OD2	2.53	0.41
1:A:149:ASN:N	1:A:149:ASN:ND2	2.67	0.41
1:C:1025:LEU:HD11	1:C:1034:PHE:HZ	1.85	0.41
1:A:862:VAL:CG1	1:A:863:GLU:OE1	2.68	0.41
2:B:913:LEU:C	2:B:913:LEU:CD2	2.88	0.41
2:B:76:ASN:CB	2:B:77:PRO:HD2	2.46	0.41
2:B:358:MET:HE2	2:B:467:LYS:HD2	2.02	0.41
2:D:811:MET:HG3	2:D:812:LYS:N	2.35	0.41
1:C:1565:ILE:HB	1:C:1614:GLY:N	2.36	0.41
1:C:1428:LEU:HA	1:C:1428:LEU:HD23	1.76	0.41
2:B:1430:VAL:HA	2:B:1436:GLU:OE2	2.21	0.41
1:C:76:GLU:O	1:C:76:GLU:CD	2.59	0.41
2:D:940:THR:O	2:D:940:THR:HG22	2.19	0.41
1:C:621:GLU:HG3	1:C:621:GLU:H	1.32	0.41
1:C:1534:GLN:HA	1:C:1608:ASN:HD22	1.85	0.41
1:C:1644:TRP:C	1:C:1645:ILE:HG12	2.39	0.41
1:A:383:VAL:CG2	1:A:383:VAL:O	2.68	0.41
2:B:1290:TYR:HD2	2:B:1301:ARG:HB3	1.85	0.41
1:C:146:TYR:CD1	1:C:182:ILE:HG23	2.55	0.41
1:A:1430:THR:O	1:A:1430:THR:HG22	2.20	0.41
2:D:476:ILE:HG23	2:D:497:ARG:HD3	2.03	0.41
2:B:221:LEU:HG	2:B:221:LEU:H	1.66	0.41
1:C:943:THR:OG1	1:C:1275:SER:OG	2.28	0.41
1:C:989:SER:O	1:C:993:SER:HB2	2.20	0.41
2:B:133:ASP:HB3	2:B:757:TRP:CZ3	2.56	0.41
3:Y:46:LEU:N	3:Y:46:LEU:HD23	2.36	0.41
1:C:185:PHE:CB	1:C:186:PRO:HD2	2.50	0.41
1:C:186:PRO:O	1:C:187:ASP:C	2.58	0.41
2:B:1524:TYR:HB3	2:B:1544:VAL:HG13	2.01	0.41
2:D:804:GLU:HA	2:D:804:GLU:OE2	2.19	0.41
1:A:1175:LEU:HB3	1:A:1195:LEU:HD11	2.02	0.41
1:C:162:THR:HB	1:C:173:MET:CE	2.50	0.41
1:C:905:ILE:O	1:C:905:ILE:HG22	2.18	0.41
1:A:20:GLU:O	1:A:21:GLN:CG	2.69	0.41
1:C:461:SER:C	1:C:463:SER:N	2.73	0.41
1:C:500:ASN:ND2	1:C:543:TYR:HE1	2.17	0.41
1:C:545:ILE:HG23	1:C:554:LEU:CD2	2.51	0.41
1:C:1560:ALA:O	1:C:1561:TYR:HB3	2.20	0.41
1:C:1610:GLU:C	1:C:1611:LEU:HD23	2.40	0.41
1:C:1629:TYR:CE1	1:C:1631:PHE:CE1	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:219:TYR:CG	2:D:220:VAL:N	2.87	0.41
2:D:224:PHE:HE1	2:D:320:VAL:HG11	1.85	0.41
1:A:1549:LYS:O	1:A:1552:ALA:N	2.46	0.41
1:A:1589:GLU:HB2	1:A:1590:ALA:H	1.69	0.41
1:C:182:ILE:HG21	1:C:601:ALA:HB2	2.01	0.41
1:A:1575:VAL:O	1:A:1601:ILE:HA	2.21	0.41
1:C:1024:TYR:HB2	1:C:1298:THR:CG2	2.50	0.41
2:B:445:LEU:HD23	2:B:533:ALA:HA	2.02	0.41
1:C:395:ILE:HG22	1:C:401:THR:HG22	2.02	0.41
2:B:219:TYR:O	2:B:220:VAL:HG13	2.20	0.41
2:B:220:VAL:O	2:B:221:LEU:C	2.59	0.41
1:C:613:GLN:C	1:C:615:GLY:N	2.73	0.41
1:A:1110:ASN:O	1:A:1111:TYR:CD1	2.73	0.41
1:C:824:PHE:CE2	1:C:846:TYR:CD1	3.04	0.41
1:C:590:LEU:CD2	1:C:774:LEU:HD11	2.50	0.41
1:C:470:THR:HG22	2:D:450:THR:HA	2.03	0.41
2:B:150:MET:SD	2:B:800:ILE:HB	2.61	0.41
2:B:511:THR:O	2:B:512:PRO:C	2.58	0.41
1:A:1179:THR:HG22	1:A:1208:ILE:HD13	2.00	0.41
2:B:1575:LEU:N	2:B:1575:LEU:HD22	2.34	0.41
2:D:275:SER:C	2:D:277:PRO:HD3	2.41	0.41
1:A:708:ASP:OD2	1:A:1476:ARG:HD3	2.20	0.41
2:D:1522:TYR:CE2	2:D:1585:GLY:N	2.77	0.41
2:B:423:GLU:CD	2:B:423:GLU:H	2.23	0.41
2:D:194:LEU:HD22	2:D:194:LEU:N	2.36	0.41
1:A:680:GLN:CG	1:A:681:LYS:H	2.32	0.41
2:B:52:LYS:HG2	2:B:111:PRO:HB2	2.01	0.41
1:C:1081:PHE:O	1:C:1084:ARG:N	2.54	0.41
2:B:280:LEU:HD22	2:B:1462:TYR:CE2	2.54	0.41
1:A:163:PHE:CD1	1:A:163:PHE:N	2.88	0.41
1:C:978:SER:O	1:C:1359:VAL:HA	2.21	0.41
1:C:439:ALA:HA	1:C:440:PRO:HD3	1.85	0.41
1:A:147:SER:OG	1:A:147:SER:O	2.38	0.41
2:B:278:ASP:OD1	2:B:278:ASP:N	2.54	0.41
1:A:20:GLU:HB2	1:A:551:THR:HB	2.01	0.41
1:A:23:TYR:CE1	1:A:655:THR:O	2.74	0.41
1:A:500:ASN:ND2	1:A:543:TYR:HE1	2.15	0.41
1:C:961:TYR:HE1	1:C:963:ILE:HG12	1.86	0.41
1:C:1570:VAL:HG22	1:C:1575:VAL:HG22	2.02	0.41
2:B:436:GLN:O	2:B:437:THR:C	2.57	0.41
2:D:965:ILE:HA	2:D:1322:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:946:PRO:O	1:C:953:ILE:HG13	2.21	0.41
1:A:238:ILE:HD11	1:A:246:PHE:CD2	2.56	0.41
2:B:628:LEU:HD12	2:B:629:THR:N	2.35	0.41
1:A:1231:ASN:OD1	1:A:1232:LEU:N	2.53	0.41
2:D:296:ARG:HD2	2:D:296:ARG:HA	1.93	0.41
2:D:306:LEU:HA	2:D:306:LEU:HD13	1.85	0.41
1:A:610:TYR:CE2	1:A:619:PRO:HG3	2.54	0.41
2:D:120:LEU:HD13	2:D:120:LEU:HA	1.78	0.41
1:C:309:GLU:CG	1:C:310:LEU:N	2.84	0.41
2:B:825:VAL:HG11	2:B:918:GLU:HB3	2.01	0.41
2:D:818:LEU:HD23	2:D:911:LYS:HB2	2.01	0.41
1:A:1156:PHE:CZ	1:A:1165:ASP:HB2	2.56	0.41
1:C:286:ALA:O	1:C:287:MET:C	2.58	0.41
1:C:1179:THR:HG22	1:C:1208:ILE:HD13	1.98	0.41
2:B:1500:LEU:C	2:B:1500:LEU:HD12	2.41	0.41
1:C:38:ASN:HA	1:C:84:ILE:CG2	2.44	0.41
1:A:151:ASP:O	1:A:152:LEU:HB2	2.21	0.41
1:A:627:LEU:HD23	1:A:627:LEU:HA	1.69	0.41
1:C:958:GLU:HG2	1:C:1347:ILE:HG12	2.01	0.41
1:C:705:VAL:CA	1:C:739:ARG:NH2	2.83	0.41
1:C:525:SER:O	2:D:401:ASN:ND2	2.54	0.41
1:A:311:SER:O	1:A:313:TYR:N	2.53	0.41
2:D:59:HIS:HA	2:D:68:LEU:HD22	2.02	0.41
1:C:1548:ARG:C	1:C:1550:GLN:N	2.74	0.41
2:B:358:MET:HA	2:B:359:PRO:HD3	1.97	0.41
2:D:1511:GLN:CG	2:D:1631:PHE:CE1	3.04	0.41
2:B:79:GLY:C	2:B:81:MET:H	2.24	0.41
2:D:257:VAL:CG1	2:D:258:GLU:N	2.82	0.41
1:A:1080:ALA:HB1	1:A:1148:THR:HA	2.01	0.41
1:A:328:THR:OG1	1:A:339:GLU:HG2	2.20	0.41
2:D:785:THR:OG1	2:D:786:THR:N	2.52	0.41
1:A:1652:THR:HG22	1:A:1653:THR:N	2.36	0.41
2:B:1370:ARG:NH1	2:B:1372:LEU:HG	2.34	0.41
1:C:1563:VAL:HG12	1:C:1581:LEU:HA	2.02	0.41
2:D:563:MET:HA	2:D:563:MET:CE	2.50	0.41
1:A:1540:ASP:CA	1:A:1660:PHE:CD1	3.03	0.41
2:D:476:ILE:CG1	2:D:524:TYR:CD2	3.03	0.41
2:B:902:GLU:O	2:B:903:ALA:HB2	2.21	0.41
1:C:1231:ASN:HB2	1:C:1235:LYS:CG	2.49	0.41
1:A:1226:ARG:HD3	1:A:1266:TYR:CE1	2.55	0.41
1:A:1267:VAL:O	1:A:1270:VAL:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:433:PHE:N	1:C:433:PHE:HD1	2.19	0.41
2:D:322:THR:HG21	2:D:326:SER:OG	2.21	0.41
2:B:1391:LEU:HA	2:B:1392:PRO:HD3	1.88	0.41
1:A:1320:LYS:CD	1:A:1321:GLY:N	2.78	0.41
1:C:1033:ILE:HG23	1:C:1034:PHE:H	1.85	0.41
2:B:810:VAL:CG1	2:B:811:MET:N	2.83	0.41
1:C:1211:ALA:HA	1:C:1214:ARG:NH1	2.34	0.41
1:A:1279:ARG:HD3	1:A:1280:TYR:H	1.85	0.41
2:D:101:ASN:ND2	2:D:641:ALA:HB2	2.36	0.41
1:A:1028:GLY:HA3	1:A:1030:HIS:CE1	2.55	0.41
1:C:1445:GLY:O	1:C:1448:GLN:HB3	2.20	0.41
2:D:610:THR:C	2:D:612:GLY:N	2.72	0.41
1:C:465:LEU:HD12	1:C:466:TYR:H	1.85	0.41
1:C:965:LEU:C	1:C:967:LEU:H	2.24	0.41
2:D:283:ILE:HA	2:D:284:PRO:HD3	1.81	0.41
1:A:804:ILE:HA	1:A:809:ILE:HA	2.02	0.41
2:B:965:ILE:HD13	2:B:1277:ILE:HD13	2.03	0.41
1:C:1093:VAL:O	1:C:1094:GLU:C	2.59	0.41
1:A:215:ALA:C	1:A:216:TYR:CD2	2.94	0.41
1:C:953:ILE:CD1	1:C:955:ARG:HH21	2.33	0.41
1:C:697:LYS:O	1:C:700:TYR:N	2.54	0.41
1:A:461:SER:C	1:A:463:SER:N	2.74	0.41
1:C:316:GLU:N	1:C:316:GLU:OE1	2.41	0.41
1:C:1234:HIS:CG	1:C:1235:LYS:N	2.88	0.41
2:D:1273:LEU:HD12	2:D:1273:LEU:O	2.20	0.41
2:B:1273:LEU:HD12	2:B:1273:LEU:C	2.41	0.41
1:A:1019:PHE:CZ	1:A:1088:GLN:HB3	2.56	0.41
1:A:1145:THR:HG22	1:A:1146:ALA:N	2.35	0.41
1:C:805:SER:O	1:C:806:ASN:C	2.59	0.41
2:B:822:TYR:CD1	2:B:822:TYR:O	2.74	0.41
2:B:276:ILE:HB	2:B:279:SER:OG	2.21	0.41
1:C:1159:CYS:O	1:C:1161:LEU:HD23	2.20	0.41
1:C:123:ASN:C	1:C:211:THR:HG21	2.39	0.41
1:A:1033:ILE:HD13	1:A:1034:PHE:CE1	2.55	0.41
2:D:541:LYS:O	2:D:543:THR:CG2	2.69	0.41
1:A:185:PHE:CB	1:A:186:PRO:HD2	2.51	0.41
3:Y:52:SER:OG	3:Y:53:GLU:N	2.53	0.41
2:B:1548:ILE:HA	2:B:1636:THR:OG1	2.21	0.41
2:B:345:ILE:O	2:B:428:LYS:HD3	2.21	0.41
2:B:1518:THR:HG23	2:B:1519:ASN:N	2.36	0.41
1:C:544:TYR:CZ	1:C:555:VAL:HG12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1538:GLU:H	1:A:1538:GLU:CD	2.23	0.41
1:C:710:THR:OG1	1:C:713:GLN:HG3	2.21	0.41
3:Y:138:VAL:HG11	3:Y:177:TYR:CD2	2.56	0.41
2:D:417:HIS:CD2	2:D:419:ASP:HB2	2.56	0.41
1:A:1195:LEU:HD23	1:A:1195:LEU:HA	1.95	0.41
2:D:748:ARG:NH1	2:D:784:ILE:HG12	2.36	0.41
1:A:1435:ASN:O	1:A:1436:GLU:C	2.58	0.41
1:A:49:ALA:HB2	1:A:74:SER:HB2	2.01	0.41
1:C:1644:TRP:NE1	1:C:1646:GLU:OE1	2.52	0.41
1:C:934:VAL:O	1:C:935:LYS:HE2	2.21	0.41
1:C:1218:VAL:CG1	1:C:1219:LYS:N	2.72	0.41
2:D:518:PHE:H	2:D:518:PHE:HD2	1.68	0.41
1:A:1090:ASN:O	1:A:1092:TYR:N	2.54	0.41
1:A:1246:ARG:HB2	1:A:1246:ARG:CZ	2.51	0.41
1:C:620:LEU:O	1:C:623:VAL:CG2	2.65	0.41
1:C:1638:PRO:HG2	1:C:1639:LEU:H	1.85	0.41
2:B:952:ASP:O	2:B:1331:ALA:CA	2.69	0.41
2:B:857:CYS:CB	2:B:885:VAL:CG2	2.99	0.41
2:D:247:ILE:HD11	2:D:318:VAL:HG21	2.03	0.41
1:A:1560:ALA:C	1:A:1561:TYR:CD2	2.95	0.41
1:A:1552:ALA:HB1	1:A:1585:TYR:OH	2.20	0.41
2:D:620:VAL:CG1	2:D:621:PHE:N	2.84	0.41
1:A:215:ALA:C	1:A:216:TYR:HD2	2.24	0.41
2:D:438:GLN:HE22	2:D:530:GLU:HA	1.86	0.41
2:B:504:VAL:O	2:B:504:VAL:HG12	2.21	0.41
1:A:849:ARG:HH22	2:B:555:LEU:C	2.24	0.41
2:B:104:VAL:HG12	2:B:121:LEU:HD13	2.02	0.41
1:C:1232:LEU:HG	1:C:1233:GLN:H	1.86	0.41
2:D:338:ILE:C	2:D:339:VAL:HG13	2.41	0.41
1:A:856:CYS:N	2:B:904:LEU:HD11	2.36	0.41
2:B:1444:LYS:HZ1	2:B:1447:GLU:HA	1.86	0.41
2:D:819:GLN:HE21	2:D:819:GLN:HA	1.85	0.41
1:C:257:ASN:HB2	1:C:848:TYR:CE2	2.56	0.41
2:B:819:GLN:HE21	2:B:819:GLN:HA	1.85	0.41
1:C:1047:LYS:O	1:C:1048:LYS:C	2.58	0.41
1:C:153:LYS:CB	1:C:154:PRO:CD	2.99	0.41
2:D:58:VAL:HG23	2:D:69:PHE:O	2.21	0.41
1:C:1342:LEU:HD23	1:C:1342:LEU:N	2.36	0.41
2:D:147:VAL:CG1	2:D:147:VAL:O	2.69	0.41
1:C:20:GLU:HG3	1:C:547:THR:OG1	2.21	0.41
1:C:1180:LEU:O	1:C:1180:LEU:HD22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1314:ASP:OD2	1:C:1325:ASN:HB3	2.20	0.41
1:C:354:LEU:H	1:C:354:LEU:HD23	1.85	0.41
2:D:1506:ILE:HB	2:D:1627:ASP:HB3	2.02	0.41
1:A:174:VAL:CG2	1:A:175:GLU:H	2.34	0.41
1:A:958:GLU:HG2	1:A:1347:ILE:HG12	2.03	0.41
2:B:615:GLN:CB	2:B:616:ASN:HD22	2.34	0.41
2:D:1459:TYR:CB	2:D:1466:GLU:HB3	2.51	0.41
2:B:1424:ILE:HG12	2:B:1426:TYR:HE2	1.80	0.41
2:D:1279:ILE:HA	2:D:1279:ILE:HD13	1.86	0.41
1:C:1669:GLU:O	1:C:1673:LEU:HG	2.21	0.41
1:C:185:PHE:CD1	1:C:186:PRO:HD2	2.56	0.41
2:B:1601:ILE:HD12	2:B:1601:ILE:N	2.36	0.41
2:B:173:VAL:HA	2:B:964:ILE:HD11	2.03	0.41
2:B:1522:TYR:HD1	2:B:1524:TYR:CE1	2.38	0.41
2:D:341:SER:HB2	2:D:426:ALA:HB2	2.03	0.41
1:C:999:ILE:O	1:C:1000:LEU:C	2.59	0.41
2:D:1423:VAL:CG1	2:D:1423:VAL:O	2.68	0.41
1:C:915:GLU:HG3	2:D:904:LEU:HG	2.03	0.41
1:A:1188:LEU:HD23	1:A:1212:LEU:CA	2.51	0.41
2:D:810:VAL:O	2:D:811:MET:HB2	2.20	0.41
2:D:902:GLU:O	2:D:903:ALA:HB2	2.20	0.41
1:A:1565:ILE:HB	1:A:1614:GLY:N	2.36	0.41
1:A:734:VAL:O	1:A:737:GLN:HB2	2.21	0.41
1:C:560:TRP:CH2	1:C:562:ASN:HB2	2.55	0.41
1:C:1661:LEU:O	1:C:1662:ALA:C	2.59	0.41
1:A:1445:GLY:O	1:A:1448:GLN:HB3	2.21	0.41
2:B:1571:GLU:O	2:B:1574:ASN:HB2	2.21	0.41
2:D:895:GLU:HA	2:D:909:VAL:O	2.21	0.41
2:D:1429:LYS:HE3	2:D:1429:LYS:H	1.85	0.41
1:C:1176:LEU:HD21	1:C:1195:LEU:HD13	2.02	0.41
2:D:751:PHE:N	2:D:751:PHE:CD2	2.88	0.41
2:B:1605:THR:HG22	2:B:1605:THR:O	2.20	0.41
1:A:505:SER:HB3	1:A:510:ILE:HD13	2.00	0.41
1:A:535:VAL:HA	1:A:563:ILE:CD1	2.50	0.41
1:C:81:ASN:CG	1:C:82:SER:N	2.74	0.41
1:C:566:LYS:O	1:C:568:GLY:N	2.54	0.41
1:A:1564:SER:HA	1:A:1616:GLN:HA	2.02	0.41
1:A:1638:PRO:HG2	1:A:1639:LEU:N	2.36	0.41
2:B:850:LEU:CD1	2:B:851:LEU:N	2.84	0.41
2:D:173:VAL:O	2:D:174:SER:HB2	2.20	0.41
1:A:967:LEU:HD12	1:A:968:VAL:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:LEU:HD11	1:C:318:LEU:HG	1.98	0.41
2:B:103:TYR:HD2	2:B:103:TYR:N	2.19	0.41
1:A:382:LEU:HA	1:A:382:LEU:HD23	1.80	0.41
1:A:1268:ASN:N	1:A:1269:PRO:HD2	2.35	0.41
1:C:255:PHE:HD1	1:C:255:PHE:O	2.04	0.41
2:B:168:PRO:CG	2:B:196:THR:N	2.84	0.41
2:B:828:GLU:O	2:B:886:PRO:HD2	2.21	0.41
1:C:1274:LEU:O	1:C:1275:SER:C	2.59	0.41
2:D:1363:LEU:HD23	2:D:1442:ILE:HG12	2.03	0.41
1:A:1161:LEU:HD12	1:C:1105:LEU:CD1	2.46	0.41
1:A:1161:LEU:CA	1:C:1102:ASN:HD21	2.26	0.41
1:A:149:ASN:HD21	1:A:153:LYS:H	1.67	0.41
2:B:1446:PHE:CD2	2:B:1448:VAL:HG13	2.56	0.41
1:A:1127:ILE:N	1:A:1127:ILE:HD12	2.28	0.41
1:A:131:ASP:OD2	1:A:132:LYS:HG3	2.21	0.41
1:A:161:LEU:HD12	1:A:161:LEU:N	2.35	0.41
1:A:88:GLN:HA	1:A:89:PRO:HD2	1.88	0.41
2:B:146:ARG:CB	2:B:146:ARG:HH11	2.34	0.41
2:B:811:MET:CE	2:B:839:TYR:HD2	2.35	0.41
1:C:734:VAL:O	1:C:737:GLN:HB2	2.21	0.41
2:D:1378:THR:O	2:D:1379:MET:C	2.59	0.41
2:B:101:ASN:ND2	2:B:641:ALA:HB2	2.36	0.41
2:B:1429:LYS:N	2:B:1429:LYS:HE3	2.36	0.41
1:C:701:ASP:CG	1:C:1446:VAL:HG23	2.41	0.41
2:D:553:ASP:N	2:D:553:ASP:OD1	2.54	0.41
2:D:370:ASP:OD1	2:D:370:ASP:N	2.47	0.41
1:A:25:ILE:HD13	1:A:25:ILE:HA	1.90	0.40
1:A:367:ILE:HD13	1:A:466:TYR:CD2	2.56	0.40
1:A:531:THR:HG23	1:A:533:ASN:N	2.35	0.40
1:A:23:TYR:CE1	1:A:655:THR:HB	2.55	0.40
1:A:74:SER:CA	1:A:79:PHE:CE1	3.04	0.40
1:C:54:ILE:HA	1:C:105:GLU:O	2.21	0.40
1:C:1246:ARG:NH1	1:C:1246:ARG:HB2	2.36	0.40
1:C:1575:VAL:O	1:C:1601:ILE:HA	2.21	0.40
1:C:601:ALA:N	1:C:802:VAL:O	2.48	0.40
2:B:235:PHE:HB3	2:B:338:ILE:CG2	2.52	0.40
1:C:569:ASN:O	1:C:570:GLN:CB	2.51	0.40
2:B:464:PHE:O	2:B:503:LEU:HA	2.20	0.40
2:B:620:VAL:CG1	2:B:621:PHE:N	2.84	0.40
2:B:58:VAL:HG23	2:B:69:PHE:O	2.21	0.40
1:C:1215:GLU:O	1:C:1217:LEU:HD23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:100:GLY:O	3:X:125:LYS:CG	2.68	0.40
1:C:100:SER:C	1:C:101:TYR:CD2	2.94	0.40
1:C:1267:VAL:HG12	1:C:1267:VAL:O	2.20	0.40
2:D:820:MET:HE2	2:D:832:ILE:HG21	2.03	0.40
2:B:148:PHE:HB2	2:B:800:ILE:HD11	2.00	0.40
1:C:1305:LYS:HD3	1:C:1305:LYS:HA	1.70	0.40
1:A:1042:LYS:HZ3	1:C:92:LEU:HD13	1.86	0.40
3:X:153:PHE:CE1	3:X:169:ILE:HD13	2.55	0.40
2:B:1494:GLY:O	2:B:1495:GLU:HB2	2.21	0.40
1:A:827:MET:HB3	1:A:829:ILE:CD1	2.52	0.40
2:B:253:TYR:HE1	2:B:839:TYR:HE2	1.69	0.40
1:A:455:ILE:CG2	1:A:456:ALA:N	2.83	0.40
1:A:1054:LEU:O	1:A:1055:SER:C	2.59	0.40
1:C:681:LYS:HD2	1:C:738:LEU:HD21	2.04	0.40
2:B:410:PRO:CB	2:B:431:THR:HG22	2.50	0.40
2:B:816:ILE:CD1	2:B:909:VAL:HG23	2.51	0.40
2:D:1571:GLU:O	2:D:1574:ASN:HB2	2.21	0.40
1:A:46:TYR:HE1	1:A:48:GLU:HB2	1.85	0.40
2:B:1410:ARG:HD2	2:B:1410:ARG:HA	1.83	0.40
1:C:404:LEU:HA	1:C:404:LEU:HD22	1.69	0.40
2:D:490:PHE:C	2:D:490:PHE:CD1	2.91	0.40
1:C:1339:GLU:OE1	1:C:1339:GLU:HA	2.21	0.40
1:A:41:ILE:HG21	1:A:41:ILE:HD13	1.68	0.40
1:A:1244:THR:HG23	1:A:1502:ASP:CG	2.40	0.40
1:C:1011:GLU:HG3	1:C:1055:SER:CB	2.51	0.40
2:B:1292:ILE:HD11	2:B:1301:ARG:HE	1.86	0.40
2:D:780:LEU:CD1	2:D:787:TRP:CD1	3.05	0.40
1:C:600:VAL:HG11	1:C:602:LEU:HD21	2.02	0.40
2:D:472:SER:O	2:D:475:GLN:HG3	2.22	0.40
1:A:971:THR:O	1:A:972:GLU:C	2.59	0.40
1:A:594:THR:O	1:A:782:ARG:CD	2.69	0.40
1:C:357:VAL:O	1:C:358:ALA:C	2.60	0.40
1:A:316:GLU:OE1	1:A:316:GLU:N	2.46	0.40
1:A:412:ARG:NE	1:A:415:ASP:OD2	2.54	0.40
1:A:1013:MET:O	1:A:1015:VAL:N	2.54	0.40
1:A:1020:TYR:CE1	1:A:1295:GLU:HA	2.56	0.40
2:D:925:VAL:HG22	2:D:1326:LEU:CD2	2.40	0.40
2:D:1367:ILE:HD13	2:D:1456:VAL:HG21	2.02	0.40
1:C:604:ALA:HB3	1:C:773:TRP:O	2.21	0.40
2:D:147:VAL:O	2:D:147:VAL:HG13	2.20	0.40
1:A:889:GLU:HB2	1:A:892:SER:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:MET:HG3	2:B:602:ILE:HD11	2.02	0.40
2:D:1331:ALA:O	2:D:1332:GLN:CB	2.58	0.40
1:C:1320:LYS:HD2	1:C:1320:LYS:HA	1.88	0.40
1:C:1180:LEU:HA	1:C:1180:LEU:HD23	1.48	0.40
2:D:1509:PRO:HA	2:D:1512:ILE:CG1	2.51	0.40
2:D:544:CYS:HB3	2:D:546:GLY:O	2.22	0.40
2:D:599:TRP:O	2:D:600:ASP:C	2.58	0.40
1:C:705:VAL:CA	1:C:739:ARG:HH22	2.33	0.40
1:A:705:VAL:CA	1:A:739:ARG:HH22	2.35	0.40
2:D:827:ASN:OD1	2:D:1490:CYS:HB2	2.22	0.40
2:D:1491:ARG:HA	2:D:1491:ARG:HD3	1.89	0.40
2:B:352:LYS:HG3	2:B:430:MET:CE	2.51	0.40
3:Y:185:LYS:HB3	3:Y:185:LYS:HE2	1.98	0.40
1:C:941:GLY:HA2	1:C:1359:VAL:O	2.22	0.40
1:C:162:THR:HG23	1:C:202:LYS:HB2	2.03	0.40
2:D:967:GLY:O	2:D:969:PRO:HD3	2.21	0.40
2:B:1635:LEU:HD23	2:B:1635:LEU:HA	1.60	0.40
1:C:1449:LEU:HD12	1:C:1449:LEU:O	2.22	0.40
1:A:510:ILE:HA	3:X:150:ILE:HG13	2.02	0.40
1:C:78:LYS:NZ	3:Y:143:GLY:O	2.47	0.40
1:A:1243:GLY:O	1:A:1285:TYR:CE2	2.74	0.40
1:C:602:LEU:HA	1:C:801:GLY:HA2	2.03	0.40
1:C:1053:MET:CE	1:C:1085:VAL:HG12	2.51	0.40
2:D:468:GLY:O	2:D:469:ASN:C	2.59	0.40
2:D:164:GLU:HB2	2:D:200:VAL:HG23	2.03	0.40
2:B:482:LEU:CB	2:B:492:VAL:HG23	2.35	0.40
2:B:464:PHE:CE2	2:B:506:MET:HE1	2.56	0.40
3:Y:61:SER:OG	3:Y:99:GLN:HA	2.20	0.40
1:A:127:PHE:HD2	1:A:623:VAL:HG22	1.85	0.40
1:A:284:GLN:HG2	1:A:310:LEU:HD11	2.03	0.40
1:A:255:PHE:HD1	1:A:255:PHE:O	2.04	0.40
1:A:1161:LEU:CD1	1:C:1105:LEU:CD1	3.00	0.40
1:C:1146:ALA:HB3	1:C:1190:ILE:CG2	2.51	0.40
1:A:116:ARG:O	1:A:117:MET:HB3	2.21	0.40
2:B:460:LEU:HD23	2:B:508:LEU:HB3	2.04	0.40
1:C:92:LEU:HA	1:C:93:PRO:HD3	1.96	0.40
1:A:153:LYS:CB	1:A:154:PRO:CD	2.99	0.40
1:C:1127:ILE:HB	1:C:1129:LEU:HD21	2.03	0.40
1:A:587:THR:HA	1:A:789:ALA:HA	2.02	0.40
2:D:943:GLU:CB	2:D:1313:VAL:HG23	2.52	0.40
1:A:1450:PHE:HB3	1:A:1463:GLN:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:283:ILE:HA	2:B:284:PRO:HD3	1.81	0.40
2:B:476:ILE:CG1	2:B:524:TYR:CD2	3.04	0.40
2:B:1539:ILE:N	2:B:1539:ILE:HD12	2.34	0.40
2:D:345:ILE:HD11	2:D:426:ALA:C	2.41	0.40
2:D:745:ILE:O	2:D:745:ILE:CG2	2.68	0.40
1:C:854:GLN:C	1:C:854:GLN:HE21	2.23	0.40
3:Y:40:LEU:HD11	3:Y:209:PHE:HZ	1.85	0.40
2:D:352:LYS:HG3	2:D:430:MET:HE1	2.03	0.40
1:A:1420:SER:O	1:A:1421:HIS:C	2.58	0.40
1:C:914:LEU:O	1:C:914:LEU:HG	2.20	0.40
2:D:45:ALA:HB3	2:D:81:MET:CE	2.51	0.40
2:B:330:VAL:HG23	2:B:330:VAL:O	2.22	0.40
1:A:1220:GLY:O	1:A:1223:PRO:HA	2.21	0.40
3:Y:67:TYR:CD1	3:Y:67:TYR:O	2.74	0.40
1:C:492:TYR:HE2	1:C:546:VAL:HG11	1.86	0.40
1:C:22:THR:HG21	1:C:657:ALA:HB2	2.04	0.40
1:C:531:THR:HG23	1:C:533:ASN:N	2.37	0.40
1:C:1430:THR:HG22	1:C:1430:THR:O	2.21	0.40
2:B:1292:ILE:HD12	2:B:1296:ASN:OD1	2.21	0.40
2:B:950:LEU:O	2:B:951:ASP:HB2	2.21	0.40
1:C:804:ILE:HA	1:C:809:ILE:HA	2.03	0.40
2:D:878:ARG:HA	2:D:878:ARG:HD2	1.92	0.40
1:A:718:ILE:HB	1:A:725:ILE:CD1	2.51	0.40
2:D:851:LEU:CD2	2:D:852:TYR:H	2.17	0.40
3:Y:113:ASN:HD21	3:Y:115:ARG:HG2	1.87	0.40
1:C:243:PHE:O	1:C:303:SER:HB2	2.21	0.40
1:C:1231:ASN:OD1	1:C:1232:LEU:N	2.54	0.40
1:C:1217:LEU:CD1	1:C:1237:SER:HA	2.52	0.40
2:D:121:LEU:HD12	2:D:121:LEU:HA	1.72	0.40
3:X:101:GLN:HB3	3:X:123:THR:O	2.22	0.40
2:D:794:PHE:CD2	2:D:795:THR:N	2.89	0.40
1:A:1300:TYR:CE2	1:A:1304:VAL:HG21	2.56	0.40
1:C:1018:VAL:HG11	1:C:1048:LYS:HB3	2.03	0.40
2:D:1383:ASP:O	2:D:1456:VAL:HA	2.22	0.40
2:D:1469:THR:O	2:D:1470:LYS:HG2	2.22	0.40
2:B:848:VAL:HG22	2:B:898:ALA:HB2	2.04	0.40
2:D:1615:GLU:O	2:D:1616:CYS:C	2.60	0.40
2:D:515:ILE:HG21	2:D:599:TRP:CZ2	2.56	0.40
1:C:789:ALA:O	1:C:790:LEU:O	2.40	0.40
1:A:1358:THR:HB	1:A:1360:HIS:HE1	1.84	0.40
2:D:64:LYS:HG3	2:D:64:LYS:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:984:VAL:O	1:C:984:VAL:HG13	2.21	0.40
2:B:1534:GLN:HB2	2:B:1539:ILE:HD11	2.04	0.40
2:D:269:ILE:HG13	2:D:272:ALA:HB3	2.02	0.40
2:D:76:ASN:CB	2:D:77:PRO:HD2	2.52	0.40
1:A:1440:LYS:O	1:A:1443:VAL:HG12	2.21	0.40
2:B:145:TYR:CD1	2:B:145:TYR:C	2.95	0.40
1:A:431:LEU:C	1:A:431:LEU:CD2	2.90	0.40
2:B:802:VAL:HG12	2:B:802:VAL:O	2.22	0.40
1:C:1248:VAL:H	1:C:1248:VAL:HG23	1.69	0.40
1:A:22:THR:CG2	1:A:23:TYR:CE1	3.04	0.40
1:A:658:ASN:O	1:A:658:ASN:OD1	2.40	0.40
1:C:489:LYS:HZ3	2:D:502:ASN:H	1.69	0.40
1:C:501:TYR:HB3	1:C:542:VAL:HG22	2.03	0.40
1:C:1228:TRP:N	1:C:1228:TRP:HE3	2.20	0.40
1:C:1008:ALA:O	1:C:1011:GLU:N	2.55	0.40
1:C:1147:PHE:C	1:C:1147:PHE:HD2	2.25	0.40
2:B:261:ALA:HB2	2:B:285:ILE:HD11	2.01	0.40
2:B:174:SER:HA	2:B:1300:ALA:HB2	2.02	0.40
1:C:923:LEU:CD2	1:C:925:LYS:HD3	2.52	0.40
1:C:1090:ASN:O	1:C:1092:TYR:N	2.54	0.40
2:D:1296:ASN:HB2	2:D:1299:LEU:HD22	2.03	0.40
2:D:23:ALA:CB	2:D:528:ASN:HD22	2.27	0.40
1:C:718:ILE:HB	1:C:725:ILE:CD1	2.51	0.40
1:C:671:GLU:HB2	1:C:672:ILE:H	1.66	0.40
2:B:397:LYS:NZ	2:B:449:ILE:O	2.55	0.40
2:B:618:LEU:CD1	2:B:635:ASN:O	2.65	0.40
1:C:849:ARG:NH2	2:D:555:LEU:HB2	2.36	0.40
2:D:1486:ILE:HG13	2:D:1486:ILE:O	2.22	0.40
1:A:316:GLU:O	1:A:349:LEU:HD21	2.21	0.40
1:A:412:ARG:HG3	1:A:413:VAL:H	1.87	0.40
2:B:795:THR:CG2	2:B:796:PRO:CD	2.98	0.40
1:A:1309:LEU:CD2	1:A:1355:GLY:HA3	2.52	0.40
1:A:644:ASN:O	1:A:647:HIS:N	2.55	0.40
1:A:127:PHE:CD2	1:A:623:VAL:HG22	2.56	0.40
1:A:127:PHE:HD1	1:A:127:PHE:N	2.20	0.40
1:C:284:GLN:HG2	1:C:310:LEU:HD11	2.02	0.40
1:C:823:VAL:HG23	1:C:846:TYR:O	2.20	0.40
1:A:160:VAL:O	1:A:160:VAL:HG12	2.20	0.40
2:B:1459:TYR:CB	2:B:1466:GLU:HB3	2.52	0.40
2:B:476:ILE:CD1	2:B:524:TYR:CD2	3.02	0.40
2:D:409:LEU:N	2:D:410:PRO:HD3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1467:ILE:HA	1:C:1468:PRO:HD3	1.83	0.40
1:A:984:VAL:HG13	1:A:984:VAL:O	2.21	0.40
3:Y:83:GLN:O	3:Y:117:SER:HA	2.22	0.40
2:B:751:PHE:CD2	2:B:751:PHE:N	2.90	0.40
1:A:1264:ILE:HD12	1:A:1264:ILE:N	2.36	0.40
2:D:891:LEU:H	2:D:891:LEU:HG	1.10	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1616/1676 (96%)	1165 (72%)	300 (19%)	151 (9%)	1	16
1	C	1616/1676 (96%)	1179 (73%)	290 (18%)	147 (9%)	1	16
2	B	1203/1642 (73%)	981 (82%)	176 (15%)	46 (4%)	4	39
2	D	1203/1642 (73%)	982 (82%)	177 (15%)	44 (4%)	4	40
3	X	189/231 (82%)	148 (78%)	31 (16%)	10 (5%)	2	30
3	Y	189/231 (82%)	150 (79%)	28 (15%)	11 (6%)	2	28
All	All	6016/7098 (85%)	4605 (76%)	1002 (17%)	409 (7%)	1	24

All (409) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	60	PRO
1	A	89	PRO
1	A	96	GLN
1	A	150	ASP
1	A	154	PRO

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Mol	Chain	Res	Type
1	A	155	ALA
1	A	208	ASP
1	A	274	ASP
1	A	285	THR
1	A	308	LYS
1	A	490	SER
1	A	495	LYS
1	A	507	GLY
1	A	522	SER
1	A	551	THR
1	A	552	ALA
1	A	570	GLN
1	A	634	CYS
1	A	643	ALA
1	A	754	MET
1	A	759	PRO
1	A	790	LEU
1	A	821	LYS
1	A	866	CYS
1	A	873	ILE
1	A	884	VAL
1	A	885	ARG
1	A	948	GLY
1	A	998	ASN
1	A	1004	PRO
1	A	1096	ASN
1	A	1232	LEU
1	A	1242	THR
1	A	1286	SER
1	A	1335	GLY
1	A	1452	ASP
1	A	1538	GLU
1	A	1573	VAL
1	A	1609	ALA
1	A	1628	LYS
1	A	1638	PRO
1	A	1639	LEU
1	A	1674	ASN
2	B	207	PRO
2	B	453	GLU
2	B	490	PHE
2	B	873	LYS

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Mol	Chain	Res	Type
2	B	1529	LEU
2	B	1548	ILE
2	B	1615	GLU
2	B	1639	GLY
1	C	60	PRO
1	C	89	PRO
1	C	96	GLN
1	C	97	ASN
1	C	150	ASP
1	C	155	ALA
1	C	208	ASP
1	C	274	ASP
1	C	285	THR
1	C	308	LYS
1	C	490	SER
1	C	495	LYS
1	C	507	GLY
1	C	522	SER
1	C	570	GLN
1	C	634	CYS
1	C	643	ALA
1	C	669	CYS
1	C	754	MET
1	C	759	PRO
1	C	790	LEU
1	C	821	LYS
1	C	873	ILE
1	C	884	VAL
1	C	885	ARG
1	C	939	TYR
1	C	948	GLY
1	C	998	ASN
1	C	1096	ASN
1	C	1232	LEU
1	C	1242	THR
1	C	1264	ILE
1	C	1286	SER
1	C	1335	GLY
1	C	1452	ASP
1	C	1538	GLU
1	C	1590	ALA
1	C	1609	ALA

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Mol	Chain	Res	Type
1	C	1628	LYS
1	C	1638	PRO
1	C	1639	LEU
1	C	1674	ASN
2	D	51	PRO
2	D	207	PRO
2	D	453	GLU
2	D	490	PHE
2	D	873	LYS
2	D	1507	ASP
2	D	1529	LEU
2	D	1548	ILE
3	X	42	ASP
3	X	72	VAL
3	X	78	LYS
3	Y	42	ASP
3	Y	72	VAL
3	Y	78	LYS
1	A	97	ASN
1	A	133	PRO
1	A	156	LYS
1	A	181	GLY
1	A	187	ASP
1	A	289	ASN
1	A	312	TYR
1	A	318	LEU
1	A	474	LYS
1	A	489	LYS
1	A	519	SER
1	A	520	ASP
1	A	565	GLU
1	A	596	MET
1	A	614	ARG
1	A	623	VAL
1	A	639	GLY
1	A	656	ASN
1	A	659	ALA
1	A	669	CYS
1	A	672	ILE
1	A	690	TYR
1	A	806	ASN
1	A	820	PHE

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Mol	Chain	Res	Type
1	A	850	THR
1	A	870	SER
1	A	939	TYR
1	A	946	PRO
1	A	1133	LEU
1	A	1134	PRO
1	A	1264	ILE
1	A	1333	PHE
1	A	1386	ILE
1	A	1471	ASP
1	A	1528	VAL
1	A	1583	ASP
1	A	1590	ALA
2	B	36	ASP
2	B	48	ASP
2	B	220	VAL
2	B	451	SER
2	B	583	ALA
2	B	604	LYS
2	B	641	ALA
2	B	821	PRO
2	B	842	GLU
2	B	1283	ASP
2	B	1449	GLY
2	B	1493	ALA
2	B	1603	LYS
2	B	1641	PRO
1	C	21	GLN
1	C	133	PRO
1	C	154	PRO
1	C	156	LYS
1	C	166	PRO
1	C	181	GLY
1	C	187	ASP
1	C	255	PHE
1	C	312	TYR
1	C	318	LEU
1	C	474	LYS
1	C	520	ASP
1	C	596	MET
1	C	614	ARG
1	C	623	VAL

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Mol	Chain	Res	Type
1	C	639	GLY
1	C	656	ASN
1	C	671	GLU
1	C	672	ILE
1	C	690	TYR
1	C	793	SER
1	C	806	ASN
1	C	820	PHE
1	C	850	THR
1	C	870	SER
1	C	917	TRP
1	C	946	PRO
1	C	1004	PRO
1	C	1134	PRO
1	C	1333	PHE
1	C	1382	ASP
1	C	1386	ILE
1	C	1573	VAL
1	C	1583	ASP
2	D	36	ASP
2	D	220	VAL
2	D	451	SER
2	D	582	LYS
2	D	583	ALA
2	D	604	LYS
2	D	641	ALA
2	D	821	PRO
2	D	842	GLU
2	D	1283	ASP
2	D	1449	GLY
2	D	1493	ALA
2	D	1603	LYS
3	Y	82	HIS
1	A	171	VAL
1	A	255	PHE
1	A	287	MET
1	A	642	ASN
1	A	671	GLU
1	A	681	LYS
1	A	699	CYS
1	A	791	PRO
1	A	793	SER

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Mol	Chain	Res	Type
1	A	917	TRP
1	A	931	PRO
1	A	1001	THR
1	A	1023	HIS
1	A	1073	SER
1	A	1122	SER
1	A	1220	GLY
1	A	1235	LYS
1	A	1241	ASN
1	A	1382	ASP
1	A	1589	GLU
2	B	51	PRO
2	B	470	ALA
2	B	582	LYS
2	B	871	PRO
2	B	1379	MET
2	B	1492	CYS
2	B	1558	ALA
1	C	171	VAL
1	C	287	MET
1	C	289	ASN
1	C	441	ASP
1	C	489	LYS
1	C	519	SER
1	C	551	THR
1	C	552	ALA
1	C	565	GLU
1	C	642	ASN
1	C	659	ALA
1	C	681	LYS
1	C	791	PRO
1	C	931	PRO
1	C	997	ILE
1	C	1001	THR
1	C	1014	SER
1	C	1073	SER
1	C	1122	SER
1	C	1133	LEU
1	C	1200	LYS
1	C	1241	ASN
1	C	1471	ASP
1	C	1589	GLU

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Mol	Chain	Res	Type
2	D	48	ASP
2	D	871	PRO
2	D	1379	MET
2	D	1492	CYS
2	D	1558	ALA
2	D	1631	PHE
3	X	82	HIS
3	X	87	LEU
3	X	125	LYS
3	X	185	LYS
3	Y	125	LYS
3	Y	185	LYS
1	A	256	TYR
1	A	441	ASP
1	A	641	ASN
1	A	663	GLN
1	A	822	ASP
1	A	863	GLU
1	A	960	PRO
1	A	997	ILE
1	A	1014	SER
1	A	1160	PRO
1	A	1181	PRO
1	A	1184	SER
1	A	1237	SER
1	A	1284	PHE
1	A	1297	LEU
1	A	1324	HIS
1	A	1488	LEU
1	A	1512	SER
1	A	1653	THR
1	A	1666	GLU
2	B	142	PRO
2	B	310	VAL
2	B	764	GLU
2	B	862	LYS
1	C	137	PRO
1	C	170	GLU
1	C	256	TYR
1	C	641	ASN
1	C	663	GLN
1	C	699	CYS

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Mol	Chain	Res	Type
1	C	752	LEU
1	C	822	ASP
1	C	960	PRO
1	C	1160	PRO
1	C	1181	PRO
1	C	1184	SER
1	C	1220	GLY
1	C	1235	LYS
1	C	1237	SER
1	C	1284	PHE
1	C	1324	HIS
1	C	1352	PHE
1	C	1488	LEU
1	C	1512	SER
1	C	1666	GLU
2	D	142	PRO
2	D	310	VAL
2	D	470	ALA
2	D	764	GLU
2	D	862	LYS
3	Y	68	ASN
3	Y	87	LEU
3	Y	124	LYS
1	A	61	ASP
1	A	475	ALA
1	A	488	PRO
1	A	506	LYS
1	A	694	VAL
1	A	720	LEU
1	A	752	LEU
1	A	994	GLN
1	A	1200	LYS
1	A	1239	VAL
1	A	1352	PHE
1	A	1398	ASP
2	B	193	SER
2	B	1286	VAL
2	B	1592	PRO
2	B	1628	PHE
1	C	61	ASP
1	C	337	SER
1	C	488	PRO

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Mol	Chain	Res	Type
1	C	685	GLU
1	C	694	VAL
1	C	1239	VAL
1	C	1398	ASP
1	C	1653	THR
1	C	1654	CYS
2	D	1435	ASP
2	D	1592	PRO
3	X	68	ASN
3	X	124	LYS
1	A	43	VAL
1	A	137	PRO
1	A	1321	GLY
1	A	1654	CYS
2	B	512	PRO
1	C	41	ILE
1	C	291	MET
1	C	1018	VAL
2	D	418	GLY
2	D	937	VAL
2	D	1286	VAL
1	A	190	ILE
1	A	440	PRO
1	A	645	VAL
1	A	760	VAL
1	A	1296	GLY
2	B	80	GLY
2	B	221	LEU
2	B	339	VAL
2	B	937	VAL
1	C	577	PRO
1	C	760	VAL
1	C	1006	GLY
1	C	1135	VAL
2	D	512	PRO
3	X	76	ASN
3	Y	76	ASN
1	A	406	PRO
1	A	577	PRO
2	B	237	ILE
1	C	43	VAL
1	C	406	PRO

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Mol	Chain	Res	Type
1	C	440	PRO
1	C	872	VAL
2	D	173	VAL
2	D	221	LEU
3	Y	143	GLY
1	A	41	ILE
1	A	231	ILE
1	A	585	GLY
1	A	1018	VAL
1	A	1135	VAL
1	A	1570	VAL
2	B	173	VAL
1	C	231	ILE
1	C	1570	VAL
2	D	47	GLY
2	D	80	GLY
2	D	237	ILE
2	D	339	VAL
1	A	618	LYS
2	B	418	GLY
1	C	618	LYS
1	C	645	VAL
1	C	1296	GLY
2	B	598	ILE
1	C	1321	GLY

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	1445/1484 (97%)	1090 (75%)	355 (25%)	1	7
1	C	1445/1484 (97%)	1098 (76%)	347 (24%)	1	7
2	B	1084/1435 (76%)	849 (78%)	235 (22%)	1	10
2	D	1084/1435 (76%)	855 (79%)	229 (21%)	1	11
3	X	175/205 (85%)	143 (82%)	32 (18%)	2	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	Y	175/205 (85%)	142 (81%)	33 (19%)	2 14
All	All	5408/6248 (87%)	4177 (77%)	1231 (23%)	1 9

All (1231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	A	21	GLN
1	A	22	THR
1	A	23	TYR
1	A	24	VAL
1	A	40	VAL
1	A	42	GLN
1	A	43	VAL
1	A	46	TYR
1	A	55	SER
1	A	58	SER
1	A	63	LYS
1	A	64	PHE
1	A	73	LEU
1	A	84	ILE
1	A	85	LEU
1	A	87	ILE
1	A	89	PRO
1	A	90	LYS
1	A	91	GLN
1	A	102	VAL
1	A	106	VAL
1	A	114	SER
1	A	125	PHE
1	A	126	LEU
1	A	128	ILE
1	A	131	ASP
1	A	136	THR
1	A	144	ARG
1	A	147	SER
1	A	149	ASN
1	A	152	LEU
1	A	157	ARG
1	A	161	LEU
1	A	162	THR
1	A	169	SER

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Mol	Chain	Res	Type
1	A	170	GLU
1	A	176	GLU
1	A	182	ILE
1	A	183	ILE
1	A	184	SER
1	A	195	ARG
1	A	200	THR
1	A	209	PHE
1	A	211	THR
1	A	212	THR
1	A	214	THR
1	A	216	TYR
1	A	219	VAL
1	A	222	TYR
1	A	223	VAL
1	A	224	LEU
1	A	228	SER
1	A	230	SER
1	A	240	TYR
1	A	242	ASN
1	A	249	THR
1	A	251	LYS
1	A	255	PHE
1	A	261	THR
1	A	264	ASP
1	A	268	THR
1	A	276	LYS
1	A	279	GLN
1	A	287	MET
1	A	289	ASN
1	A	291	MET
1	A	292	LEU
1	A	294	ASN
1	A	296	ILE
1	A	315	LEU
1	A	321	LYS
1	A	322	TYR
1	A	323	LEU
1	A	328	THR
1	A	333	THR
1	A	342	ILE
1	A	353	LYS

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Mol	Chain	Res	Type
1	A	354	LEU
1	A	355	ASN
1	A	363	LEU
1	A	371	ILE
1	A	373	VAL
1	A	375	VAL
1	A	380	ASP
1	A	383	VAL
1	A	388	VAL
1	A	389	THR
1	A	394	THR
1	A	404	LEU
1	A	414	ASP
1	A	415	ASP
1	A	422	LEU
1	A	426	SER
1	A	431	LEU
1	A	433	PHE
1	A	435	VAL
1	A	436	LYS
1	A	442	LEU
1	A	455	ILE
1	A	457	TYR
1	A	458	SER
1	A	467	ILE
1	A	469	TRP
1	A	471	ASP
1	A	474	LYS
1	A	483	ASN
1	A	487	THR
1	A	492	TYR
1	A	493	ILE
1	A	494	ASP
1	A	495	LYS
1	A	497	THR
1	A	504	LEU
1	A	506	LYS
1	A	509	ILE
1	A	510	ILE
1	A	512	PHE
1	A	522	SER
1	A	526	ILE

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Mol	Chain	Res	Type
1	A	532	GLN
1	A	534	MET
1	A	535	VAL
1	A	541	LEU
1	A	543	TYR
1	A	544	TYR
1	A	545	ILE
1	A	547	THR
1	A	549	GLU
1	A	550	GLN
1	A	559	VAL
1	A	561	LEU
1	A	563	ILE
1	A	565	GLU
1	A	569	ASN
1	A	570	GLN
1	A	583	SER
1	A	599	TRP
1	A	605	VAL
1	A	613	GLN
1	A	614	ARG
1	A	620	LEU
1	A	621	GLU
1	A	627	LEU
1	A	628	GLU
1	A	630	SER
1	A	632	LEU
1	A	640	LEU
1	A	644	ASN
1	A	648	LEU
1	A	652	THR
1	A	654	LEU
1	A	658	ASN
1	A	669	CYS
1	A	679	LEU
1	A	684	GLU
1	A	700	TYR
1	A	701	ASP
1	A	710	THR
1	A	711	CYS
1	A	713	GLN
1	A	720	LEU

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Mol	Chain	Res	Type
1	A	732	CYS
1	A	754	MET
1	A	756	THR
1	A	766	ARG
1	A	774	LEU
1	A	777	VAL
1	A	779	LEU
1	A	782	ARG
1	A	786	LEU
1	A	787	GLN
1	A	788	PHE
1	A	793	SER
1	A	795	THR
1	A	800	GLN
1	A	805	SER
1	A	813	ASP
1	A	824	PHE
1	A	825	LEU
1	A	833	VAL
1	A	838	GLN
1	A	844	THR
1	A	845	VAL
1	A	848	TYR
1	A	849	ARG
1	A	850	THR
1	A	854	GLN
1	A	856	CYS
1	A	857	VAL
1	A	859	MET
1	A	865	ILE
1	A	871	PRO
1	A	876	GLN
1	A	887	LYS
1	A	895	LEU
1	A	899	THR
1	A	901	LEU
1	A	905	ILE
1	A	916	THR
1	A	917	TRP
1	A	928	ARG
1	A	935	LYS
1	A	936	ARG

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Mol	Chain	Res	Type
1	A	942	VAL
1	A	944	LEU
1	A	945	ASP
1	A	952	THR
1	A	955	ARG
1	A	965	LEU
1	A	972	GLU
1	A	975	ARG
1	A	979	VAL
1	A	980	LYS
1	A	983	LEU
1	A	984	VAL
1	A	988	LEU
1	A	999	ILE
1	A	1001	THR
1	A	1002	HIS
1	A	1003	LEU
1	A	1007	SER
1	A	1011	GLU
1	A	1012	LEU
1	A	1013	MET
1	A	1015	VAL
1	A	1018	VAL
1	A	1021	VAL
1	A	1029	ASN
1	A	1033	ILE
1	A	1049	LEU
1	A	1054	LEU
1	A	1055	SER
1	A	1056	ILE
1	A	1061	ASN
1	A	1067	SER
1	A	1070	LYS
1	A	1079	THR
1	A	1098	ASN
1	A	1105	LEU
1	A	1110	ASN
1	A	1113	LEU
1	A	1123	GLN
1	A	1125	GLN
1	A	1127	ILE
1	A	1128	LYS

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Mol	Chain	Res	Type
1	A	1132	THR
1	A	1133	LEU
1	A	1140	ASN
1	A	1142	LEU
1	A	1144	LEU
1	A	1147	PHE
1	A	1150	ILE
1	A	1166	THR
1	A	1179	THR
1	A	1180	LEU
1	A	1184	SER
1	A	1190	ILE
1	A	1196	SER
1	A	1200	LYS
1	A	1201	THR
1	A	1202	HIS
1	A	1207	SER
1	A	1230	ASP
1	A	1232	LEU
1	A	1246	ARG
1	A	1264	ILE
1	A	1268	ASN
1	A	1275	SER
1	A	1280	TYR
1	A	1284	PHE
1	A	1286	SER
1	A	1301	SER
1	A	1302	LEU
1	A	1303	LEU
1	A	1307	LEU
1	A	1309	LEU
1	A	1313	ILE
1	A	1315	VAL
1	A	1323	LEU
1	A	1326	TYR
1	A	1329	THR
1	A	1331	LYS
1	A	1334	LEU
1	A	1336	ARG
1	A	1341	LEU
1	A	1342	LEU
1	A	1346	LEU

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Mol	Chain	Res	Type
1	A	1347	ILE
1	A	1348	VAL
1	A	1350	THR
1	A	1352	PHE
1	A	1356	LEU
1	A	1358	THR
1	A	1360	HIS
1	A	1363	THR
1	A	1366	HIS
1	A	1372	GLU
1	A	1376	SER
1	A	1401	ARG
1	A	1416	SER
1	A	1423	VAL
1	A	1430	THR
1	A	1446	VAL
1	A	1455	ILE
1	A	1459	HIS
1	A	1464	LEU
1	A	1470	SER
1	A	1475	VAL
1	A	1476	ARG
1	A	1479	ILE
1	A	1480	PHE
1	A	1483	PHE
1	A	1487	PHE
1	A	1492	THR
1	A	1493	PHE
1	A	1494	THR
1	A	1496	TYR
1	A	1500	ARG
1	A	1502	ASP
1	A	1503	LYS
1	A	1507	MET
1	A	1525	CYS
1	A	1532	CYS
1	A	1535	MET
1	A	1539	LEU
1	A	1542	THR
1	A	1548	ARG
1	A	1549	LYS
1	A	1556	GLU

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Mol	Chain	Res	Type
1	A	1557	ILE
1	A	1559	TYR
1	A	1566	THR
1	A	1569	THR
1	A	1573	VAL
1	A	1580	THR
1	A	1581	LEU
1	A	1583	ASP
1	A	1585	TYR
1	A	1589	GLU
1	A	1602	LYS
1	A	1604	VAL
1	A	1606	CYS
1	A	1618	LEU
1	A	1620	MET
1	A	1626	GLN
1	A	1629	TYR
1	A	1631	PHE
1	A	1632	SER
1	A	1634	ARG
1	A	1636	ILE
1	A	1637	TYR
1	A	1639	LEU
1	A	1654	CYS
1	A	1664	LEU
2	B	43	VAL
2	B	54	LEU
2	B	56	ILE
2	B	58	VAL
2	B	68	LEU
2	B	69	PHE
2	B	71	THR
2	B	74	ASP
2	B	82	LEU
2	B	86	THR
2	B	87	ILE
2	B	105	VAL
2	B	114	ARG
2	B	119	VAL
2	B	120	LEU
2	B	121	LEU
2	B	124	GLN

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Mol	Chain	Res	Type
2	B	146	ARG
2	B	147	VAL
2	B	161	VAL
2	B	167	THR
2	B	177	SER
2	B	178	VAL
2	B	179	ASP
2	B	183	PHE
2	B	191	LEU
2	B	196	THR
2	B	198	ARG
2	B	199	ILE
2	B	206	SER
2	B	211	THR
2	B	214	PHE
2	B	219	TYR
2	B	220	VAL
2	B	221	LEU
2	B	226	VAL
2	B	243	PHE
2	B	264	LEU
2	B	274	LYS
2	B	278	ASP
2	B	280	LEU
2	B	291	LYS
2	B	296	ARG
2	B	297	ASP
2	B	299	PHE
2	B	306	LEU
2	B	317	SER
2	B	320	VAL
2	B	328	MET
2	B	338	ILE
2	B	341	SER
2	B	344	GLN
2	B	345	ILE
2	B	349	LYS
2	B	390	THR
2	B	398	LEU
2	B	400	LEU
2	B	404	LEU
2	B	411	ILE

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Mol	Chain	Res	Type
2	B	422	ARG
2	B	435	TYR
2	B	437	THR
2	B	450	THR
2	B	458	ASP
2	B	460	LEU
2	B	469	ASN
2	B	472	SER
2	B	477	LYS
2	B	478	TYR
2	B	481	TYR
2	B	482	LEU
2	B	488	LYS
2	B	492	VAL
2	B	497	ARG
2	B	498	ARG
2	B	504	VAL
2	B	505	THR
2	B	506	MET
2	B	507	ASN
2	B	511	THR
2	B	513	ASP
2	B	518	PHE
2	B	519	ARG
2	B	520	PHE
2	B	521	VAL
2	B	523	TYR
2	B	524	TYR
2	B	525	GLN
2	B	526	VAL
2	B	528	ASN
2	B	531	ILE
2	B	543	THR
2	B	544	CYS
2	B	555	LEU
2	B	556	ILE
2	B	563	MET
2	B	567	LEU
2	B	574	ARG
2	B	582	LYS
2	B	584	VAL
2	B	588	ASN

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Mol	Chain	Res	Type
2	B	593	ILE
2	B	594	SER
2	B	599	TRP
2	B	606	ASP
2	B	620	VAL
2	B	629	THR
2	B	634	LEU
2	B	638	GLN
2	B	643	LYS
2	B	740	ILE
2	B	742	ASP
2	B	743	SER
2	B	745	ILE
2	B	746	ILE
2	B	747	SER
2	B	769	GLN
2	B	778	PHE
2	B	780	LEU
2	B	783	SER
2	B	784	ILE
2	B	789	VAL
2	B	793	SER
2	B	800	ILE
2	B	802	VAL
2	B	804	GLU
2	B	808	ILE
2	B	812	LYS
2	B	813	VAL
2	B	816	ILE
2	B	817	ASP
2	B	819	GLN
2	B	829	GLN
2	B	830	VAL
2	B	836	LEU
2	B	851	LEU
2	B	857	CYS
2	B	867	ARG
2	B	870	PHE
2	B	872	ILE
2	B	873	LYS
2	B	875	LEU
2	B	880	VAL

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Mol	Chain	Res	Type
2	B	884	ILE
2	B	889	GLN
2	B	891	LEU
2	B	893	ASP
2	B	913	LEU
2	B	914	LYS
2	B	916	VAL
2	B	918	GLU
2	B	920	VAL
2	B	926	THR
2	B	946	LYS
2	B	948	ARG
2	B	952	ASP
2	B	960	GLU
2	B	963	ILE
2	B	964	ILE
2	B	1278	THR
2	B	1279	ILE
2	B	1281	LEU
2	B	1283	ASP
2	B	1291	ARG
2	B	1292	ILE
2	B	1293	ASN
2	B	1298	LEU
2	B	1303	VAL
2	B	1305	THR
2	B	1308	ASN
2	B	1313	VAL
2	B	1324	THR
2	B	1326	LEU
2	B	1329	TYR
2	B	1330	ASN
2	B	1332	GLN
2	B	1344	HIS
2	B	1350	GLU
2	B	1351	ASN
2	B	1365	LEU
2	B	1372	LEU
2	B	1378	THR
2	B	1380	THR
2	B	1401	SER
2	B	1404	VAL

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Mol	Chain	Res	Type
2	B	1406	ARG
2	B	1423	VAL
2	B	1424	ILE
2	B	1425	ILE
2	B	1427	LEU
2	B	1429	LYS
2	B	1433	SER
2	B	1437	CYS
2	B	1438	LEU
2	B	1442	ILE
2	B	1443	LEU
2	B	1445	HIS
2	B	1448	VAL
2	B	1459	TYR
2	B	1465	ASP
2	B	1475	ASP
2	B	1480	LEU
2	B	1481	LEU
2	B	1490	CYS
2	B	1491	ARG
2	B	1492	CYS
2	B	1495	GLU
2	B	1496	THR
2	B	1497	CYS
2	B	1500	LEU
2	B	1503	GLN
2	B	1504	GLU
2	B	1505	ARG
2	B	1516	CYS
2	B	1522	TYR
2	B	1526	THR
2	B	1529	LEU
2	B	1535	ASP
2	B	1539	ILE
2	B	1561	HIS
2	B	1566	GLN
2	B	1584	TRP
2	B	1591	LEU
2	B	1594	LYS
2	B	1597	ILE
2	B	1598	SER
2	B	1604	ASN

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Mol	Chain	Res	Type
2	B	1605	THR
2	B	1606	TRP
2	B	1607	ILE
2	B	1612	HIS
2	B	1616	CYS
2	B	1617	GLN
2	B	1623	LYS
2	B	1631	PHE
1	C	20	GLU
1	C	21	GLN
1	C	22	THR
1	C	23	TYR
1	C	24	VAL
1	C	40	VAL
1	C	42	GLN
1	C	43	VAL
1	C	46	TYR
1	C	55	SER
1	C	58	SER
1	C	63	LYS
1	C	64	PHE
1	C	73	LEU
1	C	84	ILE
1	C	85	LEU
1	C	87	ILE
1	C	89	PRO
1	C	90	LYS
1	C	91	GLN
1	C	102	VAL
1	C	106	VAL
1	C	114	SER
1	C	125	PHE
1	C	126	LEU
1	C	128	ILE
1	C	131	ASP
1	C	134	VAL
1	C	136	THR
1	C	143	VAL
1	C	144	ARG
1	C	147	SER
1	C	149	ASN
1	C	152	LEU

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Mol	Chain	Res	Type
1	C	157	ARG
1	C	161	LEU
1	C	162	THR
1	C	165	ASP
1	C	169	SER
1	C	170	GLU
1	C	176	GLU
1	C	182	ILE
1	C	183	ILE
1	C	184	SER
1	C	195	ARG
1	C	200	THR
1	C	209	PHE
1	C	211	THR
1	C	212	THR
1	C	214	THR
1	C	216	TYR
1	C	219	VAL
1	C	222	TYR
1	C	223	VAL
1	C	224	LEU
1	C	228	SER
1	C	230	SER
1	C	240	TYR
1	C	242	ASN
1	C	246	PHE
1	C	249	THR
1	C	251	LYS
1	C	255	PHE
1	C	261	THR
1	C	264	ASP
1	C	268	THR
1	C	276	LYS
1	C	279	GLN
1	C	287	MET
1	C	289	ASN
1	C	291	MET
1	C	292	LEU
1	C	294	ASN
1	C	296	ILE
1	C	315	LEU
1	C	321	LYS

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Mol	Chain	Res	Type
1	C	322	TYR
1	C	323	LEU
1	C	328	THR
1	C	333	THR
1	C	342	ILE
1	C	353	LYS
1	C	354	LEU
1	C	355	ASN
1	C	363	LEU
1	C	371	ILE
1	C	373	VAL
1	C	375	VAL
1	C	383	VAL
1	C	388	VAL
1	C	389	THR
1	C	394	THR
1	C	404	LEU
1	C	414	ASP
1	C	415	ASP
1	C	422	LEU
1	C	426	SER
1	C	431	LEU
1	C	433	PHE
1	C	435	VAL
1	C	436	LYS
1	C	442	LEU
1	C	455	ILE
1	C	457	TYR
1	C	458	SER
1	C	459	SER
1	C	467	ILE
1	C	469	TRP
1	C	471	ASP
1	C	474	LYS
1	C	483	ASN
1	C	487	THR
1	C	492	TYR
1	C	493	ILE
1	C	494	ASP
1	C	495	LYS
1	C	497	THR
1	C	504	LEU

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Mol	Chain	Res	Type
1	C	506	LYS
1	C	509	ILE
1	C	510	ILE
1	C	512	PHE
1	C	522	SER
1	C	526	ILE
1	C	532	GLN
1	C	534	MET
1	C	535	VAL
1	C	541	LEU
1	C	543	TYR
1	C	544	TYR
1	C	545	ILE
1	C	547	THR
1	C	553	GLU
1	C	559	VAL
1	C	561	LEU
1	C	563	ILE
1	C	565	GLU
1	C	569	ASN
1	C	570	GLN
1	C	573	VAL
1	C	583	SER
1	C	599	TRP
1	C	605	VAL
1	C	613	GLN
1	C	614	ARG
1	C	620	LEU
1	C	621	GLU
1	C	627	LEU
1	C	628	GLU
1	C	632	LEU
1	C	640	LEU
1	C	644	ASN
1	C	648	LEU
1	C	652	THR
1	C	654	LEU
1	C	658	ASN
1	C	669	CYS
1	C	679	LEU
1	C	684	GLU
1	C	700	TYR

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Mol	Chain	Res	Type
1	C	701	ASP
1	C	710	THR
1	C	713	GLN
1	C	720	LEU
1	C	754	MET
1	C	756	THR
1	C	766	ARG
1	C	774	LEU
1	C	777	VAL
1	C	779	LEU
1	C	782	ARG
1	C	786	LEU
1	C	787	GLN
1	C	788	PHE
1	C	795	THR
1	C	800	GLN
1	C	805	SER
1	C	813	ASP
1	C	824	PHE
1	C	825	LEU
1	C	833	VAL
1	C	838	GLN
1	C	845	VAL
1	C	849	ARG
1	C	850	THR
1	C	854	GLN
1	C	856	CYS
1	C	857	VAL
1	C	859	MET
1	C	865	ILE
1	C	876	GLN
1	C	887	LYS
1	C	895	LEU
1	C	899	THR
1	C	901	LEU
1	C	905	ILE
1	C	916	THR
1	C	917	TRP
1	C	928	ARG
1	C	935	LYS
1	C	936	ARG
1	C	942	VAL

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Mol	Chain	Res	Type
1	C	944	LEU
1	C	945	ASP
1	C	952	THR
1	C	955	ARG
1	C	965	LEU
1	C	972	GLU
1	C	975	ARG
1	C	977	LEU
1	C	979	VAL
1	C	980	LYS
1	C	983	LEU
1	C	984	VAL
1	C	988	LEU
1	C	1001	THR
1	C	1002	HIS
1	C	1007	SER
1	C	1011	GLU
1	C	1012	LEU
1	C	1013	MET
1	C	1015	VAL
1	C	1018	VAL
1	C	1021	VAL
1	C	1029	ASN
1	C	1033	ILE
1	C	1049	LEU
1	C	1054	LEU
1	C	1055	SER
1	C	1056	ILE
1	C	1061	ASN
1	C	1067	SER
1	C	1070	LYS
1	C	1079	THR
1	C	1098	ASN
1	C	1105	LEU
1	C	1113	LEU
1	C	1125	GLN
1	C	1127	ILE
1	C	1128	LYS
1	C	1132	THR
1	C	1133	LEU
1	C	1140	ASN
1	C	1142	LEU

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Mol	Chain	Res	Type
1	C	1144	LEU
1	C	1150	ILE
1	C	1159	CYS
1	C	1166	THR
1	C	1179	THR
1	C	1180	LEU
1	C	1184	SER
1	C	1190	ILE
1	C	1196	SER
1	C	1200	LYS
1	C	1201	THR
1	C	1202	HIS
1	C	1207	SER
1	C	1230	ASP
1	C	1232	LEU
1	C	1246	ARG
1	C	1264	ILE
1	C	1275	SER
1	C	1280	TYR
1	C	1284	PHE
1	C	1286	SER
1	C	1301	SER
1	C	1302	LEU
1	C	1307	LEU
1	C	1309	LEU
1	C	1313	ILE
1	C	1315	VAL
1	C	1323	LEU
1	C	1326	TYR
1	C	1329	THR
1	C	1331	LYS
1	C	1334	LEU
1	C	1336	ARG
1	C	1338	VAL
1	C	1341	LEU
1	C	1342	LEU
1	C	1346	LEU
1	C	1347	ILE
1	C	1348	VAL
1	C	1350	THR
1	C	1352	PHE
1	C	1356	LEU

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Mol	Chain	Res	Type
1	C	1358	THR
1	C	1360	HIS
1	C	1363	THR
1	C	1366	HIS
1	C	1372	GLU
1	C	1376	SER
1	C	1401	ARG
1	C	1416	SER
1	C	1423	VAL
1	C	1430	THR
1	C	1446	VAL
1	C	1455	ILE
1	C	1459	HIS
1	C	1464	LEU
1	C	1470	SER
1	C	1475	VAL
1	C	1476	ARG
1	C	1479	ILE
1	C	1480	PHE
1	C	1483	PHE
1	C	1487	PHE
1	C	1492	THR
1	C	1493	PHE
1	C	1494	THR
1	C	1496	TYR
1	C	1500	ARG
1	C	1502	ASP
1	C	1503	LYS
1	C	1507	MET
1	C	1525	CYS
1	C	1531	ASP
1	C	1532	CYS
1	C	1535	MET
1	C	1539	LEU
1	C	1548	ARG
1	C	1549	LYS
1	C	1556	GLU
1	C	1557	ILE
1	C	1559	TYR
1	C	1566	THR
1	C	1569	THR
1	C	1573	VAL

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Mol	Chain	Res	Type
1	C	1580	THR
1	C	1581	LEU
1	C	1583	ASP
1	C	1585	TYR
1	C	1589	GLU
1	C	1602	LYS
1	C	1604	VAL
1	C	1606	CYS
1	C	1618	LEU
1	C	1620	MET
1	C	1626	GLN
1	C	1627	ILE
1	C	1631	PHE
1	C	1635	TYR
1	C	1636	ILE
1	C	1637	TYR
1	C	1639	LEU
1	C	1654	CYS
1	C	1664	LEU
2	D	40	GLN
2	D	43	VAL
2	D	54	LEU
2	D	56	ILE
2	D	58	VAL
2	D	68	LEU
2	D	69	PHE
2	D	71	THR
2	D	74	ASP
2	D	82	LEU
2	D	86	THR
2	D	87	ILE
2	D	105	VAL
2	D	114	ARG
2	D	119	VAL
2	D	120	LEU
2	D	121	LEU
2	D	124	GLN
2	D	146	ARG
2	D	147	VAL
2	D	150	MET
2	D	161	VAL
2	D	167	THR

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Mol	Chain	Res	Type
2	D	177	SER
2	D	178	VAL
2	D	179	ASP
2	D	183	PHE
2	D	191	LEU
2	D	196	THR
2	D	198	ARG
2	D	199	ILE
2	D	206	SER
2	D	209	ASN
2	D	211	THR
2	D	219	TYR
2	D	220	VAL
2	D	221	LEU
2	D	226	VAL
2	D	243	PHE
2	D	264	LEU
2	D	274	LYS
2	D	278	ASP
2	D	280	LEU
2	D	291	LYS
2	D	297	ASP
2	D	299	PHE
2	D	306	LEU
2	D	317	SER
2	D	320	VAL
2	D	328	MET
2	D	338	ILE
2	D	341	SER
2	D	344	GLN
2	D	345	ILE
2	D	349	LYS
2	D	390	THR
2	D	398	LEU
2	D	400	LEU
2	D	404	LEU
2	D	411	ILE
2	D	422	ARG
2	D	435	TYR
2	D	437	THR
2	D	450	THR
2	D	458	ASP

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Mol	Chain	Res	Type
2	D	460	LEU
2	D	469	ASN
2	D	472	SER
2	D	477	LYS
2	D	478	TYR
2	D	481	TYR
2	D	482	LEU
2	D	488	LYS
2	D	492	VAL
2	D	497	ARG
2	D	498	ARG
2	D	504	VAL
2	D	505	THR
2	D	506	MET
2	D	507	ASN
2	D	511	THR
2	D	513	ASP
2	D	518	PHE
2	D	519	ARG
2	D	520	PHE
2	D	521	VAL
2	D	523	TYR
2	D	524	TYR
2	D	525	GLN
2	D	526	VAL
2	D	528	ASN
2	D	531	ILE
2	D	543	THR
2	D	544	CYS
2	D	555	LEU
2	D	556	ILE
2	D	563	MET
2	D	567	LEU
2	D	574	ARG
2	D	582	LYS
2	D	584	VAL
2	D	588	ASN
2	D	593	ILE
2	D	594	SER
2	D	606	ASP
2	D	620	VAL
2	D	629	THR

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Mol	Chain	Res	Type
2	D	634	LEU
2	D	638	GLN
2	D	643	LYS
2	D	740	ILE
2	D	742	ASP
2	D	743	SER
2	D	745	ILE
2	D	746	ILE
2	D	747	SER
2	D	769	GLN
2	D	778	PHE
2	D	780	LEU
2	D	783	SER
2	D	784	ILE
2	D	789	VAL
2	D	793	SER
2	D	800	ILE
2	D	802	VAL
2	D	804	GLU
2	D	808	ILE
2	D	812	LYS
2	D	813	VAL
2	D	816	ILE
2	D	817	ASP
2	D	819	GLN
2	D	829	GLN
2	D	830	VAL
2	D	836	LEU
2	D	851	LEU
2	D	857	CYS
2	D	867	ARG
2	D	870	PHE
2	D	872	ILE
2	D	873	LYS
2	D	875	LEU
2	D	880	VAL
2	D	884	ILE
2	D	889	GLN
2	D	891	LEU
2	D	913	LEU
2	D	914	LYS
2	D	916	VAL

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Mol	Chain	Res	Type
2	D	918	GLU
2	D	920	VAL
2	D	926	THR
2	D	946	LYS
2	D	948	ARG
2	D	952	ASP
2	D	960	GLU
2	D	963	ILE
2	D	964	ILE
2	D	1278	THR
2	D	1279	ILE
2	D	1281	LEU
2	D	1283	ASP
2	D	1291	ARG
2	D	1292	ILE
2	D	1293	ASN
2	D	1298	LEU
2	D	1303	VAL
2	D	1305	THR
2	D	1308	ASN
2	D	1313	VAL
2	D	1324	THR
2	D	1326	LEU
2	D	1329	TYR
2	D	1330	ASN
2	D	1332	GLN
2	D	1344	HIS
2	D	1350	GLU
2	D	1351	ASN
2	D	1365	LEU
2	D	1367	ILE
2	D	1372	LEU
2	D	1378	THR
2	D	1401	SER
2	D	1404	VAL
2	D	1406	ARG
2	D	1423	VAL
2	D	1424	ILE
2	D	1425	ILE
2	D	1427	LEU
2	D	1429	LYS
2	D	1433	SER

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Mol	Chain	Res	Type
2	D	1437	CYS
2	D	1438	LEU
2	D	1442	ILE
2	D	1443	LEU
2	D	1445	HIS
2	D	1448	VAL
2	D	1459	TYR
2	D	1465	ASP
2	D	1475	ASP
2	D	1480	LEU
2	D	1481	LEU
2	D	1490	CYS
2	D	1491	ARG
2	D	1492	CYS
2	D	1495	GLU
2	D	1496	THR
2	D	1497	CYS
2	D	1504	GLU
2	D	1522	TYR
2	D	1526	THR
2	D	1529	LEU
2	D	1535	ASP
2	D	1539	ILE
2	D	1561	HIS
2	D	1566	GLN
2	D	1584	TRP
2	D	1591	LEU
2	D	1594	LYS
2	D	1597	ILE
2	D	1598	SER
2	D	1604	ASN
2	D	1605	THR
2	D	1607	ILE
2	D	1612	HIS
2	D	1616	CYS
2	D	1632	SER
2	D	1634	THR
2	D	1638	PHE
3	X	41	HIS
3	X	43	ILE
3	X	46	LEU
3	X	50	TYR

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Mol	Chain	Res	Type
3	X	51	SER
3	X	65	GLU
3	X	66	ASN
3	X	67	TYR
3	X	75	PHE
3	X	78	LYS
3	X	80	GLN
3	X	85	PHE
3	X	94	TYR
3	X	105	VAL
3	X	111	ASP
3	X	113	ASN
3	X	117	SER
3	X	119	VAL
3	X	123	THR
3	X	130	SER
3	X	132	THR
3	X	136	LEU
3	X	146	LEU
3	X	175	ASN
3	X	185	LYS
3	X	190	ILE
3	X	191	ILE
3	X	196	GLU
3	X	209	PHE
3	X	210	GLU
3	X	225	SER
3	X	229	ASN
3	Y	41	HIS
3	Y	43	ILE
3	Y	46	LEU
3	Y	50	TYR
3	Y	51	SER
3	Y	63	LYS
3	Y	65	GLU
3	Y	66	ASN
3	Y	67	TYR
3	Y	75	PHE
3	Y	78	LYS
3	Y	80	GLN
3	Y	85	PHE
3	Y	94	TYR

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Mol	Chain	Res	Type
3	Y	105	VAL
3	Y	111	ASP
3	Y	113	ASN
3	Y	115	ARG
3	Y	117	SER
3	Y	119	VAL
3	Y	123	THR
3	Y	132	THR
3	Y	136	LEU
3	Y	146	LEU
3	Y	175	ASN
3	Y	185	LYS
3	Y	190	ILE
3	Y	191	ILE
3	Y	196	GLU
3	Y	209	PHE
3	Y	210	GLU
3	Y	225	SER
3	Y	229	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (162) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	42	GLN
1	A	77	ASN
1	A	80	GLN
1	A	97	ASN
1	A	139	GLN
1	A	149	ASN
1	A	236	ASN
1	A	242	ASN
1	A	257	ASN
1	A	289	ASN
1	A	294	ASN
1	A	355	ASN
1	A	391	ASN
1	A	473	HIS
1	A	481	HIS
1	A	569	ASN
1	A	706	ASN
1	A	785	GLN

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Mol	Chain	Res	Type
1	A	787	GLN
1	A	800	GLN
1	A	838	GLN
1	A	854	GLN
1	A	875	HIS
1	A	876	GLN
1	A	909	ASN
1	A	1023	HIS
1	A	1029	ASN
1	A	1030	HIS
1	A	1095	GLN
1	A	1102	ASN
1	A	1112	GLN
1	A	1123	GLN
1	A	1202	HIS
1	A	1233	GLN
1	A	1241	ASN
1	A	1260	ASN
1	A	1268	ASN
1	A	1306	GLN
1	A	1360	HIS
1	A	1448	GLN
1	A	1550	GLN
1	A	1608	ASN
1	A	1658	GLN
1	A	1663	ASN
2	B	40	GLN
2	B	65	GLN
2	B	124	GLN
2	B	152	HIS
2	B	176	ASN
2	B	187	ASN
2	B	333	GLN
2	B	344	GLN
2	B	417	HIS
2	B	459	ASN
2	B	469	ASN
2	B	507	ASN
2	B	525	GLN
2	B	615	GLN
2	B	819	GLN
2	B	829	GLN

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Mol	Chain	Res	Type
2	B	869	GLN
2	B	889	GLN
2	B	901	GLN
2	B	921	GLN
2	B	1330	ASN
2	B	1341	ASN
2	B	1473	HIS
2	B	1501	ASN
2	B	1503	GLN
2	B	1562	GLN
1	C	38	ASN
1	C	42	GLN
1	C	77	ASN
1	C	80	GLN
1	C	97	ASN
1	C	110	HIS
1	C	149	ASN
1	C	236	ASN
1	C	242	ASN
1	C	257	ASN
1	C	289	ASN
1	C	294	ASN
1	C	355	ASN
1	C	391	ASN
1	C	473	HIS
1	C	481	HIS
1	C	511	HIS
1	C	550	GLN
1	C	569	ASN
1	C	658	ASN
1	C	706	ASN
1	C	785	GLN
1	C	787	GLN
1	C	800	GLN
1	C	838	GLN
1	C	854	GLN
1	C	875	HIS
1	C	876	GLN
1	C	909	ASN
1	C	1023	HIS
1	C	1029	ASN
1	C	1030	HIS

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Mol	Chain	Res	Type
1	C	1095	GLN
1	C	1102	ASN
1	C	1112	GLN
1	C	1123	GLN
1	C	1202	HIS
1	C	1233	GLN
1	C	1241	ASN
1	C	1260	ASN
1	C	1268	ASN
1	C	1306	GLN
1	C	1360	HIS
1	C	1448	GLN
1	C	1550	GLN
1	C	1608	ASN
1	C	1658	GLN
2	D	40	GLN
2	D	65	GLN
2	D	124	GLN
2	D	152	HIS
2	D	176	ASN
2	D	187	ASN
2	D	333	GLN
2	D	344	GLN
2	D	417	HIS
2	D	459	ASN
2	D	465	ASN
2	D	469	ASN
2	D	507	ASN
2	D	525	GLN
2	D	615	GLN
2	D	819	GLN
2	D	829	GLN
2	D	869	GLN
2	D	889	GLN
2	D	921	GLN
2	D	1308	ASN
2	D	1330	ASN
2	D	1341	ASN
2	D	1473	HIS
2	D	1503	GLN
2	D	1511	GLN
2	D	1562	GLN

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Mol	Chain	Res	Type
3	X	47	HIS
3	X	59	ASN
3	X	80	GLN
3	X	83	GLN
3	X	113	ASN
3	X	139	ASN
3	X	142	ASN
3	X	197	ASN
3	Y	47	HIS
3	Y	59	ASN
3	Y	71	ASN
3	Y	80	GLN
3	Y	83	GLN
3	Y	113	ASN
3	Y	139	ASN
3	Y	142	ASN
3	Y	197	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

8 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	B	2001	2,5	14,14,15	0.97	1 (7%)	15,19,21	1.67	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	2002	5	14,14,15	0.99	1 (7%)	15,19,21	2.48	5 (33%)
5	NAG	B	2003	2,5	14,14,15	2.03	7 (50%)	15,19,21	3.44	5 (33%)
5	NAG	B	2004	5	14,14,15	1.69	1 (7%)	15,19,21	1.68	4 (26%)
5	NAG	D	2001	2,5	14,14,15	0.88	1 (7%)	15,19,21	1.70	4 (26%)
5	NAG	D	2002	5	14,14,15	1.05	1 (7%)	15,19,21	1.74	3 (20%)
5	NAG	D	2003	2,5	14,14,15	1.95	6 (42%)	15,19,21	3.68	6 (40%)
5	NAG	D	2004	5	14,14,15	1.57	1 (7%)	15,19,21	1.81	4 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	2001	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	2002	5	-	0/6/23/26	0/1/1/1
5	NAG	B	2003	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	2004	5	-	0/6/23/26	0/1/1/1
5	NAG	D	2001	2,5	-	0/6/23/26	0/1/1/1
5	NAG	D	2002	5	-	0/6/23/26	0/1/1/1
5	NAG	D	2003	2,5	-	0/6/23/26	0/1/1/1
5	NAG	D	2004	5	-	0/6/23/26	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2003	NAG	C3-C2	2.02	1.57	1.52
5	B	2003	NAG	C2-N2	2.11	1.50	1.46
5	B	2002	NAG	C3-C2	2.13	1.57	1.52
5	D	2003	NAG	C3-C2	2.25	1.57	1.52
5	D	2003	NAG	C4-C5	2.43	1.58	1.53
5	B	2003	NAG	O4-C4	2.44	1.48	1.43
5	D	2001	NAG	C1-C2	2.47	1.55	1.52
5	D	2002	NAG	C1-C2	2.49	1.55	1.52
5	D	2003	NAG	O5-C1	2.55	1.48	1.43
5	D	2003	NAG	O4-C4	2.63	1.49	1.43
5	B	2003	NAG	C4-C3	2.68	1.59	1.52
5	B	2003	NAG	C4-C5	2.71	1.58	1.53
5	D	2003	NAG	C4-C3	2.88	1.59	1.52
5	B	2001	NAG	C1-C2	2.98	1.56	1.52
5	B	2003	NAG	O5-C1	2.99	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	2003	NAG	C1-C2	3.56	1.57	1.52
5	B	2003	NAG	C1-C2	4.06	1.58	1.52
5	D	2004	NAG	C1-C2	5.27	1.59	1.52
5	B	2004	NAG	C1-C2	5.44	1.60	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	2001	NAG	O3-C3-C2	-2.78	103.61	109.11
5	D	2004	NAG	O7-C7-C8	-2.49	117.50	122.06
5	D	2003	NAG	O3-C3-C2	-2.31	104.54	109.11
5	B	2004	NAG	O7-C7-C8	-2.26	117.91	122.06
5	D	2001	NAG	C3-C4-C5	-2.19	106.39	110.20
5	D	2001	NAG	C4-C3-C2	-2.13	107.92	111.23
5	B	2001	NAG	O3-C3-C2	-2.05	105.05	109.11
5	D	2003	NAG	O3-C3-C4	2.09	115.04	110.34
5	B	2002	NAG	O5-C5-C6	2.29	112.30	107.35
5	B	2003	NAG	O3-C3-C4	2.31	115.53	110.34
5	B	2001	NAG	O3-C3-C4	2.48	115.92	110.34
5	B	2002	NAG	O4-C4-C3	2.56	116.10	110.34
5	D	2002	NAG	C1-O5-C5	2.59	115.53	112.25
5	B	2003	NAG	O7-C7-N2	2.70	127.38	121.86
5	D	2004	NAG	O3-C3-C2	2.79	114.63	109.11
5	D	2004	NAG	O5-C5-C6	2.86	113.53	107.35
5	B	2002	NAG	C2-N2-C7	3.09	127.01	123.04
5	B	2004	NAG	C2-N2-C7	3.13	127.06	123.04
5	B	2004	NAG	O3-C3-C2	3.20	115.45	109.11
5	D	2003	NAG	O4-C4-C3	3.29	117.75	110.34
5	D	2002	NAG	C2-N2-C7	3.49	127.52	123.04
5	B	2004	NAG	O5-C5-C6	3.55	115.03	107.35
5	D	2002	NAG	C4-C3-C2	3.57	116.77	111.23
5	B	2003	NAG	C4-C3-C2	3.78	117.11	111.23
5	D	2001	NAG	C1-O5-C5	3.79	117.06	112.25
5	B	2001	NAG	C1-O5-C5	3.87	117.16	112.25
5	D	2004	NAG	C2-N2-C7	4.17	128.40	123.04
5	B	2002	NAG	C1-O5-C5	4.38	117.81	112.25
5	D	2003	NAG	C4-C3-C2	4.85	118.77	111.23
5	B	2003	NAG	C2-N2-C7	5.87	130.58	123.04
5	D	2003	NAG	C2-N2-C7	5.87	130.58	123.04
5	B	2002	NAG	C4-C3-C2	6.06	120.66	111.23
5	B	2003	NAG	C1-O5-C5	9.87	124.78	112.25
5	D	2003	NAG	C1-O5-C5	10.72	125.86	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2001	NAG	3	0
5	B	2002	NAG	3	0
5	B	2003	NAG	3	0
5	D	2001	NAG	4	0
5	D	2002	NAG	4	0
5	D	2003	NAG	3	0

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	2003	1	14,14,15	1.79	4 (28%)	15,19,21	3.50	11 (73%)
4	NAG	C	2003	1	14,14,15	2.01	4 (28%)	15,19,21	2.62	8 (53%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	2003	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2003	1	-	0/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2003	NAG	O4-C4	2.13	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2003	NAG	C4-C3	2.14	1.58	1.52
4	A	2003	NAG	C4-C5	2.14	1.57	1.53
4	A	2003	NAG	O4-C4	2.39	1.48	1.43
4	C	2003	NAG	C4-C5	3.06	1.59	1.53
4	C	2003	NAG	C3-C2	3.68	1.60	1.52
4	A	2003	NAG	C3-C2	4.04	1.61	1.52
4	C	2003	NAG	C1-C2	4.69	1.59	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2003	NAG	O7-C7-C8	-5.17	112.57	122.06
4	C	2003	NAG	O7-C7-C8	-3.58	115.49	122.06
4	A	2003	NAG	C3-C4-C5	-3.57	103.97	110.20
4	A	2003	NAG	O3-C3-C4	-3.23	103.06	110.34
4	C	2003	NAG	C4-C3-C2	2.03	114.38	111.23
4	C	2003	NAG	O7-C7-N2	2.17	126.30	121.86
4	A	2003	NAG	C3-C2-N2	2.57	116.71	110.56
4	C	2003	NAG	O4-C4-C3	2.65	116.30	110.34
4	A	2003	NAG	C8-C7-N2	2.89	121.64	116.11
4	A	2003	NAG	O4-C4-C5	3.17	117.64	109.24
4	C	2003	NAG	C1-O5-C5	3.22	116.33	112.25
4	C	2003	NAG	O4-C4-C5	3.27	117.91	109.24
4	C	2003	NAG	C2-N2-C7	3.40	127.41	123.04
4	A	2003	NAG	O3-C3-C2	3.43	115.91	109.11
4	A	2003	NAG	C1-O5-C5	4.20	117.58	112.25
4	A	2003	NAG	O4-C4-C3	4.34	120.10	110.34
4	A	2003	NAG	C4-C3-C2	4.42	118.10	111.23
4	C	2003	NAG	O3-C3-C2	4.75	118.53	109.11
4	A	2003	NAG	C2-N2-C7	5.75	130.43	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2003	NAG	1	0
4	C	2003	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1626/1676 (97%)	0.00	20 (1%)	81	73	72, 150, 260, 469	0
1	C	1626/1676 (97%)	0.08	58 (3%)	46	37	60, 153, 277, 515	0
2	B	1215/1642 (73%)	0.06	23 (1%)	70	61	73, 160, 235, 335	0
2	D	1215/1642 (73%)	0.01	26 (2%)	67	57	85, 155, 241, 362	0
3	X	191/231 (82%)	0.75	31 (16%)	3	4	99, 230, 333, 437	0
3	Y	191/231 (82%)	0.46	17 (8%)	12	9	95, 195, 300, 385	0
All	All	6064/7098 (85%)	0.07	175 (2%)	55	44	60, 157, 264, 515	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	X	112	PRO	12.0
3	Y	114	GLY	7.0
1	C	1651	ASP	5.9
3	X	114	GLY	5.8
3	X	113	ASN	5.7
3	Y	113	ASN	5.5
1	C	1592	ALA	5.5
1	C	1585	TYR	5.0
2	D	1272	ASP	4.6
3	X	70	SER	4.4
3	Y	115	ARG	4.3
3	X	95	LYS	4.1
2	D	100	GLN	4.1
3	Y	59	ASN	4.0
2	D	98	SER	3.9
3	Y	92	GLU	3.6
1	A	874	ASP	3.6
3	Y	71	ASN	3.6
2	B	1319	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	1318	ASP	3.6
1	A	1002	HIS	3.5
2	D	97	ASP	3.5
1	A	94	GLY	3.4
1	C	1537	GLU	3.4
1	C	1622	LYS	3.4
1	C	1002	HIS	3.3
1	C	1593	GLU	3.3
2	D	1273	LEU	3.3
2	B	1272	ASP	3.3
1	C	1586	LYS	3.3
3	Y	195	ASP	3.2
1	C	273	GLU	3.2
3	X	90	ASP	3.2
1	C	1538	GLU	3.2
1	C	1525	CYS	3.1
1	C	874	ASP	3.1
3	X	108	GLU	3.1
1	C	882	LYS	3.1
2	B	1320	LYS	3.1
3	Y	95	LYS	3.1
1	C	278	ASP	3.0
1	A	879	LYS	3.0
3	X	104	PHE	3.0
1	A	1545	ALA	3.0
1	C	712	GLU	3.0
2	B	1435	ASP	2.9
2	B	639	ARG	2.9
1	C	1609	ALA	2.9
2	B	1273	LEU	2.9
2	D	940	THR	2.9
1	A	817	ALA	2.8
1	C	1557	ILE	2.8
3	X	76	ASN	2.8
1	A	1398	ASP	2.8
3	X	71	ASN	2.8
3	X	93	GLN	2.8
1	C	159	THR	2.7
3	X	111	ASP	2.7
1	A	1399	TYR	2.7
1	C	1596	SER	2.7
1	C	1597	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
3	X	127	ASN	2.7
2	B	1344	HIS	2.7
2	D	99	ARG	2.7
3	X	126	ASN	2.6
1	C	1598	ILE	2.6
2	D	941	GLN	2.6
1	C	93	PRO	2.6
1	A	1622	LYS	2.6
1	C	1594	LYS	2.6
1	C	94	GLY	2.6
3	Y	159	GLU	2.6
2	B	1370	ARG	2.5
2	D	765	GLU	2.5
2	D	1354	LEU	2.5
3	X	128	LYS	2.5
1	C	1544	SER	2.5
2	B	1371	TYR	2.5
3	X	74	ARG	2.5
3	X	79	ASP	2.5
2	B	1376	ASP	2.5
3	X	92	GLU	2.5
1	C	403	ASP	2.5
3	X	120	GLY	2.5
1	C	255	PHE	2.5
2	B	1434	GLU	2.5
1	A	240	TYR	2.5
3	Y	196	GLU	2.4
1	C	446	ASN	2.4
3	X	195	ASP	2.4
1	A	273	GLU	2.4
2	B	1374	GLU	2.4
1	C	817	ALA	2.4
3	X	101	GLN	2.4
2	B	640	SER	2.4
1	A	1526	LYS	2.4
1	C	1241	ASN	2.4
3	Y	90	ASP	2.4
1	A	271	ILE	2.3
2	D	66	LYS	2.3
1	A	692	HIS	2.3
2	B	1375	VAL	2.3
1	C	240	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	99	ARG	2.3
1	C	1233	GLN	2.3
1	A	691	LYS	2.3
2	B	61	PHE	2.3
3	X	159	GLU	2.3
1	C	313	TYR	2.3
2	B	23	ALA	2.3
2	B	344	GLN	2.3
2	D	967	GLY	2.3
1	C	312	TYR	2.3
1	C	1545	ALA	2.3
2	D	337	HIS	2.3
3	Y	89	LYS	2.3
1	C	95	GLY	2.2
3	X	73	VAL	2.2
1	C	1595	ASP	2.2
2	D	951	ASP	2.2
3	Y	64	VAL	2.2
2	B	369	PRO	2.2
1	C	846	TYR	2.2
1	C	879	LYS	2.2
1	C	314	SER	2.2
3	X	41	HIS	2.2
3	Y	72	VAL	2.2
1	C	393	GLN	2.2
3	X	82	HIS	2.2
2	B	1537	ASN	2.2
2	D	764	GLU	2.2
3	X	116	LEU	2.2
3	Y	116	LEU	2.2
1	A	1651	ASP	2.2
1	C	274	ASP	2.2
1	A	1546	GLU	2.1
1	C	1650	ARG	2.1
1	A	311	SER	2.1
3	Y	129	THR	2.1
3	X	205	ASP	2.1
1	C	1232	LEU	2.1
1	A	1380	LYS	2.1
3	X	99	GLN	2.1
2	D	345	ILE	2.1
1	C	1548	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	52	LYS	2.1
1	C	1587	THR	2.1
1	C	598	SER	2.1
2	D	1291	ARG	2.1
2	D	1333	LEU	2.1
1	C	1579	ALA	2.1
2	D	639	ARG	2.1
2	B	242	ASN	2.1
1	C	1418	GLY	2.1
1	C	1551	THR	2.0
2	D	1376	ASP	2.0
3	X	98	LEU	2.0
1	C	272	ARG	2.0
1	C	1556	GLU	2.0
1	C	398	ASN	2.0
2	B	1271	LYS	2.0
2	D	1566	GLN	2.0
3	X	107	GLN	2.0
3	X	78	LYS	2.0
1	C	309	GLU	2.0
1	C	1327	LYS	2.0
2	D	234	PHE	2.0
1	C	1179	THR	2.0
2	D	1353	HIS	2.0
2	D	158	ASN	2.0
1	A	689	LYS	2.0
2	D	773	SER	2.0
3	Y	126	ASN	2.0
1	C	617	LYS	2.0
1	C	271	ILE	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 ⓘ

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(\AA^2)	Q<0.9
5	NAG	B	2002	14/15	0.72	0.69	-	228,239,253,257	0
5	NAG	D	2001	14/15	0.88	0.41	-	228,253,282,288	0
5	NAG	D	2002	14/15	0.66	0.60	-	228,239,251,252	0
5	NAG	B	2001	14/15	0.73	0.55	-	278,305,319,322	0
5	NAG	D	2004	14/15	0.72	0.83	-	271,274,277,278	0
5	NAG	D	2003	14/15	0.54	0.53	-	246,253,258,265	0
5	NAG	B	2003	14/15	0.24	0.78	-	225,233,240,245	0
5	NAG	B	2004	14/15	0.56	0.78	-	297,301,307,310	0

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(\AA^2)	Q<0.9
4	NAG	C	2003	14/15	0.74	0.40	0.85	177,180,183,183	0
4	NAG	A	2003	14/15	0.77	0.29	0.34	166,169,171,172	0

6.5 Other polymers [i](#)

There are no such residues in this entry.