



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 03:58 PM BST

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1



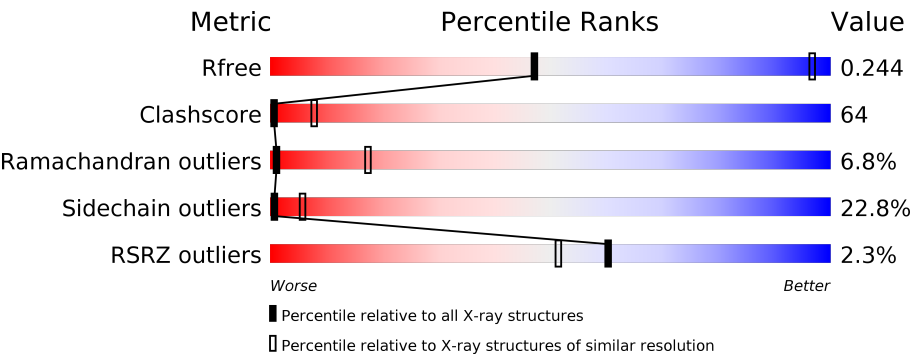
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.30 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))
$R_{free}$	130704	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)





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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1676	<div><div></div><div><div>24%</div><div>50%</div><div>21%</div><div></div></div><div></div></div>
1	C	1676	<div><div>3%</div><div><div>23%</div><div>51%</div><div>21%</div><div></div></div><div></div></div>
2	B	1642	<div><div></div><div><div>23%</div><div>38%</div><div>13%</div><div>26%</div></div><div></div></div>
2	D	1642	<div><div></div><div><div>22%</div><div>39%</div><div>12%</div><div>26%</div></div><div></div></div>
3	X	231	<div><div>11%</div><div><div>26%</div><div>44%</div><div>11%</div><div>17%</div></div><div></div></div>
3	Y	231	<div><div>6%</div><div><div>24%</div><div>45%</div><div>13%</div><div>17%</div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
4	E	2	 100%
4	F	2	 50% 50%
4	G	2	 100%
4	H	2	 50% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	E	1	-	-	-	X
4	NAG	E	2	-	-	-	X
4	NAG	F	1	-	-	-	X
4	NAG	F	2	-	-	-	X
4	NAG	G	2	-	-	-	X
4	NAG	H	1	-	-	-	X
4	NAG	H	2	-	-	-	X



## 2 Entry composition [i](#)

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 an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

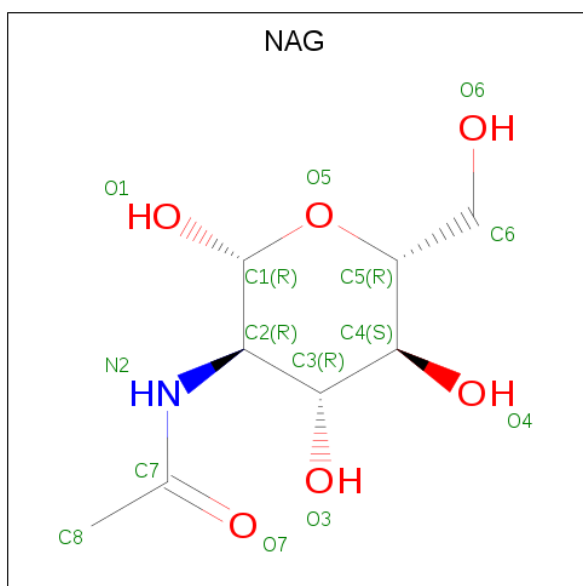
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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



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

Chain A: %

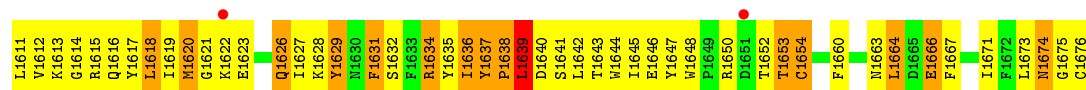
24% 50% 21%

MET	GLY	
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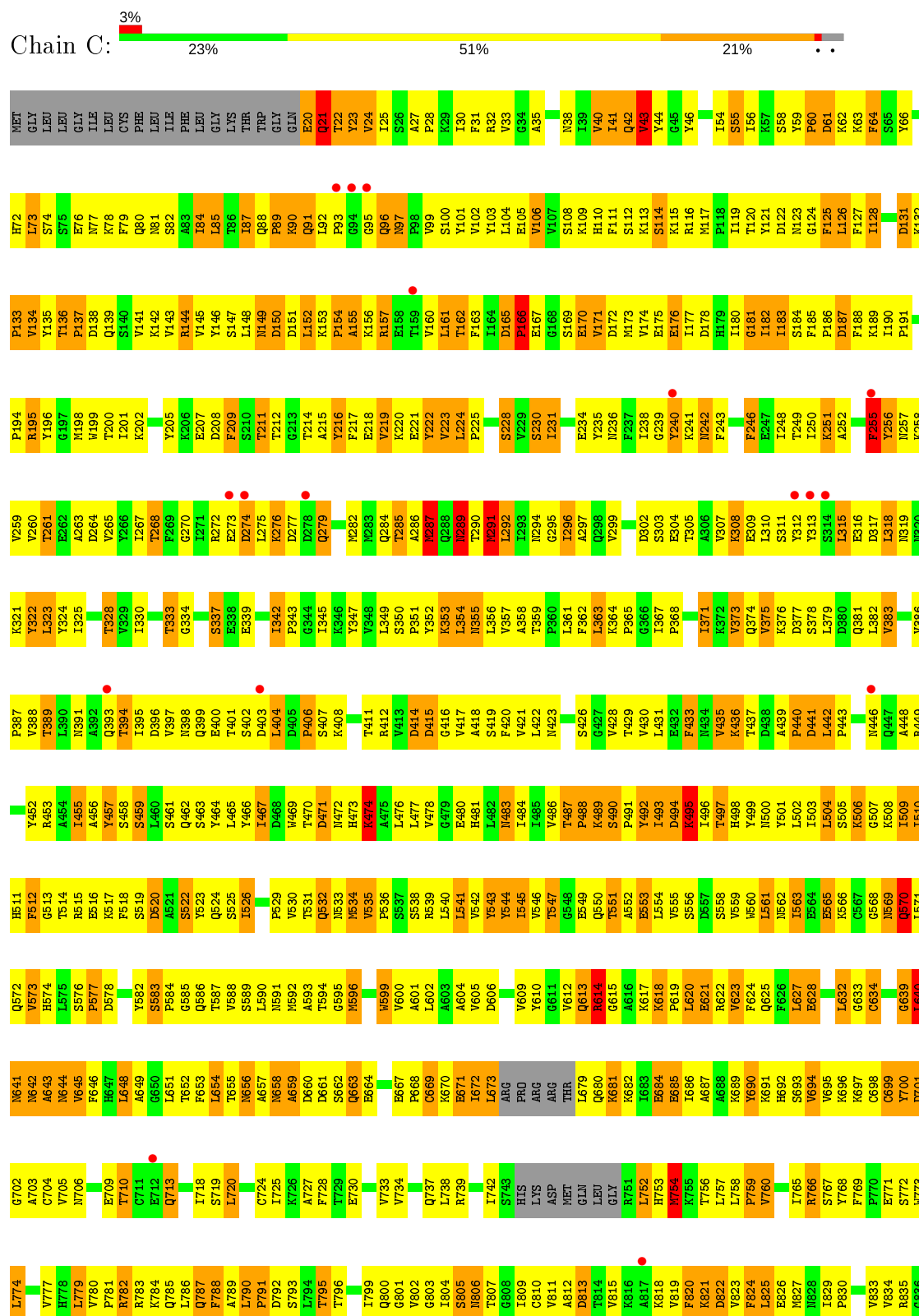


T1551	S1489	V1359	I1294	H1231	I1164	F1034	T971	L907	T644	V780	E709	F646
A1552	P1490	H1360	E1295	L1232	D1165	H1035	E972	H903	V645	F781	T740	H647
C1553	A1491	V1361	G1296	Q1233	T1166	S1036	T1167	N909	V846	R782	C711	L648
K1554	T1492	T1362	L1428	H1234	A1167	S1103	K974	N910	N847	R783	E712	A649
P1555	F1493	T1363	T1298	L1168	L1168	L1404	R975	N911	V848	K784	Q713	G650
E1556	T1494	V1364	E1299	D1236	A1171	L1405	R976	F912	V849	Q785	L651	L651
T1557	V1495	V1365	V1300	S1237	A1172	V1406	L977	S913	T850	L786	I718	T652
A1558	I1432	H1366	S1301	L1238	D1172	L1107	S978	L914	S851	Q787	S719	T653
Y1559	S1433	K1367	L1302	V1239	L1175	V1108	S979	E915	G952	F788	L720	L654
Y1498	A1434	T1368	V1303	N1241	E1110	M1109	K980	T916	N853	A789	L654	T655
H1499	A1435	S1369	K1304	N1241	M1110	E1110	G981	Q954	Q854	L790	C724	N656
P1501	E1436	Q1306	K1305	G1243	Y1111	K1048	L982	F918	F855	P791	I725	A657
S1501	S1371	G1243	G1243	G1243	L1112	K1048	L983	G919	G856	D792	K726	N658
D1502	E1372	T1244	L1307	T1244	L1113	L1049	V984	K920	V857	S793	A727	A659
K1440	E1373	R1308	R1308	A1246	D1114	K1050	G985	L923	K958	L794	F728	D660
V1443	S1376	L1309	L1309	R1246	Q1183	E1051	E986	L923	N859	T795	E730	S662
E1444	I1379	D1247	I1313	M1247	T1184	M1053	L988	V924	V662	C731	E731	Q663
G1445	L1379	E1249	D1314	F1248	T1185	M1053	L988	K925	K925	C732	C732	E664
V1446	K1380	T1250	V1315	F1186	F1187	L1054	S989	T926	E863	V733	V733	C669
D1447	I1381	T1251	S1316	T1187	L1188	S1055	A990	L927	G864	Q800	W734	K670
Q1448	D1382	L1252	K1317	A1189	S1122	M1057	S993	R928	L965	G801	I742	E671
L1449	T1383	Y1253	K1318	I1190	S1122	M1057	Q994	V929	C866	W802	HIS	L672
F1450	Q1384	A1254	H1319	S1191	Y1124	M1061	E995	V930	T867	G803	Q737	L673
T1451	D1385	L1255	K1320	A1192	D1125	Y1064	G996	P931	S868	L804	L738	L673
D1452	I1386	L1256	G1321	Y1193	F1126	Y1064	L997	V934	S870	S805	R739	L673
I1453	A1387	T1257	A1322	A1194	I1127	S1065	N998	K935	P871	R807	I742	ARG
Q1454	ALA	S1258	L1323	L1195	K1128	Y1066	L1999	R936	V872	G808	S743	PRO
S1455	SER	L1259	H1324	S1196	L1129	S1067	L1000	E937	R873	L809	ARG	ARG
K1456	HIS	N1260	N1325	L1197	D1130	V1068	T1001	S938	D874	C810	LYS	THR
D1457	TYR	L1261	K1326	G1198	L1131	M1069	H875	Y939	H875	V811	ASP	L679
G1458	ARG	K1262	K1327	D1199	T1132	K1070	L1003	S940	Q876	A812	NET	K680
H1459	GLY	T1263	M1328	K1200	L1133	G1071	P1004	G941	G877	D813	GLN	K681
V1460	TYR	T1264	T1329	H1201	P1134	G1072	S1007	V942	T878	V815	LEU	K682
L1461	GLY	N1265	D1330	H1202	V1135	S1073	T943	T943	R879	V815	GLY	L683
L1462	ASN	Y1266	K1331	P1203	Q1204	A1074	A1008	L944	C883	R816	R751	E684
S1367	S1367	Y1267	N1332	Q1203	Q1204	S1075	D945	D945	V884	A817	L752	E685
D1368	D1368	N1268	F1333	S1207	S1207	T1076	E1011	P946	R885	K818	H753	L686
Y1399	K1400	P1269	L1334	I1208	L1142	W1077	L1012	R947	Q886	V819	R754	A687
K1400	K1400	V1270	G1335	L1208	Y1143	T1078	M1013	G948	Q886	F820	K755	A688
R1401	R1401	K1272	R1336	A1211	T1144	L1144	S1014	L1949	K887	K821	R756	K689
I1402	I1402	K1273	V1340	L1212	T1145	T1145	V1015	Y950	V888	D822	L757	Y690
V1403	V1403	L1274	L1341	L1213	F1147	F1081	P1016	G951	E889	V823	L758	K691
A1404	A1404	S1275	L1342	L1214	T1148	L1082	P1017	T952	G990	F824	P759	H692
A1406	A1406	E1276	M1343	E1215	T1150	L1083	V1018	S891	S891	L825	V760	S693
S1407	S1407	E1277	D1344	A1216	T1150	V1085	F1019	S992	S893	E826	I765	V695
V1408	V1408	Q1278	D1345	L1217	G1151	L1086	Y1020	S894	S893	N827	R766	K696
K1409	K1409	R1279	L1346	V1218	T1152	G1087	V1021	H894	H828	V829	S767	K697
P1410	P1410	Y1280	V1347	K1219	R1153	Q1088	F1022	V896	V896	P830	Y768	C698
S1411	S1411	V1280	V1348	G1220	K1154	V1089	H1023	T897	T897	P830	F769	C699
F1479	F1479	G1283	V1349	N1221	A1155	N1090	Y1024	P960	F998	V833	F770	C699
E1480	E1480	F1284	T1350	P1222	F1156	K1091	L1025	Y961	F998	V834	E771	Y700
L1481	L1481	Y1285	L1351	P1223	D1157	Y1092	E1026	R962	T899	V834	E771	D701
L1482	G1351	Y1285	T1350	P1223	D1157	Y1092	E1026	R962	T899	V834	E771	D701
F1483	S1416	T1287	F1352	P1223	T1158	V1093	E1026	R962	T899	V834	E771	D701
E1484	E1484	Q1288	F1352	P1223	T1158	V1093	E1026	R962	T899	V834	E771	D701
V1485	V1485	Q1288	F1352	P1223	T1158	V1093	E1026	R962	T899	V834	E771	D701
F1486	F1486	D1289	L1356	W1228	L1161	Q1095	H1030	L967	E904	V834	E771	D701
L1488	L1488	A1293	T1358	D1230	K1163	N1096	H1030	L967	E904	V834	E771	D701
S1420	S1420	H421	G1355	F1227	L1161	Q1095	H1030	L967	E904	V834	E771	D701
H421	H421	A1293	T1358	D1230	K1163	N1096	H1030	L967	E904	V834	E771	D701
A1422	A1422	A1293	T1358	D1230	K1163	N1096	H1030	L967	E904	V834	E771	D701
V1423	V1423	A1293	T1358	D1230	K1163	N1096	H1030	L967	E904	V834	E771	D701
C1532	C1532	R1401	V1340	L1212	T1145	T1145	V1015	Y950	V888	D822	L757	Y690
G1533	G1533	S1469	S1470	L1471	F1471	F1471	F1471	F1471	F1471	F1471	F1471	F1471
Q1534	Q1534	A1404	A1404	A1404	A1404	A1404	A1404	A1404	A1404	A1404	A1404	A1404
M1535	M1535	C1405	L1342	L1342	L1342	L1342	L1342	L1342	L1342	L1342	L1342	L1342
Q1536	Q1536	A1406	M1343	E1276	E1276	E1276	E1276	E1276	E1276	E1276	E1276	E1276
E1537	E1537	S1407	D1344	E1277	E1277	E1277	E1277	E1277	E1277	E1277	E1277	E1277
I1538	I1538	Y1408	D1345	Q1278	Q1278	Q1278	Q1278	Q1278	Q1278	Q1278	Q1278	Q1278
L1539	L1539	K1409	L1346	R1279	R1279	R1279	R1279	R1279	R1279	R1279	R1279	R1279
D1540	D1540	P1410	V1347	Y1280	Y1280	Y1280	Y1280	Y1280	Y1280	Y1280	Y1280	Y1280
L1541	L1541	S1411	V1348	G1220	K1154	V1089	H1023	T897	T897	P830	F769	C699
L1542	L1542	F1479	V1349	N1221	A1155	N1090	Y1024	P960	F998	V833	F770	C699
T1543	T1543	E1414	T1350	P1222	F1156	K1091	L1025	Y961	F998	V834	E771	D701
S1544	S1544	L1482	L1351	P1223	D1157	Y1092	E1026	R962	T899	V834	E771	D701
G1545	G1545	S1416	F1352	P1223	T1158	V1093	E1026	R962	T899	V834	E771	D701
E1546	E1546	E1484	F1483	P1223	T1158	V1093	E1026	R962	T899	V834	E771	D701
T1547	T1547	V1485	V1485	P1223	T1158	V1093	E1026	R962	T899	V834	E771	D701
R1548	R1548	F1486	F1486	P1223	T1158	V1093	E1026	R962	T899	V834	E771	D701
A1609	A1609	L1487	L1487	P1223	T1158	V1093	E1026	R962	T899	V834	E771	D701
E1610	E1610	E1610	E1610	P1223	T1158	V1093	E1026	R962	T899	V834	E771	D701





● Molecule 1: Complement C5





- Molecule 2: Cobra venom factor





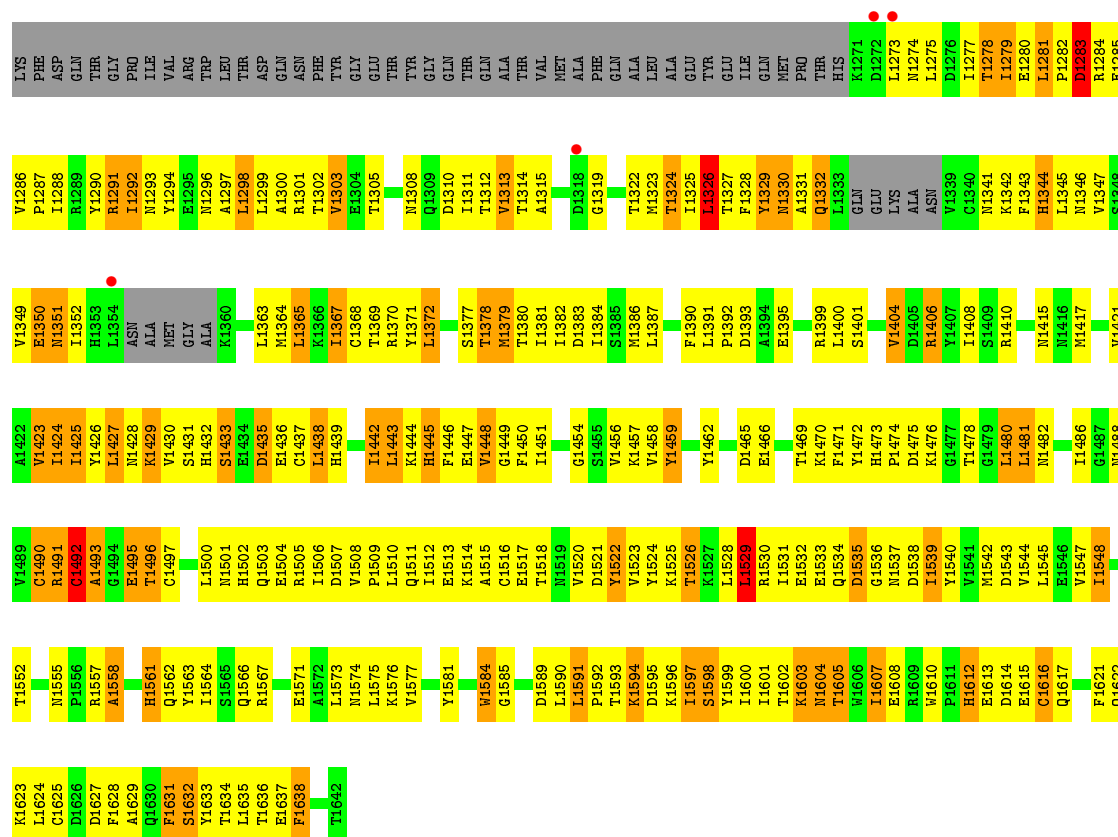




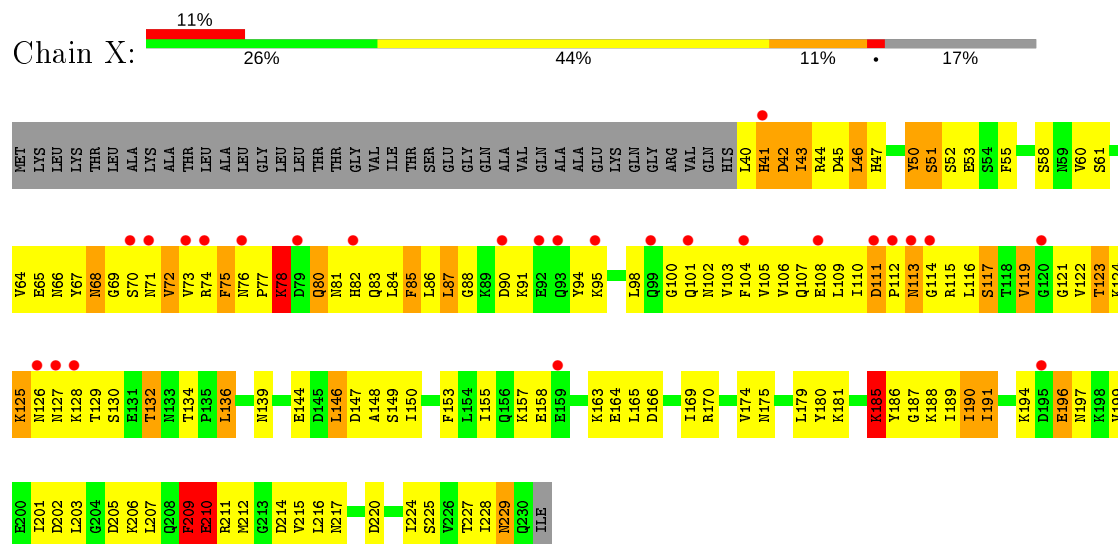




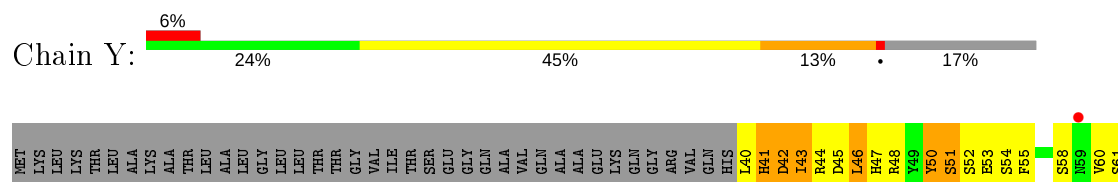




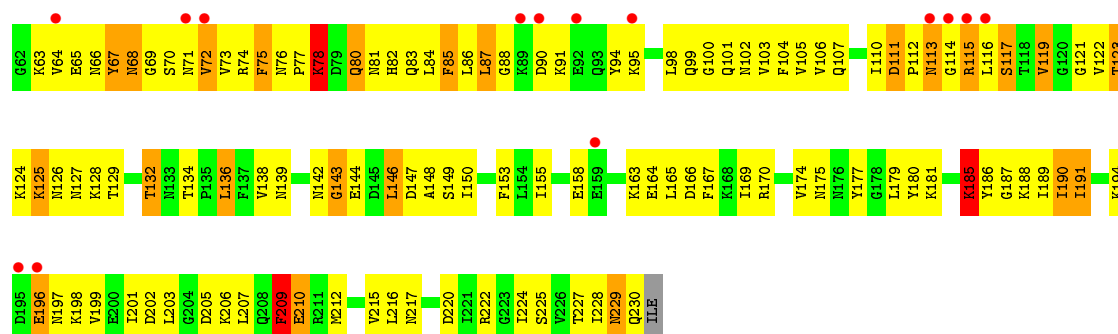
• Molecule 3: Superantigen-like protein 7



• Molecule 3: Superantigen-like protein 7







- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 100%

MAG1  
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 50%

MAG1  
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 100%

MAG1  
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 50%

MAG1  
MAG2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.83 (at 4.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.208 , 0.261 0.193 , 0.244	Depositor DCC
$R_{free}$ test set	1818 reflections (2.33%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	116.2	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 160.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	48236	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality [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	E	28	0	25	3	0
4	F	28	0	25	3	0
4	G	28	0	25	4	0
4	H	28	0	25	3	0
5	A	14	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	14	0	13	2	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:1562:LYS:HD3	1:C:1664:LEU:HD21	1.19	1.14
1:C:500:ASN:HB2	1:C:543:TYR:CE1	1.80	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:C:979:VAL:HG21	1:C:1326:TYR:CE1	1.86	1.10
1:A:25:ILE:H	1:A:655:THR:CG2	1.64	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:A:936:ARG:HG3	1:A:936:ARG:HH11	1.15	1.08
1:C:421:VAL:HG11	2:D:505:THR:HG22	1.35	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:944:LEU:HD11	1:A:1313:ILE:HD11	1.35	1.08
1:A:979:VAL:HG21	1:A:1326:TYR:CE1	1.86	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:127:PHE:HE2	1:C:623:VAL:HG13	1.21	1.05
1:C:1560:ALA:HB2	1:C:1620:MET:HG3	1.38	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
1:A:1068:VAL:HA	1:A:1078:LEU:HD12	1.36	1.02
2:D:1473:HIS:CD2	2:D:1474:PRO:HD2	1.92	1.02
2:B:1473:HIS:HD2	2:B:1474:PRO:HD2	1.22	1.02
1:C:1133:LEU:H	1:C:1133:LEU:HD12	1.20	1.02
1:A:1102:ASN:ND2	1:C:1162:VAL:HG22	1.74	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
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:B:1505:ARG:HG3	2:B:1505:ARG:HH11	1.24	1.00
2:D:263:VAL:HG22	2:D:318:VAL:HG23	1.42	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:182:ILE:HG12	1:C:804:ILE:HD11	1.40	1.00
1:C:60:PRO:HD2	1:C:61:ASP:H	1.27	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:380:VAL:HG12	2:B:387:MET:HB3	1.40	1.00
1:A:1623:GLU:HB2	1:A:1638:PRO:HG3	1.44	1.00
1:A:591:ASN:HB3	1:A:785:GLN:HE21	1.22	1.00
2:D:829:GLN:CG	2:D:1480:LEU:HD13	1.91	1.00
2:D:840:VAL:HG12	2:D:841:ASN:H	1.27	0.99
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:373:VAL:HG11	1:A:435:VAL:HG11	1.41	0.99
1:A:869:GLU:O	1:A:871:PRO:HD3	1.62	0.99
1:C:1493:PHE:HD1	1:C:1494:THR:N	1.60	0.99
2:D:482:LEU:HB3	2:D:492:VAL:HG23	1.45	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:A:371:ILE:HG22	1:A:420:PHE:HB2	1.46	0.98
2:B:851:LEU:HD23	2:B:852:TYR:H	1.28	0.98
1:C:1219:LYS:NZ	1:C:1239:VAL:HG11	1.76	0.98
1:C:1585:TYR:HD1	1:C:1671:ILE:HG21	1.28	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
1:A:60:PRO:HD2	1:A:61:ASP:H	1.25	0.97
2:B:384:PHE:CD1	2:B:400:LEU:HG	1.99	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:1008:ALA:HB3	1:A:1078:LEU:HD11	1.46	0.97
1:A:1526:LYS:O	1:A:1529:GLU:HG3	1.63	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:576:SER:HB3	1:A:577:PRO:HD3	1.45	0.97
1:A:884:VAL:O	1:A:885:ARG:HB2	1.65	0.97
1:C:33:VAL:HG21	1:C:121:TYR:CD1	1.99	0.96
1:C:1612:VAL:HB	1:C:1615:ARG:HB3	1.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:GLU:HG3	1:A:235:TYR:CD2	2.00	0.96
1:C:234:GLU:HG3	1:C:235:TYR:CD2	2.01	0.96
1:C:656:ASN:OD1	1:C:658:ASN:HB3	1.64	0.96
1:C:702:GLY:HA2	1:C:728:PHE:CE1	2.01	0.96
1:A:1612:VAL:HB	1:A:1615:ARG:HB3	1.46	0.96
1:C:292:LEU:HA	1:C:297:ALA:HB2	1.46	0.96
1:C:706:ASN:ND2	1:C:709:GLU:H	1.64	0.96
1:A:1493:PHE:HD1	1:A:1494:THR:N	1.64	0.95
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
2:B:237:ILE:HD11	2:B:309:LEU:HB2	1.46	0.95
1:C:500:ASN:HB2	1:C:543:TYR:HE1	1.20	0.95
2:B:563:MET:HG3	2:B:780:LEU:HD23	1.47	0.95
1:C:838:GLN:HA	1:C:901:LEU:HB2	1.43	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
1:C:706:ASN:HD22	1:C:709:GLU:H	1.02	0.94
2:D:380:VAL:HG12	2:D:387:MET:CB	1.96	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:419:SER:HB2	2:B:459:ASN:HD22	1.30	0.94
1:A:702:GLY:HA2	1:A:728:PHE:CE1	2.03	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:A:430:VAL:HG11	1:A:453:ARG:HH21	1.33	0.94
1:C:1124:TYR:HA	1:C:1465:ASN:OD1	1.66	0.94
1:A:24:VAL:HA	1:A:655:THR:OG1	1.66	0.94
2:B:840:VAL:HG12	2:B:841:ASN:H	1.30	0.94
1:C:1061:ASN:HB2	1:C:1065:SER:O	1.68	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
1:C:596:MET:H	1:C:782:ARG:HH11	1.03	0.93
3:Y:81:ASN:O	3:Y:115:ARG:HB2	1.68	0.93
1:A:1490:PRO:HB3	1:A:1510:SER:HB2	1.50	0.93
1:A:606:ASP:O	1:A:609:VAL:HG23	1.68	0.93
1:C:830:PRO:HG3	1:C:1483:PHE:HZ	1.33	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:353:LYS:CE	1:A:378:SER:HA	2.01	0.91
1:A:944:LEU:CD1	1:A:1313:ILE:HD11	2.00	0.91
1:C:1556:GLU:HB3	1:C:1622:LYS:HE2	1.51	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
1:A:753:HIS:O	1:A:754:MET:HB3	1.68	0.91
3:Y:166:ASP:CG	3:Y:207:LEU:CD2	2.38	0.91
1:A:1562:LYS:HD2	1:A:1648:TRP:CZ2	2.05	0.91
3:X:50:TYR:CE2	3:X:170:ARG:HD2	2.06	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:1528:LEU:HD23	2:D:1576:LYS:O	1.70	0.91
2:D:469:ASN:CG	2:D:472:SER:HB2	1.92	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:A:230:SER:HB3	1:A:251:LYS:HG3	1.50	0.90
1:A:33:VAL:HG21	1:A:121:TYR:CE1	2.06	0.90
1:C:1559:TYR:OH	1:C:1591:VAL:HA	1.71	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:221:LEU:HD11	2:B:753:LYS:HG2	1.52	0.90
2:B:435:TYR:HD1	2:B:436:GLN:H	1.11	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:C:25:ILE:H	1:C:655:THR:HG23	1.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1068:VAL:HG21	1:A:1124:TYR:CD1	2.06	0.89
1:A:502:LEU:HB2	1:A:541:LEU:CD2	2.01	0.89
1:C:1232:LEU:HD11	1:C:1233:GLN:HE21	1.35	0.89
1:C:584:PRO:HB3	1:C:792:ASP:HA	1.54	0.89
2:D:1273:LEU:HB2	2:D:1319:GLY:HA3	1.52	0.89
3:Y:50:TYR:CE2	3:Y:170:ARG:HD2	2.06	0.89
2:B:1273:LEU:HB2	2:B:1319:GLY:HA3	1.53	0.89
2:B:469:ASN:CG	2:B:472:SER:HB2	1.92	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:576:SER:HB2	1:C:589:SER:HB2	1.52	0.89
1:C:60:PRO:CD	1:C:61:ASP:H	1.86	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: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:C:23:TYR:CD1	1:C:655:THR:HB	2.09	0.88
1:A:830:PRO:HG3	1:A:1483:PHE:HZ	1.36	0.88
1:A:980:LYS:HD3	1:A:986:GLU:HA	1.55	0.88
2:D:519:ARG:NH1	2:D:608:GLY:HA3	1.89	0.88
3:X:77:PRO:HD2	3:X:80:GLN:O	1.74	0.88
1:C:511:HIS:CE1	3:Y:149:SER:OG	2.26	0.88
2:B:455:LYS:O	2:B:458:ASP:HB2	1.72	0.88
2:B:829:GLN:HE22	2:B:883:VAL:HG13	1.36	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:120:LEU:HD12	2:D:121:LEU:H	1.38	0.87
2:D:750:ASP:OD1	2:D:752:PRO:HD3	1.73	0.87
1:A:1124:TYR:HA	1:A:1465:ASN:OD1	1.74	0.87
1:A:386:VAL:N	1:A:411:THR:HG22	1.88	0.87
1:C:31:PHE:HB2	1:C:119:ILE:HG22	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:120:THR:HG22	1:A:122:ASP:N	1.88	0.87
1:A:584:PRO:HB3	1:A:792:ASP:HA	1.57	0.87
2:B:494:ARG:HG3	2:B:494:ARG:HH11	1.39	0.87
1:C:944:LEU:CD1	1:C:1313:ILE:HD11	2.05	0.87
2:D:1473:HIS:HB3	2:D:1476:LYS:HB2	1.55	0.87
2:D:1607:ILE:H	2:D:1607:ILE:CD1	1.81	0.87
3:Y:58:SER:HB3	3:Y:102:ASN:ND2	1.90	0.87
1:A:1068:VAL:HG13	1:A:1069:TRP:H	1.39	0.87
3:Y:166:ASP:CG	3:Y:207:LEU:HD21	1.95	0.87
2:B:347:PHE:O	2:B:350:THR:HG22	1.75	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
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:A:1560:ALA:CB	1:A:1620:MET:HG3	2.05	0.86
1:A:182:ILE:HG12	1:A:804:ILE:CD1	2.02	0.86
1:A:855:PHE:HA	2:B:904:LEU:HD11	1.57	0.86
2:B:750:ASP:OD1	2:B:752:PRO:HD3	1.75	0.86
1:C:1068:VAL:HG13	1:C:1069:TRP:H	1.40	0.86
1:C:1585:TYR:CD1	1:C:1671:ILE:HG21	2.10	0.86
1:C:572:GLN:HB2	1:C:593:ALA:HB3	1.56	0.86
1:C:618:LYS:H	1:C:619:PRO:HD3	1.38	0.86
1:C:934:VAL:HG22	1:C:1366:HIS:CD2	2.10	0.86
1:C:599:TRP:O	1:C:803:GLY:HA2	1.74	0.86
2:D:416:ASN:HA	2:D:425:GLN:HE22	1.40	0.86
3:X:166:ASP:CG	3:X:207:LEU:CD2	2.42	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:A:936:ARG:HG3	1:A:936:ARG:NH1	1.89	0.86
1:C:1562:LYS:HD2	1:C:1648:TRP:CZ2	2.11	0.86
1:C:127:PHE:CE2	1:C:623:VAL:HG13	2.08	0.86
1:C:1560:ALA:CB	1:C:1620:MET:HG3	2.04	0.86
1:C:463:SER:HB3	1:C:491:PRO:HA	1.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:TYR:CD1	1:A:23:TYR:N	2.40	0.86
1:C:1404:ALA:HB1	1:C:1493:PHE:CE2	2.10	0.86
1:C:504:LEU:CD1	1:C:509:ILE:HG23	2.06	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
2:B:1444:LYS:HE2	2:B:1447:GLU:HA	1.58	0.86
1:C:128:ILE:HD12	1:C:201:ILE:HG22	1.57	0.86
2:B:519:ARG:NH1	2:B:608:GLY:HA3	1.91	0.86
2:B:151:ASP:HB2	2:B:794:PHE:HZ	1.38	0.86
2:B:850:LEU:HB2	2:B:882:PHE:HE1	1.41	0.86
1:C:1068:VAL:HG21	1:C:1124:TYR:CD1	2.10	0.85
1:C:1219:LYS:HZ1	1:C:1239:VAL:HG11	1.40	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
1:C:936:ARG:HH11	1:C:936:ARG:CG	1.89	0.85
3:Y:207:LEU:CD1	3:Y:207:LEU:O	2.22	0.85
2:B:1590:LEU:HD23	2:B:1591:LEU:N	1.91	0.85
1:C:1531:ASP:OD2	1:C:1531:ASP:C	2.14	0.85
2:D:151:ASP:HB2	2:D:794:PHE:HZ	1.39	0.85
2:D:850:LEU:HB2	2:D:882:PHE:CE1	2.11	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
1:C:1576:LYS:HG2	1:C:1601:ILE:HG22	1.59	0.85
2:D:518:PHE:HE2	2:D:538:VAL:CB	1.88	0.85
3:X:170:ARG:HD3	3:X:203:LEU:HD23	1.59	0.85
1:A:1003:LEU:HD11	1:A:1286:SER:HA	1.59	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:127:PHE:HE2	1:A:623:VAL:HG13	1.40	0.85
1:A:1315:VAL:HG12	1:A:1324:HIS:O	1.76	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:1278:GLN:OE1	1:C:1283:GLY:HA2	1.76	0.85
1:C:1365:VAL:HG22	1:C:1366:HIS:H	1.40	0.85
2:D:326:SER:HB2	2:D:819:GLN:HG3	1.59	0.85
1:A:145:VAL:HB	1:A:183:ILE:HG13	1.58	0.84
1:A:391:ASN:HD21	1:A:406:PRO:HG3	1.41	0.84
2:B:1512:ILE:O	2:B:1516:CYS:HB2	1.77	0.84
2:B:380:VAL:HG12	2:B:387:MET:CB	2.06	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:518:PHE:HE2	2:B:538:VAL:CB	1.89	0.84
1:C:315:LEU:HD12	1:C:318:LEU:HG	1.59	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
1:C:641:ASN:ND2	1:C:643:ALA:HB3	1.93	0.84
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
1:A:1123:GLN:HA	1:A:1123:GLN:HE21	1.42	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
2:D:1444:LYS:HE2	2:D:1447:GLU:HA	1.59	0.84
2:D:933:ARG:HG3	2:D:933:ARG:HH11	1.40	0.84
1:A:191:PRO:HD2	1:A:194:PRO:HB3	1.60	0.83
1:C:1575:VAL:HB	1:C:1602:LYS:O	1.76	0.83
1:A:1278:GLN:OE1	1:A:1283:GLY:HA2	1.78	0.83
2:B:925:VAL:HG22	2:B:1326:LEU:HD23	1.60	0.83
1:C:145:VAL:HB	1:C:183:ILE:HG13	1.60	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
3:X:207:LEU:CD1	3:X:207:LEU:O	2.22	0.83
1:A:1061:ASN:HB2	1:A:1065:SER:O	1.77	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:1571:GLU:HB2	1:A:1574:PHE:CZ	2.13	0.83
2:B:494:ARG:NH1	2:B:494:ARG:HG3	1.91	0.83
2:D:175:SER:H	2:D:1300:ALA:HB2	1.41	0.83
2:D:347:PHE:O	2:D:350:THR:HG22	1.78	0.83
2:D:847:ARG:HG3	2:D:869:GLN:HG2	1.60	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
1:A:1056:ILE:HD11	1:A:1066:TYR:CE2	2.14	0.83
1:C:618:LYS:N	1:C:619:PRO:HD3	1.93	0.83
2:D:481:TYR:HE1	2:D:506:MET:SD	2.02	0.83
1:A:1228:TRP:N	1:A:1251:THR:HG22	1.94	0.83
1:A:572:GLN:HB2	1:A:593:ALA:HB3	1.60	0.83
1:A:895:LEU:HD12	1:A:896:VAL:H	1.42	0.83
1:C:1623:GLU:HB2	1:C:1638:PRO:CG	2.07	0.83
2:D:1500:LEU:HD12	2:D:1501:ASN:H	1.44	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:44:GLU:HG2	2:D:82:LEU:HB2	1.61	0.83
1:A:1066:TYR:H	1:A:1079:THR:HG23	1.44	0.82
2:B:1331:ALA:O	2:B:1332:GLN:HB3	1.79	0.82
1:C:391:ASN:HD21	1:C:406:PRO:HG3	1.42	0.82
2:D:563:MET:HG3	2:D:780:LEU:CD2	2.09	0.82
3:Y:86:LEU:HG	3:Y:91:LYS:HB2	1.61	0.82
1:A:1153:ARG:HD2	1:A:1197:LEU:HB3	1.58	0.82
1:C:1573:VAL:HB	1:C:1603:LYS:HD3	1.60	0.82
1:C:493:ILE:HG23	1:C:495:LYS:H	1.43	0.82
1:A:936:ARG:HH11	1:A:936:ARG:CG	1.92	0.82
1:C:250:ILE:HD11	1:C:265:VAL:HG11	1.61	0.82
1:C:824:PHE:HD2	1:C:824:PHE:H	1.27	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:B:326:SER:HB2	2:B:819:GLN:HG3	1.60	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
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:1570:VAL:HA	1:A:1574:PHE:O	1.80	0.82
1:A:1585:TYR:CE2	1:A:1586:LYS:HB3	2.15	0.82
1:A:1590:ALA:HB1	1:A:1635:TYR:CE1	2.14	0.82
1:A:546:VAL:O	1:A:553:GLU:HB3	1.78	0.82
2:D:850:LEU:HB2	2:D:882:PHE:HE1	1.41	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:A:1488:LEU:O	1:A:1488:LEU:HD12	1.80	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:C:1228:TRP:N	1:C:1251:THR:HG22	1.94	0.81
1:C:1582:LEU:HD21	1:C:1616:GLN:HG2	1.62	0.81
1:A:1582:LEU:HD21	1:A:1616:GLN:HG2	1.62	0.81
1:A:25:ILE:N	1:A:655:THR:CG2	2.44	0.81
2:B:435:TYR:HD1	2:B:436:GLN:N	1.78	0.81
2:B:933:ARG:HH11	2:B:933:ARG:HG3	1.44	0.81
1:C:696:LYS:HZ3	1:C:759:PRO:CD	1.93	0.81
2:B:168:PRO:HG3	2:B:196:THR:C	2.01	0.81
1:C:1020:TYR:HE1	1:C:1295:GLU:HG3	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1049:LEU:HD11	1:C:1089:VAL:HG13	1.63	0.81
1:C:1218:VAL:HG12	1:C:1219:LYS:H	1.46	0.81
1:A:1576:LYS:HG2	1:A:1601:ILE:CG2	2.10	0.81
1:A:500:ASN:HB2	1:A:543:TYR:CD1	2.16	0.81
2:B:795:THR:HG22	2:B:796:PRO:HD2	1.61	0.81
2:D:1607:ILE:N	2:D:1607:ILE:HD12	1.94	0.81
2:D:435:TYR:HD1	2:D:436:GLN:N	1.78	0.81
1:A:123:ASN:HB3	1:A:209:PHE:CD1	2.16	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: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
1:A:267:ILE:CD1	1:A:299:VAL:HG11	2.11	0.81
1:C:1067:SER:HA	1:C:1074:ALA:HA	1.63	0.81
1:C:87:ILE:N	1:C:87:ILE:HD13	1.96	0.81
2:D:954:VAL:HG12	2:D:955:PRO:HD2	1.63	0.81
1:C:1199:ASP:OD1	1:C:1201:THR:HG23	1.81	0.81
2:D:795:THR:HG22	2:D:796:PRO:HD2	1.63	0.81
2:B:469:ASN:HD22	2:B:470:ALA:N	1.79	0.80
1:C:149:ASN:HD22	1:C:149:ASN:H	1.26	0.80
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
1:C:523:TYR:CE1	2:D:359:PRO:HG2	2.16	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
1:A:1190:ILE:HG12	1:A:1253:TYR:CD1	2.17	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
3:X:166:ASP:CG	3:X:207:LEU:HD21	2.01	0.80
1:A:1573:VAL:HB	1:A:1603:LYS:HD3	1.63	0.80
2:B:824:VAL:HG21	2:B:830:VAL:HG11	1.62	0.80
2:D:69:PHE:CE2	2:D:71:THR:HB	2.16	0.80
1:A:1213:LYS:HG2	1:A:1266:TYR:HE2	1.45	0.80
1:A:1232:LEU:HG	1:A:1233:GLN:HG3	1.63	0.80
2:B:161:VAL:HG21	2:B:180:LEU:HD21	1.62	0.80
1:C:1152:ILE:CG2	1:C:1168:LEU:HD21	2.10	0.80
1:C:1333:PHE:O	1:C:1334:LEU:HB2	1.79	0.80
2:D:344:GLN:HA	2:D:344:GLN:HE21	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1341:ASN:HD22	2:B:1342:LYS:HG2	1.44	0.80
1:C:1571:GLU:HB2	1:C:1574:PHE:CZ	2.16	0.80
1:C:371:ILE:HD11	1:C:433:PHE:CE2	2.16	0.80
2:B:69:PHE:CE2	2:B:71:THR:HB	2.17	0.80
1:C:1067:SER:HB3	1:C:1072:GLY:O	1.81	0.80
1:C:492:TYR:CD2	1:C:493:ILE:N	2.50	0.80
1:A:243:PHE:CE1	1:A:316:GLU:HB3	2.17	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
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:C:243:PHE:CE1	1:C:316:GLU:HB3	2.16	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:1066:TYR:H	1:C:1079:THR:HG23	1.46	0.79
1:C:1570:VAL:HA	1:C:1574:PHE:O	1.82	0.79
2:D:1383:ASP:HB3	2:D:1457:LYS:HB2	1.63	0.79
2:D:344:GLN:HA	2:D:344:GLN:NE2	1.96	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
1:A:442:LEU:HD23	1:A:443:PRO:HD2	1.64	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
2:B:1284:ARG:HD2	2:B:1285:GLU:H	1.45	0.79
1:C:1341:LEU:HB2	1:C:1342:LEU:HD23	1.63	0.79
2:B:137:TYR:CZ	2:B:143:VAL:HG22	2.17	0.79
1:C:1232:LEU:HG	1:C:1233:GLN:HG3	1.62	0.79
1:C:799:ILE:HG22	1:C:815:VAL:O	1.82	0.79
2:D:1341:ASN:HD22	2:D:1342:LYS:HG2	1.48	0.79
2:D:557:GLN:HA	2:D:557:GLN:OE1	1.82	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:1562:LYS:HD3	1:C:1664:LEU:CD2	2.10	0.79
2:B:481:TYR:HE1	2:B:506:MET:SD	2.05	0.79
1:C:135:TYR:CE1	1:C:141:VAL:HA	2.17	0.79
1:C:1153:ARG:HD2	1:C:1197:LEU:HB3	1.64	0.79
1:A:78:LYS:NZ	3:X:144:GLU:HA	1.98	0.79
3:X:170:ARG:HH22	3:X:206:LYS:HA	1.47	0.79
1:C:1012:LEU:CD2	1:C:1085:VAL:HG21	2.12	0.79
1:C:191:PRO:HD2	1:C:194:PRO:HB3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:934:VAL:HG22	1:A:1366:HIS:CD2	2.17	0.79
1:A:830:PRO:CG	1:A:1483:PHE:HZ	1.95	0.79
1:A:532:GLN:HA	1:A:532:GLN:OE1	1.83	0.79
1:C:470:THR:HB	2:D:450:THR:O	1.81	0.79
2:D:1284:ARG:HD2	2:D:1285:GLU:H	1.46	0.79
2:D:872:ILE:HG22	2:D:878:ARG:HG3	1.65	0.79
2:B:961:THR:HG22	2:B:1327:THR:HG23	1.64	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
1:A:1497:GLU:OE1	1:A:1500:ARG:HD3	1.83	0.78
1:A:371:ILE:HD11	1:A:433:PHE:CE2	2.18	0.78
1:A:824:PHE:HD2	1:A:824:PHE:H	1.30	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:1133:LEU:CD1	1:A:1133:LEU:H	1.96	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
1:C:696:LYS:NZ	1:C:759:PRO:HD2	1.97	0.78
2:D:1349:VAL:HA	2:D:1364:MET:O	1.83	0.78
1:A:1573:VAL:O	1:A:1603:LYS:HG2	1.84	0.78
1:A:471:ASP:OD2	1:A:474:LYS:HB3	1.83	0.78
1:A:492:TYR:CD2	1:A:493:ILE:N	2.50	0.78
1:A:830:PRO:HG3	1:A:1483:PHE:CE2	2.18	0.78
2:B:265:PHE:CD2	2:B:294:LEU:HB2	2.18	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
2:D:494:ARG:HG3	2:D:494:ARG:NH1	1.97	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:A:1049:LEU:HD11	1:A:1089:VAL:HG13	1.65	0.78
1:A:1190:ILE:HG12	1:A:1253:TYR:CE1	2.18	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:C:23:TYR:HD1	1:C:23:TYR:N	1.81	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
2:D:385:HIS:CE1	3:Y:142:ASN:HD21	2.01	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:166:ASP:OD1	3:Y:207:LEU:HD23	1.82	0.78
1:A:284:GLN:HG2	1:A:310:LEU:CD2	2.13	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
2:D:69:PHE:HE2	2:D:71:THR:HB	1.47	0.78
1:A:1160:PRO:HG2	1:C:1098:ASN:OD1	1.83	0.78
1:A:1199:ASP:OD1	1:A:1201:THR:HG23	1.84	0.78
1:A:250:ILE:HD11	1:A:265:VAL:HG11	1.64	0.78
1:C:23:TYR:N	1:C:23:TYR:CD1	2.42	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
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
1:A:1056:ILE:HD11	1:A:1066:TYR:CD2	2.18	0.78
1:A:1535:MET:H	1:A:1608:ASN:HB3	1.49	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: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:285:ILE:N	2:D:285:ILE:HD12	1.97	0.77
2:D:422:ARG:HH12	3:Y:44:ARG:HA	1.49	0.77
2:D:218:LYS:HB3	2:D:822:TYR:CD2	2.18	0.77
1:A:22:THR:CG2	1:A:657:ALA:HB2	2.15	0.77
2:B:557:GLN:HA	2:B:557:GLN:OE1	1.82	0.77
1:C:1190:ILE:HG12	1:C:1253:TYR:CD1	2.19	0.77
1:C:1213:LYS:HG2	1:C:1266:TYR:HE2	1.48	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
1:A:20:GLU:C	1:A:21:GLN:HG3	2.04	0.77
1:A:1162:VAL:H	1:C:1102:ASN:ND2	1.82	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:C:968:VAL:HG23	1:C:971:THR:HG21	1.67	0.77
1:A:1179:THR:CG2	1:A:1208:ILE:HD13	2.15	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:1585:TYR:HD1	1:C:1671:ILE:CG2	1.97	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:1213:LYS:HG2	1:A:1266:TYR:CE2	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:471:ASP:OD2	1:C:474:LYS:HB3	1.84	0.77
1:A:765:ILE:O	1:A:765:ILE:HD12	1.84	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
1:C:42:GLN:HB2	1:C:80:GLN:NE2	1.99	0.77
1:A:23:TYR:HD1	1:A:23:TYR:N	1.79	0.77
1:A:906:GLY:H	1:A:929:VAL:HB	1.50	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:1161:LEU:HD12	1:C:1105:LEU:HD13	1.67	0.77
1:A:135:TYR:CE1	1:A:141:VAL:HA	2.17	0.77
2:B:224:PHE:CZ	2:B:329:VAL:HG22	2.20	0.77
1:C:532:GLN:OE1	1:C:532:GLN:HA	1.83	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:A:1218:VAL:HG12	1:A:1219:LYS:H	1.50	0.76
1:A:1161:LEU:HA	1:C:1102:ASN:HD21	1.49	0.76
1:C:1576:LYS:HG2	1:C:1601:ILE:CG2	2.16	0.76
1:C:128:ILE:HG13	1:C:215:ALA:HB2	1.66	0.76
1:C:25:ILE:H	1:C:655:THR:CG2	1.98	0.76
1:A:23:TYR:H	1:A:23:TYR:HD1	1.29	0.76
2:B:469:ASN:ND2	2:B:469:ASN:C	2.37	0.76
1:C:1003:LEU:HD11	1:C:1286:SER:HA	1.65	0.76
1:C:1560:ALA:HB3	1:C:1585:TYR:HE2	1.50	0.76
1:C:1573:VAL:CG1	1:C:1603:LYS:HD3	2.15	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
3:Y:170:ARG:HD3	3:Y:203:LEU:HD23	1.65	0.76
2:D:1496:THR:HG23	2:D:1603:LYS:HD2	1.66	0.76
1:C:78:LYS:HZ2	3:Y:144:GLU:HA	1.50	0.76
2:B:478:TYR:O	2:B:478:TYR:HD1	1.67	0.76
1:A:696:LYS:HZ3	1:A:759:PRO:CD	1.98	0.76
1:C:1320:LYS:CD	1:C:1321:GLY:H	1.99	0.76
1:C:1562:LYS:HD2	1:C:1648:TRP:HZ2	1.49	0.76
1:C:171:VAL:HG12	1:C:172:ASP:N	1.97	0.76
1:C:43:VAL:HG13	1:C:79:PHE:HB3	1.68	0.76
2:D:1280:GLU:HG2	2:D:1287:PRO:HB3	1.66	0.76
3:X:150:ILE:HD12	3:X:150:ILE:O	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:ARG:HG2	2:B:256:GLU:HA	1.68	0.76
2:B:422:ARG:HD3	2:B:422:ARG:H	1.49	0.76
1:C:1494:THR:HB	1:C:1506:THR:HG23	1.68	0.76
1:C:315:LEU:CD1	1:C:318:LEU:HG	2.15	0.76
1:C:849:ARG:HG2	1:C:849:ARG:NH1	1.95	0.76
3:Y:125:LYS:HA	3:Y:127:ASN:N	2.00	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:A:25:ILE:N	1:A:655:THR:HG23	1.99	0.76
1:C:1304:VAL:HG12	1:C:1305:LYS:N	2.01	0.76
1:C:351:PRO:HG2	1:C:352:TYR:CD2	2.20	0.76
1:C:830:PRO:HG3	1:C:1483:PHE:CE2	2.21	0.76
3:Y:136:LEU:O	3:Y:136:LEU:HG	1.84	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
2:D:415:THR:OG1	2:D:425:GLN:HB2	1.85	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
1:C:1179:THR:CG2	1:C:1208:ILE:HD13	2.16	0.75
2:D:954:VAL:HB	2:D:957:THR:CG2	2.15	0.75
1:A:315:LEU:CD1	1:A:318:LEU:HG	2.15	0.75
2:B:261:ALA:HB2	2:B:320:VAL:CG2	2.13	0.75
1:C:1488:LEU:HD12	1:C:1488:LEU:O	1.85	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
2:D:200:VAL:HG12	2:D:211:THR:OG1	1.87	0.75
1:A:1067:SER:HB3	1:A:1072:GLY:O	1.85	0.75
1:A:1379:LEU:HD11	1:A:1505:CYS:O	1.86	0.75
2:B:1583:ILE:HG12	2:B:1607:ILE:HG23	1.66	0.75
2:B:344:GLN:HA	2:B:344:GLN:NE2	2.02	0.75
2:B:825:VAL:O	2:B:828:GLU:HG3	1.87	0.75
1:C:1585:TYR:CE2	1:C:1586:LYS:HB3	2.22	0.75
1:C:596:MET:N	1:C:782:ARG:HD3	2.01	0.75
1:A:1108:VAL:HG21	1:A:1167:ALA:HB2	1.69	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:ILE:HB	1:C:599:TRP:CZ3	2.22	0.75
1:C:539:ARG:NH2	1:C:634:CYS:H	1.84	0.75
2:D:1424:ILE:HG12	2:D:1426:TYR:CE2	2.22	0.75
2:D:422:ARG:HD3	2:D:422:ARG:H	1.50	0.75
1:A:1244:THR:HG23	1:A:1502:ASP:OD2	1.85	0.75
1:A:433:PHE:CE1	1:A:452:TYR:HB2	2.21	0.75
1:A:539:ARG:NH2	1:A:634:CYS:H	1.85	0.75
2:B:1284:ARG:CD	2:B:1285:GLU:H	2.00	0.75
2:B:948:ARG:HH21	2:B:948:ARG:HB2	1.51	0.75
1:C:1104:LEU:O	1:C:1108:VAL:HG12	1.87	0.75
2:D:469:ASN:C	2:D:469:ASN:ND2	2.39	0.75
1:A:1638:PRO:O	1:A:1639:LEU:HB2	1.87	0.75
1:A:128:ILE:HD12	1:A:201:ILE:HG22	1.67	0.75
1:A:535:VAL:CG2	1:A:536:PRO:HD3	2.13	0.75
2:B:818:LEU:HB3	2:B:911:LYS:HD2	1.69	0.75
1:C:1504:GLN:HG3	1:C:1505:CYS:HA	1.69	0.75
1:C:260:VAL:HG12	1:C:261:THR:H	1.50	0.75
1:C:38:ASN:HA	1:C:84:ILE:HG22	1.68	0.75
2:D:1347:VAL:HG22	2:D:1367:ILE:HG23	1.69	0.75
2:D:265:PHE:CD2	2:D:294:LEU:HB2	2.21	0.75
1:A:255:PHE:HE1	1:A:258:LYS:CB	1.98	0.75
2:B:829:GLN:CG	2:B:1480:LEU:HD13	2.17	0.75
1:C:1320:LYS:HD2	1:C:1321:GLY:H	1.51	0.75
1:C:44:TYR:HB2	1:C:545:ILE:HD12	1.69	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:A:1402:ILE:HG13	1:A:1479:ILE:HD11	1.69	0.74
2:B:508:LEU:HD12	2:B:509:HIS:H	1.52	0.74
1:C:1218:VAL:HG12	1:C:1219:LYS:N	2.02	0.74
1:C:1314:ASP:HA	1:C:1325:ASN:HB2	1.68	0.74
1:A:849:ARG:HG2	1:A:849:ARG:NH1	1.94	0.74
1:C:1244:THR:HG23	1:C:1502:ASP:OD2	1.87	0.74
1:C:415:ASP:HB2	1:C:417:VAL:HB	1.69	0.74
2:D:261:ALA:CB	2:D:320:VAL:HG23	2.15	0.74
2:D:42:LEU:HD11	2:D:82:LEU:HD12	1.68	0.74
1:C:224:LEU:HD23	1:C:225:PRO:HD2	1.70	0.74
1:A:613:GLN:HG3	1:A:613:GLN:O	1.85	0.74
2:B:1473:HIS:HB3	2:B:1476:LYS:HB2	1.68	0.74
1:C:33:VAL:HG21	1:C:121:TYR:HD1	1.51	0.74
2:D:615:GLN:HB2	2:D:616:ASN:ND2	2.03	0.74
3:X:87:LEU:HA	3:X:91:LYS:HD3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:961:TYR:HE2	1:C:1343:ASN:HA	1.53	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
1:A:1562:LYS:HD3	1:A:1664:LEU:HD21	1.70	0.74
1:C:285:THR:HG22	1:C:285:THR:O	1.86	0.74
1:C:640:LEU:H	1:C:644:ASN:HB3	1.53	0.74
1:C:895:LEU:HD12	1:C:896:VAL:H	1.52	0.74
1:A:1047:LYS:HE2	1:A:1051:GLU:OE2	1.86	0.74
1:A:1402:ILE:HG13	1:A:1479:ILE:CD1	2.17	0.74
1:A:258:LYS:HD3	1:A:893:SER:OG	1.85	0.74
1:C:1056:ILE:HD11	1:C:1066:TYR:CE2	2.23	0.74
2:D:34:ARG:HD3	2:D:124:GLN:HG2	1.69	0.74
2:D:469:ASN:HD22	2:D:470:ALA:N	1.86	0.74
1:A:620:LEU:O	1:A:623:VAL:HG23	1.88	0.74
1:C:1024:TYR:HA	1:C:1302:LEU:HD21	1.69	0.74
1:C:123:ASN:HB3	1:C:209:PHE:CD1	2.23	0.74
1:C:538:SER:O	1:C:561:LEU:HB2	1.88	0.74
1:C:695:VAL:HG13	1:C:724:CYS:HA	1.70	0.74
2:D:758:LEU:HD13	2:D:760:LYS:HE2	1.69	0.74
1:A:1031:TRP:CZ2	1:A:1042:LYS:HG3	2.22	0.74
1:A:1152:ILE:CG2	1:A:1168:LEU:HD21	2.17	0.74
1:A:128:ILE:HG13	1:A:215:ALA:HB2	1.69	0.74
1:A:42:GLN:HB2	1:A:80:GLN:NE2	2.02	0.74
1:C:993:SER:C	1:C:995:GLU:H	1.91	0.74
2:D:1525:LYS:HD2	2:D:1610:TRP:CZ2	2.22	0.74
2:D:620:VAL:HG12	2:D:621:PHE:HD2	1.53	0.74
1:A:144:ARG:HD2	1:A:146:TYR:CE1	2.22	0.73
1:A:538:SER:O	1:A:561:LEU:HB2	1.86	0.73
2:B:344:GLN:HA	2:B:344:GLN:HE21	1.52	0.73
1:C:1013:MET:SD	1:C:1016:VAL:HG21	2.28	0.73
1:C:1186:PHE:HA	1:C:1250:THR:HG22	1.70	0.73
1:C:1622:LYS:HZ3	1:C:1642:LEU:HD23	1.52	0.73
3:X:132:THR:HG23	3:X:155:ILE:HB	1.70	0.73
1:A:1020:TYR:HE1	1:A:1295:GLU:HG3	1.52	0.73
1:A:503:ILE:HB	1:A:511:HIS:HB2	1.69	0.73
2:B:1435:ASP:OD1	4:F:1:NAG:H81	1.88	0.73
1:C:1627:ILE:HD12	1:C:1629:TYR:HB3	1.69	0.73
1:C:133:PRO:HD2	1:C:609:VAL:CG1	2.17	0.73
1:C:127:PHE:CD2	1:C:623:VAL:HG22	2.23	0.73
1:A:1341:LEU:HB2	1:A:1342:LEU:HD23	1.69	0.73
1:A:1370:THR:HG23	1:A:1373:GLU:OE1	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1593:GLU:HB2	1:A:1596:SER:OG	1.88	0.73
1:C:1133:LEU:H	1:C:1133:LEU:CD1	1.95	0.73
1:C:222:TYR:HE1	1:C:768:TYR:HB2	1.51	0.73
2:D:948:ARG:HB2	2:D:948:ARG:HH21	1.53	0.73
3:X:111:ASP:OD1	3:X:112:PRO:HD2	1.89	0.73
2:B:1349:VAL:HA	2:B:1364:MET:O	1.88	0.73
1:C:1190:ILE:HG12	1:C:1253:TYR:CE1	2.23	0.73
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:A:1068:VAL:HA	1:A:1078:LEU:CD1	2.17	0.73
1:A:160:VAL:HG22	1:A:175:GLU:HB3	1.71	0.73
2:B:484:LEU:HB2	2:B:519:ARG:HG3	1.70	0.73
1:C:1056:ILE:HD11	1:C:1066:TYR:CD2	2.23	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
2:B:1607:ILE:H	2:B:1607:ILE:HD12	1.53	0.73
1:C:1493:PHE:CD1	1:C:1494:THR:N	2.52	0.73
2:B:620:VAL:HG12	2:B:621:PHE:HD2	1.52	0.73
1:C:906:GLY:H	1:C:929:VAL:HB	1.53	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: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: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: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:1626:GLN:HB2	1:C:1635:TYR:HD1	1.53	0.73
1:C:255:PHE:HE1	1:C:258:LYS:CB	2.02	0.73
1:A:700:TYR:C	1:A:700:TYR:HD2	1.92	0.73
2:B:548:LEU:HD22	2:B:793:SER:HB3	1.70	0.73
1:C:1527:CYS:C	1:C:1529:GLU:N	2.34	0.73
1:C:160:VAL:HG22	1:C:175:GLU:HB3	1.71	0.73
1:C:220:LYS:HD3	1:C:765:ILE:HG23	1.69	0.73
2:D:825:VAL:O	2:D:828:GLU:HG3	1.88	0.73
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:B:844:ILE:HG13	2:B:872:ILE:HG12	1.71	0.72
1:C:494:ASP:O	1:C:496:ILE:N	2.22	0.72
2:D:1482:ASN:HB2	2:D:1495:GLU:HG2	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:THR:O	1:A:515:ARG:HD3	1.89	0.72
1:A:517:LYS:HG2	1:A:518:PHE:N	2.04	0.72
2:B:148:PHE:CE2	2:B:792:VAL:HG11	2.24	0.72
1:C:1152:ILE:HG21	1:C:1168:LEU:HD21	1.70	0.72
1:C:1213:LYS:HG2	1:C:1266:TYR:CE2	2.24	0.72
1:C:963:ILE:HG23	1:C:967:LEU:HD23	1.72	0.72
1:A:149:ASN:H	1:A:149:ASN:HD22	1.36	0.72
1:A:1573:VAL:HG12	1:A:1603:LYS:HB3	1.70	0.72
1:A:493:ILE:HG23	1:A:495:LYS:H	1.55	0.72
1:A:695:VAL:HG13	1:A:724:CYS:HA	1.70	0.72
2:B:1347:VAL:HG22	2:B:1367:ILE:HG23	1.70	0.72
1:C:1358:THR:HB	1:C:1360:HIS:CE1	2.24	0.72
1:C:365:PRO:HD2	1:C:464:TYR:CD2	2.25	0.72
1:C:700:TYR:C	1:C:700:TYR:HD2	1.92	0.72
2:D:834:ALA:O	2:D:835:ILE:HD13	1.89	0.72
2:D:850:LEU:HD12	2:D:851:LEU:H	1.53	0.72
1:A:483:ASN:ND2	2:B:399:ILE:HB	2.04	0.72
1:A:799:ILE:HG22	1:A:815:VAL:O	1.90	0.72
2:B:1279:ILE:HG22	2:B:1288:ILE:HB	1.71	0.72
2:B:34:ARG:HD3	2:B:124:GLN:HG2	1.71	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:D:844:ILE:HG13	2:D:872:ILE:HG12	1.72	0.72
1:A:148:LEU:HD23	1:A:152:LEU:CD1	2.19	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
3:X:68:ASN:CG	3:X:69:GLY:H	1.92	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:1278:GLN:OE1	1:C:1283:GLY:CA	2.37	0.72
1:C:1573:VAL:CB	1:C:1603:LYS:HD3	2.19	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:A:260:VAL:HG12	1:A:261:THR:H	1.54	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:1560:ALA:HB3	1:A:1585:TYR:CE2	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1108:VAL:HG11	1:C:1164:ILE:HG22	1.70	0.72
1:C:1329:THR:OG1	1:C:1331:LYS:HG2	1.90	0.72
2:D:1506:ILE:HD11	2:D:1628:PHE:HE1	1.53	0.72
1:A:1347:ILE:O	1:A:1347:ILE:HG22	1.89	0.72
1:A:373:VAL:HG23	1:A:418:ALA:HB3	1.70	0.72
2:B:1313:VAL:HG11	2:B:1323:MET:SD	2.29	0.72
1:C:1560:ALA:HB3	1:C:1585:TYR:CE2	2.24	0.72
3:X:64:VAL:HG11	3:X:95:LYS:O	1.90	0.72
1:A:1076:THR:CG2	1:A:1120:GLU:HA	2.18	0.72
1:A:1304:VAL:HG12	1:A:1305:LYS:N	2.03	0.72
1:A:1493:PHE:CD1	1:A:1494:THR:N	2.55	0.72
1:A:225:PRO:HG3	1:A:766:ARG:HB2	1.71	0.72
2:B:162:ILE:CG2	2:B:202:LYS:HG2	2.20	0.72
1:C:596:MET:HA	1:C:782:ARG:HG2	1.70	0.72
1:C:1163:LYS:O	1:C:1166:THR:HG22	1.90	0.71
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
2:D:481:TYR:HB2	2:D:520:PHE:CE1	2.25	0.71
2:B:563:MET:HB3	2:B:778:PHE:CE2	2.25	0.71
1:C:1068:VAL:HG13	1:C:1069:TRP:N	2.06	0.71
1:C:1567:SER:HB3	1:C:1578:LYS:HB2	1.70	0.71
1:C:386:VAL:H	1:C:411:THR:CG2	1.92	0.71
1:A:1104:LEU:O	1:A:1108:VAL:HG12	1.91	0.71
1:A:351:PRO:HG2	1:A:352:TYR:CD2	2.25	0.71
2:B:618:LEU:HD11	2:B:635:ASN:O	1.90	0.71
1:C:1423:VAL:HG13	1:C:1496:TYR:CD2	2.24	0.71
2:D:23:ALA:HB3	2:D:528:ASN:HD22	1.55	0.71
3:Y:166:ASP:OD2	3:Y:207:LEU:HG	1.89	0.71
3:Y:68:ASN:CG	3:Y:69:GLY:H	1.93	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
1:C:979:VAL:HG21	1:C:1326:TYR:HE1	1.52	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:491:PRO:O	1:A:492:TYR:C	2.28	0.71
1:A:552:ALA:HB2	1:A:657:ALA:HB3	1.73	0.71
1:A:981:GLY:CA	1:A:1333:PHE:HB2	2.21	0.71
2:B:435:TYR:CD1	2:B:436:GLN:N	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:TYR:HD2	1:C:223:VAL:N	1.88	0.71
1:C:42:GLN:HA	1:C:80:GLN:HG3	1.72	0.71
2:D:1371:TYR:CG	2:D:1377:SER:HB3	2.25	0.71
1:A:224:LEU:HD23	1:A:225:PRO:HD2	1.71	0.71
1:C:530:VAL:HG23	1:C:534:MET:HE2	1.71	0.71
2:D:1284:ARG:CD	2:D:1285:GLU:H	2.02	0.71
2:D:1562:GLN:HE22	2:D:1596:LYS:NZ	1.88	0.71
1:A:374:GLN:HA	1:A:416:GLY:O	1.91	0.71
1:A:44:TYR:HB2	1:A:545:ILE:HD12	1.71	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:961:TYR:HE2	1:A:1343:ASN:HA	1.55	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:A:774:LEU:HD12	1:A:799:ILE:HD11	1.71	0.71
1:C:1219:LYS:HZ3	1:C:1239:VAL:HG11	1.55	0.71
1:C:961:TYR:CE2	1:C:1343:ASN:HA	2.25	0.71
1:A:1268:ASN:HD22	1:A:1268:ASN:H	1.38	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
2:B:1446:PHE:HD2	2:B:1448:VAL:HG22	1.54	0.71
1:C:967:LEU:HD12	1:C:968:VAL:N	2.04	0.71
3:X:64:VAL:HG23	3:X:71:ASN:OD1	1.91	0.71
1:A:1179:THR:HG21	1:A:1208:ILE:HD13	1.72	0.71
1:A:1573:VAL:CB	1:A:1603:LYS:HD3	2.21	0.71
1:A:40:VAL:HG21	1:A:512:PHE:HD1	1.55	0.71
1:A:640:LEU:H	1:A:644:ASN:HB3	1.56	0.71
1:A:99:VAL:O	1:A:119:ILE:HD11	1.90	0.71
2:B:1593:THR:HG22	2:B:1594:LYS:N	2.06	0.71
2:B:165:PHE:CZ	2:B:199:ILE:HD11	2.26	0.71
2:B:481:TYR:HB2	2:B:520:PHE:CE1	2.25	0.71
1:C:1638:PRO:O	1:C:1639:LEU:HB2	1.89	0.71
1:A:1076:THR:HG22	1:A:1120:GLU:OE2	1.91	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:365:PRO:HD2	1:A:464:TYR:CD2	2.25	0.70
1:A:398:ASN:O	1:A:399:GLN:HB2	1.90	0.70
1:A:906:GLY:O	1:A:908:HIS:CE1	2.43	0.70
2:B:850:LEU:HD12	2:B:851:LEU:H	1.55	0.70
2:D:162:ILE:CG2	2:D:202:LYS:HG2	2.20	0.70
2:D:508:LEU:HD12	2:D:509:HIS:H	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1186:PHE:HA	1:A:1250:THR:HG22	1.73	0.70
1:A:765:ILE:HD13	1:A:767:SER:O	1.91	0.70
1:A:963:ILE:HG23	1:A:967:LEU:HD23	1.72	0.70
1:C:109:LYS:HD3	1:C:110:HIS:CE1	2.26	0.70
1:A:1013:MET:SD	1:A:1016:VAL:HG21	2.31	0.70
1:A:1127:ILE:HD11	1:A:1143:TYR:CD2	2.27	0.70
1:A:1525:CYS:C	1:A:1528:VAL:HG22	2.12	0.70
1:A:238:ILE:HD12	1:A:347:TYR:HE1	1.55	0.70
2:B:1482:ASN:HB2	2:B:1495:GLU:HG2	1.72	0.70
3:X:166:ASP:OD1	3:X:207:LEU:HD23	1.91	0.70
1:A:131:ASP:HB3	1:A:142:LYS:HB2	1.74	0.70
1:A:504:LEU:HD21	1:A:651:LEU:HG	1.74	0.70
2:B:615:GLN:HB2	2:B:616:ASN:ND2	2.06	0.70
1:C:1127:ILE:H	1:C:1127:ILE:HD12	1.56	0.70
1:C:131:ASP:O	1:C:132:LYS:HG2	1.91	0.70
1:C:968:VAL:HG12	1:C:1368:THR:HG22	1.73	0.70
1:C:152:LEU:HD11	1:C:627:LEU:HD11	1.73	0.70
1:C:491:PRO:O	1:C:492:TYR:C	2.26	0.70
1:C:503:ILE:HB	1:C:511:HIS:HB2	1.72	0.70
2:D:1381:ILE:HG21	2:D:1459:TYR:HE1	1.56	0.70
3:Y:80:GLN:HG3	3:Y:114:GLY:C	2.12	0.70
1:A:1076:THR:HG21	1:A:1120:GLU:HA	1.72	0.70
1:A:961:TYR:CE2	1:A:1343:ASN:HA	2.27	0.70
1:A:685:GLU:HA	1:A:685:GLU:OE1	1.92	0.70
2:B:950:LEU:HD22	2:B:1329:TYR:CZ	2.26	0.70
2:B:1615:GLU:HB3	2:B:1621:PHE:CD1	2.26	0.70
2:B:28:ILE:HD12	2:B:42:LEU:HD23	1.73	0.70
1:C:1112:GLN:HE21	1:C:1171:ALA:HB2	1.54	0.70
1:C:869:GLU:C	1:C:871:PRO:HD3	2.11	0.70
2:D:1445:HIS:CG	2:D:1446:PHE:N	2.59	0.70
2:D:618:LEU:HD11	2:D:635:ASN:O	1.92	0.70
3:Y:146:LEU:HD22	3:Y:147:ASP:N	2.06	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
1:A:1504:GLN:HG3	1:A:1505:CYS:HA	1.72	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:690:TYR:O	1:C:690:TYR:CG	2.43	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:262:PHE:HE1	2:D:282:ARG:HG3	1.56	0.70
1:A:285:THR:HG22	1:A:285:THR:O	1.91	0.70
2:B:954:VAL:HB	2:B:957:THR:CG2	2.19	0.70
1:C:1047:LYS:HE2	1:C:1051:GLU:OE2	1.92	0.70
1:C:419:SER:HB2	2:D:459:ASN:HD22	1.56	0.70
1:C:968:VAL:CG2	1:C:971:THR:HG21	2.22	0.70
1:A:1616:GLN:OE1	1:A:1650:ARG:HD3	1.92	0.70
1:A:330:ILE:HG22	1:A:337:SER:CB	2.21	0.70
1:C:99:VAL:O	1:C:119:ILE:HD11	1.91	0.70
1:C:1625:LEU:O	1:C:1627:ILE:HG23	1.91	0.70
1:C:639:GLY:HA2	1:C:648:LEU:HD13	1.74	0.70
1:C:938:SER:O	1:C:940:SER:N	2.25	0.70
2:D:237:ILE:O	2:D:306:LEU:HD11	1.92	0.70
3:X:136:LEU:HG	3:X:136:LEU:O	1.91	0.70
3:Y:111:ASP:OD1	3:Y:112:PRO:HD2	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
1:A:1278:GLN:OE1	1:A:1283:GLY:CA	2.40	0.69
1:A:148:LEU:HD23	1:A:152:LEU:HD12	1.74	0.69
1:A:1567:SER:HB3	1:A:1578:LYS:HB2	1.74	0.69
1:A:587:THR:HG22	1:A:789:ALA:HB2	1.72	0.69
1:C:1219:LYS:CE	1:C:1239:VAL:HG21	2.22	0.69
1:C:1370:THR:HG23	1:C:1373:GLU:OE1	1.91	0.69
2:D:484:LEU:HB2	2:D:519:ARG:HG3	1.73	0.69
3:X:73:VAL:HG23	3:X:74:ARG:N	2.07	0.69
3:Y:170:ARG:NH2	3:Y:206:LYS:HA	2.06	0.69
1:A:1543:ILE:O	1:A:1547:THR:HG23	1.91	0.69
1:A:1646:GLU:OE2	1:A:1660:PHE:HZ	1.75	0.69
1:A:495:LYS:HA	1:A:495:LYS:CE	2.17	0.69
1:A:596:MET:HA	1:A:782:ARG:HG2	1.74	0.69
1:A:849:ARG:NH2	2:B:555:LEU:HB2	2.07	0.69
2:B:834:ALA:O	2:B:835:ILE:HD13	1.92	0.69
1:C:1429:PRO:HB2	1:C:1432:ILE:CG1	2.22	0.69
1:C:1646:GLU:OE2	1:C:1660:PHE:HZ	1.75	0.69
2:D:148:PHE:HB3	2:D:800:ILE:HD11	1.75	0.69
2:D:825:VAL:N	2:D:828:GLU:OE1	2.25	0.69
1:A:33:VAL:HG21	1:A:121:TYR:HD1	1.57	0.69
1:C:1019:PHE:C	1:C:1019:PHE:CD2	2.65	0.69
1:C:1404:ALA:HB1	1:C:1493:PHE:HE2	1.57	0.69
1:C:1585:TYR:CE1	1:C:1671:ILE:HG12	2.28	0.69
2:D:435:TYR:CD1	2:D:436:GLN:N	2.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:73:VAL:HG23	3:Y:74:ARG:N	2.07	0.69
1:A:1329:THR:OG1	1:A:1331:LYS:HG2	1.92	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
2:B:1445:HIS:CG	2:B:1446:PHE:N	2.59	0.69
2:B:236:TYR:CZ	2:B:424:ARG:HD2	2.27	0.69
1:C:131:ASP:HB3	1:C:142:LYS:HB2	1.72	0.69
1:C:238:ILE:HB	1:C:347:TYR:CD1	2.28	0.69
1:C:658:ASN:O	1:C:659:ALA:HB3	1.91	0.69
2:D:422:ARG:NH1	3:Y:44:ARG:HA	2.07	0.69
2:D:859:ALA:HB1	2:D:866:TYR:CD1	2.27	0.69
1:A:1108:VAL:HG11	1:A:1164:ILE:HG22	1.73	0.69
1:A:1404:ALA:HB1	1:A:1493:PHE:HE2	1.57	0.69
1:A:234:GLU:HG3	1:A:235:TYR:CE2	2.28	0.69
1:C:1228:TRP:H	1:C:1251:THR:CG2	1.98	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
3:Y:50:TYR:HE2	3:Y:170:ARG:NH1	1.90	0.69
1:A:1423:VAL:HG13	1:A:1496:TYR:CD2	2.27	0.69
2:B:1371:TYR:CG	2:B:1377:SER:HB3	2.27	0.69
2:B:230:PRO:HG3	2:B:333:GLN:HG2	1.73	0.69
1:C:144:ARG:HD2	1:C:146:TYR:HE1	1.58	0.69
1:C:257:ASN:HD21	1:C:892:SER:HA	1.58	0.69
1:C:24:VAL:HA	1:C:655:THR:OG1	1.93	0.69
2:D:127:PHE:HE2	2:D:602:ILE:HG23	1.57	0.69
2:D:224:PHE:CZ	2:D:329:VAL:HG22	2.27	0.69
2:D:262:PHE:CE1	2:D:282:ARG:HG3	2.27	0.69
2:D:824:VAL:HG22	2:D:825:VAL:H	1.58	0.69
1:A:1429:PRO:HB2	1:A:1432:ILE:CG1	2.23	0.69
1:A:700:TYR:CD2	1:A:700:TYR:C	2.64	0.69
2:B:859:ALA:HB1	2:B:866:TYR:CD1	2.28	0.69
1:C:1347:ILE:O	1:C:1347:ILE:HG22	1.93	0.69
1:C:1423:VAL:HG13	1:C:1496:TYR:CE2	2.27	0.69
1:C:837:GLU:HG2	1:C:1488:LEU:HA	1.75	0.69
1:C:1525:CYS:O	1:C:1529:GLU:HG3	1.93	0.69
1:C:1549:LYS:NZ	1:C:1667:PHE:HB3	2.07	0.69
1:C:77:ASN:HD21	1:C:81:ASN:HB2	1.57	0.69
2:D:950:LEU:HD22	2:D:1329:TYR:CZ	2.28	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
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:C:115:LYS:HB2	1:C:654:LEU:HD21	1.74	0.69
1:C:587:THR:HG22	1:C:789:ALA:HB2	1.74	0.69
2:D:1382:ILE:HB	2:D:1425:ILE:HB	1.74	0.69
2:D:840:VAL:HG12	2:D:841:ASN:N	2.06	0.69
3:X:188:LYS:HD3	3:X:202:ASP:HA	1.75	0.69
1:A:1086:LEU:HD12	1:A:1095:GLN:HG3	1.75	0.69
1:A:549:GLU:CD	1:A:549:GLU:H	1.96	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
2:D:1593:THR:HG22	2:D:1594:LYS:N	2.07	0.69
1:A:1218:VAL:HG12	1:A:1219:LYS:N	2.07	0.69
1:A:123:ASN:HB3	1:A:209:PHE:HD1	1.56	0.69
1:A:92:LEU:HD12	1:C:1029:ASN:ND2	2.07	0.69
2:B:1381:ILE:HG21	2:B:1459:TYR:HE1	1.57	0.69
2:B:136:ILE:HA	2:B:215:ASP:O	1.92	0.69
1:C:166:PRO:HD3	1:C:199:TRP:HA	1.75	0.69
1:C:596:MET:N	1:C:782:ARG:HH11	1.85	0.69
2:D:114:ARG:O	2:D:115:LEU:HD23	1.93	0.69
2:D:1435:ASP:OD1	4:H:1:NAG:H81	1.92	0.69
2:D:1610:TRP:CD2	2:D:1628:PHE:CD2	2.81	0.69
2:D:813:VAL:HG12	2:D:840:VAL:HG22	1.75	0.69
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:222:TYR:HD2	1:A:223:VAL:N	1.90	0.68
1:A:467:ILE:CG2	1:A:486:VAL:HG22	2.23	0.68
2:B:950:LEU:HD22	2:B:1329:TYR:CE1	2.27	0.68
2:D:1446:PHE:CD2	2:D:1448:VAL:HG22	2.27	0.68
3:X:98:LEU:HD22	3:X:101:GLN:OE1	1.93	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:255:PHE:HE1	1:A:258:LYS:HB2	1.56	0.68
1:A:25:ILE:H	1:A:655:THR:HG21	1.56	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:B:1424:ILE:HG12	2:B:1426:TYR:CE2	2.28	0.68
1:C:1268:ASN:H	1:C:1268:ASN:HD22	1.42	0.68
1:C:1504:GLN:HG3	1:C:1505:CYS:N	2.09	0.68
1:C:705:VAL:N	1:C:739:ARG:HH22	1.92	0.68
1:C:91:GLN:O	1:C:92:LEU:HG	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1424:ILE:HD13	2:D:1424:ILE:H	1.59	0.68
2:D:197:TRP:HB2	2:D:214:PHE:CE1	2.28	0.68
2:D:913:LEU:HD23	2:D:914:LYS:N	2.09	0.68
1:A:1366:HIS:ND1	1:A:1366:HIS:N	2.41	0.68
1:A:228:SER:O	1:A:252:ALA:HA	1.93	0.68
1:A:543:TYR:O	1:A:543:TYR:HD1	1.77	0.68
1:A:690:TYR:CG	1:A:690:TYR:O	2.46	0.68
2:B:114:ARG:O	2:B:115:LEU:HD23	1.93	0.68
1:C:1671:ILE:HA	1:C:1675:GLY:H	1.57	0.68
3:Y:64:VAL:HG11	3:Y:95:LYS:O	1.93	0.68
1:A:1608:ASN:O	1:A:1610:GLU:N	2.27	0.68
1:A:938:SER:O	1:A:940:SER:N	2.27	0.68
2:B:1345:LEU:HA	2:B:1368:CYS:O	1.93	0.68
1:C:1226:ARG:CZ	1:C:1266:TYR:HE1	2.07	0.68
1:C:307:VAL:HG13	1:C:313:TYR:HB2	1.76	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:A:174:VAL:HG22	1:A:175:GLU:N	2.09	0.68
2:B:464:PHE:HB2	2:B:504:VAL:O	1.94	0.68
1:C:104:LEU:HD12	1:C:105:GLU:H	1.59	0.68
1:C:774:LEU:HD12	1:C:799:ILE:HD11	1.76	0.68
2:D:1313:VAL:HG11	2:D:1323:MET:SD	2.34	0.68
1:A:1068:VAL:HG13	1:A:1069:TRP:N	2.08	0.68
1:A:1127:ILE:H	1:A:1127:ILE:HD12	1.59	0.68
1:A:255:PHE:CE1	1:A:258:LYS:CB	2.77	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:C:1673:LEU:O	1:C: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:C:742:ILE:HG13	1:C:752:LEU:O	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
1:A:77:ASN:HD21	1:A:81:ASN:HB2	1.59	0.68
1:A:829:ILE:HG12	1:A:925:LYS:HG2	1.74	0.68
1:C:1034:PHE:CE2	1:C:1041:GLU:HG2	2.29	0.68
1:C:1179:THR:HG21	1:C:1208:ILE:HD13	1.76	0.68
1:A:101:TYR:CE2	1:C:1305:LYS:HE3	2.28	0.68
3:X:134:THR:HG22	3:X:153:PHE:O	1.94	0.68
3:X:228:ILE:O	3:X:228:ILE:HG22	1.94	0.68
3:Y:86:LEU:HG	3:Y:91:LYS:CB	2.24	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:1631:PHE:CD2	1:C:1631:PHE:N	2.60	0.68
1:C:382:LEU:HD13	1:C:415:ASP:C	2.14	0.68
1:C:700:TYR:C	1:C:700:TYR:CD2	2.63	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
3:X:166:ASP:OD2	3:X:207:LEU:HG	1.94	0.68
1:A:161:LEU:HD11	1:A:185:PHE:CD1	2.29	0.68
1:A:706:ASN:ND2	1:A:709:GLU:N	2.38	0.68
2:B:218:LYS:HB3	2:B:822:TYR:HD2	1.59	0.68
2:B:133:ASP:HA	2:B:757:TRP:HZ3	1.59	0.68
1:C:1266:TYR:O	1:C:1266:TYR:CD1	2.45	0.68
1:C:222:TYR:C	1:C:222:TYR:HD2	1.97	0.68
1:C:330:ILE:HG22	1:C:337:SER:HB2	1.76	0.68
1:C:373:VAL:HG23	1:C:418:ALA:HB3	1.74	0.68
1:C:938:SER:C	1:C:940:SER:H	1.96	0.68
1:A:1320:LYS:HD2	1:A:1321:GLY:H	1.58	0.67
1:A:1309:LEU:HD13	1:A:1328:MET:HG3	1.75	0.67
1:A:1450:PHE:CZ	1:A:1475:VAL:HB	2.28	0.67
1:A:365:PRO:HD2	1:A:464:TYR:CE2	2.28	0.67
1:A:40:VAL:CG2	1:A:512:PHE:HD1	2.06	0.67
2:B:243:PHE:HD1	2:B:314:LEU:HD23	1.58	0.67
1:C:1341:LEU:HB2	1:C:1342:LEU:CD2	2.24	0.67
1:C:517:LYS:HG2	1:C:518:PHE:H	1.59	0.67
3:Y:150:ILE:HD12	3:Y:150:ILE:O	1.93	0.67
1:A:1358:THR:HB	1:A:1360:HIS:CE1	2.29	0.67
1:A:517:LYS:HG2	1:A:518:PHE:H	1.58	0.67
1:A:612:VAL:HG21	1:A:769:PHE:CZ	2.29	0.67
1:C:1159:CYS:O	1:C:1161:LEU:N	2.27	0.67
1:C:1202:HIS:CD2	1:C:1203:PRO:HD2	2.28	0.67
1:C:471:ASP:OD2	1:C:474:LYS:HD2	1.94	0.67
2:D:28:ILE:HG12	2:D:628:LEU:HD13	1.75	0.67
3:X:179:LEU:HD12	3:X:180:TYR:N	2.10	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
1:A:470:THR:HG22	2:B:450:THR:CG2	2.22	0.67
2:B:261:ALA:CB	2:B:285:ILE:HD11	2.24	0.67
1:C:576:SER:HB2	1:C:589:SER:CB	2.24	0.67
1:A:1112:GLN:HE21	1:A:1171:ALA:HB2	1.59	0.67
1:A:1423:VAL:HG13	1:A:1496:TYR:CE2	2.30	0.67
1:A:704:CYS:C	1:A:739:ARG:HH22	1.98	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:GLN:O	1:A:90:LYS:HD3	1.94	0.67
1:C:1142:LEU:HD11	1:C:1179:THR:HA	1.77	0.67
3:X:80:GLN:HG3	3:X:114:GLY:C	2.15	0.67
3:Y:166:ASP:CG	3:Y:207:LEU:HD23	2.14	0.67
1:A:1034:PHE:CE2	1:A:1041:GLU:HG2	2.29	0.67
1:A:1244:THR:HG22	1:A:1246:ARG:N	2.08	0.67
1:A:1266:TYR:CD1	1:A:1266:TYR:O	2.48	0.67
1:A:207:GLU:O	1:A:209:PHE:N	2.28	0.67
1:A:640:LEU:O	1:A:640:LEU:HD12	1.93	0.67
2:B:149:SER:O	2:B:794:PHE:HE1	1.78	0.67
1:C:596:MET:H	1:C:782:ARG:NH1	1.87	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:1019:PHE:CD2	1:A:1019:PHE:C	2.67	0.67
1:A:104:LEU:HD12	1:A:105:GLU:H	1.59	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
1:A:222:TYR:C	1:A:222:TYR:HD2	1.98	0.67
1:A:586:GLN:O	1:A:586:GLN:HG3	1.95	0.67
2:B:1480:LEU:HD12	2:B:1481:LEU:N	2.10	0.67
2:B:1602:THR:C	2:B:1604:ASN:H	1.97	0.67
2:B:262:PHE:HE1	2:B:282:ARG:HG3	1.60	0.67
2:B:299:PHE:HE1	2:B:303:PHE:HD2	1.43	0.67
1:C:1049:LEU:HD11	1:C:1089:VAL:CG1	2.24	0.67
1:C:1493:PHE:CD1	1:C:1493:PHE:C	2.67	0.67
1:C:765:ILE:HD13	1:C:767:SER:O	1.94	0.67
2:D:531:ILE:HD11	2:D:634:LEU:HD23	1.76	0.67
1:A:109:LYS:HD3	1:A:110:HIS:CE1	2.30	0.67
1:A:1142:LEU:HD11	1:A:1179:THR:HA	1.77	0.67
1:A:190:ILE:HG22	1:A:191:PRO:N	2.09	0.67
1:A:742:ILE:HG13	1:A:752:LEU:O	1.94	0.67
1:A:596:MET:N	1:A:782:ARG:HD3	2.10	0.67
1:A:865:ILE:O	1:A:866:CYS:O	2.11	0.67
1:C:180:ILE:HB	1:C:599:TRP:CE3	2.30	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
3:Y:47:HIS:CE1	3:Y:181:LYS:HE2	2.30	0.67
2:B:1505:ARG:NH1	2:B:1505:ARG:HG3	1.93	0.67
2:B:1562:GLN:HE22	2:B:1596:LYS:HZ2	1.42	0.67
1:C:1077:TRP:NE1	1:C:1147:PHE:CE1	2.62	0.67
1:C:1535:MET:H	1:C:1608:ASN:HB3	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:474:LYS:H	1:C:474:LYS:HD3	1.60	0.67
3:Y:41:HIS:O	3:Y:42:ASP:HB2	1.95	0.67
2:B:30:PRO:HG3	2:B:489:ILE:HG13	1.77	0.67
2:B:783:SER:HB2	2:B:787:TRP:HZ2	1.60	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
1:C:1504:GLN:HG3	1:C:1505:CYS:CA	2.24	0.67
1:C:473:HIS:O	1:C:473:HIS:CD2	2.47	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
2:D:603:GLU:O	2:D:605:SER:N	2.27	0.67
1:A:459:SER:OG	1:A:461:SER:HB3	1.94	0.67
1:A:796:THR:HG23	1:A:818:LYS:CB	2.25	0.67
1:C:944:LEU:HD23	1:C:944:LEU:N	2.10	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
2:D:829:GLN:HG3	2:D:1480:LEU:CD1	2.07	0.67
3:X:86:LEU:HG	3:X:91:LYS:CB	2.23	0.67
1:A:1219:LYS:CE	1:A:1239:VAL:HG21	2.25	0.66
1:A:530:VAL:HG23	1:A:534:MET:HE2	1.75	0.66
1:A:947:ARG:O	1:A:949:ILE:HG12	1.95	0.66
2:B:1382:ILE:HB	2:B:1425:ILE:HB	1.77	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
1:C:1323:LEU:HD12	1:C:1324:HIS:N	2.10	0.66
1:C:222:TYR:C	1:C:222:TYR:CD2	2.68	0.66
1:C:583:SER:O	1:C:586:GLN:HG2	1.94	0.66
1:C:698:CYS:C	1:C:700:TYR:H	1.97	0.66
2:D:481:TYR:HB2	2:D:520:PHE:HE1	1.58	0.66
3:Y:128:LYS:HB2	3:Y:158:GLU:HB2	1.77	0.66
1:A:1643:THR:HG22	1:A:1644:TRP:N	2.09	0.66
1:A:474:LYS:H	1:A:474:LYS:HD3	1.59	0.66
2:B:1444:LYS:CE	2:B:1447:GLU:HA	2.25	0.66
2:B:1450:PHE:CD1	2:B:1451:ILE:N	2.64	0.66
2:B:599:TRP:HA	2:B:599:TRP:CE3	2.29	0.66
1:C:1226:ARG:HB3	1:C:1269:PRO:HB2	1.75	0.66
3:X:166:ASP:CG	3:X:207:LEU:HD23	2.14	0.66
1:A:473:HIS:CD2	1:A:473:HIS:O	2.49	0.66
1:A:115:LYS:CB	1:A:654:LEU:HD21	2.25	0.66
1:C:1113:LEU:CD2	1:C:1114:ASP:H	2.07	0.66
1:C:1643:THR:HG22	1:C:1644:TRP:N	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:480:GLU:O	1:C:530:VAL:HG12	1.95	0.66
2:D:131:GLN:OE1	2:D:146:ARG:NH1	2.28	0.66
1:C:525:SER:H	2:D:401:ASN:HD21	1.40	0.66
1:A:25:ILE:HD13	1:A:41:ILE:HB	1.77	0.66
2:B:1606:TRP:C	2:B:1606:TRP:CD1	2.69	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
1:C:640:LEU:HD12	1:C:640:LEU:O	1.95	0.66
2:D:1602:THR:C	2:D:1604:ASN:H	1.99	0.66
3:Y:205:ASP:O	3:Y:206:LYS:C	2.33	0.66
1:C:1219:LYS:HD3	1:C:1239:VAL:HG21	1.77	0.66
1:C:467:ILE:CG2	1:C:486:VAL:HG22	2.25	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:307:VAL:HG13	1:A:313:TYR:HB2	1.78	0.66
1:A:471:ASP:OD2	1:A:474:LYS:HD2	1.96	0.66
1:C:685:GLU:OE1	1:C:685:GLU:HA	1.94	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:A:238:ILE:HB	1:A:347:TYR:CD1	2.31	0.66
1:A:484:ILE:CD1	1:A:540:LEU:HD21	2.26	0.66
1:A:632:LEU:N	1:A:632:LEU:HD23	2.11	0.66
1:A:690:TYR:CD2	1:A:690:TYR:O	2.49	0.66
1:A:702:GLY:CA	1:A:728:PHE:CE1	2.78	0.66
2:B:961:THR:CG2	2:B:1327:THR:HG23	2.25	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: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
1:C:1352:PHE:CD2	1:C:1352:PHE:N	2.62	0.66
1:C:1562:LYS:CD	1:C:1664:LEU:HD21	2.12	0.66
1:C:190:ILE:HG22	1:C:191:PRO:N	2.11	0.66
1:C:234:GLU:HG3	1:C:235:TYR:CE2	2.29	0.66
1:C:931:PRO:HB2	1:C:1366:HIS:CD2	2.30	0.66
2:D:1445:HIS:CG	2:D:1446:PHE:H	2.14	0.66
2:D:964:ILE:HG13	2:D:1302:THR:HG23	1.77	0.66
1:A:869:GLU:C	1:A:871:PRO:HD3	2.15	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
1:C:255:PHE:HE1	1:C:258:LYS:HB2	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:639:GLY:H	1:C:645:VAL:HA	1.60	0.66
1:C:670:LYS:HD2	1:C:671:GLU:HG2	1.78	0.66
1:C:935:LYS:HD3	1:C:1373:GLU:OE2	1.94	0.66
2:D:961:THR:CG2	2:D:1327:THR:HG23	2.25	0.66
3:Y:98:LEU:HD22	3:Y:101:GLN:OE1	1.96	0.66
1:A:1566:THR:O	1:A:1613:LYS:HE3	1.95	0.66
1:A:1618:LEU:HD22	1:A:1619:ILE:H	1.60	0.66
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:131:GLN:OE1	2:B:146:ARG:NH1	2.29	0.66
2:B:523:TYR:CD1	2:B:523:TYR:C	2.68	0.66
1:C:1127:ILE:HD11	1:C:1143:TYR:CD2	2.31	0.66
1:C:1213:LYS:HE2	1:C:1266:TYR:CD2	2.31	0.66
1:C:436:LYS:HB2	1:C:449:ARG:HG2	1.77	0.66
2:D:1345:LEU:HA	2:D:1368:CYS:O	1.96	0.66
2:D:236:TYR:CZ	2:D:424:ARG:HD2	2.31	0.66
2:D:69:PHE:CG	2:D:87:ILE:HG22	2.31	0.66
1:A:1202:HIS:CD2	1:A:1203:PRO:HD2	2.31	0.66
1:C:1034:PHE:CD2	1:C:1041:GLU:HG2	2.30	0.66
1:C:981:GLY:CA	1:C:1333:PHE:HB2	2.25	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
2:D:230:PRO:HG3	2:D:333:GLN:HG2	1.77	0.66
2:D:57:PHE:HD1	2:D:59:HIS:HE2	1.44	0.66
1:A:62:LYS:HE2	1:A:103:TYR:CE2	2.31	0.65
1:A:955:ARG:NH1	1:A:1352:PHE:HA	2.11	0.65
2:B:194:LEU:HD12	2:B:217:ARG:HA	1.78	0.65
1:A:1163:LYS:HZ1	1:C:1109:GLU:CD	1.99	0.65
1:C:495:LYS:HE2	1:C:495:LYS:HA	1.76	0.65
1:C:705:VAL:HA	1:C:739:ARG:NH1	2.11	0.65
2:D:563:MET:HB3	2:D:778:PHE:CE2	2.31	0.65
1:A:436:LYS:HB2	1:A:449:ARG:HG2	1.78	0.65
1:A:489:LYS:HG3	1:A:490:SER:H	1.60	0.65
1:A:633:GLY:O	1:A:634:CYS:HB2	1.96	0.65
1:A:641:ASN:O	1:A:643:ALA:N	2.29	0.65
1:A:25:ILE:HB	1:A:654:LEU:HB2	1.78	0.65
1:A:87:ILE:HD13	1:A:87:ILE:H	1.61	0.65
1:A:895:LEU:HD12	1:A:896:VAL:N	2.11	0.65
1:C:704:CYS:C	1:C:739:ARG:HH22	2.00	0.65
1:C:511:HIS:CE1	3:Y:149:SER:HG	2.14	0.65
1:A:935:LYS:HD3	1:A:1373:GLU:OE2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:505:SER:OG	1:C:506:LYS:HD3	1.97	0.65
1:C:934:VAL:CG2	1:C:1366:HIS:CD2	2.79	0.65
1:A:1585:TYR:CG	1:A:1586:LYS:N	2.64	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
1:C:443:PRO:HD2	1:C:446:ASN:HB2	1.78	0.65
1:C:884:VAL:O	1:C:885:ARG:CB	2.42	0.65
2:D:128:LEU:O	2:D:129:PHE:CD1	2.49	0.65
2:D:481:TYR:CE2	2:D:493:GLY:CA	2.79	0.65
3:X:47:HIS:HE1	3:X:181:LYS:HE2	1.62	0.65
2:B:69:PHE:CG	2:B:87:ILE:HG22	2.32	0.65
1:A:875:HIS:HB3	2:B:901:GLN:NE2	2.11	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:D:133:ASP:HA	2:D:757:TRP:HZ3	1.60	0.65
3:X:41:HIS:O	3:X:42:ASP:HB2	1.96	0.65
3:Y:207:LEU:HD12	3:Y:207:LEU:C	2.14	0.65
1:A:1034:PHE:CD2	1:A:1041:GLU:HG2	2.32	0.65
1:A:505:SER:OG	1:A:506:LYS:HD3	1.97	0.65
1:A:884:VAL:O	1:A:885:ARG:CB	2.41	0.65
1:C:1123:GLN:NE2	1:C:1123:GLN:HA	2.11	0.65
1:C:1180:LEU:O	1:C:1182:ALA:N	2.29	0.65
1:C:1564:SER:HB2	1:C:1616:GLN:HG3	1.78	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
2:D:282:ARG:C	2:D:283:ILE:HD12	2.17	0.65
2:D:239:GLY:H	2:D:296:ARG:NH2	1.95	0.65
2:D:421:PRO:HB2	2:D:423:GLU:OE2	1.96	0.65
2:D:422:ARG:CD	2:D:422:ARG:H	2.08	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
3:Y:43:ILE:HG23	3:Y:44:ARG:H	1.60	0.65
1:A:1381:ILE:HG12	1:A:1382:ASP:N	2.12	0.65
1:A:222:TYR:C	1:A:222:TYR:CD2	2.70	0.65
1:A:60:PRO:CD	1:A:61:ASP:N	2.56	0.65
1:A:705:VAL:N	1:A:739:ARG:HH22	1.94	0.65
2:B:783:SER:HB2	2:B:787:TRP:CZ2	2.32	0.65
1:C:1076:THR:HG21	1:C:1120:GLU:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1075:SER:HB2	1:C:1120:GLU:OE1	1.96	0.65
1:C:24:VAL:HG11	1:C:543:TYR:CE2	2.31	0.65
1:C:936:ARG:NH2	1:C:1284:PHE:CE1	2.64	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
2:B:144:LEU:H	2:B:144:LEU:HD23	1.62	0.65
2:B:237:ILE:HD11	2:B:309:LEU:CB	2.24	0.65
2:B:460:LEU:O	2:B:460:LEU:HD23	1.97	0.65
2:B:23:ALA:HB3	2:B:528:ASN:HD22	1.61	0.65
1:C:1231:ASN:HB2	1:C:1235:LYS:HG3	1.77	0.65
1:C:863:GLU:H	1:C:863:GLU:CD	2.00	0.65
2:D:557:GLN:HE21	2:D:563:MET:CE	2.10	0.65
3:Y:53:GLU:HB3	3:Y:55:PHE:CE2	2.32	0.65
2:B:1371:TYR:O	2:B:1432:HIS:HA	1.97	0.65
2:B:1445:HIS:CG	2:B:1446:PHE:H	2.15	0.65
2:B:887:LEU:CD2	2:B:1490:CYS:HB3	2.27	0.65
2:B:262:PHE:CE1	2:B:282:ARG:HG3	2.30	0.65
2:B:825:VAL:N	2:B:828:GLU:OE1	2.29	0.65
1:C:1429:PRO:HB2	1:C:1432:ILE:HG13	1.78	0.65
1:C:492:TYR:HD2	1:C:493:ILE:H	1.44	0.65
1:C:690:TYR:CD2	1:C:690:TYR:O	2.49	0.65
2:D:1515:ALA:HB1	2:D:1523:VAL:HG21	1.79	0.65
2:D:167:THR:HG23	2:D:171:ILE:H	1.61	0.65
1:A:1259:LEU:HD11	1:A:1300:TYR:HB2	1.78	0.65
1:A:931:PRO:HB2	1:A:1366:HIS:CD2	2.32	0.65
1:A:690:TYR:C	1:A:692:HIS:H	2.00	0.65
2:B:481:TYR:HB2	2:B:520:PHE:HE1	1.59	0.65
2:B:603:GLU:O	2:B:605:SER:N	2.28	0.65
1:C:1304:VAL:CG1	1:C:1305:LYS:N	2.60	0.65
1:C:24:VAL:CG1	1:C:24:VAL:O	2.45	0.65
1:C:884:VAL:CG1	1:C:886:GLN:HG2	2.27	0.65
2:D:1387:LEU:HB2	2:D:1390:PHE:CD2	2.32	0.65
3:X:50:TYR:HE2	3:X:170:ARG:NH1	1.94	0.65
1:A:1244:THR:H	1:A:1247:MET:HE3	1.62	0.64
1:A:307:VAL:CG1	1:A:313:TYR:HB2	2.27	0.64
1:A:492:TYR:HD2	1:A:493:ILE:H	1.45	0.64
1:A:705:VAL:HA	1:A:739:ARG:NH1	2.12	0.64
2:B:364:VAL:HG21	2:B:379:VAL:HG21	1.79	0.64
2:D:299:PHE:HE1	2:D:303:PHE:HD2	1.45	0.64
2:D:433:ILE:HG22	2:D:434:ALA:O	1.96	0.64
1:A:1352:PHE:N	1:A:1352:PHE:CD2	2.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:LEU:H	1:A:658:ASN:HD22	1.43	0.64
1:A:423:ASN:HB3	2:B:501:GLN:NE2	2.13	0.64
2:B:838:ASN:OD1	2:B:840:VAL:HG23	1.97	0.64
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
1:C:1244:THR:HG22	1:C:1246:ARG:N	2.13	0.64
3:X:70:SER:CB	3:X:91:LYS:HE3	2.27	0.64
1:A:1627:ILE:HG13	1:A:1627:ILE:O	1.98	0.64
1:A:494:ASP:OD1	1:A:495:LYS:HE2	1.97	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: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:170:ARG:O	3:X:174:VAL:HG23	1.97	0.64
3:X:179:LEU:HD12	3:X:180:TYR:H	1.62	0.64
1:A:656:ASN:HB3	1:A:659:ALA:H	1.63	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:A:917:TRP:HB3	2:B:558:MET:SD	2.38	0.64
1:C:1086:LEU:HD12	1:C:1095:GLN:HG3	1.79	0.64
1:C:119:ILE:O	1:C:119:ILE:HD12	1.97	0.64
1:C:1423:VAL:CG1	1:C:1496:TYR:CE2	2.80	0.64
1:C:1566:THR:O	1:C:1613:LYS:HE3	1.98	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
2:D:26:THR:OG1	2:D:44:GLU:HB2	1.98	0.64
1:C:429:THR:HA	1:C:456:ALA:HB2	1.80	0.64
3:X:205:ASP:O	3:X:206:LYS:C	2.33	0.64
1:A:1077:TRP:NE1	1:A:1147:PHE:CE1	2.66	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
2:B:1623:LYS:HA	2:B:1623:LYS:HZ3	1.63	0.64
1:C:1548:ARG:HD3	1:C:1548:ARG:H	1.63	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
2:D:1547:VAL:HG23	2:D:1557:ARG:NH1	2.12	0.64
2:D:523:TYR:C	2:D:523:TYR:CD1	2.70	0.64
3:X:170:ARG:HD3	3:X:203:LEU:CD2	2.27	0.64
3:Y:64:VAL:HG23	3:Y:71:ASN:OD1	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:LEU:H	1:C:161:LEU:HD12	1.62	0.64
1:C:60:PRO:HD2	1:C:61:ASP:N	2.09	0.64
1:C:362:PHE:CE1	1:C:640:LEU:HB2	2.33	0.64
2:D:149:SER:O	2:D:794:PHE:HE1	1.80	0.64
1:A:1024:TYR:HA	1:A:1302:LEU:CD2	2.28	0.64
1:A:1365:VAL:CG2	1:A:1366:HIS:H	2.08	0.64
1:A:24:VAL:CG1	1:A:24:VAL:O	2.45	0.64
1:A:535:VAL:HG23	1:A:536:PRO:CD	2.16	0.64
2:B:1615:GLU:HB3	2:B:1621:PHE:HD1	1.63	0.64
1:C:260:VAL:HG12	1:C:261:THR:N	2.12	0.64
2:D:136:ILE:HA	2:D:215:ASP:O	1.97	0.64
2:D:1505:ARG:CZ	2:D:1623:LYS:NZ	2.61	0.64
2:D:130:ILE:HD13	2:D:199:ILE:HG22	1.80	0.64
2:D:464:PHE:HB2	2:D:504:VAL:O	1.98	0.64
2:D:599:TRP:HA	2:D:599:TRP:CE3	2.31	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: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:436:LYS:HA	1:C:448:ALA:O	1.97	0.64
1:C:883:CYS:O	1:C:884:VAL:O	2.16	0.64
1:A:1304:VAL:CG1	1:A:1305:LYS:N	2.61	0.64
1:A:144:ARG:HD2	1:A:146:TYR:HE1	1.62	0.64
1:C:1402:ILE:HG13	1:C:1479:ILE:CD1	2.28	0.64
1:C:632:LEU:HD23	1:C:632:LEU:N	2.13	0.64
1:C:612:VAL:HG21	1:C:769:PHE:CZ	2.32	0.64
2:D:218:LYS:HB3	2:D:822:TYR:HD2	1.59	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
3:X:194:LYS:NZ	3:X:197:ASN:HB2	2.10	0.64
3:X:73:VAL:HG22	3:X:84:LEU:HB3	1.80	0.64
3:Y:70:SER:CB	3:Y:91:LYS:HE3	2.28	0.64
2:B:1446:PHE:CD2	2:B:1448:VAL:HG22	2.33	0.63
2:B:534:ASP:HA	2:B:620:VAL:HG21	1.80	0.63
1:C:693:SER:C	1:C:695:VAL:H	2.01	0.63
2:D:1417:MET:HG2	2:D:1443:LEU:HD23	1.80	0.63
2:D:1591:LEU:HD23	2:D:1591:LEU:C	2.19	0.63
2:D:543:THR:OG1	2:D:544:CYS:N	2.30	0.63
1:A:1101:CYS:HB3	1:C:1161:LEU:HD11	1.81	0.63
1:A:653:PHE:CD1	1:A:660:ASP:HB3	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:355:LYS:O	2:D:358:MET:HB3	1.97	0.63
1:C:483:ASN:ND2	2:D:399:ILE:HB	2.14	0.63
1:A:671:GLU:O	1:A:672:ILE:HB	1.97	0.63
2:B:221:LEU:CD1	2:B:753:LYS:HG2	2.25	0.63
1:C:1286:SER:HB2	1:C:1499:HIS:HA	1.80	0.63
1:C:393:GLN:HG2	1:C:403:ASP:OD1	1.99	0.63
1:C:459:SER:OG	1:C:461:SER:HB3	1.97	0.63
1:C:633:GLY:O	1:C:634:CYS:HB2	1.98	0.63
1:C:982:LEU:C	1:C:984:VAL:H	2.01	0.63
2:D:1371:TYR:O	2:D:1432:HIS:HA	1.97	0.63
2:D:58:VAL:HG12	2:D:104:VAL:HG22	1.80	0.63
3:X:50:TYR:CE2	3:X:170:ARG:CD	2.80	0.63
3:Y:134:THR:HG22	3:Y:153:PHE:O	1.97	0.63
3:Y:179:LEU:HD12	3:Y:180:TYR:H	1.62	0.63
1:A:1219:LYS:HD3	1:A:1239:VAL:HG21	1.80	0.63
1:A:1459:HIS:CD2	1:A:1459:HIS:N	2.66	0.63
1:A:91:GLN:O	1:A:92:LEU:HG	1.96	0.63
2:B:58:VAL:HG12	2:B:104:VAL:HG22	1.80	0.63
2:B:829:GLN:HG2	2:B:885:VAL:CG1	2.28	0.63
2:D:194:LEU:HD12	2:D:217:ARG:HA	1.80	0.63
1:C:423:ASN:CG	2:D:504:VAL:HG22	2.18	0.63
3:X:207:LEU:HD12	3:X:207:LEU:C	2.14	0.63
3:X:43:ILE:HG23	3:X:44:ARG:H	1.62	0.63
1:A:1286:SER:HB2	1:A:1499:HIS:HA	1.80	0.63
1:A:153:LYS:HB3	1:A:154:PRO:HD2	1.80	0.63
1:A:1618:LEU:HD22	1:A:1619:ILE:N	2.12	0.63
1:A:330:ILE:HG22	1:A:337:SER:HB2	1.79	0.63
1:A:443:PRO:HD2	1:A:446:ASN:HB2	1.80	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:A:60:PRO:HD2	1:A:61:ASP:N	2.08	0.63
2:B:1539:ILE:H	2:B:1539:ILE:HD12	1.62	0.63
2:B:127:PHE:HE2	2:B:602:ILE:HG23	1.62	0.63
1:C:238:ILE:HB	1:C:347:TYR:HD1	1.62	0.63
1:C:473:HIS:ND1	2:D:455:LYS:HE3	2.13	0.63
1:C:512:PHE:CD2	1:C:512:PHE:O	2.51	0.63
1:C:947:ARG:O	1:C:949:ILE:N	2.31	0.63
1:A:199:TRP:HB2	1:A:217:PHE:CE1	2.34	0.63
1:A:977:LEU:HD22	1:A:978:SER:H	1.63	0.63
2:B:965:ILE:CG1	2:B:1301:ARG:HB2	2.25	0.63
1:C:104:LEU:HD12	1:C:105:GLU:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:830:PRO:CG	1:C:1483:PHE:CZ	2.74	0.63
1:C:238:ILE:HD12	1:C:347:TYR:CE1	2.33	0.63
1:C:512:PHE:HE2	3:Y:148:ALA:HB3	1.63	0.63
1:A:1236:ASP:O	1:A:1238:SER:N	2.29	0.63
1:A:1013:MET:CE	1:A:1287:THR:HB	2.28	0.63
2:B:261:ALA:HB3	2:B:285:ILE:HD11	1.80	0.63
1:C:1459:HIS:CD2	1:C:1459:HIS:N	2.66	0.63
1:C:1629:TYR:CE1	1:C:1631:PHE:CD1	2.86	0.63
1:C:614:ARG:HD2	1:C:615:GLY:H	1.63	0.63
1:C:702:GLY:CA	1:C:728:PHE:CE1	2.77	0.63
1:C:949:ILE:HG22	1:C:950:TYR:CE1	2.33	0.63
2:D:965:ILE:CG1	2:D:1301:ARG:HB2	2.26	0.63
2:D:1447:GLU:HG3	2:D:1447:GLU:O	1.98	0.63
2:D:963:ILE:HD11	2:D:1311:ILE:HG21	1.81	0.63
2:B:1591:LEU:C	2:B:1591:LEU:HD23	2.19	0.63
1:C:653:PHE:CD1	1:C:660:ASP:HB3	2.33	0.63
1:C:24:VAL:CA	1:C:655:THR:HG21	2.28	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
2:D:296:ARG:HG3	2:D:296:ARG:HH11	1.63	0.63
1:A:938:SER:C	1:A:940:SER:H	2.01	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
2:B:620:VAL:HG12	2:B:621:PHE:CD2	2.32	0.63
1:C:1229:LYS:NZ	1:C:1240:PRO:HD2	2.14	0.63
1:C:195:ARG:HD3	1:C:1058:SER:HA	1.80	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:824:PHE:CE2	1:C:846:TYR:HB2	2.34	0.63
1:C:88:GLN:O	1:C:90:LYS:HD3	1.99	0.63
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
1:A:1626:GLN:HG2	1:A:1626:GLN:O	1.98	0.62
1:A:502:LEU:HB2	1:A:541:LEU:HD23	1.79	0.62
1:C:1641:SER:C	1:C:1643:THR:H	2.03	0.62
1:C:656:ASN:HB3	1:C:659:ALA:H	1.64	0.62
1:C:752:LEU:HG	1:C:752:LEU:O	1.99	0.62
2:D:364:VAL:HG21	2:D:379:VAL:HG21	1.81	0.62
3:Y:170:ARG:O	3:Y:174:VAL:HG23	1.98	0.62
1:A:614:ARG:HD2	1:A:615:GLY:H	1.63	0.62
1:A:967:LEU:HD12	1:A:968:VAL:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1607:ILE:N	2:B:1607:ILE:HD12	2.14	0.62
1:C:101:TYR:CE1	1:C:116:ARG:NH2	2.67	0.62
1:A:92:LEU:HD12	1:C:1029:ASN:HD21	1.64	0.62
1:C:1493:PHE:HD1	1:C:1493:PHE:C	2.00	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
1:A:123:ASN:O	1:A:211:THR:HG21	1.98	0.62
1:A:1556:GLU:CB	1:A:1622:LYS:HE2	2.24	0.62
2:B:57:PHE:HD1	2:B:59:HIS:HE2	1.47	0.62
2:B:964:ILE:HG13	2:B:1302:THR:HG23	1.82	0.62
1:C:1527:CYS:O	1:C:1528:VAL:C	2.36	0.62
1:C:1622:LYS:HD2	1:C:1642:LEU:HB3	1.81	0.62
1:C:59:TYR:CD1	1:C:60:PRO:HD3	2.34	0.62
2:D:30:PRO:HG3	2:D:489:ILE:HG13	1.81	0.62
1:A:506:LYS:HE2	1:A:533:ASN:O	1.98	0.62
1:A:543:TYR:CD1	1:A:543:TYR:O	2.51	0.62
1:A:551:THR:O	1:A:552:ALA:CB	2.47	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:265:PHE:CE2	2:B:294:LEU:HB2	2.34	0.62
2:B:355:LYS:N	2:B:355:LYS:HD2	2.15	0.62
2:B:76:ASN:HB2	2:B:77:PRO:HD2	1.82	0.62
1:C:1219:LYS:HE2	1:C:1239:VAL:HG21	1.81	0.62
1:C:1627:ILE:O	1:C:1627:ILE:CG1	2.46	0.62
1:C:267:ILE:HD11	1:C:299:VAL:HG11	1.81	0.62
1:C:270:GLY:HA3	1:C:282:MET:HG2	1.80	0.62
1:C:506:LYS:HE2	1:C:533:ASN:O	1.99	0.62
1:C:834:VAL:O	1:C:837:GLU:HB2	2.00	0.62
2:D:294:LEU:HD12	2:D:295:LYS:N	2.14	0.62
2:D:384:PHE:O	2:D:385:HIS:C	2.38	0.62
2:D:524:TYR:HD1	2:D:524:TYR:O	1.83	0.62
2:D:850:LEU:HD12	2:D:851:LEU:N	2.14	0.62
1:A:938:SER:OG	1:A:1284:PHE:CZ	2.53	0.62
1:A:1423:VAL:CG1	1:A:1496:TYR:CE2	2.81	0.62
1:A:20:GLU:O	1:A:20:GLU:CD	2.37	0.62
1:A:682:LYS:HZ3	1:A:686:ILE:HD11	1.64	0.62
1:A:837:GLU:O	1:A:901:LEU:HD12	2.00	0.62
2:B:1547:VAL:HG23	2:B:1557:ARG:NH1	2.14	0.62
1:C:1386:ILE:HG13	1:C:1387:GLU:H	1.63	0.62
1:C:199:TRP:HB2	1:C:217:PHE:CE1	2.34	0.62
1:C:222:TYR:CD2	1:C:223:VAL:N	2.66	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:623:VAL:O	1:C:624:PHE:C	2.38	0.62
1:C:824:PHE:N	1:C:824:PHE:HD2	1.97	0.62
2:D:61:PHE:CG	2:D:62:PRO:HA	2.35	0.62
3:X:146:LEU:HD22	3:X:147:ASP:N	2.14	0.62
1:A:511:HIS:CE1	3:X:149:SER:OG	2.52	0.62
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:A:1056:ILE:CD1	1:A:1066:TYR:CE2	2.82	0.62
1:A:1429:PRO:HB2	1:A:1432:ILE:HG13	1.80	0.62
1:A:884:VAL:HG12	1:A:885:ARG:N	2.15	0.62
1:C:1271:ILE:O	1:C:1275:SER:HB3	2.00	0.62
1:C:412:ARG:HD2	2:D:458:ASP:OD1	2.00	0.62
1:C:968:VAL:HG23	1:C:971:THR:CG2	2.30	0.62
2:D:510:ILE:HG23	2:D:514:LEU:HD12	1.81	0.62
2:D:563:MET:CG	2:D:780:LEU:HD23	2.25	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:B:1446:PHE:HB3	2:B:1448:VAL:HG22	1.81	0.62
1:C:1142:LEU:HD13	1:C:1187:THR:HG21	1.82	0.62
1:C:1585:TYR:CD2	1:C:1586:LYS:N	2.67	0.62
2:D:1532:GLU:O	2:D:1539:ILE:HD12	1.99	0.62
2:D:162:ILE:HG21	2:D:202:LYS:HG2	1.82	0.62
2:D:355:LYS:N	2:D:355:LYS:HD2	2.14	0.62
2:D:69:PHE:CD2	2:D:70:GLN:N	2.68	0.62
2:D:221:LEU:CD1	2:D:753:LYS:HG2	2.29	0.62
2:D:923:SER:O	2:D:924:ILE:HD12	2.00	0.62
1:C:512:PHE:CE2	3:Y:148:ALA:HB3	2.35	0.62
3:Y:179:LEU:HG	3:Y:180:TYR:CD2	2.35	0.62
1:A:104:LEU:HD12	1:A:105:GLU:N	2.15	0.62
1:A:1226:ARG:CZ	1:A:1266:TYR:HE1	2.13	0.62
1:A:161:LEU:HD11	1:A:185:PHE:CE1	2.35	0.62
2:B:922:LYS:HE3	2:B:1329:TYR:CZ	2.34	0.62
2:B:1562:GLN:NE2	2:B:1596:LYS:NZ	2.48	0.62
2:B:148:PHE:CB	2:B:800:ILE:HD11	2.30	0.62
1:C:936:ARG:NH2	1:C:1284:PHE:HE1	1.98	0.62
1:C:1333:PHE:CD1	1:C:1334:LEU:HD13	2.34	0.62
1:C:442:LEU:HD23	1:C:443:PRO:CD	2.29	0.62
1:C:125:PHE:CE1	1:C:627:LEU:HD21	2.34	0.62
1:C:976:ILE:HB	1:C:1362:THR:HG22	1.82	0.62
2:D:534:ASP:HA	2:D:620:VAL:HG21	1.82	0.62
1:A:1493:PHE:CD1	1:A:1493:PHE:C	2.73	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1646:GLU:OE2	1:A:1660:PHE:CZ	2.53	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:A:488:PRO:HG3	1:A:499:TYR:OH	2.00	0.62
2:B:1431:SER:HB3	2:B:1433:SER:H	1.64	0.62
2:B:1523:VAL:HG22	2:B:1584:TRP:HB2	1.81	0.62
2:B:344:GLN:HB2	2:B:367:THR:O	2.00	0.62
2:B:829:GLN:HA	2:B:885:VAL:HG12	1.81	0.62
1:C:690:TYR:CE1	1:C:692:HIS:HA	2.34	0.62
2:D:873:LYS:HD2	2:D:873:LYS:N	2.15	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:1648:TRP:NE1	1:A:1664:LEU:HD21	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:A:779:LEU:HD12	1:A:780:VAL:N	2.15	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:C:161:LEU:HD11	1:C:185:PHE:CD1	2.35	0.61
1:C:705:VAL:HA	1:C:739:ARG:CZ	2.30	0.61
1:C:849:ARG:CG	1:C:849:ARG:HH11	2.11	0.61
2:D:380:VAL:CG1	2:D:387:MET:HB3	2.17	0.61
2:D:34:ARG:HD2	2:D:488:LYS:NZ	2.15	0.61
3:X:53:GLU:HB3	3:X:55:PHE:CE2	2.35	0.61
1:A:1076:THR:HG22	1:A:1120:GLU:CD	2.20	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
2:B:543:THR:OG1	2:B:544:CYS:N	2.31	0.61
1:C:1211:ALA:HA	1:C:1214:ARG:HH11	1.65	0.61
1:C:1381:ILE:O	1:C:1382:ASP:HB3	2.00	0.61
1:C:796:THR:HG23	1:C:818:LYS:CB	2.30	0.61
2:D:1380:THR:HG22	2:D:1381:ILE:H	1.64	0.61
2:D:1610:TRP:CE3	2:D:1628:PHE:CD2	2.87	0.61
2:D:161:VAL:HG21	2:D:180:LEU:CD2	2.28	0.61
2:D:219:TYR:CD1	2:D:220:VAL:N	2.69	0.61
2:D:620:VAL:HG12	2:D:621:PHE:CD2	2.34	0.61
3:X:58:SER:HB2	3:X:125:LYS:HE3	1.82	0.61
1:C:513:GLY:HA2	3:Y:146:LEU:HD13	1.82	0.61
1:A:1219:LYS:HZ3	1:A:1239:VAL:HG11	1.61	0.61
1:A:1504:GLN:HG3	1:A:1505:CYS:CA	2.30	0.61
1:A:393:GLN:HG2	1:A:403:ASP:OD1	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:SER:HB2	1:A:589:SER:CB	2.27	0.61
1:A:653:PHE:CE1	1:A:660:ASP:HB3	2.35	0.61
2:B:120:LEU:HD12	2:B:121:LEU:N	2.11	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:1053:MET:SD	1:C:1089:VAL:HG21	2.40	0.61
1:C:586:GLN:O	1:C:586:GLN:HG3	2.00	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
2:D:1347:VAL:HG21	2:D:1456:VAL:HG11	1.81	0.61
2:D:1511:GLN:HG2	2:D:1631:PHE:CE1	2.35	0.61
2:D:69:PHE:CD1	2:D:87:ILE:HG22	2.36	0.61
3:Y:166:ASP:CB	3:Y:207:LEU:HD21	2.30	0.61
1:A:1365:VAL:CG2	1:A:1366:HIS:N	2.60	0.61
1:A:270:GLY:HA3	1:A:282:MET:HG2	1.83	0.61
1:A:44:TYR:CE1	1:A:497:THR:HG21	2.35	0.61
1:A:824:PHE:CE2	1:A:846:TYR:HD1	2.19	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
2:B:242:ASN:OD1	2:B:295:LYS:HD2	1.99	0.61
1:A:855:PHE:HA	2:B:904:LEU:CD1	2.28	0.61
1:C:927:LEU:HD23	1:C:928:ARG:N	2.16	0.61
1:C:955:ARG:NH1	1:C:1352:PHE:HA	2.15	0.61
2:D:342:PRO:HG2	2:D:420:LEU:HD13	1.81	0.61
2:D:410:PRO:HA	2:D:431:THR:HG22	1.83	0.61
1:A:868:SER:CA	1:A:1527:CYS:HB2	2.28	0.61
1:A:1641:SER:C	1:A:1643:THR:H	2.02	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
2:B:237:ILE:O	2:B:306:LEU:HD11	1.99	0.61
1:C:149:ASN:H	1:C:149:ASN:ND2	1.97	0.61
1:C:177:ILE:HG22	1:C:178:ASP:H	1.66	0.61
1:C:317:ASP:C	1:C:319:ASN:H	2.03	0.61
2:D:1344:HIS:O	2:D:1369:THR:HA	2.01	0.61
2:D:964:ILE:O	2:D:964:ILE:HG22	2.00	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
3:Y:73:VAL:HG22	3:Y:84:LEU:HB3	1.80	0.61
1:A:1147:PHE:O	1:A:1150:ILE:HB	2.01	0.61
1:A:1163:LYS:NZ	1:C:1109:GLU:CD	2.54	0.61
1:A:871:PRO:HD2	1:A:872:VAL:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1188:LEU:HD23	1:C:1212:LEU:HD13	1.83	0.61
1:C:20:GLU:O	1:C:20:GLU:CD	2.39	0.61
1:C:481:HIS:HE1	1:C:529:PRO:HB3	1.64	0.61
1:C:742:ILE:HG21	1:C:753:HIS:HA	1.83	0.61
1:C:837:GLU:O	1:C:901:LEU:HD12	2.00	0.61
2:D:581:ASP:O	2:D:582:LYS:C	2.39	0.61
1:A:1033:ILE:HG23	1:A:1034:PHE:N	2.14	0.61
1:A:161:LEU:HD11	1:A:185:PHE:CG	2.36	0.61
1:A:260:VAL:HG12	1:A:261:THR:N	2.15	0.61
1:A:267:ILE:HD12	1:A:299:VAL:HG11	1.83	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:1583:ILE:HG12	2:B:1607:ILE:CG2	2.30	0.61
2:B:384:PHE:O	2:B:385:HIS:C	2.38	0.61
2:B:484:LEU:HD11	2:B:626:LEU:HD11	1.83	0.61
1:C:44:TYR:CE1	1:C:497:THR:HG21	2.35	0.61
1:C:653:PHE:CE1	1:C:660:ASP:HB3	2.35	0.61
2:D:1506:ILE:O	2:D:1508:VAL:N	2.34	0.61
2:D:384:PHE:HD1	2:D:400:LEU:HG	1.60	0.61
3:X:191:ILE:HD12	3:X:199:VAL:HB	1.82	0.61
1:A:1049:LEU:HD11	1:A:1089:VAL:CG1	2.30	0.61
1:A:24:VAL:HG11	1:A:543:TYR:CE2	2.35	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
1:C:1582:LEU:HD11	1:C:1648:TRP:HZ2	1.66	0.61
1:C:489:LYS:CG	1:C:490:SER:H	2.13	0.61
1:C:60:PRO:CD	1:C:61:ASP:N	2.56	0.61
2:D:34:ARG:HD2	2:D:488:LYS:HZ3	1.66	0.61
3:Y:50:TYR:CE2	3:Y:170:ARG:CD	2.81	0.61
1:A:428:VAL:HG22	1:A:429:THR:H	1.65	0.61
1:A:59:TYR:CD1	1:A:60:PRO:HD3	2.36	0.61
2:B:1610:TRP:CD2	2:B:1628:PHE:HD2	2.19	0.61
2:B:599:TRP:CZ3	2:B:602:ILE:HD12	2.36	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
3:Y:191:ILE:HD12	3:Y:199:VAL:HB	1.83	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
1:A:824:PHE:CE2	1:A:846:TYR:HB2	2.36	0.61
2:B:1447:GLU:HG3	2:B:1447:GLU:O	2.00	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:244:HIS:HB3	2:B:291:LYS:CD	2.29	0.61
2:B:433:ILE:HG22	2:B:434:ALA:O	2.01	0.61
1:C:1147:PHE:O	1:C:1150:ILE:HB	2.00	0.61
1:C:40:VAL:CG2	1:C:512:PHE:HD1	2.14	0.61
2:D:1500:LEU:HD11	2:D:1608:GLU:O	2.01	0.61
2:D:841:ASN:O	2:D:842:GLU:C	2.40	0.61
1:A:119:ILE:O	1:A:119:ILE:HD12	2.01	0.60
1:A:1535:MET:HA	1:A:1645:ILE:HB	1.83	0.60
1:A:658:ASN:OD1	1:A:658:ASN:C	2.40	0.60
2:B:1561:HIS:CE1	2:B:1597:ILE:HD13	2.35	0.60
2:B:342:PRO:HG2	2:B:420:LEU:HD13	1.83	0.60
1:C:1268:ASN:H	1:C:1268:ASN:ND2	1.98	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:822:ASP:HA	1:C:849:ARG:HD2	1.83	0.60
2:D:1391:LEU:HB2	2:D:1417:MET:HE2	1.83	0.60
2:D:829:GLN:NE2	2:D:883:VAL:HG13	2.10	0.60
1:A:1003:LEU:N	1:A:1003:LEU:HD23	2.16	0.60
1:A:1268:ASN:ND2	1:A:1268:ASN:H	1.99	0.60
1:A:1627:ILE:O	1:A:1629:TYR:N	2.34	0.60
1:A:177:ILE:HG22	1:A:178:ASP:H	1.65	0.60
1:A:532:GLN:NE2	1:A:568:GLY:HA2	2.16	0.60
2:B:167:THR:HG23	2:B:171:ILE:H	1.65	0.60
1:C:1054:LEU:HD23	1:C:1057:MET:HE2	1.83	0.60
1:C:1232:LEU:CD1	1:C:1233:GLN:HE21	2.09	0.60
1:C:256:TYR:HD2	1:C:846:TYR:CE1	2.19	0.60
1:C:873:ILE:O	1:C:873:ILE:HD12	2.01	0.60
2:D:133:ASP:OD2	2:D:134:LYS:HG2	2.01	0.60
2:D:1610:TRP:CD2	2:D:1628:PHE:HD2	2.18	0.60
2:D:581:ASP:O	2:D:583:ALA:N	2.34	0.60
2:D:814:PHE:HZ	2:D:846:VAL:HG21	1.66	0.60
3:X:170:ARG:NH2	3:X:206:LYS:HA	2.16	0.60
1:A:1211:ALA:HA	1:A:1214:ARG:HH11	1.66	0.60
1:A:987:ILE:CD1	1:A:1294:ILE:HG23	2.31	0.60
1:A:1323:LEU:HD12	1:A:1324:HIS:N	2.16	0.60
1:A:1427:SER:HB3	1:A:1492:THR:HG23	1.81	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:171:VAL:HG11	1:C:1054:LEU:HD11	1.82	0.60
1:C:243:PHE:HE2	1:C:304:GLU:HA	1.66	0.60
1:C:322:TYR:N	1:C:322:TYR:CD2	2.68	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:242:ASN:OD1	2:D:295:LYS:HD2	2.00	0.60
1:A:443:PRO:HG2	1:A:446:ASN:OD1	2.01	0.60
1:A:500:ASN:CB	1:A:543:TYR:CE1	2.61	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
2:B:756:LEU:HD12	2:B:758:LEU:HG	1.84	0.60
1:C:1487:PHE:O	1:C:1488:LEU:C	2.40	0.60
1:C:1549:LYS:HZ2	1:C:1667:PHE:HB3	1.66	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
2:D:196:THR:HG23	2:D:215:ASP:OD1	2.01	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
1:A:161:LEU:H	1:A:161:LEU:HD12	1.65	0.60
1:A:1585:TYR:HE1	1:A:1671:ILE:HG12	1.66	0.60
2:B:1381:ILE:HG21	2:B:1459:TYR:CE1	2.35	0.60
2:B:1473:HIS:CD2	2:B:1474:PRO:CD	2.84	0.60
2:B:435:TYR:OH	2:B:532:VAL:HG22	2.00	0.60
2:B:738:GLY:O	2:B:901:GLN:HA	2.02	0.60
1:C:1646:GLU:OE2	1:C:1660:PHE:CZ	2.54	0.60
1:C:209:PHE:H	1:C:209:PHE:HD2	1.48	0.60
1:C:531:THR:O	1:C:534:MET:HG3	2.01	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:A:1213:LYS:HE2	1:A:1266:TYR:CE2	2.37	0.60
1:A:1548:ARG:HD3	1:A:1548:ARG:H	1.66	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:A:503:ILE:HD11	1:A:540:LEU:HD13	1.83	0.60
1:A:670:LYS:HD2	1:A:671:GLU:HG2	1.84	0.60
2:B:127:PHE:CE2	2:B:602:ILE:HG23	2.37	0.60
2:B:556:ILE:H	2:B:556:ILE:HD12	1.65	0.60
1:C:702:GLY:CA	1:C:728:PHE:CD1	2.84	0.60
2:D:120:LEU:HD12	2:D:121:LEU:N	2.13	0.60
2:D:233:LYS:HG3	2:D:233:LYS:O	2.01	0.60
1:A:101:TYR:CE1	1:A:116:ARG:NH2	2.70	0.60
1:A:690:TYR:CE1	1:A:692:HIS:HA	2.36	0.60
2:B:61:PHE:HB3	2:B:103:TYR:HB2	1.83	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:931:PRO:HG2	1:C:1366:HIS:NE2	2.16	0.60
1:C:209:PHE:CD2	1:C:209:PHE:N	2.68	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
2:D:1561:HIS:CE1	2:D:1597:ILE:HD13	2.37	0.60
1:A:1053:MET:SD	1:A:1089:VAL:HG21	2.42	0.60
1:A:1128:LYS:C	1:A:1129:LEU:HD23	2.22	0.60
1:A:436:LYS:HA	1:A:448:ALA:O	2.01	0.60
2:B:133:ASP:OD2	2:B:134:LYS:HG2	2.01	0.60
2:B:294:LEU:HD12	2:B:295:LYS:N	2.16	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
1:C:174:VAL:HG22	1:C:175:GLU:N	2.15	0.60
1:C:25:ILE:CD1	1:C:41:ILE:HB	2.31	0.60
1:C:115:LYS:CB	1:C:654:LEU:HD21	2.32	0.60
1:C:820:PHE:O	1:C:821:LYS:HG3	2.00	0.60
1:C:824:PHE:HE2	1:C:846:TYR:HB2	1.65	0.60
2:D:1510:LEU:HD21	2:D:1514:LYS:NZ	2.15	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
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:1239:VAL:O	1:C:1239:VAL:HG12	2.02	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
1:A:1231:ASN:HB2	1:A:1235:LYS:HG3	1.83	0.60
1:A:1341:LEU:HB2	1:A:1342:LEU:CD2	2.31	0.60
1:A:1671:ILE:HA	1:A:1675:GLY:H	1.66	0.60
1:A:474:LYS:H	1:A:474:LYS:CD	2.15	0.60
1:A:55:SER:O	1:A:56:ILE:HD13	2.01	0.60
1:A:705:VAL:HA	1:A:739:ARG:CZ	2.31	0.60
2:B:197:TRP:HB2	2:B:214:PHE:CE1	2.36	0.60
2:B:296:ARG:HH11	2:B:296:ARG:HG3	1.66	0.60
2:B:510:ILE:HG23	2:B:514:LEU:HD12	1.84	0.60
2:B:557:GLN:HE21	2:B:563:MET:CE	2.14	0.60
1:C:1150:ILE:CD1	1:C:1193:TYR:CD2	2.85	0.60
1:C:1608:ASN:O	1:C:1610:GLU:N	2.35	0.60
1:C:443:PRO:HG2	1:C:446:ASN:OD1	2.02	0.60
1:C:569:ASN:ND2	1:C:570:GLN:H	2.00	0.60
1:A:443:PRO:HG2	1:A:446:ASN:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:THR:HA	1:A:456:ALA:HB2	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:A:362:PHE:HE1	1:A:640:LEU:HB2	1.67	0.59
1:A:25:ILE:HB	1:A:655:THR:HG23	1.84	0.59
1:A:824:PHE:HD2	1:A:824:PHE:N	1.99	0.59
2:B:523:TYR:HB3	2:B:533:ALA:HB2	1.83	0.59
1:C:1329:THR:H	1:C:1332:ASN:HB2	1.67	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
1:C:342:ILE:HD12	1:C:345:ILE:HD11	1.84	0.59
2:D:476:ILE:O	2:D:476:ILE:CG2	2.50	0.59
2:D:476:ILE:HD11	2:D:524:TYR:CG	2.36	0.59
1:A:1056:ILE:CD1	1:A:1066:TYR:HE2	2.15	0.59
1:A:504:LEU:HD12	1:A:509:ILE:HG23	1.85	0.59
1:A:612:VAL:HG12	1:A:612:VAL:O	2.01	0.59
1:A:25:ILE:N	1:A:655:THR:HG21	2.12	0.59
2:B:508:LEU:HD12	2:B:509:HIS:N	2.16	0.59
2:B:531:ILE:HD11	2:B:634:LEU:HD23	1.84	0.59
1:C:1152:ILE:HG22	1:C:1168:LEU:HD21	1.82	0.59
1:C:967:LEU:HD12	1:C:968:VAL:H	1.66	0.59
2:D:1486:ILE:HD11	2:D:1591:LEU:HD22	1.85	0.59
2:D:261:ALA:CB	2:D:285:ILE:HD11	2.32	0.59
3:X:179:LEU:HG	3:X:180:TYR:CD2	2.36	0.59
3:X:68:ASN:CG	3:X:69:GLY:N	2.55	0.59
3:Y:101:GLN:HA	3:Y:125:LYS:HB3	1.84	0.59
3:Y:68:ASN:CG	3:Y:69:GLY:N	2.55	0.59
1:A:1113:LEU:CD2	1:A:1114:ASP:H	2.15	0.59
1:A:1381:ILE:O	1:A:1382:ASP:HB3	2.02	0.59
1:A:1559:TYR:HH	1:A:1591:VAL:HA	1.66	0.59
1:A:1612:VAL:HB	1:A:1615:ARG:CB	2.26	0.59
1:A:209:PHE:H	1:A:209:PHE:HD2	1.50	0.59
1:A:199:TRP:CD1	1:A:219:VAL:HB	2.37	0.59
1:A:222:TYR:CD2	1:A:223:VAL:N	2.69	0.59
1:A:838:GLN:HA	1:A:901:LEU:CB	2.29	0.59
1:A:949:ILE:HG22	1:A:950:TYR:CE1	2.37	0.59
2:B:69:PHE:CD1	2:B:87:ILE:HG22	2.37	0.59
2:B:829:GLN:NE2	2:B:883:VAL:HG13	2.13	0.59
1:C:1320:LYS:CE	1:C:1321:GLY:H	2.15	0.59
1:C:493:ILE:HG23	1:C:495:LYS:HB2	1.85	0.59
1:A:623:VAL:HG12	1:A:624:PHE:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1424:ILE:H	2:B:1424:ILE:CD1	2.14	0.59
2:B:309:LEU:HB3	2:B:338:ILE:HD12	1.84	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
1:A:1011:GLU:O	1:A:1014:SER:HB3	2.02	0.59
1:A:115:LYS:HB2	1:A:654:LEU:HD21	1.85	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
1:A:874:ASP:HA	1:A:878:THR:O	2.03	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:C:1615:ARG:NH1	1:C:1647:TYR:CE1	2.70	0.59
1:C:515:ARG:NH1	1:C:526:ILE:HG22	2.16	0.59
1:A:1329:THR:H	1:A:1332:ASN:HB2	1.68	0.59
1:A:356:LEU:HG	1:A:452:TYR:CZ	2.38	0.59
1:A:503:ILE:CB	1:A:511:HIS:HB2	2.33	0.59
2:B:241:GLU:O	2:B:296:ARG:HD3	2.02	0.59
2:B:525:GLN:HA	2:B:530:GLU:O	2.03	0.59
2:B:148:PHE:HB3	2:B:800:ILE:HD11	1.83	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:243:PHE:HE1	2:D:336:ILE:HG21	1.67	0.59
2:D:61:PHE:HB3	2:D:103:TYR:HB2	1.83	0.59
2:D:738:GLY:O	2:D:901:GLN:HA	2.03	0.59
1:A:1066:TYR:N	1:A:1079:THR:HG23	2.16	0.59
1:A:1219:LYS:HE2	1:A:1239:VAL:HG21	1.85	0.59
1:A:361:LEU:N	1:A:361:LEU:HD12	2.16	0.59
1:A:936:ARG:NH2	1:A:1284:PHE:CE1	2.71	0.59
2:B:130:ILE:HD13	2:B:199:ILE:HG22	1.83	0.59
2:B:1609:ARG:HG2	2:B:1609:ARG:HH11	1.68	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:C:569:ASN:CG	1:C:570:GLN:H	2.06	0.59
1:C:680:GLN:HG3	1:C:681:LYS:N	2.17	0.59
2:D:745:ILE:HD11	2:D:907:ASP:H	1.66	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:491:PRO:C	1:A:493:ILE:N	2.51	0.59
1:A:702:GLY:CA	1:A:728:PHE:CD1	2.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:LEU:HG	1:A:752:LEU:O	2.02	0.59
1:A:774:LEU:HG	1:A:788:PHE:CE1	2.38	0.59
1:A:790:LEU:HB3	1:A:791:PRO:CD	2.32	0.59
1:A:813:ASP:O	1:A:815:VAL:HG23	2.03	0.59
2:B:316:ALA:HB3	2:B:333:GLN:HB3	1.85	0.59
2:B:746:ILE:H	2:B:746:ILE:HD13	1.68	0.59
1:C:1013:MET:CE	1:C:1287:THR:HB	2.32	0.59
1:C:1450:PHE:HZ	1:C:1475:VAL:HB	1.66	0.59
1:C:355:ASN:N	1:C:355:ASN:HD22	2.01	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
2:D:922:LYS:HE3	2:D:1329:TYR:CZ	2.38	0.59
2:D:1505:ARG:NE	2:D:1623:LYS:HZ2	2.01	0.59
1:A:505:SER:HB3	1:A:510:ILE:CD1	2.32	0.59
1:A:720:LEU:HD13	1:A:724:CYS:HB3	1.83	0.59
2:B:961:THR:HG22	2:B:1327:THR:CG2	2.32	0.59
1:A:855:PHE:CA	2:B:904:LEU:HD11	2.31	0.59
1:A:78:LYS:HZ1	3:X:144:GLU:HA	1.65	0.59
1:A:1159:CYS:N	1:A:1160:PRO:CD	2.66	0.59
1:A:1352:PHE:HD2	1:A:1352:PHE:N	2.01	0.59
1:A:1493:PHE:HE1	1:A:1495:VAL:HG12	1.67	0.59
1:A:825:LEU:HG	1:A:826:GLU:N	2.18	0.59
1:A:257:ASN:HB2	1:A:848:TYR:CE2	2.37	0.59
1:C:1402:ILE:HG13	1:C:1479:ILE:HD11	1.84	0.59
1:C:182:ILE:HG12	1:C:804:ILE:CD1	2.25	0.59
2:D:103:TYR:CD2	2:D:120:LEU:HD13	2.37	0.59
2:D:309:LEU:HB3	2:D:338:ILE:HD12	1.85	0.59
2:D:476:ILE:CG2	2:D:497:ARG:HD3	2.33	0.59
1:A:322:TYR:CD2	1:A:322:TYR:N	2.70	0.58
1:A:544:TYR:C	1:A:544:TYR:CD2	2.76	0.58
1:A:644:ASN:CG	1:A:648:LEU:HD12	2.23	0.58
1:A:84:ILE:HD12	1:A:84:ILE:H	1.68	0.58
1:A:865:ILE:C	1:A:866:CYS:O	2.41	0.58
1:A:883:CYS:O	1:A:884:VAL:O	2.21	0.58
1:A:944:LEU:N	1:A:944:LEU:HD23	2.18	0.58
1:A:955:ARG:HH12	1:A:1352:PHE:HA	1.66	0.58
2:B:820:MET:HG3	2:B:821:PRO:HD2	1.85	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:C:154:PRO:O	1:C:155:ALA:HB3	2.03	0.58
1:C:267:ILE:HG22	1:C:268:THR:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:69:PHE:CD2	2:D:69:PHE:C	2.76	0.58
4:E:1:NAG:C3	4:E:2:NAG:O5	2.51	0.58
1:A:1065:SER:HB3	1:A:1106:TRP:CD2	2.38	0.58
1:A:863:GLU:H	1:A:863:GLU:CD	2.07	0.58
2:B:481:TYR:CE2	2:B:493:GLY:CA	2.86	0.58
2:B:476:ILE:HD11	2:B:524:TYR:CD2	2.37	0.58
1:C:172:ASP:OD2	1:C:1050:LYS:HD3	2.02	0.58
1:C:1110:ASN:N	1:C:1110:ASN:OD1	2.36	0.58
1:C:1229:LYS:NZ	1:C:1238:SER:OG	2.34	0.58
1:C:1451:THR:O	1:C:1452:ASP:CB	2.51	0.58
1:C:1562:LYS:HD3	1:C:1648:TRP:HE1	1.68	0.58
1:C:838:GLN:HA	1:C:901:LEU:CB	2.28	0.58
1:A:171:VAL:CG1	1:A:172:ASP:N	2.67	0.58
1:A:126:LEU:HD11	1:A:205:TYR:CE2	2.39	0.58
1:A:512:PHE:CD2	1:A:512:PHE:O	2.56	0.58
1:A:680:GLN:HG3	1:A:681:LYS:N	2.19	0.58
1:A:702:GLY:O	1:A:732:CYS:HB2	2.03	0.58
1:A:824:PHE:N	1:A:824:PHE:CD2	2.70	0.58
2:B:1532:GLU:O	2:B:1539:ILE:HD12	2.04	0.58
2:B:243:PHE:HE1	2:B:336:ILE:HG21	1.67	0.58
1:C:1076:THR:HG22	1:C:1120:GLU:OE2	2.02	0.58
1:C:1219:LYS:CD	1:C:1239:VAL:HG21	2.33	0.58
1:C:356:LEU:HG	1:C:452:TYR:CZ	2.38	0.58
1:C:623:VAL:HG12	1:C:624:PHE:N	2.18	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:D:606:ASP:O	2:D:606:ASP:OD1	2.21	0.58
3:X:166:ASP:CB	3:X:207:LEU:HD21	2.32	0.58
1:A:1572:ASN:O	1:A:1573:VAL:HG23	2.04	0.58
1:A:25:ILE:CD1	1:A:41:ILE:HB	2.33	0.58
1:A:950:TYR:CE2	1:A:1356:LEU:HD11	2.38	0.58
2:B:1563:TYR:HB3	2:B:1601:ILE:HD11	1.86	0.58
2:B:1593:THR:CG2	2:B:1594:LYS:N	2.67	0.58
2:B:183:PHE:CD2	2:B:183:PHE:N	2.70	0.58
2:B:45:ALA:HB3	2:B:81:MET:HE3	1.85	0.58
1:C:362:PHE:HE1	1:C:640:LEU:HB2	1.66	0.58
1:C:813:ASP:O	1:C:815:VAL:HG23	2.02	0.58
2:D:344:GLN:HB2	2:D:367:THR:O	2.03	0.58
2:D:829:GLN:HG2	2:D:885:VAL:CG1	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1011:GLU:HG3	1:A:1055:SER:OG	2.03	0.58
1:A:134:VAL:C	1:A:135:TYR:HD2	2.07	0.58
1:A:504:LEU:HD23	1:A:649:ALA:O	2.03	0.58
2:B:1391:LEU:HD12	2:B:1417:MET:HE1	1.84	0.58
1:A:412:ARG:HD2	2:B:458:ASP:OD1	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
2:D:887:LEU:CD2	2:D:1490:CYS:HB3	2.34	0.58
1:A:1152:ILE:HG22	1:A:1168:LEU:HD21	1.83	0.58
1:A:1549:LYS:HD3	1:A:1667:PHE:HB3	1.85	0.58
1:A:421:VAL:HG11	2:B:505:THR:HG22	1.86	0.58
1:A:784:LYS:HG2	1:A:785:GLN:N	2.18	0.58
1:A:902:PRO:O	1:A:903:LEU:HD13	2.02	0.58
1:A:907:LEU:HG	1:A:908:HIS:N	2.17	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
2:B:851:LEU:HD23	2:B:852:TYR:N	2.10	0.58
1:C:309:GLU:HG2	1:C:310:LEU:HD12	1.86	0.58
2:D:1491:ARG:HG3	2:D:1492:CYS:H	1.67	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
2:D:24:LEU:HB3	2:D:46:HIS:HB2	1.84	0.58
2:D:615:GLN:HB2	2:D:616:ASN:HD22	1.68	0.58
3:X:119:VAL:HG21	3:X:209:PHE:HB3	1.85	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
2:B:1500:LEU:CD1	2:B:1500:LEU:C	2.72	0.58
2:B:1528:LEU:HD13	2:B:1542:MET:HE2	1.84	0.58
2:B:1624:LEU:HG	2:B:1628:PHE:CE1	2.38	0.58
2:B:348:THR:HA	2:B:352:LYS:NZ	2.19	0.58
1:C:1019:PHE:HD2	1:C:1020:TYR:N	2.01	0.58
1:C:1065:SER:HB3	1:C:1106:TRP:CD2	2.39	0.58
1:C:1618:LEU:HD22	1:C:1619:ILE:H	1.67	0.58
1:C:163:PHE:CD2	1:C:188:PHE:CD1	2.91	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:854:GLN:NE2	1:C:854:GLN:H	2.02	0.58
1:A:1333:PHE:CD1	1:A:1334:LEU:HD13	2.39	0.58
1:A:132:LYS:NZ	1:A:139:GLN:HE22	2.01	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:A:788:PHE:HD2	1:A:788:PHE:N	2.02	0.58
2:B:1278:THR:HB	2:B:1314:THR:HB	1.84	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:581:ASP:O	2:B:582:LYS:C	2.42	0.58
2:B:599:TRP:HE3	2:B:599:TRP:HA	1.68	0.58
2:B:746:ILE:HD13	2:B:746:ILE:N	2.18	0.58
2:B:844:ILE:HG13	2:B:872:ILE:CG1	2.34	0.58
1:C:936:ARG:HH12	1:C:1284:PHE:HZ	1.50	0.58
1:C:1411:SER:N	1:C:1414:GLU:HG3	2.19	0.58
1:C:350:SER:OG	1:C:352:TYR:O	2.20	0.58
1:C:361:LEU:N	1:C:361:LEU:HD12	2.18	0.58
1:C:368:PRO:HG3	2:D:505:THR:HB	1.85	0.58
1:C:364:LYS:HE3	1:C:457:TYR:HD1	1.68	0.58
1:C:484:ILE:CD1	1:C:540:LEU:HD21	2.33	0.58
1:C:967:LEU:HD13	1:C:1365:VAL:CG2	2.34	0.58
2:D:71:THR:HG23	2:D:72:ARG:N	2.18	0.58
3:Y:106:VAL:HG22	3:Y:163:LYS:CE	2.33	0.58
1:A:1255:LEU:O	1:A:1255:LEU:HD12	2.03	0.58
1:A:1411:SER:N	1:A:1414:GLU:HG3	2.19	0.58
1:A:1493:PHE:HD1	1:A:1494:THR:H	1.48	0.58
1:A:1496:TYR:CD2	1:A:1496:TYR:N	2.71	0.58
1:A:1496:TYR:N	1:A:1496:TYR:HD2	2.02	0.58
1:A:342:ILE:HG22	1:A:343:PRO:HD2	1.86	0.58
1:A:350:SER:OG	1:A:352:TYR:O	2.20	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:C:1003:LEU:N	1:C:1003:LEU:HD23	2.19	0.58
1:C:161:LEU:HD11	1:C:185:PHE:CG	2.39	0.58
2:D:1528:LEU:HD13	2:D:1542:MET:HE2	1.86	0.58
2:D:283:ILE:HD12	2:D:283:ILE:N	2.18	0.58
1:A:1035:HIS:ND1	1:A:1035:HIS:N	2.52	0.58
1:A:1159:CYS:SG	1:A:1161:LEU:HD23	2.44	0.58
1:A:1408:TYR:CE2	1:A:1410:PRO:HA	2.39	0.58
1:A:1431:GLY:HA2	1:A:1483:PHE:CE1	2.39	0.58
1:A:824:PHE:HE2	1:A:846:TYR:HB2	1.69	0.58
1:A:927:LEU:HD23	1:A:928:ARG:N	2.19	0.58
2:B:239:GLY:H	2:B:296:ARG:NH2	2.02	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
1:C:1113:LEU:HD22	1:C:1114:ASP:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1271:ILE:HD13	1:C:1300:TYR:CZ	2.39	0.58
1:C:1536:GLN:HG3	1:C:1536:GLN:O	2.04	0.58
1:C:655:THR:O	1:C:656:ASN:C	2.42	0.58
1:C:720:LEU:HD13	1:C:724:CYS:HB3	1.84	0.58
2:D:460:LEU:O	2:D:460:LEU:HD23	2.04	0.58
2:D:844:ILE:HG13	2:D:872:ILE:CG1	2.34	0.58
2:D:36:ASP:OD1	2:D:90:PRO:HA	2.04	0.58
2:D:825:VAL:HG22	2:D:916:VAL:HG13	1.85	0.58
1:A:1053:MET:CE	1:A:1086:LEU:HD13	2.33	0.57
1:A:1159:CYS:O	1:A:1161:LEU:N	2.37	0.57
1:A:1468:PRO:HD3	1:A:1473:LEU:HD13	1.85	0.57
1:A:1541:LEU:HD21	1:A:1543:ILE:HD12	1.86	0.57
1:A:1560:ALA:HB2	1:A:1620:MET:CG	2.27	0.57
1:A:265:VAL:O	1:A:289:ASN:HA	2.04	0.57
1:A:599:TRP:CD1	1:A:779:LEU:HA	2.39	0.57
2:B:167:THR:HG22	2:B:171:ILE:O	2.03	0.57
2:B:36:ASP:OD1	2:B:90:PRO:HA	2.04	0.57
2:B:964:ILE:O	2:B:964:ILE:CG2	2.51	0.57
1:C:23:TYR:C	1:C:655:THR:HG21	2.24	0.57
1:C:585:GLY:O	1:C:789:ALA:HB1	2.04	0.57
1:C:680:GLN:O	1:C:684:GLU:HG3	2.04	0.57
2:D:362:LEU:HD13	2:D:411:ILE:HD12	1.86	0.57
2:D:508:LEU:HD12	2:D:509:HIS:N	2.18	0.57
4:G:1:NAG:C3	4:G:2:NAG:O5	2.51	0.57
3:Y:110:ILE:HG22	3:Y:111:ASP:O	2.04	0.57
1:A:1093:VAL:O	1:A:1093:VAL:HG12	2.03	0.57
1:A:489:LYS:CG	1:A:490:SER:H	2.15	0.57
2:B:1536:GLY:O	2:B:1567:ARG:HG2	2.04	0.57
2:B:449:ILE:HD13	2:B:462:VAL:HG23	1.85	0.57
1:C:1011:GLU:HG3	1:C:1055:SER:OG	2.04	0.57
1:C:55:SER:C	1:C:56:ILE:HD13	2.23	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
2:D:783:SER:HB2	2:D:787:TRP:CZ2	2.39	0.57
2:D:913:LEU:HD23	2:D:913:LEU:C	2.24	0.57
2:D:916:VAL:HG23	2:D:917:PRO:HD2	1.86	0.57
1:A:512:PHE:CE2	3:X:148:ALA:HB3	2.39	0.57
3:Y:185:LYS:HG2	3:Y:186:TYR:CE2	2.38	0.57
3:Y:194:LYS:NZ	3:Y:197:ASN:HB2	2.10	0.57
1:A:1145:THR:O	1:A:1149:VAL:HG23	2.04	0.57
1:A:190:ILE:HG22	1:A:191:PRO:CD	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:VAL:O	1:A:624:PHE:C	2.38	0.57
2:B:137:TYR:CE1	2:B:143:VAL:HG22	2.40	0.57
2:B:873:LYS:N	2:B:873:LYS:HD2	2.18	0.57
1:C:1053:MET:CE	1:C:1086:LEU:HD22	2.34	0.57
1:C:1159:CYS:SG	1:C:1161:LEU:HD23	2.45	0.57
1:C:1468:PRO:HD3	1:C:1473:LEU:HD13	1.86	0.57
1:C:1560:ALA:O	1:C:1561:TYR:HD2	1.86	0.57
1:C:488:PRO:HG3	1:C:499:TYR:OH	2.03	0.57
1:C:687:ALA:O	1:C:690:TYR:HB3	2.04	0.57
2:D:1279:ILE:CG2	2:D:1288:ILE:HB	2.35	0.57
2:D:1346:ASN:HB2	2:D:1368:CYS:HB2	1.86	0.57
3:Y:78:LYS:C	3:Y:78:LYS:HD2	2.25	0.57
2:B:963:ILE:CG1	2:B:1325:ILE:HG12	2.35	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
2:B:383:ALA:C	2:B:384:PHE:CD2	2.78	0.57
1:A:1162:VAL:N	1:C:1102:ASN:HD21	2.02	0.57
1:C:503:ILE:CB	1:C:511:HIS:HB2	2.34	0.57
2:D:519:ARG:CZ	2:D:608:GLY:HA3	2.34	0.57
3:X:111:ASP:CG	3:X:112:PRO:HD2	2.24	0.57
1:A:133:PRO:HD2	1:A:609:VAL:HG11	1.86	0.57
1:A:243:PHE:HE2	1:A:304:GLU:HA	1.70	0.57
1:A:455:ILE:HG22	1:A:456:ALA:N	2.20	0.57
1:A:532:GLN:HE21	1:A:568:GLY:HA2	1.69	0.57
1:A:822:ASP:HA	1:A:849:ARG:HD2	1.87	0.57
2:B:1349:VAL:HG22	2:B:1363:LEU:HD12	1.86	0.57
2:B:1498:SER:O	2:B:1573:LEU:HD23	2.04	0.57
2:B:963:ILE:HG13	2:B:1325:ILE:HG12	1.86	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:D:244:HIS:HB3	2:D:291:LYS:CD	2.28	0.57
2:D:443:ASN:OD1	2:D:469:ASN:HB3	2.05	0.57
2:D:789:VAL:HG23	2:D:806:TYR:O	2.04	0.57
3:X:125:LYS:HA	3:X:127:ASN:H	1.69	0.57
1:A:1075:SER:HB2	1:A:1120:GLU:OE1	2.04	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:A:481:HIS:HE1	1:A:529:PRO:HB3	1.64	0.57
1:A:742:ILE:HG21	1:A:753:HIS:HA	1.86	0.57
1:A:943:THR:OG1	1:A:1275:SER:OG	2.22	0.57
1:A:980:LYS:HD3	1:A:986:GLU:CA	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:519:ARG:CZ	2:B:608:GLY:HA3	2.34	0.57
1:C:126:LEU:HD11	1:C:205:TYR:CE2	2.39	0.57
1:C:489:LYS:C	1:C:491:PRO:HD3	2.24	0.57
1:C:358:ALA:H	1:C:672:ILE:CG2	2.18	0.57
2:D:199:ILE:HG22	2:D:199:ILE:O	2.05	0.57
1:A:111:PHE:CG	1:A:112:SER:N	2.73	0.57
1:A:1130:GLN:OE1	1:A:1232:LEU:HD22	2.03	0.57
1:A:196:TYR:CE1	1:A:221:GLU:HB2	2.40	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:493:ILE:HG23	1:A:495:LYS:N	2.18	0.57
2:B:168:PRO:HG3	2:B:197:TRP:N	2.20	0.57
1:C:1562:LYS:CD	1:C:1648:TRP:HE1	2.18	0.57
1:C:571:LEU:HD12	1:C:593:ALA:O	2.05	0.57
1:C:599:TRP:O	1:C:803:GLY:CA	2.49	0.57
1:C:457:TYR:CE2	1:C:641:ASN:HA	2.39	0.57
2:D:1371:TYR:CD1	2:D:1377:SER:HB3	2.40	0.57
2:D:556:ILE:H	2:D:556:ILE:CD1	2.14	0.57
2:D:961:THR:HG22	2:D:1327:THR:CG2	2.32	0.57
1:A:1268:ASN:N	1:A:1269:PRO:CD	2.67	0.57
1:A:1526:LYS:C	1:A:1529:GLU:HG3	2.24	0.57
1:A:1552:ALA:HB2	1:A:1620:MET:CE	2.34	0.57
1:A:359:THR:HG23	1:A:359:THR:O	2.03	0.57
1:A:779:LEU:C	1:A:779:LEU:HD12	2.25	0.57
1:A:977:LEU:HD22	1:A:978:SER:N	2.19	0.57
1:A:981:GLY:HA3	1:A:1333:PHE:HB2	1.85	0.57
2:B:484:LEU:HD11	2:B:626:LEU:CD1	2.34	0.57
2:B:825:VAL:HG22	2:B:916:VAL:HG13	1.86	0.57
1:C:23:TYR:O	1:C:655:THR:HB	2.04	0.57
1:C:443:PRO:HG2	1:C:446:ASN:HB2	1.85	0.57
1:C:788:PHE:HD2	1:C:788:PHE:N	2.03	0.57
1:C:805:SER:O	1:C:807:THR:N	2.38	0.57
2:D:1450:PHE:HD1	2:D:1451:ILE:H	1.53	0.57
2:D:1381:ILE:HG21	2:D:1459:TYR:CE1	2.37	0.57
2:D:218:LYS:HD3	2:D:822:TYR:HE2	1.67	0.57
3:X:101:GLN:HA	3:X:125:LYS:HB3	1.86	0.57
1:A:1221:ASN:HA	1:A:1222:PRO:C	2.23	0.57
1:A:492:TYR:CE2	1:A:493:ILE:HB	2.39	0.57
1:A:544:TYR:C	1:A:544:TYR:HD2	2.08	0.57
1:A:571:LEU:HD23	1:A:812:ALA:HB2	1.87	0.57
1:C:610:TYR:N	1:C:610:TYR:CD1	2.71	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:100:GLY:O	3:X:125:LYS:HG2	2.04	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
1:A:1239:VAL:HG12	1:A:1239:VAL:O	2.04	0.57
1:A:1429:PRO:HB2	1:A:1432:ILE:HG12	1.86	0.57
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
1:A:22:THR:HG22	1:A:23:TYR:CE1	2.40	0.57
1:C:163:PHE:CE2	1:C:188:PHE:CD1	2.93	0.57
2:D:1544:VAL:HB	2:D:1557:ARG:HA	1.87	0.57
2:D:243:PHE:CE1	2:D:336:ILE:HG21	2.40	0.57
2:D:383:ALA:C	2:D:384:PHE:CD2	2.78	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:1213:LYS:HE2	1:A:1266:TYR:HD2	1.69	0.56
1:A:1240:PRO:HB2	1:A:1242:THR:HG23	1.86	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:512:PHE:CD2	1:A:512:PHE:C	2.77	0.56
1:A:362:PHE:CE1	1:A:640:LEU:HB2	2.40	0.56
1:A:953:ILE:HD11	1:A:955:ARG:HH21	1.69	0.56
2:B:476:ILE:O	2:B:476:ILE:CG2	2.52	0.56
1:C:1527:CYS:O	1:C:1529:GLU:N	2.38	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:84:ILE:H	1:C:84:ILE:HD12	1.70	0.56
2:D:558:MET:O	2:D:561:ALA:CB	2.53	0.56
2:D:795:THR:HG22	2:D:796:PRO:CD	2.33	0.56
1:A:1271:ILE:O	1:A:1275:SER:HB3	2.05	0.56
1:A:920:LYS:HZ3	2:B:842:GLU:CD	2.08	0.56
1:A:982:LEU:C	1:A:984:VAL:H	2.09	0.56
2:B:1562:GLN:HE22	2:B:1596:LYS:HZ1	1.52	0.56
2:B:840:VAL:HG12	2:B:841:ASN:N	2.11	0.56
2:B:964:ILE:HG22	2:B:964:ILE:O	2.04	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:C:153:LYS:HB3	1:C:154:PRO:CD	2.34	0.56
1:C:571:LEU:HD23	1:C:812:ALA:HB2	1.86	0.56
1:C:938:SER:C	1:C:940:SER:N	2.58	0.56
2:D:1424:ILE:CD1	2:D:1424:ILE:H	2.17	0.56
2:D:1631:PHE:CD2	2:D:1632:SER:N	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:844:ILE:CD1	2:D:872:ILE:HD11	2.35	0.56
3:X:185:LYS:HG2	3:X:186:TYR:CE2	2.40	0.56
3:Y:75:PHE:O	3:Y:77:PRO:HD3	2.05	0.56
1:A:1117:SER:HA	1:A:1145:THR:OG1	2.05	0.56
1:A:309:GLU:HG2	1:A:310:LEU:N	2.21	0.56
1:A:309:GLU:HG2	1:A:310:LEU:HD12	1.86	0.56
1:A:550:GLN:HG2	1:A:550:GLN:O	2.04	0.56
2:B:843:ASP:HA	2:B:873:LYS:O	2.06	0.56
1:A:915:GLU:HB2	2:B:905:TRP:CZ2	2.40	0.56
2:B:916:VAL:HG23	2:B:917:PRO:HD2	1.86	0.56
1:C:473:HIS:O	1:C:473:HIS:HD2	1.88	0.56
1:C:511:HIS:CE1	3:Y:149:SER:CB	2.87	0.56
1:C:981:GLY:HA3	1:C:1333:PHE:HB2	1.85	0.56
2:D:1273:LEU:CB	2:D:1319:GLY:HA3	2.31	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:524:GLN:HB2	2:D:401:ASN:OD1	2.05	0.56
2:D:857:CYS:HB3	2:D:885:VAL:HG22	1.87	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
1:A:979:VAL:HG21	1:A:1326:TYR:CZ	2.36	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
1:C:1000:LEU:O	1:C:1001:THR:HG23	2.06	0.56
1:C:128:ILE:HD12	1:C:201:ILE:CG2	2.32	0.56
1:C:543:TYR:CD1	1:C:543:TYR:O	2.57	0.56
1:C:742:ILE:CG2	1:C:753:HIS:HA	2.34	0.56
2:D:1288:ILE:CD1	2:D:1303:VAL:HG21	2.36	0.56
3:X:47:HIS:O	3:X:51:SER:HB2	2.06	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:A:149:ASN:N	1:A:149:ASN:HD22	1.99	0.56
1:A:267:ILE:HG22	1:A:268:THR:N	2.21	0.56
1:A:680:GLN:O	1:A:684:GLU:HG3	2.04	0.56
1:A:587:THR:CG2	1:A:789:ALA:HB2	2.34	0.56
1:C:1352:PHE:HD2	1:C:1352:PHE:N	2.01	0.56
1:C:161:LEU:HD11	1:C:185:PHE:CE1	2.39	0.56
1:C:265:VAL:O	1:C:289:ASN:HA	2.05	0.56
1:C:395:ILE:O	1:C:395:ILE:HD12	2.05	0.56
1:C:512:PHE:HD2	1:C:512:PHE:O	1.89	0.56
1:C:695:VAL:CG1	1:C:724:CYS:HA	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:235:PHE:HB3	2:D:338:ILE:HG23	1.88	0.56
1:A:1548:ARG:C	1:A:1550:GLN:H	2.09	0.56
1:A:308:LYS:HG3	1:A:309:GLU:N	2.21	0.56
1:A:355:ASN:HD22	1:A:355:ASN:N	2.03	0.56
1:A:617:LYS:HB3	1:A:619:PRO:HD2	1.88	0.56
1:A:827:MET:SD	1:A:843:GLY:HA3	2.45	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
2:B:1562:GLN:NE2	2:B:1596:LYS:HZ2	2.03	0.56
2:B:913:LEU:C	2:B:913:LEU:HD23	2.26	0.56
1:C:1217:LEU:HD13	1:C:1237:SER:HA	1.88	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:D:183:PHE:CD2	2:D:183:PHE:N	2.72	0.56
2:D:39:GLU:OE1	2:D:488:LYS:HB3	2.06	0.56
2:D:435:TYR:OH	2:D:532:VAL:HG22	2.05	0.56
2:D:484:LEU:HD11	2:D:626:LEU:CD1	2.35	0.56
3:X:77:PRO:O	3:X:78:LYS:HB3	2.06	0.56
1:A:25:ILE:CB	1:A:655:THR:HG23	2.36	0.56
2:B:1509:PRO:O	2:B:1512:ILE:HG13	2.06	0.56
1:C:149:ASN:HD22	1:C:149:ASN:N	1.92	0.56
1:C:827:MET:SD	1:C:843:GLY:HA3	2.45	0.56
2:D:1510:LEU:HD21	2:D:1514:LYS:HZ1	1.70	0.56
2:D:494:ARG:CG	2:D:494:ARG:HH11	2.15	0.56
2:D:953:ARG:CZ	2:D:959:ILE:HD11	2.36	0.56
1:A:135:TYR:CD1	1:A:141:VAL:HG22	2.41	0.56
1:A:33:VAL:HG21	1:A:121:TYR:HE1	1.66	0.56
1:A:351:PRO:HG2	1:A:352:TYR:CE2	2.40	0.56
1:A:489:LYS:C	1:A:491:PRO:HD3	2.26	0.56
1:A:655:THR:O	1:A:656:ASN:C	2.43	0.56
1:A:788:PHE:N	1:A:788:PHE:CD2	2.73	0.56
1:A:42:GLN:CA	1:A:80:GLN:HG3	2.35	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:C:874:ASP:HA	1:C:878:THR:O	2.05	0.56
1:A:1110:ASN:OD1	1:A:1110:ASN:N	2.38	0.56
1:C:1323:LEU:CD1	1:C:1324:HIS:H	2.19	0.56
1:C:135:TYR:CD1	1:C:141:VAL:HG22	2.40	0.56
1:C:1585:TYR:CD1	1:C:1671:ILE:HG12	2.41	0.56
2:D:1384:ILE:HB	2:D:1423:VAL:HG12	1.87	0.56
2:D:167:THR:HG23	2:D:171:ILE:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:518:PHE:CD2	2:D:538:VAL:HB	2.38	0.56
2:D:599:TRP:HA	2:D:599:TRP:HE3	1.70	0.56
2:D:829:GLN:HA	2:D:885:VAL:HG12	1.88	0.56
3:X:110:ILE:HG22	3:X:111:ASP:O	2.05	0.56
1:A:43:VAL:HG11	1:A:73:LEU:CD1	2.36	0.56
1:A:59:TYR:CE2	1:A:99:VAL:HG21	2.41	0.56
1:A:59:TYR:CE1	1:A:60:PRO:HG3	2.41	0.56
2:B:1288:ILE:CD1	2:B:1303:VAL:HG21	2.36	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
2:B:520:PHE:O	2:B:535:SER:HA	2.06	0.56
1:C:1429:PRO:HB2	1:C:1432:ILE:HG12	1.86	0.56
1:C:1559:TYR:CD1	1:C:1561:TYR:HE2	2.23	0.56
1:C:24:VAL:HG21	1:C:554:LEU:HD11	1.88	0.56
1:C:774:LEU:HG	1:C:788:PHE:CE1	2.41	0.56
2:D:525:GLN:HA	2:D:530:GLU:O	2.05	0.56
2:D:599:TRP:CZ3	2:D:602:ILE:HD12	2.40	0.56
2:D:824:VAL:HG22	2:D:825:VAL:N	2.20	0.56
3:Y:127:ASN:OD1	3:Y:158:GLU:HB3	2.06	0.56
1:A:1095:GLN:O	1:A:1097:GLN:N	2.39	0.56
1:A:115:LYS:HB2	1:A:654:LEU:CD2	2.35	0.56
1:A:1450:PHE:HZ	1:A:1475:VAL:HB	1.70	0.56
1:A:1598:ILE:HG22	1:A:1599:THR:H	1.70	0.56
1:A:78:LYS:HG3	3:X:146:LEU:HB2	1.87	0.56
2:B:69:PHE:C	2:B:69:PHE:CD2	2.79	0.56
2:B:789:VAL:HG23	2:B:806:TYR:O	2.05	0.56
2:B:916:VAL:HG22	2:B:917:PRO:O	2.05	0.56
1:C:1128:LYS:C	1:C:1129:LEU:HD23	2.27	0.56
1:C:1559:TYR:CD1	1:C:1561:TYR:CE2	2.94	0.56
1:C:577:PRO:CD	1:C:588:VAL:HG23	2.36	0.56
2:D:422:ARG:HH12	3:Y:44:ARG:CA	2.18	0.56
2:D:826:LYS:NZ	2:D:1488:ASN:HB3	2.21	0.56
2:D:829:GLN:HE22	2:D:883:VAL:CG1	2.14	0.56
2:D:40:GLN:HG3	2:D:86:THR:HG23	1.88	0.56
2:D:885:VAL:HG23	2:D:885:VAL:O	2.06	0.56
1:A:1132:THR:O	1:A:1134:PRO:N	2.39	0.55
1:A:1585:TYR:CE1	1:A:1671:ILE:HG12	2.40	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
1:A:610:TYR:CD1	1:A:610:TYR:N	2.73	0.55
1:A:680:GLN:HB2	1:A:684:GLU:OE2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:VAL:CG1	1:A:724:CYS:HA	2.35	0.55
2:B:1284:ARG:CG	2:B:1285:GLU:N	2.69	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
2:B:34:ARG:HD2	2:B:488:LYS:NZ	2.21	0.55
1:C:126:LEU:HD11	1:C:205:TYR:CZ	2.41	0.55
1:C:617:LYS:HB3	1:C:619:PRO:HD2	1.88	0.55
1:C:693:SER:C	1:C:695:VAL:N	2.60	0.55
2:D:1280:GLU:HG2	2:D:1287:PRO:CB	2.33	0.55
2:D:1424:ILE:HG12	2:D:1426:TYR:HE2	1.70	0.55
2:D:1612:HIS:O	2:D:1613:GLU:C	2.44	0.55
2:D:355:LYS:O	2:D:358:MET:CB	2.54	0.55
2:D:595:GLN:O	2:D:598:ILE:HB	2.07	0.55
1:A:1219:LYS:CD	1:A:1239:VAL:HG21	2.36	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
2:B:1371:TYR:CD1	2:B:1377:SER:HB3	2.41	0.55
1:C:1108:VAL:HG21	1:C:1167:ALA:CB	2.34	0.55
1:C:1274:LEU:O	1:C:1277:GLU:N	2.37	0.55
1:C:351:PRO:HG3	1:C:442:LEU:HD11	1.88	0.55
2:D:1593:THR:CG2	2:D:1594:LYS:N	2.68	0.55
3:Y:58:SER:HB2	3:Y:125:LYS:HE3	1.87	0.55
3:Y:100:GLY:O	3:Y:125:LYS:HG2	2.05	0.55
3:Y:146:LEU:HD21	3:Y:148:ALA:HB2	1.88	0.55
1:A:1053:MET:CE	1:A:1086:LEU:HD22	2.37	0.55
1:A:1190:ILE:HG22	1:A:1191:SER:N	2.20	0.55
1:A:1453:TYR:O	1:A:1453:TYR:CG	2.59	0.55
1:A:198:MET:SD	1:A:218:GLU:HG3	2.45	0.55
2:B:355:LYS:O	2:B:358:MET:HB3	2.07	0.55
1:C:1083:LEU:HD13	1:C:1104:LEU:HD23	1.89	0.55
1:C:1527:CYS:C	1:C:1529:GLU:H	2.10	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:549:GLU:CD	1:C:550:GLN:N	2.60	0.55
1:C:644:ASN:CG	1:C:648:LEU:HD12	2.26	0.55
2:D:481:TYR:CE2	2:D:493:GLY:HA3	2.41	0.55
1:C:855:PHE:HA	2:D:904:LEU:HD11	1.87	0.55
3:Y:40:LEU:HD11	3:Y:209:PHE:CZ	2.41	0.55
3:Y:41:HIS:O	3:Y:42:ASP:CB	2.54	0.55
1:A:1232:LEU:HG	1:A:1233:GLN:N	2.21	0.55
1:A:428:VAL:HG22	1:A:429:THR:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:LYS:HE3	1:A:457:TYR:HD1	1.72	0.55
2:B:42:LEU:HD22	2:B:492:VAL:HG21	1.87	0.55
1:C:1130:GLN:OE1	1:C:1232:LEU:HD22	2.05	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
1:C:77:ASN:ND2	1:C:81:ASN:HB2	2.22	0.55
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:1056:ILE:O	1:A:1056:ILE:HG12	2.05	0.55
1:A:1180:LEU:HG	1:A:1208:ILE:HG12	1.89	0.55
1:A:153:LYS:HB3	1:A:154:PRO:CD	2.35	0.55
1:A:180:ILE:HG22	1:A:181:GLY:N	2.22	0.55
1:A:532:GLN:O	1:A:535:VAL:HG13	2.07	0.55
1:A:923:LEU:HD23	1:A:924:VAL:N	2.22	0.55
1:A:934:VAL:CG2	1:A:1366:HIS:CD2	2.88	0.55
2:B:130:ILE:HG12	2:B:147:VAL:HG23	1.87	0.55
2:B:1606:TRP:C	2:B:1606:TRP:HD1	2.10	0.55
2:B:51:PRO:O	2:B:52:LYS:HG3	2.06	0.55
2:B:558:MET:O	2:B:561:ALA:CB	2.55	0.55
1:C:1108:VAL:CG2	1:C:1167:ALA:HB2	2.36	0.55
1:C:1180:LEU:HG	1:C:1208:ILE:HG12	1.88	0.55
1:C:1287:THR:OG1	1:C:1288:GLN:N	2.39	0.55
1:C:504:LEU:HD21	1:C:651:LEU:HG	1.88	0.55
2:D:1562:GLN:HB2	2:D:1598:SER:HB3	1.88	0.55
2:D:343:TYR:HE1	2:D:420:LEU:HD11	1.72	0.55
2:D:512:PRO:HA	2:D:515:ILE:HD12	1.87	0.55
2:D:76:ASN:HB2	2:D:77:PRO:HD2	1.88	0.55
2:D:826:LYS:HG3	2:D:887:LEU:O	2.05	0.55
3:X:87:LEU:HA	3:X:91:LYS:CD	2.37	0.55
3:Y:146:LEU:HD22	3:Y:146:LEU:C	2.26	0.55
1:A:1228:TRP:N	1:A:1228:TRP:CE3	2.75	0.55
1:A:1272:LYS:O	1:A:1276:GLU:HG3	2.07	0.55
1:A:811:VAL:O	1:A:811:VAL:HG12	2.05	0.55
1:A:851:SER:O	1:A:890:GLY:HA2	2.07	0.55
2:B:233:LYS:HG3	2:B:233:LYS:O	2.05	0.55
2:B:365:TYR:HA	2:B:394:GLY:O	2.07	0.55
1:C:1453:TYR:O	1:C:1453:TYR:CG	2.59	0.55
1:C:1615:ARG:HD2	1:C:1647:TYR:HD1	1.71	0.55
1:C:24:VAL:HA	1:C:655:THR:HG21	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1591:LEU:C	2:D:1591:LEU:CD2	2.75	0.55
2:D:28:ILE:HD13	2:D:621:PHE:HE1	1.70	0.55
1:A:1188:LEU:HD23	1:A:1212:LEU:HA	1.89	0.55
2:B:1594:LYS:HA	2:B:1594:LYS:CE	2.18	0.55
2:B:276:ILE:O	2:B:277:PRO:C	2.45	0.55
1:C:1132:THR:O	1:C:1134:PRO:N	2.39	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:D:261:ALA:HB3	2:D:285:ILE:HD11	1.88	0.55
2:D:476:ILE:HG23	2:D:476:ILE:O	2.06	0.55
2:D:481:TYR:HE2	2:D:493:GLY:HA3	1.71	0.55
2:D:838:ASN:OD1	2:D:840:VAL:HG23	2.07	0.55
1:A:1344:ASP:OD1	1:A:1345:ASP:N	2.40	0.55
1:A:1571:GLU:O	1:A:1574:PHE:CD2	2.60	0.55
1:A:569:ASN:ND2	1:A:570:GLN:H	2.04	0.55
1:A:596:MET:H	1:A:782:ARG:NH1	1.92	0.55
1:A:834:VAL:O	1:A:837:GLU:HB2	2.07	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:A:906:GLY:O	1:A:908:HIS:NE2	2.40	0.55
2:B:862:LYS:HD2	2:B:1588:SER:OG	2.06	0.55
2:B:1591:LEU:C	2:B:1591:LEU:CD2	2.75	0.55
2:B:343:TYR:HE1	2:B:420:LEU:HD11	1.71	0.55
2:B:847:ARG:O	2:B:898:ALA:HA	2.07	0.55
2:B:928:VAL:HG23	2:B:1323:MET:HB3	1.87	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
1:C:1383:THR:HG21	1:C:1511:THR:HG22	1.88	0.55
1:C:510:ILE:HA	3:Y:150:ILE:HG13	1.87	0.55
1:C:539:ARG:HE	1:C:633:GLY:HA3	1.71	0.55
1:C:612:VAL:O	1:C:612:VAL:HG12	2.06	0.55
1:C:599:TRP:CD1	1:C:779:LEU:HA	2.41	0.55
1:C:824:PHE:N	1:C:824:PHE:CD2	2.69	0.55
2:D:1349:VAL:HG22	2:D:1363:LEU:HD12	1.88	0.55
2:D:1602:THR:H	2:D:1605:THR:HB	1.72	0.55
2:D:42:LEU:HD22	2:D:492:VAL:HG21	1.89	0.55
3:Y:134:THR:CG2	3:Y:153:PHE:HB3	2.37	0.55
1:A:1013:MET:HA	1:A:1016:VAL:HG23	1.88	0.55
1:A:614:ARG:C	1:A:614:ARG:HD2	2.24	0.55
2:B:243:PHE:CE1	2:B:336:ILE:HG21	2.42	0.55
2:B:285:ILE:CD1	2:B:285:ILE:N	2.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:443:ASN:OD1	2:B:469:ASN:HB3	2.06	0.55
2:B:447:VAL:O	2:B:447:VAL:HG13	2.06	0.55
2:B:923:SER:O	2:B:924:ILE:HD12	2.07	0.55
1:C:1218:VAL:CG1	1:C:1219:LYS:H	2.17	0.55
1:C:145:VAL:HB	1:C:183:ILE:CG1	2.34	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:199:TRP:CB	1:C:217:PHE:CE1	2.90	0.55
1:C:290:THR:O	1:C:291:MET:HB2	2.07	0.55
1:C:697:LYS:O	1:C:700:TYR:HB3	2.06	0.55
2:D:1381:ILE:HB	2:D:1459:TYR:CD1	2.42	0.55
2:D:184:TRP:HB2	2:D:185:PRO:CD	2.37	0.55
3:Y:107:GLN:OE1	3:Y:110:ILE:HD11	2.07	0.55
1:A:1474:CYS:HB3	1:A:1476:ARG:NH1	2.22	0.55
1:A:44:TYR:CZ	1:A:497:THR:HG21	2.41	0.55
1:A:773:TRP:HZ3	1:A:788:PHE:CE1	2.25	0.55
1:A:936:ARG:HH12	1:A:1284:PHE:HZ	1.53	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
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:1227:PHE:HB2	1:C:1251:THR:HG21	1.89	0.55
1:C:134:VAL:C	1:C:135:TYR:HD2	2.10	0.55
1:C:171:VAL:CG1	1:C:172:ASP:N	2.70	0.55
1:C:308:LYS:HG3	1:C:309:GLU:N	2.21	0.55
1:C:342:ILE:HG22	1:C:343:PRO:HD2	1.88	0.55
1:C:503:ILE:HD11	1:C:540:LEU:HD13	1.89	0.55
2:D:1530:ARG:HG3	2:D:1530:ARG:HH11	1.72	0.55
3:Y:50:TYR:HE2	3:Y:170:ARG:CZ	2.19	0.55
3:Y:87:LEU:HA	3:Y:91:LYS:CD	2.36	0.55
1:A:1554:LYS:HG3	1:A:1555:PRO:HD2	1.88	0.54
1:A:42:GLN:HE21	1:A:43:VAL:C	2.11	0.54
1:A:662:SER:O	1:A:663:GLN:HG2	2.07	0.54
2:B:126:SER:O	2:B:208:GLU:HG3	2.07	0.54
2:B:1522:TYR:N	2:B:1522:TYR:CD2	2.73	0.54
2:B:1633:TYR:CE1	2:B:1637:GLU:OE1	2.59	0.54
2:B:167:THR:HG23	2:B:171:ILE:N	2.23	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
1:C:1221:ASN:HA	1:C:1222:PRO:C	2.26	0.54
1:C:127:PHE:HE2	1:C:623:VAL:CG1	2.09	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1601:ILE:O	1:C:1638:PRO:O	2.25	0.54
1:C:231:ILE:O	1:C:231:ILE:HG23	2.06	0.54
1:C:505:SER:HB3	1:C:510:ILE:CD1	2.37	0.54
1:C:705:VAL:HA	1:C:739:ARG:NH2	2.21	0.54
1:C:587:THR:CG2	1:C:789:ALA:HB2	2.37	0.54
2:D:1536:GLY:O	2:D:1567:ARG:HG2	2.07	0.54
2:D:1506:ILE:CD1	2:D:1628:PHE:CE1	2.89	0.54
2:D:96:THR:HG21	2:D:102:GLN:OE1	2.06	0.54
3:Y:111:ASP:CG	3:Y:112:PRO:HD2	2.27	0.54
3:Y:47:HIS:O	3:Y:51:SER:HB2	2.07	0.54
1:A:1013:MET:HE2	1:A:1287:THR:HB	1.88	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:316:GLU:HG2	1:A:349:LEU:HD23	1.88	0.54
1:A:494:ASP:CG	1:A:495:LYS:HE2	2.28	0.54
1:A:694:VAL:O	1:A:697:LYS:HE2	2.06	0.54
1:A:824:PHE:CZ	1:A:846:TYR:HD1	2.26	0.54
1:A:854:GLN:NE2	1:A:854:GLN:H	2.05	0.54
1:A:871:PRO:CD	1:A:872:VAL:N	2.68	0.54
2:B:410:PRO:HA	2:B:431:THR:HG22	1.89	0.54
2:B:953:ARG:CZ	2:B:959:ILE:HD11	2.37	0.54
1:C:1562:LYS:O	1:C:1563:VAL:HG13	2.06	0.54
1:C:222:TYR:CD1	1:C:768:TYR:HB2	2.42	0.54
1:C:359:THR:HG23	1:C:359:THR:O	2.08	0.54
1:C:428:VAL:HG22	1:C:429:THR:H	1.72	0.54
1:C:549:GLU:CG	1:C:550:GLN:H	2.19	0.54
1:C:967:LEU:HD13	1:C:1365:VAL:HG22	1.89	0.54
1:A:1611:LEU:HD13	1:A:1617:TYR:CD1	2.43	0.54
1:A:1562:LYS:CD	1:A:1648:TRP:CZ2	2.86	0.54
1:A:472:ASN:O	1:A:473:HIS:HB3	2.07	0.54
1:A:656:ASN:CG	1:A:658:ASN:HB3	2.27	0.54
2:B:1593:THR:CG2	2:B:1594:LYS:H	2.20	0.54
2:B:218:LYS:HD3	2:B:822:TYR:HE2	1.72	0.54
1:C:1013:MET:HA	1:C:1016:VAL:HG23	1.90	0.54
1:C:1011:GLU:O	1:C:1014:SER:HB3	2.08	0.54
1:C:1117:SER:HA	1:C:1145:THR:OG1	2.07	0.54
1:C:1236:ASP:O	1:C:1238:SER:N	2.35	0.54
1:C:455:ILE:HG22	1:C:456:ALA:N	2.22	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
2:D:1387:LEU:HD21	2:D:1472:TYR:CE1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1486:ILE:HD11	2:D:1591:LEU:CD2	2.37	0.54
2:D:559:PRO:HG2	2:D:812:LYS:HD2	1.88	0.54
3:X:125:LYS:HA	3:X:126:ASN:C	2.25	0.54
3:X:46:LEU:HD12	3:X:180:TYR:CE1	2.43	0.54
3:Y:166:ASP:HB2	3:Y:207:LEU:HD21	1.89	0.54
1:A:1279:ARG:HD3	1:A:1280:TYR:N	2.22	0.54
1:A:1020:TYR:CE1	1:A:1295:GLU:HG3	2.39	0.54
1:A:126:LEU:HD11	1:A:205:TYR:CZ	2.43	0.54
1:A:25:ILE:HD13	1:A:41:ILE:CB	2.37	0.54
1:A:490:SER:N	1:A:491:PRO:CD	2.70	0.54
1:A:44:TYR:CB	1:A:545:ILE:HD12	2.38	0.54
2:B:954:VAL:HG23	2:B:1330:ASN:O	2.07	0.54
2:B:1443:LEU:N	2:B:1443:LEU:HD13	2.23	0.54
2:B:775:THR:HG22	2:B:776:MET:H	1.72	0.54
1:C:1569:THR:O	1:C:1570:VAL:HG23	2.07	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: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:680:GLN:HG3	1:C:681:LYS:H	1.72	0.54
1:C:779:LEU:HD12	1:C:780:VAL:N	2.22	0.54
2:D:1278:THR:HB	2:D:1314:THR:HB	1.90	0.54
2:D:503:LEU:C	2:D:503:LEU:HD23	2.28	0.54
2:D:775:THR:HG22	2:D:776:MET:H	1.71	0.54
1:A:1084:ARG:HD2	1:A:1154:LYS:HG3	1.90	0.54
1:A:1188:LEU:HD23	1:A:1212:LEU:HD13	1.88	0.54
1:A:1402:ILE:HG13	1:A:1479:ILE:HD13	1.89	0.54
1:A:705:VAL:HA	1:A:739:ARG:NH2	2.22	0.54
1:A:594:THR:O	1:A:782:ARG:HD2	2.07	0.54
1:A:989:SER:O	1:A:993:SER:CB	2.56	0.54
2:B:1274:ASN:OD1	2:B:1291:ARG:NH2	2.41	0.54
1:C:234:GLU:HB3	1:C:246:PHE:HE1	1.72	0.54
1:C:662:SER:O	1:C:663:GLN:HG2	2.07	0.54
1:C:895:LEU:HD12	1:C:896:VAL:N	2.22	0.54
2:D:1636:THR:HG22	2:D:1637:GLU:HG3	1.89	0.54
3:X:119:VAL:HG21	3:X:209:PHE:CB	2.38	0.54
1:A:100:SER:O	1:A:101:TYR:HB2	2.06	0.54
1:A:1133:LEU:HD12	1:A:1133:LEU:N	2.06	0.54
1:A:1440:LYS:O	1:A:1444:GLU:HG3	2.08	0.54
1:A:145:VAL:HB	1:A:183:ILE:CG1	2.33	0.54
1:A:903:LEU:N	1:A:903:LEU:HD22	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1288:ILE:HD13	2:B:1303:VAL:HG21	1.90	0.54
2:B:1638:PHE:O	2:B:1639:GLY:O	2.26	0.54
1:C:109:LYS:HD3	1:C:110:HIS:HE1	1.73	0.54
1:C:1084:ARG:HD2	1:C:1154:LYS:HG3	1.88	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:987:ILE:HD11	1:C:1294:ILE:HG23	1.90	0.54
1:C:155:ALA:O	1:C:157:ARG:N	2.40	0.54
1:C:309:GLU:HG2	1:C:310:LEU:N	2.22	0.54
1:C:515:ARG:HG3	1:C:526:ILE:CG2	2.38	0.54
1:C:680:GLN:HB2	1:C:684:GLU:OE2	2.07	0.54
1:C:594:THR:O	1:C:782:ARG:HD2	2.08	0.54
2:D:126:SER:O	2:D:208:GLU:HG3	2.08	0.54
1:A:1549:LYS:HD3	1:A:1667:PHE:CB	2.38	0.54
1:A:154:PRO:O	1:A:155:ALA:CB	2.55	0.54
1:A:199:TRP:CB	1:A:217:PHE:CE1	2.91	0.54
1:A:316:GLU:HG2	1:A:349:LEU:CD2	2.37	0.54
1:A:398:ASN:O	1:A:399:GLN:CB	2.56	0.54
1:A:847:ASN:ND2	1:A:853:MET:HB3	2.23	0.54
1:A:917:TRP:HA	1:A:917:TRP:CE3	2.43	0.54
2:B:1279:ILE:CG2	2:B:1288:ILE:HB	2.35	0.54
2:B:184:TRP:HB2	2:B:185:PRO:CD	2.37	0.54
2:B:861:THR:O	2:B:863:GLY:N	2.41	0.54
1:C:1082:ALA:O	1:C:1086:LEU:HD23	2.07	0.54
1:C:1112:GLN:HB2	1:C:1118:PHE:CE1	2.43	0.54
1:A:1102:ASN:HD21	1:C:1162:VAL:HG22	1.67	0.54
1:C:1278:GLN:NE2	1:C:1293:ALA:HB1	2.22	0.54
1:C:1020:TYR:CE1	1:C:1295:GLU:HG3	2.35	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:614:ARG:HD2	1:C:614:ARG:C	2.24	0.54
1:C:612:VAL:HG21	1:C:769:PHE:HZ	1.72	0.54
2:D:46:HIS:ND1	2:D:525:GLN:HG2	2.22	0.54
2:D:69:PHE:CE1	2:D:87:ILE:HA	2.43	0.54
2:D:861:THR:O	2:D:863:GLY:N	2.41	0.54
3:X:50:TYR:HE2	3:X:170:ARG:CZ	2.21	0.54
3:Y:86:LEU:HG	3:Y:91:LYS:HG3	1.88	0.54
1:A:1108:VAL:CG2	1:A:1167:ALA:HB2	2.38	0.54
1:A:641:ASN:OD1	1:A:644:ASN:HB2	2.08	0.54
1:A:771:GLU:HG3	1:A:772:SER:O	2.08	0.54
2:B:1611:PRO:HD3	2:B:1624:LEU:HD23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:ILE:HD13	2:B:621:PHE:HE1	1.72	0.54
2:B:941:GLN:HE21	2:B:943:GLU:HG2	1.71	0.54
1:C:1094:GLU:CD	1:C:1094:GLU:H	2.11	0.54
1:C:190:ILE:HD12	1:C:219:VAL:HG21	1.90	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:1509:PRO:O	2:D:1512:ILE:HG13	2.08	0.54
2:D:1562:GLN:HE22	2:D:1596:LYS:HZ2	1.53	0.54
2:D:168:PRO:HG3	2:D:197:TRP:N	2.21	0.54
2:D:595:GLN:OE1	2:D:595:GLN:HA	2.07	0.54
3:X:139:ASN:HD22	3:X:148:ALA:HB1	1.72	0.54
3:Y:163:LYS:HG3	3:Y:212:MET:SD	2.48	0.54
1:A:74:SER:HA	1:A:79:PHE:HE1	1.73	0.54
2:B:175:SER:N	2:B:1300:ALA:HB2	2.20	0.54
2:B:595:GLN:OE1	2:B:595:GLN:HA	2.06	0.54
1:C:1133:LEU:HB2	1:C:1134:PRO:HD3	1.90	0.54
1:C:1286:SER:OG	1:C:1287:THR:N	2.40	0.54
1:C:1548:ARG:C	1:C:1550:GLN:H	2.11	0.54
1:C:497:THR:OG1	1:C:498:HIS:N	2.38	0.54
1:C:753:HIS:O	1:C:754:MET:CB	2.52	0.54
1:C:907:LEU:HG	1:C:908:HIS:N	2.23	0.54
1:C:950:TYR:C	1:C:952:THR:H	2.11	0.54
2:D:57:PHE:HD1	2:D:59:HIS:NE2	2.05	0.54
3:Y:125:LYS:HA	3:Y:127:ASN:H	1.72	0.54
1:A:134:VAL:C	1:A:135:TYR:CD2	2.81	0.54
1:A:1629:TYR:CE1	1:A:1634:ARG:NH2	2.76	0.54
1:A:484:ILE:HG23	1:A:526:ILE:HG13	1.88	0.54
2:B:736:GLU:CD	2:B:737:ASP:H	2.11	0.54
2:B:826:LYS:HG3	2:B:887:LEU:O	2.08	0.54
1:C:430:VAL:HG11	1:C:453:ARG:NH2	2.17	0.54
1:C:44:TYR:CB	1:C:545:ILE:HD12	2.36	0.54
1:C:490:SER:N	1:C:491:PRO:CD	2.71	0.54
1:C:773:TRP:HZ3	1:C:788:PHE:CE1	2.25	0.54
1:C:796:THR:HA	1:C:818:LYS:HA	1.89	0.54
1:C:87:ILE:N	1:C:87:ILE:CD1	2.66	0.54
2:D:1415:ASN:O	2:D:1417:MET:HG3	2.08	0.54
2:D:528:ASN:OD1	2:D:528:ASN:N	2.41	0.54
2:D:585:TYR:CD2	2:D:788:VAL:HG11	2.42	0.54
2:D:820:MET:HG3	2:D:821:PRO:HD2	1.90	0.54
2:D:952:ASP:O	2:D:1331:ALA:HA	2.08	0.54
1:A:1150:ILE:CD1	1:A:1193:TYR:CD2	2.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1623:GLU:HB2	1:A:1638:PRO:CD	2.38	0.53
1:A:287:MET:HG2	1:A:299:VAL:HG21	1.89	0.53
2:B:243:PHE:CD1	2:B:314:LEU:HD23	2.41	0.53
2:B:87:ILE:H	2:B:87:ILE:HD12	1.73	0.53
1:C:1190:ILE:HG22	1:C:1191:SER:N	2.22	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
1:C:1421:HIS:CE1	1:C:1498:TYR:CD1	2.95	0.53
1:C:24:VAL:HG11	1:C:543:TYR:CZ	2.43	0.53
1:C:625:GLN:O	1:C:628:GLU:HB3	2.08	0.53
2:D:130:ILE:HG12	2:D:147:VAL:HG23	1.89	0.53
2:D:1593:THR:CG2	2:D:1594:LYS:H	2.21	0.53
2:D:476:ILE:HD11	2:D:524:TYR:CD2	2.43	0.53
4:E:1:NAG:H3	4:E:2:NAG:O5	2.07	0.53
2:D:1344:HIS:ND1	4:H:1:NAG:H82	2.23	0.53
1:A:149:ASN:O	1:A:151:ASP:N	2.40	0.53
1:A:1631:PHE:N	1:A:1631:PHE:CD2	2.74	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
2:B:384:PHE:HD1	2:B:400:LEU:HG	1.67	0.53
2:B:546:GLY:HA3	2:B:570:ASP:OD1	2.08	0.53
2:B:606:ASP:OD1	2:B:606:ASP:O	2.26	0.53
1:C:33:VAL:CG2	1:C:121:TYR:HD1	2.20	0.53
1:C:1304:VAL:CG1	1:C:1305:LYS:H	2.21	0.53
1:C:1548:ARG:HE	1:C:1550:GLN:NE2	2.07	0.53
1:C:222:TYR:HE2	1:C:224:LEU:CA	2.21	0.53
1:C:263:ALA:HB3	1:C:292:LEU:HB3	1.90	0.53
1:C:40:VAL:HG23	1:C:41:ILE:H	1.73	0.53
1:C:25:ILE:HD13	1:C:41:ILE:CB	2.36	0.53
1:C:980:LYS:HD3	1:C:986:GLU:CA	2.37	0.53
1:C:982:LEU:C	1:C:984:VAL:N	2.61	0.53
2:D:365:TYR:HA	2:D:394:GLY:O	2.08	0.53
2:D:437:THR:HG23	2:D:444:TYR:CD1	2.43	0.53
2:D:963:ILE:HG13	2:D:1325:ILE:HG12	1.90	0.53
3:X:107:GLN:HB3	3:X:116:LEU:HD22	1.90	0.53
1:A:24:VAL:O	1:A:24:VAL:HG12	2.08	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:1384:ILE:HB	2:B:1423:VAL:HG12	1.90	0.53
2:B:1522:TYR:N	2:B:1522:TYR:HD2	2.07	0.53
2:B:218:LYS:HD3	2:B:822:TYR:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1213:LYS:HE2	1:C:1266:TYR:CE2	2.43	0.53
2:D:1386:MET:CE	2:D:1386:MET:HA	2.38	0.53
2:D:1548:ILE:HG23	2:D:1635:LEU:CB	2.39	0.53
1:A:1218:VAL:CG1	1:A:1219:LYS:H	2.20	0.53
1:A:1320:LYS:CE	1:A:1321:GLY:H	2.21	0.53
2:B:236:TYR:CE1	2:B:424:ARG:HD2	2.43	0.53
2:B:481:TYR:C	2:B:481:TYR:CD2	2.82	0.53
2:B:563:MET:HA	2:B:563:MET:HE3	1.89	0.53
2:B:885:VAL:HG23	2:B:885:VAL:O	2.08	0.53
2:B:952:ASP:N	2:B:952:ASP:OD1	2.33	0.53
1:C:1370:THR:O	1:C:1371:SER:C	2.47	0.53
1:C:149:ASN:O	1:C:150:ASP:C	2.46	0.53
1:C:1581:LEU:HD12	1:C:1592:ALA:HB1	1.91	0.53
1:C:382:LEU:HD13	1:C:415:ASP:O	2.09	0.53
1:C:600:VAL:HA	1:C:802:VAL:O	2.08	0.53
1:C:884:VAL:HG12	1:C:885:ARG:N	2.23	0.53
1:C:917:TRP:CE3	1:C:917:TRP:HA	2.43	0.53
1:C:953:ILE:HD11	1:C:955:ARG:HH21	1.73	0.53
3:X:134:THR:CG2	3:X:153:PHE:HB3	2.38	0.53
3:Y:43:ILE:O	3:Y:44:ARG:C	2.45	0.53
1:A:1180:LEU:CD2	1:A:1208:ILE:HG12	2.38	0.53
1:A:24:VAL:N	1:A:655:THR:HG21	2.23	0.53
1:A:804:ILE:CG2	1:A:809:ILE:HG13	2.36	0.53
2:B:585:TYR:CD2	2:B:788:VAL:HG11	2.44	0.53
1:C:1204:GLN:HA	1:C:1204:GLN:OE1	2.09	0.53
1:C:1620:MET:CB	1:C:1644:TRP:CB	2.85	0.53
1:C:363:LEU:HD12	1:C:456:ALA:HA	1.90	0.53
1:C:493:ILE:HG22	1:C:493:ILE:O	2.08	0.53
1:C:523:TYR:CD1	2:D:359:PRO:HG2	2.43	0.53
1:C:554:LEU:H	1:C:658:ASN:ND2	2.06	0.53
1:C:790:LEU:HB3	1:C:791:PRO:CD	2.38	0.53
1:C:916:THR:C	1:C:918:PHE:H	2.11	0.53
2:D:1400:LEU:HD22	2:D:1406:ARG:HH12	1.73	0.53
2:D:1561:HIS:CD2	2:D:1597:ILE:HD13	2.43	0.53
2:D:1615:GLU:HB3	2:D:1621:PHE:CD1	2.43	0.53
2:D:851:LEU:HD23	2:D:852:TYR:N	2.13	0.53
3:X:217:ASN:HB2	3:X:220:ASP:OD2	2.08	0.53
1:A:1274:LEU:O	1:A:1277:GLU:N	2.42	0.53
1:A:128:ILE:CG2	1:A:145:VAL:HG22	2.28	0.53
1:A:1569:THR:O	1:A:1570:VAL:CG2	2.57	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
2:B:1504:GLU:CD	2:B:1504:GLU:H	2.11	0.53
2:B:24:LEU:HB3	2:B:46:HIS:HB2	1.91	0.53
1:C:123:ASN:O	1:C:211:THR:HG21	2.07	0.53
1:C:1320:LYS:HD2	1:C:1321:GLY:N	2.21	0.53
1:C:1619:ILE:HG12	1:C:1645:ILE:CD1	2.38	0.53
1:C:250:ILE:HD11	1:C:265:VAL:CG1	2.37	0.53
1:C:655:THR:OG1	1:C:656:ASN:N	2.41	0.53
1:C:720:LEU:HD11	1:C:724:CYS:SG	2.48	0.53
2:D:175:SER:N	2:D:1300:ALA:HB2	2.19	0.53
2:D:345:ILE:HD11	2:D:427:THR:N	2.23	0.53
3:Y:107:GLN:HB3	3:Y:116:LEU:HD22	1.90	0.53
1:A:115:LYS:HB3	1:A:654:LEU:HD21	1.91	0.53
1:C:1056:ILE:CD1	1:C:1066:TYR:HE2	2.22	0.53
1:C:1159:CYS:C	1:C:1161:LEU:H	2.11	0.53
1:C:1142:LEU:HD13	1:C:1187:THR:CG2	2.38	0.53
1:C:1381:ILE:O	1:C:1382:ASP:CB	2.55	0.53
1:C:1496:TYR:N	1:C:1496:TYR:HD2	2.06	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
1:C:955:ARG:HH12	1:C:1352:PHE:HA	1.74	0.53
2:D:954:VAL:HG23	2:D:1330:ASN:O	2.08	0.53
2:D:1593:THR:HB	2:D:1596:LYS:O	2.09	0.53
2:D:204:GLU:O	2:D:205:HIS:HB2	2.08	0.53
2:D:266:GLY:HA2	2:D:276:ILE:HG13	1.90	0.53
2:D:129:PHE:CE2	2:D:598:ILE:HG23	2.44	0.53
2:D:745:ILE:CG2	2:D:897:LYS:HD3	2.39	0.53
3:Y:170:ARG:HD3	3:Y:203:LEU:CD2	2.38	0.53
1:A:1451:THR:O	1:A:1452:ASP:HB3	2.07	0.53
1:A:1615:ARG:NH1	1:A:1647:TYR:CE1	2.77	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
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:B:469:ASN:ND2	2:B:472:SER:H	2.06	0.53
2:B:46:HIS:ND1	2:B:525:GLN:HG2	2.24	0.53
2:B:824:VAL:HG22	2:B:825:VAL:N	2.24	0.53
1:C:1159:CYS:N	1:C:1160:PRO:CD	2.72	0.53
1:C:1228:TRP:N	1:C:1228:TRP:CE3	2.77	0.53
1:C:23:TYR:O	1:C:655:THR:CB	2.56	0.53
1:C:461:SER:C	1:C:463:SER:H	2.12	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
1:C:949:ILE:HG22	1:C:950:TYR:CZ	2.44	0.53
2:D:353:TYR:HA	2:D:433:ILE:O	2.09	0.53
2:D:523:TYR:HD2	2:D:621:PHE:HZ	1.54	0.53
2:D:622:GLU:OE2	2:D:637:LYS:HD3	2.09	0.53
2:D:745:ILE:HG13	2:D:906:SER:HB2	1.90	0.53
3:Y:194:LYS:NZ	3:Y:197:ASN:HD22	2.06	0.53
1:A:1204:GLN:OE1	1:A:1204:GLN:HA	2.09	0.53
1:A:968:VAL:HG22	1:A:1366:HIS:O	2.08	0.53
1:A:1454:GLN:HG3	1:A:1461:ILE:HB	1.90	0.53
1:A:149:ASN:O	1:A:150:ASP:C	2.47	0.53
1:A:702:GLY:HA2	1:A:728:PHE:HE1	1.70	0.53
1:A:979:VAL:HG11	1:A:1326:TYR:HE1	1.73	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
2:B:618:LEU:HD22	2:B:636:THR:HA	1.89	0.53
2:B:622:GLU:OE2	2:B:637:LYS:HD3	2.09	0.53
1:C:1626:GLN:HB2	1:C:1635:TYR:CD1	2.40	0.53
1:C:569:ASN:CG	1:C:570:GLN:N	2.62	0.53
1:C:694:VAL:O	1:C:697:LYS:HE2	2.09	0.53
1:C:771:GLU:HG3	1:C:772:SER:O	2.09	0.53
1:C:824:PHE:CZ	1:C:846:TYR:HD1	2.27	0.53
2:D:1480:LEU:HD12	2:D:1480:LEU:C	2.28	0.53
2:D:285:ILE:CD1	2:D:285:ILE:N	2.67	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:A:1066:TYR:H	1:A:1079:THR:CG2	2.19	0.53
1:A:1242:THR:OG1	1:A:1243:GLY:N	2.42	0.53
1:A:1559:TYR:CD1	1:A:1561:TYR:HE2	2.27	0.53
1:A:363:LEU:HD12	1:A:456:ALA:HA	1.90	0.53
1:A:612:VAL:HG21	1:A:769:PHE:HZ	1.71	0.53
1:A:655:THR:OG1	1:A:656:ASN:N	2.41	0.53
1:A:599:TRP:NE1	1:A:779:LEU:HA	2.24	0.53
2:B:1281:LEU:HB2	2:B:1283:ASP:HB2	1.89	0.53
2:B:175:SER:O	2:B:1299:LEU:HD12	2.09	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
2:B:512:PRO:HA	2:B:515:ILE:HD12	1.90	0.53
1:C:1035:HIS:N	1:C:1035:HIS:ND1	2.56	0.53
1:C:111:PHE:HE2	1:C:113:LYS:CB	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1534:GLN:HG3	2:D:1535:ASP:OD2	2.09	0.53
2:D:456:PRO:HG3	2:D:515:ILE:HD11	1.91	0.53
3:X:166:ASP:HB2	3:X:207:LEU:HD21	1.90	0.53
1:A:1097:GLN:HG3	1:A:1158:ILE:HG22	1.90	0.52
1:A:1112:GLN:NE2	1:A:1171:ALA:HB2	2.24	0.52
1:A:1226:ARG:CZ	1:A:1266:TYR:CE1	2.92	0.52
1:A:967:LEU:HD13	1:A:1365:VAL:CG2	2.39	0.52
1:A:689:LYS:HG2	1:A:699:CYS:SG	2.48	0.52
1:A:687:ALA:O	1:A:690:TYR:HB3	2.08	0.52
1:A:720:LEU:HD11	1:A:724:CYS:SG	2.49	0.52
1:A:804:ILE:HG22	1:A:809:ILE:CG1	2.37	0.52
2:B:1530:ARG:HH11	2:B:1530:ARG:HG3	1.74	0.52
2:B:1593:THR:HB	2:B:1596:LYS:O	2.09	0.52
2:B:1602:THR:C	2:B:1604:ASN:N	2.63	0.52
2:B:229:GLN:OE1	2:B:229:GLN:HA	2.09	0.52
2:B:357:GLY:HA3	2:B:404:LEU:HD12	1.91	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:C:1097:GLN:HG3	1:C:1158:ILE:HG22	1.90	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:C:576:SER:CB	1:C:589:SER:H	2.22	0.52
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:906:GLY:O	1:C:908:HIS:NE2	2.42	0.52
2:D:736:GLU:CD	2:D:737:ASP:H	2.13	0.52
2:D:941:GLN:HE21	2:D:943:GLU:HG2	1.74	0.52
3:Y:129:THR:HG22	3:Y:129:THR:O	2.09	0.52
1:A:1152:ILE:HG21	1:A:1168:LEU:CD2	2.39	0.52
1:A:680:GLN:HG3	1:A:681:LYS:H	1.75	0.52
1:A:920:LYS:NZ	2:B:842:GLU:CD	2.63	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
1:C:1232:LEU:HG	1:C:1233:GLN:N	2.24	0.52
1:C:176:GLU:HB2	1:C:185:PHE:CE1	2.43	0.52
1:C:541:LEU:HD23	1:C:541:LEU:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:610:TYR:N	1:C:610:TYR:HD1	2.06	0.52
1:C:702:GLY:HA2	1:C:728:PHE:HE1	1.67	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
2:D:469:ASN:ND2	2:D:472:SER:H	2.07	0.52
2:D:481:TYR:CD2	2:D:481:TYR:O	2.52	0.52
3:Y:217:ASN:HB2	3:Y:220:ASP:OD2	2.10	0.52
3:Y:61:SER:O	3:Y:75:PHE:CZ	2.61	0.52
1:A:1082:ALA:O	1:A:1086:LEU:HD23	2.09	0.52
1:A:1076:THR:HG22	1:A:1120:GLU:HA	1.90	0.52
1:A:1381:ILE:O	1:A:1382:ASP:CB	2.57	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
2:B:929:LYS:NZ	2:B:1322:THR:OG1	2.43	0.52
2:B:476:ILE:O	2:B:476:ILE:HG23	2.08	0.52
1:C:1093:VAL:O	1:C:1093:VAL:HG12	2.08	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: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: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:C:989:SER:O	1:C:993:SER:CB	2.57	0.52
2:D:1522:TYR:CD2	2:D:1522:TYR:N	2.76	0.52
2:D:1529:LEU:O	2:D:1577:VAL:HG13	2.10	0.52
3:X:43:ILE:HG23	3:X:44:ARG:N	2.25	0.52
1:A:1559:TYR:CD1	1:A:1561:TYR:CE2	2.97	0.52
1:A:577:PRO:CD	1:A:588:VAL:HG23	2.39	0.52
1:A:641:ASN:O	1:A:642:ASN:C	2.47	0.52
1:A:753:HIS:O	1:A:754:MET:CB	2.49	0.52
2:B:1595:ASP:OD1	2:B:1595:ASP:N	2.40	0.52
1:C:1130:GLN:NE2	1:C:1230:ASP:HB3	2.25	0.52
1:C:1013:MET:HE3	1:C:1287:THR:HB	1.89	0.52
1:C:1641:SER:O	1:C:1642:LEU:HB2	2.10	0.52
1:C:190:ILE:HG22	1:C:191:PRO:CD	2.39	0.52
1:C:238:ILE:HG23	1:C:242:ASN:HD22	1.75	0.52
1:C:577:PRO:HD2	1:C:588:VAL:HG23	1.92	0.52
1:C:59:TYR:CE1	1:C:60:PRO:HG3	2.44	0.52
1:C:645:VAL:HG12	1:C:646:PHE:N	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1284:ARG:CG	2:D:1285:GLU:N	2.72	0.52
2:D:963:ILE:CG1	2:D:1325:ILE:HG12	2.40	0.52
2:D:316:ALA:HB3	2:D:333:GLN:HB3	1.90	0.52
2:D:598:ILE:HD12	2:D:800:ILE:HG21	1.92	0.52
3:X:87:LEU:HD12	3:X:210:GLU:HA	1.91	0.52
1:A:1287:THR:OG1	1:A:1288:GLN:N	2.40	0.52
1:A:222:TYR:HE2	1:A:224:LEU:CA	2.22	0.52
1:A:239:GLY:O	1:A:241:LYS:N	2.43	0.52
1:A:512:PHE:HD2	1:A:512:PHE:O	1.93	0.52
1:A:837:GLU:O	1:A:901:LEU:HB2	2.10	0.52
2:B:528:ASN:N	2:B:528:ASN:OD1	2.41	0.52
2:B:57:PHE:HD1	2:B:59:HIS:NE2	2.07	0.52
2:B:870:PHE:CD1	2:B:878:ARG:NH2	2.78	0.52
1:C:1279:ARG:HD3	1:C:1280:TYR:N	2.25	0.52
1:C:979:VAL:HG11	1:C:1326:TYR:HE1	1.74	0.52
1:C:25:ILE:HB	1:C:654:LEU:HB2	1.90	0.52
1:C:396:ASP:HB3	1:C:398:ASN:H	1.74	0.52
1:C:702:GLY:HA3	1:C:728:PHE:CD1	2.45	0.52
1:C:599:TRP:NE1	1:C:779:LEU:HA	2.25	0.52
1:C:993:SER:C	1:C:995:GLU:N	2.59	0.52
2:D:1292:ILE:HD12	2:D:1296:ASN:OD1	2.10	0.52
2:D:144:LEU:HD23	2:D:144:LEU:N	2.25	0.52
2:D:343:TYR:CE1	2:D:420:LEU:HD11	2.45	0.52
1:C:421:VAL:HG23	2:D:507:ASN:ND2	2.24	0.52
2:D:966:GLN:HG3	2:D:966:GLN:O	2.09	0.52
3:X:139:ASN:HD22	3:X:148:ALA:CB	2.22	0.52
1:A:1532:CYS:O	1:A:1641:SER:N	2.43	0.52
1:A:161:LEU:HD11	1:A:185:PHE:CZ	2.45	0.52
1:A:610:TYR:HD1	1:A:610:TYR:N	2.08	0.52
2:B:1280:GLU:HB2	2:B:1312:THR:HB	1.91	0.52
2:B:1622:GLN:O	2:B:1625:CYS:HB2	2.10	0.52
2:B:437:THR:HG23	2:B:444:TYR:CD1	2.45	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
1:C:500:ASN:O	1:C:542:VAL:HG13	2.09	0.52
1:C:544:TYR:C	1:C:544:TYR:CD2	2.83	0.52
1:C:934:VAL:CG1	1:C:935:LYS:N	2.73	0.52
2:D:175:SER:O	2:D:1299:LEU:HD12	2.09	0.52
2:D:351:PRO:N	2:D:611:ALA:HB3	2.24	0.52
2:D:481:TYR:C	2:D:481:TYR:HD2	2.12	0.52
2:D:484:LEU:HD11	2:D:626:LEU:HG	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1019:PHE:HD2	1:A:1020:TYR:N	2.07	0.52
1:A:111:PHE:HE2	1:A:113:LYS:CB	2.23	0.52
1:A:1247:MET:O	1:A:1251:THR:HG23	2.10	0.52
1:A:1527:CYS:O	1:A:1528:VAL:C	2.48	0.52
1:A:161:LEU:HD11	1:A:185:PHE:CD2	2.44	0.52
1:A:24:VAL:CA	1:A:655:THR:HG21	2.40	0.52
1:A:396:ASP:HB3	1:A:398:ASN:HB2	1.92	0.52
1:A:543:TYR:CD1	1:A:543:TYR:C	2.81	0.52
1:A:934:VAL:CG1	1:A:935:LYS:N	2.73	0.52
2:B:1280:GLU:HG2	2:B:1287:PRO:CB	2.38	0.52
1:C:1496:TYR:N	1:C:1496:TYR:CD2	2.75	0.52
1:C:165:ASP:C	1:C:167:GLU:H	2.12	0.52
2:D:929:LYS:NZ	2:D:1322:THR:OG1	2.42	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
3:X:150:ILE:C	3:X:150:ILE:HD12	2.30	0.52
3:X:119:VAL:O	3:X:163:LYS:HD2	2.10	0.52
1:A:1161:LEU:HA	1:C:1102:ASN:ND2	2.21	0.52
1:A:1265:ASN:C	1:A:1267:VAL:H	2.12	0.52
1:A:135:TYR:CE1	1:A:141:VAL:HG22	2.44	0.52
1:A:190:ILE:HD12	1:A:219:VAL:HG21	1.92	0.52
1:A:32:ARG:O	1:A:35:ALA:HB3	2.09	0.52
1:A:377:ASP:OD2	1:A:379:LEU:HB2	2.10	0.52
2:B:216:VAL:O	2:B:216:VAL:CG1	2.57	0.52
2:B:452:THR:O	2:B:453:GLU:O	2.28	0.52
2:B:523:TYR:HD1	2:B:523:TYR:C	2.12	0.52
2:B:941:GLN:HE21	2:B:943:GLU:CG	2.22	0.52
1:C:1033:ILE:HG23	1:C:1034:PHE:N	2.24	0.52
1:C:171:VAL:CG1	1:C:1054:LEU:HD11	2.40	0.52
1:A:1163:LYS:HE3	1:C:1109:GLU:HG2	1.92	0.52
1:C:135:TYR:CE1	1:C:141:VAL:HG22	2.45	0.52
1:C:274:ASP:HA	1:C:322:TYR:CD2	2.45	0.52
2:D:1602:THR:C	2:D:1604:ASN:N	2.63	0.52
2:D:965:ILE:HG13	2:D:1301:ARG:CB	2.31	0.52
3:Y:103:VAL:HG22	3:Y:122:VAL:HG22	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
1:C:825:LEU:HG	1:C:826:GLU:N	2.25	0.52
1:C:968:VAL:HG22	1:C:1366:HIS:O	2.10	0.52
2:D:1500:LEU:HD12	2:D:1501:ASN:N	2.20	0.52
2:D:1539:ILE:HG23	2:D:1564:ILE:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:433:ILE:CG2	2:D:434:ALA:N	2.72	0.52
2:D:800:ILE:HG23	2:D:801:CYS:N	2.24	0.52
2:D:887:LEU:HD23	2:D:1490:CYS:HB3	1.91	0.52
3:X:103:VAL:HG22	3:X:122:VAL:HG22	1.91	0.52
3:Y:119:VAL:O	3:Y:163:LYS:HD2	2.10	0.52
3:Y:61:SER:O	3:Y:75:PHE:HZ	1.92	0.52
1:A:645:VAL:HG12	1:A:646:PHE:N	2.24	0.52
1:A:113:LYS:HE2	1:A:654:LEU:O	2.10	0.52
1:A:222:TYR:CD1	1:A:768:TYR:HB2	2.42	0.52
2:B:1503:GLN:NE2	2:B:1506:ILE:HG12	2.25	0.52
2:B:1593:THR:HG22	2:B:1594:LYS:H	1.73	0.52
2:B:283:ILE:N	2:B:283:ILE:HD12	2.25	0.52
2:B:437:THR:HG21	2:B:443:ASN:N	2.25	0.52
1:C:1098:ASN:O	1:C:1101:CYS:HB2	2.10	0.52
1:C:120:THR:HG22	1:C:121:TYR:N	2.24	0.52
1:C:1408:TYR:CE2	1:C:1410:PRO:HA	2.44	0.52
1:C:1431:GLY:HA2	1:C:1483:PHE:CE1	2.45	0.52
1:C:180:ILE:CB	1:C:599:TRP:CE3	2.93	0.52
2:D:1530:ARG:NH1	2:D:1530:ARG:HG3	2.25	0.52
2:D:558:MET:O	2:D:561:ALA:HB3	2.10	0.52
3:X:86:LEU:HG	3:X:91:LYS:HG3	1.92	0.52
1:A:1021:VAL:HG12	1:A:1022:PHE:N	2.26	0.51
1:A:1199:ASP:C	1:A:1201:THR:H	2.13	0.51
1:A:1013:MET:HE3	1:A:1287:THR:HB	1.91	0.51
1:A:1298:THR:O	1:A:1299:GLU:C	2.49	0.51
1:A:1385:ASP:O	1:A:1386:ILE:HB	2.09	0.51
1:A:1581:LEU:HD12	1:A:1592:ALA:HB1	1.90	0.51
1:A:1612:VAL:HG23	1:A:1617:TYR:OH	2.10	0.51
1:A:1640:ASP:O	1:A:1643:THR:HB	2.11	0.51
1:A:234:GLU:HB3	1:A:246:PHE:HE1	1.74	0.51
2:B:1351:ASN:O	2:B:1352:ILE:HG12	2.09	0.51
2:B:1381:ILE:HB	2:B:1459:TYR:CD1	2.44	0.51
1:C:1226:ARG:NE	1:C:1266:TYR:HE1	2.08	0.51
1:C:1385:ASP:O	1:C:1386:ILE:HB	2.09	0.51
1:C:1559:TYR:HH	1:C:1591:VAL:HA	1.74	0.51
1:C:219:VAL:O	1:C:219:VAL:HG12	2.10	0.51
1:C:40:VAL:CG2	1:C:41:ILE:N	2.73	0.51
1:C:436:LYS:HB2	1:C:449:ARG:CG	2.41	0.51
1:C:914:LEU:HD11	1:C:916:THR:HG22	1.92	0.51
1:C:950:TYR:CE2	1:C:1356:LEU:HD11	2.46	0.51
2:D:1595:ASP:OD1	2:D:1595:ASP:N	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:216:VAL:CG1	2:D:216:VAL:O	2.58	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
2:D:519:ARG:NH1	2:D:606:ASP:OD2	2.44	0.51
2:D:756:LEU:HD12	2:D:758:LEU:HG	1.92	0.51
1:C:78:LYS:HZ1	3:Y:144:GLU:HA	1.70	0.51
3:Y:43:ILE:HG23	3:Y:44:ARG:N	2.23	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:976:ILE:HB	1:A:1362:THR:HG22	1.92	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
1:A:949:ILE:HG22	1:A:949:ILE:O	2.09	0.51
2:B:1275:LEU:HD21	2:B:1319:GLY:O	2.10	0.51
2:B:948:ARG:NH2	2:B:948:ARG:HB2	2.23	0.51
1:C:1227:PHE:CD1	1:C:1227:PHE:C	2.84	0.51
1:C:287:MET:HG2	1:C:299:VAL:HG21	1.92	0.51
1:C:472:ASN:O	1:C:473:HIS:CB	2.57	0.51
1:C:525:SER:H	2:D:401:ASN:ND2	2.06	0.51
2:D:1466:GLU:HA	2:D:1466:GLU:OE1	2.10	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:D:87:ILE:HD12	2:D:87:ILE:H	1.75	0.51
3:Y:187:GLY:C	3:Y:203:LEU:HD12	2.31	0.51
3:Y:77:PRO:O	3:Y:78:LYS:HB3	2.10	0.51
1:A:148:LEU:HG	1:A:153:LYS:O	2.10	0.51
1:A:1560:ALA:O	1:A:1561:TYR:HD2	1.92	0.51
1:A:351:PRO:HG3	1:A:442:LEU:HD11	1.92	0.51
1:A:365:PRO:HG2	1:A:464:TYR:CE2	2.46	0.51
1:A:693:SER:C	1:A:695:VAL:N	2.63	0.51
1:A:698:CYS:HB3	1:A:728:PHE:HB2	1.92	0.51
1:A:985:GLY:O	1:A:986:GLU:C	2.49	0.51
2:B:1390:PHE:CD1	2:B:1442:ILE:HG13	2.44	0.51
2:B:188:LEU:HD13	2:B:216:VAL:HG21	1.93	0.51
2:B:745:ILE:HG13	2:B:906:SER:HB2	1.91	0.51
2:B:745:ILE:CG2	2:B:897:LYS:HD3	2.40	0.51
1:C:1017:PRO:O	1:C:1018:VAL:C	2.48	0.51
1:C:1279:ARG:NH1	1:C:1280:TYR:CD2	2.78	0.51
1:C:161:LEU:HD11	1:C:185:PHE:CD2	2.45	0.51
1:C:465:LEU:HD11	1:C:486:VAL:HG13	1.93	0.51
1:C:689:LYS:HG2	1:C:699:CYS:SG	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:HIS:C	1:C:72:HIS:CD2	2.83	0.51
2:D:946:LYS:HA	2:D:1310:ASP:OD1	2.10	0.51
2:D:1581:TYR:HD1	2:D:1608:GLU:O	1.93	0.51
2:D:239:GLY:N	2:D:296:ARG:NH2	2.59	0.51
2:D:276:ILE:O	2:D:277:PRO:C	2.47	0.51
3:X:146:LEU:C	3:X:146:LEU:HD22	2.31	0.51
3:Y:119:VAL:HG21	3:Y:209:PHE:HB3	1.92	0.51
1:A:1188:LEU:HD23	1:A:1212:LEU:CD1	2.41	0.51
1:A:936:ARG:NH2	1:A:1284:PHE:HE1	2.08	0.51
1:A:154:PRO:O	1:A:155:ALA:HB3	2.10	0.51
1:A:274:ASP:CG	1:A:275:LEU:H	2.14	0.51
2:B:58:VAL:HG12	2:B:104:VAL:CG2	2.40	0.51
2:B:1343:PHE:CD1	2:B:1458:VAL:HG11	2.46	0.51
2:B:1514:LYS:O	2:B:1517:GLU:HB2	2.09	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
2:B:952:ASP:O	2:B:1331:ALA:HA	2.10	0.51
1:C:1229:LYS:HZ3	1:C:1240:PRO:HD2	1.74	0.51
1:C:698:CYS:C	1:C:700:TYR:N	2.62	0.51
2:D:1274:ASN:OD1	2:D:1291:ARG:NH2	2.42	0.51
2:D:1381:ILE:CG2	2:D:1459:TYR:CE1	2.93	0.51
2:D:1438:LEU:O	2:D:1438:LEU:HD13	2.11	0.51
2:D:342:PRO:HG2	2:D:420:LEU:CD1	2.41	0.51
2:D:746:ILE:N	2:D:746:ILE:HD13	2.25	0.51
2:D:89:ILE:HD11	2:D:104:VAL:HG11	1.92	0.51
3:X:113:ASN:ND2	3:X:115:ARG:NH1	2.58	0.51
1:A:165:ASP:HB2	1:A:166:PRO:CD	2.40	0.51
1:A:180:ILE:O	1:A:182:ILE:N	2.44	0.51
1:A:472:ASN:O	1:A:473:HIS:CB	2.58	0.51
1:A:656:ASN:CB	1:A:659:ALA:H	2.23	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:B:1330:ASN:N	2:B:1330:ASN:ND2	2.58	0.51
2:B:1381:ILE:CG2	2:B:1459:TYR:CE1	2.94	0.51
2:B:1391:LEU:HB2	2:B:1417:MET:HE2	1.93	0.51
2:B:1561:HIS:CD2	2:B:1597:ILE:HD13	2.46	0.51
2:B:204:GLU:O	2:B:205:HIS:HB2	2.10	0.51
1:C:1188:LEU:HD23	1:C:1212:LEU:HA	1.92	0.51
1:C:1327:LYS:HG3	1:C:1328:MET:H	1.75	0.51
1:C:1124:TYR:CA	1:C:1465:ASN:OD1	2.50	0.51
2:D:122:SER:OG	2:D:124:GLN:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:231:SER:HB3	2:D:244:HIS:HB2	1.91	0.51
2:D:69:PHE:HD2	2:D:69:PHE:C	2.14	0.51
3:X:194:LYS:NZ	3:X:197:ASN:HD22	2.08	0.51
1:C:511:HIS:HE1	3:Y:149:SER:OG	1.92	0.51
1:A:193:ASN:OD1	1:A:1070:LYS:HE2	2.11	0.51
1:A:1084:ARG:HG2	1:A:1084:ARG:HH11	1.75	0.51
1:A:1217:LEU:HD13	1:A:1237:SER:HA	1.93	0.51
1:A:1234:HIS:O	1:A:1235:LYS:HB2	2.10	0.51
1:A:40:VAL:CG2	1:A:512:PHE:CD1	2.92	0.51
1:A:625:GLN:O	1:A:628:GLU:HB3	2.11	0.51
1:A:552:ALA:CB	1:A:657:ALA:HB3	2.39	0.51
1:A:875:HIS:HB3	2:B:901:GLN:HE22	1.74	0.51
1:A:914:LEU:HD11	1:A:916:THR:HG22	1.93	0.51
2:B:1530:ARG:NH1	2:B:1530:ARG:HG3	2.26	0.51
2:B:353:TYR:HA	2:B:433:ILE:O	2.11	0.51
2:B:46:HIS:CG	2:B:525:GLN:HG2	2.45	0.51
2:B:573:ALA:HB3	2:B:762:LEU:HD13	1.93	0.51
1:C:1031:TRP:CH2	1:C:1042:LYS:HG3	2.45	0.51
1:C:111:PHE:CG	1:C:112:SER:N	2.78	0.51
1:C:1440:LYS:O	1:C:1444:GLU:HG3	2.11	0.51
1:C:1544:SER:HA	1:C:1547:THR:OG1	2.11	0.51
1:C:20:GLU:C	1:C:21:GLN:CG	2.77	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
1:C:827:MET:HE2	1:C:912:PHE:CE2	2.46	0.51
2:D:1351:ASN:O	2:D:1352:ILE:HG12	2.10	0.51
2:D:189:PRO:C	2:D:191:LEU:H	2.12	0.51
2:D:795:THR:CG2	2:D:796:PRO:HD2	2.39	0.51
2:D:847:ARG:O	2:D:898:ALA:HA	2.10	0.51
3:X:88:GLY:O	3:X:91:LYS:N	2.38	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:33:VAL:CG2	1:A:121:TYR:HD1	2.23	0.51
1:A:361:LEU:HD21	1:A:452:TYR:HB3	1.92	0.51
1:A:459:SER:HG	1:A:461:SER:HB3	1.74	0.51
1:A:689:LYS:HD3	1:A:730:GLU:OE2	2.11	0.51
1:A:257:ASN:ND2	1:A:892:SER:O	2.43	0.51
2:B:343:TYR:CE1	2:B:420:LEU:HD11	2.45	0.51
2:B:870:PHE:HB2	2:B:871:PRO:CD	2.41	0.51
1:C:958:GLU:HA	1:C:1346:LEU:O	2.10	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
1:C:1571:GLU:O	1:C:1574:PHE:CD2	2.64	0.51
1:C:199:TRP:HB2	1:C:217:PHE:CD1	2.46	0.51
1:C:974:LYS:O	1:C:1364:VAL:HG12	2.11	0.51
2:D:1482:ASN:H	2:D:1495:GLU:HG2	1.76	0.51
2:D:1548:ILE:CG2	2:D:1635:LEU:HB3	2.40	0.51
2:D:603:GLU:C	2:D:605:SER:H	2.14	0.51
2:D:902:GLU:HG3	2:D:902:GLU:O	2.11	0.51
1:A:1085:VAL:O	1:A:1089:VAL:HG23	2.10	0.51
1:A:1304:VAL:CG1	1:A:1305:LYS:H	2.23	0.51
1:A:1527:CYS:C	1:A:1529:GLU:N	2.64	0.51
1:A:1536:GLN:O	1:A:1536:GLN:HG3	2.10	0.51
1:A:473:HIS:O	1:A:473:HIS:HD2	1.90	0.51
1:A:59:TYR:CD2	1:A:99:VAL:HG21	2.46	0.51
1:A:974:LYS:O	1:A:1364:VAL:HG12	2.11	0.51
2:B:1386:MET:HA	2:B:1386:MET:CE	2.40	0.51
1:A:849:ARG:HH21	2:B:556:ILE:HD12	1.76	0.51
2:B:745:ILE:HD11	2:B:907:ASP:H	1.75	0.51
2:B:862:LYS:HZ2	2:B:1519:ASN:HB3	1.75	0.51
2:B:89:ILE:HD11	2:B:104:VAL:HG11	1.93	0.51
1:C:123:ASN:OD1	1:C:123:ASN:C	2.49	0.51
1:C:1323:LEU:CG	1:C:1324:HIS:H	2.24	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:C:396:ASP:HB3	1:C:398:ASN:HB2	1.92	0.51
1:C:804:ILE:CG2	1:C:809:ILE:HG13	2.38	0.51
1:C:847:ASN:ND2	1:C:853:MET:HB3	2.26	0.51
3:X:88:GLY:C	3:X:90:ASP:H	2.14	0.51
1:C:513:GLY:CA	3:Y:146:LEU:HD13	2.41	0.51
1:A:1240:PRO:O	1:A:1242:THR:N	2.43	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
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
1:A:95:GLY:O	1:A:96:GLN:O	2.29	0.51
2:B:1387:LEU:HD21	2:B:1472:TYR:CE1	2.46	0.51
2:B:1457:LYS:HG2	2:B:1469:THR:OG1	2.10	0.51
2:B:280:LEU:HD11	2:B:1379:MET:HG3	1.93	0.51
1:C:62:LYS:HE2	1:C:103:TYR:CE2	2.45	0.51
1:C:1619:ILE:HG12	1:C:1645:ILE:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:LEU:N	1:C:477:LEU:HD22	2.25	0.51
1:C:961:TYR:C	1:C:961:TYR:CD1	2.83	0.51
2:D:1562:GLN:HE22	2:D:1596:LYS:HZ1	1.57	0.51
2:D:1538:ASP:OD2	2:D:1567:ARG:HD2	2.11	0.51
2:D:1562:GLN:NE2	2:D:1596:LYS:NZ	2.56	0.51
2:D:243:PHE:CD1	2:D:314:LEU:HD23	2.43	0.51
2:D:746:ILE:HD13	2:D:746:ILE:H	1.76	0.51
3:X:106:VAL:HG22	3:X:163:LYS:HE3	1.93	0.51
3:Y:166:ASP:OD2	3:Y:207:LEU:CD2	2.59	0.51
1:A:1033:ILE:HG23	1:A:1034:PHE:H	1.75	0.51
1:A:1232:LEU:CG	1:A:1233:GLN:HG3	2.37	0.51
1:A:977:LEU:HD23	1:A:1361:VAL:HG22	1.93	0.51
1:A:697:LYS:O	1:A:700:TYR:HB3	2.10	0.51
2:B:1526:THR:HA	2:B:1545:LEU:HD13	1.92	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
2:B:902:GLU:HG3	2:B:902:GLU:O	2.11	0.51
2:B:962:LYS:HD2	2:B:1302:THR:HG21	1.91	0.51
1:C:1031:TRP:CZ3	1:C:1042:LYS:HA	2.46	0.51
1:C:1093:VAL:HG12	1:C:1095:GLN:HE21	1.76	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:1421:HIS:C	1:C:1421:HIS:CD2	2.83	0.51
1:C:1569:THR:O	1:C:1570:VAL:CG2	2.59	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:698:CYS:HB3	1:C:728:PHE:HB2	1.93	0.51
3:X:107:GLN:OE1	3:X:110:ILE:HD11	2.10	0.51
3:X:166:ASP:OD2	3:X:207:LEU:CD2	2.57	0.51
3:Y:113:ASN:ND2	3:Y:115:ARG:NH1	2.59	0.51
1:A:220:LYS:HD3	1:A:765:ILE:HG23	1.93	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:134:LYS:HD2	2:B:584:VAL:HG11	1.93	0.50
2:B:265:PHE:O	2:B:276:ILE:HG13	2.11	0.50
2:B:351:PRO:N	2:B:611:ALA:HB3	2.26	0.50
2:B:923:SER:HB3	2:B:1328:PHE:CE1	2.47	0.50
1:C:1099:SER:O	1:C:1100:ILE:C	2.47	0.50
1:C:1648:TRP:NE1	1:C:1664:LEU:HD21	2.25	0.50
1:C:23:TYR:CD1	1:C:655:THR:CB	2.89	0.50
2:D:1343:PHE:CG	2:D:1458:VAL:HG11	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:25:ILE:HG13	1:A:106:VAL:HG21	1.92	0.50
1:A:1245:ALA:HB2	1:A:1285:TYR:HB3	1.93	0.50
1:A:1327:LYS:HG3	1:A:1328:MET:H	1.75	0.50
1:A:375:VAL:O	1:A:383:VAL:HG13	2.11	0.50
1:A:415:ASP:OD1	1:A:415:ASP:N	2.44	0.50
1:A:496:ILE:HG22	1:A:496:ILE:O	2.10	0.50
1:A:541:LEU:HD23	1:A:541:LEU:O	2.10	0.50
1:A:689:LYS:O	1:A:691:LYS:N	2.43	0.50
1:A:698:CYS:C	1:A:700:TYR:N	2.63	0.50
1:A:78:LYS:HZ2	3:X:144:GLU:HA	1.71	0.50
2:B:1330:ASN:N	2:B:1330:ASN:HD22	2.09	0.50
2:B:285:ILE:HD12	2:B:285:ILE:H	1.74	0.50
1:C:1565:ILE:HB	1:C:1614:GLY:H	1.76	0.50
1:C:1622:LYS:CD	1:C:1642:LEU:HB3	2.40	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:1624:LEU:O	2:D:1625:CYS:C	2.50	0.50
2:D:208:GLU:OE1	2:D:210:TYR:HB2	2.11	0.50
2:D:236:TYR:CE1	2:D:424:ARG:HD2	2.45	0.50
2:D:44:GLU:OE1	2:D:480:THR:HG21	2.11	0.50
3:X:41:HIS:O	3:X:42:ASP:CB	2.58	0.50
3:X:85:PHE:CD1	3:X:85:PHE:N	2.78	0.50
1:A:1064:TYR:HD2	1:A:1102:ASN:CB	2.25	0.50
1:A:1226:ARG:NE	1:A:1266:TYR:HE1	2.08	0.50
1:A:1227:PHE:HB2	1:A:1251:THR:HG21	1.92	0.50
1:A:1643:THR:CG2	1:A:1644:TRP:N	2.73	0.50
1:A:395:ILE:CG1	1:A:430:VAL:HB	2.42	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:C:1064:TYR:HD2	1:C:1102:ASN:CB	2.24	0.50
1:C:1153:ARG:CZ	1:C:1168:LEU:HD12	2.42	0.50
1:C:1226:ARG:NE	1:C:1266:TYR:CE1	2.80	0.50
1:C:1474:CYS:HB3	1:C:1476:ARG:NH1	2.26	0.50
1:C:149:ASN:O	1:C:151:ASP:N	2.44	0.50
1:C:1602:LYS:HE3	1:C:1609:ALA:O	2.11	0.50
1:C:1640:ASP:O	1:C:1643:THR:HB	2.12	0.50
1:C:180:ILE:O	1:C:182:ILE:N	2.45	0.50
1:C:54:ILE:HG12	1:C:106:VAL:HG13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:784:LYS:HG2	1:C:785:GLN:H	1.75	0.50
1:C:804:ILE:HG22	1:C:809:ILE:CG1	2.39	0.50
1:C:864:GLY:HA3	1:C:907:LEU:HD22	1.92	0.50
2:D:1288:ILE:HD13	2:D:1303:VAL:HG21	1.92	0.50
2:D:1438:LEU:HD22	2:D:1439:HIS:N	2.26	0.50
2:D:45:ALA:HB3	2:D:81:MET:HE3	1.93	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
3:X:43:ILE:O	3:X:44:ARG:C	2.48	0.50
3:Y:58:SER:HB3	3:Y:102:ASN:HD22	1.72	0.50
1:A:1130:GLN:NE2	1:A:1230:ASP:HB3	2.26	0.50
1:A:124:GLY:C	1:A:125:PHE:CG	2.84	0.50
1:A:481:HIS:ND1	1:A:529:PRO:HB3	2.26	0.50
1:A:987:ILE:HD11	1:A:1294:ILE:HG23	1.91	0.50
2:B:942:LEU:HD13	2:B:1314:THR:HG23	1.92	0.50
2:B:503:LEU:HD23	2:B:503:LEU:C	2.32	0.50
2:B:575:VAL:O	2:B:759:THR:HA	2.12	0.50
2:B:40:GLN:HG3	2:B:86:THR:HG23	1.93	0.50
1:C:1320:LYS:CD	1:C:1321:GLY:N	2.72	0.50
1:C:134:VAL:C	1:C:135:TYR:CD2	2.85	0.50
1:C:1408:TYR:O	1:C:1410:PRO:HD3	2.11	0.50
1:C:239:GLY:O	1:C:241:LYS:N	2.44	0.50
1:C:274:ASP:CG	1:C:275:LEU:H	2.15	0.50
1:C:396:ASP:HB2	1:C:400:GLU:H	1.75	0.50
1:C:670:LYS:HD2	1:C:671:GLU:H	1.76	0.50
1:C:923:LEU:HD23	1:C:924:VAL:N	2.26	0.50
2:D:1427:LEU:N	2:D:1427:LEU:HD13	2.26	0.50
2:D:565:ILE:HG22	2:D:806:TYR:HE2	1.77	0.50
3:X:61:SER:N	3:X:75:PHE:HZ	2.09	0.50
1:A:1179:THR:HG22	1:A:1180:LEU:HD23	1.94	0.50
1:A:1540:ASP:HA	1:A:1660:PHE:HD1	1.76	0.50
1:A:396:ASP:HB3	1:A:398:ASN:H	1.76	0.50
1:A:577:PRO:HD2	1:A:588:VAL:HG23	1.93	0.50
1:A:796:THR:HA	1:A:818:LYS:HA	1.93	0.50
1:A:958:GLU:HA	1:A:1346:LEU:O	2.12	0.50
2:B:1438:LEU:HD22	2:B:1439:HIS:N	2.26	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:B:484:LEU:HD11	2:B:626:LEU:HG	1.93	0.50
1:C:1456:LYS:HG3	1:C:1457:ASP:OD2	2.11	0.50
1:C:1549:LYS:HD3	1:C:1667:PHE:CG	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:PHE:CE2	1:C:304:GLU:HA	2.45	0.50
1:C:851:SER:O	1:C:890:GLY:HA2	2.10	0.50
1:C:902:PRO:O	1:C:903:LEU:HD13	2.10	0.50
2:D:204:GLU:HG3	2:D:204:GLU:O	2.12	0.50
2:D:54:LEU:N	2:D:54:LEU:HD23	2.25	0.50
2:D:745:ILE:HD11	2:D:907:ASP:N	2.26	0.50
3:X:85:PHE:N	3:X:85:PHE:HD1	2.10	0.50
1:A:1066:TYR:CD1	1:A:1066:TYR:N	2.80	0.50
1:A:1383:THR:HG21	1:A:1511:THR:HG22	1.93	0.50
1:A:1548:ARG:HE	1:A:1550:GLN:NE2	2.09	0.50
1:A:1576:LYS:CG	1:A:1601:ILE:HG22	2.33	0.50
1:A:163:PHE:CE2	1:A:188:PHE:CD1	2.99	0.50
1:A:492:TYR:CD2	1:A:493:ILE:HB	2.46	0.50
1:A:691:LYS:C	1:A:693:SER:H	2.12	0.50
1:A:691:LYS:C	1:A:693:SER:N	2.65	0.50
2:B:1343:PHE:CG	2:B:1458:VAL:HG11	2.46	0.50
2:B:558:MET:O	2:B:561:ALA:HB3	2.11	0.50
2:B:887:LEU:HD23	2:B:1490:CYS:HB3	1.92	0.50
2:B:946:LYS:H	2:B:946:LYS:CD	2.23	0.50
1:C:1056:ILE:HG12	1:C:1056:ILE:O	2.10	0.50
1:C:1433:SER:OG	1:C:1482:LEU:HD12	2.11	0.50
1:C:316:GLU:HG2	1:C:349:LEU:HD23	1.94	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
1:C:837:GLU:O	1:C:901:LEU:HB2	2.11	0.50
1:C:856:CYS:HB3	1:C:915:GLU:HG2	1.94	0.50
1:C:95:GLY:O	1:C:96:GLN:O	2.30	0.50
2:D:1610:TRP:CE3	2:D:1628:PHE:CE2	3.00	0.50
2:D:357:GLY:HA3	2:D:404:LEU:HD12	1.94	0.50
2:D:415:THR:O	2:D:425:GLN:CD	2.50	0.50
2:D:846:VAL:HG22	2:D:847:ARG:N	2.26	0.50
1:A:1408:TYR:O	1:A:1410:PRO:HD3	2.12	0.50
2:B:1346:ASN:HB2	2:B:1368:CYS:HB2	1.93	0.50
2:B:338:ILE:C	2:B:339:VAL:HG13	2.32	0.50
2:B:362:LEU:HD13	2:B:411:ILE:HD12	1.94	0.50
1:C:1021:VAL:HG12	1:C:1022:PHE:N	2.27	0.50
1:C:1084:ARG:HA	1:C:1151:GLY:HA2	1.94	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:544:TYR:C	1:C:544:TYR:HD2	2.15	0.50
1:C:614:ARG:HD2	1:C:614:ARG:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:661:ASP:OD2	1:C:663:GLN:N	2.45	0.50
1:C:911:ASN:OD1	1:C:924:VAL:HG22	2.12	0.50
1:C:985:GLY:O	1:C:986:GLU:C	2.50	0.50
2:D:1290:TYR:CD2	2:D:1301:ARG:HB3	2.46	0.50
2:D:1593:THR:HG22	2:D:1594:LYS:H	1.72	0.50
2:D:1623:LYS:HB3	2:D:1623:LYS:HZ2	1.77	0.50
2:D:476:ILE:HG12	2:D:524:TYR:CD2	2.47	0.50
2:D:565:ILE:O	2:D:776:MET:HB3	2.11	0.50
3:X:229:ASN:N	3:X:229:ASN:OD1	2.45	0.50
1:A:1147:PHE:C	1:A:1147:PHE:CD2	2.85	0.50
1:A:950:TYR:HD1	1:A:1268:ASN:OD1	1.94	0.50
1:A:1347:ILE:CG2	1:A:1347:ILE:O	2.60	0.50
1:A:199:TRP:HB2	1:A:217:PHE:CD1	2.47	0.50
1:A:234:GLU:HB3	1:A:246:PHE:CE1	2.47	0.50
1:A:530:VAL:HG23	1:A:534:MET:CE	2.39	0.50
1:A:23:TYR:O	1:A:655:THR:HB	2.12	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:B:857:CYS:HB3	2:B:885:VAL:HG22	1.93	0.50
1:C:1033:ILE:HD13	1:C:1034:PHE:CE1	2.47	0.50
1:C:33:VAL:HG23	1:C:120:THR:O	2.11	0.50
1:C:1245:ALA:HB2	1:C:1285:TYR:HB3	1.94	0.50
1:C:32:ARG:O	1:C:35:ALA:HB3	2.12	0.50
1:C:523:TYR:CE1	2:D:359:PRO:CG	2.93	0.50
2:D:46:HIS:CG	2:D:525:GLN:HG2	2.46	0.50
2:D:780:LEU:HD11	2:D:787:TRP:CD1	2.47	0.50
2:D:952:ASP:N	2:D:952:ASP:OD1	2.31	0.50
3:Y:107:GLN:CD	3:Y:110:ILE:HD11	2.32	0.50
1:C:78:LYS:HG3	3:Y:146:LEU:HB2	1.92	0.50
3:Y:166:ASP:OD2	3:Y:207:LEU:CG	2.58	0.50
1:A:1012:LEU:HD22	1:A:1085:VAL:CG2	2.25	0.50
1:A:1370:THR:O	1:A:1371:SER:C	2.49	0.50
1:A:1540:ASP:CA	1:A:1660:PHE:HD1	2.25	0.50
1:A:155:ALA:O	1:A:157:ARG:N	2.45	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:236:ASN:HD22	1:A:379:LEU:HD21	1.76	0.50
1:A:24:VAL:HA	1:A:655:THR:CB	2.42	0.50
1:A:612:VAL:HG21	1:A:769:PHE:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:916:THR:C	1:A:918:PHE:H	2.15	0.50
2:B:1427:LEU:N	2:B:1427:LEU:HD13	2.27	0.50
2:B:1601:ILE:HD12	2:B:1601:ILE:H	1.76	0.50
2:B:1609:ARG:NH1	2:B:1609:ARG:HG2	2.25	0.50
2:B:881:PRO:O	2:B:882:PHE:CD2	2.65	0.50
1:C:1240:PRO:C	1:C:1242:THR:N	2.65	0.50
1:C:1263:ASP:O	1:C:1265:ASN:N	2.45	0.50
1:C:1582:LEU:O	1:C:1583:ASP:C	2.50	0.50
1:C:74:SER:HA	1:C:79:PHE:HE1	1.77	0.50
2:D:1381:ILE:HB	2:D:1459:TYR:HD1	1.77	0.50
3:X:61:SER:O	3:X:75:PHE:CZ	2.65	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:A:149:ASN:H	1:A:149:ASN:ND2	2.05	0.49
1:A:560:TRP:HH2	1:A:673:LEU:HD22	1.77	0.49
1:A:805:SER:O	1:A:807:THR:N	2.45	0.49
2:B:1539:ILE:HG23	2:B:1564:ILE:HG12	1.94	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:1147:PHE:CD2	1:C:1147:PHE:C	2.86	0.49
1:C:1365:VAL:CG2	1:C:1366:HIS:N	2.73	0.49
1:C:161:LEU:HD11	1:C:185:PHE:CZ	2.47	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:C:820:PHE:CG	1:C:821:LYS:N	2.80	0.49
2:D:1529:LEU:HD11	2:D:1543:ASP:HB2	1.94	0.49
3:Y:215:VAL:C	3:Y:216:LEU:HD22	2.32	0.49
1:A:1053:MET:HE2	1:A:1086:LEU:CD1	2.42	0.49
1:A:1215:GLU:O	1:A:1217:LEU:HD23	2.12	0.49
1:A:1544:SER:HA	1:A:1547:THR:OG1	2.12	0.49
1:A:1598:ILE:HG22	1:A:1599:THR:N	2.27	0.49
1:A:484:ILE:HD12	1:A:540:LEU:CD2	2.42	0.49
1:A:55:SER:C	1:A:56:ILE:HD13	2.32	0.49
1:A:571:LEU:CD2	1:A:812:ALA:HB2	2.41	0.49
2:B:147:VAL:HG12	2:B:183:PHE:CE1	2.45	0.49
2:B:1480:LEU:C	2:B:1480:LEU:HD12	2.33	0.49
2:B:199:ILE:O	2:B:199:ILE:HG22	2.11	0.49
1:C:1162:VAL:HG23	1:C:1163:LYS:N	2.27	0.49
1:C:42:GLN:HE21	1:C:44:TYR:N	2.10	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:C:998:ASN:HB3	1:C:1000:LEU:HG	1.94	0.49
2:D:923:SER:HB3	2:D:1328:PHE:CE1	2.47	0.49
2:D:1391:LEU:HD12	2:D:1417:MET:HE1	1.92	0.49
3:X:146:LEU:HD21	3:X:148:ALA:HB2	1.94	0.49
3:Y:41:HIS:ND1	3:Y:41:HIS:N	2.60	0.49
1:A:1323:LEU:CD1	1:A:1324:HIS:H	2.24	0.49
1:A:658:ASN:O	1:A:659:ALA:HB3	2.11	0.49
1:A:680:GLN:O	1:A:682:LYS:N	2.45	0.49
1:A:983:LEU:HD21	1:A:1271:ILE:HD12	1.94	0.49
2:B:1611:PRO:HG3	2:B:1624:LEU:HB3	1.94	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
1:C:1537:GLU:O	1:C:1539:LEU:N	2.44	0.49
1:C:398:ASN:O	1:C:399:GLN:HB2	2.13	0.49
1:C:757:LEU:O	1:C:758:LEU:HD23	2.12	0.49
2:D:963:ILE:CD1	2:D:1311:ILE:HG21	2.41	0.49
2:D:1522:TYR:N	2:D:1522:TYR:HD2	2.10	0.49
2:D:167:THR:HG22	2:D:171:ILE:O	2.12	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
3:X:61:SER:N	3:X:75:PHE:CZ	2.80	0.49
3:Y:71:ASN:O	3:Y:72:VAL:HG23	2.13	0.49
1:A:1019:PHE:CD2	1:A:1020:TYR:N	2.80	0.49
1:A:1068:VAL:CG1	1:A:1069:TRP:H	2.17	0.49
1:A:196:TYR:HE2	1:A:1070:LYS:NZ	2.10	0.49
1:A:1077:TRP:NE1	1:A:1147:PHE:CD1	2.80	0.49
1:A:1327:LYS:O	1:A:1332:ASN:ND2	2.46	0.49
1:A:1487:PHE:O	1:A:1488:LEU:C	2.50	0.49
1:A:1537:GLU:O	1:A:1539:LEU:N	2.45	0.49
1:A:23:TYR:HA	1:A:43:VAL:HA	1.94	0.49
1:A:987:ILE:HD13	1:A:1294:ILE:HG23	1.94	0.49
1:A:998:ASN:HB3	1:A:1000:LEU:HG	1.93	0.49
2:B:1415:ASN:O	2:B:1417:MET:HG3	2.12	0.49
2:B:1522:TYR:CD2	2:B:1522:TYR:O	2.65	0.49
2:B:1506:ILE:CD1	2:B:1628:PHE:CE1	2.95	0.49
2:B:481:TYR:HE2	2:B:493:GLY:CA	2.24	0.49
2:B:643:LYS:HG3	2:B:644:CYS:N	2.27	0.49
2:B:963:ILE:CD1	2:B:1311:ILE:HG21	2.42	0.49
1:C:1541:LEU:HD21	1:C:1543:ILE:HD12	1.93	0.49
1:C:1643:THR:CG2	1:C:1644:TRP:N	2.74	0.49
1:C:296:ILE:CG2	1:C:297:ALA:N	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:PHE:HE2	1:C:304:GLU:CA	2.25	0.49
1:C:515:ARG:CZ	1:C:526:ILE:HG22	2.42	0.49
1:C:541:LEU:HB2	1:C:558:SER:HB3	1.95	0.49
1:C:613:GLN:O	1:C:615:GLY:N	2.46	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
1:C:903:LEU:HD22	1:C:903:LEU:N	2.27	0.49
1:C:916:THR:O	1:C:918:PHE:N	2.46	0.49
2:D:1371:TYR:CD1	2:D:1377:SER:CB	2.95	0.49
2:D:322:THR:HG21	2:D:327:ASP:H	1.78	0.49
2:D:564:LYS:HA	2:D:776:MET:O	2.12	0.49
2:D:643:LYS:HG3	2:D:644:CYS:N	2.27	0.49
2:D:916:VAL:CG2	2:D:917:PRO:N	2.76	0.49
3:X:104:PHE:CE1	3:X:164:GLU:HG3	2.47	0.49
3:Y:106:VAL:HG22	3:Y:163:LYS:HE3	1.93	0.49
3:Y:85:PHE:CE1	3:Y:117:SER:HB3	2.47	0.49
3:Y:119:VAL:HG13	3:Y:212:MET:SD	2.52	0.49
1:A:1423:VAL:HG11	1:A:1496:TYR:CZ	2.47	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
2:B:168:PRO:HD3	2:B:197:TRP:CD1	2.47	0.49
2:B:565:ILE:HG22	2:B:806:TYR:HE2	1.77	0.49
2:B:59:HIS:HB3	2:B:64:LYS:HA	1.95	0.49
1:C:1226:ARG:CB	1:C:1269:PRO:HB2	2.42	0.49
1:C:234:GLU:HB3	1:C:246:PHE:CE1	2.47	0.49
1:C:377:ASP:OD2	1:C:379:LEU:HB2	2.12	0.49
1:C:758:LEU:HB3	1:C:759:PRO:HD2	1.93	0.49
1:C:85:LEU:HD22	1:C:85:LEU:N	2.27	0.49
2:D:235:PHE:HB3	2:D:338:ILE:CG2	2.43	0.49
2:D:408:SER:HB3	2:D:410:PRO:HD3	1.95	0.49
2:D:511:THR:O	2:D:513:ASP:N	2.46	0.49
2:D:825:VAL:HB	2:D:828:GLU:CD	2.33	0.49
2:D:942:LEU:HD13	2:D:1314:THR:HG23	1.95	0.49
3:X:71:ASN:O	3:X:72:VAL:HG23	2.12	0.49
1:A:123:ASN:N	1:A:211:THR:HG23	2.27	0.49
1:A:1249:GLU:O	1:A:1253:TYR:HD2	1.96	0.49
1:A:1286:SER:OG	1:A:1287:THR:N	2.46	0.49
1:A:1318:LYS:HB2	1:A:1345:ASP:HB2	1.94	0.49
1:A:1564:SER:CB	1:A:1616:GLN:HG3	2.43	0.49
1:A:719:SER:OG	1:A:1123:GLN:HG3	2.12	0.49
1:A:74:SER:HA	1:A:79:PHE:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:PHE:CG	1:A:821:LYS:N	2.81	0.49
2:B:1400:LEU:HD22	2:B:1406:ARG:HH12	1.77	0.49
2:B:1347:VAL:HG21	2:B:1456:VAL:HG11	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
2:B:916:VAL:CG2	2:B:917:PRO:N	2.74	0.49
1:C:100:SER:O	1:C:101:TYR:HB2	2.11	0.49
1:C:1557:ILE:HD13	1:C:1622:LYS:HG3	1.93	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:C:719:SER:OG	1:C:1123:GLN:HG3	2.13	0.49
2:D:280:LEU:HD22	2:D:1462:TYR:HE2	1.76	0.49
2:D:1526:THR:HA	2:D:1545:LEU:HD13	1.95	0.49
2:D:1533:GLU:OE1	2:D:1533:GLU:HA	2.13	0.49
2:D:26:THR:HG22	2:D:630:THR:HG22	1.94	0.49
1:A:100:SER:C	1:A:101:TYR:HD2	2.16	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
1:A:514:THR:HG22	1:A:515:ARG:N	2.27	0.49
1:A:766:ARG:H	1:A:766:ARG:HD3	1.78	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
2:B:1529:LEU:HD11	2:B:1543:ASP:HB2	1.93	0.49
2:B:494:ARG:CG	2:B:494:ARG:HH11	2.12	0.49
2:B:620:VAL:HG12	2:B:621:PHE:N	2.28	0.49
1:C:1454:GLN:HG3	1:C:1461:ILE:HB	1.94	0.49
1:C:1475:VAL:CG2	1:C:1476:ARG:N	2.75	0.49
1:C:1620:MET:CB	1:C:1644:TRP:HB3	2.27	0.49
1:C:257:ASN:HD21	1:C:892:SER:CA	2.23	0.49
2:D:1502:HIS:ND1	2:D:1503:GLN:N	2.51	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
2:D:63:ARG:HB3	2:D:65:GLN:HG3	1.95	0.49
2:D:218:LYS:HB3	2:D:822:TYR:CE2	2.47	0.49
2:D:948:ARG:HB2	2:D:948:ARG:NH2	2.25	0.49
3:X:88:GLY:C	3:X:90:ASP:N	2.66	0.49
3:Y:86:LEU:HG	3:Y:91:LYS:CG	2.43	0.49
1:A:1204:GLN:O	1:A:1208:ILE:HG13	2.13	0.49
1:A:174:VAL:HG22	1:A:175:GLU:H	1.77	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:469:ASN:CB	2:B:472:SER:HB2	2.42	0.49
2:B:519:ARG:NH1	2:B:606:ASP:OD2	2.45	0.49
2:B:825:VAL:HB	2:B:828:GLU:CD	2.32	0.49
2:B:933:ARG:NH1	2:B:933:ARG:HG3	2.18	0.49
1:C:1140:ASN:O	1:C:1143:TYR:HB3	2.13	0.49
1:C:1265:ASN:C	1:C:1267:VAL:H	2.15	0.49
1:C:1411:SER:H	1:C:1414:GLU:HG3	1.78	0.49
1:C:272:ARG:HG3	1:C:279:GLN:O	2.13	0.49
1:C:296:ILE:HG23	1:C:297:ALA:N	2.26	0.49
1:C:518:PHE:O	1:C:520:ASP:N	2.42	0.49
1:C:571:LEU:CD2	1:C:812:ALA:HB2	2.43	0.49
1:C:682:LYS:NZ	1:C:686:ILE:CD1	2.75	0.49
1:C:862:VAL:O	1:C:863:GLU:C	2.51	0.49
1:C:945:ASP:OD1	1:C:945:ASP:C	2.48	0.49
2:D:1443:LEU:CD1	2:D:1443:LEU:N	2.76	0.49
2:D:1602:THR:O	2:D:1604:ASN:N	2.41	0.49
2:D:1621:PHE:O	2:D:1622:GLN:C	2.50	0.49
2:D:189:PRO:C	2:D:191:LEU:N	2.66	0.49
2:D:322:THR:CG2	2:D:327:ASP:H	2.25	0.49
2:D:463:ASN:OD1	2:D:505:THR:OG1	2.31	0.49
2:D:573:ALA:HB3	2:D:762:LEU:HD13	1.93	0.49
2:D:847:ARG:HG3	2:D:869:GLN:CG	2.36	0.49
1:A:1386:ILE:HG13	1:A:1387:GLU:N	2.27	0.49
1:A:1456:LYS:HG3	1:A:1457:ASP:OD2	2.13	0.49
1:A:757:LEU:O	1:A:758:LEU:HD23	2.12	0.49
1:A:849:ARG:HH11	1:A:849:ARG:CG	2.12	0.49
2:B:1299:LEU:HB3	2:B:1301:ARG:HD3	1.94	0.49
2:B:144:LEU:HD23	2:B:144:LEU:N	2.28	0.49
2:B:531:ILE:O	2:B:617:ASN:ND2	2.39	0.49
2:B:946:LYS:N	2:B:946:LYS:HD3	2.27	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
1:C:148:LEU:HA	1:C:154:PRO:O	2.12	0.49
1:C:1562:LYS:HD3	1:C:1648:TRP:NE1	2.27	0.49
1:C:165:ASP:C	1:C:167:GLU:N	2.66	0.49
1:C:395:ILE:CG1	1:C:430:VAL:HB	2.43	0.49
2:D:58:VAL:HG12	2:D:104:VAL:CG2	2.41	0.49
2:D:1281:LEU:HB2	2:D:1283:ASP:HB2	1.95	0.49
2:D:1390:PHE:CD1	2:D:1442:ILE:HG13	2.47	0.49
2:D:462:VAL:HG21	2:D:520:PHE:CE2	2.48	0.49
2:D:548:LEU:HD23	2:D:803:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:87:LEU:HD12	3:Y:210:GLU:HA	1.95	0.49
1:A:1190:ILE:CG1	1:A:1253:TYR:CE1	2.94	0.49
1:A:1069:TRP:HH2	1:A:1465:ASN:ND2	2.10	0.49
1:A:1475:VAL:CG2	1:A:1476:ARG:N	2.76	0.49
1:A:1566:THR:HG23	1:A:1578:LYS:O	2.13	0.49
1:A:189:LYS:HG3	1:A:190:ILE:O	2.13	0.49
1:A:123:ASN:C	1:A:211:THR:HG21	2.32	0.49
1:A:515:ARG:NH1	1:A:526:ILE:HG22	2.27	0.49
1:A:682:LYS:NZ	1:A:686:ILE:CD1	2.76	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
2:B:239:GLY:N	2:B:296:ARG:NH2	2.61	0.49
1:A:423:ASN:CG	2:B:504:VAL:HG22	2.33	0.49
1:C:1085:VAL:O	1:C:1089:VAL:HG23	2.13	0.49
1:C:1128:LYS:HD3	1:C:1414:GLU:OE1	2.13	0.49
1:C:115:LYS:HB2	1:C:654:LEU:CD2	2.42	0.49
1:C:1255:LEU:C	1:C:1255:LEU:HD12	2.31	0.49
1:C:1318:LYS:HB2	1:C:1345:ASP:HB2	1.95	0.49
1:C:1493:PHE:HD1	1:C:1494:THR:H	1.50	0.49
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:C:96:GLN:O	1:C:97:ASN:O	2.31	0.49
2:D:1280:GLU:HB2	2:D:1312:THR:HB	1.95	0.49
2:D:1567:ARG:NH1	2:D:1567:ARG:HG3	2.28	0.49
2:D:188:LEU:HD13	2:D:216:VAL:HG21	1.95	0.49
2:D:481:TYR:CE1	2:D:506:MET:SD	2.93	0.49
2:D:889:GLN:HA	2:D:915:VAL:HB	1.95	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: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
1:A:1565:ILE:HB	1:A:1614:GLY:H	1.78	0.48
1:A:354:LEU:HB2	1:A:374:GLN:O	2.13	0.48
1:A:963:ILE:CG2	1:A:967:LEU:HD23	2.41	0.48
2:B:1344:HIS:ND1	4:F:1:NAG:H82	2.27	0.48
2:B:1610:TRP:CD2	2:B:1628:PHE:CD2	2.99	0.48
2:B:830:VAL:CG2	2:B:831:GLU:N	2.74	0.48
1:C:1234:HIS:O	1:C:1235:LYS:HB2	2.12	0.48
1:C:1559:TYR:CE1	1:C:1587:THR:HA	2.47	0.48
1:C:371:ILE:CG2	1:C:420:PHE:HB2	2.34	0.48
1:C:596:MET:SD	1:C:782:ARG:HG2	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1601:ILE:HD12	2:D:1601:ILE:H	1.78	0.48
1:C:523:TYR:CZ	2:D:359:PRO:HD2	2.48	0.48
2:D:945:ILE:N	2:D:945:ILE:HD12	2.28	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:A:1017:PRO:O	1:A:1018:VAL:C	2.51	0.48
1:A:1231:ASN:O	1:A:1233:GLN:N	2.46	0.48
1:A:1376:SER:OG	1:A:1503:LYS:HG3	2.13	0.48
1:A:163:PHE:CD2	1:A:188:PHE:CD1	3.00	0.48
1:A:1641:SER:O	1:A:1642:LEU:HB2	2.14	0.48
1:A:24:VAL:HG11	1:A:543:TYR:CZ	2.48	0.48
1:A:272:ARG:HG3	1:A:279:GLN:O	2.13	0.48
1:A:477:LEU:HD23	1:A:480:GLU:OE1	2.14	0.48
1:A:54:ILE:HG12	1:A:106:VAL:HG13	1.94	0.48
1:A:560:TRP:CH2	1:A:673:LEU:CD2	2.96	0.48
1:A:613:GLN:O	1:A:615:GLY:N	2.46	0.48
1:A:689:LYS:CG	1:A:699:CYS:SG	3.01	0.48
1:A:734:VAL:HA	1:A:737:GLN:HG2	1.94	0.48
1:A:853:MET:O	1:A:888:VAL:HG12	2.13	0.48
2:B:1533:GLU:OE1	2:B:1533:GLU:HA	2.12	0.48
2:B:1614:ASP:O	2:B:1616:CYS:N	2.46	0.48
2:B:216:VAL:O	2:B:216:VAL:HG13	2.13	0.48
2:B:580:VAL:CG1	2:B:584:VAL:HG23	2.43	0.48
2:B:615:GLN:HB2	2:B:616:ASN:HD22	1.75	0.48
2:B:598:ILE:HD12	2:B:800:ILE:HG21	1.92	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
1:C:136:THR:O	1:C:139:GLN:HG3	2.12	0.48
1:C:1377:PHE:CD2	1:C:1495:VAL:HG22	2.48	0.48
1:C:1622:LYS:HZ2	1:C:1642:LEU:HB3	1.78	0.48
1:C:1562:LYS:CD	1:C:1648:TRP:NE1	2.76	0.48
1:C:248:ILE:HB	1:C:299:VAL:HG13	1.93	0.48
1:C:496:ILE:HG22	1:C:496:ILE:O	2.12	0.48
2:D:853:ASN:C	2:D:853:ASN:OD1	2.52	0.48
3:X:103:VAL:HG22	3:X:122:VAL:HG13	1.94	0.48
3:X:81:ASN:O	3:X:115:ARG:CB	2.53	0.48
3:Y:125:LYS:HA	3:Y:126:ASN:C	2.27	0.48
1:A:1000:LEU:O	1:A:1001:THR:HG23	2.13	0.48
1:A:1240:PRO:C	1:A:1242:THR:N	2.67	0.48
1:A:1671:ILE:CD1	1:A:1676:CYS:SG	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:GLN:H	1:A:310:LEU:HD22	1.78	0.48
1:A:997:ILE:O	1:A:997:ILE:HG13	2.13	0.48
2:B:322:THR:HG21	2:B:327:ASP:H	1.79	0.48
1:C:1077:TRP:NE1	1:C:1147:PHE:CD1	2.79	0.48
1:C:1142:LEU:HD21	1:C:1179:THR:OG1	2.14	0.48
1:C:977:LEU:HD23	1:C:1361:VAL:HG22	1.96	0.48
1:C:222:TYR:HE2	1:C:224:LEU:HA	1.79	0.48
1:C:443:PRO:CD	1:C:446:ASN:HB2	2.42	0.48
1:C:514:THR:CG2	1:C:515:ARG:N	2.77	0.48
1:C:695:VAL:HG12	1:C:727:ALA:CB	2.44	0.48
1:C:43:VAL:HG12	1:C:79:PHE:O	2.13	0.48
2:D:580:VAL:CG1	2:D:584:VAL:HG23	2.43	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
3:X:187:GLY:C	3:X:203:LEU:HD12	2.33	0.48
3:Y:85:PHE:CD1	3:Y:85:PHE:N	2.81	0.48
1:A:1057:MET:HE2	1:A:1057:MET:HB3	1.77	0.48
1:A:1226:ARG:NE	1:A:1266:TYR:CE1	2.82	0.48
1:A:1320:LYS:HD2	1:A:1321:GLY:N	2.27	0.48
1:A:1431:GLY:HA2	1:A:1483:PHE:HE1	1.78	0.48
1:A:1286:SER:CB	1:A:1499:HIS:HA	2.44	0.48
1:A:493:ILE:O	1:A:493:ILE:HG22	2.12	0.48
1:A:500:ASN:ND2	1:A:543:TYR:CE1	2.77	0.48
1:A:576:SER:CB	1:A:589:SER:H	2.27	0.48
1:A:825:LEU:HB2	1:A:845:VAL:HG23	1.96	0.48
2:B:1611:PRO:CD	2:B:1624:LEU:HD23	2.44	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:132:LYS:NZ	1:C:139:GLN:HE22	2.11	0.48
1:C:1563:VAL:HA	1:C:1582:LEU:H	1.78	0.48
1:C:322:TYR:N	1:C:322:TYR:HD2	2.10	0.48
1:C:236:ASN:HD22	1:C:379:LEU:HD21	1.78	0.48
1:C:494:ASP:OD1	1:C:495:LYS:HE2	2.13	0.48
1:C:481:HIS:ND1	1:C:529:PRO:HB3	2.27	0.48
1:C:950:TYR:HD1	1:C:1268:ASN:OD1	1.96	0.48
1:C:964:PRO:HG2	1:C:1365:VAL:HG11	1.95	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
2:D:210:TYR:CG	2:D:211:THR:N	2.81	0.48
2:D:32:VAL:HB	2:D:607:PHE:CZ	2.48	0.48
2:D:853:ASN:HA	2:D:854:PRO:HD3	1.58	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:860:SER:OG	2:D:866:TYR:N	2.39	0.48
2:D:941:GLN:HE21	2:D:943:GLU:CG	2.26	0.48
1:A:1084:ARG:HA	1:A:1151:GLY:HA2	1.94	0.48
1:A:1411:SER:H	1:A:1414:GLU:HG3	1.78	0.48
1:A:1563:VAL:HG12	1:A:1581:LEU:HA	1.96	0.48
1:A:174:VAL:CG2	1:A:175:GLU:N	2.74	0.48
1:A:430:VAL:HG11	1:A:453:ARG:NH2	2.14	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
1:A:663:GLN:CG	1:A:664:GLU:N	2.76	0.48
1:A:690:TYR:C	1:A:692:HIS:N	2.67	0.48
1:A:911:ASN:OD1	1:A:924:VAL:HG22	2.14	0.48
1:A:92:LEU:HD13	1:C:1026:GLU:OE2	2.13	0.48
2:B:548:LEU:HD23	2:B:803:ALA:HB2	1.96	0.48
2:B:32:VAL:HB	2:B:607:PHE:CZ	2.48	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:C:554:LEU:H	1:C:658:ASN:HD22	1.61	0.48
1:C:545:ILE:HG23	1:C:554:LEU:HD21	1.95	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:C:883:CYS:O	1:C:884:VAL:C	2.51	0.48
1:A:1042:LYS:HZ1	1:C:92:LEU:HD13	1.77	0.48
2:D:1344:HIS:ND1	4:H:1:NAG:C8	2.77	0.48
3:X:50:TYR:CE2	3:X:170:ARG:CZ	2.96	0.48
1:A:1142:LEU:HD13	1:A:1187:THR:HG21	1.95	0.48
1:A:981:GLY:HA3	1:A:1333:PHE:CD1	2.49	0.48
1:A:25:ILE:CD1	1:A:41:ILE:HG13	2.43	0.48
1:A:461:SER:CB	1:A:553:GLU:OE2	2.61	0.48
1:A:541:LEU:HB2	1:A:557:ASP:O	2.13	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
2:B:1624:LEU:O	2:B:1625:CYS:C	2.52	0.48
2:B:384:PHE:CD2	2:B:384:PHE:N	2.81	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:C:119:ILE:C	1:C:119:ILE:HD12	2.34	0.48
1:C:1255:LEU:HD13	1:C:1267:VAL:HG13	1.95	0.48
1:C:1421:HIS:HD2	1:C:1422:ALA:N	2.11	0.48
1:C:367:ILE:HD13	1:C:466:TYR:CD2	2.48	0.48
1:C:539:ARG:NH2	1:C:634:CYS:N	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:971:THR:O	1:C:971:THR:OG1	2.23	0.48
2:D:870:PHE:HB2	2:D:871:PRO:CD	2.42	0.48
3:X:41:HIS:ND1	3:X:41:HIS:N	2.62	0.48
1:A:20:GLU:C	1:A:21:GLN:CG	2.77	0.48
2:B:224:PHE:CE1	2:B:320:VAL:CG1	2.96	0.48
2:B:570:ASP:O	2:B:573:ALA:HB2	2.14	0.48
1:C:1068:VAL:CG1	1:C:1069:TRP:H	2.18	0.48
1:C:1066:TYR:N	1:C:1079:THR:HG23	2.21	0.48
1:A:1161:LEU:CD1	1:C:1105:LEU:HD13	2.41	0.48
1:C:161:LEU:HD21	1:C:185:PHE:CD2	2.49	0.48
1:C:1622:LYS:NZ	1:C:1642:LEU:HB3	2.29	0.48
1:C:23:TYR:CE2	1:C:111:PHE:CD2	3.01	0.48
1:C:243:PHE:CE2	1:C:304:GLU:CA	2.96	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:C:871:PRO:CD	1:C:872:VAL:N	2.75	0.48
2:D:1631:PHE:HD2	2:D:1632:SER:N	2.11	0.48
2:D:216:VAL:HG13	2:D:216:VAL:O	2.13	0.48
2:D:229:GLN:HA	2:D:229:GLN:OE1	2.14	0.48
2:D:27:LEU:O	2:D:628:LEU:HD12	2.14	0.48
2:D:345:ILE:HG13	2:D:428:LYS:HB3	1.96	0.48
2:D:524:TYR:CE1	2:D:532:VAL:HG12	2.49	0.48
2:D:61:PHE:CD1	2:D:62:PRO:HA	2.48	0.48
3:X:77:PRO:O	3:X:78:LYS:CB	2.61	0.48
1:A:1090:ASN:ND2	1:A:1158:ILE:HG12	2.29	0.48
1:A:1234:HIS:CG	1:A:1235:LYS:H	2.31	0.48
1:A:964:PRO:HG2	1:A:1365:VAL:HG11	1.95	0.48
1:A:30:ILE:HG22	1:A:31:PHE:N	2.29	0.48
1:A:494:ASP:OD2	1:A:495:LYS:HE2	2.14	0.48
1:A:59:TYR:CD2	1:A:60:PRO:HD3	2.49	0.48
2:B:25:TYR:CE2	2:B:113:VAL:HG22	2.48	0.48
2:B:130:ILE:HD13	2:B:199:ILE:CG2	2.44	0.48
2:B:441:SER:HB2	2:B:443:ASN:ND2	2.29	0.48
2:B:462:VAL:HG21	2:B:520:PHE:CE2	2.48	0.48
2:B:575:VAL:HG23	2:B:762:LEU:CD1	2.44	0.48
2:B:853:ASN:C	2:B:853:ASN:OD1	2.52	0.48
2:B:866:TYR:HE2	2:B:868:GLN:OE1	1.96	0.48
1:C:1066:TYR:H	1:C:1079:THR:CG2	2.23	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:1573:VAL:HG12	1:C:1603:LYS:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:ILE:HG22	1:C:31:PHE:N	2.28	0.48
1:C:354:LEU:HB2	1:C:374:GLN:O	2.14	0.48
1:C:532:GLN:O	1:C:535:VAL:HG13	2.14	0.48
2:D:1442:ILE:C	2:D:1443:LEU:HD13	2.34	0.48
2:D:59:HIS:HB3	2:D:64:LYS:HA	1.96	0.48
1:A:465:LEU:HD11	1:A:486:VAL:HG13	1.95	0.48
1:A:548:GLY:HA3	1:A:550:GLN:OE1	2.14	0.48
2:B:1504:GLU:CD	2:B:1505:ARG:H	2.15	0.48
2:B:1534:GLN:OE1	2:B:1534:GLN:HA	2.13	0.48
2:B:1610:TRP:HA	2:B:1628:PHE:CE2	2.49	0.48
2:B:224:PHE:HE1	2:B:320:VAL:HG11	1.79	0.48
2:B:235:PHE:HB3	2:B:338:ILE:HG23	1.96	0.48
2:B:603:GLU:C	2:B:605:SER:H	2.16	0.48
1:C:999:ILE:HD12	1:C:1001:THR:O	2.14	0.48
1:C:153:LYS:HG2	1:C:806:ASN:O	2.13	0.48
1:C:500:ASN:O	1:C:542:VAL:HA	2.14	0.48
2:D:1345:LEU:HD21	2:D:1456:VAL:HG12	1.96	0.48
2:D:1535:ASP:C	2:D:1537:ASN:H	2.17	0.48
2:D:1628:PHE:O	2:D:1629:ALA:C	2.51	0.48
2:D:285:ILE:HD12	2:D:285:ILE:H	1.71	0.48
3:Y:88:GLY:C	3:Y:90:ASP:N	2.66	0.48
1:A:1022:PHE:O	1:A:1024:TYR:N	2.47	0.48
1:A:1140:ASN:O	1:A:1143:TYR:HB3	2.14	0.48
1:A:1244:THR:HG22	1:A:1246:ARG:H	1.75	0.48
1:A:1323:LEU:CG	1:A:1324:HIS:H	2.27	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
1:A:243:PHE:CE2	1:A:304:GLU:HA	2.48	0.48
1:A:274:ASP:HA	1:A:322:TYR:CE2	2.49	0.48
1:A:436:LYS:HB2	1:A:449:ARG:CG	2.43	0.48
1:A:965:LEU:C	1:A:967:LEU:H	2.17	0.48
2:B:370:ASP:N	2:B:370:ASP:OD1	2.46	0.48
2:B:478:TYR:CD1	2:B:478:TYR:O	2.58	0.48
2:B:541:LYS:O	2:B:543:THR:CG2	2.62	0.48
1:C:1376:SER:OG	1:C:1503:LYS:HG3	2.14	0.48
1:C:198:MET:SD	1:C:218:GLU:HG3	2.54	0.48
1:C:397:VAL:O	1:C:399:GLN:NE2	2.46	0.48
1:C:371:ILE:CD1	1:C:433:PHE:CE2	2.93	0.48
1:C:525:SER:CB	2:D:399:ILE:HG21	2.44	0.48
1:C:543:TYR:CD1	1:C:543:TYR:C	2.86	0.48
1:C:576:SER:HB2	1:C:589:SER:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:504:LEU:HD23	1:C:649:ALA:O	2.14	0.48
1:C:680:GLN:O	1:C:684:GLU:CG	2.62	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
2:D:1381:ILE:CG2	2:D:1459:TYR:HE1	2.25	0.48
2:D:56:ILE:O	2:D:70:GLN:HA	2.14	0.48
2:D:618:LEU:HD22	2:D:636:THR:HA	1.95	0.48
2:D:760:LYS:HE3	2:D:776:MET:SD	2.54	0.48
4:G:1:NAG:H3	4:G:2:NAG:O5	2.14	0.48
3:Y:132:THR:CG2	3:Y:155:ILE:HB	2.41	0.48
1:A:1108:VAL:HG21	1:A:1167:ALA:CB	2.40	0.47
1:A:1113:LEU:HD22	1:A:1114:ASP:H	1.77	0.47
1:A:1379:LEU:HD21	1:A:1495:VAL:HG13	1.95	0.47
1:A:1583:ASP:N	1:A:1594:LYS:HZ1	2.12	0.47
1:A:614:ARG:CD	1:A:614:ARG:N	2.76	0.47
1:A:43:VAL:HG12	1:A:79:PHE:O	2.13	0.47
1:A:986:GLU:HG2	1:A:987:ILE:N	2.29	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
2:B:69:PHE:CE1	2:B:87:ILE:HA	2.49	0.47
1:A:883:CYS:N	2:B:902:GLU:OE2	2.46	0.47
1:C:1076:THR:HG22	1:C:1120:GLU:HA	1.94	0.47
1:C:1186:PHE:HA	1:C:1250:THR:CG2	2.41	0.47
1:C:1247:MET:O	1:C:1251:THR:HG23	2.14	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:682:LYS:HZ3	1:C:686:ILE:HD11	1.79	0.47
1:C:977:LEU:HD22	1:C:978:SER:H	1.78	0.47
2:D:165:PHE:CZ	2:D:199:ILE:CD1	2.96	0.47
2:D:482:LEU:CD1	2:D:521:VAL:HB	2.44	0.47
2:D:52:LYS:HE3	2:D:111:PRO:O	2.13	0.47
2:D:69:PHE:HD2	2:D:70:GLN:N	2.12	0.47
1:A:1053:MET:HE1	1:A:1086:LEU:HD13	1.95	0.47
1:A:123:ASN:C	1:A:123:ASN:OD1	2.53	0.47
1:A:38:ASN:ND2	3:X:150:ILE:HG12	2.28	0.47
1:A:682:LYS:NZ	1:A:686:ILE:HD11	2.29	0.47
1:A:837:GLU:OE2	1:A:1430:THR:HB	2.14	0.47
2:B:1371:TYR:CD1	2:B:1377:SER:CB	2.98	0.47
2:B:1506:ILE:HB	2:B:1627:ASP:HB3	1.97	0.47
2:B:220:VAL:O	2:B:222:PRO:N	2.47	0.47
2:B:322:THR:CG2	2:B:327:ASP:H	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:544:CYS:HB3	2:B:546:GLY:O	2.13	0.47
2:B:56:ILE:O	2:B:70:GLN:HA	2.14	0.47
2:B:862:LYS:HZ2	2:B:1519:ASN:CB	2.27	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:C:285:THR:O	1:C:285:THR:CG2	2.59	0.47
1:C:394:THR:HG23	1:C:402:SER:O	2.14	0.47
1:C:871:PRO:HD2	1:C:872:VAL:N	2.29	0.47
1:C:944:LEU:HD23	1:C:944:LEU:H	1.78	0.47
2:D:237:ILE:HD11	2:D:309:LEU:CB	2.36	0.47
2:D:575:VAL:O	2:D:759:THR:HA	2.14	0.47
1:A:1562:LYS:O	1:A:1563:VAL:CG1	2.62	0.47
1:A:1562:LYS:HD3	1:A:1648:TRP:HE1	1.80	0.47
1:A:42:GLN:HE22	1:A:44:TYR:HB2	1.78	0.47
1:A:569:ASN:CG	1:A:570:GLN:N	2.68	0.47
2:B:1279:ILE:HG22	2:B:1288:ILE:CB	2.43	0.47
2:B:41:ILE:O	2:B:85:PRO:HD2	2.14	0.47
2:B:955:PRO:O	2:B:957:THR:HG23	2.14	0.47
1:C:1003:LEU:HA	1:C:1004:PRO:HD2	1.51	0.47
1:C:1506:THR:HG22	1:C:1507:MET:N	2.29	0.47
1:C:1583:ASP:N	1:C:1594:LYS:NZ	2.63	0.47
1:C:216:TYR:N	1:C:216:TYR:CD2	2.82	0.47
1:C:489:LYS:HG2	1:C:490:SER:OG	2.14	0.47
2:D:25:TYR:CE2	2:D:113:VAL:HG22	2.49	0.47
2:D:1370:ARG:NH1	2:D:1372:LEU:HG	2.29	0.47
2:D:386:SER:O	2:D:398:LEU:HD11	2.14	0.47
2:D:148:PHE:CZ	2:D:792:VAL:HG11	2.48	0.47
3:X:42:ASP:HB3	3:X:45:ASP:HB2	1.95	0.47
3:Y:88:GLY:C	3:Y:90:ASP:H	2.15	0.47
1:A:1018:VAL:HG11	1:A:1048:LYS:HB3	1.95	0.47
1:A:1559:TYR:O	1:A:1621:GLY:N	2.47	0.47
1:A:72:HIS:CD2	1:A:72:HIS:C	2.87	0.47
1:A:87:ILE:CD1	1:A:87:ILE:N	2.55	0.47
2:B:1386:MET:HE2	2:B:1386:MET:HA	1.96	0.47
2:B:1482:ASN:H	2:B:1495:GLU:HG2	1.79	0.47
2:B:1567:ARG:HD2	2:B:1567:ARG:HA	1.63	0.47
2:B:1506:ILE:CD1	2:B:1628:PHE:HE1	2.27	0.47
2:B:575:VAL:CG2	2:B:762:LEU:HD11	2.44	0.47
1:C:1069:TRP:HH2	1:C:1465:ASN:ND2	2.12	0.47
1:C:1637:TYR:N	1:C:1637:TYR:CD2	2.83	0.47
1:C:1663:ASN:O	1:C:1666:GLU:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:GLU:HG2	1:C:349:LEU:CD2	2.43	0.47
1:C:560:TRP:CH2	1:C:673:LEU:CD2	2.98	0.47
1:C:592:MET:O	1:C:783:ARG:HA	2.15	0.47
1:C:641:ASN:O	1:C:642:ASN:C	2.53	0.47
2:D:1330:ASN:ND2	2:D:1330:ASN:N	2.62	0.47
2:D:1399:ARG:HG2	2:D:1399:ARG:HH11	1.79	0.47
2:D:1638:PHE:N	2:D:1638:PHE:CD2	2.82	0.47
2:D:161:VAL:CG2	2:D:180:LEU:HD21	2.38	0.47
2:D:531:ILE:O	2:D:617:ASN:ND2	2.41	0.47
3:X:103:VAL:HA	3:X:121:GLY:O	2.15	0.47
1:A:1271:ILE:HD13	1:A:1300:TYR:CZ	2.50	0.47
1:A:617:LYS:HD2	1:A:622:ARG:NH2	2.22	0.47
1:A:695:VAL:HG12	1:A:727:ALA:CB	2.44	0.47
2:B:120:LEU:HA	2:B:120:LEU:HD13	1.76	0.47
2:B:1446:PHE:C	2:B:1448:VAL:H	2.18	0.47
2:B:1575:LEU:N	2:B:1575:LEU:CD2	2.77	0.47
2:B:1575:LEU:HD13	2:B:1581:TYR:CZ	2.49	0.47
2:B:1614:ASP:C	2:B:1616:CYS:N	2.67	0.47
2:B:148:PHE:CZ	2:B:792:VAL:HG11	2.50	0.47
2:B:173:VAL:HA	2:B:964:ILE:CD1	2.44	0.47
1:C:1572:ASN:O	1:C:1573:VAL:HG23	2.14	0.47
1:C:284:GLN:H	1:C:310:LEU:HD22	1.79	0.47
1:C:968:VAL:HG23	1:C:971:THR:OG1	2.14	0.47
2:D:1482:ASN:HB2	2:D:1495:GLU:HA	1.96	0.47
2:D:778:PHE:N	2:D:778:PHE:CD2	2.83	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:1328:MET:HE2	1:A:1328:MET:HA	1.97	0.47
1:A:231:ILE:HG23	1:A:231:ILE:O	2.14	0.47
1:A:243:PHE:HE2	1:A:304:GLU:CA	2.28	0.47
1:A:443:PRO:CD	1:A:446:ASN:HB2	2.44	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:A:892:SER:HB3	1:A:893:SER:H	1.41	0.47
2:B:35:THR:HB	2:B:91:ALA:HB2	1.97	0.47
1:A:419:SER:CB	2:B:459:ASN:HD22	2.15	0.47
1:C:1079:THR:HB	1:C:1107:LEU:HD11	1.96	0.47
1:C:1427:SER:CB	1:C:1492:THR:HG23	2.44	0.47
1:C:1468:PRO:CD	1:C:1473:LEU:HD13	2.44	0.47
1:C:224:LEU:CD2	1:C:225:PRO:HD2	2.43	0.47
1:C:614:ARG:CD	1:C:614:ARG:N	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:680:GLN:O	1:C:682:LYS:N	2.48	0.47
1:C:840:GLN:HE21	1:C:897:THR:HG21	1.80	0.47
1:C:963:ILE:HA	1:C:973:ILE:HD11	1.97	0.47
2:D:1438:LEU:C	2:D:1438:LEU:HD13	2.34	0.47
2:D:1517:GLU:O	2:D:1518:THR:C	2.53	0.47
2:D:1523:VAL:O	2:D:1548:ILE:HB	2.14	0.47
2:D:280:LEU:HD11	2:D:1379:MET:HG3	1.97	0.47
2:D:433:ILE:HG22	2:D:434:ALA:N	2.28	0.47
2:D:484:LEU:HD11	2:D:626:LEU:CG	2.45	0.47
2:D:543:THR:O	2:D:599:TRP:NE1	2.39	0.47
2:D:794:PHE:C	2:D:794:PHE:CD2	2.88	0.47
2:D:870:PHE:CD1	2:D:878:ARG:NH2	2.83	0.47
3:X:119:VAL:HG13	3:X:212:MET:SD	2.55	0.47
3:Y:136:LEU:HA	3:Y:224:ILE:O	2.14	0.47
1:A:1159:CYS:O	1:A:1161:LEU:HD23	2.14	0.47
1:A:1279:ARG:NH1	1:A:1280:TYR:CD2	2.83	0.47
1:A:1307:LEU:HD22	1:A:1307:LEU:H	1.79	0.47
1:A:394:THR:HG23	1:A:402:SER:O	2.14	0.47
1:A:518:PHE:O	1:A:520:ASP:N	2.43	0.47
2:B:189:PRO:C	2:B:191:LEU:H	2.17	0.47
2:B:511:THR:O	2:B:513:ASP:N	2.48	0.47
2:B:563:MET:HB3	2:B:778:PHE:HE2	1.78	0.47
2:B:83:VAL:C	2:B:85:PRO:HD3	2.35	0.47
2:B:846:VAL:HG22	2:B:847:ARG:N	2.28	0.47
1:C:1249:GLU:O	1:C:1253:TYR:HD2	1.98	0.47
1:C:240:TYR:CD2	1:C:241:LYS:N	2.82	0.47
1:C:383:VAL:O	1:C:383:VAL:CG2	2.62	0.47
1:C:42:GLN:HE22	1:C:44:TYR:HB2	1.80	0.47
1:C:670:LYS:HD2	1:C:671:GLU:N	2.29	0.47
1:C:923:LEU:C	1:C:923:LEU:HD23	2.34	0.47
2:D:143:VAL:O	2:D:143:VAL:HG12	2.14	0.47
2:D:168:PRO:HD3	2:D:197:TRP:CD1	2.49	0.47
2:D:206:SER:O	2:D:208:GLU:N	2.47	0.47
2:D:249:ALA:O	2:D:257:VAL:HB	2.15	0.47
2:D:314:LEU:HD12	2:D:314:LEU:HA	1.71	0.47
2:D:478:TYR:CD1	2:D:478:TYR:O	2.58	0.47
3:X:166:ASP:OD2	3:X:207:LEU:CG	2.62	0.47
1:A:1031:TRP:CZ3	1:A:1042:LYS:HA	2.50	0.47
1:A:1186:PHE:HA	1:A:1250:THR:CG2	2.43	0.47
1:A:1293:ALA:O	1:A:1294:ILE:C	2.51	0.47
1:A:1309:LEU:CD1	1:A:1328:MET:HG3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:59:TYR:CD1	1:A:60:PRO:HG3	2.49	0.47
1:A:656:ASN:OD1	1:A:658:ASN:CB	2.51	0.47
2:B:108:VAL:O	2:B:114:ARG:HA	2.14	0.47
2:B:280:LEU:HD22	2:B:1462:TYR:HE2	1.78	0.47
2:B:34:ARG:HD2	2:B:488:LYS:HZ3	1.79	0.47
2:B:642:ALA:O	2:B:643:LYS:HB3	2.15	0.47
2:B:794:PHE:C	2:B:794:PHE:CD2	2.88	0.47
1:C:1179:THR:HG22	1:C:1180:LEU:HD23	1.97	0.47
1:C:1215:GLU:OE1	1:C:1235:LYS:HD3	2.15	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
1:C:1504:GLN:OE1	1:C:1506:THR:OG1	2.28	0.47
1:C:1552:ALA:HB2	1:C:1620:MET:CE	2.45	0.47
1:C:576:SER:CB	1:C:577:PRO:CD	2.91	0.47
1:C:595:GLY:O	1:C:596:MET:C	2.52	0.47
2:D:108:VAL:O	2:D:114:ARG:HA	2.15	0.47
2:D:1387:LEU:O	2:D:1390:PHE:HB2	2.14	0.47
2:D:1506:ILE:HD12	2:D:1628:PHE:CE1	2.49	0.47
2:D:1623:LYS:NZ	2:D:1623:LYS:CB	2.78	0.47
2:D:173:VAL:HG11	2:D:186:TYR:OH	2.13	0.47
2:D:566:LYS:O	2:D:567:LEU:HD23	2.15	0.47
1:A:1047:LYS:O	1:A:1048:LYS:C	2.53	0.47
1:A:1585:TYR:CZ	1:A:1586:LYS:HB3	2.49	0.47
1:A:576:SER:CB	1:A:577:PRO:CD	2.91	0.47
1:A:680:GLN:O	1:A:684:GLU:CG	2.62	0.47
1:A:802:VAL:HG12	1:A:803:GLY:N	2.29	0.47
2:B:1567:ARG:NH1	2:B:1567:ARG:HG3	2.29	0.47
2:B:230:PRO:HG3	2:B:333:GLN:CG	2.44	0.47
2:B:482:LEU:HD11	2:B:521:VAL:HB	1.96	0.47
2:B:79:GLY:O	2:B:81:MET:N	2.47	0.47
1:C:1076:THR:HG23	1:C:1077:TRP:N	2.29	0.47
1:C:1240:PRO:HB2	1:C:1242:THR:CG2	2.45	0.47
1:C:1402:ILE:HG13	1:C:1479:ILE:HD13	1.95	0.47
1:C:532:GLN:O	1:C:534:MET:N	2.47	0.47
1:C:993:SER:O	1:C:995:GLU:N	2.48	0.47
2:D:173:VAL:HG13	2:D:964:ILE:HD11	1.95	0.47
1:C:473:HIS:CE1	2:D:455:LYS:NZ	2.83	0.47
2:D:482:LEU:HD11	2:D:521:VAL:HB	1.97	0.47
2:D:813:VAL:CG1	2:D:840:VAL:HG22	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:150:ILE:HD12	3:Y:150:ILE:C	2.34	0.47
3:Y:85:PHE:N	3:Y:85:PHE:HD1	2.13	0.47
1:A:1084:ARG:CA	1:A:1151:GLY:HA2	2.45	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
1:A:239:GLY:O	1:A:240:TYR:C	2.52	0.47
1:A:530:VAL:CG2	1:A:563:ILE:HD12	2.45	0.47
1:A:25:ILE:HG12	1:A:655:THR:CG2	2.45	0.47
2:B:1517:GLU:O	2:B:1518:THR:C	2.53	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
2:B:466:VAL:HG12	2:B:524:TYR:HE2	1.79	0.47
1:C:25:ILE:HG13	1:C:106:VAL:HG21	1.96	0.47
1:C:1215:GLU:HA	1:C:1215:GLU:OE1	2.15	0.47
1:C:148:LEU:HG	1:C:153:LYS:O	2.14	0.47
1:C:263:ALA:O	1:C:291:MET:HE3	2.14	0.47
1:C:407:SER:O	1:C:420:PHE:HE1	1.98	0.47
1:C:997:ILE:HG13	1:C:997:ILE:O	2.15	0.47
2:D:1593:THR:HG21	2:D:1596:LYS:HE3	1.97	0.47
3:Y:128:LYS:HD3	3:Y:158:GLU:CD	2.35	0.47
3:Y:194:LYS:HZ2	3:Y:197:ASN:HD22	1.63	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: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
1:A:186:PRO:O	1:A:187:ASP:C	2.53	0.47
1:A:543:TYR:HB3	1:A:556:SER:HB3	1.97	0.47
2:B:433:ILE:CG2	2:B:434:ALA:N	2.78	0.47
2:B:787:TRP:HB2	2:B:808:ILE:HG22	1.97	0.47
2:B:829:GLN:HE22	2:B:883:VAL:CG1	2.19	0.47
1:C:323:LEU:HD22	1:C:324:TYR:N	2.30	0.47
1:C:510:ILE:O	1:C:511:HIS:ND1	2.48	0.47
2:D:1367:ILE:HB	2:D:1438:LEU:CD1	2.45	0.47
2:D:1522:TYR:O	2:D:1522:TYR:CD2	2.68	0.47
2:D:1561:HIS:NE2	2:D:1597:ILE:CD1	2.78	0.47
1:C:525:SER:HB2	2:D:399:ILE:HG21	1.96	0.47
3:X:85:PHE:CE1	3:X:117:SER:HB3	2.50	0.47
3:X:52:SER:OG	3:X:53:GLU:N	2.48	0.47
3:X:86:LEU:HG	3:X:91:LYS:CG	2.45	0.47
3:Y:46:LEU:HD12	3:Y:180:TYR:CE1	2.50	0.47
1:A:1583:ASP:N	1:A:1594:LYS:NZ	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:24:VAL:HG11	1:A:543:TYR:HE2	1.79	0.46
2:B:1486:ILE:HD11	2:B:1591:LEU:CD2	2.45	0.46
2:B:1602:THR:O	2:B:1604:ASN:N	2.43	0.46
2:B:236:TYR:C	2:B:238:ASP:H	2.18	0.46
2:B:338:ILE:O	2:B:339:VAL:CG1	2.64	0.46
2:B:342:PRO:HG2	2:B:420:LEU:CD1	2.44	0.46
2:B:563:MET:HA	2:B:563:MET:CE	2.45	0.46
1:C:1083:LEU:HD22	1:C:1104:LEU:HD21	1.96	0.46
1:C:1453:TYR:O	1:C:1453:TYR:CD1	2.67	0.46
1:C:219:VAL:CG1	1:C:219:VAL:O	2.63	0.46
1:C:239:GLY:O	1:C:240:TYR:C	2.53	0.46
1:C:302:ASP:HB3	1:C:305:THR:HB	1.97	0.46
1:C:23:TYR:HA	1:C:43:VAL:HA	1.96	0.46
1:C:481:HIS:HB2	2:D:388:GLY:HA2	1.96	0.46
1:C:461:SER:HB2	1:C:553:GLU:CD	2.34	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:D:1457:LYS:HG2	2:D:1469:THR:OG1	2.15	0.46
2:D:263:VAL:HG21	2:D:292:ALA:CB	2.45	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
2:D:750:ASP:OD1	2:D:750:ASP:C	2.53	0.46
2:D:866:TYR:HE2	2:D:868:GLN:OE1	1.99	0.46
3:X:166:ASP:O	3:X:170:ARG:HG3	2.15	0.46
1:A:1031:TRP:CH2	1:A:1042:LYS:HG3	2.51	0.46
1:A:975:ARG:NH2	1:A:1346:LEU:HD22	2.30	0.46
1:A:1453:TYR:CD1	1:A:1453:TYR:O	2.69	0.46
1:A:1506:THR:HG22	1:A:1507:MET:N	2.31	0.46
1:A:152:LEU:HD13	1:A:152:LEU:HA	1.49	0.46
1:A:287:MET:SD	1:A:299:VAL:HG23	2.55	0.46
2:B:961:THR:HG22	2:B:1327:THR:CB	2.45	0.46
2:B:143:VAL:O	2:B:143:VAL:HG12	2.15	0.46
2:B:45:ALA:HB3	2:B:81:MET:CE	2.46	0.46
2:B:52:LYS:HE3	2:B:111:PRO:O	2.14	0.46
2:B:541:LYS:O	2:B:543:THR:HG23	2.15	0.46
2:B:613:SER:HA	2:B:620:VAL:HG23	1.96	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
1:C:1232:LEU:CG	1:C:1233:GLN:HG3	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1616:GLN:OE1	1:C:1650:ARG:HD3	2.15	0.46
1:C:189:LYS:HG3	1:C:190:ILE: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:906:GLY:N	1:C:929:VAL:HB	2.24	0.46
1:C:963:ILE:CG2	1:C:967:LEU:HD23	2.42	0.46
2:D:1299:LEU:HB3	2:D:1301:ARG:HD3	1.96	0.46
2:D:452:THR:O	2:D:453:GLU:O	2.34	0.46
2:D:481:TYR:CE2	2:D:493:GLY:N	2.83	0.46
2:D:39:GLU:O	2:D:87:ILE:HD12	2.15	0.46
1:A:1068:VAL:CG1	1:A:1069:TRP:N	2.78	0.46
1:A:127:PHE:CE1	1:A:626:PHE:CD2	3.04	0.46
1:A:1304:VAL:HG12	1:A:1305:LYS:H	1.80	0.46
1:A:20:GLU:OE2	1:A:20:GLU:O	2.33	0.46
1:A:773:TRP:CE3	1:A:774:LEU:HB2	2.51	0.46
1:A:74:SER:C	1:A:79:PHE:CE1	2.89	0.46
1:A:923:LEU:HD23	1:A:923:LEU:C	2.35	0.46
2:B:1504:GLU:O	2:B:1624:LEU:HD13	2.14	0.46
2:B:1535:ASP:C	2:B:1537:ASN:H	2.18	0.46
2:B:44:GLU:OE1	2:B:480:THR:HG21	2.15	0.46
2:B:953:ARG:CG	2:B:954:VAL:N	2.78	0.46
1:C:1622:LYS:HD2	1:C:1642:LEU:CB	2.44	0.46
1:C:365:PRO:HG2	1:C:464:TYR:HE2	1.79	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:949:ILE:O	1:C:949:ILE:HG22	2.14	0.46
2:D:1294:TYR:O	2:D:1294:TYR:CD2	2.67	0.46
2:D:1589:ASP:HB3	2:D:1600:ILE:HG13	1.97	0.46
2:D:449:ILE:HD13	2:D:462:VAL:HG23	1.97	0.46
2:D:575:VAL:CG2	2:D:762:LEU:HD11	2.46	0.46
2:D:810:VAL:CG1	2:D:811:MET:N	2.79	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:500:ASN:O	1:A:542:VAL:HG13	2.16	0.46
1:A:680:GLN:O	1:A:681:LYS:C	2.53	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
2:B:1367:ILE:HD13	2:B:1456:VAL:HG21	1.96	0.46
2:B:137:TYR:HB2	2:B:216:VAL:HG23	1.98	0.46
2:B:1399:ARG:HG2	2:B:1399:ARG:HH11	1.79	0.46
2:B:1496:THR:HG23	2:B:1603:LYS:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1499:SER:HA	2:B:1572:ALA:O	2.16	0.46
2:B:129:PHE:CE2	2:B:598:ILE:HG23	2.50	0.46
2:B:69:PHE:C	2:B:69:PHE:HD2	2.19	0.46
2:B:778:PHE:CD2	2:B:778:PHE:N	2.82	0.46
2:B:850:LEU:HB2	2:B:882:PHE:CD1	2.50	0.46
2:B:940:THR:HG22	2:B:940:THR:O	2.15	0.46
1:C:1080:ALA:HB1	1:C:1148:THR:HA	1.97	0.46
1:C:174:VAL:HG22	1:C:175:GLU:H	1.80	0.46
1:C:20:GLU:HG3	1:C:547:THR:CB	2.45	0.46
1:C:241:LYS:NZ	1:C:351:PRO:HB3	2.30	0.46
1:C:428:VAL:HG22	1:C:429:THR:N	2.29	0.46
1:C:489:LYS:NZ	2:D:502:ASN:H	2.13	0.46
1:C:680:GLN:O	1:C:681:LYS:C	2.54	0.46
1:C:811:VAL:O	1:C:811:VAL:HG12	2.16	0.46
1:C:829:ILE:HA	1:C:830:PRO:HD3	1.78	0.46
2:D:296:ARG:HG3	2:D:296:ARG:NH1	2.29	0.46
2:D:466:VAL:HG12	2:D:524:TYR:HE2	1.80	0.46
2:D:787:TRP:HB2	2:D:808:ILE:HG22	1.96	0.46
2:D:920:VAL:O	2:D:1330:ASN:HA	2.15	0.46
2:D:929:LYS:HD3	2:D:929:LYS:HA	1.70	0.46
3:Y:185:LYS:HG2	3:Y:186:TYR:CD2	2.51	0.46
3:Y:119:VAL:HG21	3:Y:209:PHE:CB	2.44	0.46
3:Y:77:PRO:O	3:Y:78:LYS:CB	2.63	0.46
1:A:1159:CYS:C	1:A:1161:LEU:H	2.18	0.46
1:A:1255:LEU:HD13	1:A:1267:VAL:HG13	1.97	0.46
1:A:161:LEU:HD21	1:A:185:PHE:CD2	2.51	0.46
1:A:274:ASP:CG	1:A:275:LEU:N	2.69	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:A:787:GLN:O	1:A:788:PHE:HB3	2.15	0.46
2:B:1363:LEU:HD23	2:B:1442:ILE:HG12	1.98	0.46
2:B:1573:LEU:HB3	2:B:1575:LEU:HD23	1.97	0.46
2:B:361:GLU:HB3	2:B:399:ILE:HD13	1.98	0.46
2:B:352:LYS:HG3	2:B:430:MET:HE1	1.98	0.46
2:B:481:TYR:HE2	2:B:493:GLY:HA3	1.81	0.46
2:B:599:TRP:CE3	2:B:602:ILE:HD12	2.51	0.46
2:B:750:ASP:C	2:B:750:ASP:OD1	2.53	0.46
1:C:1022:PHE:CE2	1:C:1092:TYR:CD1	3.04	0.46
1:C:1535:MET:HA	1:C:1645:ILE:HB	1.98	0.46
1:C:42:GLN:CA	1:C:80:GLN:HG3	2.42	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
2:D:1567:ARG:HG3	2:D:1567:ARG:HH11	1.80	0.46
2:D:1561:HIS:NE2	2:D:1597:ILE:HD13	2.29	0.46
2:D:825:VAL:HG11	2:D:918:GLU:HB3	1.97	0.46
3:X:136:LEU:HA	3:X:224:ILE:O	2.14	0.46
3:X:179:LEU:HD11	3:X:180:TYR:CE1	2.50	0.46
1:A:119:ILE:C	1:A:119:ILE:HD12	2.36	0.46
1:A:1244:THR:O	1:A:1245:ALA:C	2.54	0.46
1:A:125:PHE:N	1:A:125:PHE:CD1	2.83	0.46
1:A:128:ILE:HD12	1:A:201:ILE:CG2	2.41	0.46
1:A:1671:ILE:HD13	1:A:1676:CYS:SG	2.56	0.46
1:A:216:TYR:CD2	1:A:216:TYR:N	2.82	0.46
1:A:374:GLN:HG2	1:A:382:LEU:CD2	2.45	0.46
1:A:371:ILE:CD1	1:A:433:PHE:CE2	2.96	0.46
1:A:42:GLN:OE1	1:A:500:ASN:ND2	2.48	0.46
1:A:644:ASN:O	1:A:645:VAL:C	2.54	0.46
1:A:86:THR:C	1:A:87:ILE:HD13	2.35	0.46
1:A:982:LEU:C	1:A:984:VAL:N	2.68	0.46
2:B:1424:ILE:HD13	2:B:1424:ILE:N	2.27	0.46
2:B:1500:LEU:HD22	2:B:1607:ILE:HB	1.98	0.46
2:B:398:LEU:HA	2:B:398:LEU:HD23	1.50	0.46
2:B:476:ILE:HG12	2:B:524:TYR:CD2	2.50	0.46
2:B:525:GLN:NE2	2:B:528:ASN:H	2.13	0.46
1:C:1093:VAL:HG12	1:C:1095:GLN:NE2	2.30	0.46
1:C:1426:ILE:O	1:C:1426:ILE:HG22	2.16	0.46
1:C:1572:ASN:C	1:C:1573:VAL:HG23	2.35	0.46
1:C:909:ASN:HD21	5:C:2003:NAG:H83	1.81	0.46
1:C:705:VAL:HA	1:C:739:ARG:HH12	1.80	0.46
1:C:78:LYS:O	1:C:80:GLN:N	2.49	0.46
1:C:853:MET:O	1:C:888:VAL:HG12	2.15	0.46
2:D:1351:ASN:N	2:D:1351:ASN:OD1	2.44	0.46
2:D:1573:LEU:HB3	2:D:1575:LEU:HD23	1.98	0.46
2:D:398:LEU:HA	2:D:398:LEU:HD23	1.53	0.46
2:D:933:ARG:HH11	2:D:933:ARG:CG	2.18	0.46
3:Y:42:ASP:HB3	3:Y:45:ASP:HB2	1.98	0.46
1:A:1025:LEU:HD13	1:A:1031:TRP:CZ3	2.51	0.46
1:A:1227:PHE:HA	1:A:1228:TRP:CE3	2.51	0.46
1:A:938:SER:OG	1:A:1284:PHE:CE2	2.68	0.46
1:A:1561:TYR:CD1	1:A:1581:LEU:HD21	2.50	0.46
1:A:219:VAL:HG12	1:A:219:VAL:O	2.15	0.46
1:A:25:ILE:CG2	1:A:654:LEU:HB2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ILE:CG2	1:A:297:ALA:N	2.77	0.46
1:A:248:ILE:HB	1:A:299:VAL:HG13	1.97	0.46
1:A:383:VAL:HG23	1:A:386:VAL:HG23	1.98	0.46
1:A:554:LEU:H	1:A:658:ASN:ND2	2.11	0.46
1:A:827:MET:HE2	1:A:912:PHE:CE2	2.51	0.46
2:B:1508:VAL:HG13	2:B:1631:PHE:HB2	1.97	0.46
2:B:267:VAL:HG22	2:B:314:LEU:CD1	2.46	0.46
2:B:338:ILE:O	2:B:339:VAL:HG13	2.16	0.46
2:B:345:ILE:HG13	2:B:428:LYS:HB3	1.98	0.46
2:B:557:GLN:OE1	2:B:557:GLN:CA	2.58	0.46
2:B:582:LYS:O	2:B:583:ALA:C	2.53	0.46
1:C:1133:LEU:N	1:C:1133:LEU:CD1	2.71	0.46
1:C:1246:ARG:HB2	1:C:1246:ARG:CZ	2.46	0.46
1:C:1309:LEU:CD1	1:C:1328:MET:HG3	2.45	0.46
1:C:1406:ALA:O	1:C:1472:PHE:HA	2.16	0.46
1:C:1622:LYS:HZ2	1:C:1642:LEU:HD23	1.80	0.46
1:C:25:ILE:CD1	1:C:41:ILE:HG13	2.46	0.46
1:C:560:TRP:HH2	1:C:673:LEU:HD22	1.80	0.46
2:D:275:SER:O	2:D:277:PRO:HD3	2.16	0.46
2:D:384:PHE:CD2	2:D:384:PHE:N	2.84	0.46
4:G:1:NAG:HO3	4:G:2:NAG:C5	2.29	0.46
1:A:1128:LYS:O	1:A:1129:LEU:HD23	2.15	0.46
1:A:1127:ILE:HD11	1:A:1143:TYR:CE2	2.50	0.46
1:A:1641:SER:C	1:A:1643:THR:N	2.69	0.46
1:A:374:GLN:HG2	1:A:382:LEU:HD21	1.96	0.46
1:A:993:SER:C	1:A:995:GLU:N	2.60	0.46
2:B:122:SER:OG	2:B:124:GLN:HB3	2.15	0.46
2:B:148:PHE:CZ	2:B:792:VAL:CG1	2.99	0.46
2:B:1510:LEU:O	2:B:1513:GLU:N	2.48	0.46
2:B:484:LEU:HD11	2:B:626:LEU:CG	2.45	0.46
2:B:953:ARG:CG	2:B:954:VAL:H	2.29	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
1:C:1305:LYS:O	1:C:1307:LEU:HD13	2.16	0.46
1:C:1582:LEU:C	1:C:1594:LYS:HZ2	2.19	0.46
1:C:291:MET:HE2	1:C:291:MET:HB3	1.79	0.46
1:C:351:PRO:CG	1:C:442:LEU:HD11	2.45	0.46
1:C:766:ARG:H	1:C:766:ARG:HD3	1.80	0.46
2:D:1284:ARG:HG3	2:D:1285:GLU:N	2.30	0.46
2:D:1506:ILE:HD11	2:D:1628:PHE:CE1	2.43	0.46
2:D:164:GLU:HA	2:D:174:SER:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:511:THR:O	2:D:512:PRO:C	2.54	0.46
2:D:806:TYR:CD1	2:D:806:TYR:C	2.89	0.46
2:D:830:VAL:CG2	2:D:831:GLU:N	2.75	0.46
2:D:191:LEU:HD12	2:D:958:GLU:HG2	1.98	0.46
3:Y:174:VAL:O	3:Y:174:VAL:HG12	2.15	0.46
1:A:100:SER:C	1:A:101:TYR:CD2	2.89	0.46
1:A:1637:TYR:HD2	1:A:1637:TYR:N	2.14	0.46
1:A:164:ILE:HG22	1:A:165:ASP:O	2.16	0.46
1:A:186:PRO:O	1:A:187:ASP:O	2.33	0.46
1:A:296:ILE:HG23	1:A:297:ALA:N	2.30	0.46
1:A:592:MET:O	1:A:783:ARG:HA	2.15	0.46
1:A:909:ASN:HD21	5:A:2003:NAG:C8	2.29	0.46
2:B:1505:ARG:CG	2:B:1505:ARG:HH11	2.07	0.46
2:B:1529:LEU:CD1	2:B:1529:LEU:N	2.79	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
2:B:566:LYS:O	2:B:567:LEU:HD23	2.16	0.46
2:B:87:ILE:H	2:B:87:ILE:CD1	2.26	0.46
2:B:954:VAL:O	2:B:957:THR:HG23	2.16	0.46
1:C:1379:LEU:HD21	1:C:1495:VAL:HG13	1.97	0.46
1:C:1436:GLU:HG2	1:C:1453:TYR:HE2	1.81	0.46
1:C:307:VAL:O	1:C:311:SER:HB2	2.16	0.46
1:C:382:LEU:HA	1:C:382:LEU:HD23	1.80	0.46
1:C:477:LEU:HD23	1:C:480:GLU:OE1	2.15	0.46
1:C:493:ILE:CG2	1:C:495:LYS:HB2	2.46	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
3:X:58:SER:HB3	3:X:102:ASN:HD22	1.75	0.46
1:A:1079:THR:HB	1:A:1107:LEU:HD11	1.98	0.46
1:A:22:THR:HG21	1:A:657:ALA:CB	2.39	0.46
1:A:285:THR:CG2	1:A:285:THR:O	2.63	0.46
1:A:322:TYR:N	1:A:322:TYR:HD2	2.13	0.46
1:A:382:LEU:HD22	1:A:416:GLY:HA3	1.97	0.46
1:A:20:GLU:HB2	1:A:551:THR:HG22	1.98	0.46
1:A:690:TYR:CZ	1:A:692:HIS:CB	2.99	0.46
1:A:862:VAL:O	1:A:863:GLU:C	2.53	0.46
2:B:105:VAL:HG12	2:B:118:VAL:HA	1.97	0.46
2:B:139:PRO:HG2	2:B:218:LYS:HE2	1.96	0.46
2:B:1429:LYS:H	2:B:1429:LYS:HE3	1.80	0.46
2:B:1631:PHE:CD2	2:B:1632:SER:N	2.84	0.46
2:B:210:TYR:CG	2:B:211:THR:N	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:524:TYR:CD1	2:B:524:TYR:C	2.89	0.46
2:B:525:GLN:CD	2:B:525:GLN:O	2.54	0.46
2:B:640:SER:O	2:B:641:ALA:HB2	2.16	0.46
2:B:916:VAL:HG22	2:B:917:PRO:N	2.31	0.46
2:B:96:THR:HG22	2:B:97:ASP:N	2.31	0.46
1:C:1068:VAL:CG1	1:C:1069:TRP:N	2.76	0.46
1:C:1156:PHE:O	1:C:1160:PRO:HD3	2.16	0.46
1:C:1298:THR:O	1:C:1299:GLU:C	2.53	0.46
1:C:1332:ASN:O	1:C:1333:PHE:O	2.34	0.46
1:C:1346:LEU:HA	1:C:1346:LEU:HD12	1.48	0.46
1:C:1582:LEU:C	1:C:1594:LYS:NZ	2.70	0.46
1:C:161:LEU:HD11	1:C:185:PHE:CE2	2.50	0.46
1:C:1627:ILE:O	1:C:1627:ILE:HG13	2.16	0.46
1:C:165:ASP:HA	1:C:166:PRO:HD2	1.76	0.46
1:C:545:ILE:HG12	1:C:545:ILE:H	1.41	0.46
1:C:569:ASN:H	1:C:569:ASN:HD22	1.64	0.46
1:C:553:GLU:HA	1:C:658:ASN:HD22	1.81	0.46
2:D:1347:VAL:CG2	2:D:1456:VAL:HG11	2.43	0.46
2:D:1525:LYS:HE3	2:D:1610:TRP:CE2	2.51	0.46
2:D:873:LYS:CD	2:D:873:LYS:N	2.79	0.46
2:D:857:CYS:HB3	2:D:885:VAL:CG2	2.45	0.46
2:D:954:VAL:CG1	2:D:955:PRO:HD2	2.38	0.46
3:X:128:LYS:HD3	3:X:158:GLU:CD	2.36	0.46
3:X:190:ILE:HG12	3:X:190:ILE:O	2.16	0.46
3:Y:215:VAL:O	3:Y:216:LEU:HD13	2.15	0.46
1:A:999:ILE:HD12	1:A:1001:THR:O	2.16	0.45
1:A:148:LEU:HA	1:A:154:PRO:O	2.15	0.45
1:A:364:LYS:HD2	1:A:364:LYS:N	2.32	0.45
1:A:376:LYS:HA	1:A:381:GLN:O	2.15	0.45
1:A:560:TRP:CH2	1:A:562:ASN:HB2	2.51	0.45
1:A:25:ILE:CB	1:A:654:LEU:HB2	2.46	0.45
2:B:1290:TYR:CD2	2:B:1301:ARG:HB3	2.51	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
2:B:416:ASN:CA	2:B:425:GLN:HE22	2.20	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:1162:VAL:CG2	1:C:1163:LYS:N	2.79	0.45
1:C:1234:HIS:CG	1:C:1235:LYS:H	2.34	0.45
1:C:1317:TYR:CE1	1:C:1342:LEU:HD12	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:328:THR:HG22	1:C:328:THR:O	2.16	0.45
2:D:1393:ASP:OD1	2:D:1395:GLU:HB3	2.15	0.45
2:D:758:LEU:HD23	2:D:758:LEU:HA	1.70	0.45
2:D:575:VAL:HG23	2:D:762:LEU:CD1	2.46	0.45
2:D:851:LEU:HD21	2:D:865:ARG:HH21	1.81	0.45
3:Y:68:ASN:OD1	3:Y:69:GLY:N	2.40	0.45
1:A:57:LYS:O	1:A:102:VAL:HG22	2.16	0.45
1:A:1022:PHE:HE2	1:A:1092:TYR:CD1	2.34	0.45
1:A:1213:LYS:CG	1:A:1266:TYR:HE2	2.22	0.45
1:A:1562:LYS:O	1:A:1563:VAL:HG13	2.16	0.45
1:A:263:ALA:O	1:A:291:MET:HE3	2.16	0.45
1:A:455:ILE:HG22	1:A:456:ALA:H	1.79	0.45
1:A:705:VAL:HA	1:A:739:ARG:HH12	1.81	0.45
1:A:718:ILE:HD11	1:A:728:PHE:CD2	2.51	0.45
1:A:733:VAL:O	1:A:737:GLN:HG2	2.15	0.45
1:A:76:GLU:O	1:A:76:GLU:CD	2.55	0.45
1:A:871:PRO:HD2	1:A:872:VAL:H	1.78	0.45
1:A:883:CYS:O	1:A:884:VAL:C	2.54	0.45
2:B:132:THR:O	2:B:133:ASP:C	2.55	0.45
2:B:1482:ASN:HB2	2:B:1495:GLU:HA	1.97	0.45
2:B:570:ASP:O	2:B:573:ALA:CB	2.64	0.45
2:B:756:LEU:HD22	2:B:778:PHE:CD1	2.51	0.45
1:C:1525:CYS:C	1:C:1528:VAL:HG22	2.28	0.45
1:C:185:PHE:HD1	1:C:186:PRO:HD2	1.82	0.45
1:C:20:GLU:HG3	1:C:547:THR:HB	1.98	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:690:TYR:CZ	1:C:692:HIS:CB	2.98	0.45
1:C:590:LEU:HD21	1:C:774:LEU:HD11	1.99	0.45
2:D:107:GLN:HG3	2:D:116:GLU:HG3	1.98	0.45
2:D:208:GLU:O	2:D:209:ASN:C	2.55	0.45
2:D:618:LEU:HG	2:D:634:LEU:HD11	1.98	0.45
2:D:79:GLY:O	2:D:81:MET:N	2.50	0.45
3:X:107:GLN:CD	3:X:110:ILE:HD11	2.36	0.45
3:X:119:VAL:HG22	3:X:212:MET:HB2	1.99	0.45
1:A:1249:GLU:HG3	1:A:1289:ASP:CA	2.46	0.45
1:A:1300:TYR:CD2	1:A:1300:TYR:C	2.89	0.45
1:A:1128:LYS:HD3	1:A:1414:GLU:OE1	2.16	0.45
1:A:1646:GLU:HG2	1:A:1660:PHE:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:TYR:CD2	1:A:241:LYS:N	2.85	0.45
1:A:436:LYS:CB	1:A:449:ARG:HG2	2.45	0.45
1:A:365:PRO:HG2	1:A:464:TYR:HE2	1.80	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:A:710:THR:OG1	1:A:713:GLN:HG3	2.16	0.45
1:A:961:TYR:CD1	1:A:961:TYR:C	2.89	0.45
2:B:1371:TYR:HB2	2:B:1377:SER:HB3	1.99	0.45
2:B:760:LYS:HE3	2:B:776:MET:SD	2.55	0.45
2:B:853:ASN:HA	2:B:854:PRO:HD3	1.56	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
1:C:150:ASP:CG	1:C:151:ASP:N	2.70	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:96:GLN:HG3	1:C:97:ASN:N	2.31	0.45
2:D:103:TYR:N	2:D:103:TYR:CD2	2.85	0.45
2:D:130:ILE:HG21	2:D:199:ILE:HG21	1.98	0.45
2:D:1380:THR:HG22	2:D:1381:ILE:N	2.31	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
2:D:63:ARG:CB	2:D:65:GLN:HG3	2.46	0.45
2:D:954:VAL:O	2:D:957:THR:HG23	2.15	0.45
1:A:1215:GLU:HA	1:A:1215:GLU:OE1	2.16	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:A:224:LEU:CD2	1:A:225:PRO:HD2	2.44	0.45
1:A:61:ASP:O	1:A:62:LYS:CB	2.64	0.45
1:A:661:ASP:OD2	1:A:663:GLN:N	2.50	0.45
1:A:855:PHE:HB2	1:A:914:LEU:HD11	1.98	0.45
1:A:909:ASN:HA	1:A:926:THR:HA	1.98	0.45
1:A:989:SER:O	1:A:993:SER:HB3	2.16	0.45
2:B:962:LYS:HD2	2:B:1302:THR:CG2	2.46	0.45
2:B:178:VAL:HG21	2:B:183:PHE:CD1	2.52	0.45
2:B:531:ILE:HD11	2:B:634:LEU:CD2	2.45	0.45
2:B:778:PHE:N	2:B:778:PHE:HD2	2.13	0.45
1:C:484:ILE:HD13	1:C:540:LEU:HD21	1.96	0.45
1:C:690:TYR:CE1	1:C:696:LYS:HD2	2.52	0.45
1:C:773:TRP:CE3	1:C:774:LEU:HB2	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1313:VAL:HG21	2:D:1323:MET:HE2	1.98	0.45
2:D:1633:TYR:CE1	2:D:1637:GLU:OE1	2.69	0.45
2:D:778:PHE:N	2:D:778:PHE:HD2	2.14	0.45
2:D:953:ARG:CG	2:D:954:VAL:H	2.29	0.45
3:X:60:VAL:O	3:X:60:VAL:HG23	2.17	0.45
1:A:1023:HIS:O	1:A:1027:THR:HB	2.15	0.45
1:A:1328:MET:HB2	1:A:1328:MET:HE3	1.85	0.45
1:A:136:THR:O	1:A:139:GLN:HG3	2.17	0.45
1:A:1468:PRO:CD	1:A:1473:LEU:HD13	2.45	0.45
1:A:1557:ILE:HD13	1:A:1622:LYS:HG3	1.99	0.45
1:A:248:ILE:HD13	1:A:325:ILE:HD13	1.99	0.45
1:A:407:SER:O	1:A:420:PHE:HE1	1.99	0.45
2:B:103:TYR:CD2	2:B:103:TYR:N	2.83	0.45
2:B:188:LEU:HD13	2:B:216:VAL:CG2	2.47	0.45
2:B:162:ILE:HG22	2:B:202:LYS:O	2.16	0.45
1:A:481:HIS:CD2	2:B:387:MET:HG3	2.51	0.45
2:B:456:PRO:CG	2:B:515:ILE:HD11	2.46	0.45
2:B:842:GLU:O	2:B:844:ILE:HG23	2.17	0.45
2:B:922:LYS:NZ	2:B:952:ASP:OD2	2.50	0.45
1:C:1561:TYR:HE1	1:C:1581:LEU:HG	1.82	0.45
1:C:420:PHE:CD2	1:C:420:PHE:N	2.84	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:970:LYS:C	1:C:971:THR:CG2	2.85	0.45
2:D:105:VAL:HG12	2:D:118:VAL:HA	1.99	0.45
2:D:1529:LEU:N	2:D:1529:LEU:CD1	2.80	0.45
2:D:315:TYR:CD1	2:D:315:TYR:C	2.89	0.45
2:D:44:GLU:OE2	2:D:523:TYR:OH	2.33	0.45
1:C:473:HIS:CE1	2:D:455:LYS:HE3	2.51	0.45
2:D:570:ASP:O	2:D:573:ALA:CB	2.65	0.45
2:B:1344:HIS:ND1	4:F:1:NAG:C8	2.79	0.45
3:X:139:ASN:HB2	3:X:227:THR:HG23	1.98	0.45
1:A:1180:LEU:HD21	1:A:1208:ILE:HA	1.98	0.45
1:A:1488:LEU:HD12	1:A:1488:LEU:C	2.37	0.45
1:A:1570:VAL:HG22	1:A:1575:VAL:HA	1.99	0.45
1:A:1648:TRP:NE1	1:A:1664:LEU:CD2	2.79	0.45
1:A:222:TYR:HE2	1:A:224:LEU:HA	1.81	0.45
1:A:288:GLN:O	1:A:289:ASN:C	2.55	0.45
1:A:419:SER:HB2	2:B:459:ASN:ND2	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:TYR:CE1	1:A:696:LYS:HD2	2.52	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:B:1391:LEU:HB2	2:B:1417:MET:CE	2.47	0.45
2:B:159:LYS:HE2	2:B:180:LEU:HD12	1.99	0.45
2:B:410:PRO:CA	2:B:431:THR:HG22	2.46	0.45
2:B:518:PHE:CD2	2:B:518:PHE:O	2.70	0.45
2:B:613:SER:HA	2:B:620:VAL:CG2	2.46	0.45
2:B:780:LEU:HD11	2:B:787:TRP:HD1	1.82	0.45
2:B:862:LYS:NZ	2:B:1519:ASN:HB3	2.32	0.45
1:C:1113:LEU:HD23	1:C:1114:ASP:H	1.81	0.45
1:C:20:GLU:O	1:C:20:GLU:OE2	2.34	0.45
1:C:224:LEU:HD23	1:C:225:PRO:CD	2.44	0.45
1:C:892:SER:HB3	1:C:893:SER:H	1.41	0.45
2:D:184:TRP:CE3	2:D:184:TRP:N	2.81	0.45
2:D:378:PRO:HA	2:D:389:THR:HA	1.99	0.45
3:Y:222:ARG:HB2	3:Y:222:ARG:HE	1.60	0.45
1:A:1226:ARG:CD	1:A:1266:TYR:HE1	2.29	0.45
1:A:1186:PHE:HD1	1:A:1250:THR:HG22	1.82	0.45
1:A:1332:ASN:O	1:A:1333:PHE:O	2.35	0.45
1:A:532:GLN:HA	1:A:535:VAL:HG13	1.98	0.45
1:A:532:GLN:O	1:A:534:MET:N	2.49	0.45
1:A:256:TYR:HB3	1:A:848:TYR:OH	2.17	0.45
1:A:916:THR:O	1:A:918:PHE:N	2.50	0.45
2:B:1567:ARG:HH11	2:B:1567:ARG:HG3	1.82	0.45
2:B:208:GLU:O	2:B:209:ASN:C	2.55	0.45
2:B:267:VAL:HG22	2:B:314:LEU:HD12	1.99	0.45
2:B:481:TYR:CE1	2:B:506:MET:SD	2.97	0.45
2:B:855:ALA:O	2:B:856:PHE:CD1	2.70	0.45
1:C:1106:TRP:CZ2	1:C:1111:TYR:HE2	2.34	0.45
1:C:274:ASP:OD1	1:C:277:ASP:CG	2.55	0.45
1:C:284:GLN:HG2	1:C:310:LEU:CD1	2.47	0.45
1:C:374:GLN:HG2	1:C:382:LEU:CD2	2.47	0.45
1:C:376:LYS:HA	1:C:381:GLN:O	2.16	0.45
1:C:382:LEU:HD22	1:C:416:GLY:HA3	1.97	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
1:C:612:VAL:HG21	1:C:769:PHE:CE2	2.52	0.45
2:D:1382:ILE:CD1	2:D:1458:VAL:HG22	2.47	0.45
2:D:1524:TYR:HB3	2:D:1544:VAL:HG13	1.98	0.45
2:D:378:PRO:HB2	2:D:416:ASN:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:83:VAL:C	2:D:85:PRO:HD3	2.36	0.45
1:A:1142:LEU:HD13	1:A:1187:THR:CG2	2.47	0.45
1:A:120:THR:CG2	1:A:121:TYR:N	2.80	0.45
1:A:1636:ILE:HG22	1:A:1636:ILE:O	2.16	0.45
1:A:274:ASP:OD1	1:A:277:ASP:CG	2.55	0.45
1:A:505:SER:O	1:A:506:LYS:C	2.55	0.45
1:A:560:TRP:CH2	1:A:673:LEU:HD22	2.51	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:107:GLN:HG3	2:B:116:GLU:HG3	1.98	0.45
2:B:173:VAL:HG13	2:B:964:ILE:HD11	1.98	0.45
2:B:415:THR:O	2:B:425:GLN:CD	2.55	0.45
2:B:44:GLU:OE2	2:B:523:TYR:OH	2.31	0.45
2:B:891:LEU:H	2:B:891:LEU:HG	1.21	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
1:C:1272:LYS:O	1:C:1276:GLU:HG3	2.16	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
1:C:356:LEU:HG	1:C:452:TYR:CE2	2.51	0.45
1:C:847:ASN:OD1	1:C:847:ASN:C	2.55	0.45
1:C:977:LEU:HD22	1:C:978:SER:N	2.32	0.45
2:D:615:GLN:CB	2:D:616:ASN:HD22	2.29	0.45
2:D:953:ARG:CG	2:D:954:VAL:N	2.80	0.45
1:A:1053:MET:HE2	1:A:1086:LEU:HD13	1.98	0.45
1:A:1080:ALA:CB	1:A:1148:THR:HG22	2.47	0.45
1:A:1093:VAL:HG12	1:A:1095:GLN:NE2	2.31	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
1:A:23:TYR:CE2	1:A:111:PHE:CD2	3.05	0.45
1:A:477:LEU:N	1:A:477:LEU:HD22	2.31	0.45
1:A:481:HIS:CE1	2:B:387:MET:CE	3.00	0.45
1:A:491:PRO:O	1:A:491:PRO:HG2	2.17	0.45
1:A:760:VAL:HG22	1:A:760:VAL:O	2.17	0.45
1:A:96:GLN:O	1:A:97:ASN:O	2.35	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
2:B:297:ASP:N	2:B:297:ASP:OD2	2.49	0.45
2:B:481:TYR:CE2	2:B:493:GLY:HA3	2.51	0.45
2:B:598:ILE:HD13	2:B:800:ILE:HG21	1.95	0.45
1:C:1013:MET:HE2	1:C:1287:THR:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1629:TYR:HD2	1:C:1629:TYR:H	1.65	0.45
1:C:491:PRO:O	1:C:493:ILE:N	2.48	0.45
1:C:606:ASP:OD2	1:C:795:THR:HG21	2.17	0.45
2:D:1386:MET:HE2	2:D:1386:MET:HA	1.99	0.45
2:D:1623:LYS:HA	2:D:1623:LYS:HD2	1.68	0.45
2:D:524:TYR:CD1	2:D:524:TYR:C	2.90	0.45
2:D:824:VAL:CG2	2:D:828:GLU:OE1	2.64	0.45
2:D:96:THR:HG22	2:D:97:ASP:O	2.16	0.45
3:Y:191:ILE:O	3:Y:198:LYS:HA	2.17	0.45
1:A:1054:LEU:HD23	1:A:1057:MET:HE1	1.98	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
1:A:190:ILE:CG2	1:A:191:PRO:CD	2.95	0.45
1:A:489:LYS:NZ	2:B:502:ASN:H	2.14	0.45
1:A:506:LYS:O	1:A:508:LYS:N	2.49	0.45
1:A:523:TYR:CE2	2:B:465:ASN:CG	2.90	0.45
1:A:596:MET:SD	1:A:782:ARG:HG2	2.57	0.45
1:A:862:VAL:HG12	1:A:863:GLU:OE1	2.16	0.45
1:A:840:GLN:HE21	1:A:897:THR:HG21	1.81	0.45
1:A:950:TYR:C	1:A:952:THR:H	2.20	0.45
1:A:96:GLN:HG3	1:A:97:ASN:N	2.32	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
2:B:1631:PHE:CD2	2:B:1631:PHE:C	2.90	0.45
2:B:628:LEU:HD12	2:B:629:THR:H	1.81	0.45
2:B:63:ARG:CB	2:B:65:GLN:HG3	2.47	0.45
2:B:133:ASP:CA	2:B:757:TRP:HZ3	2.28	0.45
1:C:1013:MET:O	1:C:1015:VAL:N	2.50	0.45
1:C:1250:THR:O	1:C:1252:ALA:N	2.50	0.45
1:C:1646:GLU:HG2	1:C:1660:PHE:CZ	2.52	0.45
1:C:190:ILE:CG2	1:C:191:PRO:N	2.80	0.45
1:C:259:VAL:HB	1:C:295:GLY:CA	2.46	0.45
1:C:439:ALA:O	1:C:441:ASP:N	2.43	0.45
1:C:473:HIS:CE1	2:D:455:LYS:CE	3.00	0.45
1:C:24:VAL:HG11	1:C:543:TYR:HE2	1.75	0.45
1:C:577:PRO:HD2	1:C:588:VAL:CG2	2.47	0.45
1:C:923:LEU:HD21	1:C:925:LYS:HD3	1.99	0.45
2:D:965:ILE:HD13	2:D:1277:ILE:HD13	1.99	0.45
2:D:176:ASN:HB3	2:D:184:TRP:HZ2	1.82	0.45
2:D:224:PHE:CE1	2:D:320:VAL:CG1	3.01	0.45
2:D:436:GLN:O	2:D:437:THR:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:525:GLN:CD	2:D:525:GLN:O	2.55	0.45
2:D:810:VAL:HG12	2:D:811:MET:N	2.31	0.45
2:D:173:VAL:HA	2:D:964:ILE:CD1	2.47	0.45
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:1240:PRO:HB2	1:A:1242:THR:CG2	2.47	0.44
1:A:149:ASN:O	1:A:152:LEU:N	2.25	0.44
1:A:476:LEU:HA	1:A:476:LEU:HD23	1.83	0.44
1:A:491:PRO:HB2	1:A:493:ILE:C	2.36	0.44
1:A:60:PRO:CG	1:A:61:ASP:H	2.30	0.44
2:B:1609:ARG:O	2:B:1611:PRO:HD3	2.17	0.44
2:B:1637:GLU:O	2:B:1638:PHE:CG	2.70	0.44
2:B:176:ASN:HB3	2:B:184:TRP:HZ2	1.82	0.44
2:B:189:PRO:C	2:B:191:LEU:N	2.69	0.44
2:B:280:LEU:HG	2:B:280:LEU:O	2.16	0.44
2:B:523:TYR:CB	2:B:533:ALA:HB2	2.47	0.44
2:B:580:VAL:HG13	2:B:584:VAL:CG2	2.47	0.44
2:B:61:PHE:CD1	2:B:62:PRO:HA	2.52	0.44
1:C:1386:ILE:HG13	1:C:1387:GLU:N	2.29	0.44
1:C:506:LYS:O	1:C:508:LYS:N	2.51	0.44
1:C:554:LEU:HB2	1:C:642:ASN:OD1	2.17	0.44
1:C:662:SER:O	1:C:663:GLN:C	2.56	0.44
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
2:D:1343:PHE:CZ	2:D:1371:TYR:HD1	2.35	0.44
2:D:1382:ILE:HG12	2:D:1427:LEU:HD11	1.99	0.44
2:D:1425:ILE:HG22	2:D:1427:LEU:HD12	1.98	0.44
2:D:31:ALA:O	2:D:119:VAL:HG12	2.17	0.44
2:D:525:GLN:NE2	2:D:528:ASN:H	2.15	0.44
2:D:640:SER:O	2:D:641:ALA:HB2	2.16	0.44
2:D:946:LYS:N	2:D:946:LYS:HD3	2.32	0.44
3:X:40:LEU:HD11	3:X:209:PHE:CZ	2.52	0.44
1:A:1033:ILE:CG2	1:A:1034:PHE:N	2.80	0.44
1:A:1259:LEU:HD21	1:A:1267:VAL:HG11	1.98	0.44
1:A:134:VAL:HA	1:A:218:GLU:O	2.17	0.44
1:A:356:LEU:HG	1:A:452:TYR:CE2	2.53	0.44
1:A:653:PHE:CE1	1:A:660:ASP:CB	3.00	0.44
1:A:694:VAL:HG12	1:A:694:VAL:O	2.16	0.44
2:B:1284:ARG:CG	2:B:1285:GLU:H	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1611:PRO:HA	2:B:1615:GLU:OE1	2.17	0.44
2:B:1617:GLN:HG2	2:B:1617:GLN:H	1.66	0.44
1:C:330:ILE:HG22	1:C:337:SER:HB3	1.99	0.44
1:C:374:GLN:HG2	1:C:382:LEU:HD21	1.98	0.44
1:C:500:ASN:OD1	1:C:514:THR:HG23	2.18	0.44
1:C:624:PHE:CD1	1:C:625:GLN:N	2.85	0.44
1:C:639:GLY:HA2	1:C:648:LEU:CD1	2.44	0.44
1:C:700:TYR:O	1:C:703:ALA:N	2.50	0.44
1:C:584:PRO:CB	1:C:792:ASP:HA	2.37	0.44
2:D:111:PRO:O	2:D:113:VAL:HG23	2.18	0.44
2:D:235:PHE:CE2	2:D:299:PHE:CE2	3.05	0.44
2:D:336:ILE:HD13	2:D:336:ILE:HA	1.79	0.44
2:D:739:PHE:CE2	2:D:847:ARG:NE	2.85	0.44
3:X:201:ILE:HD13	3:X:207:LEU:HD23	2.00	0.44
1:A:1153:ARG:CZ	1:A:1168:LEU:HD12	2.47	0.44
1:A:1226:ARG:CD	1:A:1266:TYR:CE1	3.01	0.44
1:A:1525:CYS:N	1:A:1528:VAL:CG1	2.79	0.44
1:A:243:PHE:CE2	1:A:304:GLU:CA	3.00	0.44
1:A:414:ASP:OD1	1:A:414:ASP:N	2.50	0.44
1:A:421:VAL:HG23	2:B:507:ASN:ND2	2.32	0.44
1:A:351:PRO:CG	1:A:442:LEU:HD11	2.48	0.44
1:A:535:VAL:O	1:A:563:ILE:HG12	2.17	0.44
1:A:576:SER:HB2	1:A:589:SER:H	1.81	0.44
1:A:624:PHE:CD1	1:A:625:GLN:N	2.85	0.44
2:B:111:PRO:O	2:B:113:VAL:HG23	2.18	0.44
2:B:345:ILE:HD11	2:B:427:THR:CA	2.47	0.44
1:C:1022:PHE:O	1:C:1024:TYR:N	2.50	0.44
1:C:1286:SER:CB	1:C:1499:HIS:HA	2.46	0.44
1:C:1532:CYS:O	1:C:1641:SER:N	2.51	0.44
1:C:502:LEU:HB2	1:C:541:LEU:HD21	1.97	0.44
1:C:667:GLU:HA	1:C:668:PRO:HD3	1.79	0.44
2:D:1345:LEU:HD12	2:D:1368:CYS:O	2.17	0.44
2:D:148:PHE:CZ	2:D:792:VAL:CG1	3.00	0.44
2:D:1597:ILE:HD11	2:D:1599:TYR:CE1	2.53	0.44
2:D:1610:TRP:CE2	2:D:1628:PHE:HD2	2.35	0.44
2:D:344:GLN:O	2:D:366:VAL:HA	2.17	0.44
2:D:838:ASN:HB2	2:D:844:ILE:HD11	1.98	0.44
3:Y:179:LEU:HD11	3:Y:180:TYR:CE1	2.51	0.44
1:A:977:LEU:CD2	1:A:1361:VAL:HG22	2.48	0.44
1:A:1069:TRP:CH2	1:A:1465:ASN:ND2	2.85	0.44
1:A:1573:VAL:HG12	1:A:1603:LYS:HD3	1.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:LEU:HD12	1:A:466:TYR:H	1.83	0.44
1:A:493:ILE:CG2	1:A:495:LYS:HB2	2.45	0.44
1:A:632:LEU:N	1:A:632:LEU:CD2	2.68	0.44
1:A:981:GLY:O	1:A:1356:LEU:O	2.35	0.44
2:B:515:ILE:HG21	2:B:599:TRP:CZ2	2.52	0.44
2:B:847:ARG:HG3	2:B:869:GLN:CG	2.42	0.44
2:B:739:PHE:CE2	2:B:847:ARG:NE	2.86	0.44
1:C:1219:LYS:HE2	1:C:1239:VAL:CG2	2.45	0.44
1:C:1268:ASN:N	1:C:1269:PRO:HD2	2.33	0.44
1:C:1298:THR:O	1:C:1301:SER:N	2.51	0.44
1:C:398:ASN:O	1:C:399:GLN:CB	2.64	0.44
1:C:532:GLN:O	1:C:533:ASN:C	2.53	0.44
1:C:854:GLN:NE2	1:C:854:GLN:N	2.65	0.44
1:C:257:ASN:ND2	1:C:892:SER:HA	2.27	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: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
2:D:570:ASP:O	2:D:573:ALA:HB2	2.17	0.44
2:D:642:ALA:O	2:D:643:LYS:HB3	2.17	0.44
3:X:185:LYS:HG2	3:X:186:TYR:CD2	2.53	0.44
3:Y:139:ASN:HB2	3:Y:227:THR:HG23	2.00	0.44
3:Y:88:GLY:O	3:Y:91:LYS:N	2.43	0.44
1:A:1421:HIS:CD2	1:A:1422:ALA:N	2.85	0.44
1:A:1559:TYR:HE2	1:A:1590:ALA:O	1.98	0.44
1:A:1561:TYR:HE1	1:A:1598:ILE:HD11	1.83	0.44
1:A:333:THR:OG1	1:A:334:GLY:N	2.50	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
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:A:421:VAL:HG23	2:B:507:ASN:HD22	1.81	0.44
2:B:558:MET:HA	2:B:559:PRO:HD3	1.85	0.44
2:B:830:VAL:HG23	2:B:831:GLU:N	2.32	0.44
1:C:120:THR:CG2	1:C:121:TYR:N	2.81	0.44
1:C:1459:HIS:HD2	1:C:1459:HIS:N	2.15	0.44
1:C:1549:LYS:H	1:C:1549:LYS:HG2	1.41	0.44
1:C:1637:TYR:N	1:C:1637:TYR:HD2	2.15	0.44
1:C:316:GLU:HA	1:C:319:ASN:HB2	1.99	0.44
1:C:909:ASN:HA	1:C:926:THR:HA	1.99	0.44
1:C:930:VAL:HA	1:C:931:PRO:HD3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:962:LYS:HD2	2:D:1302:THR:CG2	2.47	0.44
2:D:134:LYS:HD2	2:D:584:VAL:HG11	1.99	0.44
1:C:480:GLU:HG2	2:D:389:THR:HB	2.00	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:41:ILE:O	2:D:85:PRO:HD2	2.18	0.44
2:D:89:ILE:CD1	2:D:104:VAL:HG11	2.48	0.44
2:D:946:LYS:CD	2:D:946:LYS:H	2.29	0.44
4:G:1:NAG:O3	4:G:2:NAG:O5	2.34	0.44
3:Y:188:LYS:HD3	3:Y:202:ASP:CA	2.42	0.44
1:A:1003:LEU:HA	1:A:1004:PRO:HD2	1.49	0.44
1:A:1663:ASN:O	1:A:1666:GLU:HB3	2.18	0.44
1:A:284:GLN:HG2	1:A:310:LEU:CD1	2.47	0.44
1:A:569:ASN:HD22	1:A:569:ASN:H	1.64	0.44
1:A:606:ASP:OD2	1:A:795:THR:HG21	2.18	0.44
1:A:60:PRO:CG	1:A:61:ASP:N	2.81	0.44
1:A:671:GLU:HB2	1:A:672:ILE:H	1.66	0.44
1:A:979:VAL:C	1:A:980:LYS:HG2	2.37	0.44
2:B:1282:PRO:O	2:B:1283:ASP:C	2.56	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
2:B:1438:LEU:HD13	2:B:1438:LEU:C	2.37	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: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:1200:LYS:HE3	1:C:1200:LYS:HB3	1.79	0.44
1:C:1268:ASN:ND2	1:C:1268:ASN:N	2.66	0.44
1:C:1428:LEU:HD11	1:C:1434:ALA:HB2	1.99	0.44
1:C:152:LEU:HA	1:C:152:LEU:HD13	1.48	0.44
1:C:1636:ILE:O	1:C:1636:ILE:HG22	2.17	0.44
1:C:415:ASP:N	1:C:415:ASP:OD1	2.48	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
1:C:60:PRO:CG	1:C:61:ASP:H	2.30	0.44
1:C:694:VAL:O	1:C:694:VAL:HG12	2.18	0.44
1:C:779:LEU:O	1:C:781:PRO:HD3	2.18	0.44
2:D:1330:ASN:N	2:D:1330:ASN:HD22	2.15	0.44
2:D:1444:LYS:NZ	2:D:1447:GLU:HA	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1525:LYS:HE3	2:D:1610:TRP:NE1	2.32	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
2:D:818:LEU:HG	2:D:820:MET:HE3	2.00	0.44
2:D:824:VAL:HG21	2:D:830:VAL:CG1	2.41	0.44
1:A:1016:VAL:O	1:A:1020:TYR:HD2	2.01	0.44
1:A:1024:TYR:HB2	1:A:1298:THR:CG2	2.48	0.44
1:A:1066:TYR:CD1	1:A:1079:THR:HG23	2.53	0.44
1:A:1096:ASN:O	1:A:1097:GLN:C	2.55	0.44
1:A:955:ARG:O	1:A:1349:SER:HA	2.18	0.44
1:A:1627:ILE:HD12	1:A:1629:TYR:HB3	2.00	0.44
1:A:1540:ASP:HA	1:A:1660:PHE:CD1	2.53	0.44
1:A:180:ILE:CG2	1:A:181:GLY:N	2.81	0.44
1:A:250:ILE:HG13	1:A:250:ILE:O	2.17	0.44
1:A:273:GLU:O	1:A:274:ASP:HB3	2.17	0.44
1:A:307:VAL:O	1:A:311:SER:HB2	2.18	0.44
1:A:316:GLU:HA	1:A:319:ASN:HB2	1.99	0.44
1:A:383:VAL:HG23	1:A:386:VAL:CG2	2.48	0.44
1:A:42:GLN:HE21	1:A:44:TYR:N	2.10	0.44
1:A:599:TRP:O	1:A:803:GLY:CA	2.58	0.44
2:B:922:LYS:HE3	2:B:1329:TYR:OH	2.18	0.44
2:B:1486:ILE:HG13	2:B:1486:ILE:O	2.18	0.44
2:B:1522:TYR:CE2	2:B:1585:GLY:N	2.79	0.44
1:A:483:ASN:HD21	2:B:399:ILE:HB	1.81	0.44
2:B:518:PHE:CD2	2:B:538:VAL:HB	2.42	0.44
2:B:63:ARG:HD2	2:B:65:GLN:NE2	2.33	0.44
1:C:1180:LEU:HD21	1:C:1208:ILE:HA	2.00	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:C:180:ILE:HG22	1:C:181:GLY:N	2.32	0.44
1:C:238:ILE:HB	1:C:347:TYR:CE1	2.52	0.44
1:C:33:VAL:HG21	1:C:121:TYR:HE1	1.73	0.44
1:C:41:ILE:HD13	1:C:41:ILE:HG21	1.63	0.44
1:C:40:VAL:HG23	1:C:41:ILE:N	2.32	0.44
1:C:443:PRO:CG	1:C:446:ASN:HB2	2.48	0.44
1:C:436:LYS:CB	1:C:449:ARG:HG2	2.43	0.44
1:C:492:TYR:CD2	1:C:493:ILE:HB	2.53	0.44
1:C:491:PRO:HB2	1:C:493:ILE:C	2.37	0.44
1:C:180:ILE:HG13	1:C:599:TRP:CZ3	2.52	0.44
1:C:59:TYR:CD1	1:C:60:PRO:HG3	2.53	0.44
2:D:1567:ARG:HA	2:D:1567:ARG:HD2	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1594:LYS:O	2:D:1596:LYS:HG2	2.17	0.44
2:D:178:VAL:HG21	2:D:183:PHE:CD1	2.53	0.44
2:D:834:ALA:C	2:D:835:ILE:HD13	2.38	0.44
2:D:857:CYS:CB	2:D:885:VAL:CG2	2.95	0.44
2:D:35:THR:HB	2:D:91:ALA:HB2	1.99	0.44
3:Y:73:VAL:CG2	3:Y:74:ARG:N	2.78	0.44
1:A:1023:HIS:CD2	1:A:1023:HIS:O	2.70	0.44
1:A:1031:TRP:CE2	1:A:1042:LYS:HG3	2.52	0.44
1:A:1156:PHE:CE1	1:A:1164:ILE:HG13	2.53	0.44
1:A:1234:HIS:CG	1:A:1235:LYS:N	2.85	0.44
1:A:1317:TYR:CE1	1:A:1342:LEU:HD12	2.53	0.44
1:A:132:LYS:HZ1	1:A:139:GLN:HE22	1.65	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:A:238:ILE:HB	1:A:347:TYR:CE1	2.53	0.44
1:A:302:ASP:HB3	1:A:305:THR:HB	2.00	0.44
1:A:321:LYS:O	1:A:347:TYR:HB2	2.18	0.44
1:A:804:ILE:HG22	1:A:809:ILE:CB	2.48	0.44
1:A:915:GLU:CB	2:B:905:TRP:CZ2	3.00	0.44
1:A:856:CYS:HB3	1:A:915:GLU:HG2	1.99	0.44
2:B:1404:VAL:O	2:B:1428:ASN:ND2	2.50	0.44
2:B:1438:LEU:HD13	2:B:1438:LEU:O	2.18	0.44
2:B:1443:LEU:CD1	2:B:1443:LEU:N	2.80	0.44
2:B:263:VAL:HG21	2:B:292:ALA:CB	2.47	0.44
2:B:345:ILE:H	2:B:345:ILE:HG12	1.60	0.44
2:B:524:TYR:C	2:B:524:TYR:HD1	2.19	0.44
2:B:949:LYS:H	2:B:949:LYS:HG3	1.54	0.44
1:C:1023:HIS:O	1:C:1027:THR:HB	2.17	0.44
1:A:1163:LYS:CE	1:C:1109:GLU:HG2	2.48	0.44
1:C:1020:TYR:CE1	1:C:1295:GLU:HA	2.52	0.44
1:C:375:VAL:O	1:C:383:VAL:HG13	2.16	0.44
1:C:787:GLN:O	1:C:788:PHE:HB3	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:C:917:TRP:HB3	2:D:558:MET:SD	2.58	0.44
2:D:855:ALA:O	2:D:856:PHE:CD1	2.71	0.44
3:X:91:LYS:NZ	3:X:95:LYS:HE3	2.33	0.44
1:A:1007:SER:OG	1:A:1008:ALA:N	2.50	0.44
1:A:1305:LYS:HG3	1:C:101:TYR:OH	2.17	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:GLU:HB2	1:A:185:PHE:CE1	2.52	0.44
1:A:382:LEU:HD13	1:A:415:ASP:O	2.18	0.44
1:A:383:VAL:CG2	1:A:386:VAL:HG21	2.48	0.44
1:A:42:GLN:HG2	1:A:43:VAL:H	1.83	0.44
1:A:443:PRO:CG	1:A:446:ASN:HB2	2.48	0.44
1:A:513:GLY:HA2	3:X:146:LEU:HD13	2.00	0.44
1:A:506:LYS:HD2	1:A:536:PRO:CD	2.48	0.44
1:A:643:ALA:O	1:A:644:ASN:C	2.55	0.44
1:A:949:ILE:HG22	1:A:950:TYR:CZ	2.53	0.44
2:B:1442:ILE:C	2:B:1443:LEU:HD13	2.38	0.44
2:B:243:PHE:C	2:B:243:PHE:HD2	2.20	0.44
2:B:275:SER:O	2:B:277:PRO:HD3	2.17	0.44
2:B:309:LEU:O	2:B:310:VAL:C	2.54	0.44
2:B:889:GLN:HA	2:B:915:VAL:HB	1.99	0.44
1:C:1069:TRP:CH2	1:C:1465:ASN:ND2	2.86	0.44
1:C:1019:PHE:CZ	1:C:1088:GLN:HB3	2.53	0.44
1:C:137:PRO:O	1:C:138:ASP:HB2	2.18	0.44
1:C:1629:TYR:HE1	1:C:1631:PHE:CD1	2.34	0.44
1:C:223:VAL:O	1:C:225:PRO:HD3	2.18	0.44
1:C:317:ASP:O	1:C:319:ASN:N	2.50	0.44
1:C:248:ILE:HD13	1:C:325:ILE:HD13	2.00	0.44
1:C:532:GLN:CA	1:C:532:GLN:OE1	2.59	0.44
1:C:24:VAL:CG2	1:C:554:LEU:HD11	2.48	0.44
1:C:60:PRO:CG	1:C:61:ASP:N	2.81	0.44
1:C:680:GLN:CG	1:C:681:LYS:H	2.31	0.44
1:C:989:SER:O	1:C:993:SER:HB3	2.17	0.44
2:D:966:GLN:OE1	2:D:1298:LEU:HD13	2.17	0.44
2:D:1521:ASP:OD1	2:D:1552:THR:OG1	2.36	0.44
2:D:1539:ILE:HD12	2:D:1539:ILE:N	2.32	0.44
2:D:1637:GLU:C	2:D:1638:PHE:CD2	2.91	0.44
2:D:397:LYS:NZ	2:D:449:ILE:O	2.51	0.44
3:X:215:VAL:O	3:X:216:LEU:HD13	2.18	0.44
1:A:1320:LYS:HA	1:A:1320:LYS:HD2	1.90	0.43
1:A:150:ASP:CG	1:A:151:ASP:N	2.72	0.43
1:A:1627:ILE:O	1:A:1627:ILE:CG1	2.63	0.43
1:A:472:ASN:HA	1:A:474:LYS:HD2	1.99	0.43
1:A:578:ASP:CG	1:A:578:ASP:O	2.56	0.43
1:A:856:CYS:HB2	2:B:904:LEU:HG	1.99	0.43
2:B:783:SER:HB3	2:B:785:THR:HG22	2.00	0.43
2:B:881:PRO:C	2:B:882:PHE:CD2	2.91	0.43
1:C:1090:ASN:ND2	1:C:1158:ILE:HG12	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1227:PHE:HA	1:C:1228:TRP:CE3	2.53	0.43
1:C:1257:THR:O	1:C:1261:LEU:HD23	2.17	0.43
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
1:C:682:LYS:HZ2	1:C:686:ILE:HD12	1.81	0.43
1:C:713:GLN:HG3	1:C:713:GLN:H	1.44	0.43
2:D:137:TYR:HB2	2:D:216:VAL:HG23	2.00	0.43
2:D:1575:LEU:HD13	2:D:1581:TYR:CZ	2.53	0.43
2:D:1610:TRP:CD2	2:D:1628:PHE:CE2	3.06	0.43
2:D:1635:LEU:O	2:D:1636:THR:C	2.55	0.43
2:D:243:PHE:HD2	2:D:243:PHE:C	2.22	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
2:D:736:GLU:HA	2:D:847:ARG:NH2	2.33	0.43
2:D:850:LEU:CD1	2:D:851:LEU:N	2.81	0.43
2:D:875:LEU:HG	2:D:875:LEU:O	2.18	0.43
2:D:913:LEU:C	2:D:913:LEU:CD2	2.86	0.43
2:D:932:PRO:HB3	2:D:939:GLY:O	2.18	0.43
1:A:1075:SER:OG	1:A:1078:LEU:HB2	2.18	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:317:ASP:C	1:A:319:ASN:N	2.71	0.43
1:A:359:THR:CG2	1:A:359:THR:O	2.65	0.43
1:A:387:PRO:HB2	1:A:438:ASP:HB3	2.00	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:577:PRO:HD2	1:A:588:VAL:CG2	2.48	0.43
1:A:855:PHE:HB2	1:A:914:LEU:CD1	2.48	0.43
2:B:961:THR:HG22	2:B:1327:THR:OG1	2.18	0.43
2:B:234:PHE:CE1	2:B:236:TYR:CE1	3.06	0.43
2:B:326:SER:OG	2:B:327:ASP:N	2.51	0.43
2:B:361:GLU:HB3	2:B:399:ILE:CD1	2.48	0.43
1:C:1084:ARG:CA	1:C:1151:GLY:HA2	2.48	0.43
1:C:1293:ALA:O	1:C:1294:ILE:C	2.56	0.43
1:C:131:ASP:OD2	1:C:132:LYS:HG3	2.18	0.43
1:C:1364:VAL:HG13	1:C:1364:VAL:O	2.18	0.43
1:C:1638:PRO:O	1:C:1639:LEU:CB	2.62	0.43
1:C:273:GLU:O	1:C:274:ASP:HB3	2.17	0.43
1:C:276:LYS:HA	1:C:276:LYS:HD2	1.76	0.43
1:C:419:SER:C	1:C:420:PHE:CD2	2.92	0.43
1:C:955:ARG:O	1:C:1349:SER:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:142:PRO:HB3	2:D:187:ASN:HD22	1.83	0.43
2:D:930:LEU:HD13	2:D:1315:ALA:HB2	1.99	0.43
2:D:943:GLU:HB2	2:D:1313:VAL:HG23	2.00	0.43
1:A:1112:GLN:HB2	1:A:1118:PHE:CE1	2.54	0.43
1:A:1156:PHE:CE2	1:A:1160:PRO:HB3	2.54	0.43
1:A:1189:ALA:O	1:A:1192:ALA:HB3	2.19	0.43
1:A:1215:GLU:OE1	1:A:1235:LYS:HD3	2.18	0.43
1:A:1249:GLU:O	1:A:1253:TYR:CD2	2.71	0.43
1:A:1257:THR:O	1:A:1261:LEU:HD23	2.19	0.43
1:A:127:PHE:CD1	1:A:127:PHE:N	2.85	0.43
1:A:165:ASP:CB	1:A:166:PRO:CD	2.96	0.43
1:A:231:ILE:HG12	1:A:231:ILE:O	2.18	0.43
1:A:241:LYS:NZ	1:A:351:PRO:HB3	2.34	0.43
1:A:465:LEU:HD12	1:A:487:THR:O	2.19	0.43
1:A:40:VAL:HG12	1:A:509:ILE:HD12	2.01	0.43
1:A:990:ALA:HB1	1:A:1000:LEU:HD11	2.01	0.43
2:B:1296:ASN:O	2:B:1297:ALA:C	2.56	0.43
2:B:1566:GLN:H	2:B:1566:GLN:HG2	1.50	0.43
2:B:1506:ILE:HD11	2:B:1628:PHE:HE1	1.84	0.43
2:B:161:VAL:CG2	2:B:180:LEU:HD21	2.43	0.43
2:B:456:PRO:HG3	2:B:515:ILE:HD11	2.01	0.43
2:B:745:ILE:O	2:B:745:ILE:CG2	2.66	0.43
2:B:736:GLU:HA	2:B:847:ARG:NH2	2.33	0.43
2:B:89:ILE:CD1	2:B:104:VAL:HG11	2.48	0.43
2:B:951:ASP:C	2:B:953:ARG:H	2.13	0.43
1:C:1226:ARG:HD3	1:C:1266:TYR:CE1	2.54	0.43
1:C:1439:LEU:O	1:C:1440:LYS:C	2.57	0.43
1:C:389:THR:OG1	1:C:408:LYS:HE2	2.18	0.43
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
1:C:742:ILE:CG1	1:C:752:LEU:O	2.65	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:D:265:PHE:O	2:D:276:ILE:HG13	2.18	0.43
2:D:361:GLU:HB3	2:D:399:ILE:CD1	2.47	0.43
2:D:449:ILE:HG23	2:D:449:ILE:O	2.18	0.43
2:D:358:MET:HE2	2:D:467:LYS:HD2	1.99	0.43
2:D:518:PHE:CE2	2:D:538:VAL:CB	2.71	0.43
2:D:580:VAL:HG13	2:D:584:VAL:HG23	2.00	0.43
2:D:628:LEU:HD12	2:D:629:THR:H	1.82	0.43
3:X:169:ILE:HG21	3:X:189:ILE:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:54:SER:HB2	3:Y:167:PHE:CE1	2.54	0.43
3:Y:81:ASN:O	3:Y:115:ARG:CB	2.53	0.43
1:A:1076:THR:HG23	1:A:1077:TRP:N	2.34	0.43
1:A:1439:LEU:HA	1:A:1439:LEU:HD23	1.64	0.43
1:A:1546:GLU:HG2	1:A:1663:ASN:HD21	1.80	0.43
1:A:1573:VAL:HB	1:A:1603:LYS:CD	2.43	0.43
1:A:317:ASP:O	1:A:319:ASN:N	2.51	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
1:A:595:GLY:O	1:A:596:MET:C	2.57	0.43
2:B:1378:THR:O	2:B:1379:MET:C	2.57	0.43
2:B:1454:GLY:O	2:B:1471:PHE:HD1	2.00	0.43
2:B:269:ILE:HG13	2:B:272:ALA:HB3	2.01	0.43
2:B:224:PHE:HE1	2:B:320:VAL:CG1	2.31	0.43
2:B:319:THR:HG23	2:B:330:VAL:CG1	2.48	0.43
2:B:433:ILE:HG22	2:B:434:ALA:N	2.33	0.43
2:B:851:LEU:HD11	2:B:865:ARG:NH2	2.33	0.43
2:B:191:LEU:HD12	2:B:958:GLU:HG2	1.99	0.43
1:C:1300:TYR:C	1:C:1300:TYR:CD2	2.91	0.43
1:C:1317:TYR:CZ	1:C:1342:LEU:HG	2.53	0.43
1:C:1327:LYS:C	1:C:1332:ASN:HD22	2.22	0.43
1:C:1358:THR:HB	1:C:1360:HIS:HE1	1.77	0.43
1:C:274:ASP:HA	1:C:322:TYR:CE2	2.53	0.43
1:C:433:PHE:N	1:C:433:PHE:CD1	2.87	0.43
1:C:671:GLU:HG2	1:C:671:GLU:H	1.62	0.43
1:C:847:ASN:OD1	1:C:849:ARG:N	2.51	0.43
1:C:949:ILE:HA	1:C:949:ILE:HD13	1.81	0.43
2:D:124:GLN:HG3	2:D:124:GLN:O	2.18	0.43
2:D:1404:VAL:O	2:D:1428:ASN:ND2	2.51	0.43
2:D:1528:LEU:HD11	2:D:1540:TYR:HB3	1.99	0.43
2:D:1614:ASP:O	2:D:1617:GLN:HG2	2.18	0.43
2:D:580:VAL:HG13	2:D:584:VAL:CG2	2.49	0.43
2:D:613:SER:HA	2:D:620:VAL:CG2	2.49	0.43
3:Y:138:VAL:O	3:Y:138:VAL:HG12	2.18	0.43
3:Y:196:GLU:CD	3:Y:196:GLU:N	2.72	0.43
3:Y:201:ILE:HD13	3:Y:207:LEU:HD23	2.00	0.43
1:A:1025:LEU:HD11	1:A:1034:PHE:HZ	1.82	0.43
1:A:1072:GLY:O	1:A:1073:SER:C	2.55	0.43
1:A:109:LYS:HD3	1:A:110:HIS:HE1	1.77	0.43
1:A:33:VAL:CG2	1:A:121:TYR:CD1	2.88	0.43
1:A:1428:LEU:HD11	1:A:1434:ALA:HB2	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:461:SER:O	1:A:462:GLN:HB2	2.17	0.43
1:A:829:ILE:CG1	1:A:925:LYS:HG2	2.47	0.43
1:A:984:VAL:HG12	1:A:988:LEU:HD12	2.01	0.43
2:B:1459:TYR:HB3	2:B:1466:GLU:HB3	1.99	0.43
2:B:800:ILE:HG23	2:B:801:CYS:N	2.31	0.43
2:B:954:VAL:CG1	2:B:955:PRO:HD2	2.42	0.43
1:C:987:ILE:HD13	1:C:1294:ILE:HG23	2.00	0.43
1:C:837:GLU:OE2	1:C:1430:THR:HB	2.19	0.43
1:C:1538:GLU:O	1:C:1539:LEU:C	2.57	0.43
1:C:222:TYR:HE2	1:C:224:LEU:N	2.17	0.43
1:C:290:THR:CG2	1:C:297:ALA:HB1	2.48	0.43
1:C:259:VAL:HB	1:C:295:GLY:HA2	2.00	0.43
1:C:916:THR:C	1:C:918:PHE:N	2.71	0.43
2:D:1292:ILE:CD1	2:D:1301:ARG:HE	2.31	0.43
2:D:961:THR:HG22	2:D:1327:THR:CB	2.48	0.43
2:D:1391:LEU:HA	2:D:1392:PRO:HD3	1.85	0.43
2:D:1408:ILE:HD13	2:D:1425:ILE:HA	2.00	0.43
2:D:355:LYS:HE2	2:D:445:LEU:O	2.18	0.43
2:D:56:ILE:HD11	2:D:73:VAL:HG23	2.01	0.43
2:D:830:VAL:HG23	2:D:831:GLU:N	2.33	0.43
2:D:881:PRO:O	2:D:882:PHE:CD2	2.71	0.43
3:X:185:LYS:CG	3:X:186:TYR:CE2	3.01	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:A:680:GLN:CG	1:A:681:LYS:N	2.81	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
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
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:C:131:ASP:OD2	1:C:132:LYS:CG	2.66	0.43
1:C:177:ILE:HD13	1:C:177:ILE:N	2.33	0.43
1:C:23:TYR:HD1	1:C:23:TYR:H	1.31	0.43
1:C:472:ASN:HA	1:C:474:LYS:HD2	2.01	0.43
1:C:113:LYS:HE2	1:C:654:LEU:O	2.19	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
1:C:996:GLY:O	1:C:998:ASN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1273:LEU:C	2:D:1273:LEU:HD12	2.39	0.43
2:D:326:SER:OG	2:D:327:ASP:N	2.52	0.43
2:D:476:ILE:O	2:D:497:ARG:HG2	2.18	0.43
2:D:47:GLY:O	2:D:48:ASP:HB2	2.19	0.43
2:D:518:PHE:CD2	2:D:518:PHE:O	2.72	0.43
2:D:618:LEU:CD1	2:D:635:ASN:O	2.65	0.43
3:X:108:GLU:O	3:X:109:LEU:HG	2.18	0.43
3:Y:166:ASP:O	3:Y:170:ARG:HG3	2.18	0.43
3:Y:229:ASN:C	3:Y:230:GLN:HG3	2.39	0.43
1:A:1043:GLN:O	1:A:1044:LYS:C	2.54	0.43
1:A:1106:TRP:CZ2	1:A:1111:TYR:HE2	2.37	0.43
1:A:133:PRO:HD2	1:A:609:VAL:CG1	2.48	0.43
1:A:1646:GLU:HG2	1:A:1660:PHE:HZ	1.84	0.43
1:A:503:ILE:O	1:A:510:ILE:HG12	2.19	0.43
1:A:631:ASP:C	1:A:633:GLY:H	2.22	0.43
1:A:670:LYS:HD2	1:A:671:GLU:H	1.83	0.43
1:A:864:GLY:HA3	1:A:907:LEU:HD22	2.00	0.43
1:A:953:ILE:CD1	1:A:955:ARG:HH21	2.32	0.43
2:B:1367:ILE:HB	2:B:1438:LEU:CD1	2.49	0.43
2:B:1486:ILE:HD11	2:B:1591:LEU:HD21	2.00	0.43
1:A:523:TYR:CE2	2:B:465:ASN:ND2	2.86	0.43
2:B:490:PHE:C	2:B:490:PHE:CD1	2.90	0.43
1:C:1023:HIS:O	1:C:1023:HIS:CD2	2.71	0.43
1:C:1213:LYS:HE2	1:C:1266:TYR:HD2	1.78	0.43
1:C:1249:GLU:O	1:C:1253:TYR:CD2	2.72	0.43
1:C:1665:ASP:O	1:C:1668:ALA:HB3	2.19	0.43
1:C:274:ASP:CG	1:C:275:LEU:N	2.70	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:C:501:TYR:O	1:C:512:PHE:HA	2.19	0.43
1:C:532:GLN:HA	1:C:535:VAL:HG13	2.00	0.43
1:C:551:THR:HB	1:C:657:ALA:HB1	2.00	0.43
1:C:980:LYS:HB3	1:C:980:LYS:HE2	1.79	0.43
2:D:1430:VAL:HA	2:D:1436:GLU:OE2	2.19	0.43
2:D:551:LYS:HE2	2:D:551:LYS:HB2	1.91	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
2:D:951:ASP:C	2:D:953:ARG:H	2.19	0.43
3:X:211:ARG:O	3:X:214:ASP:HB2	2.18	0.43
1:A:1037:ASP:HA	1:A:1038:PRO:HD3	1.62	0.43
1:A:33:VAL:HG23	1:A:120:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1263:ASP:O	1:A:1265:ASN:N	2.52	0.43
1:A:1317:TYR:CZ	1:A:1342:LEU:HG	2.54	0.43
1:A:1426:ILE:O	1:A:1426:ILE:HG22	2.18	0.43
1:A:1403:VAL:HG22	1:A:1476:ARG:HB3	2.01	0.43
1:A:1571:GLU:O	1:A:1574:PHE:N	2.46	0.43
1:A:539:ARG:HE	1:A:633:GLY:HA3	1.83	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
2:B:345:ILE:HD11	2:B:426:ALA:C	2.38	0.43
1:C:1053:MET:O	1:C:1056:ILE:HG22	2.19	0.43
1:C:1012:LEU:HD11	1:C:1056:ILE:HG13	2.01	0.43
1:C:938:SER:OG	1:C:1284:PHE:CE2	2.71	0.43
1:C:1566:THR:HG23	1:C:1578:LYS:O	2.18	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:587:THR:HA	1:C:789:ALA:HA	2.00	0.43
1:C:64:PHE:HD2	1:C:66:TYR:CE1	2.36	0.43
1:C:258:LYS:HD3	1:C:893:SER:OG	2.17	0.43
2:D:1275:LEU:HD21	2:D:1319:GLY:O	2.19	0.43
2:D:1528:LEU:HD21	2:D:1531:ILE:HD11	2.01	0.43
2:D:144:LEU:HB3	2:D:185:PRO:HB3	2.01	0.43
2:D:384:PHE:CE1	2:D:400:LEU:HG	2.51	0.43
2:D:582:LYS:O	2:D:583:ALA:C	2.56	0.43
2:D:933:ARG:NH1	2:D:933:ARG:CG	2.79	0.43
3:Y:163:LYS:HG3	3:Y:212:MET:CE	2.49	0.43
1:A:1016:VAL:N	1:A:1017:PRO:CD	2.81	0.43
1:A:1208:ILE:HG22	1:A:1208:ILE:O	2.19	0.43
1:A:1309:LEU:O	1:A:1329:THR:HA	2.19	0.43
1:A:931:PRO:CB	1:A:1366:HIS:CD2	3.02	0.43
1:A:1538:GLU:O	1:A:1539:LEU:C	2.54	0.43
1:A:1602:LYS:HE3	1:A:1609:ALA:O	2.18	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:484:ILE:CD1	1:A:540:LEU:CD2	2.97	0.43
1:A:701:ASP:CG	1:A:1446:VAL:HG23	2.39	0.43
2:B:114:ARG:O	2:B:114:ARG:NE	2.51	0.43
2:B:1564:ILE:O	2:B:1601:ILE:HD12	2.19	0.43
2:B:247:ILE:CD1	2:B:318:VAL:HG21	2.49	0.43
2:B:794:PHE:CD2	2:B:795:THR:N	2.86	0.43
2:B:810:VAL:O	2:B:811:MET:HB2	2.19	0.43
1:C:1072:GLY:O	1:C:1073:SER:C	2.57	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
1:C:132:LYS:HZ1	1:C:139:GLN:HE22	1.67	0.43
1:C:492:TYR:CE2	1:C:546:VAL:HG11	2.53	0.43
1:C:653:PHE:CE1	1:C:660:ASP:CB	3.00	0.43
1:C:701:ASP:N	1:C:701:ASP:OD1	2.52	0.43
1:C:802:VAL:HG12	1:C:803:GLY:N	2.34	0.43
1:C:855:PHE:HB2	1:C:914:LEU:HD11	2.00	0.43
2:D:1424:ILE:HD13	2:D:1424:ILE:N	2.29	0.43
2:D:1459:TYR:HB3	2:D:1466:GLU:HB3	1.99	0.43
2:D:146:ARG:CB	2:D:146:ARG:HH11	2.32	0.43
2:D:1482:ASN:HB3	2:D:1493:ALA:CB	2.49	0.43
2:D:1544:VAL:C	2:D:1545:LEU:HD12	2.40	0.43
2:D:1562:GLN:NE2	2:D:1596:LYS:HZ2	2.15	0.43
2:D:222:PRO:HG2	2:D:329:VAL:HG12	1.99	0.43
2:D:341:SER:HA	2:D:342:PRO:HD3	1.72	0.43
2:D:40:GLN:O	2:D:489:ILE:HD12	2.18	0.43
2:D:481:TYR:HE2	2:D:493:GLY:N	2.16	0.43
2:D:780:LEU:HD11	2:D:787:TRP:HD1	1.84	0.43
1:A:1083:LEU:HD13	1:A:1104:LEU:HD23	2.00	0.43
1:A:1084:ARG:HG2	1:A:1084:ARG:NH1	2.33	0.43
1:A:1219:LYS:HB2	1:A:1219:LYS:HE3	1.76	0.43
1:A:1406:ALA:O	1:A:1472:PHE:HA	2.18	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
1:A:582:TYR:O	1:A:819:VAL:HG13	2.18	0.43
2:B:1454:GLY:HA3	2:B:1472:TYR:CE2	2.54	0.43
2:B:315:TYR:CD1	2:B:315:TYR:C	2.91	0.43
2:B:764:GLU:HG3	2:B:772:SER:HB3	2.01	0.43
2:B:840:VAL:CG1	2:B:841:ASN:N	2.77	0.43
2:B:851:LEU:HD21	2:B:865:ARG:HH21	1.83	0.43
2:B:895:GLU:HA	2:B:909:VAL:O	2.19	0.43
1:C:1127:ILE:HD11	1:C:1143:TYR:CE2	2.54	0.43
1:C:1175:LEU:HD23	1:C:1175:LEU:HA	1.88	0.43
1:C:1244:THR:O	1:C:1245:ALA:C	2.57	0.43
1:C:1639:LEU:HA	1:C:1639:LEU:HD22	1.76	0.43
1:C:1643:THR:HG22	1:C:1644:TRP:H	1.84	0.43
1:C:317:ASP:C	1:C:319:ASN:N	2.70	0.43
1:C:487:THR:HA	1:C:488:PRO:HD3	1.83	0.43
1:C:511:HIS:CE1	3:Y:149:SER:HB3	2.54	0.43
1:C:628:GLU:HG3	1:C:628:GLU:O	2.18	0.43
1:C:837:GLU:O	1:C:901:LEU:CD1	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1454:GLY:O	2:D:1471:PHE:HD1	2.01	0.43
2:D:1635:LEU:HD23	2:D:1635:LEU:HA	1.70	0.43
2:D:550:VAL:HG22	2:D:567:LEU:HD21	2.01	0.43
3:X:174:VAL:HG12	3:X:174:VAL:O	2.19	0.43
3:X:196:GLU:N	3:X:196:GLU:CD	2.72	0.43
3:Y:45:ASP:OD1	3:Y:48:ARG:NH1	2.51	0.43
1:A:1093:VAL:O	1:A:1094:GLU:C	2.57	0.42
1:A:1245:ALA:O	1:A:1246:ARG:C	2.56	0.42
1:A:223:VAL:O	1:A:225:PRO:HD3	2.19	0.42
1:A:40:VAL:HG23	1:A:41:ILE:H	1.83	0.42
1:A:522:SER:HB2	1:A:523:TYR:H	1.54	0.42
1:A:640:LEU:H	1:A:644:ASN:CB	2.28	0.42
1:A:710:THR:N	1:A:713:GLN:OE1	2.50	0.42
1:A:824:PHE:CE2	1:A:846:TYR:CD1	3.05	0.42
1:A:997:ILE:O	1:A:998:ASN:O	2.37	0.42
2:B:1469:THR:O	2:B:1470:LYS:HG2	2.19	0.42
2:B:1522:TYR:HD1	2:B:1524:TYR:CZ	2.36	0.42
2:B:1631:PHE:HD2	2:B:1632:SER:N	2.16	0.42
2:B:235:PHE:CE2	2:B:299:PHE:CE2	3.06	0.42
2:B:247:ILE:HD11	2:B:318:VAL:HG21	2.01	0.42
2:B:345:ILE:HG13	2:B:428:LYS:CB	2.49	0.42
2:B:875:LEU:O	2:B:875:LEU:HG	2.19	0.42
1:C:1075:SER:OG	1:C:1078:LEU:HB2	2.18	0.42
1:A:1163:LYS:NZ	1:C:1109:GLU:HG2	2.34	0.42
1:C:117:MET:HE2	1:C:117:MET:HB2	1.71	0.42
1:C:33:VAL:CG2	1:C:121:TYR:CD1	2.87	0.42
1:C:1402:ILE:CG2	1:C:1403:VAL:N	2.82	0.42
1:C:1562:LYS:C	1:C:1563:VAL:HG13	2.38	0.42
1:C:161:LEU:HD12	1:C:161:LEU:N	2.32	0.42
1:C:515:ARG:HG3	1:C:515:ARG:NH1	2.33	0.42
1:C:569:ASN:HD21	1:C:810:CYS:HB2	1.84	0.42
1:C:869:GLU:HB2	1:C:871:PRO:HG3	2.01	0.42
2:D:1471:PHE:O	2:D:1478:THR:O	2.37	0.42
2:D:267:VAL:HG22	2:D:314:LEU:CD1	2.49	0.42
2:D:63:ARG:HD2	2:D:65:GLN:NE2	2.33	0.42
2:D:878:ARG:HE	2:D:1421:VAL:CG2	2.32	0.42
3:Y:194:LYS:HG2	3:Y:197:ASN:HB3	2.01	0.42
1:A:108:SER:HG	1:A:111:PHE:C	2.22	0.42
1:A:1146:ALA:HB3	1:A:1190:ILE:CG2	2.48	0.42
1:A:1219:LYS:HE2	1:A:1239:VAL:CG2	2.49	0.42
1:A:1560:ALA:O	1:A:1561:TYR:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:PHE:O	1:A:256:TYR:HB2	2.19	0.42
1:A:291:MET:HB3	1:A:291:MET:HE2	1.75	0.42
1:A:364:LYS:HE2	1:A:465:LEU:O	2.18	0.42
1:A:491:PRO:CG	1:A:491:PRO:O	2.67	0.42
1:A:461:SER:HB3	1:A:553:GLU:OE2	2.19	0.42
1:A:639:GLY:HA2	1:A:648:LEU:CD1	2.45	0.42
1:A:689:LYS:CD	1:A:730:GLU:OE2	2.67	0.42
1:A:821:LYS:HB3	1:A:822:ASP:H	1.34	0.42
1:A:862:VAL:O	1:A:865:ILE:HG13	2.19	0.42
1:A:949:ILE:O	1:A:949:ILE:CG2	2.66	0.42
2:B:1538:ASP:OD2	2:B:1567:ARG:HD2	2.19	0.42
2:B:1544:VAL:C	2:B:1545:LEU:HD12	2.40	0.42
2:B:449:ILE:HA	2:B:449:ILE:HD12	1.71	0.42
2:B:967:GLY:O	2:B:969:PRO:HD3	2.18	0.42
1:C:100:SER:C	1:C:101:TYR:HD2	2.22	0.42
1:C:108:SER:HG	1:C:111:PHE:C	2.23	0.42
1:C:1110:ASN:O	1:C:1111:TYR:CD1	2.72	0.42
1:C:1344:ASP:OD1	1:C:1345:ASP:N	2.52	0.42
1:C:1622:LYS:HZ3	1:C:1642:LEU:CD2	2.27	0.42
1:C:1673:LEU:O	1:C:1674:ASN:CB	2.65	0.42
1:C:190:ILE:CG2	1:C:191:PRO:CD	2.97	0.42
1:C:73:LEU:HB2	1:C:79:PHE:HA	2.01	0.42
1:C:871:PRO:O	1:C:873:ILE:N	2.52	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
2:D:126:SER:OG	2:D:152:HIS:HD2	2.02	0.42
2:D:1370:ARG:HG3	2:D:1431:SER:O	2.19	0.42
2:D:1548:ILE:CG2	2:D:1635:LEU:CB	2.95	0.42
2:D:417:HIS:O	2:D:419:ASP:N	2.52	0.42
2:D:820:MET:HA	2:D:821:PRO:HD3	1.73	0.42
3:Y:91:LYS:NZ	3:Y:95:LYS:HE3	2.34	0.42
1:A:1244:THR:N	1:A:1247:MET:HE3	2.33	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:1348:VAL:HG11	1:A:1359:VAL:HG21	2.01	0.42
1:A:1559:TYR:HB3	1:A:1637:TYR:HE1	1.84	0.42
1:A:185:PHE:HD1	1:A:186:PRO:HD2	1.84	0.42
1:A:290:THR:CG2	1:A:297:ALA:HB1	2.48	0.42
1:A:420:PHE:N	1:A:420:PHE:CD2	2.86	0.42
1:A:489:LYS:HZ3	2:B:501:GLN:HA	1.85	0.42
1:A:949:ILE:O	1:A:950:TYR:CD1	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:946:PRO:O	1:A:953:ILE:HG13	2.19	0.42
2:B:878:ARG:HE	2:B:1421:VAL:CG2	2.32	0.42
2:B:1583:ILE:CG1	2:B:1607:ILE:HG23	2.42	0.42
1:C:1080:ALA:HB2	1:C:1148:THR:HG22	2.02	0.42
1:C:1468:PRO:HD2	1:C:1473:LEU:HB2	2.01	0.42
1:C:1644:TRP:O	1:C:1645:ILE:CD1	2.66	0.42
1:C:909:ASN:HD21	5:C:2003:NAG:C8	2.32	0.42
1:C:354:LEU:HD22	1:C:448:ALA:HB1	2.01	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
2:D:451:SER:O	2:D:452:THR:HG23	2.19	0.42
2:D:482:LEU:CB	2:D:492:VAL:HG23	2.33	0.42
2:D:568:GLU:HA	2:D:772:SER:O	2.19	0.42
3:X:217:ASN:ND2	3:X:220:ASP:OD2	2.48	0.42
3:Y:153:PHE:CE1	3:Y:169:ILE:HD13	2.55	0.42
3:Y:71:ASN:HD22	3:Y:91:LYS:CD	2.33	0.42
1:A:111:PHE:O	1:A:112:SER:OG	2.30	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
1:A:216:TYR:N	1:A:216:TYR:HD2	2.16	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:386:VAL:HA	1:A:387:PRO:HD3	1.82	0.42
1:A:433:PHE:N	1:A:433:PHE:CD1	2.88	0.42
1:A:49:ALA:CB	1:A:74:SER:HB2	2.50	0.42
1:A:662:SER:O	1:A:663:GLN:C	2.57	0.42
1:A:683:ILE:O	1:A:687:ALA:HB3	2.19	0.42
1:A:829:ILE:HD12	1:A:829:ILE:N	2.34	0.42
1:A:968:VAL:CG2	1:A:971:THR:HG21	2.49	0.42
2:B:1626:ASP:O	2:B:1627:ASP:C	2.58	0.42
2:B:1610:TRP:CE3	2:B:1628:PHE:CD2	3.08	0.42
2:B:236:TYR:O	2:B:238:ASP:N	2.52	0.42
2:B:344:GLN:O	2:B:366:VAL:HA	2.18	0.42
2:B:449:ILE:HG23	2:B:449:ILE:O	2.18	0.42
2:B:74:ASP:OD1	2:B:74:ASP:N	2.45	0.42
2:B:563:MET:SD	2:B:808:ILE:HD11	2.60	0.42
1:C:1189:ALA:O	1:C:1192:ALA:HB3	2.19	0.42
1:C:1188:LEU:CD2	1:C:1212:LEU:HA	2.49	0.42
1:C:1328:MET:HE2	1:C:1328:MET:HA	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:ILE:HG22	1:C:456:ALA:H	1.83	0.42
1:C:969:PRO:O	1:C:971:THR:HG23	2.19	0.42
2:D:964:ILE:HG22	2:D:1324:THR:OG1	2.18	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:D:174:SER:HA	2:D:1300:ALA:HB2	2.02	0.42
2:D:247:ILE:CD1	2:D:318:VAL:HG21	2.48	0.42
2:D:345:ILE:HD11	2:D:427:THR:CA	2.49	0.42
2:D:616:ASN:OD1	2:D:618:LEU:HB2	2.20	0.42
2:D:781:ARG:HD3	2:D:781:ARG:HA	1.53	0.42
2:D:859:ALA:CB	2:D:866:TYR:CD1	3.00	0.42
3:X:194:LYS:HG2	3:X:197:ASN:HB3	2.00	0.42
3:Y:217:ASN:ND2	3:Y:220:ASP:OD2	2.51	0.42
1:A:114:SER:O	1:A:115:LYS:HE2	2.20	0.42
1:A:571:LEU:HG	1:A:812:ALA:HB2	2.02	0.42
1:A:837:GLU:O	1:A:901:LEU:CD1	2.65	0.42
2:B:1284:ARG:HD2	2:B:1285:GLU:N	2.24	0.42
2:B:1444:LYS:NZ	2:B:1447:GLU:HA	2.34	0.42
2:B:1383:ASP:O	2:B:1456:VAL:HA	2.18	0.42
2:B:781:ARG:HA	2:B:781:ARG:HD3	1.53	0.42
1:C:1161:LEU:O	1:C:1164:ILE:HG12	2.19	0.42
1:C:1267:VAL:O	1:C:1270:VAL:HB	2.19	0.42
1:C:134:VAL:HA	1:C:218:GLU:O	2.19	0.42
1:C:981:GLY:O	1:C:1356:LEU:O	2.38	0.42
1:C:1637:TYR:HB3	1:C:1638:PRO:HD2	2.01	0.42
1:C:191:PRO:O	1:C:194:PRO:HD3	2.20	0.42
1:C:215:ALA:C	1:C:216:TYR:CD2	2.93	0.42
1:C:328:THR:OG1	1:C:339:GLU:HG2	2.19	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
1:C:693:SER:O	1:C:695:VAL:N	2.53	0.42
1:C:804:ILE:HG22	1:C:809:ILE:CB	2.49	0.42
1:C:997:ILE:O	1:C:998:ASN:O	2.37	0.42
2:D:280:LEU:HD22	2:D:1462:TYR:CE2	2.54	0.42
2:D:147:VAL:HG12	2:D:183:PHE:CE1	2.50	0.42
2:D:188:LEU:HD13	2:D:216:VAL:CG2	2.50	0.42
2:D:224:PHE:HE1	2:D:320:VAL:CG1	2.33	0.42
2:D:455:LYS:O	2:D:458:ASP:CB	2.58	0.42
3:X:153:PHE:CZ	3:X:169:ILE:HD13	2.55	0.42
3:Y:103:VAL:HA	3:Y:121:GLY:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:125:LYS:HD2	3:Y:126:ASN:HA	2.02	0.42
3:Y:190:ILE:O	3:Y:190:ILE:HG12	2.18	0.42
1:A:1239:VAL:N	1:A:1240:PRO:CD	2.82	0.42
1:A:1298:THR:O	1:A:1301:SER:N	2.53	0.42
1:A:160:VAL:HG11	1:A:204:LYS:HE3	2.01	0.42
1:A:205:TYR:HA	1:A:205:TYR:HD2	1.73	0.42
1:A:545:ILE:HG12	1:A:545:ILE:H	1.44	0.42
1:A:129:HIS:CE1	1:A:620:LEU:HD21	2.54	0.42
1:A:622:ARG:HD3	1:A:622:ARG:HA	1.73	0.42
1:A:905:ILE:O	1:A:905:ILE:HG22	2.19	0.42
2:B:1610:TRP:CE3	2:B:1628:PHE:HD2	2.38	0.42
2:B:164:GLU:HB2	2:B:200:VAL:HG23	2.02	0.42
2:B:296:ARG:NH1	2:B:296:ARG:HG3	2.32	0.42
2:B:599:TRP:O	2:B:600:ASP:C	2.55	0.42
2:B:785:THR:OG1	2:B:786:THR:N	2.51	0.42
2:B:873:LYS:CD	2:B:873:LYS:N	2.82	0.42
2:B:965:ILE:O	2:B:1301:ARG:HG2	2.19	0.42
2:B:968:ASP:O	2:B:1273:LEU:HD23	2.20	0.42
1:C:1283:GLY:HA3	1:C:1290:THR:HG23	2.02	0.42
1:C:1560:ALA:C	1:C:1561:TYR:CD2	2.93	0.42
1:C:1571:GLU:O	1:C:1574:PHE:N	2.49	0.42
1:C:216:TYR:HD2	1:C:216:TYR:N	2.17	0.42
1:C:287:MET:SD	1:C:299:VAL:HG23	2.60	0.42
1:C:383:VAL:HG23	1:C:386:VAL:CG2	2.49	0.42
1:C:40:VAL:HG12	1:C:509:ILE:HD12	2.00	0.42
1:C:461:SER:O	1:C:462:GLN:HB2	2.19	0.42
1:C:680:GLN:CG	1:C:681:LYS:N	2.80	0.42
1:C:718:ILE:HD11	1:C:728:PHE:CD2	2.54	0.42
1:C:752:LEU:CG	1:C:752:LEU:O	2.67	0.42
1:C:74:SER:C	1:C:79:PHE:CE1	2.93	0.42
1:C:582:TYR:O	1:C:819:VAL:HG13	2.20	0.42
1:C:829:ILE:HD12	1:C:829:ILE:N	2.33	0.42
1:C:829:ILE:CD1	1:C:829:ILE:N	2.82	0.42
1:C:839:ILE:HD12	1:C:1485:VAL:HG12	2.01	0.42
1:C:949:ILE:O	1:C:950:TYR:CD1	2.73	0.42
1:C:96:GLN:CG	1:C:97:ASN:H	2.29	0.42
2:D:200:VAL:HG12	2:D:211:THR:HG1	1.80	0.42
2:D:504:VAL:HG12	2:D:504:VAL:O	2.19	0.42
2:D:523:TYR:CB	2:D:533:ALA:HB2	2.48	0.42
2:D:736:GLU:C	2:D:738:GLY:H	2.22	0.42
2:D:80:GLY:O	2:D:81:MET:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:838:ASN:CG	2:D:838:ASN:O	2.58	0.42
2:D:952:ASP:O	2:D:1331:ALA:CA	2.67	0.42
2:D:955:PRO:O	2:D:957:THR:HG23	2.20	0.42
3:X:83:GLN:HG2	3:X:85:PHE:HE1	1.85	0.42
3:Y:101:GLN:HB3	3:Y:123:THR:O	2.20	0.42
3:Y:119:VAL:HG22	3:Y:212:MET:HB2	2.01	0.42
1:A:1083:LEU:HD22	1:A:1104:LEU:HD21	2.00	0.42
1:A:1147:PHE:HD2	1:A:1147:PHE:C	2.23	0.42
1:A:115:LYS:HB2	1:A:115:LYS:HE2	1.82	0.42
1:A:1639:LEU:HD22	1:A:1639:LEU:HA	1.76	0.42
1:A:259:VAL:HB	1:A:295:GLY:CA	2.49	0.42
1:A:309:GLU:CG	1:A:310:LEU:N	2.83	0.42
1:A:700:TYR:O	1:A:703:ALA:N	2.52	0.42
1:A:255:PHE:HB2	1:A:846:TYR:OH	2.20	0.42
1:A:883:CYS:HB2	2:B:902:GLU:OE2	2.20	0.42
2:B:1371:TYR:CB	2:B:1377:SER:HB3	2.50	0.42
2:B:1423:VAL:CG1	2:B:1423:VAL:O	2.67	0.42
2:B:1491:ARG:HG3	2:B:1492:CYS:N	2.33	0.42
2:B:1521:ASP:OD1	2:B:1552:THR:OG1	2.35	0.42
2:B:1528:LEU:HD21	2:B:1531:ILE:HD11	2.02	0.42
2:B:203:TYR:O	2:B:204:GLU:C	2.57	0.42
2:B:275:SER:C	2:B:277:PRO:HD3	2.40	0.42
2:B:355:LYS:N	2:B:355:LYS:CD	2.82	0.42
2:B:516:PRO:HG2	2:B:603:GLU:HG3	2.00	0.42
2:B:580:VAL:HG13	2:B:584:VAL:HG23	2.00	0.42
2:B:806:TYR:C	2:B:806:TYR:CD1	2.90	0.42
2:B:811:MET:HG3	2:B:812:LYS:N	2.35	0.42
2:B:933:ARG:HH11	2:B:933:ARG:CG	2.21	0.42
1:C:1022:PHE:HE2	1:C:1092:TYR:CD1	2.37	0.42
1:C:1239:VAL:O	1:C:1240:PRO:C	2.58	0.42
1:C:1190:ILE:CG1	1:C:1253:TYR:CE1	2.99	0.42
1:C:1386:ILE:HG22	1:C:1399:TYR:O	2.19	0.42
1:C:1440:LYS:O	1:C:1443:VAL:HG12	2.20	0.42
1:C:123:ASN:N	1:C:211:THR:HG23	2.33	0.42
1:C:506:LYS:HD2	1:C:536:PRO:HG2	2.01	0.42
1:C:821:LYS:HB3	1:C:822:ASP:H	1.31	0.42
2:D:114:ARG:O	2:D:114:ARG:NE	2.52	0.42
2:D:1290:TYR:HD2	2:D:1301:ARG:HB3	1.83	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:D:159:LYS:HE2	2:D:180:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:764:GLU:O	2:D:765:GLU:C	2.58	0.42
3:Y:194:LYS:HZ2	3:Y:197:ASN:CB	2.15	0.42
1:A:1161:LEU:O	1:A:1164:ILE:HG12	2.20	0.42
1:A:1246:ARG:HG3	1:A:1246:ARG:O	2.18	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:1643:THR:HG22	1:A:1644:TRP:H	1.82	0.42
1:A:308:LYS:CG	1:A:309:GLU:N	2.81	0.42
1:A:829:ILE:N	1:A:829:ILE:CD1	2.82	0.42
2:B:121:LEU:HA	2:B:121:LEU:HD12	1.72	0.42
2:B:1594:LYS:O	2:B:1596:LYS:HG2	2.20	0.42
2:B:234:PHE:CD1	2:B:234:PHE:C	2.93	0.42
2:B:513:ASP:OD2	2:B:513:ASP:N	2.52	0.42
2:B:745:ILE:HD11	2:B:907:ASP:N	2.34	0.42
2:B:838:ASN:OD1	2:B:838:ASN:C	2.58	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: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
1:C:773:TRP:CZ3	1:C:788:PHE:CE1	3.08	0.42
2:D:1279:ILE:HG22	2:D:1288:ILE:CB	2.44	0.42
2:D:1513:GLU:O	2:D:1516:CYS:N	2.53	0.42
2:D:1522:TYR:HE2	2:D:1585:GLY:C	2.23	0.42
2:D:1575:LEU:CD2	2:D:1575:LEU:N	2.83	0.42
2:D:1598:SER:C	2:D:1599:TYR:HD1	2.23	0.42
3:X:157:LYS:HA	3:X:157:LYS:HD3	1.83	0.42
3:X:215:VAL:C	3:X:216:LEU:HD22	2.40	0.42
3:Y:60:VAL:HG23	3:Y:60:VAL:O	2.19	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
1:A:1159:CYS:SG	1:A:1161:LEU:CD2	3.07	0.42
1:A:1297:LEU:CD1	1:A:1297:LEU:H	2.33	0.42
1:A:354:LEU:HD22	1:A:448:ALA:HB1	2.02	0.42
1:A:500:ASN:O	1:A:542:VAL:HA	2.19	0.42
1:A:569:ASN:HD21	1:A:810:CYS:HB2	1.84	0.42
1:A:604:ALA:O	1:A:772:SER:HB3	2.19	0.42
1:A:644:ASN:ND2	1:A:648:LEU:HD12	2.35	0.42
1:A:698:CYS:O	1:A:700:TYR:N	2.52	0.42
1:A:590:LEU:HD21	1:A:774:LEU:HD11	2.01	0.42
1:A:825:LEU:HB2	1:A:845:VAL:CG2	2.50	0.42
1:A:854:GLN:NE2	1:A:854:GLN:N	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1294:TYR:O	2:B:1294:TYR:CD2	2.73	0.42
2:B:141:SER:HA	2:B:142:PRO:HD3	1.85	0.42
2:B:618:LEU:HG	2:B:634:LEU:HD11	2.01	0.42
2:B:736:GLU:OE1	2:B:737:ASP:N	2.51	0.42
2:B:56:ILE:HD11	2:B:73:VAL:HG23	2.01	0.42
2:B:780:LEU:CD1	2:B:787:TRP:CD1	3.03	0.42
2:B:834:ALA:C	2:B:835:ILE:HD13	2.39	0.42
1:C:1066:TYR:HD1	1:C:1066:TYR:N	2.18	0.42
1:C:1069:TRP:HH2	1:C:1465:ASN:CG	2.24	0.42
1:C:1652:THR:HG22	1:C:1653:THR:N	2.35	0.42
1:C:352:TYR:HE2	1:C:442:LEU:CD1	2.33	0.42
1:C:436:LYS:HG3	1:C:437:THR:N	2.34	0.42
1:C:781:PRO:C	1:C:783:ARG:H	2.20	0.42
1:C:971:THR:O	1:C:972:GLU:C	2.58	0.42
2:D:1511:GLN:O	2:D:1514:LYS:HB2	2.20	0.42
2:D:1555:ASN:O	2:D:1558:ALA:HB3	2.20	0.42
2:D:1520:VAL:HG11	2:D:1584:TRP:CD1	2.55	0.42
2:D:220:VAL:O	2:D:221:LEU:C	2.57	0.42
2:D:869:GLN:O	2:D:870:PHE:HB3	2.20	0.42
1:A:1156:PHE:HZ	1:A:1165:ASP:HB2	1.84	0.42
1:A:1090:ASN:HD22	1:A:1158:ILE:HG12	1.85	0.42
1:A:117:MET:HB2	1:A:117:MET:HE2	1.68	0.42
1:A:1232:LEU:HG	1:A:1233:GLN:H	1.83	0.42
1:A:1245:ALA:O	1:A:1247:MET:N	2.52	0.42
1:A:1548:ARG:C	1:A:1550:GLN:N	2.73	0.42
1:A:177:ILE:N	1:A:177:ILE:HD13	2.35	0.42
1:A:259:VAL:HB	1:A:295:GLY:HA2	2.01	0.42
1:A:417:VAL:HG12	1:A:417:VAL:O	2.20	0.42
1:A:502:LEU:O	1:A:503:ILE:HD13	2.19	0.42
1:A:989:SER:O	1:A:993:SER:HB2	2.19	0.42
2:B:1518:THR:HG23	2:B:1519:ASN:H	1.85	0.42
2:B:341:SER:HB2	2:B:426:ALA:HB2	2.02	0.42
2:B:460:LEU:CD2	2:B:508:LEU:HB3	2.50	0.42
2:B:518:PHE:HE2	2:B:538:VAL:CG1	2.33	0.42
2:B:844:ILE:O	2:B:871:PRO:HA	2.20	0.42
2:B:932:PRO:HB3	2:B:939:GLY:O	2.20	0.42
2:B:946:LYS:N	2:B:946:LYS:CD	2.82	0.42
1:C:977:LEU:CD2	1:C:1361:VAL:HG22	2.49	0.42
1:C:931:PRO:CB	1:C:1366:HIS:CD2	3.00	0.42
1:C:215:ALA:C	1:C:216:TYR:HD2	2.23	0.42
1:C:267:ILE:CG2	1:C:268:THR:N	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:644:ASN:HD22	1:C:644:ASN:HA	1.59	0.42
1:C:651:LEU:HD23	1:C:651:LEU:HA	1.69	0.42
1:C:698:CYS:O	1:C:700:TYR:N	2.53	0.42
1:C:689:LYS:CD	1:C:730:GLU:OE2	2.68	0.42
1:C:839:ILE:HD12	1:C:839:ILE:HA	1.78	0.42
1:C:835:ARG:HH22	1:C:971:THR:HG22	1.84	0.42
2:D:1282:PRO:O	2:D:1283:ASP:C	2.57	0.42
2:D:1349:VAL:O	2:D:1350:GLU:HB3	2.20	0.42
2:D:1615:GLU:HB3	2:D:1621:PHE:CE1	2.54	0.42
2:D:416:ASN:CA	2:D:425:GLN:HE22	2.22	0.42
2:D:581:ASP:C	2:D:583:ALA:N	2.73	0.42
1:A:1011:GLU:HG3	1:A:1055:SER:CB	2.50	0.41
1:A:1069:TRP:HH2	1:A:1465:ASN:CG	2.23	0.41
1:A:1113:LEU:HD23	1:A:1114:ASP:H	1.85	0.41
1:A:123:ASN:O	1:A:211:THR:CG2	2.66	0.41
1:A:1554:LYS:CG	1:A:1555:PRO:HD2	2.50	0.41
1:A:961:TYR:CE2	1:A:1343:ASN:CA	3.00	0.41
2:B:1331:ALA:O	2:B:1332:GLN:CB	2.55	0.41
2:B:1349:VAL:O	2:B:1350:GLU:HB3	2.20	0.41
2:B:438:GLN:HE22	2:B:530:GLU:HA	1.85	0.41
2:B:632:THR:O	2:B:633:ASN:C	2.56	0.41
1:C:1022:PHE:O	1:C:1023:HIS:C	2.58	0.41
1:C:1108:VAL:CG2	1:C:1167:ALA:CB	2.97	0.41
1:C:1208:ILE:HG22	1:C:1208:ILE:O	2.19	0.41
1:C:1243:GLY:O	1:C:1285:TYR:CE2	2.73	0.41
1:C:1307:LEU:H	1:C:1307:LEU:HD22	1.85	0.41
1:C:1573:VAL:HG12	1:C:1603:LYS:CB	2.45	0.41
1:C:1559:TYR:HE1	1:C:1587:THR:HA	1.85	0.41
1:C:1576:LYS:CG	1:C:1601:ILE:HG22	2.40	0.41
1:C:308:LYS:CG	1:C:309:GLU:N	2.82	0.41
1:C:505:SER:O	1:C:506:LYS:C	2.56	0.41
1:C:943:THR:CG2	1:C:1356:LEU:HD21	2.50	0.41
2:D:1329:TYR:CD2	2:D:1329:TYR:N	2.88	0.41
2:D:276:ILE:HB	2:D:279:SER:OG	2.20	0.41
2:D:946:LYS:CD	2:D:946:LYS:N	2.83	0.41
4:E:1:NAG:O3	4:E:2:NAG:O5	2.38	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:510:ILE:HG22	3:Y:150:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:209:PHE:O	3:Y:212:MET:HB2	2.20	0.41
1:A:1084:ARG:HB2	1:A:1151:GLY:HA2	2.00	0.41
1:A:979:VAL:CG2	1:A:1326:TYR:HE1	2.27	0.41
1:A:1423:VAL:HG22	1:A:1496:TYR:HE2	1.85	0.41
1:A:544:TYR:HD2	1:A:544:TYR:O	2.04	0.41
1:A:613:GLN:C	1:A:615:GLY:N	2.73	0.41
1:A:602:LEU:HA	1:A:801:GLY:HA2	2.02	0.41
1:A:839:ILE:CD1	1:A:1485:VAL:HG12	2.50	0.41
2:B:126:SER:OG	2:B:152:HIS:HD2	2.02	0.41
2:B:1529:LEU:O	2:B:1577:VAL:HG13	2.20	0.41
2:B:1581:TYR:HA	2:B:1608:GLU:O	2.20	0.41
2:B:355:LYS:HA	2:B:356:PRO:HD3	1.85	0.41
2:B:506:MET:O	2:B:506:MET:HG2	2.17	0.41
2:B:816:ILE:HD12	2:B:909:VAL:HG23	2.02	0.41
2:B:966:GLN:HG3	2:B:966:GLN:O	2.20	0.41
1:C:1016:VAL:N	1:C:1017:PRO:CD	2.83	0.41
1:C:1033:ILE:HG23	1:C:1034:PHE:CD1	2.55	0.41
1:C:1342:LEU:H	1:C:1342:LEU:HG	1.50	0.41
1:C:260:VAL:CG1	1:C:261:THR:N	2.82	0.41
1:C:644:ASN:O	1:C:645:VAL:C	2.58	0.41
1:C:984:VAL:HG12	1:C:988:LEU:HD12	2.01	0.41
2:D:961:THR:HG22	2:D:1327:THR:OG1	2.19	0.41
2:D:1410:ARG:HA	2:D:1410:ARG:HD2	1.81	0.41
2:D:203:TYR:O	2:D:204:GLU:C	2.59	0.41
2:D:355:LYS:HA	2:D:356:PRO:HD3	1.85	0.41
2:D:524:TYR:HD1	2:D:524:TYR:C	2.22	0.41
2:D:874:ALA:C	2:D:876:SER:N	2.72	0.41
3:Y:169:ILE:HG21	3:Y:189:ILE:HD13	2.02	0.41
1:A:1153:ARG:NH2	1:A:1172:ASP:OD2	2.53	0.41
1:A:149:ASN:N	1:A:149:ASN:ND2	2.67	0.41
1:A:1571:GLU:O	1:A:1574:PHE:CG	2.73	0.41
1:A:222:TYR:HE2	1:A:224:LEU:N	2.18	0.41
1:A:491:PRO:O	1:A:493:ILE:N	2.52	0.41
1:A:862:VAL:CG1	1:A:863:GLU:OE1	2.68	0.41
2:B:1430:VAL:HA	2:B:1436:GLU:OE2	2.21	0.41
2:B:1476:LYS:HB3	2:B:1476:LYS:HE3	1.90	0.41
2:B:1598:SER:C	2:B:1599:TYR:HD1	2.22	0.41
2:B:358:MET:HE2	2:B:467:LYS:HD2	2.02	0.41
2:B:481:TYR:CE2	2:B:493:GLY:N	2.88	0.41
2:B:76:ASN:CB	2:B:77:PRO:HD2	2.46	0.41
2:B:913:LEU:C	2:B:913:LEU:CD2	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1025:LEU:HD11	1:C:1034:PHE:HZ	1.85	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:1428:LEU:HA	1:C:1428:LEU:HD23	1.76	0.41
1:C:149:ASN:O	1:C:152:LEU:N	2.23	0.41
1:C:1565:ILE:HB	1:C:1614:GLY:N	2.36	0.41
1:C:196:TYR:HA	1:C:219:VAL:HG12	2.02	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
1:C:604:ALA:O	1:C:772:SER:HB3	2.21	0.41
1:C:621:GLU:HG3	1:C:621:GLU:H	1.32	0.41
1:C:622:ARG:HD3	1:C:622:ARG:HA	1.73	0.41
1:C:76:GLU:O	1:C:76:GLU:CD	2.59	0.41
2:D:235:PHE:CZ	2:D:296:ARG:NE	2.87	0.41
2:D:355:LYS:CD	2:D:355:LYS:N	2.81	0.41
2:D:469:ASN:ND2	2:D:472:SER:N	2.69	0.41
2:D:811:MET:HG3	2:D:812:LYS:N	2.35	0.41
2:D:940:THR:O	2:D:940:THR:HG22	2.19	0.41
2:D:922:LYS:NZ	2:D:952:ASP:OD2	2.53	0.41
3:X:194:LYS:HZ2	3:X:197:ASN:HD22	1.68	0.41
1:A:1175:LEU:HB3	1:A:1195:LEU:HD11	2.02	0.41
1:A:1430:THR:O	1:A:1430:THR:HG22	2.20	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
2:B:1524:TYR:HB3	2:B:1544:VAL:HG13	2.01	0.41
2:B:221:LEU:HG	2:B:221:LEU:H	1.66	0.41
2:B:133:ASP:HB3	2:B:757:TRP:CZ3	2.56	0.41
1:C:146:TYR:CD1	1:C:182:ILE:HG23	2.55	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:C:162:THR:HB	1:C:173:MET:CE	2.50	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
1:C:905:ILE:O	1:C:905:ILE:HG22	2.18	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:D:476:ILE:HG23	2:D:497:ARG:HD3	2.03	0.41
2:D:804:GLU:HA	2:D:804:GLU:OE2	2.19	0.41
3:Y:46:LEU:N	3:Y:46:LEU:HD23	2.36	0.41
1:A:1110:ASN:O	1:A:1111:TYR:CD1	2.73	0.41
1:A:1179:THR:HG22	1:A:1208:ILE:HD13	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:ASP:OD2	1:A:1476:ARG:HD3	2.20	0.41
1:A:147:SER:OG	1:A:147:SER:O	2.38	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:A:1575:VAL:O	1:A:1601:ILE:HA	2.21	0.41
1:A:163:PHE:CD1	1:A:163:PHE:N	2.88	0.41
1:A:20:GLU:O	1:A:21:GLN:CG	2.69	0.41
1:A:680:GLN:CG	1:A:681:LYS:H	2.32	0.41
2:B:1575:LEU:N	2:B:1575:LEU:HD22	2.34	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
2:B:278:ASP:OD1	2:B:278:ASP:N	2.54	0.41
2:B:280:LEU:HD22	2:B:1462:TYR:CE2	2.54	0.41
2:B:423:GLU:CD	2:B:423:GLU:H	2.23	0.41
2:B:511:THR:O	2:B:512:PRO:C	2.58	0.41
2:B:52:LYS:HG2	2:B:111:PRO:HB2	2.01	0.41
2:B:445:LEU:HD23	2:B:533:ALA:HA	2.02	0.41
2:B:150:MET:SD	2:B:800:ILE:HB	2.61	0.41
1:C:1024:TYR:HB2	1:C:1298:THR:CG2	2.50	0.41
1:C:1081:PHE:O	1:C:1084:ARG:N	2.54	0.41
1:C:978:SER:O	1:C:1359:VAL:HA	2.21	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
1:C:395:ILE:HG22	1:C:401:THR:HG22	2.02	0.41
1:C:439:ALA:HA	1:C:440:PRO:HD3	1.85	0.41
1:C:461:SER:C	1:C:463:SER:N	2.73	0.41
1:C:470:THR:HG22	2:D:450:THR:HA	2.03	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:590:LEU:CD2	1:C:774:LEU:HD11	2.50	0.41
1:C:182:ILE:HG21	1:C:601:ALA:HB2	2.01	0.41
1:C:613:GLN:C	1:C:615:GLY:N	2.73	0.41
1:C:824:PHE:CE2	1:C:846:TYR:CD1	3.04	0.41
2:D:1522:TYR:CE2	2:D:1585:GLY:N	2.77	0.41
2:D:194:LEU:HD22	2:D:194:LEU:N	2.36	0.41
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
2:D:275:SER:C	2:D:277:PRO:HD3	2.41	0.41
1:A:1080:ALA:HB1	1:A:1148:THR:HA	2.01	0.41
1:A:1156:PHE:CZ	1:A:1165:ASP:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1231:ASN:OD1	1:A:1232:LEU:N	2.53	0.41
1:A:151:ASP:O	1:A:152:LEU:HB2	2.21	0.41
1:A:1652:THR:HG22	1:A:1653:THR:N	2.36	0.41
1:A:238:ILE:HD11	1:A:246:PHE:CD2	2.56	0.41
1:A:23:TYR:CE1	1:A:655:THR:O	2.74	0.41
1:A:311:SER:O	1:A:313:TYR:N	2.53	0.41
1:A:328:THR:OG1	1:A:339:GLU:HG2	2.20	0.41
1:A:500:ASN:ND2	1:A:543:TYR:HE1	2.15	0.41
1:A:20:GLU:HB2	1:A:551:THR:HB	2.01	0.41
1:A:610:TYR:CE2	1:A:619:PRO:HG3	2.54	0.41
1:A:627:LEU:HD23	1:A:627:LEU:HA	1.69	0.41
2:B:1370:ARG:NH1	2:B:1372:LEU:HG	2.34	0.41
2:B:1500:LEU:C	2:B:1500:LEU:HD12	2.41	0.41
2:B:358:MET:HA	2:B:359:PRO:HD3	1.97	0.41
2:B:436:GLN:O	2:B:437:THR:C	2.57	0.41
2:B:628:LEU:HD12	2:B:629:THR:N	2.35	0.41
2:B:79:GLY:C	2:B:81:MET:H	2.24	0.41
2:B:825:VAL:HG11	2:B:918:GLU:HB3	2.01	0.41
1:C:1179:THR:HG22	1:C:1208:ILE:HD13	1.98	0.41
1:C:1548:ARG:C	1:C:1550:GLN:N	2.74	0.41
1:C:1570:VAL:HG22	1:C:1575:VAL:HG22	2.02	0.41
1:C:286:ALA:O	1:C:287:MET:C	2.58	0.41
1:C:309:GLU:CG	1:C:310:LEU:N	2.84	0.41
1:C:38:ASN:HA	1:C:84:ILE:CG2	2.44	0.41
1:C:525:SER:O	2:D:401:ASN:ND2	2.54	0.41
1:C:705:VAL:CA	1:C:739:ARG:NH2	2.83	0.41
1:C:946:PRO:O	1:C:953:ILE:HG13	2.21	0.41
1:C:958:GLU:HG2	1:C:1347:ILE:HG12	2.01	0.41
1:C:961:TYR:HE1	1:C:963:ILE:HG12	1.86	0.41
2:D:120:LEU:HA	2:D:120:LEU:HD13	1.78	0.41
2:D:965:ILE:HA	2:D:1322:THR:O	2.20	0.41
2:D:1511:GLN:CG	2:D:1631:PHE:CE1	3.04	0.41
2:D:257:VAL:CG1	2:D:258:GLU:N	2.82	0.41
2:D:296:ARG:HA	2:D:296:ARG:HD2	1.93	0.41
2:D:306:LEU:HA	2:D:306:LEU:HD13	1.85	0.41
2:D:59:HIS:HA	2:D:68:LEU:HD22	2.02	0.41
2:D:785:THR:OG1	2:D:786:THR:N	2.52	0.41
2:D:818:LEU:HD23	2:D:911:LYS:HB2	2.01	0.41
1:A:1028:GLY:HA3	1:A:1030:HIS:CE1	2.55	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:A:1279:ARG:HD3	1:A:1280:TYR:H	1.85	0.41
1:A:1320:LYS:CD	1:A:1321:GLY:N	2.78	0.41
1:A:1540:ASP:CA	1:A:1660:PHE:CD1	3.03	0.41
2:B:1391:LEU:HA	2:B:1392:PRO:HD3	1.88	0.41
2:B:810:VAL:CG1	2:B:811:MET:N	2.83	0.41
2:B:902:GLU:O	2:B:903:ALA:HB2	2.21	0.41
1:C:1033:ILE:HG23	1:C:1034:PHE:H	1.85	0.41
1:C:1211:ALA:HA	1:C:1214:ARG:NH1	2.34	0.41
1:C:1231:ASN:HB2	1:C:1235:LYS:CG	2.49	0.41
1:C:1445:GLY:O	1:C:1448:GLN:HB3	2.20	0.41
1:C:1563:VAL:HG12	1:C:1581:LEU:HA	2.02	0.41
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:D:476:ILE:CG1	2:D:524:TYR:CD2	3.03	0.41
2:D:563:MET:HA	2:D:563:MET:CE	2.50	0.41
2:D:610:THR:C	2:D:612:GLY:N	2.72	0.41
2:D:101:ASN:ND2	2:D:641:ALA:HB2	2.36	0.41
1:A:1019:PHE:CZ	1:A:1088:GLN:HB3	2.56	0.41
1:A:1033:ILE:HD13	1:A:1034:PHE:CE1	2.55	0.41
1:A:1145:THR:HG22	1:A:1146:ALA:N	2.35	0.41
1:A:1195:LEU:HD23	1:A:1195:LEU:HA	1.95	0.41
1:A:1435:ASN:O	1:A:1436:GLU:C	2.58	0.41
1:A:1538:GLU:H	1:A:1538:GLU:CD	2.23	0.41
1:A:185:PHE:CB	1:A:186:PRO:HD2	2.51	0.41
1:A:215:ALA:C	1:A:216:TYR:CD2	2.94	0.41
1:A:461:SER:C	1:A:463:SER:N	2.74	0.41
1:A:804:ILE:HA	1:A:809:ILE:HA	2.02	0.41
2:B:1273:LEU:HD12	2:B:1273:LEU:C	2.41	0.41
2:B:965:ILE:HD13	2:B:1277:ILE:HD13	2.03	0.41
2:B:1518:THR:HG23	2:B:1519:ASN:N	2.36	0.41
2:B:1548:ILE:HA	2:B:1636:THR:OG1	2.21	0.41
2:B:276:ILE:HB	2:B:279:SER:OG	2.21	0.41
2:B:345:ILE:O	2:B:428:LYS:HD3	2.21	0.41
2:B:822:TYR:CD1	2:B:822:TYR:O	2.74	0.41
1:C:1093:VAL:O	1:C:1094:GLU:C	2.59	0.41
1:C:1159:CYS:O	1:C:1161:LEU:HD23	2.20	0.41
1:C:1234:HIS:CG	1:C:1235:LYS:N	2.88	0.41
1:C:123:ASN:C	1:C:211:THR:HG21	2.39	0.41
1:C:316:GLU:N	1:C:316:GLU:OE1	2.41	0.41
1:C:465:LEU:HD12	1:C:466:TYR:H	1.85	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:C:697:LYS:O	1:C:700:TYR:N	2.54	0.41
1:C:710:THR:OG1	1:C:713:GLN:HG3	2.21	0.41
1:C:805:SER:O	1:C:806:ASN:C	2.59	0.41
1:C:953:ILE:CD1	1:C:955:ARG:HH21	2.33	0.41
1:C:965:LEU:C	1:C:967:LEU:H	2.24	0.41
2:D:1273:LEU:HD12	2:D:1273:LEU:O	2.20	0.41
2:D:283:ILE:HA	2:D:284:PRO:HD3	1.81	0.41
2:D:417:HIS:CD2	2:D:419:ASP:HB2	2.56	0.41
2:D:541:LYS:O	2:D:543:THR:CG2	2.69	0.41
2:D:748:ARG:NH1	2:D:784:ILE:HG12	2.36	0.41
3:Y:138:VAL:HG11	3:Y:177:TYR:CD2	2.56	0.41
3:Y:52:SER:OG	3:Y:53:GLU:N	2.53	0.41
1:A:1188:LEU:HD23	1:A:1212:LEU:CA	2.51	0.41
1:A:1445:GLY:O	1:A:1448:GLN:HB3	2.21	0.41
1:A:1552:ALA:HB1	1:A:1585:TYR:OH	2.20	0.41
1:A:1560:ALA:C	1:A:1561:TYR:CD2	2.95	0.41
1:A:1565:ILE:HB	1:A:1614:GLY:N	2.36	0.41
1:A:174:VAL:CG2	1:A:175:GLU:H	2.34	0.41
1:A:215:ALA:C	1:A:216:TYR:HD2	2.24	0.41
1:A:49:ALA:HB2	1:A:74:SER:HB2	2.01	0.41
2:B:1424:ILE:HG12	2:B:1426:TYR:HE2	1.80	0.41
2:B:1522:TYR:HD1	2:B:1524:TYR:CE1	2.38	0.41
2:B:1571:GLU:O	2:B:1574:ASN:HB2	2.21	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:615:GLN:CB	2:B:616:ASN:HD22	2.34	0.41
2:B:819:GLN:HE21	2:B:819:GLN:HA	1.85	0.41
2:B:857:CYS:CB	2:B:885:VAL:CG2	2.99	0.41
1:C:1047:LYS:O	1:C:1048:LYS:C	2.58	0.41
1:C:1180:LEU:O	1:C:1180:LEU:HD22	2.20	0.41
1:C:1218:VAL:CG1	1:C:1219:LYS:N	2.72	0.41
1:C:1314:ASP:OD2	1:C:1325:ASN:HB3	2.20	0.41
1:C:1342:LEU:HD23	1:C:1342:LEU:N	2.36	0.41
1:C:153:LYS:CB	1:C:154:PRO:CD	2.99	0.41
1:C:1638:PRO:HG2	1:C:1639:LEU:H	1.85	0.41
1:C:1661:LEU:O	1:C:1662:ALA:C	2.59	0.41
1:C:185:PHE:CD1	1:C:186:PRO:HD2	2.56	0.41
1:C:20:GLU:HG3	1:C:547:THR:OG1	2.21	0.41
1:C:560:TRP:CH2	1:C:562:ASN:HB2	2.55	0.41
1:C:999:ILE:O	1:C:1000:LEU:C	2.59	0.41
2:D:1429:LYS:HE3	2:D:1429:LYS:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:338:ILE:C	2:D:339:VAL:HG13	2.41	0.41
2:D:518:PHE:H	2:D:518:PHE:HD2	1.68	0.41
2:D:620:VAL:CG1	2:D:621:PHE:N	2.84	0.41
2:D:819:GLN:HE21	2:D:819:GLN:HA	1.85	0.41
2:D:895:GLU:HA	2:D:909:VAL:O	2.21	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:A:734:VAL:O	1:A:737:GLN:HB2	2.21	0.41
1:A:849:ARG:HH22	2:B:555:LEU:C	2.24	0.41
1:A:958:GLU:HG2	1:A:1347:ILE:HG12	2.03	0.41
2:B:104:VAL:HG12	2:B:121:LEU:HD13	2.02	0.41
2:B:952:ASP:O	2:B:1331:ALA:CA	2.69	0.41
2:B:1444:LYS:HZ1	2:B:1447:GLU:HA	1.86	0.41
2:B:1605:THR:HG22	2:B:1605:THR:O	2.20	0.41
2:B:504:VAL:O	2:B:504:VAL:HG12	2.21	0.41
1:A:856:CYS:N	2:B:904:LEU:HD11	2.36	0.41
1:C:1176:LEU:HD21	1:C:1195:LEU:HD13	2.02	0.41
1:C:1232:LEU:HG	1:C:1233:GLN:H	1.86	0.41
1:C:1644:TRP:NE1	1:C:1646:GLU:OE1	2.52	0.41
1:C:1669:GLU:O	1:C:1673:LEU:HG	2.21	0.41
1:C:354:LEU:H	1:C:354:LEU:HD23	1.85	0.41
1:C:620:LEU:O	1:C:623:VAL:CG2	2.65	0.41
1:C:257:ASN:HB2	1:C:848:TYR:CE2	2.56	0.41
1:C:934:VAL:O	1:C:935:LYS:HE2	2.21	0.41
2:D:1279:ILE:HD13	2:D:1279:ILE:HA	1.86	0.41
2:D:1423:VAL:CG1	2:D:1423:VAL:O	2.68	0.41
2:D:1459:TYR:CB	2:D:1466:GLU:HB3	2.51	0.41
2:D:147:VAL:O	2:D:147:VAL:CG1	2.69	0.41
2:D:1506:ILE:HB	2:D:1627:ASP:HB3	2.02	0.41
2:D:247:ILE:HD11	2:D:318:VAL:HG21	2.03	0.41
2:D:341:SER:HB2	2:D:426:ALA:HB2	2.03	0.41
2:D:438:GLN:HE22	2:D:530:GLU:HA	1.86	0.41
2:D:58:VAL:HG23	2:D:69:PHE:O	2.21	0.41
2:D:751:PHE:N	2:D:751:PHE:CD2	2.88	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:C:915:GLU:HG3	2:D:904:LEU:HG	2.03	0.41
1:A:1127:ILE:N	1:A:1127:ILE:HD12	2.28	0.41
1:A:1161:LEU:HD12	1:C:1105:LEU:CD1	2.46	0.41
1:A:1268:ASN:N	1:A:1269:PRO:HD2	2.35	0.41
1:A:131:ASP:OD2	1:A:132:LYS:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ASN:HD21	1:A:153:LYS:H	1.67	0.41
1:A:1564:SER:HA	1:A:1616:GLN:HA	2.02	0.41
1:A:161:LEU:HD12	1:A:161:LEU:N	2.35	0.41
1:A:1638:PRO:HG2	1:A:1639:LEU:N	2.36	0.41
1:A:382:LEU:HA	1:A:382:LEU:HD23	1.80	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:A:88:GLN:HA	1:A:89:PRO:HD2	1.88	0.41
1:A:967:LEU:HD12	1:A:968:VAL:H	1.86	0.41
2:B:103:TYR:HD2	2:B:103:TYR:N	2.19	0.41
2:B:1429:LYS:N	2:B:1429:LYS:HE3	2.36	0.41
2:B:1446:PHE:CD2	2:B:1448:VAL:HG13	2.56	0.41
2:B:146:ARG:HH11	2:B:146:ARG:CB	2.34	0.41
2:B:168:PRO:CG	2:B:196:THR:N	2.84	0.41
2:B:101:ASN:ND2	2:B:641:ALA:HB2	2.36	0.41
2:B:811:MET:CE	2:B:839:TYR:HD2	2.35	0.41
2:B:850:LEU:CD1	2:B:851:LEU:N	2.84	0.41
2:B:828:GLU:O	2:B:886:PRO:HD2	2.21	0.41
1:A:1161:LEU:CA	1:C:1102:ASN:HD21	2.26	0.41
1:C:1274:LEU:O	1:C:1275:SER:C	2.59	0.41
1:C:701:ASP:CG	1:C:1446:VAL:HG23	2.41	0.41
1:C:255:PHE:HD1	1:C:255:PHE:O	2.04	0.41
1:C:315:LEU:HD11	1:C:318:LEU:HG	1.98	0.41
1:C:566:LYS:O	1:C:568:GLY:N	2.54	0.41
1:C:734:VAL:O	1:C:737:GLN:HB2	2.21	0.41
1:C:81:ASN:CG	1:C:82:SER:N	2.74	0.41
2:D:1363:LEU:HD23	2:D:1442:ILE:HG12	2.03	0.41
2:D:1378:THR:O	2:D:1379:MET:C	2.59	0.41
2:D:173:VAL:O	2:D:174:SER:HB2	2.20	0.41
2:D:370:ASP:OD1	2:D:370:ASP:N	2.47	0.41
2:D:553:ASP:N	2:D:553:ASP:OD1	2.54	0.41
1:A:1054:LEU:O	1:A:1055:SER:C	2.59	0.40
1:A:25:ILE:HD13	1:A:25:ILE:HA	1.90	0.40
1:A:455:ILE:CG2	1:A:456:ALA:N	2.83	0.40
1:A:367:ILE:HD13	1:A:466:TYR:CD2	2.56	0.40
1:A:46:TYR:HE1	1:A:48:GLU:HB2	1.85	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:A:827:MET:HB3	1:A:829:ILE:CD1	2.52	0.40
2:B:1410:ARG:HD2	2:B:1410:ARG:HA	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1494:GLY:O	2:B:1495:GLU:HB2	2.21	0.40
2:B:235:PHE:HB3	2:B:338:ILE:CG2	2.52	0.40
2:B:410:PRO:CB	2:B:431:THR:HG22	2.50	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
2:B:148:PHE:HB2	2:B:800:ILE:HD11	2.00	0.40
2:B:816:ILE:CD1	2:B:909:VAL:HG23	2.51	0.40
2:B:253:TYR:HE1	2:B:839:TYR:HE2	1.69	0.40
1:C:100:SER:C	1:C:101:TYR:CD2	2.94	0.40
1:C:54:ILE:HA	1:C:105:GLU:O	2.21	0.40
1:C:1215:GLU:O	1:C:1217:LEU:HD23	2.21	0.40
1:C:1246:ARG:NH1	1:C:1246:ARG:HB2	2.36	0.40
1:C:1267:VAL:HG12	1:C:1267:VAL:O	2.20	0.40
1:C:1305:LYS:HD3	1:C:1305:LYS:HA	1.70	0.40
1:C:1339:GLU:OE1	1:C:1339:GLU:HA	2.21	0.40
1:C:1575:VAL:O	1:C:1601:ILE:HA	2.21	0.40
1:C:404:LEU:HA	1:C:404:LEU:HD22	1.69	0.40
1:C:569:ASN:O	1:C:570:GLN:CB	2.51	0.40
1:C:681:LYS:HD2	1:C:738:LEU:HD21	2.04	0.40
1:C:601:ALA:N	1:C:802:VAL:O	2.48	0.40
1:A:1042:LYS:HZ3	1:C:92:LEU:HD13	1.86	0.40
2:D:1571:GLU:O	2:D:1574:ASN:HB2	2.21	0.40
2:D:490:PHE:C	2:D:490:PHE:CD1	2.91	0.40
2:D:820:MET:HE2	2:D:832:ILE:HG21	2.03	0.40
3:X:100:GLY:O	3:X:125:LYS:CG	2.68	0.40
3:X:153:PHE:CE1	3:X:169:ILE:HD13	2.55	0.40
1:A:1013:MET:O	1:A:1015:VAL:N	2.54	0.40
1:A:1244:THR:HG23	1:A:1502:ASP:CG	2.40	0.40
1:A:1020:TYR:CE1	1:A:1295:GLU:HA	2.56	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:41:ILE:HG21	1:A:41:ILE:HD13	1.68	0.40
1:A:594:THR:O	1:A:782:ARG:CD	2.69	0.40
1:A:705:VAL:CA	1:A:739:ARG:HH22	2.35	0.40
1:A:889:GLU:HB2	1:A:892:SER:HB2	2.04	0.40
1:A:971:THR:O	1:A:972:GLU:C	2.59	0.40
2:B:1292:ILE:HD11	2:B:1301:ARG:HE	1.86	0.40
2:B:1635:LEU:HD23	2:B:1635:LEU:HA	1.60	0.40
2:B:352:LYS:HG3	2:B:430:MET:CE	2.51	0.40
2:B:150:MET:HG3	2:B:602:ILE:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1011:GLU:HG3	1:C:1055:SER:CB	2.51	0.40
1:C:1180:LEU:HA	1:C:1180:LEU:HD23	1.48	0.40
1:C:1320:LYS:HD2	1:C:1320:LYS:HA	1.88	0.40
1:C:1449:LEU:HD12	1:C:1449:LEU:O	2.22	0.40
1:C:162:THR:HG23	1:C:202:LYS:HB2	2.03	0.40
1:C:357:VAL:O	1:C:358:ALA:C	2.60	0.40
1:C:600:VAL:HG11	1:C:602:LEU:HD21	2.02	0.40
1:C:705:VAL:CA	1:C:739:ARG:HH22	2.33	0.40
1:C:604:ALA:HB3	1:C:773:TRP:O	2.21	0.40
1:C:941:GLY:HA2	1:C:1359:VAL:O	2.22	0.40
2:D:1331:ALA:O	2:D:1332:GLN:CB	2.58	0.40
2:D:1367:ILE:HD13	2:D:1456:VAL:HG21	2.02	0.40
2:D:147:VAL:O	2:D:147:VAL:HG13	2.20	0.40
2:D:1491:ARG:HD3	2:D:1491:ARG:HA	1.89	0.40
2:D:1509:PRO:HA	2:D:1512:ILE:CG1	2.51	0.40
2:D:472:SER:O	2:D:475:GLN:HG3	2.22	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
2:D:780:LEU:CD1	2:D:787:TRP:CD1	3.05	0.40
2:D:827:ASN:OD1	2:D:1490:CYS:HB2	2.22	0.40
2:D:925:VAL:HG22	2:D:1326:LEU:CD2	2.40	0.40
2:D:967:GLY:O	2:D:969:PRO:HD3	2.21	0.40
3:Y:185:LYS:HB3	3:Y:185:LYS:HE2	1.98	0.40
1:A:1161:LEU:CD1	1:C:1105:LEU:CD1	3.00	0.40
1:A:116:ARG:O	1:A:117:MET:HB3	2.21	0.40
1:A:1220:GLY:O	1:A:1223:PRO:HA	2.21	0.40
1:A:127:PHE:HD2	1:A:623:VAL:HG22	1.85	0.40
1:A:1243:GLY:O	1:A:1285:TYR:CE2	2.74	0.40
1:A:1420:SER:O	1:A:1421:HIS:C	2.58	0.40
1:A:1450:PHE:HB3	1:A:1463:GLN:O	2.21	0.40
1:A:153:LYS:CB	1:A:154:PRO:CD	2.99	0.40
1:A:255:PHE:HD1	1:A:255:PHE:O	2.04	0.40
1:A:284:GLN:HG2	1:A:310:LEU:HD11	2.03	0.40
1:A:510:ILE:HA	3:X:150:ILE:HG13	2.02	0.40
1:A:587:THR:HA	1:A:789:ALA:HA	2.02	0.40
2:B:1539:ILE:N	2:B:1539:ILE:HD12	2.34	0.40
2:B:283:ILE:HA	2:B:284:PRO:HD3	1.81	0.40
2:B:330:VAL:HG23	2:B:330:VAL:O	2.22	0.40
2:B:460:LEU:HD23	2:B:508:LEU:HB3	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:476:ILE:CG1	2:B:524:TYR:CD2	3.04	0.40
1:C:1053:MET:CE	1:C:1085:VAL:HG12	2.51	0.40
1:C:1127:ILE:HB	1:C:1129:LEU:HD21	2.03	0.40
1:C:1146:ALA:HB3	1:C:1190:ILE:CG2	2.51	0.40
1:C:602:LEU:HA	1:C:801:GLY:HA2	2.03	0.40
1:C:854:GLN:HE21	1:C:854:GLN:C	2.23	0.40
1:C:914:LEU:O	1:C:914:LEU:HG	2.20	0.40
1:C:92:LEU:HA	1:C:93:PRO:HD3	1.96	0.40
2:D:164:GLU:HB2	2:D:200:VAL:HG23	2.03	0.40
2:D:345:ILE:HD11	2:D:426:ALA:C	2.41	0.40
2:D:352:LYS:HG3	2:D:430:MET:HE1	2.03	0.40
2:D:45:ALA:HB3	2:D:81:MET:CE	2.51	0.40
2:D:468:GLY:O	2:D:469:ASN:C	2.59	0.40
2:D:745:ILE:O	2:D:745:ILE:CG2	2.68	0.40
2:D:943:GLU:CB	2:D:1313:VAL:HG23	2.52	0.40
1:C:78:LYS:NZ	3:Y:143:GLY:O	2.47	0.40
3:Y:40:LEU:HD11	3:Y:209:PHE:HZ	1.85	0.40
3:Y:67:TYR:CD1	3:Y:67:TYR:O	2.74	0.40
3:Y:61:SER:OG	3:Y:99:GLN:HA	2.20	0.40
1:A:1300:TYR:CE2	1:A:1304:VAL:HG21	2.56	0.40
1:A:1358:THR:HB	1:A:1360:HIS:HE1	1.84	0.40
1:A:1440:LYS:O	1:A:1443:VAL:HG12	2.21	0.40
1:A:431:LEU:C	1:A:431:LEU:CD2	2.90	0.40
1:A:718:ILE:HB	1:A:725:ILE:CD1	2.51	0.40
2:B:1292:ILE:HD12	2:B:1296:ASN:OD1	2.21	0.40
2:B:145:TYR:CD1	2:B:145:TYR:C	2.95	0.40
2:B:1534:GLN:HB2	2:B:1539:ILE:HD11	2.04	0.40
2:B:802:VAL:HG12	2:B:802:VAL:O	2.22	0.40
2:B:848:VAL:HG22	2:B:898:ALA:HB2	2.04	0.40
2:B:950:LEU:O	2:B:951:ASP:HB2	2.21	0.40
1:C:1018:VAL:HG11	1:C:1048:LYS:HB3	2.03	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
1:C:1248:VAL:H	1:C:1248:VAL:HG23	1.69	0.40
1:C:1430:THR:HG22	1:C:1430:THR:O	2.21	0.40
1:C:243:PHE:O	1:C:303:SER:HB2	2.21	0.40
1:C:492:TYR:HE2	1:C:546:VAL:HG11	1.86	0.40
1:C:531:THR:HG23	1:C:533:ASN:N	2.37	0.40
1:C:22:THR:HG21	1:C:657:ALA:HB2	2.04	0.40
1:C:789:ALA:O	1:C:790:LEU:O	2.40	0.40
1:C:804:ILE:HA	1:C:809:ILE:HA	2.03	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:D:121:LEU:HD12	2:D:121:LEU:HA	1.72	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:D:1615:GLU:O	2:D:1616:CYS:C	2.60	0.40
2:D:269:ILE:HG13	2:D:272:ALA:HB3	2.02	0.40
2:D:515:ILE:HG21	2:D:599:TRP:CZ2	2.56	0.40
2:D:64:LYS:HG3	2:D:64:LYS:O	2.22	0.40
2:D:76:ASN:CB	2:D:77:PRO:HD2	2.52	0.40
2:D:794:PHE:CD2	2:D:795:THR:N	2.89	0.40
2:D:851:LEU:CD2	2:D:852:TYR:H	2.17	0.40
2:D:878:ARG:HA	2:D:878:ARG:HD2	1.92	0.40
3:X:101:GLN:HB3	3:X:123:THR:O	2.22	0.40
3:Y:113:ASN:HD21	3:Y:115:ARG:HG2	1.87	0.40
1:A:1264:ILE:HD12	1:A:1264:ILE:N	2.36	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:A:1309:LEU:CD2	1:A:1355:GLY:HA3	2.52	0.40
1:A:160:VAL:O	1:A:160:VAL:HG12	2.20	0.40
1:A:22:THR:CG2	1:A:23:TYR:CE1	3.04	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
1:A:644:ASN:O	1:A:647:HIS:N	2.55	0.40
1:A:658:ASN:O	1:A:658:ASN:OD1	2.40	0.40
1:A:984:VAL:HG13	1:A:984:VAL:O	2.21	0.40
2:B:174:SER:HA	2:B:1300:ALA:HB2	2.02	0.40
2:B:1459:TYR:CB	2:B:1466:GLU:HB3	2.52	0.40
2:B:261:ALA:HB2	2:B:285:ILE:HD11	2.01	0.40
2:B:397:LYS:NZ	2:B:449:ILE:O	2.55	0.40
2:B:476:ILE:CD1	2:B:524:TYR:CD2	3.02	0.40
2:B:618:LEU:CD1	2:B:635:ASN:O	2.65	0.40
2:B:751:PHE:CD2	2:B:751:PHE:N	2.90	0.40
2:B:795:THR:CG2	2:B:796:PRO:CD	2.98	0.40
1:C:1008:ALA:O	1:C:1011:GLU:N	2.55	0.40
1:C:1090:ASN:O	1:C:1092:TYR:N	2.54	0.40
1:C:1147:PHE:C	1:C:1147:PHE:HD2	2.25	0.40
1:C:1228:TRP:N	1:C:1228:TRP:HE3	2.20	0.40
1:C:1467:ILE:HA	1:C:1468:PRO:HD3	1.83	0.40
1:C:284:GLN:HG2	1:C:310:LEU:HD11	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:671:GLU:HB2	1:C:672:ILE:H	1.66	0.40
1:C:718:ILE:HB	1:C:725:ILE:CD1	2.51	0.40
1:C:823:VAL:HG23	1:C:846:TYR:O	2.20	0.40
1:C:923:LEU:CD2	1:C:925:LYS:HD3	2.52	0.40
2:D:1296:ASN:HB2	2:D:1299:LEU:HD22	2.03	0.40
2:D:1486:ILE:O	2:D:1486:ILE:HG13	2.22	0.40
2:D:409:LEU:N	2:D:410:PRO:HD3	2.36	0.40
2:D:23:ALA:CB	2:D:528:ASN:HD22	2.27	0.40
1:C:849:ARG:NH2	2:D:555:LEU:HB2	2.36	0.40
2:D:891:LEU:H	2:D:891:LEU:HG	1.10	0.40
3:Y:83:GLN:O	3:Y:117:SER:HA	2.22	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%)	0	12
1	C	1616/1676 (96%)	1179 (73%)	290 (18%)	147 (9%)	1	12
2	B	1203/1642 (73%)	981 (82%)	176 (15%)	46 (4%)	3	27
2	D	1203/1642 (73%)	982 (82%)	177 (15%)	44 (4%)	3	28
3	X	189/231 (82%)	148 (78%)	31 (16%)	10 (5%)	2	22
3	Y	189/231 (82%)	150 (79%)	28 (15%)	11 (6%)	1	20
All	All	6016/7098 (85%)	4605 (76%)	1002 (17%)	409 (7%)	1	17

All (409) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	GLN

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

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Mol	Chain	Res	Type
1	A	1674	ASN
2	B	207	PRO
2	B	453	GLU
2	B	490	PHE
2	B	873	LYS
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

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Mol	Chain	Res	Type
1	C	1335	GLY
1	C	1452	ASP
1	C	1538	GLU
1	C	1590	ALA
1	C	1609	ALA
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

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Mol	Chain	Res	Type
1	A	669	CYS
1	A	672	ILE
1	A	690	TYR
1	A	806	ASN
1	A	820	PHE
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

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Mol	Chain	Res	Type
1	C	474	LYS
1	C	520	ASP
1	C	596	MET
1	C	614	ARG
1	C	623	VAL
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

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Mol	Chain	Res	Type
1	A	671	GLU
1	A	681	LYS
1	A	699	CYS
1	A	791	PRO
1	A	793	SER
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

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Mol	Chain	Res	Type
1	C	1133	LEU
1	C	1200	LYS
1	C	1241	ASN
1	C	1471	ASP
1	C	1589	GLU
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

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Mol	Chain	Res	Type
1	C	170	GLU
1	C	256	TYR
1	C	641	ASN
1	C	663	GLN
1	C	699	CYS
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

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Mol	Chain	Res	Type
2	B	1592	PRO
2	B	1628	PHE
1	C	61	ASP
1	C	337	SER
1	C	488	PRO
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

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Mol	Chain	Res	Type
1	A	406	PRO
1	A	577	PRO
2	B	237	ILE
1	C	43	VAL
1	C	406	PRO
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%)	<span style="border: 2px solid red; padding: 2px;">0</span> <span style="border: 2px solid red; padding: 2px;">4</span>

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	1445/1484 (97%)	1098 (76%)	347 (24%)	0	5
2	B	1084/1435 (76%)	849 (78%)	235 (22%)	1	6
2	D	1084/1435 (76%)	855 (79%)	229 (21%)	1	7
3	X	175/205 (85%)	143 (82%)	32 (18%)	1	11
3	Y	175/205 (85%)	142 (81%)	33 (19%)	1	10
All	All	5408/6248 (87%)	4177 (77%)	1231 (23%)	1	6

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

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Mol	Chain	Res	Type
1	A	149	ASN
1	A	152	LEU
1	A	157	ARG
1	A	161	LEU
1	A	162	THR
1	A	169	SER
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

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Mol	Chain	Res	Type
1	A	322	TYR
1	A	323	LEU
1	A	328	THR
1	A	333	THR
1	A	342	ILE
1	A	353	LYS
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

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Mol	Chain	Res	Type
1	A	506	LYS
1	A	509	ILE
1	A	510	ILE
1	A	512	PHE
1	A	522	SER
1	A	526	ILE
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

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Mol	Chain	Res	Type
1	A	700	TYR
1	A	701	ASP
1	A	710	THR
1	A	711	CYS
1	A	713	GLN
1	A	720	LEU
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

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Mol	Chain	Res	Type
1	A	905	ILE
1	A	916	THR
1	A	917	TRP
1	A	928	ARG
1	A	935	LYS
1	A	936	ARG
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

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Mol	Chain	Res	Type
1	A	1110	ASN
1	A	1113	LEU
1	A	1123	GLN
1	A	1125	GLN
1	A	1127	ILE
1	A	1128	LYS
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

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Mol	Chain	Res	Type
1	A	1331	LYS
1	A	1334	LEU
1	A	1336	ARG
1	A	1341	LEU
1	A	1342	LEU
1	A	1346	LEU
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

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Mol	Chain	Res	Type
1	A	1535	MET
1	A	1539	LEU
1	A	1542	THR
1	A	1548	ARG
1	A	1549	LYS
1	A	1556	GLU
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

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Mol	Chain	Res	Type
2	B	105	VAL
2	B	114	ARG
2	B	119	VAL
2	B	120	LEU
2	B	121	LEU
2	B	124	GLN
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

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Mol	Chain	Res	Type
2	B	349	LYS
2	B	390	THR
2	B	398	LEU
2	B	400	LEU
2	B	404	LEU
2	B	411	ILE
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

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Mol	Chain	Res	Type
2	B	563	MET
2	B	567	LEU
2	B	574	ARG
2	B	582	LYS
2	B	584	VAL
2	B	588	ASN
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

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Mol	Chain	Res	Type
2	B	867	ARG
2	B	870	PHE
2	B	872	ILE
2	B	873	LYS
2	B	875	LEU
2	B	880	VAL
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

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Mol	Chain	Res	Type
2	B	1365	LEU
2	B	1372	LEU
2	B	1378	THR
2	B	1380	THR
2	B	1401	SER
2	B	1404	VAL
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

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Mol	Chain	Res	Type
2	B	1584	TRP
2	B	1591	LEU
2	B	1594	LYS
2	B	1597	ILE
2	B	1598	SER
2	B	1604	ASN
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

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Mol	Chain	Res	Type
1	C	136	THR
1	C	143	VAL
1	C	144	ARG
1	C	147	SER
1	C	149	ASN
1	C	152	LEU
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

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Mol	Chain	Res	Type
1	C	291	MET
1	C	292	LEU
1	C	294	ASN
1	C	296	ILE
1	C	315	LEU
1	C	321	LYS
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

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Mol	Chain	Res	Type
1	C	492	TYR
1	C	493	ILE
1	C	494	ASP
1	C	495	LYS
1	C	497	THR
1	C	504	LEU
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

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Mol	Chain	Res	Type
1	C	654	LEU
1	C	658	ASN
1	C	669	CYS
1	C	679	LEU
1	C	684	GLU
1	C	700	TYR
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

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Mol	Chain	Res	Type
1	C	916	THR
1	C	917	TRP
1	C	928	ARG
1	C	935	LYS
1	C	936	ARG
1	C	942	VAL
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

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Mol	Chain	Res	Type
1	C	1127	ILE
1	C	1128	LYS
1	C	1132	THR
1	C	1133	LEU
1	C	1140	ASN
1	C	1142	LEU
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

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Mol	Chain	Res	Type
1	C	1346	LEU
1	C	1347	ILE
1	C	1348	VAL
1	C	1350	THR
1	C	1352	PHE
1	C	1356	LEU
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

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Mol	Chain	Res	Type
1	C	1556	GLU
1	C	1557	ILE
1	C	1559	TYR
1	C	1566	THR
1	C	1569	THR
1	C	1573	VAL
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

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Mol	Chain	Res	Type
2	D	124	GLN
2	D	146	ARG
2	D	147	VAL
2	D	150	MET
2	D	161	VAL
2	D	167	THR
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

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Mol	Chain	Res	Type
2	D	411	ILE
2	D	422	ARG
2	D	435	TYR
2	D	437	THR
2	D	450	THR
2	D	458	ASP
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

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Mol	Chain	Res	Type
2	D	588	ASN
2	D	593	ILE
2	D	594	SER
2	D	606	ASP
2	D	620	VAL
2	D	629	THR
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

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Mol	Chain	Res	Type
2	D	884	ILE
2	D	889	GLN
2	D	891	LEU
2	D	913	LEU
2	D	914	LYS
2	D	916	VAL
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

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Mol	Chain	Res	Type
2	D	1423	VAL
2	D	1424	ILE
2	D	1425	ILE
2	D	1427	LEU
2	D	1429	LYS
2	D	1433	SER
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

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Mol	Chain	Res	Type
2	D	1634	THR
2	D	1638	PHE
3	X	41	HIS
3	X	43	ILE
3	X	46	LEU
3	X	50	TYR
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

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Mol	Chain	Res	Type
3	Y	67	TYR
3	Y	75	PHE
3	Y	78	LYS
3	Y	80	GLN
3	Y	85	PHE
3	Y	94	TYR
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

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Mol	Chain	Res	Type
1	A	391	ASN
1	A	473	HIS
1	A	481	HIS
1	A	569	ASN
1	A	706	ASN
1	A	785	GLN
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

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Mol	Chain	Res	Type
2	B	469	ASN
2	B	507	ASN
2	B	525	GLN
2	B	615	GLN
2	B	819	GLN
2	B	829	GLN
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

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Mol	Chain	Res	Type
1	C	875	HIS
1	C	876	GLN
1	C	909	ASN
1	C	1023	HIS
1	C	1029	ASN
1	C	1030	HIS
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

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Mol	Chain	Res	Type
2	D	1330	ASN
2	D	1341	ASN
2	D	1473	HIS
2	D	1503	GLN
2	D	1511	GLN
2	D	1562	GLN
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 monosaccharides 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	E	1	2,4	14,14,15	0.96	1 (7%)	17,19,21	2.06	6 (35%)
4	NAG	E	2	4	14,14,15	1.04	1 (7%)	17,19,21	2.50	6 (35%)
4	NAG	F	1	2,4	14,14,15	2.05	7 (50%)	17,19,21	3.28	8 (47%)
4	NAG	F	2	4	14,14,15	1.64	1 (7%)	17,19,21	2.34	6 (35%)
4	NAG	G	1	2,4	14,14,15	0.88	1 (7%)	17,19,21	1.97	6 (35%)
4	NAG	G	2	4	14,14,15	1.07	1 (7%)	17,19,21	1.74	4 (23%)
4	NAG	H	1	2,4	14,14,15	1.99	6 (42%)	17,19,21	3.46	9 (52%)
4	NAG	H	2	4	14,14,15	1.52	1 (7%)	17,19,21	2.32	6 (35%)

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	E	1	2,4	-	4/6/23/26	0/1/1/1
4	NAG	E	2	4	-	5/6/23/26	0/1/1/1
4	NAG	F	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	6/6/23/26	0/1/1/1
4	NAG	G	1	2,4	-	3/6/23/26	0/1/1/1
4	NAG	G	2	4	-	5/6/23/26	0/1/1/1
4	NAG	H	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	6/6/23/26	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	2	NAG	C1-C2	5.13	1.60	1.52
4	H	2	NAG	C1-C2	4.97	1.59	1.52
4	F	1	NAG	C1-C2	3.85	1.58	1.52
4	H	1	NAG	C1-C2	3.38	1.57	1.52
4	F	1	NAG	O5-C1	3.13	1.48	1.43
4	H	1	NAG	C4-C3	2.99	1.59	1.52
4	E	1	NAG	C1-C2	2.84	1.56	1.52
4	F	1	NAG	C4-C3	2.79	1.59	1.52
4	F	1	NAG	C4-C5	2.75	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	NAG	O5-C1	2.68	1.48	1.43
4	H	1	NAG	O4-C4	2.67	1.49	1.43
4	F	1	NAG	O4-C4	2.48	1.48	1.43
4	H	1	NAG	C4-C5	2.47	1.58	1.53
4	H	1	NAG	C3-C2	2.41	1.57	1.52
4	G	2	NAG	C1-C2	2.39	1.55	1.52
4	G	1	NAG	C1-C2	2.37	1.55	1.52
4	E	2	NAG	C3-C2	2.27	1.57	1.52
4	F	1	NAG	C2-N2	2.20	1.50	1.46
4	F	1	NAG	C3-C2	2.16	1.57	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	NAG	C1-O5-C5	10.09	125.86	112.19
4	F	1	NAG	C1-O5-C5	9.29	124.78	112.19
4	E	2	NAG	C4-C3-C2	6.58	120.66	111.02
4	H	2	NAG	C1-C2-N2	5.47	119.84	110.49
4	F	2	NAG	C1-C2-N2	5.45	119.79	110.49
4	H	1	NAG	C2-N2-C7	5.39	130.58	122.90
4	F	1	NAG	C2-N2-C7	5.39	130.58	122.90
4	H	1	NAG	C4-C3-C2	5.29	118.77	111.02
4	F	2	NAG	O5-C5-C6	4.99	115.03	107.20
4	F	1	NAG	C4-C3-C2	4.16	117.11	111.02
4	E	2	NAG	C1-O5-C5	4.14	117.81	112.19
4	H	2	NAG	O5-C5-C6	4.03	113.53	107.20
4	E	1	NAG	O5-C1-C2	3.99	117.58	111.29
4	G	2	NAG	C4-C3-C2	3.93	116.77	111.02
4	H	2	NAG	C2-N2-C7	3.86	128.40	122.90
4	E	1	NAG	C1-O5-C5	3.67	117.16	112.19
4	G	1	NAG	C1-O5-C5	3.59	117.06	112.19
4	G	1	NAG	O5-C1-C2	3.50	116.81	111.29
4	E	1	NAG	C1-C2-N2	3.26	116.05	110.49
4	E	2	NAG	O5-C5-C6	3.25	112.30	107.20
4	G	2	NAG	C2-N2-C7	3.25	127.52	122.90
4	G	1	NAG	C1-C2-N2	3.22	115.99	110.49
4	H	1	NAG	O4-C4-C3	3.20	117.75	110.35
4	F	1	NAG	O5-C5-C4	3.12	118.42	110.83
4	H	1	NAG	O5-C5-C4	3.09	118.34	110.83
4	F	1	NAG	O5-C1-C2	3.03	116.07	111.29
4	F	1	NAG	O7-C7-N2	2.95	127.38	121.95
4	F	2	NAG	C2-N2-C7	2.92	127.06	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	2	NAG	O3-C3-C2	2.89	115.45	109.47
4	E	2	NAG	C2-N2-C7	2.88	127.01	122.90
4	G	1	NAG	O3-C3-C2	-2.83	103.61	109.47
4	F	2	NAG	O5-C1-C2	-2.83	106.82	111.29
4	H	2	NAG	O5-C1-C2	-2.73	106.97	111.29
4	E	1	NAG	O5-C5-C6	2.63	111.33	107.20
4	H	2	NAG	O3-C3-C2	2.50	114.63	109.47
4	E	2	NAG	O4-C4-C3	2.49	116.10	110.35
4	G	2	NAG	C1-O5-C5	2.47	115.53	112.19
4	H	2	NAG	O7-C7-C8	-2.45	117.50	122.06
4	E	2	NAG	O5-C5-C4	-2.44	104.89	110.83
4	E	1	NAG	O3-C3-C4	2.41	115.92	110.35
4	H	1	NAG	O3-C3-C2	-2.38	104.54	109.47
4	F	1	NAG	O3-C3-C4	2.24	115.53	110.35
4	F	2	NAG	O7-C7-C8	-2.23	117.91	122.06
4	H	1	NAG	O5-C1-C2	2.18	114.73	111.29
4	G	1	NAG	C3-C4-C5	-2.16	106.39	110.24
4	E	1	NAG	O3-C3-C2	-2.13	105.05	109.47
4	G	2	NAG	O7-C7-N2	2.13	125.87	121.95
4	F	1	NAG	C8-C7-N2	-2.13	112.50	116.10
4	G	1	NAG	C4-C3-C2	-2.11	107.92	111.02
4	H	1	NAG	O3-C3-C4	2.03	115.04	110.35
4	H	1	NAG	O7-C7-N2	2.00	125.63	121.95

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	H	2	NAG	C8-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2
4	G	2	NAG	C1-C2-N2-C7
4	F	2	NAG	C1-C2-N2-C7
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
4	E	2	NAG	C1-C2-N2-C7
4	E	2	NAG	O7-C7-N2-C2
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	E	2	NAG	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	F	1	NAG	C8-C7-N2-C2
4	H	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
4	E	1	NAG	C4-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
4	H	2	NAG	C1-C2-N2-C7
4	F	2	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	H	2	NAG	C3-C2-N2-C7
4	F	2	NAG	C3-C2-N2-C7
4	E	1	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6

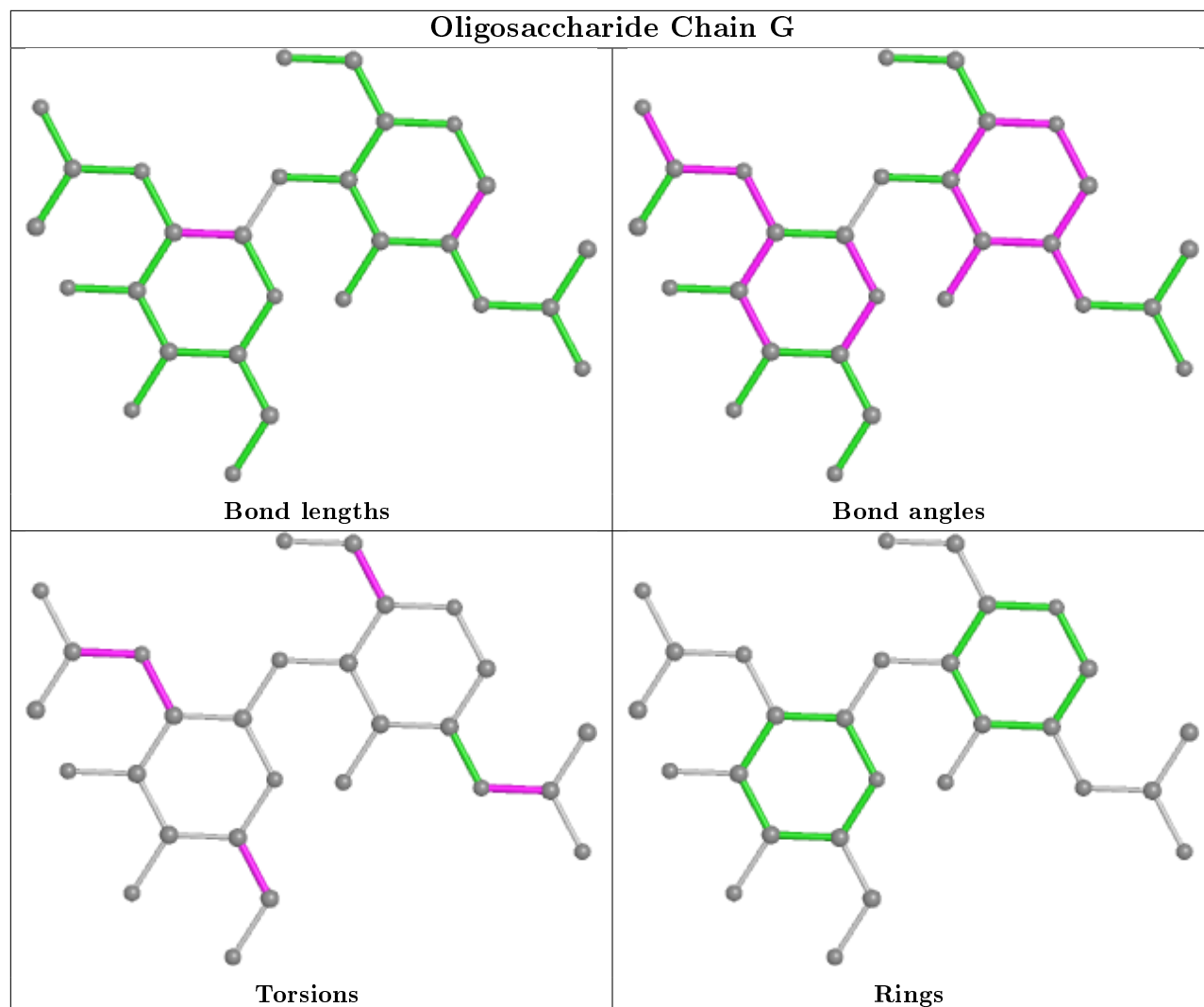
There are no ring outliers.

6 monomers are involved in 13 short contacts:

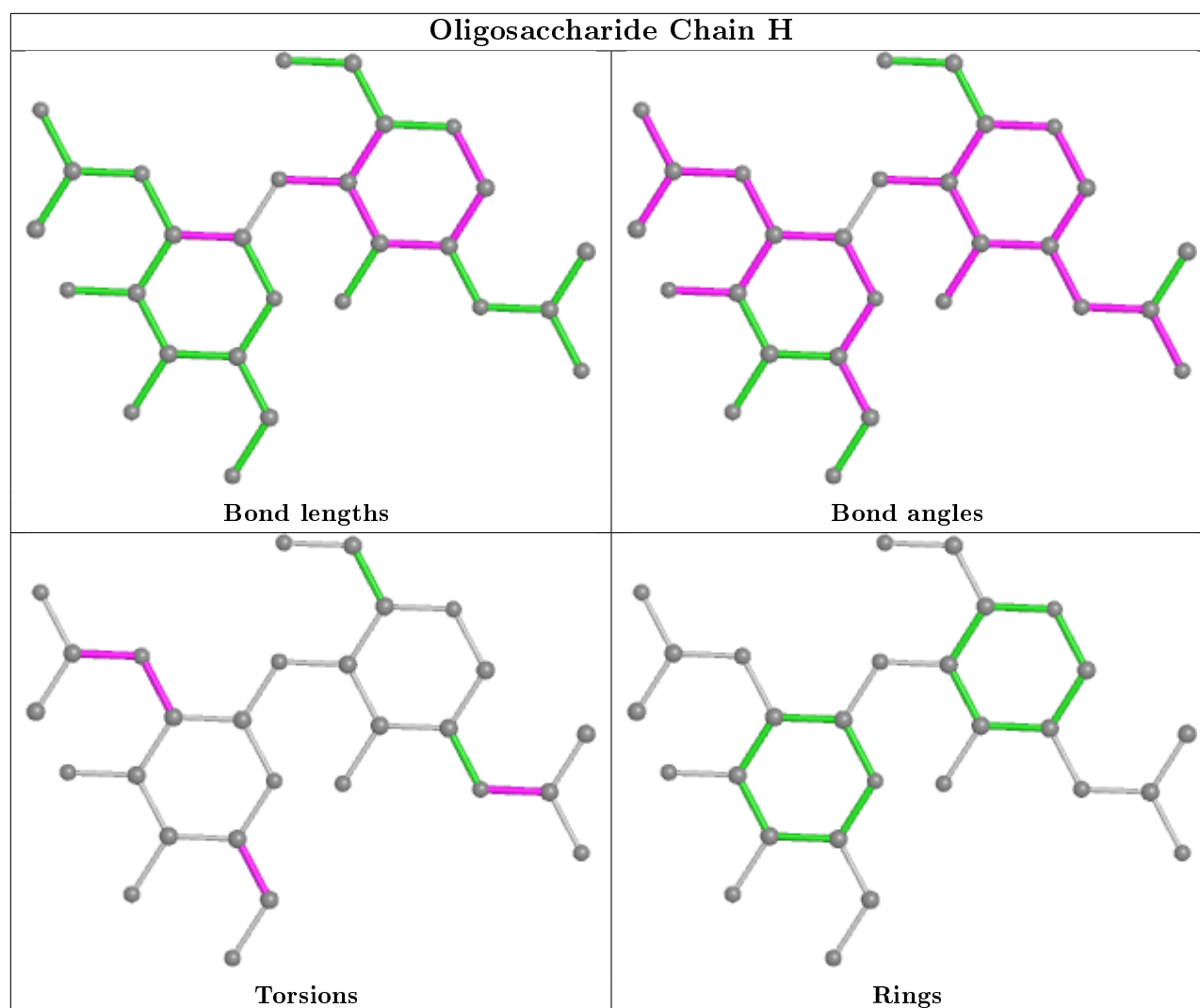
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	NAG	3	0
4	F	1	NAG	3	0
4	G	2	NAG	4	0
4	H	1	NAG	3	0
4	E	2	NAG	3	0
4	G	1	NAG	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









## 5.6 Ligand geometry ⓘ

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	$\# Z  > 2$
5	NAG	C	2003	1	14,14,15	2.04	4 (28%)	17,19,21	2.60	10 (58%)
5	NAG	A	2003	1	14,14,15	1.89	5 (35%)	17,19,21	3.34	13 (76%)



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	C	2003	1	-	4/6/23/26	0/1/1/1
5	NAG	A	2003	1	-	2/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2003	NAG	C1-C2	4.43	1.59	1.52
5	A	2003	NAG	C3-C2	4.37	1.61	1.52
5	C	2003	NAG	C3-C2	3.97	1.60	1.52
5	C	2003	NAG	C4-C5	3.10	1.59	1.53
5	A	2003	NAG	O4-C4	2.43	1.48	1.43
5	A	2003	NAG	C4-C3	2.23	1.58	1.52
5	A	2003	NAG	C4-C5	2.18	1.57	1.53
5	C	2003	NAG	O4-C4	2.16	1.48	1.43
5	A	2003	NAG	O5-C5	2.13	1.47	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2003	NAG	C2-N2-C7	5.28	130.43	122.90
5	A	2003	NAG	O7-C7-C8	-5.11	112.57	122.06
5	A	2003	NAG	C4-C3-C2	4.83	118.10	111.02
5	C	2003	NAG	O3-C3-C2	4.38	118.53	109.47
5	A	2003	NAG	O4-C4-C3	4.22	120.10	110.35
5	A	2003	NAG	C1-O5-C5	3.97	117.58	112.19
5	C	2003	NAG	O7-C7-C8	-3.54	115.49	122.06
5	A	2003	NAG	C3-C4-C5	-3.51	103.97	110.24
5	C	2003	NAG	O4-C4-C5	3.47	117.91	109.30
5	A	2003	NAG	O4-C4-C5	3.36	117.64	109.30
5	A	2003	NAG	C8-C7-N2	3.27	121.64	116.10
5	C	2003	NAG	C2-N2-C7	3.17	127.41	122.90
5	A	2003	NAG	O3-C3-C4	-3.15	103.06	110.35
5	A	2003	NAG	O3-C3-C2	3.11	115.91	109.47
5	C	2003	NAG	C1-O5-C5	3.06	116.33	112.19
5	C	2003	NAG	O5-C5-C4	3.00	118.14	110.83
5	C	2003	NAG	C1-C2-N2	-2.77	105.75	110.49
5	A	2003	NAG	C1-C2-N2	-2.71	105.86	110.49
5	A	2003	NAG	O5-C5-C6	2.66	111.37	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	2003	NAG	O4-C4-C3	2.57	116.30	110.35
5	C	2003	NAG	O7-C7-N2	2.36	126.30	121.95
5	C	2003	NAG	C4-C3-C2	2.30	114.38	111.02
5	A	2003	NAG	O7-C7-N2	2.09	125.79	121.95

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	2003	NAG	O5-C5-C6-O6
5	A	2003	NAG	O5-C5-C6-O6
5	C	2003	NAG	C4-C5-C6-O6
5	A	2003	NAG	C4-C5-C6-O6
5	C	2003	NAG	C8-C7-N2-C2
5	C	2003	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	2003	NAG	2	0
5	A	2003	NAG	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1626/1676 (97%)	-0.04	19 (1%) 79 70	72, 150, 260, 469	0
1	C	1626/1676 (97%)	0.03	42 (2%) 56 46	60, 153, 277, 515	0
2	B	1215/1642 (73%)	0.02	21 (1%) 70 61	73, 160, 235, 335	0
2	D	1215/1642 (73%)	-0.03	16 (1%) 77 68	85, 155, 241, 362	0
3	X	191/231 (82%)	0.68	26 (13%) 3 3	99, 230, 333, 437	0
3	Y	191/231 (82%)	0.41	15 (7%) 12 11	95, 195, 300, 385	0
All	All	6064/7098 (85%)	0.03	139 (2%) 60 51	60, 157, 264, 515	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	X	112	PRO	11.8
3	Y	114	GLY	6.8
3	X	113	ASN	5.6
1	C	1651	ASP	5.6
3	X	114	GLY	5.6
3	Y	113	ASN	5.4
1	C	1592	ALA	5.1
1	C	1585	TYR	4.6
2	D	1272	ASP	4.4
3	X	70	SER	4.2
3	Y	115	ARG	4.1
3	X	95	LYS	4.0
3	Y	59	ASN	4.0
2	D	100	GLN	3.9
2	D	98	SER	3.7
3	Y	71	ASN	3.5
1	A	874	ASP	3.5
2	B	1319	GLY	3.4
2	D	1318	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	97	ASP	3.4
3	Y	92	GLU	3.4
1	A	1002	HIS	3.3
1	C	1622	LYS	3.3
1	A	94	GLY	3.3
1	C	1537	GLU	3.2
1	C	1586	LYS	3.2
2	B	1272	ASP	3.2
1	C	1593	GLU	3.2
1	C	1525	CYS	3.1
3	Y	195	ASP	3.1
1	C	1002	HIS	3.1
1	C	882	LYS	3.1
1	C	273	GLU	3.1
2	B	1320	LYS	3.0
3	X	90	ASP	3.0
2	D	1273	LEU	3.0
1	C	874	ASP	3.0
3	Y	95	LYS	3.0
1	C	1538	GLU	3.0
3	X	108	GLU	3.0
1	C	278	ASP	2.9
1	A	879	LYS	2.9
2	B	639	ARG	2.8
2	B	1435	ASP	2.8
1	C	712	GLU	2.8
3	X	104	PHE	2.8
2	B	1273	LEU	2.7
2	D	940	THR	2.7
1	A	1545	ALA	2.7
2	D	99	ARG	2.7
3	X	76	ASN	2.7
3	X	93	GLN	2.7
1	C	93	PRO	2.6
1	C	1609	ALA	2.6
1	C	1596	SER	2.6
3	X	71	ASN	2.6
3	X	127	ASN	2.6
1	C	1597	GLU	2.6
1	A	1398	ASP	2.6
1	C	159	THR	2.6
3	X	111	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
3	X	126	ASN	2.6
1	C	1594	LYS	2.6
1	C	1557	ILE	2.6
1	A	817	ALA	2.5
1	A	1622	LYS	2.5
2	D	941	GLN	2.5
3	X	128	LYS	2.5
2	B	1344	HIS	2.5
3	Y	159	GLU	2.5
2	D	765	GLU	2.5
1	C	94	GLY	2.5
1	C	1598	ILE	2.4
1	A	1399	TYR	2.4
2	B	1370	ARG	2.4
2	B	1376	ASP	2.4
3	X	92	GLU	2.4
3	X	79	ASP	2.4
3	X	74	ARG	2.4
1	C	403	ASP	2.4
2	B	640	SER	2.4
2	D	1354	LEU	2.4
1	C	1544	SER	2.3
3	X	101	GLN	2.3
1	C	446	ASN	2.3
3	X	120	GLY	2.3
3	X	195	ASP	2.3
1	A	273	GLU	2.3
1	A	1526	LYS	2.3
2	B	1434	GLU	2.3
1	A	691	LYS	2.3
1	C	255	PHE	2.3
1	C	1241	ASN	2.3
2	D	66	LYS	2.3
3	Y	196	GLU	2.3
2	B	99	ARG	2.2
2	B	1371	TYR	2.2
3	Y	89	LYS	2.2
3	Y	90	ASP	2.2
1	A	240	TYR	2.2
2	B	1374	GLU	2.2
3	X	159	GLU	2.2
1	C	879	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	344	GLN	2.2
1	A	692	HIS	2.2
2	B	369	PRO	2.2
1	C	817	ALA	2.2
2	B	61	PHE	2.2
1	C	1595	ASP	2.1
1	C	1233	GLN	2.1
2	B	1375	VAL	2.1
1	A	271	ILE	2.1
2	D	337	HIS	2.1
2	D	967	GLY	2.1
1	C	95	GLY	2.1
2	D	951	ASP	2.1
1	C	314	SER	2.1
1	C	1548	ARG	2.1
1	C	393	GLN	2.1
1	C	274	ASP	2.1
2	B	23	ALA	2.1
2	B	1537	ASN	2.1
1	A	1380	LYS	2.1
3	X	99	GLN	2.1
3	Y	72	VAL	2.1
1	C	313	TYR	2.1
1	C	240	TYR	2.1
1	A	311	SER	2.1
3	Y	64	VAL	2.0
3	X	82	HIS	2.0
3	X	41	HIS	2.0
1	C	312	TYR	2.0
3	X	73	VAL	2.0
2	B	52	LYS	2.0
1	A	1651	ASP	2.0
1	A	1546	GLU	2.0
3	Y	116	LEU	2.0
1	C	846	TYR	2.0
2	D	764	GLU	2.0

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

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

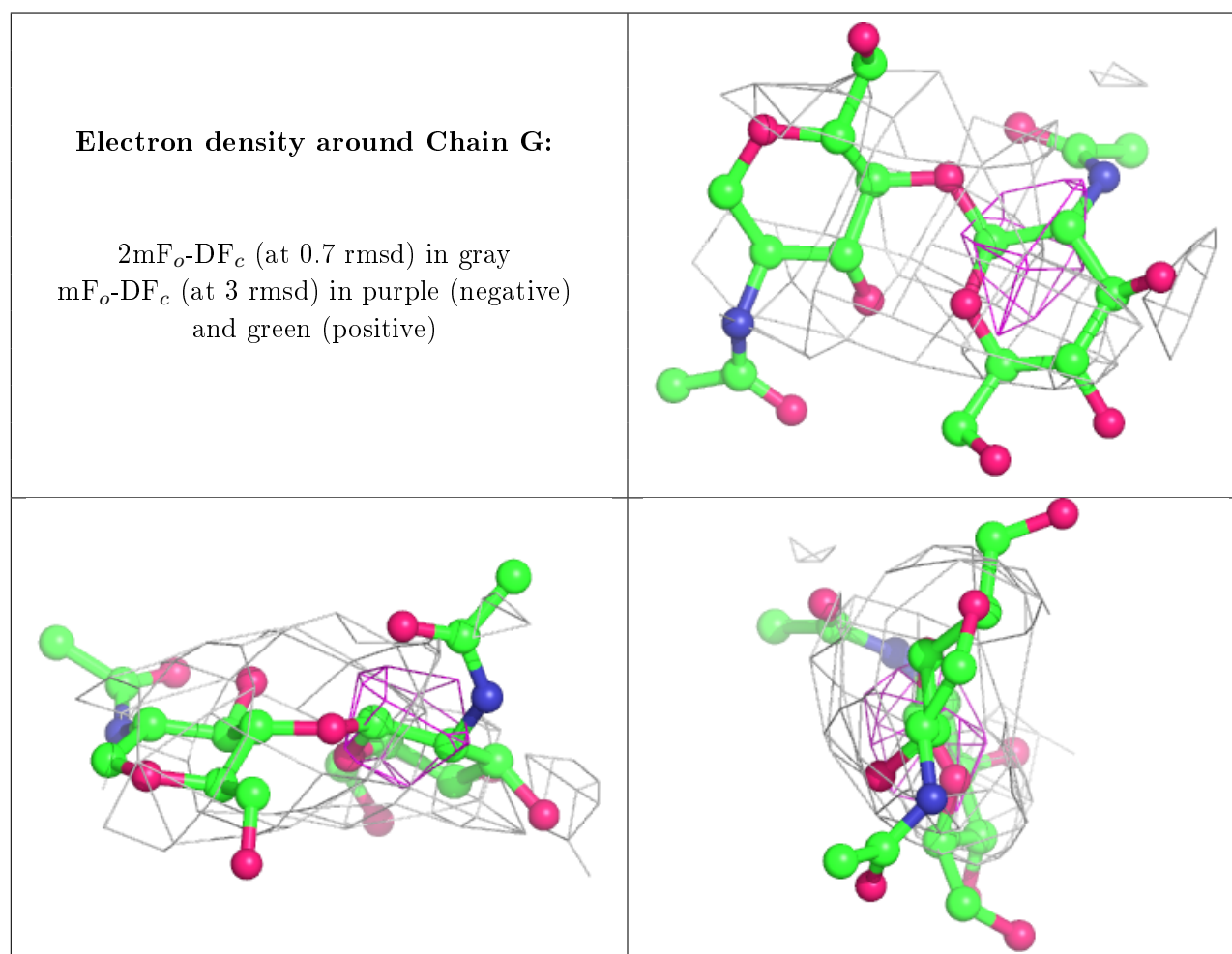


### 6.3 Carbohydrates ⓘ

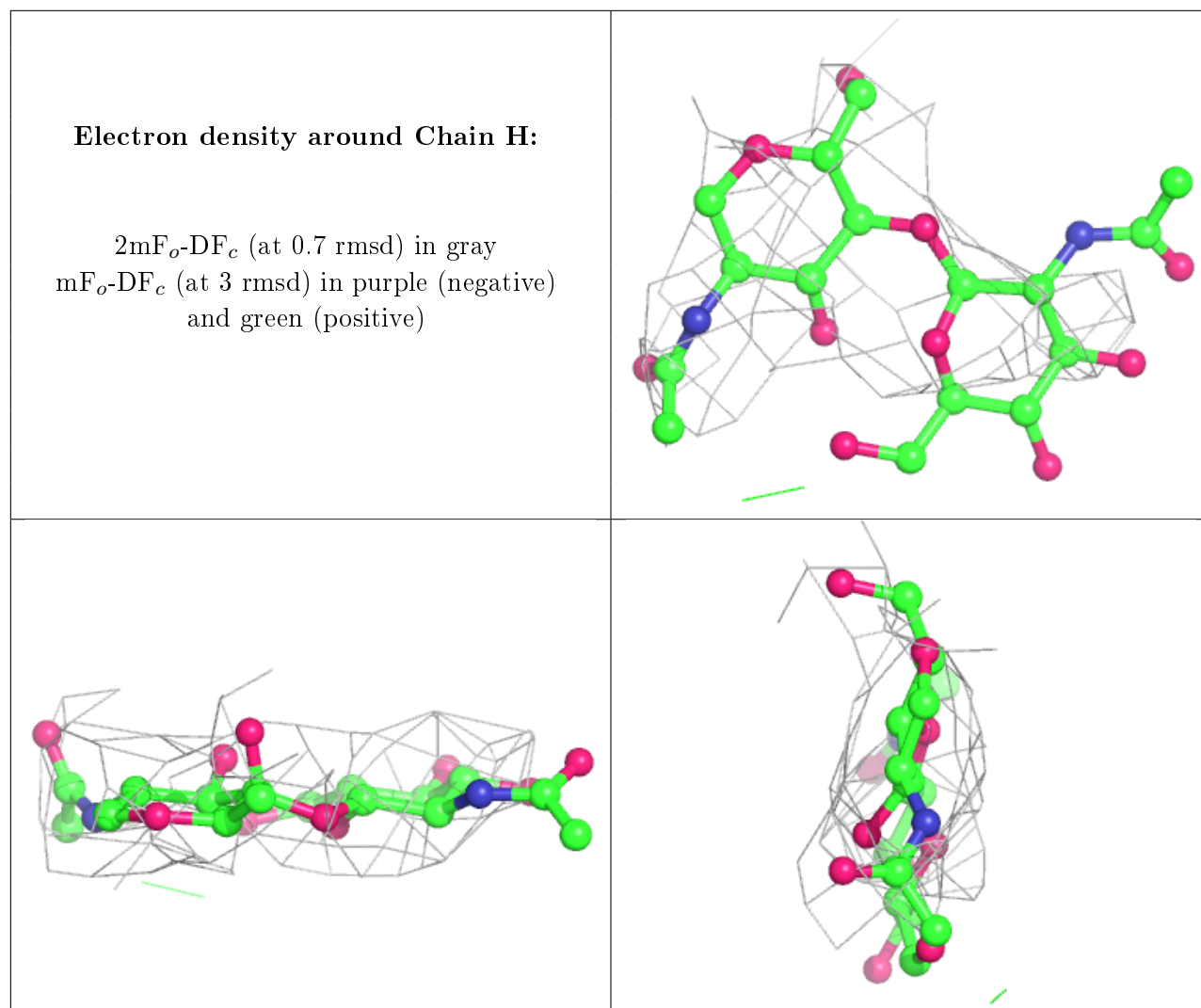
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	F	1	14/15	0.24	0.78	225,233,240,245	0
4	NAG	H	1	14/15	0.54	0.54	246,253,258,265	0
4	NAG	F	2	14/15	0.55	0.79	297,301,307,310	0
4	NAG	G	2	14/15	0.66	0.60	228,239,251,252	0
4	NAG	H	2	14/15	0.72	0.85	271,274,277,278	0
4	NAG	E	2	14/15	0.72	0.69	228,239,253,257	0
4	NAG	E	1	14/15	0.73	0.55	278,305,319,322	0
4	NAG	G	1	14/15	0.89	0.41	228,253,282,288	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.







## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	C	2003	14/15	0.73	0.39	177,180,183,183	0
5	NAG	A	2003	14/15	0.78	0.29	166,169,171,172	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.