



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:18 AM GMT

PDB ID : 3HOW  
Title : Complete RNA polymerase II elongation complex III with a T-U mismatch and a frayed RNA 3'-uridine  
Authors : Sydow, J.F.; Brueckner, F.; Cheung, A.C.M.; Damsma, G.E.; Dengl, S.; Lehmann, E.; Vassylyev, D.; Cramer, P.  
Deposited on : 2009-06-03  
Resolution : 3.60 Å(reported)

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

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

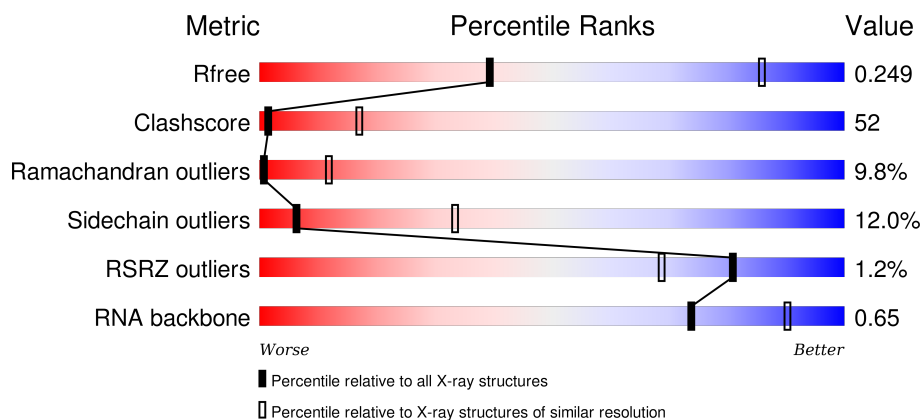
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 Å.

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





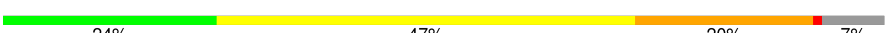
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)
RNA backbone	2183	1058 (4.40-2.80)

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. 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	1733	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 29%, yellow 41%, orange 10%, grey 18%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>29%</span> <span>41%</span> <span>10%</span> <span>18%</span> </div> </div>
2	B	1224	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 28%, yellow 49%, orange 13%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>28%</span> <span>49%</span> <span>13%</span> <span>9%</span> </div> </div>
3	C	347	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 20%, yellow 44%, orange 12%, grey 23%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span></span> <span>20%</span> <span>44%</span> <span>12%</span> <span>23%</span> </div> </div>
4	D	221	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 25%, yellow 41%, orange 12%, grey 19%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span></span> <span>25%</span> <span>41%</span> <span>12%</span> <span>19%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	2	12	
14	1	26	
15	3	18	

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 31876 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1416	Total	C	N	O	S	0	0	0
			11143	7021	1949	2111	62			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1112	Total	C	N	O	S	0	0	0
			8838	5594	1550	1639	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-28	MET	-	EXPRESSION TAG	UNP P16370
C	-27	GLY	-	EXPRESSION TAG	UNP P16370
C	-26	SER	-	EXPRESSION TAG	UNP P16370
C	-25	HIS	-	EXPRESSION TAG	UNP P16370
C	-24	HIS	-	EXPRESSION TAG	UNP P16370
C	-23	HIS	-	EXPRESSION TAG	UNP P16370
C	-22	HIS	-	EXPRESSION TAG	UNP P16370
C	-21	HIS	-	EXPRESSION TAG	UNP P16370
C	-20	HIS	-	EXPRESSION TAG	UNP P16370
C	-19	SER	-	EXPRESSION TAG	UNP P16370
C	-18	ASN	-	EXPRESSION TAG	UNP P16370
C	-17	SER	-	EXPRESSION TAG	UNP P16370
C	-16	GLY	-	EXPRESSION TAG	UNP P16370
C	-15	LEU	-	EXPRESSION TAG	UNP P16370

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	ASN	-	EXPRESSION TAG	UNP P16370
C	-13	ASP	-	EXPRESSION TAG	UNP P16370
C	-12	ILE	-	EXPRESSION TAG	UNP P16370
C	-11	PHE	-	EXPRESSION TAG	UNP P16370
C	-10	GLU	-	EXPRESSION TAG	UNP P16370
C	-9	ALA	-	EXPRESSION TAG	UNP P16370
C	-8	GLN	-	EXPRESSION TAG	UNP P16370
C	-7	LYS	-	EXPRESSION TAG	UNP P16370
C	-6	ILE	-	EXPRESSION TAG	UNP P16370
C	-5	GLU	-	EXPRESSION TAG	UNP P16370
C	-4	TRP	-	EXPRESSION TAG	UNP P16370
C	-3	HIS	-	EXPRESSION TAG	UNP P16370
C	-2	GLU	-	EXPRESSION TAG	UNP P16370
C	-1	ASP	-	EXPRESSION TAG	UNP P16370
C	0	THR	-	EXPRESSION TAG	UNP P16370
C	1	GLY	-	EXPRESSION TAG	UNP P16370

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	134	Total	C	N	O	S	0	0	0
			1076	677	182	213	4			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	114	Total	C	N	O	S	0	0	0
			927	571	168	178	10			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	44	Total	C	N	O	S	0	0	0
			351	217	70	60	4			

- Molecule 13 is a DNA chain called 5'-D(\*AP\*CP\*TP\*AP\*CP\*TP\*TP\*GP\*AP\*GP\*CP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	2	7	Total	C	N	O	P	0	0	0
			137	68	22	41	6			

- Molecule 14 is a DNA chain called 5'-D(\*AP\*GP\*CP\*TP\*C\*AP\*AP\*GP\*TP\*AP\*GP\*TP\*TP\*AP\*TP\*GP\*CP\*CP\*(BRU)P\*GP\*GP\*TP\*CP\*AP\*TP\*T)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
14	1	19	Total	Br	C	N	O	P	0	0	0
			389	1	186	71	113	18			

- Molecule 15 is a RNA chain called 5'-R(\*UP\*GP\*CP\*AP\*UP\*UP\*U\*CP\*AP\*AP\*CP\*CP

\*AP\*GP\*GP\*CP\*UP\*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	3	11	Total	C	N	O	P	0	0	0
			229	104	41	74	10			

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	J	1	Total	Zn	0	0
			1	1		
16	B	1	Total	Zn	0	0
			1	1		
16	I	2	Total	Zn	0	0
			2	2		
16	C	1	Total	Zn	0	0
			1	1		
16	A	2	Total	Zn	0	0
			2	2		
16	L	1	Total	Zn	0	0
			1	1		

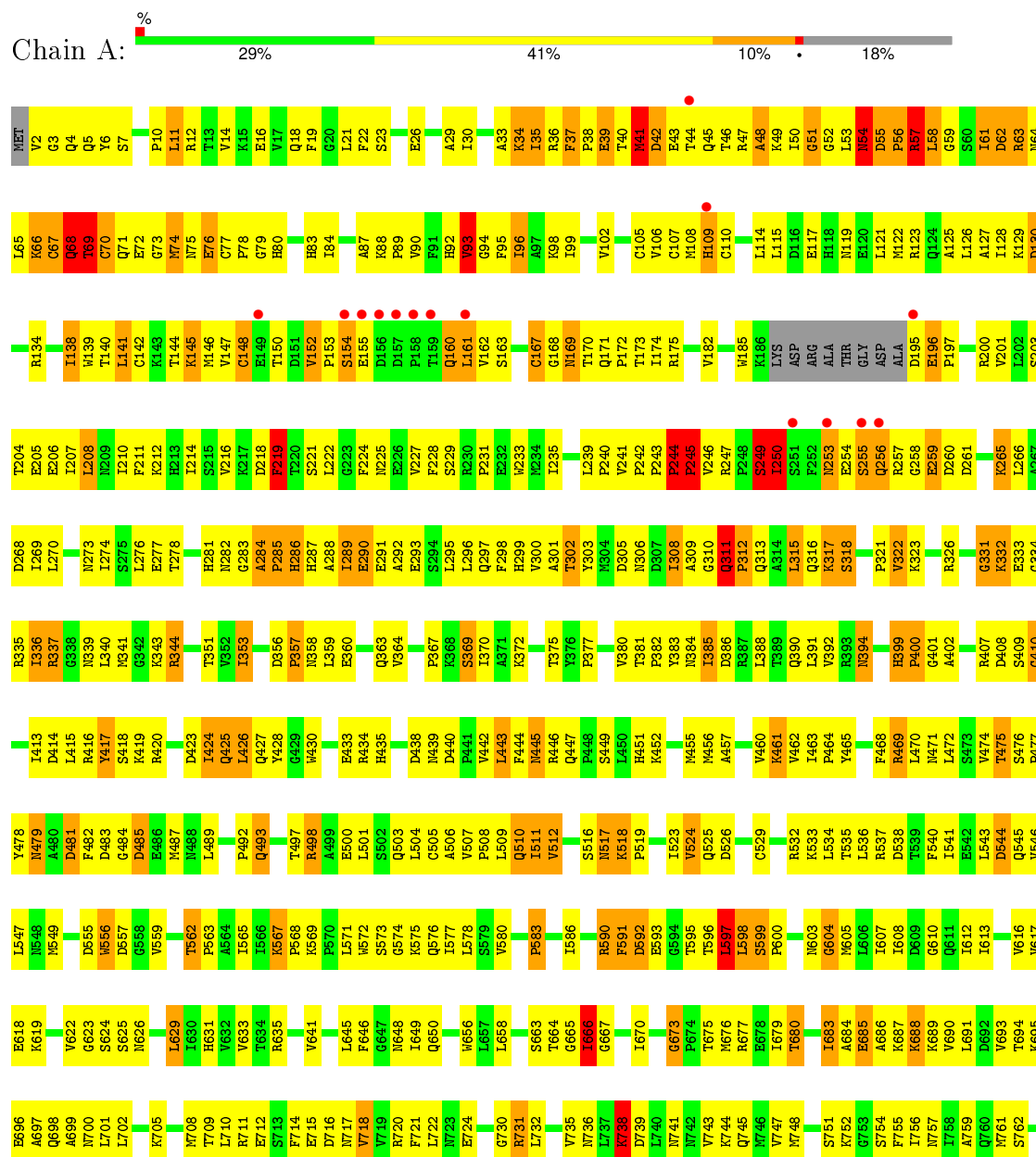
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Mg	0	0
			1	1		

### 3 Residue-property plots

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

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



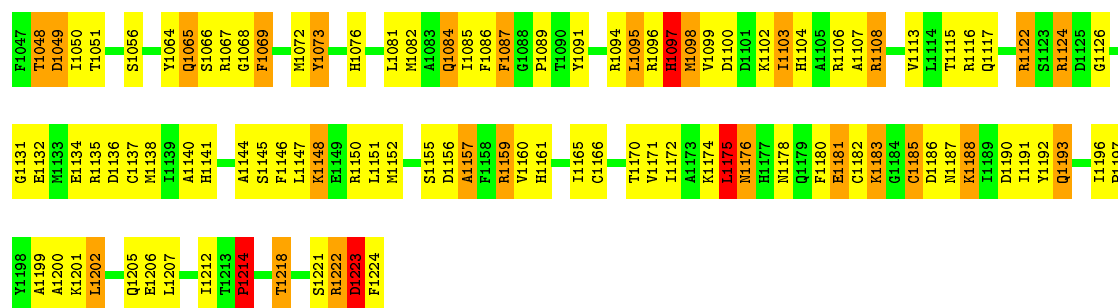


PRO	LYS	PRO	LEU	L1409	I1333	M1267	D1206	H1140	E1074	G1002	S915	V842	Q767
ALA	GLN	VAL	VAL	F1410	D1334	L1288	L1207	T1141	P1075	K1003	G916	K843	Q769
TYR	ASN	ASN	ASN		I1335	E1289	M1209	T1142	A1076	M1004	E1919	L345	K773
SER	ALA	PHE	ALA	A1414	M1336		M1208	S1145	M1079	E1005	E1920	E846	R774
PRO	GLU	SER	ASP	S1415	V1337	T1272	Q1211	T1146	T1080	I1006	G921	E846	I775
THR	THR	PRO	THR	A1416	E1338	L1173	Q1212	T1147	L1081	M1009	D922	M849	A776
SER	TYR	ASP	ASP		L1339	R1274	V1212	T1148	ASN	A1010	E1923	V850	F777
PRO	VAL	VAL	VAL	D1419	G1340	E1277	G1213	I1148	THR	Q1011	G924	H851	F778
ASN	PRO	VAL	VAL	D1420	I1341	E1278	E1214	A1149	PHE	Q1011	E1925	D853	F779
GLU	TYR	ASP	ASP	C1421	E1342	M1278	R1215	S1150	HIS		Q926	D853	V780
SER	TYR	GLU	GLU	R1422	A1343	I1279	I1216	E1151	ALA		L929	T854	D781
PRO	PRO	LEU	LEU		G1344	E1280	K1217	I1152	PHE	V1015		T855	R782
THR	THR	MET	MET	S1425	R1345	R1281	Q1218	I1153	ALA	T1016		T856	T783
SER	SER	PHE	PHE	E1426		V1282	T1219	T1154	GLY	L1017		R857	T783
PRO	PRO	THR	THR		L1348	V1283	F1220	D1155	VAL	F1018		R857	L784
PRO	SER	SER	SER		I1349	M1284	K1221	P1158	ALA	C1019		N858	P785
TYR	ALA	LEU	ALA		K1350	M1285	M1222	P1159	SER	C1020		S859	H786
SER	VAL	VAL	VAL	Q1432	E1351	D1286	D1223	R1159	K1092	L1021		L860	G861
PRO	THR	TYR	TYR		I1352	V1287	L1224	T1161	K1093	R1022		G861	K789
THR	PRO	PRO	ASP		Y1353	D1288	F1225	T1162	V1094	R1023		N862	
SER	THR	THR	GLY	I1436	Y1354	R1289	V1226	V1163		R1024		F866	S793
PRO	PRO	SER	GLY	G1437	T1438	V1290	I1227	I1163	A1027	T1028		F867	P794
PRO	SER	PRO	SER	T1439	G1439	K1290	M1228	I1163	R1029	F942		Y868	E795
TYR	TYR	PRO	ASN	A1440		V1291	V1228	T1164	R1030	L943		G869	S796
SER	PRO	PRO	ASP	F1441		P1292	S1229	P1165	R1100			E870	K797
THR	THR	PRO	ALA		Y1362	S1293	E1230	D1166		Y946			G798
THR	THR	PRO	MET		N1364	P1294	D1231	E1167	T1104	F947		D871	F799
THR	THR	PRO	ALA	M1444	Y1365	T1295	M1232	E1168		V1031		G872	V800
PRO	TYR	THR	GLY	I1445	K1367	G1296	D1233	T1169	L1105	E1034		M873	E801
PRO	GLY	THR	GLY	D1446	H1367	E1297		I1170	M1106	Y1035		D874	N802
SER	PRO	PRO	PHE	E1447	M1368	Y1298	L1236	Q1171	V1107	R1036		A875	S803
TYR	TYR	THR	THR		A1369	V1299	I1237	L1172		P955			Y804
SER	THR	THR	THR	L1450	L1370	K1300	I1238		M1110	L1037		E879	L805
PRO	PRO	PRO	ALA	V1451	L1371	E1303	R1239	S1175	M1111	T1038		L883	R806
THR	THR	GLY	GLY	K1452	D1372	M1304	C1240	LEU	K1112	Q1039		D884	T809
PRO	GLY	THR	GLY	Y1453	V1373	V1305	R1241	ASP	T1113	A1041		T885	
ASN	ALA	SER	ALA	M1454	V1374	L1306	V1242	GLU	S1115	F1042		I886	E812
TYR	TYR	PRO	ASP	P1455	M1375	E1307	R1244	GLU	L1116			G887	F815
PRO	PRO	THR	TYR	GLU	T1376			ALA	T1117	L1046		S888	H816
PRO	GLN	GLY	GLY	L1381	T1377	T1308	PRO	GLU	Y1118	S1047		D890	
THR	ILE	LEU	ILE			D1309	LYS	GLN	Y1119	N1048		A891	K821
THR	THR	THR	THR	THR		G1310	SER	SER	L1120	I1049			
PRO	GLU	SER	SER	GLU	T1385	M1312	ASP	PHE	E1121	E1050		R896	D826
PRO	ILE	PRO	PRO	ILE	H1386	S1314	ALA	ASP	P1122	F1053		Y897	T827
GLY	GLU	THR	PHE	GLU	H1387	E1315	GLU	Q1187	G1123	L1054		R898	A828
GLY	ASP	GLY	GLY	GLY	R1391	V1316	THR	S1189	H1124	R1055		V899	X829
THR	GLY	PRO	PRO	GLY			GLU			S1056		D900	K830
THR	ASP	THR	THR	ASP	T1394	V1319	A1254	L1192	D1127	V1057		L901	T831
PRO	GLY	SER	SER	GLY	G1395	P1320	E1256	L1193	Q1128	V1058		L902	A832
GLY	THR	PRO	PRO	GLY	A1396	G1321	D1287	R1194	Q1130	P1099		N903	
THR	VAL	THR	THR	VAL	L1397	D1323	H1288	L1195	A1131			T904	E833
PRO	PRO	THR	THR	THR	G1400	M1324	M1259	D1198	K1132	K984		D905	T834
PRO	PRO	PRO	PRO	PRO	T1325	T1324	K1261	L1133	L1133	D985		H906	G835
GLY	TYR	PRO	PRO	TYR	S1401	K1262	K1262	R1199	T1134	V1064		T907	Y836
SER	GLY	THR	THR	SER	F1402	K1263		A1200	R1135			L908	T837
PRO	SER	THR	PHE	GLY	E1403	T1263	I1263		S1136	L1087			Q838
ALA	PRO	PRO	PHE	GLY	E1404	E1264	E1264	M1203	A1137			L913	R840
TYR	THR	THR	VAL	SER	S1331	M1265	M1265	D1204	I1138	I1072			R839
SER	SER	TYR	SER	GLY	T1405	F1332	T1266	K1205	G1073			E914	L841

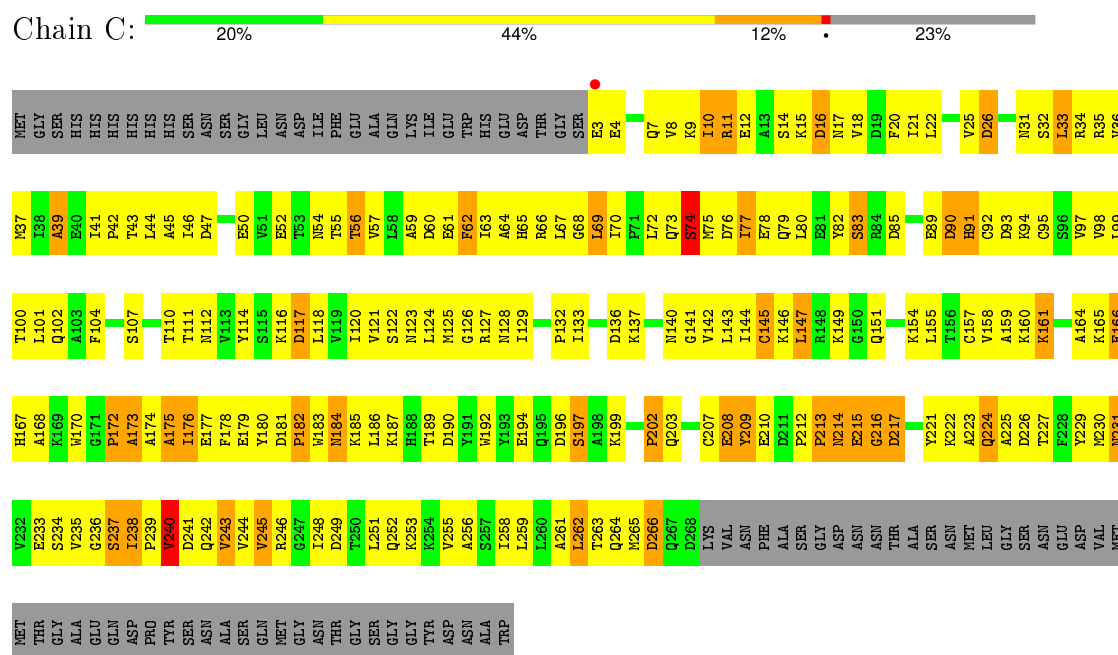
● Molecule 2: DNA-directed RNA polymerase II subunit RPB2



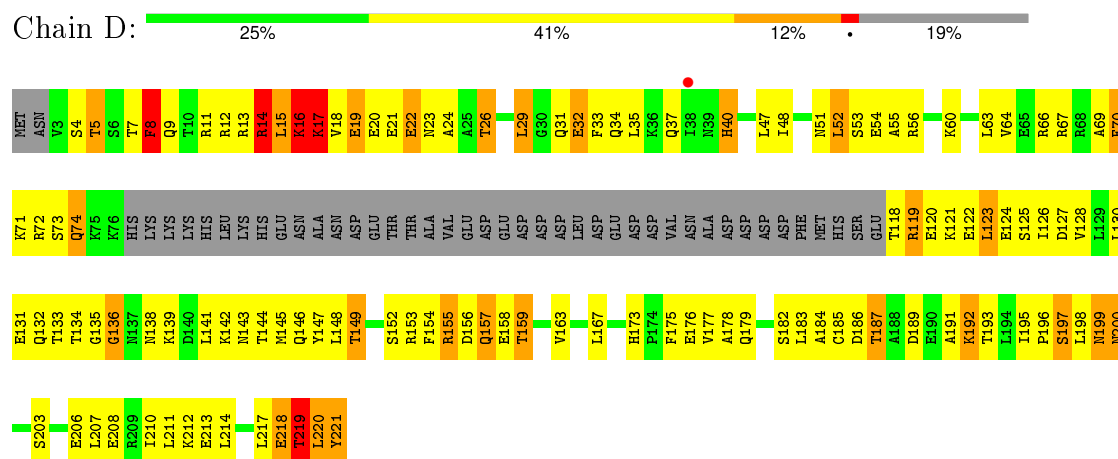




- Molecule 3: DNA-directed RNA polymerase II subunit RPB3



- Molecule 4: DNA-directed RNA polymerase II subunit RPB4

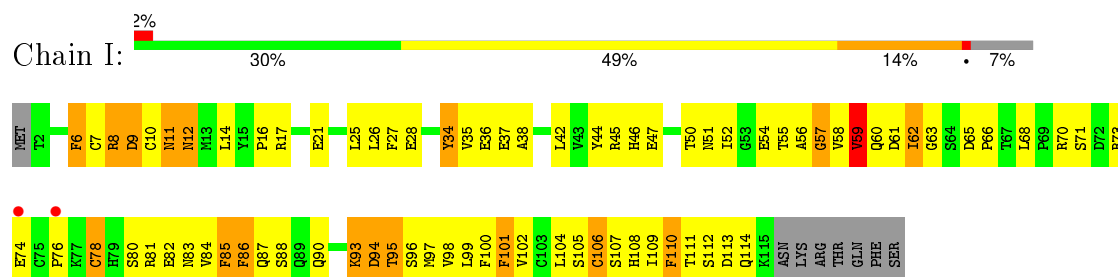


- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

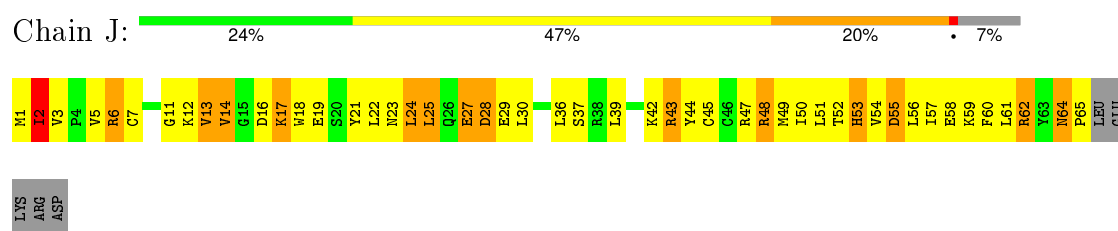




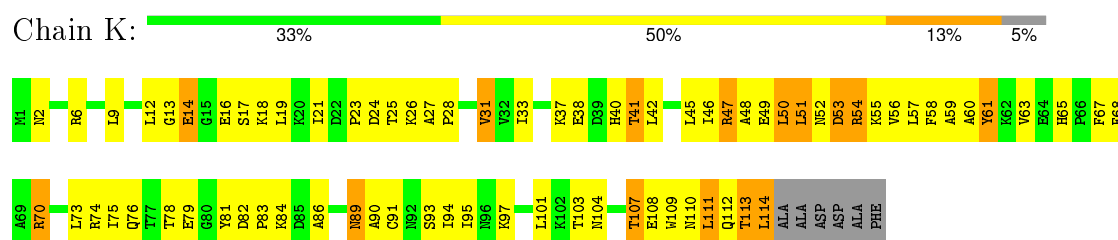
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



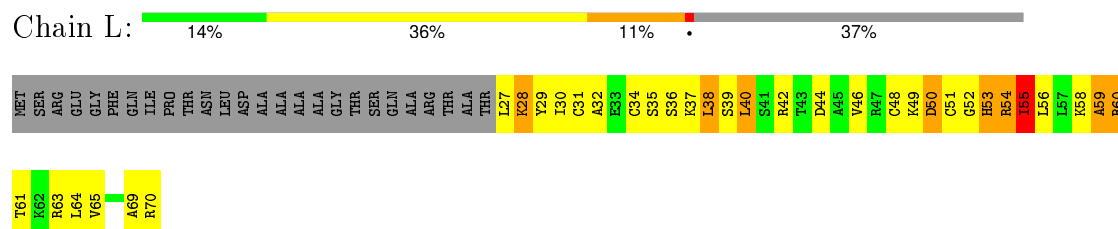
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



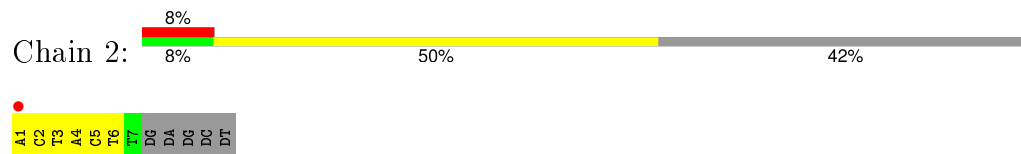
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

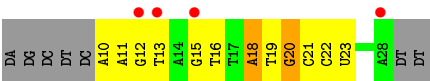


- Molecule 13: 5'-D(\*AP\*CP\*TP\*AP\*CP\*TP\*TP\*GP\*AP\*GP\*CP\*T)-3'

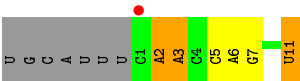


- Molecule 14: 5'-D(\*AP\*GP\*CP\*TP\*C\*AP\*AP\*GP\*TP\*AP\*GP\*TP\*TP\*AP\*TP\*GP\*CP\*C  
P\*(BRU)P\*GP\*GP\*TP\*CP\*AP\*TP\*T)-3'





● Molecule 15: 5'-R(\*UP\*GP\*CP\*AP\*UP\*UP\*U\*CP\*AP\*AP\*CP\*CP\*AP\*GP\*GP\*CP\*UP\*U)-3'



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	222.65Å 395.96Å 283.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 48.95 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.60) 99.9 (48.95-3.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 3.57Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.214 , 0.254 0.212 , 0.249	Depositor DCC
$R_{free}$ test set	2843 reflections (2.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	91.4	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 91.3	EDS
Estimated twinning fraction	0.011 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.018 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 144004 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	31876	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.53	0/11342	0.80	4/15337 (0.0%)
2	B	0.51	0/9009	0.75	2/12146 (0.0%)
3	C	0.53	0/2133	0.78	1/2891 (0.0%)
4	D	0.48	0/1444	0.76	2/1935 (0.1%)
5	E	0.50	0/1788	0.70	0/2406
6	F	0.60	0/717	0.85	0/967
7	G	0.54	0/1368	0.81	0/1844
8	H	0.48	0/1094	0.77	1/1481 (0.1%)
9	I	0.46	0/945	0.74	0/1273
10	J	0.53	0/541	0.88	0/727
11	K	0.54	0/937	0.72	0/1265
12	L	0.45	0/353	0.77	0/468
13	2	0.68	0/152	0.89	0/232
14	1	0.59	0/413	0.80	0/634
15	3	0.60	0/255	0.89	0/395
All	All	0.52	0/32491	0.78	10/44001 (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
3	C	0	1
14	1	0	3
All	All	0	4

There are no bond length outliers.

All (10) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	26	THR	N-CA-C	-6.09	94.56	111.00
1	A	56	PRO	N-CA-C	-6.08	96.28	112.10
1	A	55	ASP	N-CA-CB	6.07	121.52	110.60
1	A	311	GLN	N-CA-C	5.98	127.14	111.00
2	B	43	LEU	CA-CB-CG	-5.82	101.91	115.30
3	C	39	ALA	N-CA-C	5.75	126.51	111.00
2	B	335	GLY	N-CA-C	-5.74	98.74	113.10
1	A	54	ASN	C-N-CA	5.27	134.87	121.70
4	D	8	PHE	N-CA-C	5.17	124.97	111.00
8	H	89	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	1	18	DA	Sidechain
14	1	20	DG	Sidechain
14	1	21	DC	Sidechain
3	C	229	TYR	Sidechain

## 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	11143	0	11217	1115	0
2	B	8838	0	8870	1052	0
3	C	2095	0	2051	258	0
4	D	1434	0	1460	178	0
5	E	1752	0	1776	175	0
6	F	705	0	731	64	0
7	G	1340	0	1357	142	0
8	H	1076	0	1046	152	0
9	I	927	0	882	122	0
10	J	532	0	542	98	0
11	K	919	0	929	98	0
12	L	351	0	376	59	0
13	2	137	0	82	12	0
14	1	389	0	214	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	3	229	0	121	12	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	1	0	0	0	0
All	All	31876	0	31654	3273	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 52.

All (3273) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:882:THR:HG21	2:B:935:ARG:HA	1.24	1.19
1:A:53:LEU:HD23	1:A:54:ASN:N	1.59	1.18
4:D:71:LYS:HA	4:D:74:GLN:HB2	1.23	1.13
7:G:26:LEU:HD12	7:G:56:ILE:HD11	1.22	1.11
1:A:567:LYS:CD	1:A:568:PRO:HD2	1.80	1.11
2:B:622:LYS:HE2	9:I:59:VAL:HG22	1.19	1.11
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.31	1.10
1:A:225:ASN:ND2	1:A:228:PHE:H	1.48	1.10
4:D:14:ARG:HB3	4:D:14:ARG:HH11	1.13	1.10
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.32	1.09
2:B:744:HIS:HD2	2:B:745:PRO:HD2	1.10	1.08
2:B:559:SER:HA	2:B:563:MET:HB3	1.11	1.07
4:D:220:LEU:HD23	4:D:221:TYR:H	1.17	1.07
1:A:855:THR:HG21	1:A:857:ARG:HE	1.20	1.06
5:E:117:THR:HG22	5:E:119:SER:H	1.19	1.06
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.37	1.04
2:B:542:MET:HG2	2:B:747:MET:HE3	1.39	1.04
1:A:1420:ASP:HB3	1:A:1422:ARG:HG3	1.40	1.03
2:B:806:THR:HG22	2:B:808:ALA:H	1.18	1.03
1:A:351:THR:HG22	2:B:1103:ILE:HA	1.34	1.03
1:A:1116:LEU:HB3	1:A:1308:THR:HG21	1.37	1.03
1:A:41:MET:HB3	1:A:49:LYS:HA	1.40	1.02
1:A:53:LEU:CD2	1:A:54:ASN:H	1.69	1.02
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.40	1.02
2:B:850:LEU:HD12	2:B:851:PHE:N	1.74	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:510:LYS:HB3	2:B:511:PRO:HD3	1.42	1.02
1:A:567:LYS:HB3	8:H:96:VAL:H	1.21	1.02
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.40	1.02
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.22	1.02
8:H:4:THR:HA	8:H:60:ALA:HB2	1.41	1.01
12:L:40:LEU:HD13	12:L:44:ASP:HB3	1.37	1.01
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.38	1.01
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.42	1.00
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.40	1.00
1:A:1116:LEU:HB3	1:A:1308:THR:CG2	1.92	0.99
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.43	0.99
1:A:913:LEU:HD12	1:A:914:GLU:H	1.24	0.99
6:F:119:ARG:HG3	6:F:119:ARG:HH11	1.27	0.99
1:A:858:ASN:ND2	1:A:860:LEU:H	1.60	0.99
2:B:430:ARG:HB3	2:B:430:ARG:HH11	1.25	0.98
1:A:541:ILE:HD13	1:A:549:MET:HE1	1.42	0.98
3:C:66:ARG:HH12	10:J:2:ILE:CG2	1.76	0.98
2:B:737:THR:HG21	9:I:66:PRO:HA	1.45	0.98
1:A:321:PRO:O	1:A:322:VAL:HB	1.64	0.97
1:A:315:LEU:H	1:A:315:LEU:HD23	1.30	0.97
2:B:168:GLY:H	2:B:450:ALA:HB1	1.30	0.96
2:B:744:HIS:CD2	2:B:745:PRO:HD2	2.00	0.96
1:A:779:PHE:HE1	1:A:785:PRO:HD3	1.30	0.95
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.46	0.95
9:I:111:THR:HG22	9:I:112:SER:H	1.31	0.95
1:A:901:LEU:H	1:A:926:GLN:NE2	1.65	0.95
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.47	0.95
2:B:589:VAL:HG12	2:B:590:HIS:H	1.30	0.95
1:A:61:ILE:HG22	1:A:62:ASP:H	1.29	0.95
1:A:1364:ASN:OD1	1:A:1366:ARG:HG2	1.66	0.95
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.46	0.95
6:F:82:THR:HG22	6:F:84:TYR:H	1.30	0.94
9:I:34:TYR:HD2	9:I:35:VAL:N	1.63	0.94
2:B:559:SER:HA	2:B:563:MET:CB	1.96	0.94
2:B:244:LEU:HD11	2:B:366:GLN:NE2	1.81	0.94
1:A:567:LYS:CG	1:A:568:PRO:HD2	1.98	0.94
1:A:738:LYS:H	1:A:738:LYS:HD3	1.33	0.94
1:A:1127:ASP:OD2	1:A:1130:GLN:HB2	1.68	0.94
2:B:708:GLU:HG3	2:B:709:ASP:H	1.30	0.94
1:A:353:ILE:HD12	1:A:487:MET:HE2	1.51	0.93
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:15:PRO:HA	7:G:18:PHE:CD1	2.03	0.93
2:B:130:VAL:HG23	2:B:167:ILE:HD13	1.49	0.93
6:F:77:ASP:O	6:F:78:GLN:HB2	1.67	0.93
1:A:21:LEU:HD12	1:A:229:SER:HB2	1.48	0.93
2:B:1065:GLN:HE21	2:B:1067:ARG:H	0.98	0.92
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.49	0.92
8:H:130:ARG:HB2	8:H:130:ARG:NH1	1.84	0.92
1:A:567:LYS:HB3	8:H:96:VAL:N	1.84	0.92
2:B:995:ARG:HH12	3:C:165:LYS:HG2	1.33	0.92
9:I:7:CYS:HB3	9:I:14:LEU:HD21	1.50	0.92
1:A:1100:ARG:NH2	1:A:1351:GLU:HG2	1.85	0.91
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.35	0.91
2:B:879:ARG:CD	2:B:879:ARG:H	1.84	0.90
8:H:81:PRO:HB2	8:H:82:PRO:HD2	1.51	0.90
3:C:56:THR:HG21	3:C:145:CYS:SG	2.12	0.90
1:A:567:LYS:HD3	8:H:95:TYR:CD2	2.05	0.90
1:A:1308:THR:HG23	1:A:1309:ASP:N	1.87	0.90
3:C:252:GLN:HE21	11:K:95:ILE:HG23	1.36	0.90
4:D:220:LEU:CD2	4:D:221:TYR:H	1.83	0.90
2:B:842:ASN:HD22	2:B:845:SER:H	1.19	0.90
2:B:345:LYS:HG2	2:B:346:GLU:H	1.35	0.90
1:A:899:VAL:HB	1:A:929:LEU:HD12	1.52	0.90
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.53	0.89
2:B:638:PHE:HB3	2:B:651:LEU:HD21	1.52	0.89
2:B:810:GLU:HB2	2:B:815:ARG:HH22	1.35	0.89
1:A:53:LEU:HD23	1:A:54:ASN:H	0.77	0.89
2:B:770:GLN:OE1	2:B:983:ARG:HA	1.71	0.89
2:B:879:ARG:HD2	2:B:879:ARG:H	1.35	0.89
9:I:6:PHE:HB3	9:I:12:ASN:O	1.72	0.89
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.55	0.89
8:H:84:ALA:HB1	8:H:87:ARG:HB3	1.55	0.89
1:A:567:LYS:HD3	8:H:95:TYR:CG	2.08	0.89
1:A:629:LEU:O	1:A:633:VAL:HG23	1.72	0.89
5:E:56:LYS:HE2	5:E:84:ASP:HB2	1.54	0.89
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.07	0.89
3:C:177:GLU:HG3	3:C:231:ASN:HD22	1.38	0.89
3:C:69:LEU:H	3:C:69:LEU:HD12	1.38	0.88
2:B:307:ASP:OD2	2:B:310:MET:HB2	1.74	0.88
2:B:805:THR:HG22	2:B:806:THR:H	1.35	0.88
7:G:7:LEU:HB2	7:G:74:TYR:CE2	2.08	0.88
2:B:850:LEU:HD12	2:B:851:PHE:H	1.34	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:549:THR:HG22	2:B:550:ASP:H	1.36	0.88
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.55	0.88
1:A:14:VAL:H	1:A:1432:GLN:HE22	0.91	0.88
1:A:41:MET:CB	1:A:49:LYS:HA	2.04	0.88
4:D:130:LEU:HD13	4:D:142:LYS:HD3	1.56	0.87
2:B:766:ARG:NH1	2:B:1020:ARG:HD2	1.89	0.87
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	1.57	0.87
4:D:155:ARG:HG2	4:D:219:THR:HG21	1.55	0.86
1:A:416:ARG:HH11	1:A:417:TYR:HE2	1.23	0.86
1:A:323:LYS:H	1:A:323:LYS:HD2	1.41	0.86
7:G:1:MET:SD	7:G:79:PHE:HD1	1.98	0.86
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.58	0.86
11:K:65:HIS:HD2	11:K:67:PHE:H	1.19	0.86
4:D:66:ARG:HD2	4:D:133:THR:HB	1.57	0.86
10:J:1:MET:N	10:J:57:ILE:H	1.73	0.86
11:K:65:HIS:CD2	11:K:67:PHE:H	1.92	0.86
9:I:34:TYR:CD2	9:I:35:VAL:N	2.43	0.86
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.05	0.86
1:A:107:CYS:HA	1:A:171:GLN:NE2	1.90	0.86
8:H:42:ILE:HG23	8:H:95:TYR:HE1	1.38	0.86
3:C:66:ARG:HH12	10:J:2:ILE:HG21	1.37	0.85
2:B:805:THR:HA	2:B:809:MET:HE1	1.59	0.85
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.58	0.85
2:B:890:TYR:O	2:B:893:LEU:HB2	1.76	0.85
1:A:11:LEU:O	1:A:11:LEU:HD23	1.76	0.85
1:A:225:ASN:HD22	1:A:228:PHE:H	1.18	0.85
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.58	0.85
2:B:291:ILE:HD13	2:B:300:HIS:NE2	1.91	0.85
4:D:156:ASP:HB2	4:D:159:THR:HG23	1.58	0.85
2:B:102:VAL:CG2	2:B:112:LEU:HD22	2.06	0.85
1:A:858:ASN:HD22	1:A:858:ASN:C	1.78	0.85
1:A:353:ILE:HD12	1:A:487:MET:CE	2.06	0.85
2:B:842:ASN:ND2	2:B:845:SER:H	1.75	0.85
2:B:863:GLU:OE2	2:B:873:THR:HA	1.77	0.85
2:B:345:LYS:HA	2:B:348:ARG:HE	1.38	0.85
8:H:104:PHE:CZ	8:H:136:LYS:HA	2.12	0.85
1:A:63:ARG:HA	1:A:74:MET:HE2	1.58	0.85
2:B:944:THR:HG21	2:B:1122:ARG:NH2	1.92	0.85
2:B:603:LEU:HD13	2:B:608:ASP:HB2	1.59	0.84
2:B:1124:ARG:NH1	2:B:1124:ARG:HB3	1.92	0.84
1:A:381:THR:HG23	1:A:382:PRO:HD2	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:244:VAL:O	3:C:248:ILE:HG13	1.76	0.84
1:A:1312:ASN:HD21	1:A:1315:GLU:HG3	1.40	0.84
7:G:138:THR:HG22	7:G:139:ILE:N	1.92	0.84
2:B:289:LEU:HD13	2:B:375:ALA:HB2	1.58	0.84
2:B:806:THR:HG22	2:B:808:ALA:N	1.91	0.84
4:D:154:PHE:CD1	4:D:163:VAL:HG21	2.13	0.84
4:D:159:THR:O	4:D:163:VAL:HG23	1.77	0.84
1:A:853:ASP:OD1	1:A:855:THR:HB	1.78	0.84
7:G:126:ASN:HD22	7:G:127:PRO:HA	1.42	0.83
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	1.78	0.83
7:G:34:VAL:HG11	7:G:74:TYR:HE1	1.43	0.83
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.61	0.83
1:A:1107:VAL:HG12	1:A:1107:VAL:O	1.78	0.83
3:C:242:GLN:HA	3:C:245:VAL:HG23	1.60	0.83
10:J:64:ASN:HB3	10:J:65:PRO:CD	2.08	0.83
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.58	0.83
1:A:107:CYS:HB2	1:A:114:LEU:HD21	1.60	0.83
3:C:83:SER:OG	3:C:160:LYS:HD3	1.79	0.83
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.60	0.83
8:H:130:ARG:HH11	8:H:130:ARG:HB2	1.40	0.83
2:B:345:LYS:HG2	2:B:346:GLU:N	1.94	0.83
12:L:49:LYS:O	12:L:50:ASP:HB2	1.77	0.83
2:B:862:GLN:HG2	2:B:963:PHE:HD1	1.44	0.82
2:B:126:SER:OG	2:B:172:ILE:HD11	1.78	0.82
1:A:942:PHE:HZ	5:E:207:ARG:HG3	1.42	0.82
1:A:55:ASP:N	1:A:56:PRO:HD3	1.93	0.82
1:A:567:LYS:CB	8:H:95:TYR:HA	2.09	0.82
1:A:1409:LEU:HD13	2:B:1207:LEU:HD11	1.61	0.82
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.08	0.82
7:G:1:MET:SD	7:G:79:PHE:CD1	2.72	0.82
5:E:114:ASN:O	5:E:115:ASN:HB3	1.78	0.82
11:K:47:ARG:HB3	11:K:47:ARG:HH11	1.44	0.82
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.60	0.82
1:A:503:GLN:NE2	6:F:90:ARG:NH2	2.28	0.82
2:B:654:ARG:HH11	2:B:654:ARG:HG3	1.45	0.82
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.19	0.82
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.77	0.82
2:B:865:LYS:HG2	2:B:961:LEU:HD21	1.62	0.82
1:A:866:PHE:O	1:A:867:ILE:HD12	1.78	0.82
1:A:1170:ILE:HD12	1:A:1170:ILE:H	1.41	0.82
1:A:145:LYS:HA	1:A:145:LYS:HE3	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.77	0.82
1:A:839:ARG:HG2	1:A:839:ARG:HH11	1.42	0.82
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.14	0.81
1:A:901:LEU:H	1:A:926:GLN:HE21	1.26	0.81
1:A:381:THR:HG22	1:A:383:TYR:H	1.43	0.81
5:E:79:TRP:HE1	5:E:81:GLU:HB2	1.43	0.81
2:B:261:ARG:HH11	2:B:261:ARG:HB3	1.44	0.81
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.61	0.81
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.77	0.81
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.62	0.81
1:A:858:ASN:HD22	1:A:860:LEU:H	1.24	0.81
1:A:288:ALA:HA	1:A:291:GLU:OE1	1.80	0.81
1:A:40:THR:HG22	1:A:41:MET:HG3	1.61	0.81
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.61	0.81
1:A:1116:LEU:N	1:A:1308:THR:HG22	1.95	0.81
2:B:800:GLN:HB3	10:J:52:THR:HG22	1.61	0.81
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.63	0.81
7:G:30:LEU:HD22	7:G:72:VAL:HG11	1.62	0.81
3:C:32:SER:O	3:C:36:VAL:HG23	1.80	0.81
2:B:589:VAL:HG12	2:B:590:HIS:N	1.96	0.81
15:3:11:U:OP1	15:3:11:U:H4'	1.80	0.81
1:A:154:SER:HB3	1:A:162:VAL:HG21	1.63	0.81
1:A:1214:GLU:O	1:A:1218:GLN:HG2	1.81	0.80
1:A:534:LEU:O	1:A:574:GLY:HA3	1.81	0.80
1:A:244:PRO:HB2	1:A:245:PRO:CD	2.11	0.80
11:K:57:LEU:HB2	11:K:76:GLN:HG2	1.61	0.80
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.62	0.80
1:A:754:SER:H	1:A:757:ASN:HD22	1.28	0.80
12:L:32:ALA:CB	12:L:55:ILE:HG13	2.11	0.80
1:A:534:LEU:O	1:A:534:LEU:HG	1.79	0.80
1:A:98:LYS:O	1:A:102:VAL:HG23	1.82	0.80
1:A:1445:ILE:H	1:A:1445:ILE:HD12	1.45	0.79
12:L:32:ALA:HB2	12:L:55:ILE:HG13	1.61	0.79
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.17	0.79
8:H:95:TYR:HE2	8:H:97:MET:HG3	1.47	0.79
2:B:232:SER:HA	14:1:11:DA:OP1	1.82	0.79
1:A:115:LEU:HD12	1:A:142:CYS:HB3	1.65	0.79
11:K:46:ILE:O	11:K:50:LEU:HB2	1.82	0.79
1:A:889:SER:HB3	1:A:1297:GLU:HG3	1.63	0.79
12:L:61:THR:HG22	12:L:63:ARG:HG3	1.64	0.79
1:A:35:ILE:O	1:A:35:ILE:HG22	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1444:MET:HG3	7:G:60:ARG:HA	1.65	0.79
2:B:613:VAL:HG13	2:B:627:PHE:O	1.82	0.79
2:B:549:THR:HG22	2:B:550:ASP:N	1.98	0.79
4:D:47:LEU:HD13	4:D:48:ILE:N	1.98	0.78
1:A:69:THR:HG21	2:B:1174:LYS:NZ	1.97	0.78
12:L:30:ILE:O	12:L:56:LEU:HA	1.82	0.78
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.65	0.78
1:A:69:THR:O	1:A:71:GLN:N	2.16	0.78
2:B:796:LEU:HD21	2:B:821:GLN:HE21	1.48	0.78
1:A:855:THR:CG2	1:A:857:ARG:HE	1.96	0.78
7:G:15:PRO:HA	7:G:18:PHE:CE1	2.18	0.78
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.19	0.78
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.45	0.78
2:B:1165:ILE:HG22	4:D:15:LEU:HA	1.65	0.78
2:B:944:THR:HG21	2:B:1122:ARG:HH21	1.47	0.78
11:K:107:THR:HG22	11:K:108:GLU:N	1.97	0.78
3:C:112:ASN:HB3	3:C:114:TYR:CE1	2.19	0.78
1:A:855:THR:HG21	1:A:857:ARG:NE	1.99	0.78
4:D:220:LEU:HD23	4:D:221:TYR:N	1.97	0.78
8:H:89:LEU:C	8:H:91:ASP:H	1.86	0.78
7:G:14:HIS:CD2	7:G:16:SER:H	2.02	0.78
5:E:112:TYR:O	5:E:137:GLU:HG3	1.84	0.78
1:A:250:ILE:HG22	1:A:250:ILE:O	1.83	0.77
2:B:798:TYR:HE2	3:C:62:PHE:CZ	2.02	0.77
1:A:754:SER:N	1:A:757:ASN:HD22	1.82	0.77
10:J:23:ASN:C	10:J:25:LEU:H	1.87	0.77
4:D:155:ARG:CG	4:D:219:THR:HG21	2.15	0.77
1:A:1135:ARG:HG2	1:A:1136:SER:N	1.98	0.77
1:A:1329:THR:HG22	1:A:1331:SER:H	1.49	0.77
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.20	0.77
2:B:816:GLU:O	2:B:817:LEU:HD23	1.85	0.77
1:A:470:LEU:HD23	1:A:470:LEU:H	1.50	0.77
15:3:5:C:O2'	15:3:6:A:H5'	1.84	0.77
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.00	0.77
5:E:117:THR:HG22	5:E:119:SER:N	1.99	0.77
1:A:903:ASN:HD22	1:A:904:THR:N	1.82	0.77
1:A:49:LYS:HZ1	1:A:61:ILE:N	1.83	0.77
2:B:1187:ASN:O	2:B:1188:LYS:HB2	1.84	0.77
9:I:50:THR:CG2	9:I:52:ILE:HG12	2.15	0.77
6:F:89:GLU:O	6:F:93:ILE:HD12	1.85	0.77
2:B:469:GLN:O	2:B:472:ALA:HB3	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:914:LYS:HG2	2:B:937:ALA:HB3	1.67	0.77
2:B:995:ARG:NH1	3:C:165:LYS:HG2	1.99	0.77
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.67	0.77
2:B:799:PRO:HB2	2:B:818:PRO:HG2	1.67	0.77
1:A:503:GLN:HE21	6:F:90:ARG:NH2	1.83	0.76
5:E:5:ASN:O	5:E:9:ILE:HG13	1.84	0.76
1:A:42:ASP:O	1:A:44:THR:N	2.18	0.76
2:B:1020:ARG:HG2	2:B:1020:ARG:HH11	1.48	0.76
1:A:683:ILE:HD13	1:A:801:GLU:HG3	1.67	0.76
2:B:1084:GLN:NE2	2:B:1084:GLN:N	2.32	0.76
12:L:60:ARG:HG2	12:L:61:THR:H	1.50	0.76
1:A:535:THR:HG21	1:A:616:VAL:HA	1.68	0.76
3:C:89:GLU:O	3:C:90:ASP:HB3	1.85	0.76
8:H:42:ILE:HG23	8:H:95:TYR:CE1	2.21	0.76
2:B:294:ASP:O	2:B:296:GLU:N	2.18	0.76
2:B:278:GLN:HG2	2:B:279:ASP:N	2.00	0.76
10:J:53:HIS:HD2	10:J:54:VAL:N	1.84	0.76
8:H:30:SER:HB2	8:H:36:CYS:HB3	1.68	0.76
3:C:249:ASP:O	3:C:252:GLN:HB3	1.86	0.76
3:C:128:ASN:O	3:C:129:ILE:HG13	1.85	0.76
2:B:227:LYS:HG3	2:B:395:GLN:HG3	1.68	0.76
2:B:193:LYS:NZ	12:L:32:ALA:HB1	2.01	0.76
2:B:401:PHE:HA	2:B:404:LYS:HG3	1.68	0.76
1:A:709:THR:HG22	1:A:710:LEU:H	1.51	0.76
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	1.99	0.75
2:B:706:GLN:HB2	2:B:709:ASP:HB3	1.68	0.75
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	1.86	0.75
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.26	0.75
2:B:996:ARG:HH12	3:C:174:ALA:HA	1.49	0.75
2:B:278:GLN:HG2	2:B:279:ASP:H	1.51	0.75
2:B:577:ALA:CB	2:B:589:VAL:HG11	2.15	0.75
2:B:806:THR:HB	2:B:809:MET:HG3	1.67	0.75
1:A:399:HIS:HB3	1:A:400:PRO:CD	2.16	0.75
9:I:55:THR:HG22	9:I:58:VAL:HG21	1.68	0.75
1:A:1130:GLN:O	1:A:1134:ILE:HG13	1.86	0.75
1:A:316:GLN:HE21	1:A:317:LYS:HD2	1.52	0.75
1:A:1279:ILE:HD11	1:A:1316:VAL:HG21	1.69	0.75
5:E:22:MET:HE3	5:E:26:ARG:HE	1.52	0.75
1:A:523:ILE:HG13	1:A:622:VAL:HG22	1.69	0.75
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.68	0.75
2:B:288:ALA:HB1	2:B:331:LEU:HD12	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:THR:O	1:A:698:GLN:HG3	1.87	0.75
2:B:815:ARG:HH11	2:B:815:ARG:HB2	1.52	0.74
1:A:167:CYS:HB2	1:A:169:ASN:ND2	2.01	0.74
1:A:34:LYS:NZ	1:A:57:ARG:NH2	2.35	0.74
1:A:590:ARG:HG2	1:A:590:ARG:HH11	1.50	0.74
3:C:221:TYR:CE1	3:C:222:LYS:HG3	2.23	0.74
4:D:14:ARG:HB3	4:D:14:ARG:NH1	1.97	0.74
2:B:637:LEU:HB2	2:B:693:ILE:HD11	1.67	0.74
1:A:343:LYS:HZ2	2:B:1151:LEU:HG	1.52	0.74
2:B:803:LEU:HD12	2:B:1032:SER:HB3	1.69	0.74
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.03	0.74
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.68	0.74
8:H:26:ILE:HD11	8:H:49:VAL:HG11	1.70	0.74
8:H:59:ILE:HG22	8:H:60:ALA:N	2.00	0.74
7:G:7:LEU:HB2	7:G:74:TYR:HE2	1.51	0.74
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.51	0.74
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.69	0.74
2:B:1175:LEU:O	2:B:1176:ASN:HB2	1.85	0.74
8:H:58:THR:HG22	8:H:59:ILE:H	1.52	0.74
2:B:244:LEU:HD11	2:B:366:GLN:HE22	1.49	0.74
3:C:43:THR:HG22	3:C:44:LEU:N	2.00	0.74
1:A:767:GLN:NE2	1:A:774:ARG:HB3	2.02	0.74
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.18	0.74
1:A:372:LYS:HA	1:A:435:HIS:ND1	2.01	0.74
8:H:11:GLN:HA	8:H:53:ASP:O	1.88	0.74
1:A:117:GLU:H	1:A:117:GLU:CD	1.90	0.74
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.80	0.74
2:B:957:ASN:O	2:B:959:ASP:N	2.21	0.74
10:J:1:MET:H1	10:J:57:ILE:H	1.33	0.74
3:C:208:GLU:O	3:C:210:GLU:N	2.20	0.74
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.70	0.74
2:B:39:ARG:NH2	2:B:665:GLU:HG2	2.03	0.74
2:B:345:LYS:O	2:B:347:LYS:HG2	1.88	0.73
1:A:388:LEU:O	1:A:392:VAL:HG23	1.88	0.73
8:H:40:LEU:HD12	8:H:123:MET:HB2	1.70	0.73
2:B:1001:PHE:HE2	3:C:34:ARG:NE	1.86	0.73
12:L:61:THR:CG2	12:L:63:ARG:HG3	2.17	0.73
1:A:399:HIS:O	1:A:401:GLY:N	2.21	0.73
2:B:516:ASN:N	2:B:516:ASN:HD22	1.84	0.73
1:A:722:LEU:H	1:A:722:LEU:HD12	1.51	0.73
1:A:946:VAL:HG12	1:A:947:PHE:CD2	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:CYS:O	1:A:72:GLU:HG2	1.88	0.73
8:H:130:ARG:HD3	8:H:130:ARG:N	2.03	0.73
1:A:1161:THR:HG21	1:A:1163:ILE:HD12	1.69	0.73
10:J:14:VAL:CG1	10:J:50:ILE:HD11	2.19	0.73
2:B:873:THR:O	2:B:914:LYS:HA	1.87	0.73
1:A:55:ASP:C	1:A:57:ARG:H	1.91	0.73
11:K:47:ARG:HB3	11:K:47:ARG:NH1	2.03	0.73
5:E:2:ASP:O	5:E:3:GLN:HG2	1.87	0.73
3:C:147:LEU:HD23	3:C:147:LEU:N	2.04	0.73
12:L:58:LYS:O	12:L:59:ALA:O	2.06	0.73
1:A:981:LEU:HD21	1:A:1039:LYS:HA	1.69	0.73
1:A:443:LEU:HD12	2:B:1146:PHE:CE2	2.24	0.73
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.24	0.73
11:K:113:THR:O	11:K:114:LEU:HB2	1.87	0.73
8:H:127:GLY:O	8:H:128:ASN:HB2	1.89	0.73
5:E:99:HIS:HE1	5:E:103:LYS:HD2	1.54	0.73
1:A:134:ARG:HD2	1:A:221:SER:O	1.89	0.72
2:B:705:MET:HB3	2:B:706:GLN:OE1	1.89	0.72
9:I:111:THR:HG22	9:I:112:SER:N	2.02	0.72
2:B:1182:CYS:SG	2:B:1182:CYS:O	2.47	0.72
1:A:567:LYS:NZ	8:H:46:LEU:HB2	2.05	0.72
1:A:1422:ARG:HD3	2:B:1224:PHE:CZ	2.24	0.72
1:A:482:PHE:O	2:B:989:THR:HG23	1.89	0.72
1:A:857:ARG:HD3	1:A:861:GLY:O	1.88	0.72
2:B:345:LYS:CG	2:B:346:GLU:H	2.01	0.72
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.29	0.72
1:A:129:LYS:O	1:A:130:ASP:HB2	1.89	0.72
1:A:590:ARG:O	1:A:591:PHE:HB2	1.89	0.72
12:L:55:ILE:HG12	12:L:56:LEU:H	1.53	0.72
1:A:873:MET:C	1:A:1058:VAL:HG23	2.10	0.72
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.71	0.72
8:H:130:ARG:HH11	8:H:130:ARG:CB	2.03	0.72
2:B:1122:ARG:HB3	14:1:22:DC:OP1	1.90	0.72
6:F:86:THR:HG23	6:F:89:GLU:OE1	1.90	0.72
3:C:133:ILE:HD12	3:C:237:SER:N	2.04	0.72
2:B:351:TYR:CE1	2:B:355:ILE:HD11	2.25	0.72
3:C:144:ILE:HG22	3:C:145:CYS:HB3	1.72	0.72
4:D:153:ARG:HB3	4:D:154:PHE:CE2	2.24	0.72
2:B:1183:LYS:HE3	2:B:1183:LYS:N	2.05	0.72
1:A:512:VAL:HA	1:A:519:PRO:HA	1.70	0.72
5:E:213:ILE:HG12	5:E:214:CYS:H	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:805:THR:HG22	2:B:806:THR:N	2.04	0.72
1:A:913:LEU:CD1	1:A:914:GLU:H	2.00	0.72
7:G:126:ASN:HD22	7:G:127:PRO:CA	2.03	0.72
15:3:2:A:H2'	15:3:3:A:H8	1.54	0.72
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.20	0.71
1:A:425:GLN:N	1:A:425:GLN:CD	2.43	0.71
1:A:446:ARG:HB2	1:A:487:MET:SD	2.30	0.71
2:B:705:MET:N	2:B:710:LEU:HD12	2.04	0.71
2:B:810:GLU:CB	2:B:815:ARG:HH22	2.03	0.71
2:B:351:TYR:O	2:B:355:ILE:HG13	1.90	0.71
1:A:1397:LEU:HB2	1:A:1426:GLU:OE1	1.91	0.71
9:I:50:THR:HG22	9:I:51:ASN:H	1.56	0.71
1:A:470:LEU:HD23	1:A:470:LEU:N	2.04	0.71
11:K:65:HIS:HD2	11:K:67:PHE:N	1.87	0.71
3:C:67:LEU:HD11	3:C:155:LEU:CD1	2.19	0.71
1:A:709:THR:HG22	1:A:710:LEU:N	2.05	0.71
2:B:1034:VAL:HG12	2:B:1035:ALA:N	2.05	0.71
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.21	0.71
6:F:119:ARG:NH1	6:F:119:ARG:HG3	2.03	0.71
1:A:369:SER:HB3	11:K:2:ASN:HD21	1.56	0.71
2:B:839:MET:HE1	2:B:980:PHE:HB2	1.73	0.71
2:B:299:GLU:HB3	2:B:571:PRO:HG3	1.72	0.71
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.72	0.71
2:B:172:ILE:HD13	2:B:178:ASN:HD22	1.54	0.71
2:B:1095:LEU:H	2:B:1095:LEU:HD12	1.53	0.71
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.26	0.71
1:A:830:LYS:O	1:A:834:THR:HB	1.91	0.71
5:E:84:ASP:O	5:E:86:PRO:HD3	1.89	0.71
4:D:4:SER:O	4:D:5:THR:HB	1.90	0.71
5:E:23:VAL:O	5:E:28:TYR:HB2	1.90	0.71
2:B:745:PRO:O	2:B:747:MET:N	2.24	0.71
2:B:227:LYS:H	2:B:395:GLN:NE2	1.89	0.71
2:B:999:MET:CE	2:B:999:MET:HA	2.20	0.71
7:G:158:HIS:HD2	7:G:159:ALA:H	1.36	0.71
1:A:1094:VAL:HG22	1:A:1113:THR:HG21	1.71	0.71
2:B:918:ILE:HD12	2:B:935:ARG:NH1	2.06	0.71
1:A:62:ASP:O	1:A:63:ARG:C	2.28	0.71
8:H:95:TYR:CE2	8:H:97:MET:HG3	2.26	0.71
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.71	0.71
2:B:622:LYS:HE2	9:I:59:VAL:CG2	2.11	0.71
3:C:46:ILE:HD12	3:C:67:LEU:HB3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:PRO:O	1:A:57:ARG:HG3	1.91	0.70
9:I:44:TYR:CD1	9:I:45:ARG:N	2.59	0.70
1:A:384:ASN:OD1	1:A:388:LEU:HD12	1.91	0.70
11:K:40:HIS:HD1	11:K:61:TYR:HH	1.39	0.70
9:I:34:TYR:HE2	9:I:36:GLU:HB3	1.56	0.70
7:G:128:PRO:O	7:G:138:THR:HG23	1.91	0.70
2:B:642:ASP:HA	2:B:649:LYS:HA	1.72	0.70
2:B:601:ARG:O	2:B:605:ARG:HG3	1.91	0.70
1:A:908:LEU:HD12	1:A:983:ILE:HD11	1.72	0.70
2:B:359:GLU:O	2:B:362:PRO:HD3	1.91	0.70
2:B:882:THR:HG22	2:B:884:ARG:H	1.54	0.70
1:A:34:LYS:HZ2	1:A:57:ARG:NH2	1.89	0.70
8:H:59:ILE:HG22	8:H:60:ALA:H	1.56	0.70
2:B:364:ILE:HG13	2:B:585:VAL:HG13	1.73	0.70
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.74	0.70
2:B:1001:PHE:HE2	3:C:34:ARG:CZ	2.02	0.70
3:C:203:GLN:HG3	3:C:207:CYS:SG	2.31	0.70
4:D:123:LEU:HD13	4:D:123:LEU:O	1.91	0.70
2:B:313:MET:HE2	2:B:390:LEU:HD21	1.73	0.70
3:C:145:CYS:HA	10:J:2:ILE:HD12	1.73	0.70
2:B:955:THR:HG22	2:B:956:THR:N	2.05	0.70
1:A:535:THR:CG2	1:A:616:VAL:HA	2.22	0.70
1:A:335:ARG:NH1	2:B:1206:GLU:OE1	2.24	0.70
15:3:2:A:H2'	15:3:3:A:C8	2.27	0.70
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.72	0.70
9:I:50:THR:HG22	9:I:51:ASN:N	2.07	0.70
2:B:483:LEU:HD11	2:B:491:THR:CG2	2.21	0.70
12:L:55:ILE:HD13	12:L:55:ILE:H	1.57	0.70
2:B:469:GLN:HG2	2:B:470:LYS:H	1.57	0.70
8:H:101:ALA:HB2	8:H:116:TYR:HE2	1.57	0.70
2:B:170:LEU:HD23	2:B:170:LEU:O	1.91	0.70
9:I:98:VAL:HG13	9:I:100:PHE:HE1	1.57	0.70
3:C:66:ARG:NH1	10:J:2:ILE:HG21	2.05	0.70
1:A:249:SER:O	1:A:250:ILE:HG13	1.91	0.70
1:A:549:MET:SD	1:A:577:ILE:HD11	2.32	0.70
3:C:3:GLU:HG2	3:C:4:GLU:HG3	1.72	0.70
1:A:69:THR:HG21	2:B:1174:LYS:HZ2	1.57	0.69
2:B:1002:THR:HG22	2:B:1072:MET:HG2	1.74	0.69
2:B:798:TYR:HE2	3:C:62:PHE:CE2	2.10	0.69
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.26	0.69
1:A:335:ARG:HD3	1:A:339:ASN:HD22	1.54	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.26	0.69
7:G:34:VAL:HG11	7:G:74:TYR:CE1	2.25	0.69
1:A:718:VAL:O	1:A:721:PHE:HB2	1.92	0.69
2:B:258:LEU:O	2:B:258:LEU:HG	1.92	0.69
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.72	0.69
4:D:144:THR:O	4:D:148:LEU:HB2	1.91	0.69
1:A:182:VAL:HG22	1:A:201:VAL:HA	1.74	0.69
1:A:208:LEU:HD21	1:A:212:LYS:HE3	1.74	0.69
1:A:591:PHE:HA	1:A:595:THR:HG21	1.75	0.69
2:B:637:LEU:HD12	2:B:693:ILE:HD11	1.74	0.69
14:1:12:DG:H2''	14:1:13:DT:H5'	1.75	0.69
3:C:183:TRP:O	3:C:185:LYS:N	2.25	0.69
7:G:112:LYS:HA	7:G:115:MET:HE3	1.73	0.69
6:F:109:VAL:HG12	6:F:110:ASP:N	2.08	0.69
1:A:66:LYS:NZ	1:A:68:GLN:H	1.90	0.69
3:C:221:TYR:CD1	3:C:222:LYS:HG3	2.28	0.69
4:D:12:ARG:HH12	4:D:14:ARG:HA	1.57	0.69
2:B:562:GLY:HA3	2:B:590:HIS:ND1	2.07	0.69
3:C:184:ASN:OD1	3:C:187:LYS:HA	1.92	0.69
4:D:60:LYS:HE3	4:D:126:ILE:HD11	1.73	0.69
2:B:559:SER:CA	2:B:563:MET:HB3	2.06	0.69
1:A:50:ILE:C	1:A:52:GLY:H	1.96	0.69
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.22	0.69
2:B:1096:ARG:O	2:B:1097:HIS:HB2	1.91	0.69
2:B:521:LEU:HB3	2:B:633:VAL:HG11	1.75	0.69
10:J:53:HIS:C	10:J:53:HIS:CD2	2.66	0.69
2:B:1084:GLN:HE21	2:B:1084:GLN:N	1.89	0.69
6:F:111:LEU:O	6:F:113:GLY:N	2.25	0.69
5:E:171:LYS:HG2	5:E:174:GLN:HG3	1.75	0.69
9:I:8:ARG:HG3	9:I:9:ASP:OD1	1.92	0.69
2:B:95:ILE:HG13	2:B:130:VAL:HG22	1.74	0.69
2:B:549:THR:HB	2:B:628:THR:OG1	1.93	0.69
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.57	0.69
4:D:12:ARG:HG2	4:D:12:ARG:HH11	1.58	0.68
1:A:265:LYS:O	1:A:269:ILE:HG13	1.92	0.68
1:A:913:LEU:HD12	1:A:914:GLU:N	2.05	0.68
2:B:102:VAL:HG23	2:B:112:LEU:HD22	1.74	0.68
2:B:39:ARG:HH21	2:B:665:GLU:CG	2.06	0.68
1:A:134:ARG:HG2	1:A:138:ILE:HD11	1.75	0.68
1:A:1370:LEU:O	1:A:1374:VAL:HG23	1.93	0.68
1:A:1193:LEU:HD12	1:A:1194:ARG:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:810:GLU:HB2	2:B:815:ARG:NH2	2.07	0.68
11:K:101:LEU:O	11:K:101:LEU:HD23	1.94	0.68
5:E:22:MET:CE	5:E:26:ARG:HH21	2.07	0.68
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.57	0.68
7:G:1:MET:SD	7:G:2:PHE:N	2.67	0.68
8:H:14:GLU:HG2	8:H:15:VAL:N	2.09	0.68
3:C:189:THR:HG22	3:C:190:ASP:N	2.08	0.68
2:B:39:ARG:HH21	2:B:665:GLU:HG2	1.58	0.68
2:B:53:GLN:HG2	2:B:547:VAL:CG2	2.23	0.68
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.20	0.68
14:1:18:DA:OP1	14:1:18:DA:H3'	1.93	0.68
2:B:427:ASP:HA	2:B:430:ARG:HG3	1.75	0.68
6:F:111:LEU:N	6:F:111:LEU:HD12	2.09	0.68
7:G:165:GLU:HB2	7:G:168:LEU:HD12	1.75	0.68
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	1.74	0.68
8:H:63:LEU:HD23	8:H:90:ALA:HB3	1.76	0.68
5:E:127:ILE:O	5:E:127:ILE:HG13	1.94	0.68
2:B:914:LYS:HE2	2:B:937:ALA:HB1	1.75	0.68
1:A:860:LEU:HA	1:A:1422:ARG:NH2	2.09	0.68
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.75	0.68
2:B:363:HIS:O	2:B:364:ILE:HB	1.92	0.68
1:A:942:PHE:CZ	5:E:207:ARG:HG3	2.28	0.68
2:B:25:ILE:CG2	2:B:658:ILE:HD12	2.24	0.68
2:B:865:LYS:HB2	2:B:961:LEU:HD11	1.76	0.68
12:L:30:ILE:HG22	12:L:31:CYS:N	2.08	0.68
5:E:19:VAL:O	5:E:23:VAL:HG23	1.93	0.68
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.75	0.68
2:B:1099:VAL:HG13	2:B:1100:ASP:N	2.09	0.68
1:A:934:LYS:O	1:A:937:VAL:HG12	1.94	0.68
2:B:1187:ASN:O	2:B:1188:LYS:CB	2.43	0.67
1:A:1348:LEU:O	1:A:1352:VAL:HG23	1.94	0.67
2:B:664:THR:HA	2:B:667:GLN:HE21	1.59	0.67
1:A:66:LYS:HD3	1:A:67:CYS:N	2.09	0.67
4:D:66:ARG:O	4:D:70:PHE:HB2	1.94	0.67
1:A:427:GLN:HG3	1:A:430:TRP:CZ2	2.29	0.67
3:C:243:VAL:HG12	3:C:243:VAL:O	1.94	0.67
8:H:89:LEU:HB2	8:H:91:ASP:OD1	1.95	0.67
4:D:139:LYS:HG2	4:D:143:ASN:ND2	2.09	0.67
8:H:143:LEU:N	8:H:143:LEU:HD12	2.09	0.67
1:A:108:MET:HA	1:A:210:ILE:HD13	1.75	0.67
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:VAL:HG12	1:A:153:PRO:HD2	1.75	0.67
1:A:283:GLY:O	1:A:285:PRO:HD2	1.93	0.67
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.74	0.67
7:G:138:THR:O	7:G:140:LYS:N	2.27	0.67
6:F:97:ARG:O	6:F:101:ILE:HG13	1.93	0.67
1:A:1436:ILE:O	1:A:1437:GLY:C	2.33	0.67
2:B:707:PRO:HG2	2:B:708:GLU:H	1.59	0.67
2:B:705:MET:H	2:B:710:LEU:HD12	1.59	0.67
4:D:52:LEU:HD12	4:D:182:SER:HB2	1.74	0.67
12:L:34:CYS:O	12:L:34:CYS:SG	2.53	0.67
3:C:112:ASN:CB	3:C:114:TYR:HE1	2.07	0.67
2:B:882:THR:HG22	2:B:884:ARG:N	2.10	0.67
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.77	0.67
1:A:315:LEU:N	1:A:315:LEU:HD23	2.08	0.67
1:A:219:PHE:O	1:A:222:LEU:HB2	1.94	0.67
10:J:16:ASP:OD1	10:J:17:LYS:HD2	1.95	0.67
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.30	0.67
1:A:57:ARG:O	1:A:68:GLN:HG2	1.95	0.67
1:A:1444:MET:CG	7:G:60:ARG:HA	2.24	0.67
4:D:14:ARG:CB	4:D:14:ARG:HH11	2.01	0.67
3:C:145:CYS:HA	10:J:2:ILE:CD1	2.25	0.67
3:C:252:GLN:NE2	11:K:95:ILE:HG23	2.07	0.67
2:B:637:LEU:HD21	2:B:742:GLU:HA	1.76	0.67
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.77	0.67
7:G:115:MET:HB3	7:G:116:PRO:HD2	1.76	0.67
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.29	0.67
2:B:1221:SER:O	2:B:1223:ASP:N	2.26	0.67
2:B:807:ARG:HG2	2:B:1045:SER:OG	1.95	0.67
1:A:1095:THR:HG21	1:A:1112:LYS:HB2	1.76	0.67
1:A:34:LYS:HB3	1:A:36:ARG:NH1	2.09	0.67
7:G:59:GLY:HA3	7:G:70:PHE:CD2	2.30	0.67
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.18	0.67
7:G:51:TYR:O	7:G:54:ILE:HG13	1.94	0.67
5:E:77:SER:O	5:E:105:PHE:HB3	1.94	0.67
1:A:23:SER:HA	1:A:233:TRP:NE1	2.09	0.67
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.30	0.66
8:H:82:PRO:C	8:H:84:ALA:H	1.98	0.66
1:A:323:LYS:HD2	1:A:323:LYS:N	2.09	0.66
1:A:626:ASN:O	1:A:631:HIS:HD2	1.77	0.66
2:B:955:THR:CG2	2:B:956:THR:N	2.58	0.66
11:K:40:HIS:ND1	11:K:61:TYR:OH	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ASN:ND2	1:A:228:PHE:N	2.33	0.66
2:B:510:LYS:CB	2:B:511:PRO:HD3	2.23	0.66
11:K:63:VAL:HG23	11:K:63:VAL:O	1.94	0.66
1:A:88:LYS:HG3	1:A:276:LEU:HD21	1.76	0.66
7:G:14:HIS:HD2	7:G:16:SER:H	1.43	0.66
3:C:184:ASN:ND2	3:C:189:THR:HB	2.11	0.66
2:B:408:LEU:HD12	2:B:408:LEU:N	2.10	0.66
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.61	0.66
8:H:84:ALA:HB2	8:H:87:ARG:CZ	2.26	0.66
1:A:903:ASN:C	1:A:903:ASN:HD22	1.98	0.66
8:H:15:VAL:HG22	8:H:26:ILE:CG1	2.25	0.66
9:I:61:ASP:C	9:I:63:GLY:H	1.99	0.66
2:B:64:CYS:HA	2:B:67:SER:OG	1.95	0.66
1:A:596:THR:O	1:A:598:LEU:N	2.29	0.66
4:D:130:LEU:C	4:D:132:GLN:H	1.99	0.66
1:A:134:ARG:HH11	1:A:221:SER:HA	1.61	0.66
2:B:980:PHE:HE1	2:B:990:ILE:HD11	1.61	0.66
2:B:597:MET:HA	2:B:597:MET:CE	2.26	0.66
2:B:294:ASP:H	9:I:12:ASN:ND2	1.94	0.66
4:D:208:GLU:O	4:D:212:LYS:HG3	1.95	0.66
2:B:847:ASP:C	2:B:849:GLY:H	1.99	0.66
1:A:265:LYS:HD3	1:A:302:THR:CG2	2.25	0.66
2:B:25:ILE:HG21	2:B:658:ILE:HD12	1.76	0.66
5:E:22:MET:HE3	5:E:26:ARG:NE	2.11	0.66
1:A:62:ASP:O	1:A:64:ASN:HB2	1.96	0.66
2:B:745:PRO:C	2:B:747:MET:H	1.99	0.65
1:A:866:PHE:C	1:A:867:ILE:HD12	2.16	0.65
1:A:443:LEU:HD12	2:B:1146:PHE:CZ	2.30	0.65
5:E:180:ARG:HB2	5:E:215:MET:OXT	1.95	0.65
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.76	0.65
2:B:53:GLN:HG2	2:B:547:VAL:HG22	1.77	0.65
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.30	0.65
1:A:30:ILE:HG23	2:B:1170:THR:HG23	1.78	0.65
2:B:216:GLU:OE1	2:B:537:LYS:HE3	1.96	0.65
2:B:464:GLY:O	2:B:477:ALA:HA	1.96	0.65
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.62	0.65
2:B:847:ASP:HB3	3:C:167:HIS:NE2	2.12	0.65
1:A:1258:HIS:O	1:A:1262:LYS:HE3	1.97	0.65
4:D:123:LEU:O	4:D:127:ASP:HB2	1.97	0.65
4:D:118:THR:HB	4:D:121:LYS:HB2	1.78	0.65
1:A:61:ILE:HG22	1:A:62:ASP:N	2.08	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.78	0.65
2:B:891:ASP:O	2:B:893:LEU:N	2.29	0.65
8:H:104:PHE:HZ	8:H:136:LYS:HA	1.61	0.65
8:H:44:VAL:O	8:H:44:VAL:HG12	1.97	0.65
1:A:424:ILE:HG22	1:A:425:GLN:N	2.11	0.65
7:G:112:LYS:HA	7:G:115:MET:CE	2.26	0.65
5:E:48:ASP:CG	5:E:49:SER:H	1.98	0.65
4:D:124:GLU:HA	4:D:127:ASP:HB2	1.77	0.65
1:A:203:SER:HB3	1:A:206:GLU:HB2	1.79	0.65
2:B:291:ILE:HD13	2:B:300:HIS:CD2	2.32	0.65
5:E:176:PRO:O	5:E:212:ARG:HA	1.96	0.65
4:D:8:PHE:CE1	4:D:37:GLN:HB2	2.32	0.65
1:A:982:THR:C	1:A:984:LYS:H	1.98	0.65
2:B:875:GLU:O	2:B:877:PRO:HD3	1.97	0.65
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.79	0.65
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.25	0.65
1:A:666:ILE:N	1:A:666:ILE:HD12	2.12	0.65
2:B:773:MET:SD	2:B:987:LYS:HD3	2.37	0.65
1:A:106:VAL:HG12	1:A:107:CYS:N	2.11	0.65
7:G:122:ASN:ND2	7:G:125:SER:HB3	2.11	0.65
2:B:1001:PHE:CE2	3:C:34:ARG:NE	2.64	0.65
3:C:10:ILE:HG22	3:C:11:ARG:O	1.97	0.65
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.11	0.65
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.26	0.65
4:D:29:LEU:N	4:D:29:LEU:HD22	2.12	0.65
9:I:102:VAL:HG22	9:I:109:ILE:HG12	1.78	0.65
1:A:1445:ILE:N	1:A:1445:ILE:HD12	2.12	0.65
2:B:976:ILE:O	2:B:990:ILE:HB	1.97	0.65
2:B:282:ILE:HG21	2:B:382:ILE:HD11	1.78	0.65
1:A:344:ARG:HH11	1:A:344:ARG:HB3	1.62	0.65
4:D:13:ARG:C	4:D:15:LEU:H	1.99	0.65
2:B:542:MET:CG	2:B:747:MET:HE3	2.22	0.65
3:C:165:LYS:O	11:K:6:ARG:NH1	2.29	0.65
2:B:815:ARG:HD3	2:B:1041:GLU:OE2	1.97	0.65
4:D:7:THR:O	4:D:9:GLN:N	2.29	0.65
2:B:955:THR:HG22	2:B:956:THR:O	1.97	0.65
7:G:88:ASP:HB3	7:G:144:ARG:HA	1.77	0.65
1:A:481:ASP:OD1	1:A:485:ASP:OD2	2.15	0.65
2:B:497:ARG:NH2	2:B:775:LYS:NZ	2.45	0.65
4:D:154:PHE:HE1	4:D:163:VAL:HG11	1.62	0.65
1:A:1189:SER:O	1:A:1241:ARG:HD3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:178:ILE:HG22	5:E:213:ILE:O	1.96	0.65
1:A:19:PHE:O	1:A:1416:ALA:HA	1.96	0.65
10:J:53:HIS:CD2	10:J:54:VAL:N	2.66	0.64
1:A:626:ASN:O	1:A:631:HIS:CD2	2.50	0.64
6:F:135:ARG:HG2	6:F:137:TYR:CE1	2.32	0.64
2:B:465:ASN:HD22	2:B:465:ASN:N	1.93	0.64
1:A:567:LYS:CB	8:H:96:VAL:H	2.03	0.64
2:B:34:ILE:HG12	2:B:542:MET:HE1	1.79	0.64
2:B:705:MET:H	2:B:710:LEU:CD1	2.11	0.64
2:B:801:LYS:O	10:J:52:THR:HG23	1.96	0.64
7:G:116:PRO:HG2	7:G:119:LEU:HB3	1.78	0.64
2:B:796:LEU:HD12	2:B:852:ARG:O	1.96	0.64
1:A:255:SER:OG	2:B:918:ILE:HD13	1.96	0.64
1:A:567:LYS:HD2	1:A:568:PRO:CD	2.21	0.64
1:A:853:ASP:OD1	1:A:855:THR:CB	2.45	0.64
2:B:168:GLY:HA2	2:B:450:ALA:O	1.96	0.64
7:G:138:THR:HG22	7:G:139:ILE:H	1.62	0.64
1:A:154:SER:HB3	1:A:162:VAL:CG2	2.27	0.64
10:J:24:LEU:O	10:J:30:LEU:HB2	1.97	0.64
1:A:590:ARG:HG2	1:A:590:ARG:NH1	2.10	0.64
2:B:430:ARG:CB	2:B:430:ARG:HH11	2.07	0.64
2:B:708:GLU:HG3	2:B:709:ASP:N	2.10	0.64
1:A:382:PRO:HD3	1:A:428:TYR:CD2	2.32	0.64
3:C:238:ILE:HD11	3:C:246:ARG:NH1	2.13	0.64
2:B:387:LEU:HD12	2:B:387:LEU:H	1.63	0.64
2:B:916:THR:HB	2:B:935:ARG:HD2	1.79	0.64
1:A:225:ASN:ND2	1:A:227:VAL:H	1.95	0.64
1:A:768:GLN:CG	1:A:816:HIS:HA	2.26	0.64
1:A:108:MET:HB3	1:A:210:ILE:HD11	1.78	0.64
2:B:181:LEU:HD22	2:B:189:LEU:CD2	2.27	0.64
1:A:1076:ALA:HA	1:A:1079:MET:CE	2.27	0.64
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.61	0.64
1:A:33:ALA:HA	1:A:57:ARG:NH1	2.12	0.64
2:B:364:ILE:O	2:B:365:THR:HB	1.97	0.64
3:C:236:GLY:O	3:C:238:ILE:N	2.30	0.64
7:G:120:THR:HG22	7:G:131:GLN:O	1.97	0.64
2:B:1001:PHE:CE2	3:C:34:ARG:CZ	2.80	0.64
1:A:1230:GLU:O	1:A:1232:ASN:N	2.30	0.64
1:A:332:LYS:O	1:A:333:GLU:HB2	1.98	0.64
1:A:195:ASP:O	1:A:196:GLU:HB3	1.97	0.64
2:B:284:ILE:HD13	2:B:333:PHE:HD2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:112:ASN:CB	3:C:114:TYR:CE1	2.80	0.64
3:C:43:THR:CG2	3:C:44:LEU:N	2.60	0.64
5:E:15:ALA:O	5:E:19:VAL:HG23	1.96	0.64
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.79	0.64
1:A:567:LYS:CB	1:A:568:PRO:CD	2.75	0.64
2:B:589:VAL:CG1	2:B:590:HIS:H	2.09	0.64
2:B:333:PHE:O	2:B:334:ILE:HG13	1.98	0.64
2:B:987:LYS:HE3	15:3:11:U:O2'	1.98	0.64
1:A:114:LEU:O	1:A:115:LEU:HG	1.98	0.64
1:A:1313:LEU:HD23	1:A:1338:VAL:HG21	1.80	0.64
2:B:211:VAL:O	2:B:480:SER:HA	1.97	0.64
2:B:525:ALA:O	2:B:768:THR:HG23	1.97	0.64
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.33	0.64
1:A:1205:LYS:O	1:A:1207:LEU:HG	1.97	0.64
2:B:1124:ARG:HH11	2:B:1124:ARG:HB3	1.62	0.64
7:G:158:HIS:CD2	7:G:159:ALA:H	2.15	0.64
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.13	0.64
5:E:179:GLN:HB2	5:E:182:ASP:HB2	1.80	0.64
8:H:8:ASP:OD2	8:H:9:ILE:N	2.27	0.64
4:D:18:VAL:O	4:D:19:GLU:HB2	1.95	0.64
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.80	0.64
2:B:996:ARG:NH2	3:C:175:ALA:H	1.96	0.64
7:G:1:MET:C	7:G:1:MET:SD	2.76	0.64
3:C:11:ARG:HD3	3:C:21:ILE:HD11	1.80	0.64
8:H:100:THR:HG23	8:H:138:GLU:HG2	1.79	0.64
1:A:390:GLN:O	1:A:394:ASN:HB2	1.98	0.64
2:B:30:SER:HB3	2:B:743:ILE:O	1.98	0.64
4:D:119:ARG:HD3	4:D:221:TYR:CE2	2.32	0.63
1:A:316:GLN:HG2	1:A:317:LYS:N	2.13	0.63
2:B:842:ASN:HD22	2:B:845:SER:N	1.93	0.63
2:B:497:ARG:HH21	2:B:775:LYS:HZ3	1.45	0.63
12:L:28:LYS:HE3	12:L:39:SER:OG	1.97	0.63
5:E:99:HIS:CE1	5:E:103:LYS:HD2	2.34	0.63
1:A:1076:ALA:HA	1:A:1079:MET:HE2	1.80	0.63
5:E:29:PHE:O	5:E:30:ILE:HG13	1.98	0.63
3:C:91:HIS:O	3:C:91:HIS:HD2	1.80	0.63
4:D:35:LEU:N	4:D:35:LEU:HD12	2.13	0.63
1:A:571:LEU:HD22	8:H:46:LEU:HD11	1.80	0.63
3:C:39:ALA:O	3:C:164:ALA:HB3	1.98	0.63
1:A:427:GLN:HG3	1:A:430:TRP:CE2	2.33	0.63
2:B:60:GLN:O	2:B:63:ILE:HG22	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:611:PRO:HB3	2:B:685:LEU:HD11	1.79	0.63
3:C:248:ILE:HD13	11:K:101:LEU:HD22	1.80	0.63
7:G:138:THR:CG2	7:G:139:ILE:N	2.59	0.63
1:A:1259:MET:HE2	1:A:1263:ILE:HG13	1.79	0.63
9:I:105:SER:O	9:I:106:CYS:HB3	1.98	0.63
2:B:953:LEU:O	2:B:953:LEU:HD23	1.98	0.63
2:B:582:VAL:HG22	2:B:626:ILE:CG2	2.29	0.63
3:C:221:TYR:HE1	3:C:222:LYS:HE3	1.63	0.63
2:B:549:THR:CG2	2:B:550:ASP:H	2.08	0.63
1:A:343:LYS:NZ	2:B:1151:LEU:HG	2.13	0.63
4:D:29:LEU:HB3	7:G:82:PHE:CE2	2.34	0.63
2:B:34:ILE:HG12	2:B:542:MET:CE	2.28	0.63
2:B:797:TYR:O	10:J:1:MET:HG2	1.99	0.63
5:E:202:SER:OG	5:E:204:THR:HG22	1.99	0.63
2:B:345:LYS:HB2	2:B:348:ARG:HH21	1.64	0.63
3:C:253:LYS:O	3:C:256:ALA:HB3	1.98	0.63
1:A:37:PHE:N	1:A:37:PHE:CD1	2.66	0.63
3:C:242:GLN:C	3:C:244:VAL:H	2.01	0.63
7:G:116:PRO:HG2	7:G:119:LEU:CB	2.28	0.63
8:H:26:ILE:CD1	8:H:49:VAL:HG11	2.28	0.63
1:A:332:LYS:C	1:A:334:GLY:H	2.00	0.63
1:A:1353:TYR:C	1:A:1353:TYR:HD2	2.02	0.63
2:B:1176:ASN:C	2:B:1178:ASN:H	2.02	0.63
1:A:481:ASP:OD1	1:A:483:ASP:OD2	2.17	0.63
1:A:698:GLN:HA	9:I:97:MET:O	1.97	0.63
4:D:154:PHE:CE1	4:D:163:VAL:HG21	2.34	0.63
5:E:69:ILE:N	5:E:69:ILE:HD12	2.13	0.63
1:A:472:LEU:O	1:A:475:THR:HB	1.98	0.63
7:G:91:VAL:HG12	7:G:92:VAL:N	2.12	0.63
6:F:119:ARG:CG	6:F:119:ARG:HH11	2.05	0.62
8:H:130:ARG:H	8:H:130:ARG:HD3	1.63	0.62
2:B:800:GLN:HB3	10:J:52:THR:HG21	1.81	0.62
7:G:129:SER:CB	7:G:138:THR:OG1	2.47	0.62
3:C:98:VAL:C	3:C:99:LEU:HD22	2.20	0.62
5:E:22:MET:HE3	5:E:26:ARG:HH21	1.62	0.62
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.34	0.62
9:I:58:VAL:HG13	9:I:62:ILE:HD13	1.81	0.62
1:A:858:ASN:ND2	1:A:858:ASN:C	2.52	0.62
5:E:94:LYS:CE	5:E:98:ILE:HD11	2.22	0.62
1:A:380:VAL:HG12	1:A:428:TYR:HA	1.80	0.62
1:A:289:ILE:HG22	1:A:290:GLU:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:69:ILE:H	5:E:69:ILE:HD12	1.64	0.62
1:A:57:ARG:HB2	1:A:57:ARG:HH11	1.64	0.62
1:A:1107:VAL:CG1	1:A:1107:VAL:O	2.47	0.62
2:B:616:ILE:HG12	2:B:697:GLU:HA	1.80	0.62
1:A:308:ILE:HG22	1:A:309:ALA:H	1.63	0.62
4:D:14:ARG:NH1	4:D:16:LYS:HD2	2.15	0.62
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.80	0.62
2:B:282:ILE:HD11	2:B:317:CYS:SG	2.40	0.62
1:A:34:LYS:NZ	1:A:57:ARG:HH21	1.98	0.62
2:B:345:LYS:CG	2:B:346:GLU:N	2.62	0.62
1:A:425:GLN:N	1:A:425:GLN:OE1	2.33	0.62
5:E:207:ARG:HB3	5:E:207:ARG:HH11	1.64	0.62
12:L:53:HIS:HB3	12:L:55:ILE:CD1	2.28	0.62
3:C:258:ILE:HD11	11:K:42:LEU:HD21	1.82	0.62
2:B:505:ASP:CG	13:2:1:DA:H8	2.03	0.62
5:E:117:THR:HB	5:E:120:ALA:HB2	1.81	0.62
6:F:89:GLU:OE2	6:F:134:ILE:HG21	1.99	0.62
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.31	0.62
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.80	0.62
1:A:1095:THR:HG21	1:A:1112:LYS:HD2	1.80	0.62
5:E:46:TYR:CE2	5:E:58:MET:HA	2.35	0.62
4:D:12:ARG:NH1	4:D:14:ARG:HA	2.13	0.62
1:A:351:THR:CG2	2:B:1103:ILE:HA	2.21	0.62
1:A:1308:THR:CG2	1:A:1309:ASP:N	2.59	0.62
1:A:722:LEU:HD21	1:A:794:PRO:HB3	1.82	0.62
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.34	0.62
11:K:13:GLY:O	11:K:16:GLU:HG3	2.00	0.62
1:A:1293:SER:OG	1:A:1294:PRO:HD2	2.00	0.62
2:B:1095:LEU:N	2:B:1095:LEU:HD12	2.14	0.62
2:B:615:MET:HG2	2:B:626:ILE:HG12	1.81	0.62
1:A:172:PRO:HD3	1:A:185:TRP:NE1	2.14	0.62
2:B:882:THR:HB	2:B:934:LYS:O	2.00	0.62
1:A:305:ASP:OD1	1:A:306:ASN:N	2.32	0.62
8:H:89:LEU:C	8:H:91:ASP:N	2.52	0.62
2:B:642:ASP:O	2:B:644:GLU:N	2.30	0.62
2:B:547:VAL:HG12	2:B:612:GLU:OE2	1.99	0.62
3:C:123:ASN:CG	3:C:125:MET:H	2.03	0.62
9:I:8:ARG:HG3	9:I:9:ASP:N	2.15	0.62
7:G:129:SER:HB3	7:G:138:THR:OG1	2.00	0.62
1:A:369:SER:HB3	11:K:2:ASN:ND2	2.14	0.62
1:A:216:VAL:O	1:A:219:PHE:HB2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1385:THR:HG22	1:A:1386:ARG:N	2.15	0.62
11:K:68:PHE:HD1	11:K:70:ARG:HH12	1.47	0.62
1:A:73:GLY:O	1:A:75:ASN:N	2.33	0.61
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.29	0.61
4:D:153:ARG:HB3	4:D:154:PHE:CD2	2.34	0.61
5:E:207:ARG:NH1	5:E:207:ARG:HB3	2.15	0.61
2:B:868:MET:O	2:B:870:ILE:HG13	2.00	0.61
8:H:76:THR:O	8:H:77:ARG:HB2	2.00	0.61
2:B:686:ASN:C	2:B:688:GLY:H	2.03	0.61
2:B:983:ARG:NH1	2:B:1028:GLU:OE1	2.33	0.61
3:C:189:THR:HG22	3:C:190:ASP:H	1.64	0.61
3:C:124:LEU:O	3:C:127:ARG:HG2	2.00	0.61
3:C:33:LEU:HG	3:C:37:MET:HE1	1.81	0.61
1:A:7:SER:HB3	2:B:1193:GLN:HE22	1.65	0.61
3:C:76:ASP:OD2	3:C:128:ASN:N	2.32	0.61
2:B:226:PHE:HA	2:B:395:GLN:HG2	1.83	0.61
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.00	0.61
2:B:261:ARG:NH1	2:B:261:ARG:HB3	2.13	0.61
1:A:1036:ARG:HG2	1:A:1036:ARG:HH11	1.64	0.61
2:B:290:GLY:O	2:B:292:ILE:HG13	1.99	0.61
6:F:69:LEU:HD22	6:F:71:GLU:OE2	1.99	0.61
2:B:167:ILE:HG22	2:B:453:ILE:HD12	1.82	0.61
2:B:1159:ARG:HB3	2:B:1159:ARG:NH1	2.15	0.61
1:A:1161:THR:C	1:A:1163:ILE:H	2.01	0.61
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.82	0.61
1:A:1450:LEU:O	1:A:1450:LEU:HG	1.99	0.61
1:A:351:THR:HG22	2:B:1103:ILE:CA	2.21	0.61
1:A:353:ILE:HG13	1:A:470:LEU:HD21	1.82	0.61
8:H:87:ARG:HG2	8:H:88:SER:N	2.16	0.61
4:D:51:ASN:O	4:D:52:LEU:O	2.19	0.61
2:B:1084:GLN:HE21	2:B:1084:GLN:H	1.47	0.61
2:B:63:ILE:HD12	2:B:421:PHE:CE2	2.35	0.61
2:B:277:LYS:HE2	2:B:336:ARG:HD3	1.82	0.61
12:L:42:ARG:HG3	12:L:42:ARG:HH11	1.65	0.61
7:G:26:LEU:HD12	7:G:56:ILE:CD1	2.15	0.61
4:D:153:ARG:NH2	4:D:184:ALA:HA	2.15	0.61
10:J:23:ASN:C	10:J:25:LEU:N	2.53	0.61
1:A:105:CYS:SG	1:A:139:TRP:HA	2.41	0.61
9:I:85:PHE:HD2	9:I:85:PHE:H	1.47	0.61
1:A:853:ASP:O	1:A:854:ASN:HB2	1.99	0.61
2:B:289:LEU:HD13	2:B:375:ALA:CB	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:136:ASN:OD1	5:E:137:GLU:N	2.34	0.61
2:B:469:GLN:HG2	2:B:470:LYS:N	2.16	0.61
8:H:15:VAL:HG22	8:H:26:ILE:HG13	1.82	0.61
1:A:1141:THR:CG2	1:A:1205:LYS:HD3	2.30	0.61
8:H:139:ASN:O	8:H:140:ALA:CB	2.48	0.61
1:A:2:VAL:HG11	2:B:1157:ALA:HB1	1.82	0.61
1:A:1444:MET:N	1:A:1444:MET:HE2	2.14	0.61
10:J:57:ILE:HA	10:J:60:PHE:CD2	2.27	0.61
2:B:95:ILE:HB	2:B:130:VAL:HG13	1.82	0.61
2:B:332:ASP:O	2:B:334:ILE:N	2.32	0.61
2:B:1001:PHE:CD1	2:B:1001:PHE:C	2.74	0.61
2:B:278:GLN:CG	2:B:279:ASP:H	2.13	0.61
1:A:1341:ILE:CG2	1:A:1342:GLU:N	2.63	0.61
4:D:124:GLU:HA	4:D:127:ASP:CB	2.31	0.61
1:A:886:ILE:HD12	1:A:943:LEU:HB3	1.83	0.61
9:I:111:THR:HG21	9:I:113:ASP:HB2	1.83	0.61
1:A:870:GLU:HB2	5:E:204:THR:HG21	1.83	0.61
1:A:382:PRO:HD3	1:A:428:TYR:CE2	2.35	0.61
1:A:1353:TYR:CD2	1:A:1353:TYR:C	2.74	0.61
1:A:1395:GLY:HA3	1:A:1419:ASP:OD2	1.99	0.61
1:A:979:SER:OG	1:A:980:ASP:N	2.33	0.61
2:B:175:ARG:HB2	2:B:200:GLY:HA3	1.82	0.61
1:A:597:LEU:N	1:A:597:LEU:HD12	2.16	0.60
9:I:85:PHE:HD1	9:I:99:LEU:HD22	1.65	0.60
8:H:4:THR:HG22	8:H:5:LEU:N	2.16	0.60
2:B:247:GLY:C	2:B:249:ARG:H	2.04	0.60
3:C:112:ASN:HB2	3:C:114:TYR:HE1	1.66	0.60
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	2.89	0.60
2:B:398:ARG:NH1	2:B:398:ARG:HB2	2.16	0.60
1:A:225:ASN:HD22	1:A:228:PHE:N	1.94	0.60
2:B:510:LYS:HB3	2:B:511:PRO:CD	2.27	0.60
1:A:317:LYS:O	1:A:318:SER:HB3	1.99	0.60
2:B:516:ASN:ND2	2:B:516:ASN:N	2.49	0.60
6:F:103:MET:O	6:F:104:ASN:HB2	2.01	0.60
8:H:31:THR:HG22	8:H:31:THR:O	1.99	0.60
1:A:665:GLY:HA2	2:B:1026:LEU:CD2	2.31	0.60
2:B:583:ASN:ND2	2:B:628:THR:HG22	2.16	0.60
4:D:154:PHE:CD2	4:D:154:PHE:N	2.68	0.60
1:A:35:ILE:HA	1:A:52:GLY:O	2.01	0.60
2:B:288:ALA:CB	2:B:331:LEU:HD12	2.30	0.60
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:871:THR:HG22	2:B:872:GLU:O	2.01	0.60
7:G:26:LEU:CD1	7:G:56:ILE:HD11	2.15	0.60
1:A:335:ARG:NH1	2:B:1202:LEU:HD13	2.16	0.60
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.31	0.60
3:C:101:LEU:HB2	3:C:118:LEU:HD23	1.83	0.60
4:D:138:ASN:HD21	7:G:35:GLU:HB3	1.64	0.60
2:B:883:LEU:O	2:B:885:MET:N	2.34	0.60
1:A:66:LYS:HZ2	1:A:68:GLN:H	1.49	0.60
8:H:23:VAL:HG22	8:H:42:ILE:O	2.01	0.60
5:E:117:THR:HB	5:E:120:ALA:CB	2.32	0.60
1:A:288:ALA:HA	1:A:291:GLU:CD	2.22	0.60
1:A:794:PRO:HG2	1:A:795:GLU:OE2	2.01	0.60
1:A:1095:THR:CG2	1:A:1112:LYS:HD2	2.32	0.60
11:K:21:ILE:HG12	11:K:33:ILE:HG23	1.82	0.60
3:C:261:ALA:HA	3:C:264:GLN:OE1	2.01	0.60
1:A:49:LYS:HE2	1:A:61:ILE:HD12	1.84	0.60
2:B:1069:PHE:HA	2:B:1085:ILE:O	2.00	0.60
10:J:1:MET:H1	10:J:57:ILE:N	2.00	0.60
2:B:773:MET:C	2:B:775:LYS:H	2.04	0.60
2:B:811:TYR:N	2:B:811:TYR:CD1	2.70	0.60
2:B:193:LYS:HZ1	12:L:32:ALA:HB1	1.67	0.60
3:C:258:ILE:O	3:C:262:LEU:HB2	2.01	0.60
3:C:7:GLN:HG3	11:K:104:ASN:HD22	1.67	0.60
1:A:809:THR:OG1	1:A:812:GLU:HG3	2.01	0.60
1:A:1027:ALA:O	1:A:1031:VAL:HG23	2.00	0.60
2:B:1174:LYS:O	2:B:1175:LEU:C	2.40	0.60
1:A:21:LEU:HD11	1:A:1414:ALA:HA	1.83	0.60
2:B:1156:ASP:O	2:B:1157:ALA:O	2.20	0.60
5:E:44:ALA:O	5:E:45:LYS:HB2	1.99	0.60
2:B:65:GLU:OE1	2:B:418:LYS:HE3	2.01	0.60
8:H:87:ARG:HG2	8:H:88:SER:H	1.67	0.60
2:B:652:LYS:HB3	2:B:689:LEU:CD2	2.31	0.60
2:B:1095:LEU:H	2:B:1095:LEU:CD1	2.12	0.60
1:A:284:ALA:O	1:A:286:HIS:N	2.35	0.60
2:B:734:HIS:O	2:B:735:ALA:HB2	2.02	0.60
5:E:135:PHE:HD2	5:E:140:LEU:HD21	1.66	0.60
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.82	0.60
1:A:7:SER:OG	2:B:1161:HIS:HE1	1.84	0.60
2:B:553:PRO:O	2:B:557:PHE:HB2	2.02	0.60
3:C:17:ASN:N	3:C:240:VAL:HG11	2.16	0.60
2:B:505:ASP:HA	13:2:1:DA:C8	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:185:CYS:O	4:D:211:LEU:HD22	2.01	0.60
3:C:161:LYS:O	3:C:170:TRP:NE1	2.34	0.59
1:A:839:ARG:NH1	1:A:839:ARG:HG2	2.12	0.59
2:B:189:LEU:HD13	2:B:196:PRO:HA	1.83	0.59
1:A:709:THR:HB	1:A:712:GLU:H	1.67	0.59
9:I:105:SER:O	9:I:106:CYS:CB	2.50	0.59
2:B:1096:ARG:HG2	2:B:1097:HIS:ND1	2.16	0.59
2:B:235:SER:OG	2:B:236:HIS:HD2	1.85	0.59
2:B:882:THR:HG21	2:B:935:ARG:CA	2.16	0.59
4:D:14:ARG:HH12	4:D:16:LYS:HD2	1.67	0.59
12:L:38:LEU:HD11	12:L:49:LYS:HE2	1.84	0.59
2:B:36:ALA:HA	2:B:39:ARG:HD2	1.84	0.59
1:A:850:VAL:HG12	1:A:850:VAL:O	2.03	0.59
1:A:605:MET:HE1	1:A:612:ILE:HG23	1.84	0.59
1:A:438:ASP:O	1:A:439:ASN:HB2	2.02	0.59
1:A:266:LEU:HD21	1:A:303:TYR:CZ	2.37	0.59
4:D:134:THR:HG22	4:D:135:GLY:N	2.17	0.59
1:A:741:ASN:HD22	1:A:744:LYS:H	1.48	0.59
1:A:744:LYS:HG2	1:A:748:MET:CE	2.31	0.59
3:C:66:ARG:NH1	10:J:2:ILE:CG2	2.57	0.59
2:B:770:GLN:CD	2:B:983:ARG:HA	2.22	0.59
2:B:1147:LEU:CD2	2:B:1151:LEU:HD22	2.32	0.59
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.84	0.59
1:A:1042:PHE:CE2	1:A:1046:LEU:HD11	2.37	0.59
1:A:67:CYS:O	1:A:70:CYS:HB3	2.01	0.59
4:D:155:ARG:NE	4:D:221:TYR:CE1	2.68	0.59
10:J:3:VAL:HA	10:J:53:HIS:CE1	2.37	0.59
12:L:38:LEU:CD1	12:L:49:LYS:HE2	2.32	0.59
2:B:687:GLU:O	2:B:689:LEU:HG	2.02	0.59
5:E:79:TRP:NE1	5:E:81:GLU:HB2	2.15	0.59
2:B:1001:PHE:HD1	2:B:1001:PHE:C	2.05	0.59
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.37	0.59
2:B:35:SER:HA	2:B:811:TYR:HE2	1.68	0.59
2:B:473:MET:HE3	2:B:474:SER:HA	1.85	0.59
10:J:27:GLU:O	10:J:29:GLU:N	2.35	0.59
1:A:567:LYS:HB3	8:H:95:TYR:CA	2.32	0.59
2:B:847:ASP:O	2:B:849:GLY:N	2.35	0.59
2:B:637:LEU:HD22	2:B:741:CYS:O	2.02	0.59
5:E:56:LYS:NZ	5:E:84:ASP:H	2.00	0.59
1:A:869:GLY:O	5:E:204:THR:HG21	2.02	0.59
7:G:119:LEU:HD11	7:G:130:TYR:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1153:TYR:CD2	1:A:1163:ILE:HD11	2.37	0.59
1:A:146:MET:O	1:A:147:VAL:HG23	2.03	0.59
2:B:864:LYS:HG3	2:B:872:GLU:OE1	2.02	0.59
2:B:273:LEU:O	2:B:276:ILE:HB	2.03	0.59
2:B:583:ASN:HD21	2:B:628:THR:CG2	2.14	0.59
6:F:109:VAL:HG12	6:F:110:ASP:H	1.65	0.59
4:D:8:PHE:HE1	4:D:37:GLN:HB2	1.66	0.59
2:B:418:LYS:HG2	2:B:422:LYS:HE3	1.85	0.59
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.83	0.59
9:I:82:GLU:HB3	9:I:104:LEU:HG	1.83	0.59
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.33	0.59
2:B:460:ALA:O	2:B:462:ALA:N	2.35	0.59
1:A:67:CYS:C	1:A:68:GLN:HG3	2.22	0.59
5:E:90:VAL:HA	5:E:120:ALA:HB2	1.84	0.59
2:B:806:THR:N	2:B:809:MET:HE3	2.17	0.59
1:A:1316:VAL:O	1:A:1316:VAL:HG12	2.02	0.59
4:D:139:LYS:HG2	4:D:143:ASN:HD22	1.67	0.59
1:A:675:THR:OG1	1:A:736:ASN:ND2	2.36	0.59
2:B:57:TYR:N	2:B:57:TYR:CD1	2.71	0.59
2:B:999:MET:HA	2:B:999:MET:HE3	1.84	0.59
4:D:198:LEU:O	4:D:200:ASN:N	2.35	0.59
8:H:30:SER:CB	8:H:36:CYS:HB3	2.32	0.59
2:B:770:GLN:HG2	2:B:983:ARG:O	2.03	0.59
1:A:676:MET:O	1:A:679:ILE:HB	2.03	0.59
2:B:241:ARG:HG2	2:B:253:THR:HG22	1.85	0.59
1:A:10:PRO:HG2	2:B:1192:TYR:HD2	1.68	0.59
1:A:964:ILE:O	1:A:967:ALA:HB3	2.02	0.59
2:B:622:LYS:HZ3	9:I:59:VAL:HG13	1.68	0.58
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.85	0.58
1:A:107:CYS:HB2	1:A:114:LEU:CD2	2.30	0.58
3:C:73:GLN:HE21	3:C:75:MET:H	1.51	0.58
2:B:936:ASP:OD1	2:B:937:ALA:N	2.36	0.58
3:C:164:ALA:HA	3:C:167:HIS:O	2.02	0.58
2:B:637:LEU:CD2	2:B:742:GLU:HA	2.33	0.58
2:B:638:PHE:HD2	2:B:690:VAL:HG22	1.68	0.58
2:B:102:VAL:HG21	2:B:112:LEU:HD22	1.85	0.58
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.33	0.58
5:E:48:ASP:HB3	5:E:54:GLN:NE2	2.19	0.58
2:B:282:ILE:CG2	2:B:382:ILE:HD11	2.32	0.58
2:B:756:ILE:O	2:B:759:PRO:HD3	2.02	0.58
2:B:90:ILE:HD12	2:B:432:MET:SD	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:GLY:O	1:A:332:LYS:O	2.21	0.58
2:B:882:THR:CG2	2:B:884:ARG:H	2.15	0.58
7:G:13:LEU:CD2	7:G:17:PHE:HB2	2.32	0.58
7:G:122:ASN:HB2	7:G:131:GLN:HE21	1.69	0.58
7:G:138:THR:CG2	7:G:139:ILE:H	2.16	0.58
2:B:20:ASP:O	2:B:22:SER:N	2.33	0.58
10:J:23:ASN:O	10:J:25:LEU:N	2.36	0.58
1:A:1241:ARG:O	1:A:1242:VAL:HG23	2.03	0.58
7:G:111:THR:HG22	7:G:114:LEU:HD22	1.85	0.58
2:B:787:VAL:O	2:B:787:VAL:HG12	2.03	0.58
2:B:918:ILE:HG21	2:B:935:ARG:NH2	2.17	0.58
1:A:65:LEU:O	1:A:66:LYS:C	2.41	0.58
8:H:40:LEU:HD13	8:H:123:MET:CE	2.33	0.58
1:A:577:ILE:HA	1:A:580:VAL:HG23	1.86	0.58
6:F:82:THR:HG22	6:F:84:TYR:N	2.11	0.58
1:A:1129:GLU:OE1	1:A:1132:LYS:HD2	2.03	0.58
1:A:50:ILE:O	1:A:52:GLY:N	2.36	0.58
1:A:129:LYS:O	1:A:130:ASP:CB	2.51	0.58
4:D:24:ALA:HB3	4:D:26:THR:HG23	1.85	0.58
1:A:372:LYS:HA	1:A:435:HIS:HD1	1.67	0.58
4:D:130:LEU:O	4:D:132:GLN:N	2.34	0.58
5:E:22:MET:HE3	5:E:26:ARG:NH2	2.18	0.58
1:A:2:VAL:HG11	2:B:1157:ALA:CB	2.33	0.58
2:B:418:LYS:HE2	2:B:422:LYS:NZ	2.18	0.58
1:A:673:GLY:O	1:A:676:MET:HB2	2.02	0.58
1:A:310:GLY:O	1:A:312:PRO:HD2	2.03	0.58
3:C:52:GLU:OE1	3:C:154:LYS:HE3	2.03	0.58
1:A:40:THR:HB	1:A:41:MET:HE2	1.84	0.58
8:H:4:THR:HA	8:H:60:ALA:CB	2.27	0.58
9:I:7:CYS:SG	9:I:8:ARG:O	2.61	0.58
8:H:84:ALA:O	8:H:85:GLY:C	2.41	0.58
2:B:100:PRO:HB2	2:B:180:TYR:HE1	1.67	0.58
2:B:429:PHE:HA	2:B:432:MET:HE3	1.85	0.58
7:G:49:LEU:HD21	7:G:77:VAL:HG23	1.86	0.58
2:B:629:ASP:HB3	2:B:632:ARG:HD3	1.85	0.58
5:E:98:ILE:HG22	5:E:102:GLU:HG3	1.84	0.58
2:B:604:ARG:NH2	2:B:614:SER:HA	2.19	0.58
1:A:535:THR:HG23	1:A:575:LYS:HE2	1.85	0.58
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.34	0.58
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.51	0.58
4:D:29:LEU:HD12	7:G:82:PHE:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:182:ASP:HB3	5:E:185:ALA:HB2	1.85	0.58
3:C:196:ASP:HB3	3:C:199:LYS:HD2	1.85	0.58
5:E:94:LYS:HE2	5:E:98:ILE:CD1	2.23	0.58
2:B:798:TYR:CE2	3:C:62:PHE:CE2	2.91	0.58
10:J:2:ILE:CG2	10:J:3:VAL:N	2.65	0.58
1:A:317:LYS:O	1:A:318:SER:CB	2.52	0.58
2:B:246:LYS:HA	2:B:249:ARG:HE	1.69	0.58
5:E:144:ILE:HG13	5:E:145:THR:N	2.17	0.58
5:E:3:GLN:NE2	5:E:52:ARG:HH22	2.02	0.58
1:A:511:ILE:HG22	1:A:512:VAL:N	2.18	0.58
3:C:124:LEU:HD12	3:C:124:LEU:N	2.18	0.58
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.86	0.58
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.86	0.58
7:G:12:THR:HG23	7:G:67:SER:HB3	1.85	0.58
1:A:993:LEU:HD12	1:A:993:LEU:O	2.04	0.58
2:B:1115:THR:HG22	2:B:1117:GLN:H	1.69	0.58
2:B:847:ASP:C	2:B:849:GLY:N	2.57	0.58
2:B:1221:SER:C	2:B:1223:ASP:H	2.08	0.58
1:A:982:THR:C	1:A:984:LYS:N	2.57	0.58
1:A:675:THR:O	1:A:679:ILE:HG13	2.04	0.58
3:C:117:ASP:N	3:C:117:ASP:OD1	2.36	0.58
4:D:64:VAL:C	4:D:66:ARG:N	2.57	0.58
2:B:639:ILE:HG22	2:B:641:GLU:HG2	1.86	0.58
2:B:192:LEU:O	2:B:193:LYS:HB2	2.04	0.58
1:A:683:ILE:HD13	1:A:801:GLU:CG	2.32	0.58
3:C:186:LEU:HD21	3:C:225:ALA:HB2	1.84	0.58
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.86	0.58
9:I:73:ARG:HD2	9:I:101:PHE:CE2	2.38	0.58
12:L:40:LEU:HD22	12:L:44:ASP:CG	2.25	0.57
8:H:84:ALA:HB2	8:H:87:ARG:NE	2.19	0.57
2:B:637:LEU:HD12	2:B:693:ILE:CD1	2.34	0.57
2:B:211:VAL:CG2	2:B:483:LEU:HB2	2.34	0.57
2:B:189:LEU:O	2:B:192:LEU:N	2.36	0.57
2:B:966:VAL:HG12	2:B:967:ARG:N	2.18	0.57
1:A:903:ASN:ND2	1:A:905:ASP:H	2.02	0.57
1:A:1241:ARG:O	1:A:1242:VAL:CB	2.51	0.57
1:A:369:SER:CB	11:K:2:ASN:HD21	2.16	0.57
4:D:118:THR:HG22	4:D:118:THR:O	2.03	0.57
4:D:29:LEU:HD12	7:G:82:PHE:CZ	2.39	0.57
1:A:332:LYS:O	1:A:333:GLU:CB	2.52	0.57
6:F:69:LEU:HB3	6:F:71:GLU:CD	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:196:PRO:O	4:D:198:LEU:N	2.36	0.57
1:A:1120:LEU:O	1:A:1323:ASP:HB2	2.04	0.57
2:B:287:ARG:NH1	2:B:324:ILE:O	2.37	0.57
5:E:7:ARG:HD2	5:E:7:ARG:C	2.25	0.57
2:B:357:GLN:O	2:B:366:GLN:HA	2.03	0.57
3:C:186:LEU:HD12	3:C:186:LEU:N	2.19	0.57
7:G:81:PRO:HG3	7:G:106:MET:SD	2.44	0.57
1:A:1021:LEU:O	1:A:1024:SER:HB3	2.04	0.57
8:H:139:ASN:O	8:H:140:ALA:HB2	2.04	0.57
6:F:96:THR:O	6:F:100:GLN:HG3	2.04	0.57
7:G:53:ASN:HD22	7:G:53:ASN:N	2.01	0.57
1:A:549:MET:SD	1:A:577:ILE:CD1	2.92	0.57
3:C:82:TYR:O	3:C:83:SER:C	2.42	0.57
5:E:180:ARG:HH21	5:E:192:ARG:HB2	1.69	0.57
3:C:183:TRP:O	3:C:184:ASN:C	2.42	0.57
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.24	0.57
1:A:23:SER:HA	1:A:233:TRP:CD1	2.39	0.57
3:C:263:THR:O	3:C:266:ASP:HB2	2.04	0.57
2:B:1197:PRO:O	2:B:1200:ALA:N	2.36	0.57
9:I:50:THR:HG22	9:I:52:ILE:H	1.69	0.57
2:B:1102:LYS:O	2:B:1103:ILE:C	2.42	0.57
2:B:638:PHE:CD2	2:B:690:VAL:HG22	2.40	0.57
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.62	0.57
1:A:41:MET:HE3	1:A:41:MET:H	1.69	0.57
1:A:55:ASP:CG	1:A:55:ASP:O	2.42	0.57
1:A:66:LYS:O	1:A:67:CYS:HB2	2.03	0.57
4:D:64:VAL:C	4:D:66:ARG:H	2.07	0.57
4:D:155:ARG:HE	4:D:221:TYR:HE1	1.47	0.57
4:D:217:LEU:O	4:D:219:THR:N	2.38	0.57
2:B:737:THR:O	2:B:739:THR:HG23	2.05	0.57
8:H:127:GLY:O	8:H:128:ASN:CB	2.52	0.57
2:B:954:VAL:O	12:L:55:ILE:O	2.21	0.57
3:C:181:ASP:OD1	3:C:185:LYS:HB2	2.05	0.57
2:B:241:ARG:HG2	2:B:253:THR:CG2	2.35	0.57
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	2.05	0.57
1:A:75:ASN:O	1:A:76:GLU:CB	2.52	0.57
2:B:309:GLN:OE1	9:I:52:ILE:HD11	2.05	0.57
10:J:1:MET:H2	10:J:57:ILE:H	1.52	0.57
1:A:1120:LEU:HD12	1:A:1120:LEU:O	2.03	0.57
2:B:852:ARG:HH22	12:L:70:ARG:C	2.06	0.57
2:B:222:ILE:H	2:B:240:ILE:CD1	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1037:LEU:HD21	2:B:1064:TYR:HE1	1.69	0.57
2:B:975:GLN:HG2	2:B:976:ILE:H	1.69	0.57
4:D:203:SER:OG	4:D:206:GLU:HB2	2.05	0.57
2:B:622:LYS:NZ	9:I:59:VAL:HG13	2.19	0.57
1:A:861:GLY:HA3	5:E:174:GLN:HE22	1.70	0.57
2:B:805:THR:HA	2:B:809:MET:CE	2.33	0.57
1:A:399:HIS:CB	1:A:400:PRO:CD	2.79	0.57
1:A:316:GLN:HG2	1:A:317:LYS:HD2	1.87	0.57
1:A:786:HIS:CD2	1:A:786:HIS:N	2.68	0.57
7:G:116:PRO:HD2	7:G:119:LEU:HD23	1.87	0.57
5:E:195:VAL:HG22	5:E:213:ILE:HG13	1.87	0.57
1:A:1283:VAL:HG12	1:A:1284:MET:N	2.19	0.57
13:2:5:DC:H2"	13:2:6:DT:OP2	2.03	0.57
1:A:524:VAL:HG12	1:A:525:GLN:H	1.68	0.57
1:A:1286:LYS:HD2	1:A:1304:TRP:CZ2	2.40	0.57
2:B:916:THR:O	2:B:935:ARG:HG2	2.05	0.57
2:B:916:THR:HB	2:B:935:ARG:CG	2.34	0.57
1:A:51:GLY:C	1:A:56:PRO:HB3	2.26	0.57
1:A:49:LYS:NZ	1:A:61:ILE:HG13	2.20	0.57
1:A:1420:ASP:O	1:A:1421:CYS:HB2	2.03	0.57
10:J:1:MET:O	10:J:2:ILE:O	2.23	0.57
1:A:1312:ASN:HD21	1:A:1315:GLU:CG	2.16	0.57
1:A:1445:ILE:H	1:A:1445:ILE:CD1	2.07	0.57
3:C:43:THR:CG2	3:C:44:LEU:H	2.17	0.57
1:A:1161:THR:CG2	1:A:1163:ILE:HD12	2.33	0.57
2:B:839:MET:HE1	2:B:980:PHE:CB	2.35	0.57
2:B:1222:ARG:O	2:B:1222:ARG:HG2	2.05	0.57
2:B:1115:THR:O	2:B:1116:ARG:HB2	2.05	0.56
2:B:737:THR:CG2	9:I:66:PRO:HA	2.26	0.56
8:H:82:PRO:O	8:H:84:ALA:N	2.34	0.56
2:B:955:THR:CG2	2:B:956:THR:H	2.18	0.56
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.70	0.56
1:A:1305:VAL:HG12	1:A:1306:LEU:N	2.19	0.56
1:A:1261:LYS:O	1:A:1264:GLU:HB3	2.05	0.56
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.87	0.56
2:B:298:LEU:N	2:B:298:LEU:CD2	2.67	0.56
2:B:1172:ILE:O	2:B:1172:ILE:HG22	2.05	0.56
8:H:123:MET:HE3	8:H:142:LEU:CD2	2.35	0.56
1:A:861:GLY:HA3	5:E:174:GLN:NE2	2.20	0.56
2:B:840:ILE:HG21	2:B:994:TYR:HD1	1.71	0.56
3:C:43:THR:HG22	3:C:44:LEU:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:LEU:HD22	1:A:1374:VAL:HG21	1.85	0.56
2:B:241:ARG:HA	2:B:253:THR:HG22	1.86	0.56
3:C:196:ASP:CB	3:C:199:LYS:HD2	2.35	0.56
1:A:780:VAL:O	1:A:782:ARG:HG2	2.05	0.56
2:B:846:ILE:CG2	2:B:974:PRO:HG2	2.34	0.56
2:B:293:PRO:O	2:B:294:ASP:O	2.24	0.56
5:E:56:LYS:CE	5:E:84:ASP:HB2	2.32	0.56
2:B:557:PHE:O	2:B:557:PHE:HD2	1.88	0.56
2:B:557:PHE:CZ	2:B:603:LEU:HD11	2.41	0.56
1:A:265:LYS:HD3	1:A:302:THR:HG23	1.87	0.56
2:B:644:GLU:C	2:B:646:LEU:H	2.08	0.56
2:B:839:MET:HE3	2:B:1010:LEU:HD23	1.87	0.56
8:H:63:LEU:CD2	8:H:90:ALA:HB3	2.35	0.56
2:B:1048:THR:OG1	2:B:1050:ILE:HG13	2.05	0.56
1:A:879:GLU:O	1:A:955:PRO:HA	2.04	0.56
2:B:46:GLN:HE21	2:B:539:LEU:HD12	1.70	0.56
4:D:12:ARG:HG2	4:D:12:ARG:NH1	2.17	0.56
1:A:1256:GLU:O	1:A:1259:MET:HB3	2.05	0.56
1:A:207:ILE:O	1:A:208:LEU:C	2.42	0.56
11:K:53:ASP:HB3	11:K:56:VAL:HG23	1.87	0.56
2:B:235:SER:OG	2:B:236:HIS:CD2	2.59	0.56
1:A:777:PHE:CD1	1:A:781:ASP:HA	2.39	0.56
10:J:1:MET:N	10:J:56:LEU:N	2.53	0.56
10:J:3:VAL:N	10:J:53:HIS:HE1	2.03	0.56
1:A:919:ILE:HD13	1:A:983:ILE:HD12	1.88	0.56
2:B:361:LEU:O	2:B:363:HIS:O	2.22	0.56
3:C:16:ASP:C	3:C:240:VAL:HG11	2.26	0.56
2:B:1050:ILE:HG22	2:B:1051:THR:N	2.20	0.56
2:B:1106:ARG:HH11	2:B:1126:GLY:HA2	1.70	0.56
1:A:225:ASN:HD21	1:A:228:PHE:H	1.45	0.56
1:A:908:LEU:CD1	1:A:983:ILE:HD11	2.36	0.56
2:B:891:ASP:C	2:B:893:LEU:N	2.59	0.56
2:B:897:GLY:O	2:B:898:LEU:HD23	2.06	0.56
14:1:10:DA:H2"	14:1:11:DA:C8	2.41	0.56
3:C:186:LEU:HD21	3:C:224:GLN:O	2.05	0.56
2:B:597:MET:HE2	2:B:597:MET:HA	1.86	0.56
1:A:41:MET:HB2	1:A:48:ALA:O	2.06	0.56
4:D:156:ASP:O	4:D:158:GLU:N	2.39	0.56
1:A:1242:VAL:CG1	1:A:1243:VAL:N	2.68	0.56
4:D:9:GLN:O	4:D:9:GLN:HG3	2.05	0.56
5:E:182:ASP:HB3	5:E:185:ALA:CB	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:874:PHE:HA	2:B:913:GLY:O	2.04	0.56
2:B:906:SER:O	2:B:907:GLY:O	2.24	0.56
2:B:918:ILE:HD12	2:B:935:ARG:CZ	2.36	0.56
10:J:3:VAL:HA	10:J:53:HIS:ND1	2.20	0.56
9:I:111:THR:HG22	9:I:113:ASP:H	1.69	0.56
2:B:33:VAL:HG21	2:B:638:PHE:HZ	1.70	0.56
2:B:652:LYS:HB3	2:B:689:LEU:HD23	1.88	0.56
2:B:1183:LYS:HE3	2:B:1183:LYS:O	2.06	0.56
1:A:1092:LYS:O	1:A:1094:VAL:HG23	2.06	0.56
4:D:148:LEU:O	4:D:152:SER:OG	2.22	0.56
4:D:8:PHE:HD2	7:G:6:ASP:O	1.88	0.56
3:C:33:LEU:HG	3:C:37:MET:CE	2.36	0.56
1:A:68:GLN:O	1:A:68:GLN:OE1	2.23	0.56
9:I:111:THR:CG2	9:I:112:SER:H	2.12	0.56
1:A:21:LEU:CD1	1:A:1414:ALA:HA	2.36	0.56
2:B:497:ARG:NH2	2:B:775:LYS:HZ3	2.04	0.56
1:A:11:LEU:HB2	2:B:1193:GLN:HG2	1.88	0.56
2:B:22:SER:O	2:B:654:ARG:HD2	2.06	0.56
2:B:657:HIS:CE1	2:B:689:LEU:HD11	2.41	0.56
1:A:2:VAL:HG22	1:A:3:GLY:N	2.21	0.56
11:K:23:PRO:HA	11:K:31:VAL:HG13	1.88	0.56
1:A:399:HIS:O	1:A:400:PRO:C	2.44	0.56
2:B:766:ARG:HH12	2:B:1020:ARG:HD2	1.66	0.56
4:D:153:ARG:C	4:D:154:PHE:CD2	2.79	0.56
3:C:236:GLY:O	3:C:237:SER:C	2.44	0.56
2:B:39:ARG:CZ	2:B:665:GLU:HG2	2.36	0.56
1:A:1155:ASP:OD2	1:A:1161:THR:HA	2.06	0.56
1:A:830:LYS:HE3	1:A:1081:LEU:HD12	1.88	0.56
2:B:405:ARG:NE	2:B:632:ARG:HG2	2.21	0.56
7:G:153:GLN:HG3	7:G:154:VAL:HG23	1.87	0.56
3:C:93:ASP:OD1	3:C:122:SER:HB2	2.05	0.56
8:H:4:THR:HG22	8:H:5:LEU:H	1.72	0.55
1:A:1313:LEU:O	1:A:1315:GLU:N	2.38	0.55
11:K:107:THR:O	11:K:111:LEU:HG	2.05	0.55
2:B:1202:LEU:HD22	2:B:1206:GLU:CD	2.26	0.55
1:A:981:LEU:CD2	1:A:1039:LYS:HA	2.36	0.55
1:A:1229:SER:HB2	1:A:1233:ASP:OD2	2.06	0.55
4:D:138:ASN:HB3	4:D:141:LEU:HB3	1.86	0.55
1:A:1029:ARG:HG3	1:A:1029:ARG:HH11	1.71	0.55
1:A:540:PHE:HZ	8:H:121:LEU:HD11	1.71	0.55
2:B:745:PRO:C	2:B:747:MET:N	2.60	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:430:ARG:HB3	2:B:430:ARG:NH1	2.09	0.55
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.41	0.55
2:B:363:HIS:O	2:B:364:ILE:CB	2.54	0.55
1:A:738:LYS:H	1:A:738:LYS:CD	2.09	0.55
1:A:108:MET:O	1:A:109:HIS:CB	2.52	0.55
3:C:258:ILE:N	3:C:258:ILE:HD12	2.22	0.55
2:B:278:GLN:CG	2:B:279:ASP:N	2.68	0.55
2:B:1182:CYS:SG	2:B:1185:CYS:HB2	2.46	0.55
5:E:213:ILE:HG12	5:E:214:CYS:N	2.20	0.55
1:A:472:LEU:HD11	2:B:835:GLN:NE2	2.21	0.55
2:B:696:GLU:O	2:B:699:GLU:HB2	2.06	0.55
2:B:186:GLU:CG	10:J:62:ARG:HH22	2.18	0.55
2:B:891:ASP:C	2:B:893:LEU:H	2.09	0.55
8:H:91:ASP:O	8:H:93:TYR:N	2.36	0.55
2:B:759:PRO:C	2:B:761:HIS:H	2.10	0.55
2:B:615:MET:HB3	2:B:626:ILE:HG12	1.89	0.55
1:A:1322:ILE:O	1:A:1324:PRO:HD3	2.07	0.55
4:D:119:ARG:HD3	4:D:221:TYR:CD2	2.41	0.55
2:B:172:ILE:HD13	2:B:178:ASN:ND2	2.21	0.55
2:B:29:ASP:OD1	2:B:658:ILE:HG21	2.05	0.55
5:E:22:MET:CE	5:E:26:ARG:NH2	2.70	0.55
1:A:335:ARG:HD3	1:A:339:ASN:ND2	2.22	0.55
2:B:50:SER:OG	2:B:411:PRO:HD3	2.07	0.55
5:E:89:GLY:C	5:E:91:LYS:H	2.08	0.55
1:A:883:LEU:HD11	1:A:1017:LEU:HD11	1.89	0.55
1:A:316:GLN:NE2	1:A:317:LYS:HD2	2.19	0.55
2:B:1020:ARG:HG2	2:B:1020:ARG:NH1	2.14	0.55
2:B:126:SER:HG	2:B:172:ILE:HD11	1.69	0.55
1:A:1241:ARG:O	1:A:1242:VAL:HB	2.06	0.55
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.71	0.55
3:C:186:LEU:CD2	3:C:225:ALA:HB2	2.37	0.55
4:D:4:SER:O	4:D:5:THR:CB	2.54	0.55
2:B:616:ILE:N	2:B:616:ILE:HD12	2.21	0.55
1:A:557:ASP:OD2	1:A:559:VAL:HB	2.06	0.55
1:A:40:THR:HB	1:A:41:MET:CE	2.37	0.55
3:C:69:LEU:HB3	10:J:6:ARG:HD3	1.88	0.55
2:B:294:ASP:C	2:B:296:GLU:H	2.07	0.55
2:B:222:ILE:N	2:B:240:ILE:CD1	2.70	0.55
2:B:778:MET:HE2	2:B:1094:ARG:O	2.07	0.55
1:A:442:VAL:CG2	1:A:489:LEU:HD11	2.37	0.55
2:B:378:LEU:O	2:B:378:LEU:HD12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:ILE:HD11	2:B:1067:ARG:O	2.07	0.55
12:L:30:ILE:HG22	12:L:31:CYS:H	1.71	0.55
2:B:408:LEU:O	2:B:411:PRO:HD2	2.05	0.55
2:B:785:TYR:CD1	2:B:786:ASN:N	2.74	0.55
9:I:55:THR:HG22	9:I:58:VAL:CG2	2.36	0.55
8:H:128:ASN:ND2	8:H:131:ASN:OD1	2.39	0.55
2:B:773:MET:CE	2:B:985:GLY:HA2	2.36	0.55
2:B:1124:ARG:HB3	2:B:1124:ARG:CZ	2.37	0.55
1:A:547:LEU:HD22	11:K:58:PHE:CE1	2.42	0.55
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.89	0.55
6:F:103:MET:CE	7:G:66:GLY:H	2.19	0.55
2:B:315:LYS:N	2:B:316:PRO:HD2	2.21	0.55
12:L:38:LEU:O	12:L:39:SER:HB3	2.07	0.55
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.37	0.55
1:A:1199:ARG:HG2	1:A:1236:LEU:HD11	1.89	0.55
1:A:87:ALA:CB	1:A:276:LEU:HD23	2.36	0.55
1:A:756:ILE:O	1:A:759:ALA:HB3	2.06	0.55
1:A:69:THR:HB	2:B:1174:LYS:HE2	1.89	0.55
7:G:13:LEU:HD21	7:G:17:PHE:HB2	1.89	0.55
5:E:124:VAL:N	5:E:125:PRO:HD2	2.22	0.55
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.87	0.55
3:C:100:THR:HG21	3:C:102:GLN:HE21	1.71	0.55
9:I:101:PHE:N	9:I:101:PHE:CD1	2.72	0.55
1:A:402:ALA:CB	1:A:434:ARG:HA	2.37	0.55
2:B:311:LEU:O	2:B:314:LEU:N	2.35	0.55
1:A:717:ASN:HA	1:A:720:ARG:NH2	2.23	0.55
2:B:744:HIS:HD2	2:B:745:PRO:CD	2.02	0.54
10:J:36:LEU:HB2	10:J:47:ARG:HH12	1.72	0.54
6:F:119:ARG:CG	6:F:119:ARG:NH1	2.65	0.54
1:A:1437:GLY:O	1:A:1439:GLY:N	2.40	0.54
3:C:91:HIS:C	3:C:91:HIS:CD2	2.80	0.54
6:F:94:LEU:HD21	6:F:122:MET:HA	1.89	0.54
1:A:518:LYS:HE2	1:A:624:SER:O	2.06	0.54
2:B:326:ASP:OD2	2:B:328:GLU:HB3	2.07	0.54
2:B:555:ILE:O	2:B:558:LEU:HB2	2.06	0.54
2:B:554:ILE:O	2:B:558:LEU:HG	2.08	0.54
1:A:65:LEU:O	1:A:66:LYS:O	2.25	0.54
8:H:40:LEU:HD13	8:H:123:MET:HE2	1.90	0.54
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.89	0.54
6:F:86:THR:OG1	6:F:89:GLU:HG3	2.06	0.54
2:B:637:LEU:CB	2:B:693:ILE:HD11	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.91	0.54
1:A:664:THR:HG22	2:B:1014:PRO:HB3	1.89	0.54
1:A:1339:LEU:HD13	5:E:147:HIS:CD2	2.42	0.54
2:B:165:VAL:HG11	2:B:448:ILE:HD13	1.89	0.54
1:A:596:THR:C	1:A:597:LEU:HD12	2.27	0.54
8:H:38:LEU:HD12	8:H:39:THR:H	1.71	0.54
1:A:1428:VAL:HG13	2:B:1151:LEU:CD2	2.33	0.54
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.88	0.54
2:B:39:ARG:NH2	2:B:665:GLU:CG	2.67	0.54
15:3:2:A:O2'	15:3:3:A:O5'	2.18	0.54
11:K:61:TYR:C	11:K:61:TYR:CD2	2.81	0.54
1:A:500:GLU:O	1:A:504:LEU:HB2	2.07	0.54
5:E:154:ILE:HG22	5:E:155:ARG:O	2.08	0.54
2:B:899:ILE:HG22	2:B:900:ALA:N	2.21	0.54
9:I:93:LYS:HD3	9:I:93:LYS:N	2.22	0.54
1:A:35:ILE:CD1	1:A:241:VAL:HG11	2.37	0.54
8:H:89:LEU:O	8:H:91:ASP:N	2.41	0.54
4:D:7:THR:HG23	4:D:7:THR:O	2.06	0.54
2:B:303:TYR:N	2:B:303:TYR:CD2	2.74	0.54
1:A:1048:ASN:O	1:A:1049:ILE:C	2.44	0.54
10:J:7:CYS:SG	10:J:49:MET:HE3	2.47	0.54
1:A:1158:PRO:HG2	1:A:1159:ARG:HD2	1.89	0.54
2:B:467:GLY:CA	2:B:475:SER:HB3	2.38	0.54
2:B:55:VAL:HG13	2:B:97:VAL:HG21	1.89	0.54
2:B:710:LEU:O	2:B:711:GLU:HG2	2.06	0.54
2:B:95:ILE:CG1	2:B:130:VAL:HG22	2.38	0.54
2:B:519:TRP:C	2:B:519:TRP:CD1	2.80	0.54
1:A:106:VAL:HG12	1:A:107:CYS:H	1.73	0.54
2:B:25:ILE:HD13	2:B:653:VAL:HG12	1.89	0.54
1:A:250:ILE:CG2	1:A:250:ILE:O	2.52	0.54
1:A:87:ALA:HB1	1:A:276:LEU:HD23	1.87	0.54
7:G:111:THR:CG2	7:G:114:LEU:HB2	2.38	0.54
1:A:730:GLY:O	1:A:732:LEU:N	2.41	0.54
4:D:207:LEU:O	4:D:207:LEU:HD12	2.07	0.54
12:L:46:VAL:HG12	12:L:46:VAL:O	2.08	0.54
4:D:14:ARG:HH12	4:D:16:LYS:CD	2.20	0.54
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.21	0.54
3:C:8:VAL:HG12	3:C:9:LYS:N	2.22	0.54
5:E:82:PHE:O	5:E:83:CYS:HB2	2.08	0.54
2:B:827:ILE:HD12	2:B:1086:PHE:CD2	2.42	0.54
2:B:847:ASP:HB3	3:C:167:HIS:CD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ILE:HG22	1:A:425:GLN:H	1.71	0.54
9:I:78:CYS:SG	9:I:105:SER:O	2.66	0.54
1:A:1237:ILE:HG22	1:A:1238:ILE:N	2.22	0.54
4:D:35:LEU:H	4:D:35:LEU:HD12	1.73	0.54
2:B:57:TYR:N	2:B:57:TYR:HD1	2.06	0.54
1:A:898:ARG:O	1:A:1029:ARG:NH1	2.40	0.54
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.23	0.54
1:A:705:LYS:HD2	1:A:708:MET:HE3	1.88	0.54
3:C:209:TYR:H	3:C:209:TYR:HD1	1.55	0.54
1:A:567:LYS:CG	1:A:568:PRO:CD	2.81	0.54
1:A:567:LYS:CD	8:H:95:TYR:HA	2.38	0.54
2:B:526:GLU:OE1	2:B:752:ALA:HB3	2.08	0.54
2:B:110:HIS:HB3	12:L:54:ARG:HH22	1.71	0.54
2:B:916:THR:HB	2:B:935:ARG:CD	2.38	0.54
4:D:52:LEU:O	4:D:54:GLU:N	2.40	0.54
7:G:120:THR:OG1	7:G:121:PHE:N	2.38	0.54
8:H:12:VAL:HA	8:H:28:ALA:HB2	1.88	0.54
4:D:145:MET:O	4:D:149:THR:HB	2.08	0.54
2:B:582:VAL:O	2:B:582:VAL:HG12	2.08	0.54
3:C:226:ASP:O	3:C:227:THR:HB	2.08	0.54
1:A:471:ASN:O	1:A:474:VAL:HG12	2.08	0.54
1:A:858:ASN:HD21	1:A:860:LEU:HB2	1.71	0.54
2:B:423:LYS:O	2:B:427:ASP:HB2	2.08	0.54
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.43	0.54
3:C:22:LEU:HD22	3:C:230:MET:HE3	1.90	0.54
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.43	0.54
1:A:535:THR:HG21	1:A:617:VAL:H	1.73	0.54
7:G:146:LYS:HB2	7:G:168:LEU:HD11	1.90	0.54
1:A:1046:LEU:N	1:A:1046:LEU:HD23	2.23	0.54
10:J:27:GLU:C	10:J:29:GLU:H	2.12	0.54
9:I:71:SER:OG	9:I:83:ASN:HB2	2.08	0.54
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.89	0.53
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.43	0.53
1:A:879:GLU:OE1	1:A:962:ARG:NH2	2.40	0.53
1:A:623:GLY:C	1:A:625:SER:H	2.12	0.53
2:B:871:THR:HG22	2:B:872:GLU:N	2.23	0.53
8:H:94:ASP:O	8:H:95:TYR:HB2	2.09	0.53
2:B:859:TYR:OH	2:B:941:LEU:HD12	2.08	0.53
1:A:49:LYS:HZ1	1:A:61:ILE:HG13	1.73	0.53
9:I:68:LEU:HB3	9:I:84:VAL:HG23	1.91	0.53
12:L:40:LEU:HD13	12:L:44:ASP:CB	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1366:ARG:HG2	1:A:1366:ARG:HH11	1.72	0.53
11:K:45:LEU:HG	11:K:94:ILE:CD1	2.36	0.53
2:B:193:LYS:HZ3	12:L:32:ALA:HB1	1.72	0.53
1:A:102:VAL:HB	1:A:211:PHE:CZ	2.43	0.53
1:A:95:PHE:O	1:A:98:LYS:N	2.39	0.53
11:K:42:LEU:HD11	11:K:46:ILE:HD11	1.91	0.53
3:C:114:TYR:CD2	3:C:140:ASN:CB	2.91	0.53
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.43	0.53
1:A:946:VAL:HG22	5:E:201:LYS:HB3	1.90	0.53
3:C:235:VAL:HG13	10:J:13:VAL:HG22	1.90	0.53
2:B:282:ILE:HG21	2:B:382:ILE:CD1	2.38	0.53
1:A:447:GLN:NE2	14:1:20:DG:H4'	2.23	0.53
2:B:505:ASP:OD2	13:2:1:DA:H5''	2.09	0.53
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.91	0.53
1:A:90:VAL:CG1	1:A:297:GLN:HA	2.38	0.53
5:E:143:ASN:HD22	5:E:146:HIS:CE1	2.26	0.53
2:B:509:ALA:O	2:B:510:LYS:C	2.47	0.53
1:A:1104:ILE:O	1:A:1106:ASN:N	2.41	0.53
3:C:66:ARG:HA	3:C:69:LEU:CD1	2.38	0.53
1:A:444:PHE:CE2	1:A:487:MET:HE1	2.43	0.53
2:B:837:ASP:OD2	2:B:1020:ARG:NH2	2.40	0.53
12:L:49:LYS:O	12:L:50:ASP:CB	2.54	0.53
12:L:55:ILE:HG12	12:L:56:LEU:N	2.22	0.53
2:B:110:HIS:CB	12:L:54:ARG:HH22	2.22	0.53
2:B:906:SER:O	2:B:907:GLY:C	2.46	0.53
1:A:973:ILE:HD13	1:A:1037:LEU:HA	1.91	0.53
10:J:53:HIS:NE2	10:J:55:ASP:HA	2.23	0.53
4:D:154:PHE:HB3	4:D:159:THR:OG1	2.07	0.53
2:B:654:ARG:HH11	2:B:654:ARG:CG	2.19	0.53
1:A:90:VAL:HG11	1:A:297:GLN:HA	1.91	0.53
2:B:661:LEU:HD23	2:B:679:TYR:O	2.08	0.53
1:A:1006:ILE:HD12	5:E:163:GLU:HG3	1.90	0.53
1:A:322:VAL:HG12	1:A:322:VAL:O	2.06	0.53
5:E:17:ARG:O	5:E:20:LYS:HB2	2.08	0.53
2:B:805:THR:CG2	2:B:806:THR:H	2.14	0.53
1:A:1278:ASN:O	1:A:1310:GLY:HA3	2.08	0.53
3:C:18:VAL:O	3:C:18:VAL:HG12	2.09	0.53
1:A:714:PHE:O	1:A:718:VAL:HG23	2.09	0.53
5:E:180:ARG:O	5:E:186:LEU:HD21	2.09	0.53
2:B:287:ARG:HG3	2:B:292:ILE:HA	1.91	0.53
1:A:874:ASP:N	1:A:1058:VAL:HG23	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:973:ILE:HD11	1:A:1041:ALA:HB2	1.91	0.53
2:B:570:VAL:CG2	2:B:573:GLN:HB3	2.38	0.53
1:A:71:GLN:O	1:A:73:GLY:N	2.36	0.53
8:H:123:MET:HE3	8:H:142:LEU:HD21	1.90	0.53
2:B:842:ASN:HD22	2:B:845:SER:CB	2.21	0.53
2:B:333:PHE:O	2:B:334:ILE:CG1	2.56	0.53
2:B:893:LEU:HD22	2:B:897:GLY:HA2	1.91	0.53
11:K:50:LEU:HD11	11:K:75:ILE:CD1	2.38	0.53
1:A:50:ILE:C	1:A:52:GLY:N	2.62	0.53
11:K:107:THR:CG2	11:K:108:GLU:N	2.66	0.53
1:A:332:LYS:HG2	1:A:333:GLU:HG2	1.91	0.53
1:A:720:ARG:O	1:A:724:GLU:HB2	2.09	0.53
1:A:364:VAL:HG13	1:A:364:VAL:O	2.08	0.53
8:H:27:GLU:HA	8:H:38:LEU:O	2.09	0.53
10:J:2:ILE:C	10:J:53:HIS:HE1	2.12	0.53
1:A:517:ASN:ND2	1:A:1364:ASN:HB2	2.24	0.53
2:B:377:PHE:O	2:B:380:TYR:N	2.42	0.53
1:A:367:PRO:HG2	1:A:370:ILE:HD12	1.89	0.53
2:B:603:LEU:CD1	2:B:608:ASP:HB2	2.36	0.53
1:A:1313:LEU:HD23	1:A:1338:VAL:CG2	2.38	0.53
3:C:67:LEU:HD11	3:C:155:LEU:HD13	1.89	0.53
1:A:117:GLU:HA	1:A:123:ARG:HG3	1.90	0.53
1:A:134:ARG:HG2	1:A:138:ILE:CD1	2.39	0.53
4:D:53:SER:HA	4:D:56:ARG:HB3	1.91	0.53
11:K:53:ASP:OD1	11:K:55:LYS:HB2	2.09	0.53
2:B:515:HIS:O	2:B:518:HIS:HB2	2.08	0.53
1:A:696:GLU:HG2	1:A:696:GLU:O	2.09	0.53
2:B:458:LYS:O	2:B:459:TYR:C	2.46	0.53
2:B:622:LYS:CE	9:I:59:VAL:HG22	2.13	0.53
4:D:15:LEU:O	4:D:15:LEU:HD12	2.09	0.53
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.39	0.53
3:C:179:GLU:HG2	3:C:180:TYR:N	2.24	0.53
2:B:64:CYS:HA	2:B:67:SER:HG	1.74	0.53
5:E:212:ARG:HH11	5:E:212:ARG:HG3	1.73	0.52
1:A:1081:LEU:HD11	1:A:1098:VAL:HG23	1.90	0.52
1:A:1094:VAL:HG13	1:A:1113:THR:HG21	1.91	0.52
7:G:90:THR:HG22	7:G:91:VAL:N	2.23	0.52
1:A:829:VAL:HG22	2:B:507:LYS:HD2	1.91	0.52
7:G:61:ILE:HG22	7:G:62:LEU:O	2.09	0.52
1:A:567:LYS:HB2	8:H:95:TYR:HA	1.90	0.52
9:I:50:THR:CG2	9:I:51:ASN:H	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:LEU:N	1:A:926:GLN:NE2	2.46	0.52
5:E:56:LYS:HZ3	5:E:84:ASP:H	1.57	0.52
7:G:34:VAL:HG13	7:G:45:ILE:HG21	1.92	0.52
1:A:481:ASP:CG	15:3:11:U:H5"	2.30	0.52
2:B:26:THR:O	2:B:29:ASP:HB2	2.09	0.52
1:A:95:PHE:O	1:A:96:ILE:C	2.46	0.52
11:K:12:LEU:HD11	11:K:18:LYS:HE2	1.91	0.52
5:E:68:SER:HB3	5:E:75:MET:CE	2.39	0.52
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.29	0.52
1:A:2:VAL:HG22	1:A:3:GLY:H	1.74	0.52
1:A:144:THR:O	1:A:146:MET:HG3	2.07	0.52
2:B:298:LEU:HD22	2:B:298:LEU:N	2.23	0.52
5:E:35:VAL:C	5:E:37:LEU:H	2.11	0.52
2:B:879:ARG:N	2:B:879:ARG:CD	2.61	0.52
2:B:427:ASP:CA	2:B:430:ARG:HG3	2.37	0.52
7:G:115:MET:O	7:G:164:LYS:HD3	2.09	0.52
2:B:233:PRO:CD	14:1:11:DA:OP1	2.57	0.52
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.90	0.52
2:B:830:TYR:O	2:B:831:SER:C	2.45	0.52
2:B:1034:VAL:O	2:B:1036:ALA:N	2.42	0.52
1:A:1081:LEU:HD11	1:A:1098:VAL:H	1.73	0.52
2:B:521:LEU:HB3	2:B:633:VAL:CG1	2.39	0.52
1:A:1264:GLU:OE2	9:I:46:HIS:HD2	1.92	0.52
2:B:969:ARG:CD	3:C:61:GLU:OE2	2.58	0.52
1:A:41:MET:O	1:A:42:ASP:O	2.27	0.52
1:A:108:MET:H	1:A:171:GLN:HE22	1.58	0.52
1:A:385:ILE:HG22	1:A:386:ASP:N	2.24	0.52
2:B:862:GLN:HG2	2:B:963:PHE:CD1	2.34	0.52
2:B:222:ILE:H	2:B:240:ILE:HD12	1.74	0.52
2:B:778:MET:HE1	2:B:1094:ARG:HD3	1.91	0.52
2:B:235:SER:C	2:B:236:HIS:HD2	2.12	0.52
1:A:663:SER:OG	1:A:664:THR:N	2.41	0.52
1:A:783:THR:HG21	1:A:815:PHE:CZ	2.45	0.52
2:B:860:MET:HG2	2:B:861:ASP:H	1.74	0.52
2:B:259:TYR:H	2:B:259:TYR:HD1	1.58	0.52
2:B:619:ILE:O	2:B:622:LYS:N	2.41	0.52
2:B:376:PHE:CE2	2:B:569:TYR:HD2	2.28	0.52
12:L:30:ILE:CG2	12:L:31:CYS:N	2.72	0.52
1:A:1203:ASN:O	1:A:1204:ASP:C	2.47	0.52
2:B:560:GLU:O	2:B:561:TRP:CD1	2.62	0.52
4:D:192:LYS:HD2	4:D:199:ASN:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:25:VAL:HG12	3:C:26:ASP:H	1.74	0.52
1:A:1402:PHE:CE2	1:A:1403:GLU:HG3	2.45	0.52
2:B:620:ARG:NH2	9:I:68:LEU:HD21	2.25	0.52
2:B:603:LEU:HB3	2:B:609:ILE:HD11	1.91	0.52
1:A:889:SER:CB	1:A:1297:GLU:HG3	2.38	0.52
2:B:39:ARG:HG2	2:B:39:ARG:HH11	1.74	0.52
1:A:1438:THR:HB	2:B:1144:ALA:HB3	1.92	0.52
1:A:886:ILE:CG2	1:A:887:GLY:N	2.73	0.52
1:A:954:TRP:HB3	1:A:955:PRO:HD2	1.90	0.52
8:H:43:ASN:OD1	8:H:45:GLU:HB3	2.10	0.52
4:D:120:GLU:O	4:D:120:GLU:HG2	2.10	0.52
1:A:1444:MET:HG2	7:G:59:GLY:O	2.10	0.52
4:D:17:LYS:HD2	4:D:17:LYS:C	2.29	0.52
2:B:578:THR:C	2:B:589:VAL:HG13	2.29	0.52
4:D:219:THR:HG22	4:D:220:LEU:O	2.10	0.52
1:A:168:GLY:O	1:A:169:ASN:C	2.48	0.52
1:A:335:ARG:HH12	2:B:1206:GLU:CD	2.13	0.52
3:C:208:GLU:C	3:C:210:GLU:H	2.11	0.52
1:A:1161:THR:C	1:A:1163:ILE:N	2.63	0.52
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.10	0.52
1:A:512:VAL:HG12	1:A:512:VAL:O	2.08	0.52
1:A:677:ARG:HA	1:A:680:THR:OG1	2.10	0.52
1:A:1308:THR:HG23	1:A:1310:GLY:H	1.74	0.52
10:J:3:VAL:HA	10:J:53:HIS:HD1	1.73	0.52
11:K:50:LEU:HD11	11:K:75:ILE:HD13	1.92	0.52
1:A:722:LEU:HD23	1:A:799:PHE:CG	2.44	0.52
1:A:509:LEU:O	1:A:511:ILE:N	2.43	0.52
2:B:990:ILE:HG22	2:B:991:GLY:N	2.25	0.52
5:E:182:ASP:O	5:E:185:ALA:HB3	2.10	0.52
2:B:505:ASP:CG	13:2:1:DA:C8	2.82	0.52
12:L:42:ARG:NH1	12:L:42:ARG:HG3	2.25	0.52
1:A:434:ARG:NH2	1:A:440:ASP:OD1	2.42	0.52
1:A:1215:ARG:NH1	1:A:1272:THR:O	2.43	0.52
1:A:751:SER:O	1:A:752:LYS:HG2	2.09	0.52
1:A:399:HIS:CG	1:A:400:PRO:N	2.77	0.52
1:A:353:ILE:HD12	1:A:487:MET:HE3	1.90	0.52
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.93	0.52
12:L:32:ALA:HB3	12:L:55:ILE:HG13	1.88	0.52
1:A:665:GLY:HA2	2:B:1026:LEU:HD21	1.92	0.52
1:A:962:ARG:O	1:A:965:GLN:N	2.43	0.52
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:155:ARG:NH1	5:E:194:GLU:OE2	2.43	0.52
11:K:52:ASN:O	11:K:54:ARG:N	2.42	0.52
9:I:34:TYR:CE2	9:I:36:GLU:HB3	2.41	0.52
2:B:357:GLN:HA	2:B:374:LYS:NZ	2.25	0.52
2:B:842:ASN:ND2	2:B:845:SER:N	2.53	0.52
3:C:242:GLN:C	3:C:244:VAL:N	2.63	0.52
10:J:14:VAL:HG12	10:J:14:VAL:O	2.08	0.52
8:H:100:THR:HG23	8:H:138:GLU:HA	1.92	0.52
1:A:1209:MET:SD	1:A:1236:LEU:HB3	2.50	0.52
5:E:21:GLU:O	5:E:24:LYS:HG2	2.10	0.52
2:B:68:THR:CG2	2:B:91:SER:HB3	2.39	0.52
9:I:93:LYS:H	9:I:93:LYS:CD	2.23	0.52
4:D:73:SER:CB	7:G:21:ARG:HH21	2.23	0.52
2:B:461:LEU:HD12	2:B:461:LEU:H	1.75	0.52
2:B:203:PHE:N	2:B:203:PHE:CD1	2.77	0.52
2:B:916:THR:CG2	2:B:935:ARG:HD2	2.40	0.51
3:C:221:TYR:CD1	3:C:222:LYS:N	2.78	0.51
8:H:59:ILE:CG2	8:H:60:ALA:N	2.73	0.51
2:B:847:ASP:OD2	11:K:6:ARG:NH2	2.41	0.51
8:H:83:GLN:C	8:H:85:GLY:H	2.14	0.51
1:A:107:CYS:HA	1:A:171:GLN:HE22	1.74	0.51
2:B:233:PRO:HD2	14:1:11:DA:OP1	2.10	0.51
1:A:868:TYR:HE1	1:A:1064:VAL:CG1	2.23	0.51
7:G:111:THR:HG23	7:G:114:LEU:HB2	1.91	0.51
13:2:2:DC:H2"	13:2:3:DT:H71	1.91	0.51
9:I:88:SER:C	9:I:90:GLN:H	2.12	0.51
2:B:879:ARG:HH22	2:B:885:MET:CE	2.23	0.51
2:B:509:ALA:O	2:B:511:PRO:N	2.44	0.51
1:A:666:ILE:HD12	1:A:667:GLY:H	1.73	0.51
6:F:111:LEU:CD1	6:F:111:LEU:N	2.73	0.51
1:A:1095:THR:CG2	1:A:1112:LYS:HB2	2.40	0.51
1:A:1385:THR:O	1:A:1387:HIS:N	2.43	0.51
2:B:134:LYS:HD3	2:B:134:LYS:H	1.74	0.51
3:C:176:ILE:HG22	3:C:176:ILE:O	2.09	0.51
2:B:308:TRP:CH2	9:I:45:ARG:HG2	2.45	0.51
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.43	0.51
1:A:1293:SER:HB3	1:A:1297:GLU:OE1	2.10	0.51
5:E:177:ARG:O	5:E:212:ARG:HD3	2.10	0.51
1:A:831:THR:O	1:A:834:THR:HG22	2.09	0.51
3:C:91:HIS:O	3:C:91:HIS:CD2	2.62	0.51
1:A:744:LYS:HG2	1:A:748:MET:HE1	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:48:ARG:HE	10:J:49:MET:HE2	1.75	0.51
2:B:481:GLN:NE2	15:3:7:G:H4'	2.25	0.51
6:F:76:LYS:O	6:F:79:ARG:HD3	2.10	0.51
1:A:685:GLU:HG3	1:A:686:ALA:H	1.74	0.51
3:C:66:ARG:O	3:C:69:LEU:HD12	2.10	0.51
10:J:2:ILE:C	10:J:53:HIS:CE1	2.84	0.51
1:A:93:VAL:HG21	1:A:301:ALA:HA	1.90	0.51
2:B:327:ARG:HH22	2:B:371:GLU:HG2	1.76	0.51
9:I:61:ASP:O	9:I:63:GLY:N	2.43	0.51
11:K:55:LYS:HB2	11:K:81:TYR:CE1	2.45	0.51
1:A:648:ASN:O	1:A:649:ILE:C	2.49	0.51
1:A:555:ASP:O	1:A:556:TRP:O	2.28	0.51
1:A:806:ARG:HH22	2:B:729:ILE:HD11	1.75	0.51
1:A:670:ILE:HG23	1:A:805:LEU:HD21	1.92	0.51
7:G:87:VAL:CG2	7:G:103:VAL:HG21	2.40	0.51
10:J:53:HIS:C	10:J:53:HIS:HD2	2.12	0.51
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.40	0.51
1:A:503:GLN:NE2	6:F:90:ARG:HH21	2.09	0.51
2:B:469:GLN:CG	2:B:470:LYS:H	2.21	0.51
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.44	0.51
5:E:192:ARG:HH11	5:E:192:ARG:HG3	1.76	0.51
1:A:523:ILE:HG13	1:A:622:VAL:CG2	2.38	0.51
1:A:1148:ILE:CG1	1:A:1198:ASP:HB2	2.40	0.51
2:B:31:TRP:CD1	2:B:807:ARG:NH2	2.78	0.51
1:A:341:MET:HE1	2:B:1135:ARG:NH1	2.26	0.51
6:F:138:LEU:O	6:F:140:ASP:N	2.44	0.51
2:B:885:MET:HA	2:B:936:ASP:CB	2.41	0.51
1:A:598:LEU:HA	8:H:122:LEU:HD13	1.91	0.51
1:A:16:GLU:OE1	4:D:13:ARG:NH2	2.42	0.51
2:B:377:PHE:C	2:B:379:GLY:N	2.64	0.51
2:B:638:PHE:O	2:B:740:HIS:HA	2.11	0.51
2:B:773:MET:C	2:B:775:LYS:N	2.63	0.51
2:B:773:MET:HE1	2:B:985:GLY:HA2	1.93	0.51
1:A:115:LEU:CD1	1:A:142:CYS:HB3	2.40	0.51
7:G:115:MET:HB3	7:G:116:PRO:CD	2.40	0.51
3:C:35:ARG:NH1	11:K:41:THR:OG1	2.44	0.51
13:2:4:DA:H2"	13:2:5:DC:C6	2.45	0.51
7:G:111:THR:O	7:G:114:LEU:N	2.39	0.51
1:A:695:LYS:C	1:A:697:ALA:H	2.14	0.51
2:B:251:ILE:O	2:B:251:ILE:HG22	2.11	0.51
2:B:879:ARG:HH22	2:B:885:MET:HE2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:55:THR:O	9:I:55:THR:HG22	2.09	0.51
10:J:53:HIS:HD2	10:J:54:VAL:C	2.14	0.51
1:A:983:ILE:O	1:A:983:ILE:HG23	2.11	0.51
1:A:1127:ASP:CG	1:A:1130:GLN:HB2	2.29	0.51
2:B:526:GLU:HG3	2:B:771:SER:HB3	1.92	0.51
2:B:641:GLU:C	2:B:643:ASP:H	2.13	0.51
1:A:276:LEU:HD13	1:A:293:GLU:HA	1.92	0.51
2:B:90:ILE:CD1	2:B:432:MET:SD	2.98	0.51
1:A:984:LYS:HG2	1:A:988:LEU:HD12	1.91	0.51
1:A:886:ILE:HG23	1:A:887:GLY:N	2.25	0.51
1:A:665:GLY:HA2	2:B:1026:LEU:HD22	1.93	0.51
3:C:7:GLN:HE21	11:K:104:ASN:ND2	2.09	0.51
1:A:537:ARG:NH1	8:H:120:GLY:O	2.44	0.51
12:L:36:SER:O	12:L:37:LYS:C	2.49	0.51
1:A:470:LEU:CD2	1:A:470:LEU:N	2.74	0.51
7:G:129:SER:CB	7:G:138:THR:HG1	2.24	0.51
1:A:690:VAL:HG13	1:A:691:LEU:N	2.25	0.51
1:A:433:GLU:OE1	2:B:1108:ARG:NH2	2.42	0.51
2:B:230:ALA:HB3	2:B:231:PRO:HD3	1.93	0.51
9:I:74:GLU:HB3	9:I:81:ARG:HD2	1.92	0.51
2:B:305:VAL:HG12	2:B:305:VAL:O	2.10	0.51
9:I:17:ARG:HG3	9:I:28:GLU:CD	2.31	0.51
2:B:996:ARG:HH22	3:C:175:ALA:H	1.59	0.51
1:A:356:ASP:O	1:A:358:ASN:N	2.43	0.51
3:C:242:GLN:CA	3:C:245:VAL:HG23	2.37	0.51
2:B:90:ILE:HD12	2:B:432:MET:CE	2.41	0.51
7:G:91:VAL:CG1	7:G:92:VAL:N	2.74	0.51
1:A:1006:ILE:CD1	5:E:163:GLU:HG3	2.41	0.51
2:B:593:PRO:HG2	2:B:617:ARG:CZ	2.41	0.51
10:J:51:LEU:HD12	10:J:51:LEU:O	2.11	0.51
2:B:1056:SER:HB3	2:B:1066:SER:OG	2.10	0.51
3:C:69:LEU:HB3	10:J:6:ARG:CD	2.41	0.50
10:J:53:HIS:CD2	10:J:55:ASP:N	2.79	0.50
2:B:750:GLY:O	2:B:751:VAL:C	2.49	0.50
8:H:26:ILE:HD11	8:H:49:VAL:CG1	2.38	0.50
3:C:213:PRO:O	3:C:214:ASN:HB3	2.11	0.50
2:B:642:ASP:CA	2:B:649:LYS:HA	2.41	0.50
2:B:235:SER:C	2:B:236:HIS:CD2	2.84	0.50
2:B:402:GLY:HA2	2:B:695:ALA:HB3	1.93	0.50
4:D:155:ARG:HH11	4:D:155:ARG:CB	2.23	0.50
1:A:858:ASN:ND2	1:A:860:LEU:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:GLN:O	1:A:428:TYR:C	2.50	0.50
1:A:443:LEU:CD1	2:B:1146:PHE:CE2	2.93	0.50
4:D:5:THR:O	4:D:5:THR:HG23	2.11	0.50
1:A:533:LYS:CE	1:A:745:GLN:HE22	2.24	0.50
5:E:157:SER:O	5:E:159:ASP:N	2.44	0.50
8:H:95:TYR:HE2	8:H:97:MET:CG	2.19	0.50
2:B:196:PRO:HG2	2:B:197:PHE:H	1.76	0.50
1:A:1329:THR:HG22	1:A:1331:SER:N	2.21	0.50
7:G:144:ARG:O	7:G:168:LEU:HD23	2.12	0.50
2:B:408:LEU:HD21	2:B:545:ILE:HD12	1.93	0.50
1:A:836:TYR:CD2	1:A:840:ARG:HD2	2.46	0.50
2:B:277:LYS:CE	2:B:336:ARG:HD3	2.42	0.50
2:B:552:MET:HE1	2:B:555:ILE:HB	1.94	0.50
2:B:134:LYS:HZ1	2:B:164:LYS:HE2	1.76	0.50
1:A:1343:ALA:HB2	5:E:150:VAL:HG22	1.94	0.50
3:C:80:LEU:HD11	3:C:95:CYS:C	2.31	0.50
1:A:544:ASP:CG	1:A:545:GLN:N	2.64	0.50
2:B:575:PRO:HG2	2:B:576:ASP:H	1.77	0.50
9:I:55:THR:HG23	9:I:86:PHE:CZ	2.46	0.50
9:I:62:ILE:HG12	9:I:62:ILE:O	2.12	0.50
2:B:399:ASP:OD2	2:B:510:LYS:HG3	2.12	0.50
2:B:705:MET:CE	2:B:705:MET:HA	2.41	0.50
6:F:77:ASP:O	6:F:78:GLN:CB	2.50	0.50
2:B:893:LEU:HD21	2:B:897:GLY:C	2.32	0.50
11:K:12:LEU:H	11:K:12:LEU:HD12	1.77	0.50
12:L:60:ARG:HG2	12:L:61:THR:N	2.23	0.50
5:E:106:GLN:HE22	5:E:129:PRO:HB2	1.76	0.50
1:A:1376:THR:O	1:A:1377:THR:C	2.49	0.50
4:D:179:GLN:O	4:D:183:LEU:HB2	2.11	0.50
4:D:219:THR:CG2	4:D:220:LEU:O	2.60	0.50
1:A:298:PHE:O	1:A:302:THR:HB	2.12	0.50
2:B:957:ASN:HD22	2:B:961:LEU:HB2	1.75	0.50
2:B:1187:ASN:HD21	2:B:1190:ASP:HB3	1.77	0.50
2:B:1201:LYS:HE2	2:B:1205:GLN:CD	2.31	0.50
4:D:53:SER:H	4:D:148:LEU:CD2	2.24	0.50
1:A:1112:LYS:O	1:A:1114:PRO:HD3	2.11	0.50
3:C:100:THR:CG2	3:C:102:GLN:HE21	2.24	0.50
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.93	0.50
1:A:89:PRO:HB2	1:A:204:THR:HG22	1.93	0.50
1:A:326:ARG:HH11	1:A:326:ARG:HG2	1.76	0.50
1:A:63:ARG:CA	1:A:74:MET:HE2	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1117:GLN:HE21	2:B:1199:ALA:HB2	1.76	0.50
8:H:30:SER:HB3	8:H:33:GLN:O	2.12	0.50
2:B:822:ASN:ND2	10:J:52:THR:HG21	2.27	0.50
3:C:18:VAL:O	3:C:20:PHE:HD2	1.94	0.50
2:B:25:ILE:HG21	2:B:658:ILE:CD1	2.42	0.50
2:B:27:ALA:O	2:B:29:ASP:N	2.45	0.50
1:A:684:ALA:O	1:A:687:LYS:N	2.45	0.50
2:B:39:ARG:NE	2:B:665:GLU:HG2	2.27	0.50
10:J:13:VAL:O	10:J:14:VAL:HG23	2.12	0.50
9:I:61:ASP:C	9:I:63:GLY:N	2.64	0.50
2:B:1197:PRO:HG2	2:B:1200:ALA:CB	2.42	0.50
7:G:153:GLN:CG	7:G:154:VAL:HG23	2.41	0.50
2:B:185:THR:O	2:B:186:GLU:C	2.50	0.50
1:A:478:TYR:O	1:A:479:ASN:CB	2.60	0.50
1:A:646:PHE:O	1:A:650:GLN:HB2	2.12	0.50
8:H:129:TYR:CE1	8:H:130:ARG:HD2	2.46	0.50
8:H:81:PRO:HB2	8:H:82:PRO:CD	2.33	0.50
2:B:653:VAL:HG23	2:B:689:LEU:HB3	1.93	0.50
12:L:53:HIS:O	12:L:55:ILE:HD13	2.12	0.50
10:J:14:VAL:HG13	10:J:50:ILE:HD11	1.94	0.50
2:B:1182:CYS:O	2:B:1183:LYS:C	2.50	0.50
1:A:12:ARG:NH2	2:B:1192:TYR:CE2	2.80	0.50
1:A:89:PRO:C	1:A:204:THR:HG21	2.32	0.50
2:B:424:LEU:O	2:B:428:ILE:HG13	2.12	0.50
1:A:55:ASP:OD2	1:A:55:ASP:O	2.28	0.50
8:H:123:MET:HG2	8:H:124:ARG:N	2.26	0.50
4:D:13:ARG:C	4:D:15:LEU:N	2.63	0.50
2:B:1102:LYS:O	2:B:1122:ARG:NH1	2.43	0.50
1:A:463:ILE:HD11	1:A:469:ARG:HG3	1.94	0.50
1:A:1030:ARG:NH1	1:A:1035:TYR:OH	2.45	0.50
7:G:111:THR:O	7:G:111:THR:HG23	2.11	0.50
1:A:311:GLN:O	1:A:312:PRO:C	2.49	0.50
1:A:1402:PHE:CD1	1:A:1403:GLU:HG2	2.46	0.50
2:B:37:PHE:C	2:B:37:PHE:CD1	2.85	0.50
4:D:16:LYS:O	4:D:18:VAL:N	2.36	0.50
9:I:17:ARG:HG3	9:I:28:GLU:OE1	2.12	0.50
2:B:983:ARG:HD2	2:B:1091:TYR:HB3	1.93	0.50
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.92	0.50
3:C:83:SER:HG	3:C:160:LYS:HD3	1.77	0.50
2:B:469:GLN:O	2:B:470:LYS:HB2	2.12	0.50
2:B:35:SER:O	2:B:39:ARG:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:PHE:C	1:A:484:GLY:H	2.14	0.50
5:E:122:LYS:O	5:E:123:LEU:HD23	2.11	0.50
6:F:74:ILE:HD12	6:F:144:GLU:HG2	1.93	0.50
1:A:1142:THR:O	1:A:1145:SER:OG	2.30	0.50
3:C:215:GLU:O	3:C:216:GLY:C	2.49	0.50
2:B:1115:THR:CG2	2:B:1117:GLN:HB2	2.42	0.49
2:B:710:LEU:CA	2:B:733:HIS:HB3	2.36	0.49
2:B:284:ILE:HD13	2:B:333:PHE:CD2	2.44	0.49
2:B:766:ARG:NH2	15:3:11:U:O2	2.43	0.49
2:B:893:LEU:CD2	2:B:897:GLY:C	2.80	0.49
3:C:242:GLN:O	3:C:244:VAL:N	2.45	0.49
1:A:295:LEU:O	1:A:298:PHE:HB3	2.11	0.49
1:A:1210:GLY:O	1:A:1214:GLU:HG2	2.12	0.49
12:L:55:ILE:O	12:L:56:LEU:HB2	2.12	0.49
1:A:794:PRO:C	1:A:796:SER:H	2.16	0.49
2:B:1180:PHE:HB3	2:B:1191:ILE:CD1	2.42	0.49
2:B:936:ASP:CG	2:B:937:ALA:N	2.66	0.49
1:A:563:PRO:HG3	1:A:572:TRP:CE2	2.46	0.49
7:G:1:MET:SD	7:G:79:PHE:CE1	3.05	0.49
2:B:98:THR:O	2:B:126:SER:HB2	2.12	0.49
2:B:482:VAL:O	2:B:483:LEU:C	2.49	0.49
7:G:51:TYR:C	7:G:51:TYR:CD2	2.85	0.49
12:L:34:CYS:HB3	12:L:51:CYS:SG	2.52	0.49
3:C:114:TYR:OH	10:J:19:GLU:OE1	2.29	0.49
2:B:254:LEU:HD12	2:B:272:THR:O	2.13	0.49
5:E:177:ARG:HD3	5:E:215:MET:SD	2.52	0.49
2:B:758:PHE:HE1	2:B:1027:ILE:HG22	1.77	0.49
1:A:219:PHE:CE2	1:A:231:PRO:HD2	2.47	0.49
2:B:429:PHE:CD1	2:B:432:MET:HE3	2.47	0.49
2:B:461:LEU:HD12	2:B:461:LEU:N	2.27	0.49
1:A:336:ILE:HD13	1:A:340:LEU:HD12	1.93	0.49
11:K:51:LEU:HD22	11:K:59:ALA:HB3	1.93	0.49
1:A:600:PRO:HA	8:H:25:ARG:NH1	2.27	0.49
1:A:1280:GLU:O	1:A:1281:ARG:C	2.50	0.49
2:B:570:VAL:HG23	2:B:573:GLN:HB3	1.94	0.49
11:K:37:LYS:O	11:K:38:GLU:HG2	2.12	0.49
11:K:60:ALA:O	11:K:73:LEU:HD12	2.12	0.49
1:A:41:MET:O	1:A:42:ASP:C	2.51	0.49
1:A:598:LEU:O	1:A:599:SER:C	2.50	0.49
1:A:1308:THR:HG23	1:A:1309:ASP:H	1.73	0.49
2:B:995:ARG:HH11	3:C:165:LYS:HA	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1259:MET:CE	1:A:1263:ILE:HG13	2.43	0.49
1:A:718:VAL:O	1:A:722:LEU:HD12	2.12	0.49
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	2.27	0.49
1:A:1166:ASP:OD2	1:A:1239:ARG:NE	2.44	0.49
2:B:504:ARG:C	2:B:506:GLY:H	2.15	0.49
1:A:809:THR:H	1:A:812:GLU:HB2	1.77	0.49
2:B:1196:ILE:HB	2:B:1197:PRO:HD2	1.93	0.49
2:B:125:SER:HA	2:B:171:PRO:HA	1.94	0.49
1:A:69:THR:O	1:A:71:GLN:HG3	2.12	0.49
2:B:497:ARG:NH2	2:B:775:LYS:HZ2	2.10	0.49
1:A:171:GLN:OE1	1:A:171:GLN:HA	2.12	0.49
12:L:30:ILE:CG2	12:L:31:CYS:H	2.25	0.49
2:B:830:TYR:O	2:B:832:GLY:N	2.46	0.49
10:J:12:LYS:O	10:J:14:VAL:HG23	2.13	0.49
2:B:1182:CYS:C	2:B:1183:LYS:HE3	2.32	0.49
2:B:839:MET:CE	2:B:1010:LEU:HD23	2.42	0.49
5:E:28:TYR:C	5:E:65:THR:HG22	2.32	0.49
2:B:295:GLY:N	2:B:298:LEU:HD23	2.28	0.49
4:D:73:SER:HB3	7:G:21:ARG:HH21	1.77	0.49
2:B:59:LEU:HD11	2:B:417:PHE:CZ	2.48	0.49
12:L:61:THR:HG22	12:L:63:ARG:H	1.77	0.49
9:I:78:CYS:SG	9:I:106:CYS:SG	3.11	0.49
5:E:28:TYR:CE1	5:E:78:LEU:HD13	2.47	0.49
2:B:313:MET:HE2	2:B:390:LEU:CD2	2.42	0.49
7:G:106:MET:HG2	7:G:107:LYS:N	2.28	0.49
1:A:311:GLN:O	1:A:313:GLN:N	2.45	0.49
5:E:89:GLY:C	5:E:91:LYS:N	2.66	0.49
1:A:90:VAL:HG13	1:A:297:GLN:CD	2.33	0.49
11:K:24:ASP:OD1	11:K:26:LYS:N	2.46	0.49
1:A:54:ASN:HA	1:A:58:LEU:HD12	1.93	0.49
1:A:590:ARG:NH1	1:A:592:ASP:OD1	2.46	0.49
10:J:36:LEU:HD12	10:J:47:ARG:NH1	2.28	0.49
10:J:2:ILE:HG22	10:J:3:VAL:N	2.27	0.49
2:B:842:ASN:ND2	2:B:845:SER:OG	2.45	0.49
15:3:11:U:H2'	15:3:11:U:O2	2.12	0.49
1:A:464:PRO:HG2	1:A:465:TYR:CD1	2.48	0.49
1:A:1329:THR:HG22	1:A:1330:ASN:N	2.28	0.49
1:A:1242:VAL:CG1	1:A:1243:VAL:H	2.26	0.49
2:B:642:ASP:HB3	2:B:649:LYS:CG	2.43	0.49
6:F:69:LEU:HB3	6:F:71:GLU:OE2	2.13	0.49
4:D:134:THR:CG2	4:D:135:GLY:N	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ALA:HB1	1:A:433:GLU:O	2.13	0.49
1:A:739:ASP:OD2	8:H:19:ARG:HD2	2.12	0.49
1:A:323:LYS:H	1:A:323:LYS:CD	2.21	0.49
2:B:640:VAL:O	2:B:641:GLU:C	2.50	0.49
3:C:179:GLU:O	3:C:180:TYR:HB3	2.13	0.49
1:A:897:TYR:HB3	1:A:936:LEU:CD1	2.43	0.49
2:B:642:ASP:C	2:B:644:GLU:H	2.14	0.49
2:B:778:MET:CE	2:B:1094:ARG:HG2	2.43	0.49
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.94	0.49
2:B:615:MET:CB	2:B:626:ILE:HG12	2.43	0.49
5:E:7:ARG:HD2	5:E:8:ASN:N	2.28	0.49
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.13	0.49
2:B:48:LEU:O	2:B:51:PHE:N	2.43	0.49
1:A:969:GLN:O	1:A:969:GLN:HG3	2.12	0.49
1:A:1067:LEU:HD12	1:A:1067:LEU:O	2.12	0.49
8:H:99:GLY:HA3	8:H:117:SER:O	2.12	0.49
1:A:55:ASP:C	1:A:57:ARG:N	2.62	0.49
2:B:542:MET:HE3	2:B:747:MET:HG3	1.95	0.49
2:B:129:PHE:CE2	2:B:166:PHE:HB2	2.48	0.49
8:H:128:ASN:C	8:H:128:ASN:HD22	2.16	0.49
4:D:128:VAL:C	4:D:130:LEU:N	2.66	0.49
1:A:416:ARG:NH1	1:A:417:TYR:HE2	2.02	0.49
12:L:52:GLY:O	12:L:53:HIS:C	2.50	0.49
1:A:167:CYS:HB2	1:A:169:ASN:HD21	1.75	0.49
1:A:774:ARG:CZ	1:A:797:LYS:HG3	2.43	0.49
5:E:27:GLY:O	5:E:65:THR:HG23	2.12	0.49
8:H:100:THR:CG2	8:H:138:GLU:HG2	2.43	0.49
2:B:258:LEU:CG	2:B:258:LEU:O	2.57	0.49
5:E:93:MET:HG2	5:E:123:LEU:HD12	1.95	0.49
6:F:118:LEU:O	6:F:122:MET:HG3	2.13	0.49
2:B:467:GLY:N	2:B:475:SER:HB3	2.28	0.49
1:A:38:PRO:HG2	1:A:39:GLU:OE2	2.12	0.49
1:A:583:PRO:HG2	1:A:586:ILE:HG13	1.95	0.49
1:A:34:LYS:HZ1	1:A:57:ARG:NH2	2.11	0.49
3:C:173:ALA:O	3:C:174:ALA:HB3	2.12	0.49
1:A:106:VAL:CG1	1:A:107:CYS:N	2.76	0.49
3:C:14:SER:OG	3:C:15:LYS:N	2.44	0.49
2:B:912:ILE:O	2:B:938:SER:HB3	2.13	0.49
1:A:904:THR:HG22	1:A:904:THR:O	2.13	0.49
1:A:37:PHE:HD1	1:A:37:PHE:N	2.10	0.49
2:B:134:LYS:N	2:B:134:LYS:HD3	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:PRO:O	1:A:204:THR:HG21	2.13	0.49
11:K:48:ALA:O	11:K:51:LEU:N	2.37	0.49
1:A:603:ASN:O	1:A:604:GLY:C	2.50	0.49
1:A:833:GLU:O	1:A:837:ILE:HG13	2.13	0.49
11:K:93:SER:O	11:K:97:LYS:HG3	2.13	0.49
6:F:136:ARG:O	6:F:143:PHE:HA	2.13	0.49
1:A:34:LYS:CB	1:A:36:ARG:NH1	2.75	0.48
7:G:26:LEU:O	7:G:29:LYS:N	2.45	0.48
1:A:1422:ARG:HD3	2:B:1224:PHE:CE2	2.47	0.48
5:E:98:ILE:O	5:E:102:GLU:HG3	2.13	0.48
10:J:16:ASP:OD1	10:J:16:ASP:N	2.46	0.48
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.46	0.48
2:B:654:ARG:NH1	2:B:654:ARG:HG3	2.21	0.48
4:D:126:ILE:HD13	4:D:145:MET:CE	2.43	0.48
1:A:500:GLU:OE1	2:B:1145:SER:N	2.46	0.48
2:B:63:ILE:HD12	2:B:421:PHE:CZ	2.47	0.48
1:A:578:LEU:HD23	1:A:612:ILE:CD1	2.43	0.48
11:K:24:ASP:OD2	11:K:74:ARG:NH1	2.45	0.48
1:A:1053:PHE:O	1:A:1056:SER:N	2.46	0.48
5:E:164:LEU:HD22	5:E:211:TYR:CD2	2.48	0.48
1:A:173:THR:O	1:A:173:THR:HG23	2.13	0.48
4:D:13:ARG:O	4:D:15:LEU:N	2.47	0.48
2:B:744:HIS:CD2	2:B:745:PRO:CD	2.86	0.48
4:D:155:ARG:HB3	4:D:155:ARG:HH11	1.78	0.48
2:B:704:ALA:HB1	2:B:710:LEU:HB2	1.95	0.48
2:B:361:LEU:CD2	2:B:377:PHE:CD2	2.96	0.48
11:K:53:ASP:HB3	11:K:56:VAL:CG2	2.43	0.48
1:A:744:LYS:HG2	1:A:748:MET:HE2	1.94	0.48
1:A:1264:GLU:OE2	9:I:46:HIS:CD2	2.66	0.48
1:A:720:ARG:HG2	1:A:720:ARG:O	2.13	0.48
3:C:8:VAL:HG12	3:C:9:LYS:H	1.78	0.48
2:B:461:LEU:CD1	2:B:461:LEU:H	2.26	0.48
1:A:506:ALA:O	1:A:507:VAL:C	2.51	0.48
2:B:792:MET:H	2:B:857:ARG:HA	1.77	0.48
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.48	0.48
7:G:132:SER:O	7:G:133:SER:C	2.52	0.48
2:B:709:ASP:OD1	2:B:710:LEU:HD23	2.13	0.48
1:A:785:PRO:HG2	1:A:786:HIS:CD2	2.48	0.48
2:B:973:ILE:HG23	2:B:974:PRO:HD2	1.94	0.48
3:C:239:PRO:O	3:C:241:ASP:N	2.45	0.48
3:C:248:ILE:CD1	11:K:101:LEU:HD22	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:125:SER:OG	7:G:128:PRO:HA	2.13	0.48
1:A:1161:THR:HG22	1:A:1163:ILE:HG13	1.95	0.48
5:E:69:ILE:HA	5:E:72:PHE:O	2.13	0.48
2:B:506:GLY:O	2:B:507:LYS:CB	2.61	0.48
2:B:827:ILE:HG22	2:B:827:ILE:O	2.13	0.48
1:A:46:THR:O	1:A:47:ARG:C	2.52	0.48
2:B:1068:GLY:O	2:B:1069:PHE:O	2.31	0.48
2:B:771:SER:O	2:B:775:LYS:HE3	2.14	0.48
1:A:356:ASP:HB2	1:A:469:ARG:NH1	2.29	0.48
6:F:90:ARG:HG3	6:F:91:ALA:N	2.27	0.48
5:E:192:ARG:NH1	5:E:192:ARG:HG3	2.29	0.48
2:B:63:ILE:HG13	2:B:63:ILE:O	2.14	0.48
1:A:38:PRO:HA	1:A:270:LEU:HD23	1.95	0.48
1:A:658:LEU:O	1:A:658:LEU:HD12	2.13	0.48
9:I:55:THR:OG1	9:I:100:PHE:HD2	1.96	0.48
2:B:639:ILE:CG2	2:B:641:GLU:HG2	2.43	0.48
1:A:1277:GLU:C	1:A:1279:ILE:H	2.16	0.48
1:A:1120:LEU:HD12	1:A:1120:LEU:C	2.33	0.48
1:A:145:LYS:HA	1:A:145:LYS:CE	2.35	0.48
2:B:956:THR:CG2	2:B:960:GLY:HA2	2.43	0.48
5:E:191:LYS:O	5:E:192:ARG:C	2.50	0.48
1:A:774:ARG:HB2	1:A:797:LYS:O	2.13	0.48
2:B:860:MET:O	2:B:861:ASP:HB2	2.13	0.48
1:A:418:SER:C	1:A:420:ARG:H	2.16	0.48
9:I:16:PRO:HB3	9:I:27:PHE:CE2	2.48	0.48
1:A:852:TYR:O	6:F:81:THR:HG22	2.14	0.48
1:A:391:LEU:HD23	1:A:401:GLY:N	2.29	0.48
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.94	0.48
7:G:27:LYS:HD3	7:G:51:TYR:CE2	2.48	0.48
2:B:120:ARG:NH1	12:L:54:ARG:HD2	2.29	0.48
5:E:22:MET:HE3	5:E:26:ARG:CZ	2.43	0.48
1:A:1241:ARG:O	1:A:1242:VAL:CG2	2.61	0.48
5:E:48:ASP:CG	5:E:49:SER:N	2.66	0.48
2:B:827:ILE:HD12	2:B:1086:PHE:HD2	1.79	0.48
1:A:1453:TYR:O	1:A:1454:MET:HB3	2.13	0.48
4:D:32:GLU:OE1	7:G:41:LYS:HE2	2.14	0.48
2:B:885:MET:HA	2:B:936:ASP:HB2	1.96	0.48
9:I:34:TYR:C	9:I:34:TYR:CD2	2.87	0.48
2:B:364:ILE:O	2:B:365:THR:CB	2.61	0.48
2:B:846:ILE:HG23	2:B:974:PRO:CG	2.41	0.48
5:E:190:LEU:C	5:E:191:LYS:HG2	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1244:ARG:O	1:A:1244:ARG:HG2	2.14	0.48
1:A:802:ASN:ND2	1:A:812:GLU:OE1	2.37	0.48
2:B:48:LEU:HD23	2:B:173:MET:SD	2.53	0.48
1:A:715:GLU:O	1:A:716:ASP:C	2.52	0.48
4:D:155:ARG:CG	4:D:155:ARG:HH11	2.27	0.48
1:A:372:LYS:HA	1:A:435:HIS:CE1	2.48	0.48
8:H:82:PRO:C	8:H:84:ALA:N	2.67	0.48
1:A:106:VAL:HG21	1:A:214:ILE:CD1	2.43	0.48
2:B:483:LEU:CD1	2:B:491:THR:HG23	2.38	0.48
2:B:327:ARG:O	2:B:331:LEU:HD13	2.13	0.48
2:B:831:SER:HB2	2:B:833:TYR:HD1	1.79	0.48
9:I:80:SER:OG	9:I:105:SER:HB2	2.14	0.48
11:K:13:GLY:O	11:K:14:GLU:C	2.53	0.48
2:B:473:MET:CE	2:B:474:SER:HA	2.43	0.48
2:B:1006:ILE:HG22	10:J:45:CYS:HB3	1.95	0.48
4:D:153:ARG:C	4:D:154:PHE:HD2	2.16	0.48
4:D:154:PHE:HE1	4:D:163:VAL:CG1	2.26	0.48
2:B:126:SER:CB	2:B:172:ILE:HD11	2.44	0.48
2:B:654:ARG:O	2:B:657:HIS:N	2.47	0.48
2:B:479:VAL:O	2:B:480:SER:HB3	2.13	0.48
11:K:18:LYS:C	11:K:19:LEU:HD23	2.34	0.48
5:E:6:GLU:HA	5:E:9:ILE:HD12	1.95	0.48
2:B:1099:VAL:CG1	2:B:1100:ASP:N	2.76	0.48
1:A:147:VAL:HG22	1:A:170:THR:HA	1.95	0.48
2:B:1135:ARG:O	2:B:1136:ASP:C	2.52	0.48
2:B:210:LYS:HD2	2:B:481:GLN:O	2.13	0.48
5:E:157:SER:C	5:E:159:ASP:N	2.66	0.48
2:B:309:GLN:CD	9:I:52:ILE:HD11	2.34	0.48
2:B:708:GLU:CG	2:B:709:ASP:H	2.09	0.48
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.96	0.48
2:B:941:LEU:O	2:B:942:ARG:C	2.52	0.48
3:C:99:LEU:HD22	3:C:99:LEU:N	2.27	0.48
1:A:688:LYS:HE3	1:A:691:LEU:HD23	1.96	0.48
5:E:13:TRP:O	5:E:16:PHE:HB3	2.14	0.48
2:B:68:THR:HA	2:B:90:ILE:O	2.14	0.48
2:B:582:VAL:HG22	2:B:626:ILE:HG22	1.95	0.48
2:B:449:ASN:C	2:B:451:LYS:H	2.18	0.48
1:A:254:GLU:O	1:A:256:GLN:N	2.47	0.47
4:D:63:LEU:HD22	4:D:133:THR:OG1	2.13	0.47
9:I:55:THR:HG23	9:I:86:PHE:HZ	1.79	0.47
7:G:127:PRO:HG3	7:G:139:ILE:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:THR:HA	1:A:305:ASP:O	2.14	0.47
2:B:470:LYS:C	2:B:472:ALA:N	2.67	0.47
1:A:709:THR:CG2	1:A:710:LEU:H	2.25	0.47
1:A:1243:VAL:HG12	1:A:1244:ARG:N	2.29	0.47
2:B:39:ARG:HH21	2:B:665:GLU:CD	2.17	0.47
3:C:147:LEU:CD2	3:C:147:LEU:N	2.73	0.47
7:G:90:THR:HG22	7:G:91:VAL:O	2.13	0.47
2:B:732:SER:HB2	2:B:734:HIS:NE2	2.29	0.47
11:K:31:VAL:HG23	11:K:83:PRO:HG3	1.95	0.47
1:A:84:ILE:CD1	1:A:270:LEU:HD13	2.44	0.47
2:B:875:GLU:O	2:B:877:PRO:CD	2.60	0.47
9:I:86:PHE:CE1	9:I:100:PHE:HB2	2.49	0.47
2:B:944:THR:CG2	2:B:1122:ARG:NH2	2.72	0.47
8:H:58:THR:HG22	8:H:59:ILE:N	2.25	0.47
2:B:773:MET:O	2:B:775:LYS:N	2.46	0.47
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.40	0.47
11:K:108:GLU:O	11:K:112:GLN:HG2	2.14	0.47
1:A:1036:ARG:HG2	1:A:1036:ARG:NH1	2.29	0.47
1:A:332:LYS:C	1:A:334:GLY:N	2.66	0.47
1:A:886:ILE:CG2	1:A:952:ALA:HB2	2.44	0.47
1:A:1322:ILE:O	1:A:1322:ILE:HG13	2.14	0.47
6:F:94:LEU:HD22	6:F:122:MET:HG2	1.96	0.47
4:D:20:GLU:CD	4:D:20:GLU:H	2.17	0.47
1:A:567:LYS:CE	8:H:46:LEU:HB2	2.44	0.47
8:H:96:VAL:HA	8:H:142:LEU:O	2.14	0.47
1:A:914:GLU:C	1:A:916:GLY:H	2.18	0.47
1:A:547:LEU:HD22	11:K:58:PHE:CD1	2.49	0.47
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.96	0.47
1:A:1153:TYR:CE1	9:I:42:LEU:HD13	2.49	0.47
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.95	0.47
2:B:31:TRP:CZ2	2:B:807:ARG:HB2	2.49	0.47
1:A:474:VAL:HG22	1:A:474:VAL:O	2.14	0.47
14:1:15:DG:H2'	14:1:16:DT:H71	1.95	0.47
2:B:307:ASP:C	2:B:309:GLN:N	2.64	0.47
1:A:108:MET:HB3	1:A:210:ILE:CD1	2.44	0.47
2:B:654:ARG:H	2:B:657:HIS:HD2	1.60	0.47
12:L:34:CYS:SG	12:L:51:CYS:SG	3.13	0.47
11:K:109:TRP:O	11:K:112:GLN:HB2	2.15	0.47
1:A:1015:VAL:O	1:A:1016:THR:C	2.53	0.47
3:C:111:THR:O	3:C:147:LEU:HD23	2.14	0.47
4:D:53:SER:C	4:D:55:ALA:N	2.64	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:VAL:HG23	2:B:109:THR:N	2.29	0.47
2:B:54:PHE:HE1	2:B:414:ALA:HA	1.78	0.47
1:A:1168:GLU:OE2	1:A:1172:LEU:HD11	2.14	0.47
3:C:50:GLU:OE1	12:L:64:LEU:HD12	2.14	0.47
1:A:55:ASP:H	1:A:56:PRO:HD3	1.76	0.47
9:I:99:LEU:C	9:I:100:PHE:HD1	2.16	0.47
2:B:1103:ILE:O	2:B:1103:ILE:HG23	2.14	0.47
1:A:901:LEU:HA	1:A:907:THR:OG1	2.14	0.47
2:B:376:PHE:HB2	2:B:566:LEU:HD21	1.96	0.47
3:C:39:ALA:HA	3:C:164:ALA:CB	2.44	0.47
7:G:127:PRO:HG2	7:G:138:THR:HG21	1.95	0.47
2:B:859:TYR:CD1	2:B:859:TYR:N	2.83	0.47
2:B:831:SER:CB	2:B:994:TYR:OH	2.63	0.47
2:B:644:GLU:C	2:B:646:LEU:N	2.68	0.47
2:B:1010:LEU:N	2:B:1010:LEU:HD12	2.29	0.47
1:A:831:THR:HG23	1:A:832:ALA:N	2.29	0.47
4:D:29:LEU:N	4:D:29:LEU:CD2	2.77	0.47
2:B:505:ASP:HA	13:2:1:DA:N7	2.29	0.47
1:A:1450:LEU:HD21	7:G:19:GLY:O	2.15	0.47
3:C:100:THR:HG22	3:C:101:LEU:N	2.29	0.47
3:C:73:GLN:HE21	3:C:75:MET:N	2.10	0.47
1:A:1048:ASN:HD22	1:A:1048:ASN:N	2.13	0.47
2:B:855:PHE:HZ	2:B:857:ARG:NH1	2.13	0.47
1:A:608:ILE:HD12	1:A:613:ILE:HD12	1.97	0.47
4:D:69:ALA:HA	4:D:72:ARG:HG3	1.96	0.47
1:A:907:THR:HG23	1:A:908:LEU:N	2.30	0.47
2:B:25:ILE:HD11	2:B:653:VAL:O	2.14	0.47
3:C:89:GLU:O	3:C:90:ASP:CB	2.58	0.47
3:C:181:ASP:N	3:C:182:PRO:CD	2.76	0.47
1:A:826:ASP:HB2	1:A:830:LYS:HD3	1.96	0.47
5:E:10:SER:O	5:E:13:TRP:HB3	2.15	0.47
1:A:293:GLU:O	1:A:296:LEU:N	2.47	0.47
2:B:225:VAL:HA	2:B:237:VAL:O	2.14	0.47
1:A:664:THR:HG22	2:B:1014:PRO:CB	2.44	0.47
7:G:87:VAL:HG23	7:G:103:VAL:HG21	1.95	0.47
2:B:792:MET:HA	2:B:856:PHE:O	2.14	0.47
1:A:743:VAL:O	1:A:747:VAL:HG23	2.14	0.47
1:A:244:PRO:CB	1:A:245:PRO:CD	2.84	0.47
1:A:49:LYS:HD3	1:A:55:ASP:HB3	1.97	0.47
4:D:63:LEU:HD23	4:D:63:LEU:HA	1.74	0.47
1:A:569:LYS:HD3	1:A:571:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:HZ1	8:H:46:LEU:HB2	1.75	0.47
9:I:44:TYR:HD1	9:I:45:ARG:H	1.62	0.47
2:B:619:ILE:HG22	2:B:620:ARG:N	2.29	0.47
9:I:51:ASN:O	9:I:54:GLU:HG3	2.15	0.47
2:B:620:ARG:CZ	9:I:68:LEU:HD21	2.44	0.47
2:B:745:PRO:O	2:B:748:ILE:HG13	2.14	0.47
5:E:172:GLU:C	5:E:174:GLN:H	2.18	0.47
1:A:577:ILE:O	1:A:580:VAL:HG23	2.15	0.47
2:B:996:ARG:HH22	3:C:175:ALA:N	2.12	0.47
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.34	0.47
4:D:130:LEU:C	4:D:132:GLN:N	2.67	0.47
1:A:108:MET:HA	1:A:210:ILE:CD1	2.43	0.47
3:C:22:LEU:HD21	11:K:101:LEU:HD11	1.97	0.47
1:A:381:THR:CG2	1:A:382:PRO:HD2	2.38	0.47
1:A:382:PRO:HB3	1:A:428:TYR:HE2	1.80	0.47
7:G:27:LYS:CE	7:G:54:ILE:HB	2.40	0.47
2:B:859:TYR:CZ	2:B:941:LEU:HD12	2.49	0.47
2:B:466:TRP:O	2:B:468:GLU:N	2.48	0.47
1:A:687:LYS:HE2	1:A:795:GLU:OE2	2.15	0.47
1:A:711:ARG:HH21	9:I:87:GLN:NE2	2.11	0.47
3:C:44:LEU:HD21	3:C:159:ALA:CB	2.44	0.47
3:C:184:ASN:OD1	3:C:187:LYS:CA	2.61	0.47
2:B:1034:VAL:O	2:B:1037:LEU:N	2.48	0.47
4:D:118:THR:HG21	4:D:121:LYS:HE3	1.95	0.47
1:A:842:VAL:HG11	2:B:1136:ASP:OD2	2.14	0.47
5:E:153:HIS:O	5:E:154:ILE:HG13	2.13	0.47
2:B:969:ARG:HD3	3:C:61:GLU:OE2	2.15	0.47
1:A:1451:VAL:O	1:A:1454:MET:HG2	2.14	0.47
5:E:31:THR:HG1	5:E:34:GLU:H	1.62	0.47
1:A:53:LEU:CD2	1:A:54:ASN:N	2.48	0.47
5:E:171:LYS:HE2	5:E:174:GLN:CD	2.34	0.47
8:H:59:ILE:O	8:H:60:ALA:HB3	2.14	0.47
1:A:316:GLN:HB2	1:A:322:VAL:HG23	1.96	0.47
2:B:360:PHE:HD2	2:B:374:LYS:HD3	1.80	0.47
8:H:128:ASN:ND2	8:H:128:ASN:C	2.68	0.47
2:B:638:PHE:HB2	2:B:741:CYS:O	2.14	0.47
2:B:113:TYR:HE2	2:B:192:LEU:HD21	1.80	0.47
5:E:134:THR:C	5:E:135:PHE:HD1	2.17	0.47
4:D:200:ASN:N	4:D:200:ASN:OD1	2.47	0.47
7:G:114:LEU:HG	7:G:162:SER:HB3	1.97	0.47
2:B:405:ARG:HA	2:B:631:GLY:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.97	0.47
2:B:48:LEU:HA	2:B:173:MET:SD	2.55	0.47
5:E:164:LEU:HD13	5:E:211:TYR:CE2	2.49	0.47
1:A:174:ILE:HG22	1:A:175:ARG:N	2.30	0.47
1:A:1365:TYR:C	1:A:1365:TYR:CD2	2.88	0.47
11:K:78:THR:HG22	11:K:79:GLU:N	2.30	0.47
12:L:29:TYR:CD2	12:L:29:TYR:N	2.83	0.47
2:B:1115:THR:HG22	2:B:1117:GLN:HB2	1.96	0.47
1:A:1132:LYS:O	1:A:1135:ARG:HD2	2.15	0.47
1:A:709:THR:CG2	1:A:710:LEU:N	2.75	0.47
2:B:644:GLU:HA	2:B:644:GLU:OE1	2.15	0.47
2:B:1076:HIS:CD2	11:K:40:HIS:NE2	2.83	0.47
8:H:7:ASP:O	8:H:8:ASP:HB2	2.15	0.47
4:D:176:GLU:OE2	4:D:197:SER:HB2	2.14	0.47
2:B:1107:ALA:O	2:B:1108:ARG:O	2.33	0.47
2:B:552:MET:C	2:B:554:ILE:H	2.19	0.47
1:A:695:LYS:C	1:A:697:ALA:N	2.67	0.47
1:A:419:LYS:HG3	1:A:420:ARG:HG3	1.96	0.47
2:B:935:ARG:O	2:B:935:ARG:HG3	2.15	0.47
1:A:53:LEU:O	1:A:54:ASN:C	2.53	0.47
1:A:56:PRO:HD2	1:A:58:LEU:HG	1.97	0.47
9:I:50:THR:CG2	9:I:51:ASN:N	2.75	0.47
9:I:62:ILE:HD11	9:I:86:PHE:HE2	1.80	0.47
2:B:704:ALA:HB2	2:B:738:PHE:CD2	2.49	0.47
1:A:870:GLU:HG2	5:E:208:TYR:CD2	2.49	0.47
2:B:1138:MET:HE2	2:B:1146:PHE:HD2	1.80	0.47
5:E:136:ASN:OD1	5:E:138:ALA:N	2.48	0.47
5:E:198:ILE:CD1	5:E:212:ARG:HG3	2.45	0.47
1:A:167:CYS:HB2	1:A:169:ASN:HD22	1.79	0.47
1:A:1141:THR:HG23	1:A:1205:LYS:HD3	1.96	0.47
1:A:1005:GLU:O	1:A:1009:ASN:HB2	2.15	0.47
1:A:34:LYS:HZ1	1:A:57:ARG:HH21	1.62	0.46
3:C:177:GLU:HG3	3:C:231:ASN:ND2	2.18	0.46
4:D:51:ASN:C	4:D:52:LEU:O	2.52	0.46
1:A:903:ASN:C	1:A:903:ASN:ND2	2.66	0.46
1:A:711:ARG:HA	9:I:97:MET:HE1	1.96	0.46
3:C:120:ILE:HG21	3:C:124:LEU:HD11	1.97	0.46
1:A:1029:ARG:CG	1:A:1029:ARG:HH11	2.28	0.46
1:A:773:LYS:H	1:A:773:LYS:HD2	1.80	0.46
1:A:225:ASN:ND2	1:A:227:VAL:N	2.63	0.46
1:A:228:PHE:CE2	4:D:15:LEU:HD23	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:983:ILE:CG2	1:A:983:ILE:O	2.63	0.46
1:A:1132:LYS:HA	1:A:1135:ARG:HD2	1.97	0.46
1:A:11:LEU:HD23	1:A:11:LEU:C	2.35	0.46
7:G:116:PRO:HG2	7:G:119:LEU:HB2	1.97	0.46
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.55	0.46
12:L:61:THR:HG21	12:L:63:ARG:HG3	1.96	0.46
1:A:1019:CYS:O	1:A:1020:CYS:C	2.54	0.46
3:C:212:PRO:HB3	3:C:213:PRO:HD2	1.96	0.46
4:D:124:GLU:CD	4:D:124:GLU:H	2.18	0.46
6:F:111:LEU:H	6:F:111:LEU:HD12	1.81	0.46
1:A:1149:ALA:CB	9:I:47:GLU:HA	2.45	0.46
3:C:73:GLN:NE2	3:C:74:SER:H	2.13	0.46
2:B:1106:ARG:NH1	2:B:1126:GLY:HA2	2.30	0.46
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.97	0.46
1:A:278:THR:HG22	1:A:278:THR:O	2.16	0.46
1:A:33:ALA:HA	1:A:57:ARG:HH12	1.80	0.46
1:A:41:MET:HE3	1:A:41:MET:N	2.29	0.46
1:A:42:ASP:HB3	1:A:45:GLN:H	1.81	0.46
1:A:56:PRO:O	1:A:57:ARG:NH1	2.48	0.46
1:A:64:ASN:O	1:A:65:LEU:C	2.52	0.46
1:A:785:PRO:HG2	1:A:786:HIS:HD2	1.81	0.46
9:I:111:THR:HG22	9:I:113:ASP:N	2.31	0.46
2:B:1067:ARG:NH2	3:C:194:GLU:OE2	2.49	0.46
8:H:84:ALA:C	8:H:86:ASP:N	2.68	0.46
12:L:38:LEU:HG	12:L:39:SER:H	1.80	0.46
1:A:1198:ASP:OD2	1:A:1200:ALA:HB3	2.15	0.46
1:A:1194:ARG:NH2	1:A:1237:ILE:HD13	2.30	0.46
2:B:1048:THR:OG1	2:B:1049:ASP:N	2.48	0.46
5:E:35:VAL:O	5:E:37:LEU:N	2.47	0.46
7:G:22:MET:O	7:G:25:TYR:N	2.48	0.46
9:I:110:PHE:CD2	9:I:110:PHE:N	2.84	0.46
1:A:1349:TYR:C	1:A:1349:TYR:CD2	2.89	0.46
1:A:595:THR:C	1:A:596:THR:HG23	2.36	0.46
2:B:247:GLY:C	2:B:249:ARG:N	2.68	0.46
7:G:7:LEU:CB	7:G:74:TYR:HE2	2.23	0.46
1:A:463:ILE:HB	1:A:464:PRO:CD	2.45	0.46
1:A:385:ILE:CD1	1:A:426:LEU:HB2	2.46	0.46
5:E:112:TYR:CE1	5:E:136:ASN:HA	2.50	0.46
2:B:843:GLN:N	2:B:994:TYR:O	2.23	0.46
1:A:182:VAL:CG2	1:A:201:VAL:HG22	2.46	0.46
1:A:845:LEU:O	1:A:846:GLU:C	2.52	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:55:LYS:HB3	11:K:81:TYR:HD1	1.76	0.46
2:B:303:TYR:HH	2:B:586:TRP:HH2	1.62	0.46
2:B:481:GLN:HE21	15:3:7:G:H4'	1.79	0.46
2:B:1180:PHE:HB3	2:B:1191:ILE:HD13	1.96	0.46
6:F:72:LYS:HG2	6:F:72:LYS:H	1.49	0.46
1:A:41:MET:HB2	1:A:49:LYS:HA	1.94	0.46
9:I:84:VAL:O	9:I:84:VAL:HG22	2.16	0.46
1:A:1116:LEU:HD12	1:A:1116:LEU:C	2.36	0.46
2:B:850:LEU:HD12	2:B:850:LEU:C	2.33	0.46
3:C:66:ARG:HH12	10:J:2:ILE:CB	2.29	0.46
3:C:164:ALA:O	3:C:165:LYS:C	2.53	0.46
1:A:1120:LEU:HD13	1:A:1124:HIS:O	2.14	0.46
3:C:258:ILE:HG23	11:K:19:LEU:HD11	1.98	0.46
1:A:1030:ARG:HG3	1:A:1034:GLU:OE2	2.15	0.46
1:A:1057:VAL:HG12	1:A:1058:VAL:N	2.31	0.46
6:F:128:LYS:HD3	6:F:149:GLU:O	2.15	0.46
1:A:1385:THR:C	1:A:1387:HIS:N	2.69	0.46
1:A:139:TRP:O	1:A:140:THR:C	2.54	0.46
4:D:134:THR:HG22	4:D:136:GLY:H	1.80	0.46
1:A:533:LYS:HE3	1:A:745:GLN:HE22	1.80	0.46
2:B:875:GLU:OE2	2:B:934:LYS:HE2	2.16	0.46
1:A:69:THR:HG22	2:B:1174:LYS:HD3	1.98	0.46
8:H:27:GLU:HG3	8:H:39:THR:HA	1.98	0.46
1:A:315:LEU:H	1:A:315:LEU:CD2	2.04	0.46
8:H:32:THR:HG22	8:H:33:GLN:OE1	2.16	0.46
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.96	0.46
3:C:238:ILE:HG22	3:C:243:VAL:HG23	1.98	0.46
3:C:22:LEU:HD11	11:K:101:LEU:HD21	1.98	0.46
2:B:221:ASN:OD1	2:B:242:SER:HA	2.16	0.46
9:I:93:LYS:H	9:I:93:LYS:HD3	1.79	0.46
9:I:74:GLU:HB3	9:I:81:ARG:CD	2.44	0.46
6:F:116:ASP:O	6:F:117:PRO:C	2.54	0.46
2:B:44:VAL:O	2:B:45:SER:C	2.54	0.46
8:H:106:GLU:C	8:H:108:SER:H	2.16	0.46
10:J:37:SER:OG	10:J:47:ARG:NH2	2.49	0.46
2:B:172:ILE:CD1	2:B:178:ASN:HD22	2.26	0.46
1:A:709:THR:HG22	1:A:711:ARG:H	1.79	0.46
2:B:644:GLU:OE2	2:B:646:LEU:HB2	2.16	0.46
7:G:158:HIS:CD2	7:G:159:ALA:N	2.83	0.46
3:C:3:GLU:CG	3:C:4:GLU:HG3	2.41	0.46
1:A:218:ASP:O	1:A:219:PHE:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:465:ASN:ND2	2:B:465:ASN:N	2.62	0.46
1:A:1206:ASP:O	1:A:1274:ARG:CZ	2.63	0.46
9:I:82:GLU:HB3	9:I:104:LEU:CG	2.46	0.46
1:A:962:ARG:O	1:A:964:ILE:N	2.49	0.46
3:C:52:GLU:OE1	3:C:154:LYS:CE	2.63	0.46
2:B:1006:ILE:HG23	10:J:43:ARG:HG3	1.98	0.46
8:H:106:GLU:O	8:H:108:SER:N	2.35	0.46
4:D:191:ALA:O	4:D:193:THR:N	2.48	0.46
1:A:841:LEU:HA	1:A:841:LEU:HD23	1.79	0.46
1:A:75:ASN:O	1:A:76:GLU:HB2	2.16	0.46
4:D:119:ARG:HD3	4:D:221:TYR:HE2	1.79	0.46
5:E:90:VAL:HB	5:E:117:THR:HG21	1.97	0.46
1:A:401:GLY:C	1:A:435:HIS:HD2	2.18	0.46
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.98	0.46
12:L:38:LEU:HG	12:L:39:SER:N	2.31	0.46
2:B:658:ILE:HG22	2:B:662:MET:HE2	1.98	0.46
11:K:91:CYS:O	11:K:94:ILE:N	2.49	0.46
2:B:1181:GLU:H	2:B:1188:LYS:HA	1.80	0.46
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.97	0.46
9:I:94:ASP:O	9:I:95:THR:O	2.34	0.46
2:B:38:PHE:HD1	2:B:811:TYR:CD2	2.34	0.46
5:E:50:MET:HG2	5:E:52:ARG:HE	1.79	0.46
3:C:33:LEU:HD12	3:C:33:LEU:O	2.15	0.46
10:J:62:ARG:HG2	10:J:62:ARG:O	2.15	0.46
1:A:555:ASP:O	1:A:556:TRP:C	2.54	0.46
1:A:608:ILE:C	1:A:610:GLY:N	2.69	0.46
2:B:1003:ALA:HA	3:C:178:PHE:O	2.16	0.46
2:B:204:ILE:C	2:B:205:ILE:HD12	2.35	0.46
7:G:13:LEU:HD22	7:G:17:PHE:HB2	1.96	0.46
10:J:56:LEU:O	10:J:59:LYS:N	2.47	0.46
4:D:52:LEU:HD21	4:D:147:TYR:HE2	1.81	0.46
12:L:38:LEU:C	12:L:38:LEU:HD12	2.35	0.46
2:B:969:ARG:HD2	3:C:61:GLU:OE2	2.15	0.46
9:I:76:PRO:HD2	9:I:108:HIS:HD2	1.81	0.46
2:B:383:ASN:O	2:B:384:ARG:C	2.54	0.46
2:B:914:LYS:HE2	2:B:937:ALA:CB	2.46	0.46
2:B:377:PHE:O	2:B:379:GLY:N	2.49	0.46
8:H:130:ARG:HA	8:H:133:ASN:HB2	1.98	0.46
3:C:243:VAL:CG1	3:C:243:VAL:O	2.64	0.46
1:A:687:LYS:C	1:A:690:VAL:HG12	2.36	0.46
1:A:1342:GLU:HG3	5:E:198:ILE:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:11:GLN:HE21	8:H:52:GLN:HA	1.80	0.46
5:E:105:PHE:O	5:E:106:GLN:HB2	2.16	0.46
1:A:88:LYS:HG3	1:A:276:LEU:CD2	2.45	0.46
1:A:1203:ASN:O	1:A:1206:ASP:N	2.49	0.46
4:D:35:LEU:HD11	4:D:173:HIS:CD2	2.50	0.46
1:A:761:MET:O	1:A:803:SER:HB2	2.16	0.46
1:A:61:ILE:CG2	1:A:62:ASP:H	2.14	0.45
12:L:48:CYS:HB3	12:L:51:CYS:O	2.17	0.45
1:A:1293:SER:OG	1:A:1295:THR:CG2	2.65	0.45
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.97	0.45
1:A:897:TYR:CD1	1:A:897:TYR:N	2.84	0.45
5:E:198:ILE:HD11	5:E:212:ARG:HG3	1.97	0.45
2:B:408:LEU:CD1	2:B:408:LEU:N	2.77	0.45
1:A:12:ARG:HB3	2:B:1218:THR:CG2	2.47	0.45
2:B:46:GLN:OE1	2:B:47:GLN:HG2	2.15	0.45
2:B:899:ILE:CG2	2:B:900:ALA:N	2.79	0.45
2:B:37:PHE:C	2:B:37:PHE:HD1	2.19	0.45
8:H:108:SER:O	8:H:109:LYS:HB3	2.16	0.45
2:B:872:GLU:CD	2:B:914:LYS:HE3	2.36	0.45
8:H:38:LEU:HD12	8:H:39:THR:N	2.30	0.45
2:B:578:THR:O	2:B:589:VAL:HG13	2.15	0.45
1:A:1104:ILE:C	1:A:1106:ASN:N	2.70	0.45
11:K:6:ARG:O	11:K:9:LEU:HG	2.16	0.45
2:B:637:LEU:HD11	2:B:703:ILE:HD13	1.98	0.45
2:B:751:VAL:O	2:B:752:ALA:C	2.54	0.45
1:A:343:LYS:NZ	2:B:1151:LEU:O	2.42	0.45
1:A:289:ILE:O	1:A:292:ALA:N	2.43	0.45
1:A:1293:SER:OG	1:A:1295:THR:HG23	2.16	0.45
5:E:161:LYS:HD2	5:E:195:VAL:HG23	1.98	0.45
6:F:111:LEU:H	6:F:111:LEU:CD1	2.29	0.45
5:E:29:PHE:C	5:E:30:ILE:HG13	2.37	0.45
4:D:186:ASP:O	4:D:211:LEU:HD13	2.16	0.45
1:A:608:ILE:C	1:A:610:GLY:H	2.18	0.45
2:B:826:ALA:HB2	2:B:1087:PHE:HE2	1.81	0.45
2:B:1176:ASN:C	2:B:1178:ASN:N	2.66	0.45
8:H:41:ASP:C	8:H:42:ILE:HG13	2.37	0.45
9:I:68:LEU:CB	9:I:84:VAL:HG23	2.46	0.45
1:A:541:ILE:HD13	1:A:549:MET:CE	2.30	0.45
1:A:481:ASP:OD1	15:3:11:U:H5"	2.17	0.45
2:B:604:ARG:HB2	2:B:609:ILE:HG13	1.98	0.45
1:A:688:LYS:O	1:A:690:VAL:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:75:MET:O	5:E:76:GLY:O	2.35	0.45
2:B:313:MET:CE	2:B:386:LEU:HD22	2.47	0.45
6:F:109:VAL:HG13	6:F:127:GLU:OE1	2.16	0.45
2:B:429:PHE:HA	2:B:432:MET:CE	2.45	0.45
2:B:1197:PRO:HG2	2:B:1200:ALA:HB2	1.98	0.45
8:H:135:LEU:HD13	8:H:137:GLN:OE1	2.16	0.45
8:H:62:SER:OG	8:H:64:ASN:ND2	2.47	0.45
1:A:568:PRO:HB2	3:C:221:TYR:CZ	2.52	0.45
2:B:1081:LEU:HD12	2:B:1085:ILE:HD11	1.99	0.45
14:1:22:DC:H2"	14:1:23:BRU:OP2	2.16	0.45
3:C:144:ILE:HG22	3:C:145:CYS:N	2.32	0.45
2:B:243:ALA:CB	2:B:250:PHE:O	2.64	0.45
4:D:52:LEU:H	4:D:182:SER:HB3	1.82	0.45
7:G:139:ILE:HG23	7:G:140:LYS:N	2.31	0.45
2:B:25:ILE:HG22	2:B:658:ILE:HD12	1.97	0.45
3:C:112:ASN:N	3:C:112:ASN:HD22	2.12	0.45
2:B:1032:SER:HB3	2:B:1089:PRO:HG2	1.99	0.45
5:E:48:ASP:HB3	5:E:54:GLN:CD	2.36	0.45
1:A:369:SER:CB	11:K:2:ASN:OD1	2.64	0.45
1:A:828:ALA:C	1:A:831:THR:HG22	2.35	0.45
1:A:843:LYS:NZ	1:A:1401:SER:OG	2.49	0.45
1:A:1353:TYR:O	1:A:1353:TYR:HD2	2.00	0.45
1:A:1387:HIS:CE1	13:2:4:DA:H4'	2.52	0.45
4:D:138:ASN:HD21	7:G:35:GLU:CB	2.29	0.45
1:A:442:VAL:HG21	1:A:489:LEU:HD11	1.99	0.45
8:H:37:LYS:HD2	8:H:126:GLU:OE1	2.16	0.45
1:A:150:THR:O	1:A:150:THR:HG22	2.17	0.45
2:B:370:PHE:HD2	2:B:373:ARG:HD3	1.82	0.45
12:L:55:ILE:CG1	12:L:56:LEU:H	2.23	0.45
2:B:1073:TYR:OH	3:C:179:GLU:HG3	2.15	0.45
8:H:92:ASP:C	8:H:93:TYR:CD1	2.89	0.45
3:C:99:LEU:CD2	3:C:99:LEU:N	2.80	0.45
1:A:709:THR:HG23	9:I:94:ASP:HA	1.98	0.45
2:B:39:ARG:HG2	2:B:39:ARG:NH1	2.31	0.45
4:D:206:GLU:O	4:D:210:ILE:HG13	2.16	0.45
1:A:1289:ARG:HD2	1:A:1303:GLU:OE2	2.16	0.45
2:B:916:THR:HB	2:B:935:ARG:HG3	1.97	0.45
8:H:124:ARG:HD3	8:H:124:ARG:C	2.37	0.45
8:H:129:TYR:HA	8:H:131:ASN:HD21	1.82	0.45
1:A:93:VAL:CG1	1:A:301:ALA:HB1	2.45	0.45
2:B:549:THR:CG2	2:B:550:ASP:N	2.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:20:PHE:HE1	3:C:22:LEU:HD13	1.82	0.45
3:C:31:ASN:O	3:C:32:SER:C	2.52	0.45
2:B:758:PHE:N	2:B:759:PRO:CD	2.80	0.45
4:D:35:LEU:CD1	4:D:35:LEU:N	2.80	0.45
2:B:507:LYS:C	2:B:508:LEU:HD23	2.37	0.45
2:B:860:MET:HG2	2:B:861:ASP:N	2.32	0.45
12:L:29:TYR:N	12:L:29:TYR:HD2	2.13	0.45
10:J:22:LEU:HD12	10:J:22:LEU:HA	1.71	0.45
1:A:53:LEU:O	1:A:56:PRO:HG3	2.17	0.45
1:A:57:ARG:O	1:A:58:LEU:O	2.34	0.45
1:A:596:THR:C	1:A:598:LEU:N	2.70	0.45
9:I:55:THR:OG1	9:I:100:PHE:CD2	2.69	0.45
2:B:1068:GLY:O	2:B:1069:PHE:C	2.54	0.45
2:B:797:TYR:HE1	2:B:854:LEU:CD2	2.29	0.45
2:B:244:LEU:HD13	2:B:247:GLY:O	2.16	0.45
2:B:842:ASN:O	2:B:846:ILE:HG13	2.17	0.45
7:G:121:PHE:HB2	7:G:130:TYR:CE2	2.52	0.45
14:1:12:DG:H2'	14:1:13:DT:H72	1.98	0.45
1:A:80:HIS:O	1:A:243:PRO:HB3	2.15	0.45
1:A:843:LYS:HD3	1:A:846:GLU:OE2	2.16	0.45
1:A:1199:ARG:CG	1:A:1236:LEU:HD11	2.46	0.45
1:A:1438:THR:O	1:A:1438:THR:HG22	2.17	0.45
2:B:1050:ILE:CG2	2:B:1051:THR:N	2.79	0.45
2:B:615:MET:CG	2:B:626:ILE:HG12	2.46	0.45
11:K:68:PHE:CD2	11:K:68:PHE:N	2.80	0.45
1:A:90:VAL:HG13	1:A:297:GLN:OE1	2.16	0.45
1:A:693:VAL:HA	1:A:696:GLU:HB3	1.98	0.45
5:E:59:SER:O	5:E:60:PHE:HB3	2.17	0.45
8:H:39:THR:O	8:H:123:MET:HA	2.17	0.45
3:C:70:ILE:HD11	3:C:144:ILE:HD11	1.99	0.45
1:A:688:LYS:C	1:A:690:VAL:N	2.70	0.45
2:B:642:ASP:CA	2:B:649:LYS:HG3	2.47	0.45
2:B:68:THR:HG22	2:B:91:SER:HB3	1.97	0.45
4:D:195:ILE:HB	4:D:198:LEU:HD12	1.99	0.45
10:J:48:ARG:HE	10:J:49:MET:CE	2.29	0.45
1:A:685:GLU:HG3	1:A:686:ALA:N	2.32	0.45
1:A:645:LEU:HG	1:A:649:ILE:CD1	2.47	0.45
1:A:418:SER:C	1:A:420:ARG:N	2.71	0.45
1:A:573:SER:O	1:A:576:GLN:HB2	2.16	0.45
1:A:853:ASP:OD1	1:A:855:THR:CG2	2.65	0.45
10:J:58:GLU:HA	10:J:61:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:LEU:HD11	2:B:366:GLN:HE21	1.74	0.45
2:B:847:ASP:HB3	3:C:167:HIS:HE2	1.81	0.45
2:B:603:LEU:HB3	2:B:609:ILE:CD1	2.47	0.45
1:A:424:ILE:CG2	1:A:425:GLN:N	2.79	0.45
2:B:113:TYR:CE2	2:B:192:LEU:HD21	2.51	0.45
5:E:49:SER:OG	5:E:50:MET:N	2.48	0.45
2:B:269:ILE:HG22	2:B:282:ILE:HG23	1.99	0.45
3:C:123:ASN:OD1	3:C:124:LEU:N	2.50	0.45
2:B:218:SER:O	2:B:241:ARG:NH1	2.50	0.45
2:B:515:HIS:CD2	2:B:517:THR:HG23	2.52	0.45
2:B:794:ASN:C	2:B:795:ILE:HD12	2.37	0.45
1:A:731:ARG:O	1:A:735:VAL:HG23	2.17	0.45
2:B:848:ARG:HD3	10:J:11:GLY:HA2	1.97	0.45
2:B:1115:THR:HG22	2:B:1117:GLN:N	2.30	0.45
9:I:98:VAL:HG13	9:I:100:PHE:CE1	2.44	0.45
9:I:7:CYS:HB2	9:I:34:TYR:CD1	2.51	0.45
2:B:865:LYS:C	2:B:866:TYR:HD1	2.20	0.45
1:A:1208:THR:O	1:A:1211:GLN:HB2	2.17	0.45
2:B:840:ILE:CG2	2:B:994:TYR:HD1	2.31	0.45
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.99	0.45
11:K:40:HIS:O	11:K:41:THR:C	2.54	0.45
4:D:53:SER:HA	4:D:56:ARG:CB	2.47	0.45
2:B:63:ILE:HA	2:B:421:PHE:CE2	2.52	0.45
1:A:1410:PHE:HA	2:B:1212:ILE:HD11	1.98	0.45
1:A:1362:TYR:CD1	1:A:1363:VAL:N	2.85	0.45
1:A:476:SER:HB2	1:A:477:PRO:HD3	1.98	0.45
1:A:821:ARG:HB2	1:A:821:ARG:HH11	1.81	0.45
1:A:856:THR:O	1:A:856:THR:HG22	2.16	0.45
2:B:542:MET:CE	2:B:747:MET:HG3	2.47	0.44
1:A:1115:SER:C	1:A:1308:THR:HG22	2.37	0.44
2:B:361:LEU:HD21	2:B:377:PHE:HD2	1.82	0.44
1:A:367:PRO:HB3	1:A:465:TYR:O	2.18	0.44
1:A:443:LEU:HD22	1:A:455:MET:HE2	1.98	0.44
2:B:1001:PHE:HD1	2:B:1001:PHE:O	2.00	0.44
1:A:946:VAL:HG12	1:A:947:PHE:CE2	2.50	0.44
2:B:686:ASN:C	2:B:688:GLY:N	2.70	0.44
1:A:12:ARG:NH2	2:B:1192:TYR:CZ	2.83	0.44
5:E:121:MET:C	5:E:123:LEU:H	2.20	0.44
1:A:122:MET:HA	1:A:141:LEU:CD1	2.47	0.44
1:A:1291:VAL:HG22	1:A:1292:PRO:CD	2.47	0.44
5:E:92:THR:O	5:E:95:THR:HB	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:GLU:HB2	2:B:935:ARG:HH22	1.82	0.44
1:A:351:THR:H	1:A:468:PHE:HE1	1.65	0.44
5:E:124:VAL:N	5:E:125:PRO:CD	2.80	0.44
10:J:53:HIS:CD2	10:J:54:VAL:C	2.91	0.44
2:B:273:LEU:HD22	2:B:360:PHE:HD1	1.82	0.44
2:B:519:TRP:HE1	2:B:635:ARG:NH2	2.16	0.44
4:D:51:ASN:O	4:D:52:LEU:C	2.53	0.44
5:E:207:ARG:CB	5:E:207:ARG:NH1	2.80	0.44
5:E:167:ARG:HD3	5:E:167:ARG:HA	1.81	0.44
3:C:147:LEU:HB2	3:C:151:GLN:HB2	1.99	0.44
11:K:53:ASP:C	11:K:55:LYS:H	2.20	0.44
1:A:988:LEU:O	1:A:992:ASP:HB2	2.17	0.44
1:A:1206:ASP:HB3	1:A:1274:ARG:HH12	1.83	0.44
2:B:506:GLY:O	2:B:507:LYS:HB2	2.16	0.44
2:B:506:GLY:O	2:B:507:LYS:HG2	2.17	0.44
6:F:103:MET:HE3	7:G:66:GLY:N	2.32	0.44
2:B:311:LEU:O	2:B:312:GLU:C	2.55	0.44
1:A:806:ARG:HH12	2:B:729:ILE:HD12	1.81	0.44
2:B:916:THR:CB	2:B:935:ARG:HD2	2.44	0.44
1:A:244:PRO:O	1:A:246:VAL:N	2.51	0.44
2:B:620:ARG:NH2	9:I:86:PHE:HB3	2.33	0.44
1:A:913:LEU:CG	1:A:914:GLU:N	2.80	0.44
2:B:708:GLU:O	2:B:709:ASP:C	2.54	0.44
1:A:470:LEU:HD13	1:A:487:MET:HE1	1.99	0.44
1:A:115:LEU:HD22	1:A:119:ASN:CB	2.48	0.44
1:A:289:ILE:C	1:A:291:GLU:H	2.21	0.44
5:E:144:ILE:HG13	5:E:145:THR:H	1.83	0.44
3:C:182:PRO:HD2	3:C:210:GLU:OE1	2.17	0.44
1:A:1094:VAL:HG13	1:A:1113:THR:CG2	2.47	0.44
1:A:239:LEU:HD12	1:A:239:LEU:HA	1.66	0.44
2:B:579:ARG:CB	2:B:586:TRP:HE1	2.30	0.44
1:A:196:GLU:HG2	1:A:197:PRO:N	2.32	0.44
4:D:35:LEU:H	4:D:35:LEU:CD1	2.30	0.44
6:F:99:LEU:O	6:F:103:MET:HG3	2.17	0.44
1:A:1150:SER:HB3	1:A:1195:LEU:CD2	2.48	0.44
2:B:186:GLU:HG3	10:J:62:ARG:HH22	1.81	0.44
1:A:326:ARG:HG2	1:A:326:ARG:NH1	2.32	0.44
2:B:171:PRO:HD2	2:B:457:LEU:HD13	2.00	0.44
4:D:20:GLU:O	4:D:20:GLU:HG2	2.17	0.44
2:B:1214:PRO:O	2:B:1214:PRO:HG2	2.18	0.44
5:E:63:ASN:HB3	5:E:64:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:522:VAL:CG1	2:B:523:CYS:N	2.79	0.44
1:A:498:ARG:O	1:A:501:LEU:N	2.51	0.44
6:F:154:ASP:HB3	6:F:155:LEU:H	1.64	0.44
7:G:56:ILE:O	7:G:57:GLN:HB2	2.18	0.44
2:B:309:GLN:HG3	9:I:52:ILE:HD12	2.00	0.44
2:B:1072:MET:HB2	2:B:1085:ILE:HD12	2.00	0.44
1:A:1116:LEU:HD12	1:A:1117:THR:N	2.32	0.44
2:B:797:TYR:HE1	2:B:854:LEU:HD23	1.83	0.44
1:A:899:VAL:CB	1:A:929:LEU:HD12	2.36	0.44
4:D:153:ARG:CZ	4:D:184:ALA:HA	2.47	0.44
14:I:11:DA:H2''	14:I:12:DG:H5'	1.99	0.44
1:A:774:ARG:H	1:A:774:ARG:HG2	1.59	0.44
3:C:214:ASN:O	3:C:217:ASP:OD2	2.33	0.44
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.83	0.44
5:E:11:ARG:O	5:E:13:TRP:N	2.50	0.44
11:K:53:ASP:OD2	11:K:81:TYR:OH	2.35	0.44
1:A:1205:LYS:O	1:A:1206:ASP:C	2.55	0.44
1:A:172:PRO:HB3	1:A:185:TRP:CD2	2.53	0.44
4:D:185:CYS:HB2	4:D:211:LEU:HD21	2.00	0.44
5:E:37:LEU:CD1	5:E:41:ASP:HB2	2.47	0.44
1:A:89:PRO:CG	1:A:205:GLU:HG3	2.47	0.44
1:A:1254:ALA:O	1:A:1255:GLU:CB	2.66	0.44
1:A:300:VAL:HG12	1:A:300:VAL:O	2.18	0.44
2:B:426:LYS:O	2:B:426:LYS:HG3	2.17	0.44
3:C:69:LEU:N	3:C:69:LEU:HD12	2.20	0.44
6:F:89:GLU:C	6:F:93:ILE:HD12	2.38	0.44
8:H:33:GLN:NE2	8:H:129:TYR:CE2	2.85	0.44
2:B:801:LYS:N	10:J:52:THR:HG22	2.33	0.44
2:B:912:ILE:HD11	2:B:966:VAL:HG23	2.00	0.44
1:A:688:LYS:CE	1:A:691:LEU:HD23	2.47	0.44
1:A:523:ILE:CG1	1:A:622:VAL:HG22	2.44	0.44
2:B:882:THR:O	2:B:883:LEU:HB2	2.17	0.44
2:B:1040:ASN:O	2:B:1041:GLU:C	2.56	0.44
2:B:1020:ARG:CG	2:B:1020:ARG:NH1	2.80	0.44
11:K:90:ALA:O	11:K:94:ILE:HG13	2.18	0.44
3:C:233:GLU:OE1	10:J:12:LYS:HE2	2.18	0.44
1:A:224:PHE:CD2	1:A:231:PRO:HG3	2.53	0.44
2:B:505:ASP:O	2:B:506:GLY:C	2.55	0.44
3:C:124:LEU:H	3:C:124:LEU:HD12	1.81	0.44
2:B:56:ASP:HB3	2:B:57:TYR:CD1	2.53	0.44
4:D:195:ILE:HG22	4:D:198:LEU:HG	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:GLU:CD	2:B:1108:ARG:HH22	2.21	0.44
1:A:442:VAL:HG23	1:A:489:LEU:HD11	1.99	0.44
1:A:38:PRO:CA	1:A:270:LEU:HD23	2.47	0.44
1:A:699:ALA:O	1:A:700:ASN:HB3	2.18	0.44
1:A:700:ASN:C	1:A:701:LEU:HD23	2.38	0.44
1:A:77:CYS:C	1:A:78:PRO:O	2.54	0.44
1:A:360:GLU:HB2	1:A:363:GLN:HG3	1.99	0.44
4:D:70:PHE:O	4:D:71:LYS:HG3	2.17	0.44
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.98	0.44
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.47	0.44
10:J:14:VAL:HG12	10:J:50:ILE:HD11	1.98	0.44
7:G:145:VAL:HG12	7:G:146:LYS:N	2.33	0.44
5:E:16:PHE:O	5:E:17:ARG:C	2.55	0.44
11:K:53:ASP:O	11:K:56:VAL:N	2.49	0.44
2:B:460:ALA:C	2:B:462:ALA:H	2.21	0.44
1:A:525:GLN:O	1:A:526:ASP:C	2.56	0.44
2:B:593:PRO:C	2:B:595:ARG:N	2.69	0.44
8:H:38:LEU:HD13	8:H:125:LEU:HD12	1.99	0.44
3:C:66:ARG:O	3:C:68:GLY:N	2.51	0.44
2:B:707:PRO:HG2	2:B:708:GLU:N	2.30	0.44
9:I:14:LEU:HA	9:I:28:GLU:O	2.18	0.44
1:A:1134:ILE:HG13	1:A:1134:ILE:H	1.52	0.44
2:B:293:PRO:C	2:B:294:ASP:O	2.55	0.44
1:A:562:THR:HA	1:A:563:PRO:HD3	1.90	0.44
2:B:801:LYS:H	10:J:52:THR:HG22	1.82	0.44
3:C:15:LYS:O	3:C:240:VAL:HG22	2.18	0.44
2:B:652:LYS:HB3	2:B:689:LEU:HD22	1.99	0.44
2:B:866:TYR:HB2	2:B:870:ILE:HB	2.00	0.44
2:B:212:LEU:HD23	2:B:480:SER:HB2	2.00	0.44
2:B:272:THR:HG23	2:B:279:ASP:OD1	2.18	0.44
1:A:793:SER:HB2	1:A:794:PRO:HD2	1.99	0.44
2:B:999:MET:HA	2:B:999:MET:HE2	1.98	0.44
1:A:850:VAL:HG12	1:A:1060:PRO:HA	2.00	0.44
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.53	0.44
7:G:88:ASP:N	7:G:88:ASP:OD2	2.45	0.44
1:A:1450:LEU:CD2	7:G:19:GLY:O	2.65	0.44
5:E:157:SER:C	5:E:159:ASP:H	2.20	0.44
11:K:78:THR:HG22	11:K:79:GLU:H	1.83	0.44
1:A:122:MET:CE	1:A:126:LEU:HD21	2.47	0.44
11:K:27:ALA:HB1	11:K:28:PRO:HD2	1.99	0.44
2:B:948:ILE:O	2:B:968:VAL:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:64:VAL:O	4:D:66:ARG:N	2.50	0.44
1:A:789:LYS:CD	2:B:620:ARG:HH12	2.30	0.44
10:J:16:ASP:O	10:J:18:TRP:N	2.51	0.44
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.53	0.44
2:B:953:LEU:HD22	2:B:965:LYS:HB2	2.00	0.44
1:A:433:GLU:OE2	2:B:1108:ARG:NH2	2.51	0.44
2:B:185:THR:H	2:B:188:ASP:HB2	1.83	0.44
1:A:516:SER:O	1:A:518:LYS:N	2.51	0.44
2:B:1131:GLY:N	2:B:1134:GLU:OE1	2.50	0.44
5:E:67:GLU:O	5:E:70:SER:HB2	2.18	0.44
1:A:1171:GLN:H	1:A:1171:GLN:HG3	1.49	0.44
4:D:67:ARG:HD3	4:D:71:LYS:HZ1	1.82	0.43
1:A:92:HIS:O	1:A:93:VAL:C	2.56	0.43
1:A:1259:MET:HA	1:A:1262:LYS:CD	2.41	0.43
12:L:38:LEU:CG	12:L:39:SER:N	2.81	0.43
1:A:1167:GLU:O	1:A:1170:ILE:HD12	2.17	0.43
2:B:966:VAL:HG12	2:B:967:ARG:H	1.82	0.43
1:A:1237:ILE:CG2	1:A:1238:ILE:N	2.80	0.43
2:B:1045:SER:O	2:B:1046:PRO:O	2.35	0.43
5:E:100:ILE:HG23	5:E:105:PHE:HB2	2.00	0.43
2:B:616:ILE:CG1	2:B:697:GLU:HA	2.48	0.43
2:B:418:LYS:HE2	2:B:422:LYS:CE	2.48	0.43
2:B:186:GLU:HG3	10:J:62:ARG:NH2	2.33	0.43
2:B:186:GLU:CG	10:J:62:ARG:HH12	2.30	0.43
5:E:154:ILE:O	5:E:196:VAL:HA	2.17	0.43
1:A:730:GLY:C	1:A:732:LEU:N	2.71	0.43
9:I:25:LEU:HB3	9:I:38:ALA:CB	2.48	0.43
6:F:152:ILE:HG22	6:F:153:VAL:N	2.33	0.43
1:A:67:CYS:O	1:A:68:GLN:HG3	2.18	0.43
9:I:8:ARG:HG2	9:I:34:TYR:CE1	2.52	0.43
2:B:604:ARG:CA	2:B:609:ILE:HG13	2.47	0.43
8:H:11:GLN:O	8:H:28:ALA:HB1	2.18	0.43
1:A:1397:LEU:CB	1:A:1426:GLU:OE1	2.65	0.43
5:E:80:VAL:HG12	5:E:82:PHE:HE1	1.83	0.43
2:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.48	0.43
1:A:608:ILE:HD12	1:A:613:ILE:CD1	2.48	0.43
1:A:122:MET:HA	1:A:141:LEU:HD11	2.00	0.43
2:B:522:VAL:HG12	2:B:523:CYS:N	2.31	0.43
10:J:21:TYR:HB2	10:J:39:LEU:CD1	2.48	0.43
3:C:136:ASP:OD2	3:C:137:LYS:N	2.52	0.43
2:B:535:LEU:HA	2:B:535:LEU:HD23	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:ILE:CD1	3:C:144:ILE:HD11	2.49	0.43
1:A:915:SER:O	1:A:919:ILE:HB	2.18	0.43
9:I:34:TYR:C	9:I:34:TYR:HD2	2.18	0.43
1:A:356:ASP:HA	1:A:357:PRO:HD2	1.78	0.43
1:A:381:THR:O	1:A:382:PRO:C	2.55	0.43
3:C:241:ASP:CG	3:C:242:GLN:N	2.71	0.43
10:J:64:ASN:CB	10:J:65:PRO:CD	2.89	0.43
2:B:831:SER:HB3	2:B:994:TYR:OH	2.18	0.43
2:B:351:TYR:CD1	2:B:355:ILE:HD11	2.53	0.43
5:E:68:SER:HB3	5:E:75:MET:HE1	1.99	0.43
3:C:263:THR:C	3:C:265:MET:N	2.70	0.43
6:F:79:ARG:CG	6:F:144:GLU:HB3	2.49	0.43
2:B:880:THR:O	2:B:880:THR:HG22	2.17	0.43
1:A:34:LYS:HD3	1:A:57:ARG:NH2	2.32	0.43
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.18	0.43
7:G:127:PRO:O	7:G:138:THR:HG21	2.17	0.43
3:C:172:PRO:O	3:C:235:VAL:HG23	2.18	0.43
11:K:55:LYS:CB	11:K:81:TYR:CD1	3.01	0.43
10:J:24:LEU:HA	10:J:28:ASP:HB2	1.99	0.43
1:A:1076:ALA:HA	1:A:1079:MET:HE3	2.01	0.43
1:A:1387:HIS:NE2	13:2:4:DA:H5'	2.33	0.43
2:B:134:LYS:NZ	2:B:164:LYS:HE2	2.33	0.43
4:D:177:VAL:HG12	4:D:177:VAL:O	2.19	0.43
2:B:589:VAL:HG12	2:B:590:HIS:O	2.19	0.43
2:B:542:MET:HE2	2:B:747:MET:HE2	2.00	0.43
8:H:130:ARG:H	8:H:130:ARG:HH11	1.65	0.43
1:A:108:MET:SD	1:A:210:ILE:HD13	2.58	0.43
4:D:156:ASP:C	4:D:158:GLU:N	2.70	0.43
8:H:24:CYS:SG	8:H:44:VAL:HG21	2.58	0.43
1:A:896:ARG:NH2	1:A:1030:ARG:NH2	2.66	0.43
1:A:718:VAL:HG12	1:A:722:LEU:HD11	2.00	0.43
5:E:186:LEU:O	5:E:187:TYR:C	2.56	0.43
2:B:840:ILE:HG21	2:B:994:TYR:CD1	2.53	0.43
2:B:1037:LEU:CD2	2:B:1064:TYR:HE1	2.32	0.43
2:B:980:PHE:HD2	2:B:1094:ARG:HA	1.82	0.43
2:B:520:GLY:O	2:B:521:LEU:HD23	2.18	0.43
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.66	0.43
2:B:1045:SER:O	2:B:1048:THR:CG2	2.67	0.43
1:A:233:TRP:C	1:A:235:ILE:N	2.71	0.43
2:B:63:ILE:HG23	2:B:64:CYS:SG	2.58	0.43
6:F:103:MET:CE	7:G:66:GLY:N	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:VAL:HG11	2:B:448:ILE:CD1	2.48	0.43
1:A:920:LEU:HD23	1:A:920:LEU:C	2.38	0.43
9:I:98:VAL:CG1	9:I:100:PHE:HE1	2.29	0.43
9:I:50:THR:HG21	9:I:52:ILE:HG12	1.96	0.43
1:A:1129:GLU:O	1:A:1130:GLN:C	2.56	0.43
8:H:104:PHE:CD2	8:H:114:VAL:HG12	2.54	0.43
1:A:942:PHE:HE1	5:E:207:ARG:HD3	1.83	0.43
2:B:468:GLU:HB3	2:B:469:GLN:H	1.32	0.43
3:C:185:LYS:HE2	3:C:213:PRO:HA	1.99	0.43
2:B:282:ILE:HG13	2:B:283:VAL:N	2.33	0.43
2:B:582:VAL:HG22	2:B:626:ILE:HG21	2.01	0.43
13:2:4:DA:H2''	13:2:5:DC:H6	1.83	0.43
3:C:101:LEU:HD12	3:C:118:LEU:CD2	2.47	0.43
9:I:104:LEU:HD23	9:I:104:LEU:N	2.33	0.43
7:G:21:ARG:HD2	7:G:24:GLN:CB	2.49	0.43
4:D:31:GLN:C	4:D:33:PHE:H	2.22	0.43
1:A:1365:TYR:CE2	1:A:1369:ALA:HB2	2.54	0.43
1:A:849:MET:HB3	1:A:1063:MET:SD	2.58	0.43
2:B:887:HIS:CD2	2:B:887:HIS:N	2.87	0.43
1:A:255:SER:O	1:A:256:GLN:HG3	2.19	0.43
1:A:49:LYS:CD	1:A:55:ASP:HB3	2.49	0.43
7:G:13:LEU:HD21	7:G:17:PHE:CB	2.49	0.43
9:I:55:THR:HG21	9:I:109:ILE:HD13	2.00	0.43
1:A:414:ASP:OD1	1:A:416:ARG:HG2	2.19	0.43
3:C:77:ILE:HG23	3:C:161:LYS:HE3	1.99	0.43
3:C:97:VAL:HG12	3:C:99:LEU:CD2	2.48	0.43
9:I:95:THR:HG22	9:I:96:SER:N	2.34	0.43
3:C:233:GLU:CG	3:C:234:SER:N	2.82	0.43
9:I:60:GLN:CD	9:I:107:SER:HG	2.21	0.43
4:D:118:THR:HG21	4:D:121:LYS:CE	2.48	0.43
14:1:19:DT:H2''	14:1:20:DG:O5'	2.18	0.43
2:B:874:PHE:HB3	2:B:896:ASP:O	2.19	0.43
11:K:31:VAL:CG2	11:K:83:PRO:HG3	2.49	0.43
2:B:729:ILE:O	2:B:729:ILE:HG22	2.18	0.43
3:C:64:ALA:O	3:C:65:HIS:C	2.57	0.43
2:B:1148:LYS:HE3	7:G:64:THR:OG1	2.19	0.43
6:F:133:VAL:HG13	6:F:146:TRP:O	2.18	0.43
1:A:598:LEU:CD1	8:H:124:ARG:HB2	2.48	0.43
2:B:244:LEU:HD12	2:B:250:PHE:HD1	1.84	0.43
2:B:287:ARG:HB3	2:B:330:ALA:HB2	2.01	0.43
3:C:235:VAL:CG1	10:J:13:VAL:HG22	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:GLU:HG3	2:B:66:ASP:H	1.84	0.43
9:I:82:GLU:OE2	9:I:104:LEU:HD12	2.19	0.43
5:E:91:LYS:O	5:E:93:MET:N	2.51	0.43
5:E:157:SER:OG	5:E:160:GLU:HG3	2.19	0.43
1:A:1451:VAL:HG12	1:A:1452:LYS:N	2.34	0.43
2:B:1069:PHE:HD1	2:B:1069:PHE:H	1.66	0.43
2:B:711:GLU:H	2:B:712:PRO:HD2	1.83	0.43
6:F:84:TYR:N	6:F:84:TYR:CD1	2.87	0.43
3:C:174:ALA:O	3:C:175:ALA:HB3	2.19	0.43
2:B:635:ARG:NH2	2:B:742:GLU:OE2	2.52	0.43
1:A:754:SER:O	1:A:757:ASN:HB2	2.18	0.43
2:B:469:GLN:CG	2:B:470:LYS:N	2.80	0.43
1:A:79:GLY:H	2:B:1205:GLN:HE22	1.67	0.43
3:C:213:PRO:HG2	3:C:214:ASN:H	1.83	0.43
2:B:57:TYR:H	2:B:57:TYR:HD1	1.65	0.43
1:A:1018:PHE:O	1:A:1021:LEU:HB3	2.18	0.43
7:G:53:ASN:ND2	7:G:53:ASN:N	2.67	0.43
3:C:80:LEU:HD12	3:C:94:LYS:O	2.18	0.43
1:A:270:LEU:O	1:A:274:ILE:HG13	2.19	0.43
1:A:457:ALA:HB3	1:A:506:ALA:HA	2.00	0.43
4:D:32:GLU:O	4:D:33:PHE:CG	2.72	0.43
1:A:372:LYS:O	1:A:435:HIS:HE1	2.02	0.43
7:G:126:ASN:HD22	7:G:127:PRO:N	2.17	0.43
1:A:1120:LEU:H	1:A:1120:LEU:HG	1.37	0.43
11:K:91:CYS:O	11:K:94:ILE:HB	2.19	0.43
1:A:162:VAL:HG12	1:A:163:SER:N	2.34	0.43
1:A:605:MET:HE2	1:A:607:ILE:CG1	2.49	0.43
1:A:939:ASP:OD1	1:A:1023:ARG:NH1	2.52	0.43
1:A:69:THR:O	1:A:70:CYS:C	2.57	0.42
8:H:113:ALA:HB1	8:H:124:ARG:HE	1.83	0.42
4:D:14:ARG:O	4:D:16:LYS:N	2.44	0.42
2:B:509:ALA:HB1	2:B:513:GLN:CD	2.39	0.42
1:A:401:GLY:C	1:A:435:HIS:CD2	2.92	0.42
2:B:737:THR:O	2:B:738:PHE:C	2.57	0.42
1:A:106:VAL:CG1	1:A:107:CYS:H	2.31	0.42
1:A:6:TYR:CD1	1:A:7:SER:N	2.87	0.42
2:B:654:ARG:H	2:B:657:HIS:CD2	2.36	0.42
12:L:59:ALA:O	12:L:60:ARG:O	2.37	0.42
2:B:1187:ASN:OD1	2:B:1188:LYS:N	2.52	0.42
8:H:12:VAL:CG2	8:H:53:ASP:HB2	2.49	0.42
2:B:39:ARG:HE	2:B:665:GLU:HG2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:72:PHE:CD1	5:E:72:PHE:N	2.86	0.42
8:H:100:THR:HG22	8:H:101:ALA:N	2.34	0.42
7:G:142:ARG:C	7:G:143:ILE:HG13	2.39	0.42
2:B:67:SER:O	2:B:68:THR:O	2.36	0.42
2:B:610:ASN:HA	2:B:611:PRO:HD3	1.90	0.42
2:B:508:LEU:HD23	2:B:508:LEU:N	2.34	0.42
3:C:263:THR:C	3:C:265:MET:H	2.17	0.42
1:A:341:MET:CE	2:B:1135:ARG:NH1	2.81	0.42
1:A:478:TYR:O	1:A:479:ASN:HB3	2.19	0.42
1:A:1050:GLU:O	1:A:1053:PHE:HB3	2.19	0.42
1:A:1410:PHE:HD2	2:B:1212:ILE:CD1	2.32	0.42
3:C:63:ILE:O	3:C:64:ALA:C	2.57	0.42
1:A:244:PRO:O	1:A:247:ARG:N	2.51	0.42
1:A:372:LYS:O	1:A:435:HIS:CE1	2.72	0.42
2:B:770:GLN:OE1	2:B:983:ARG:CA	2.56	0.42
2:B:29:ASP:CB	2:B:658:ILE:HD13	2.49	0.42
8:H:16:ASP:O	8:H:24:CYS:HA	2.18	0.42
1:A:1035:TYR:O	1:A:1036:ARG:HB2	2.18	0.42
1:A:690:VAL:HG23	1:A:718:VAL:HG13	2.00	0.42
8:H:11:GLN:C	8:H:28:ALA:HB1	2.39	0.42
3:C:213:PRO:O	3:C:214:ASN:CB	2.67	0.42
1:A:1283:VAL:O	1:A:1306:LEU:HA	2.18	0.42
7:G:88:ASP:HA	7:G:143:ILE:O	2.19	0.42
2:B:407:ASP:C	2:B:408:LEU:HD12	2.39	0.42
4:D:196:PRO:O	4:D:197:SER:C	2.58	0.42
1:A:888:GLY:O	1:A:940:ARG:NH2	2.52	0.42
11:K:86:ALA:HA	11:K:89:ASN:ND2	2.34	0.42
4:D:155:ARG:HG3	4:D:219:THR:HG21	1.96	0.42
8:H:33:GLN:C	8:H:35:GLN:H	2.22	0.42
1:A:107:CYS:CB	1:A:114:LEU:HD21	2.40	0.42
4:D:156:ASP:O	4:D:157:GLN:C	2.57	0.42
2:B:866:TYR:HB3	2:B:870:ILE:HD12	2.01	0.42
2:B:466:TRP:CE3	2:B:466:TRP:HA	2.54	0.42
3:C:97:VAL:HG21	3:C:129:ILE:HG22	2.00	0.42
2:B:1082:MET:HA	3:C:189:THR:HA	2.01	0.42
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.52	0.42
2:B:1099:VAL:HG13	2:B:1100:ASP:H	1.84	0.42
2:B:579:ARG:HG2	2:B:579:ARG:HH11	1.82	0.42
2:B:398:ARG:CB	2:B:398:ARG:HH11	2.32	0.42
2:B:103:ASN:ND2	2:B:108:VAL:O	2.52	0.42
2:B:841:MET:O	2:B:993:THR:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:935:GLN:O	1:A:938:LYS:N	2.52	0.42
1:A:359:LEU:HD23	1:A:359:LEU:HA	1.80	0.42
1:A:861:GLY:O	1:A:862:ASN:C	2.58	0.42
10:J:57:ILE:HG23	10:J:58:GLU:N	2.34	0.42
1:A:549:MET:CE	1:A:656:TRP:HD1	2.32	0.42
2:B:600:LEU:HA	2:B:603:LEU:HB2	2.00	0.42
2:B:603:LEU:HD13	2:B:608:ASP:CB	2.40	0.42
11:K:47:ARG:CB	11:K:47:ARG:HH11	2.23	0.42
1:A:1011:GLN:HE22	1:A:1015:VAL:HG21	1.85	0.42
1:A:774:ARG:HG3	1:A:797:LYS:HB3	2.01	0.42
4:D:29:LEU:HB3	7:G:82:PHE:HE2	1.82	0.42
2:B:398:ARG:NH1	2:B:398:ARG:CB	2.82	0.42
2:B:65:GLU:HG3	2:B:66:ASP:N	2.35	0.42
5:E:153:HIS:CE1	5:E:184:VAL:HG11	2.54	0.42
2:B:1212:ILE:O	2:B:1214:PRO:HD3	2.19	0.42
1:A:49:LYS:HZ1	1:A:61:ILE:H	1.62	0.42
3:C:221:TYR:HD1	3:C:222:LYS:N	2.17	0.42
2:B:806:THR:H	2:B:809:MET:HE3	1.82	0.42
2:B:1104:HIS:HB2	2:B:1122:ARG:HD2	2.01	0.42
2:B:798:TYR:CE2	3:C:62:PHE:CZ	2.94	0.42
4:D:40:HIS:HE1	7:G:7:LEU:O	2.01	0.42
3:C:258:ILE:CD1	3:C:258:ILE:N	2.83	0.42
1:A:1232:ASN:O	1:A:1233:ASP:O	2.38	0.42
1:A:1387:HIS:CD2	13:2:4:DA:H5'	2.54	0.42
2:B:734:HIS:O	2:B:735:ALA:CB	2.66	0.42
7:G:49:LEU:HG	7:G:76:ALA:HA	2.02	0.42
7:G:154:VAL:HB	7:G:155:SER:H	1.41	0.42
2:B:498:THR:O	2:B:536:VAL:HA	2.18	0.42
1:A:253:ASN:ND2	2:B:884:ARG:HD2	2.35	0.42
2:B:878:GLN:HB3	2:B:879:ARG:HH11	1.85	0.42
1:A:75:ASN:HD22	2:B:1116:ARG:NH1	2.17	0.42
8:H:102:TYR:OH	8:H:122:LEU:HD22	2.20	0.42
3:C:66:ARG:C	3:C:68:GLY:N	2.73	0.42
2:B:360:PHE:CE2	2:B:361:LEU:HD13	2.54	0.42
2:B:95:ILE:CD1	2:B:130:VAL:HG22	2.50	0.42
2:B:703:ILE:HA	2:B:740:HIS:O	2.20	0.42
1:A:381:THR:HG23	1:A:382:PRO:CD	2.39	0.42
1:A:904:THR:CG2	1:A:904:THR:O	2.68	0.42
1:A:1155:ASP:OD2	1:A:1162:VAL:N	2.47	0.42
2:B:758:PHE:CE1	2:B:1027:ILE:CG2	3.02	0.42
2:B:236:HIS:O	2:B:237:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:82:ASP:OD1	11:K:84:LYS:N	2.53	0.42
1:A:141:LEU:HD23	1:A:141:LEU:HA	1.84	0.42
9:I:10:CYS:O	9:I:11:ASN:C	2.55	0.42
7:G:59:GLY:CA	7:G:70:PHE:CD2	3.01	0.42
1:A:316:GLN:O	1:A:317:LYS:C	2.57	0.42
1:A:784:LEU:HB3	1:A:785:PRO:HD2	2.02	0.42
9:I:8:ARG:HG2	9:I:34:TYR:CD1	2.54	0.42
2:B:637:LEU:O	2:B:690:VAL:HG13	2.19	0.42
1:A:382:PRO:HD3	1:A:428:TYR:HD2	1.81	0.42
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.18	0.42
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.85	0.42
2:B:469:GLN:O	2:B:472:ALA:CB	2.62	0.42
3:C:98:VAL:HG13	3:C:157:CYS:O	2.17	0.42
1:A:710:LEU:O	1:A:714:PHE:N	2.53	0.42
2:B:280:ILE:HG23	2:B:281:PRO:HD2	2.02	0.42
1:A:1287:TYR:CD1	1:A:1305:VAL:HG21	2.54	0.42
7:G:90:THR:CG2	7:G:91:VAL:N	2.83	0.42
2:B:1025:HIS:O	2:B:1026:LEU:C	2.57	0.42
1:A:12:ARG:HB3	2:B:1218:THR:HG22	2.02	0.42
2:B:210:LYS:HE2	2:B:461:LEU:O	2.20	0.42
1:A:1454:MET:O	1:A:1454:MET:HG3	2.20	0.42
1:A:409:SER:O	1:A:410:GLY:C	2.57	0.42
4:D:122:GLU:HA	4:D:125:SER:HB3	2.00	0.42
3:C:79:GLN:O	3:C:79:GLN:HG3	2.18	0.42
1:A:377:PRO:HG2	1:A:377:PRO:O	2.20	0.42
2:B:736:THR:O	2:B:736:THR:HG22	2.19	0.42
2:B:34:ILE:HG12	2:B:542:MET:HE2	2.01	0.42
9:I:111:THR:CG2	9:I:113:ASP:H	2.32	0.42
2:B:557:PHE:HZ	2:B:603:LEU:HD11	1.85	0.42
14:1:10:DA:C2'	14:1:11:DA:C8	3.02	0.42
12:L:58:LYS:O	12:L:58:LYS:HG2	2.19	0.42
5:E:22:MET:HG3	5:E:187:TYR:CD1	2.55	0.42
2:B:831:SER:HB2	2:B:833:TYR:CD1	2.55	0.42
1:A:1305:VAL:CG1	1:A:1306:LEU:N	2.83	0.42
1:A:153:PRO:HD3	1:A:161:LEU:HD13	2.01	0.42
7:G:90:THR:O	7:G:102:GLN:N	2.45	0.42
2:B:460:ALA:C	2:B:462:ALA:N	2.72	0.42
2:B:552:MET:HA	2:B:552:MET:CE	2.49	0.42
8:H:109:LYS:HG2	8:H:110:ASP:N	2.34	0.42
1:A:1334:ASP:O	1:A:1337:GLU:N	2.43	0.42
5:E:39:LEU:HG	5:E:43:LYS:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:47:CYS:HB3	5:E:51:GLY:HA2	2.02	0.42
2:B:1098:MET:HE2	2:B:1098:MET:N	2.34	0.42
2:B:487:THR:O	2:B:490:SER:HB3	2.20	0.42
1:A:492:PRO:O	1:A:493:GLN:NE2	2.52	0.42
1:A:277:GLU:O	1:A:277:GLU:HG2	2.20	0.42
7:G:13:LEU:HD12	7:G:26:LEU:HD21	2.01	0.42
1:A:851:HIS:O	1:A:853:ASP:N	2.53	0.42
3:C:59:ALA:O	3:C:62:PHE:HB3	2.19	0.42
2:B:247:GLY:O	2:B:248:SER:HB3	2.20	0.42
1:A:92:HIS:O	1:A:94:GLY:N	2.53	0.42
2:B:294:ASP:HB2	9:I:12:ASN:HA	2.02	0.42
4:D:51:ASN:O	4:D:54:GLU:HB3	2.20	0.42
2:B:641:GLU:O	2:B:643:ASP:N	2.51	0.42
1:A:1277:GLU:O	1:A:1279:ILE:N	2.52	0.42
7:G:126:ASN:ND2	7:G:127:PRO:HA	2.23	0.42
2:B:98:THR:HG23	2:B:127:GLY:O	2.20	0.42
2:B:189:LEU:O	2:B:190:TYR:C	2.58	0.42
2:B:1187:ASN:OD1	2:B:1190:ASP:N	2.53	0.42
5:E:145:THR:HG21	5:E:187:TYR:CE2	2.54	0.42
1:A:369:SER:HB3	11:K:2:ASN:OD1	2.19	0.42
1:A:1148:ILE:HD11	1:A:1198:ASP:HB2	2.01	0.42
1:A:1195:LEU:HD11	1:A:1267:MET:HE3	2.00	0.42
11:K:83:PRO:O	11:K:84:LYS:C	2.57	0.42
7:G:61:ILE:C	7:G:62:LEU:O	2.57	0.42
3:C:50:GLU:OE1	12:L:64:LEU:CD1	2.68	0.42
2:B:244:LEU:HD21	2:B:366:GLN:HE21	1.84	0.42
8:H:129:TYR:HA	8:H:131:ASN:ND2	2.35	0.42
3:C:160:LYS:O	3:C:161:LYS:O	2.38	0.42
1:A:241:VAL:HA	1:A:242:PRO:HD2	1.95	0.42
1:A:687:LYS:CE	1:A:795:GLU:OE2	2.68	0.42
1:A:1166:ASP:OD2	1:A:1239:ARG:CD	2.68	0.42
5:E:68:SER:O	5:E:72:PHE:O	2.37	0.42
7:G:88:ASP:CB	7:G:144:ARG:HA	2.49	0.42
7:G:101:VAL:CG1	7:G:102:GLN:N	2.80	0.42
7:G:102:GLN:HG3	7:G:106:MET:O	2.20	0.42
4:D:176:GLU:C	4:D:178:ALA:N	2.72	0.42
9:I:101:PHE:HD1	9:I:101:PHE:N	2.16	0.42
2:B:785:TYR:CD1	2:B:785:TYR:C	2.93	0.42
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.35	0.42
1:A:1332:PHE:CE1	1:A:1381:LEU:HD13	2.55	0.42
7:G:44:TYR:CE2	7:G:105:PRO:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1165:GLU:H	1:A:1165:GLU:HG3	1.61	0.42
1:A:565:ILE:HG12	8:H:97:MET:HG2	2.02	0.41
4:D:218:GLU:O	4:D:219:THR:C	2.58	0.41
1:A:351:THR:N	1:A:468:PHE:HE1	2.17	0.41
1:A:1308:THR:HG21	1:A:1310:GLY:O	2.20	0.41
2:B:223:VAL:HG21	2:B:380:TYR:HE2	1.85	0.41
2:B:370:PHE:HD2	2:B:373:ARG:CD	2.33	0.41
8:H:130:ARG:HH11	8:H:130:ARG:CA	2.32	0.41
8:H:130:ARG:CA	8:H:133:ASN:HB2	2.50	0.41
1:A:356:ASP:C	1:A:358:ASN:H	2.22	0.41
3:C:20:PHE:CE1	3:C:22:LEU:HD13	2.55	0.41
3:C:146:LYS:C	3:C:147:LEU:HD23	2.39	0.41
5:E:129:PRO:O	5:E:130:ALA:C	2.59	0.41
1:A:1225:PHE:CE2	1:A:1227:ILE:HD11	2.55	0.41
4:D:35:LEU:HD11	4:D:173:HIS:NE2	2.35	0.41
1:A:1027:ALA:O	1:A:1028:THR:C	2.58	0.41
2:B:1222:ARG:CG	2:B:1222:ARG:O	2.68	0.41
1:A:1402:PHE:CG	1:A:1403:GLU:HG2	2.55	0.41
4:D:167:LEU:HB3	4:D:177:VAL:HG13	2.02	0.41
2:B:978:ASP:OD1	2:B:1098:MET:HB3	2.20	0.41
6:F:120:ILE:O	6:F:123:LYS:HB3	2.20	0.41
8:H:41:ASP:O	8:H:42:ILE:HG13	2.20	0.41
9:I:54:GLU:HB3	9:I:100:PHE:CE2	2.54	0.41
6:F:75:PRO:O	6:F:77:ASP:O	2.38	0.41
1:A:21:LEU:HD11	1:A:1414:ALA:CA	2.49	0.41
2:B:637:LEU:CD1	2:B:693:ILE:HD11	2.47	0.41
1:A:1239:ARG:HH22	1:A:1241:ARG:HH22	1.67	0.41
2:B:758:PHE:O	2:B:761:HIS:HB2	2.19	0.41
1:A:1199:ARG:O	1:A:1200:ALA:C	2.57	0.41
11:K:55:LYS:CB	11:K:81:TYR:CE1	3.03	0.41
1:A:966:ASN:O	1:A:967:ALA:C	2.59	0.41
1:A:479:ASN:HA	1:A:479:ASN:HD22	1.70	0.41
2:B:123:THR:OG1	2:B:458:LYS:HE2	2.19	0.41
1:A:1217:LYS:O	1:A:1221:LYS:HA	2.19	0.41
1:A:1072:ILE:O	1:A:1075:PRO:HG2	2.20	0.41
2:B:1022:THR:HG23	2:B:1022:THR:O	2.20	0.41
1:A:160:GLN:H	1:A:160:GLN:HG3	1.53	0.41
2:B:871:THR:O	2:B:917:PRO:HG3	2.20	0.41
2:B:1115:THR:HG22	2:B:1117:GLN:CB	2.49	0.41
5:E:124:VAL:HB	5:E:125:PRO:HD3	2.00	0.41
1:A:1135:ARG:C	1:A:1137:ALA:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:GLN:O	1:A:426:LEU:O	2.38	0.41
1:A:1208:THR:HB	1:A:1211:GLN:HG3	2.01	0.41
2:B:38:PHE:CD1	2:B:811:TYR:CD2	3.08	0.41
10:J:14:VAL:CG1	10:J:14:VAL:O	2.69	0.41
2:B:642:ASP:HB3	2:B:649:LYS:HG3	2.02	0.41
6:F:127:GLU:O	6:F:128:LYS:C	2.58	0.41
4:D:126:ILE:HD13	4:D:145:MET:HE2	2.01	0.41
2:B:432:MET:C	2:B:434:ARG:H	2.24	0.41
2:B:835:GLN:HB2	2:B:835:GLN:HE21	1.58	0.41
1:A:1265:ASN:C	1:A:1267:MET:N	2.72	0.41
5:E:153:HIS:O	5:E:154:ILE:CG1	2.68	0.41
1:A:456:MET:HE1	1:A:474:VAL:HG23	2.01	0.41
1:A:645:LEU:HG	1:A:649:ILE:HD12	2.01	0.41
1:A:507:VAL:HB	1:A:508:PRO:HD3	2.01	0.41
1:A:460:VAL:CG1	1:A:461:LYS:N	2.83	0.41
4:D:119:ARG:CD	4:D:221:TYR:HE2	2.34	0.41
1:A:855:THR:HA	1:A:866:PHE:O	2.20	0.41
8:H:4:THR:CG2	8:H:5:LEU:N	2.83	0.41
3:C:62:PHE:O	3:C:66:ARG:HG3	2.19	0.41
10:J:3:VAL:N	10:J:53:HIS:CE1	2.86	0.41
10:J:52:THR:O	10:J:52:THR:HG22	2.20	0.41
1:A:427:GLN:HB2	1:A:430:TRP:CD1	2.55	0.41
2:B:100:PRO:HG3	2:B:172:ILE:HD12	2.03	0.41
3:C:10:ILE:CD1	11:K:108:GLU:HB3	2.51	0.41
5:E:69:ILE:HG22	5:E:69:ILE:O	2.21	0.41
2:B:1152:MET:SD	2:B:1157:ALA:HA	2.61	0.41
2:B:903:VAL:HG12	2:B:904:ARG:N	2.35	0.41
1:A:595:THR:O	1:A:596:THR:CG2	2.69	0.41
10:J:1:MET:HE2	10:J:60:PHE:HE2	1.84	0.41
3:C:166:GLU:C	11:K:6:ARG:NH1	2.74	0.41
3:C:167:HIS:CD2	3:C:168:ALA:H	2.37	0.41
1:A:691:LEU:O	1:A:694:THR:HB	2.21	0.41
5:E:22:MET:O	5:E:26:ARG:HG3	2.20	0.41
1:A:850:VAL:CG2	1:A:868:TYR:HB2	2.50	0.41
4:D:123:LEU:HD13	4:D:123:LEU:C	2.38	0.41
6:F:109:VAL:CG1	6:F:110:ASP:N	2.78	0.41
2:B:265:SER:O	2:B:266:ALA:HB3	2.21	0.41
1:A:635:ARG:HH11	1:A:635:ARG:HA	1.84	0.41
2:B:546:SER:O	2:B:546:SER:OG	2.38	0.41
9:I:56:ALA:O	9:I:57:GLY:O	2.38	0.41
1:A:567:LYS:HB3	8:H:95:TYR:C	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:857:ARG:CZ	6:F:139:PRO:HG3	2.50	0.41
2:B:365:THR:HG21	2:B:370:PHE:CG	2.54	0.41
8:H:80:ARG:HB3	8:H:81:PRO:HD2	2.03	0.41
2:B:638:PHE:HD2	2:B:638:PHE:HA	1.79	0.41
9:I:6:PHE:CD2	9:I:6:PHE:N	2.89	0.41
2:B:603:LEU:HD22	2:B:603:LEU:HA	1.84	0.41
1:A:102:VAL:CG1	1:A:211:PHE:CE1	3.03	0.41
2:B:90:ILE:HD12	2:B:432:MET:HE1	2.02	0.41
2:B:387:LEU:HD12	2:B:387:LEU:N	2.32	0.41
1:A:804:TYR:OH	2:B:763:GLN:HA	2.20	0.41
2:B:504:ARG:C	2:B:506:GLY:N	2.74	0.41
1:A:961:ARG:HG2	1:A:965:GLN:HE21	1.85	0.41
1:A:1029:ARG:CG	1:A:1029:ARG:NH1	2.83	0.41
1:A:720:ARG:HB3	1:A:720:ARG:CZ	2.51	0.41
1:A:699:ALA:HB3	1:A:701:LEU:HG	2.03	0.41
1:A:492:PRO:HB2	1:A:497:THR:HG22	2.01	0.41
1:A:257:ARG:HB3	1:A:258:GLY:H	1.60	0.41
2:B:908:GLU:O	2:B:909:ASP:C	2.57	0.41
1:A:510:GLN:HA	1:A:510:GLN:OE1	2.18	0.41
3:C:143:LEU:O	3:C:143:LEU:HG	2.21	0.41
1:A:253:ASN:HB3	2:B:935:ARG:NH1	2.36	0.41
4:D:66:ARG:CD	4:D:133:THR:HB	2.39	0.41
4:D:155:ARG:CG	4:D:155:ARG:NH1	2.82	0.41
1:A:316:GLN:HB2	1:A:322:VAL:CG2	2.51	0.41
3:C:252:GLN:HE21	11:K:95:ILE:CG2	2.21	0.41
2:B:637:LEU:HD23	2:B:637:LEU:HA	1.81	0.41
4:D:154:PHE:CE1	4:D:163:VAL:CG2	3.03	0.41
8:H:44:VAL:O	8:H:44:VAL:CG1	2.67	0.41
7:G:51:TYR:O	7:G:51:TYR:CD2	2.73	0.41
3:C:189:THR:CG2	3:C:190:ASP:N	2.78	0.41
9:I:106:CYS:O	9:I:107:SER:HB2	2.21	0.41
2:B:759:PRO:C	2:B:761:HIS:N	2.74	0.41
4:D:196:PRO:C	4:D:198:LEU:N	2.74	0.41
2:B:1106:ARG:HG3	2:B:1107:ALA:N	2.35	0.41
2:B:661:LEU:C	2:B:663:ALA:N	2.73	0.41
2:B:860:MET:CG	2:B:861:ASP:N	2.83	0.41
6:F:98:ALA:HB1	6:F:117:PRO:HB2	2.03	0.41
1:A:1319:VAL:HG13	1:A:1320:PRO:HD2	2.02	0.41
2:B:496:ARG:HB3	2:B:496:ARG:HH11	1.86	0.41
2:B:307:ASP:O	2:B:308:TRP:C	2.58	0.41
8:H:58:THR:HB	8:H:143:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:66:ARG:HH22	10:J:2:ILE:CG2	2.32	0.41
2:B:95:ILE:HG13	2:B:129:PHE:O	2.21	0.41
2:B:635:ARG:HH22	2:B:742:GLU:CD	2.23	0.41
1:A:629:LEU:HD22	1:A:633:VAL:CG2	2.50	0.41
4:D:146:GLN:O	4:D:147:TYR:C	2.58	0.41
7:G:112:LYS:HA	7:G:115:MET:HE2	2.02	0.41
3:C:82:TYR:O	3:C:85:ASP:N	2.46	0.41
2:B:1073:TYR:N	2:B:1073:TYR:CD1	2.89	0.41
11:K:110:ASN:C	11:K:112:GLN:H	2.23	0.41
1:A:535:THR:HG21	1:A:617:VAL:N	2.36	0.41
3:C:186:LEU:CD1	3:C:186:LEU:N	2.82	0.41
5:E:128:PRO:HA	5:E:129:PRO:C	2.41	0.41
2:B:507:LYS:HD3	2:B:507:LYS:HA	1.96	0.41
1:A:1385:THR:CG2	1:A:1386:ARG:N	2.83	0.41
2:B:237:VAL:CG1	2:B:238:ALA:N	2.84	0.41
14:1:15:DG:C8	14:1:16:DT:C7	3.03	0.41
1:A:452:LYS:HB2	2:B:1141:HIS:CE1	2.56	0.41
2:B:263:GLY:O	2:B:264:SER:C	2.59	0.41
2:B:648:HIS:ND1	2:B:648:HIS:N	2.64	0.41
2:B:882:THR:HG22	2:B:883:LEU:N	2.35	0.41
1:A:596:THR:C	1:A:598:LEU:H	2.23	0.41
1:A:567:LYS:HZ2	8:H:46:LEU:C	2.24	0.41
1:A:789:LYS:HD3	2:B:620:ARG:HH12	1.86	0.41
5:E:108:GLY:O	5:E:132:ILE:HG23	2.21	0.41
10:J:2:ILE:HG13	10:J:57:ILE:HD12	2.03	0.41
1:A:919:ILE:CD1	1:A:983:ILE:HD12	2.49	0.41
1:A:900:ASP:HA	1:A:926:GLN:NE2	2.36	0.41
3:C:164:ALA:O	3:C:167:HIS:O	2.38	0.41
2:B:332:ASP:OD1	2:B:348:ARG:HD2	2.20	0.41
2:B:700:SER:O	2:B:701:ILE:HG22	2.21	0.41
1:A:416:ARG:NH1	1:A:417:TYR:CE2	2.84	0.41
4:D:156:ASP:O	4:D:159:THR:N	2.54	0.41
3:C:242:GLN:HA	3:C:245:VAL:CG2	2.42	0.41
3:C:16:ASP:OD1	3:C:16:ASP:N	2.53	0.41
11:K:57:LEU:CB	11:K:76:GLN:HG2	2.42	0.41
2:B:654:ARG:O	2:B:657:HIS:HB2	2.20	0.41
2:B:654:ARG:O	2:B:656:GLY:N	2.54	0.41
3:C:251:LEU:O	3:C:255:VAL:HG23	2.20	0.41
2:B:912:ILE:O	2:B:938:SER:CB	2.69	0.41
5:E:111:VAL:CG1	5:E:137:GLU:HG2	2.51	0.41
2:B:240:ILE:HG23	2:B:240:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:LYS:H	2:B:395:GLN:CD	2.23	0.41
8:H:48:PRO:O	8:H:49:VAL:HG23	2.21	0.41
3:C:234:SER:OG	3:C:235:VAL:N	2.54	0.41
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.36	0.41
4:D:123:LEU:HB3	4:D:124:GLU:OE2	2.20	0.41
2:B:1096:ARG:CG	2:B:1097:HIS:N	2.84	0.41
1:A:1192:LEU:HG	1:A:1193:LEU:N	2.36	0.41
2:B:63:ILE:HD12	2:B:421:PHE:CD2	2.56	0.41
3:C:100:THR:CG2	3:C:101:LEU:N	2.84	0.41
9:I:70:ARG:HA	9:I:83:ASN:O	2.21	0.41
8:H:61:SER:O	8:H:62:SER:HB2	2.20	0.41
1:A:1334:ASP:O	1:A:1336:MET:N	2.54	0.41
2:B:1137:CYS:O	2:B:1140:ALA:HB3	2.21	0.41
5:E:74:ASP:N	5:E:74:ASP:OD1	2.53	0.41
2:B:591:ARG:O	2:B:592:ASN:C	2.57	0.41
4:D:187:THR:C	4:D:189:ASP:N	2.72	0.41
1:A:569:LYS:HB3	1:A:571:LEU:HD13	2.02	0.41
4:D:17:LYS:HD2	4:D:18:VAL:HG13	2.02	0.41
2:B:345:LYS:CA	2:B:348:ARG:HE	2.20	0.41
2:B:113:TYR:CE2	2:B:192:LEU:CD2	3.04	0.41
1:A:96:ILE:HA	1:A:99:ILE:HD12	2.03	0.41
11:K:17:SER:O	11:K:18:LYS:C	2.60	0.41
1:A:897:TYR:HB3	1:A:936:LEU:HD12	2.01	0.41
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.51	0.41
5:E:65:THR:O	5:E:69:ILE:CD1	2.69	0.41
1:A:846:GLU:OE1	1:A:1425:SER:OG	2.39	0.41
1:A:1148:ILE:HG12	1:A:1198:ASP:HB2	2.03	0.41
7:G:137:ILE:CG2	7:G:143:ILE:HD11	2.51	0.41
1:A:1436:ILE:O	1:A:1438:THR:N	2.54	0.41
2:B:597:MET:CE	2:B:624:LEU:HD11	2.51	0.41
4:D:208:GLU:O	4:D:212:LYS:HE3	2.21	0.41
3:C:91:HIS:ND1	3:C:158:VAL:HG11	2.36	0.41
1:A:1387:HIS:O	1:A:1391:ARG:HG3	2.21	0.41
2:B:558:LEU:O	2:B:561:TRP:N	2.54	0.41
2:B:679:TYR:CE1	2:B:683:SER:HB3	2.56	0.41
1:A:39:GLU:OE2	1:A:39:GLU:N	2.54	0.41
1:A:869:GLY:C	1:A:871:ASP:H	2.24	0.40
2:B:377:PHE:C	2:B:379:GLY:H	2.24	0.40
2:B:995:ARG:O	2:B:996:ARG:C	2.59	0.40
2:B:583:ASN:OD1	2:B:628:THR:HG22	2.20	0.40
1:A:464:PRO:O	1:A:465:TYR:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:LEU:HA	2:B:192:LEU:HB2	2.02	0.40
2:B:911:ILE:CG2	2:B:966:VAL:HG11	2.52	0.40
3:C:10:ILE:HG13	3:C:10:ILE:H	1.70	0.40
2:B:292:ILE:HD11	2:B:327:ARG:H	1.86	0.40
1:A:774:ARG:O	1:A:775:ILE:C	2.58	0.40
1:A:1193:LEU:HB2	1:A:1260:LEU:CD2	2.50	0.40
5:E:20:LYS:O	5:E:21:GLU:C	2.59	0.40
1:A:982:THR:HB	1:A:985:ASP:H	1.86	0.40
1:A:456:MET:HE2	1:A:478:TYR:CZ	2.56	0.40
2:B:400:HIS:O	2:B:402:GLY:N	2.54	0.40
1:A:533:LYS:HE3	1:A:745:GLN:NE2	2.36	0.40
8:H:99:GLY:CA	8:H:117:SER:O	2.70	0.40
7:G:22:MET:O	7:G:23:LYS:C	2.59	0.40
1:A:125:ALA:C	1:A:127:ALA:N	2.75	0.40
4:D:22:GLU:HG3	4:D:22:GLU:H	1.68	0.40
7:G:26:LEU:HD11	7:G:70:PHE:CD1	2.55	0.40
1:A:598:LEU:HD23	1:A:598:LEU:O	2.22	0.40
2:B:347:LYS:H	2:B:347:LYS:HG2	1.67	0.40
4:D:142:LYS:O	4:D:146:GLN:HG3	2.22	0.40
1:A:532:ARG:O	1:A:535:THR:HB	2.21	0.40
1:A:110:CYS:HB3	1:A:167:CYS:SG	2.61	0.40
4:D:124:GLU:CD	4:D:124:GLU:N	2.74	0.40
1:A:332:LYS:NZ	14:I:19:DT:OP2	2.53	0.40
1:A:1450:LEU:CD1	6:F:131:PRO:HG3	2.51	0.40
9:I:101:PHE:HD1	9:I:101:PHE:H	1.69	0.40
9:I:93:LYS:CD	9:I:93:LYS:N	2.83	0.40
3:C:92:CYS:SG	3:C:94:LYS:HB2	2.61	0.40
1:A:603:ASN:HB3	1:A:604:GLY:H	1.74	0.40
1:A:41:MET:HB2	1:A:42:ASP:H	1.64	0.40
2:B:307:ASP:O	2:B:309:GLN:N	2.53	0.40
1:A:1100:ARG:O	1:A:1104:ILE:HG13	2.21	0.40
2:B:708:GLU:O	2:B:710:LEU:N	2.54	0.40
8:H:103:LYS:HG2	8:H:104:PHE:N	2.37	0.40
2:B:654:ARG:CG	2:B:654:ARG:NH1	2.78	0.40
1:A:1193:LEU:HD12	1:A:1194:ARG:H	1.81	0.40
4:D:8:PHE:CD2	7:G:6:ASP:O	2.71	0.40
7:G:114:LEU:HD12	7:G:114:LEU:HA	1.94	0.40
2:B:405:ARG:CZ	2:B:632:ARG:HG2	2.51	0.40
2:B:203:PHE:HD1	2:B:203:PHE:N	2.18	0.40
1:A:536:LEU:O	1:A:537:ARG:C	2.58	0.40
11:K:24:ASP:OD1	11:K:24:ASP:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:ARG:HG2	2:B:204:ILE:HD13	2.04	0.40
1:A:939:ASP:OD2	1:A:1023:ARG:NH1	2.55	0.40
2:B:393:LYS:HA	2:B:393:LYS:HE3	2.02	0.40
1:A:259:GLU:HA	1:A:259:GLU:OE1	2.22	0.40
1:A:1404:GLU:O	1:A:1405:THR:C	2.60	0.40
1:A:1138:ILE:HG13	1:A:1139:GLU:N	2.36	0.40
1:A:1444:MET:O	6:F:133:VAL:N	2.52	0.40
9:I:50:THR:HG22	9:I:52:ILE:N	2.35	0.40
4:D:128:VAL:O	4:D:130:LEU:N	2.54	0.40
1:A:416:ARG:C	1:A:417:TYR:CD2	2.95	0.40
3:C:239:PRO:HB2	3:C:241:ASP:OD1	2.22	0.40
3:C:77:ILE:HD13	3:C:77:ILE:HA	1.85	0.40
2:B:966:VAL:CG1	2:B:967:ARG:N	2.85	0.40
1:A:711:ARG:HH21	9:I:87:GLN:HE22	1.67	0.40
5:E:175:LEU:HA	5:E:176:PRO:HD3	1.86	0.40
3:C:184:ASN:HD22	3:C:189:THR:HB	1.83	0.40
2:B:281:PRO:O	2:B:282:ILE:C	2.59	0.40
7:G:137:ILE:HG23	7:G:143:ILE:HD11	2.03	0.40
1:A:985:ASP:O	1:A:986:ILE:C	2.58	0.40
1:A:954:TRP:N	1:A:954:TRP:CD1	2.89	0.40
7:G:21:ARG:HD2	7:G:24:GLN:HB3	2.03	0.40
2:B:44:VAL:HG21	2:B:199:MET:O	2.21	0.40
1:A:1291:VAL:HG22	1:A:1292:PRO:HD2	2.04	0.40
1:A:920:LEU:HD23	1:A:921:GLY:N	2.37	0.40
1:A:1212:VAL:O	1:A:1213:GLY:C	2.60	0.40
3:C:41:ILE:HA	3:C:42:PRO:HD3	1.86	0.40
1:A:281:HIS:C	1:A:282:ASN:HD22	2.24	0.40
1:A:922:ASP:OD1	1:A:924:LYS:HB2	2.20	0.40
10:J:36:LEU:HB2	10:J:47:ARG:NH1	2.35	0.40
1:A:786:HIS:HD2	1:A:786:HIS:N	2.18	0.40
5:E:56:LYS:HE2	5:E:84:ASP:CB	2.39	0.40
1:A:414:ASP:OD1	1:A:416:ARG:CG	2.70	0.40
2:B:889:THR:HG23	2:B:891:ASP:H	1.86	0.40
2:B:866:TYR:O	2:B:867:GLY:C	2.60	0.40
1:A:1208:THR:HG22	1:A:1210:GLY:N	2.36	0.40
7:G:27:LYS:O	7:G:31:LEU:HD23	2.22	0.40
1:A:767:GLN:NE2	1:A:774:ARG:CB	2.79	0.40
5:E:28:TYR:O	5:E:65:THR:HG22	2.21	0.40
1:A:1283:VAL:CG1	1:A:1284:MET:N	2.83	0.40
1:A:1152:ILE:HA	1:A:1192:LEU:O	2.21	0.40
1:A:1206:ASP:O	1:A:1274:ARG:NH2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:507:LYS:HA	2:B:512:ARG:HE	1.87	0.40
3:C:120:ILE:HG22	3:C:121:VAL:N	2.35	0.40
3:C:7:GLN:HG3	11:K:104:ASN:ND2	2.34	0.40
1:A:741:ASN:ND2	1:A:744:LYS:H	2.18	0.40
2:B:221:ASN:N	2:B:241:ARG:O	2.53	0.40
2:B:558:LEU:O	2:B:560:GLU:N	2.54	0.40
1:A:273:ASN:O	1:A:274:ILE:C	2.59	0.40
1:A:260:ASP:O	1:A:261:ASP:C	2.58	0.40
1:A:26:GLU:O	1:A:29:ALA:N	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1406/1733 (81%)	1004 (71%)	279 (20%)	123 (9%)	1	14
2	B	1094/1224 (89%)	774 (71%)	202 (18%)	118 (11%)	0	10
3	C	264/347 (76%)	181 (69%)	48 (18%)	35 (13%)	0	6
4	D	174/221 (79%)	124 (71%)	33 (19%)	17 (10%)	1	12
5	E	212/215 (99%)	144 (68%)	46 (22%)	22 (10%)	1	11
6	F	85/155 (55%)	72 (85%)	8 (9%)	5 (6%)	2	24
7	G	169/171 (99%)	137 (81%)	24 (14%)	8 (5%)	3	30
8	H	130/146 (89%)	84 (65%)	27 (21%)	19 (15%)	0	5
9	I	112/122 (92%)	77 (69%)	26 (23%)	9 (8%)	1	16
10	J	63/70 (90%)	38 (60%)	14 (22%)	11 (18%)	0	3
11	K	112/120 (93%)	86 (77%)	22 (20%)	4 (4%)	4	39
12	L	42/70 (60%)	20 (48%)	13 (31%)	9 (21%)	0	2
All	All	3863/4594 (84%)	2741 (71%)	742 (19%)	380 (10%)	1	12

All (380) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	48	ALA
1	A	57	ARG
1	A	58	LEU
1	A	67	CYS
1	A	70	CYS
1	A	74	MET
1	A	93	VAL
1	A	96	ILE
1	A	130	ASP
1	A	154	SER
1	A	167	CYS
1	A	219	PHE
1	A	250	ILE
1	A	255	SER
1	A	286	HIS
1	A	331	GLY
1	A	332	LYS
1	A	399	HIS
1	A	410	GLY
1	A	424	ILE
1	A	517	ASN
1	A	556	TRP
1	A	567	LYS
1	A	597	LEU
1	A	598	LEU
1	A	1002	GLY
1	A	1112	LYS
1	A	1114	PRO
1	A	1115	SER
1	A	1223	ASP
1	A	1231	ASP
1	A	1233	ASP
1	A	1242	VAL
1	A	1255	GLU
1	A	1314	SER
1	A	1405	THR
2	B	21	GLU
2	B	67	SER
2	B	68	THR
2	B	100	PRO
2	B	108	VAL

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Mol	Chain	Res	Type
2	B	186	GLU
2	B	294	ASP
2	B	295	GLY
2	B	334	ILE
2	B	365	THR
2	B	367	LEU
2	B	466	TRP
2	B	502	ILE
2	B	507	LYS
2	B	510	LYS
2	B	641	GLU
2	B	643	ASP
2	B	708	GLU
2	B	709	ASP
2	B	731	VAL
2	B	746	SER
2	B	751	VAL
2	B	879	ARG
2	B	907	GLY
2	B	958	GLN
2	B	1046	PRO
2	B	1069	PHE
2	B	1097	HIS
2	B	1108	ARG
2	B	1157	ALA
2	B	1171	VAL
2	B	1176	ASN
2	B	1188	LYS
2	B	1222	ARG
3	C	90	ASP
3	C	110	THR
3	C	142	VAL
3	C	149	LYS
3	C	161	LYS
3	C	184	ASN
3	C	209	TYR
3	C	215	GLU
3	C	216	GLY
3	C	237	SER
3	C	240	VAL
4	D	5	THR
4	D	8	PHE

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Mol	Chain	Res	Type
4	D	17	LYS
4	D	19	GLU
4	D	52	LEU
4	D	199	ASN
4	D	218	GLU
5	E	36	GLU
5	E	115	ASN
7	G	112	LYS
7	G	139	ILE
8	H	17	PRO
8	H	77	ARG
8	H	92	ASP
8	H	107	VAL
8	H	128	ASN
8	H	134	ASN
8	H	140	ALA
9	I	11	ASN
9	I	57	GLY
9	I	95	THR
10	J	2	ILE
10	J	6	ARG
10	J	17	LYS
10	J	28	ASP
10	J	64	ASN
12	L	50	ASP
12	L	59	ALA
12	L	60	ARG
1	A	5	GLN
1	A	43	GLU
1	A	54	ASN
1	A	59	GLY
1	A	63	ARG
1	A	66	LYS
1	A	76	GLU
1	A	128	ILE
1	A	244	PRO
1	A	318	SER
1	A	322	VAL
1	A	357	PRO
1	A	400	PRO
1	A	426	LEU
1	A	510	GLN

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Mol	Chain	Res	Type
1	A	543	LEU
1	A	583	PRO
1	A	619	LYS
1	A	673	GLY
1	A	731	ARG
1	A	755	PHE
1	A	846	GLU
1	A	852	TYR
1	A	891	ALA
1	A	1105	LEU
1	A	1124	HIS
1	A	1281	ARG
1	A	1438	THR
2	B	27	ALA
2	B	28	GLU
2	B	45	SER
2	B	259	TYR
2	B	282	ILE
2	B	364	ILE
2	B	401	PHE
2	B	435	THR
2	B	449	ASN
2	B	450	ALA
2	B	460	ALA
2	B	461	LEU
2	B	467	GLY
2	B	506	GLY
2	B	509	ALA
2	B	619	ILE
2	B	642	ASP
2	B	655	LYS
2	B	728	ARG
2	B	735	ALA
2	B	792	MET
2	B	848	ARG
2	B	869	SER
2	B	881	ASN
2	B	892	LYS
2	B	1035	ALA
2	B	1103	ILE
3	C	74	SER
3	C	126	GLY

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Mol	Chain	Res	Type
3	C	141	GLY
3	C	224	GLN
3	C	231	ASN
4	D	14	ARG
4	D	32	GLU
4	D	119	ARG
4	D	131	GLU
4	D	136	GLY
4	D	157	GLN
4	D	192	LYS
4	D	197	SER
5	E	45	LYS
5	E	59	SER
5	E	74	ASP
5	E	76	GLY
5	E	104	ASN
5	E	106	GLN
6	F	128	LYS
6	F	139	PRO
7	G	154	VAL
8	H	21	ASN
8	H	32	THR
8	H	59	ILE
8	H	82	PRO
8	H	95	TYR
9	I	9	ASP
9	I	62	ILE
9	I	106	CYS
10	J	14	VAL
10	J	24	LEU
10	J	55	ASP
11	K	53	ASP
12	L	28	LYS
12	L	35	SER
12	L	53	HIS
1	A	41	MET
1	A	109	HIS
1	A	138	ILE
1	A	148	CYS
1	A	253	ASN
1	A	259	GLU
1	A	308	ILE

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Mol	Chain	Res	Type
1	A	311	GLN
1	A	423	ASP
1	A	591	PHE
1	A	718	VAL
1	A	738	LYS
1	A	789	LYS
1	A	795	GLU
1	A	963	ILE
1	A	968	GLN
1	A	1016	THR
1	A	1122	PRO
1	A	1206	ASP
1	A	1221	LYS
1	A	1277	GLU
1	A	1278	ASN
1	A	1309	ASP
1	A	1386	ARG
2	B	24	PRO
2	B	56	ASP
2	B	221	ASN
2	B	249	ARG
2	B	258	LEU
2	B	277	LYS
2	B	322	PHE
2	B	323	VAL
2	B	333	PHE
2	B	383	ASN
2	B	433	GLN
2	B	468	GLU
2	B	559	SER
2	B	567	GLU
2	B	575	PRO
2	B	694	ASP
2	B	711	GLU
2	B	810	GLU
2	B	884	ARG
2	B	906	SER
2	B	1065	GLN
2	B	1155	SER
2	B	1175	LEU
2	B	1186	ASP
2	B	1214	PRO

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Mol	Chain	Res	Type
3	C	12	GLU
3	C	78	GLU
3	C	172	PRO
3	C	197	SER
3	C	208	GLU
3	C	214	ASN
3	C	243	VAL
5	E	73	PRO
5	E	92	THR
5	E	167	ARG
5	E	173	SER
5	E	183	PRO
6	F	112	GLU
6	F	154	ASP
12	L	40	LEU
12	L	54	ARG
1	A	42	ASP
1	A	169	ASN
1	A	249	SER
1	A	256	GLN
1	A	592	ASP
1	A	689	LYS
1	A	821	ARG
1	A	884	ASP
1	A	885	THR
1	A	1054	LEU
1	A	1127	ASP
1	A	1229	SER
2	B	58	THR
2	B	106	ASP
2	B	257	LYS
2	B	267	ARG
2	B	384	ARG
2	B	648	HIS
2	B	752	ALA
2	B	818	PRO
2	B	937	ALA
2	B	1003	ALA
2	B	1017	ILE
2	B	1223	ASP
3	C	173	ALA
3	C	182	PRO

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Mol	Chain	Res	Type
3	C	202	PRO
3	C	213	PRO
4	D	16	LYS
4	D	219	THR
5	E	65	THR
5	E	130	ALA
5	E	158	SER
5	E	192	ARG
7	G	20	PRO
7	G	63	PRO
8	H	62	SER
8	H	91	ASP
8	H	129	TYR
9	I	8	ARG
10	J	27	GLU
11	K	14	GLU
1	A	68	GLN
1	A	69	THR
1	A	284	ALA
1	A	958	VAL
1	A	1204	ASP
1	A	1365	TYR
2	B	22	SER
2	B	114	PRO
2	B	115	GLN
2	B	250	PHE
2	B	251	ILE
2	B	309	GLN
2	B	480	SER
2	B	636	PRO
2	B	945	GLU
2	B	1181	GLU
3	C	11	ARG
3	C	60	ASP
3	C	107	SER
3	C	132	PRO
3	C	175	ALA
5	E	12	LEU
5	E	83	CYS
6	F	78	GLN
7	G	115	MET
8	H	90	ALA

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Mol	Chain	Res	Type
8	H	109	LYS
9	I	78	CYS
10	J	42	LYS
10	J	62	ARG
11	K	41	THR
11	K	54	ARG
1	A	35	ILE
1	A	599	SER
1	A	986	ILE
1	A	1130	GLN
2	B	483	LEU
2	B	688	GLY
2	B	774	GLY
3	C	223	ALA
5	E	122	LYS
8	H	8	ASP
1	A	51	GLY
1	A	285	PRO
1	A	312	PRO
1	A	683	ILE
1	A	1104	ILE
2	B	758	PHE
2	B	1034	VAL
12	L	55	ILE
1	A	604	GLY
1	A	666	ILE
1	A	1335	ILE
1	A	1454	MET
2	B	283	VAL
2	B	992	ILE
3	C	10	ILE
5	E	51	GLY
5	E	129	PRO
7	G	128	PRO
1	A	245	PRO
7	G	136	VAL
1	A	61	ILE
1	A	336	ILE
2	B	712	PRO
2	B	901	PRO
3	C	176	ILE
9	I	59	VAL

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Mol	Chain	Res	Type
2	B	1018	PRO
8	H	44	VAL

### 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	1239/1520 (82%)	1091 (88%)	148 (12%)	6	34
2	B	964/1061 (91%)	846 (88%)	118 (12%)	6	32
3	C	234/299 (78%)	207 (88%)	27 (12%)	7	36
4	D	160/200 (80%)	136 (85%)	24 (15%)	3	25
5	E	196/197 (100%)	176 (90%)	20 (10%)	9	42
6	F	77/137 (56%)	67 (87%)	10 (13%)	5	30
7	G	152/152 (100%)	141 (93%)	11 (7%)	18	58
8	H	118/128 (92%)	99 (84%)	19 (16%)	3	21
9	I	108/116 (93%)	96 (89%)	12 (11%)	8	38
10	J	60/65 (92%)	54 (90%)	6 (10%)	9	43
11	K	99/102 (97%)	86 (87%)	13 (13%)	5	30
12	L	39/57 (68%)	35 (90%)	4 (10%)	9	42
All	All	3446/4034 (85%)	3034 (88%)	412 (12%)	6	33

All (412) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	18	GLN
1	A	22	PHE
1	A	34	LYS
1	A	37	PHE
1	A	39	GLU
1	A	41	MET
1	A	54	ASN

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Mol	Chain	Res	Type
1	A	57	ARG
1	A	62	ASP
1	A	68	GLN
1	A	69	THR
1	A	83	HIS
1	A	93	VAL
1	A	121	LEU
1	A	141	LEU
1	A	145	LYS
1	A	152	VAL
1	A	155	GLU
1	A	160	GLN
1	A	161	LEU
1	A	196	GLU
1	A	200	ARG
1	A	208	LEU
1	A	219	PHE
1	A	244	PRO
1	A	245	PRO
1	A	249	SER
1	A	250	ILE
1	A	265	LYS
1	A	287	HIS
1	A	289	ILE
1	A	290	GLU
1	A	302	THR
1	A	315	LEU
1	A	317	LYS
1	A	337	ARG
1	A	344	ARG
1	A	353	ILE
1	A	369	SER
1	A	375	THR
1	A	385	ILE
1	A	394	ASN
1	A	408	ASP
1	A	417	TYR
1	A	425	GLN
1	A	443	LEU
1	A	445	ASN
1	A	449	SER
1	A	461	LYS

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Mol	Chain	Res	Type
1	A	462	VAL
1	A	469	ARG
1	A	475	THR
1	A	479	ASN
1	A	481	ASP
1	A	485	ASP
1	A	493	GLN
1	A	498	ARG
1	A	505	CYS
1	A	511	ILE
1	A	512	VAL
1	A	518	LYS
1	A	524	VAL
1	A	529	CYS
1	A	538	ASP
1	A	544	ASP
1	A	562	THR
1	A	590	ARG
1	A	593	GLU
1	A	597	LEU
1	A	618	GLU
1	A	629	LEU
1	A	641	VAL
1	A	666	ILE
1	A	680	THR
1	A	685	GLU
1	A	688	LYS
1	A	702	LEU
1	A	738	LYS
1	A	762	SER
1	A	768	GLN
1	A	774	ARG
1	A	779	PHE
1	A	783	THR
1	A	805	LEU
1	A	821	ARG
1	A	827	THR
1	A	834	THR
1	A	838	GLN
1	A	839	ARG
1	A	858	ASN
1	A	871	ASP

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Mol	Chain	Res	Type
1	A	873	MET
1	A	903	ASN
1	A	906	HIS
1	A	907	THR
1	A	937	VAL
1	A	941	LYS
1	A	955	PRO
1	A	963	ILE
1	A	969	GLN
1	A	983	ILE
1	A	1004	ASN
1	A	1009	ASN
1	A	1029	ARG
1	A	1067	LEU
1	A	1074	GLU
1	A	1110	ASN
1	A	1114	PRO
1	A	1116	LEU
1	A	1122	PRO
1	A	1124	HIS
1	A	1129	GLU
1	A	1134	ILE
1	A	1135	ARG
1	A	1146	VAL
1	A	1159	ARG
1	A	1170	ILE
1	A	1171	GLN
1	A	1187	GLN
1	A	1193	LEU
1	A	1199	ARG
1	A	1217	LYS
1	A	1260	LEU
1	A	1269	GLU
1	A	1280	GLU
1	A	1288	ASP
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1308	THR
1	A	1333	ILE
1	A	1345	ARG
1	A	1349	TYR

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Mol	Chain	Res	Type
1	A	1353	TYR
1	A	1355	VAL
1	A	1365	TYR
1	A	1366	ARG
1	A	1368	MET
1	A	1370	LEU
1	A	1386	ARG
1	A	1394	THR
1	A	1400	CYS
1	A	1436	ILE
1	A	1444	MET
1	A	1445	ILE
1	A	1447	GLU
1	A	1451	VAL
2	B	20	ASP
2	B	22	SER
2	B	25	ILE
2	B	30	SER
2	B	35	SER
2	B	37	PHE
2	B	46	GLN
2	B	57	TYR
2	B	61	ASP
2	B	68	THR
2	B	98	THR
2	B	100	PRO
2	B	103	ASN
2	B	130	VAL
2	B	134	LYS
2	B	175	ARG
2	B	194	GLU
2	B	203	PHE
2	B	217	ARG
2	B	218	SER
2	B	222	ILE
2	B	225	VAL
2	B	261	ARG
2	B	262	GLU
2	B	267	ARG
2	B	272	THR
2	B	287	ARG
2	B	298	LEU

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Mol	Chain	Res	Type
2	B	364	ILE
2	B	371	GLU
2	B	393	LYS
2	B	401	PHE
2	B	416	LEU
2	B	425	THR
2	B	430	ARG
2	B	446	LEU
2	B	452	THR
2	B	465	ASN
2	B	466	TRP
2	B	473	MET
2	B	479	VAL
2	B	485	ARG
2	B	493	SER
2	B	505	ASP
2	B	508	LEU
2	B	516	ASN
2	B	518	HIS
2	B	552	MET
2	B	557	PHE
2	B	572	HIS
2	B	597	MET
2	B	603	LEU
2	B	610	ASN
2	B	616	ILE
2	B	618	ASP
2	B	635	ARG
2	B	636	PRO
2	B	644	GLU
2	B	678	GLU
2	B	693	ILE
2	B	705	MET
2	B	714	GLU
2	B	737	THR
2	B	743	ILE
2	B	748	ILE
2	B	754	SER
2	B	766	ARG
2	B	786	ASN
2	B	790	ASP
2	B	805	THR

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Mol	Chain	Res	Type
2	B	811	TYR
2	B	815	ARG
2	B	830	TYR
2	B	835	GLN
2	B	837	ASP
2	B	839	MET
2	B	857	ARG
2	B	859	TYR
2	B	868	MET
2	B	878	GLN
2	B	879	ARG
2	B	887	HIS
2	B	894	ASP
2	B	915	THR
2	B	946	ASN
2	B	953	LEU
2	B	957	ASN
2	B	959	ASP
2	B	987	LYS
2	B	989	THR
2	B	997	GLU
2	B	999	MET
2	B	1001	PHE
2	B	1007	VAL
2	B	1022	THR
2	B	1048	THR
2	B	1049	ASP
2	B	1073	TYR
2	B	1084	GLN
2	B	1087	PHE
2	B	1095	LEU
2	B	1097	HIS
2	B	1098	MET
2	B	1113	VAL
2	B	1122	ARG
2	B	1124	ARG
2	B	1148	LYS
2	B	1150	ARG
2	B	1159	ARG
2	B	1160	VAL
2	B	1175	LEU
2	B	1183	LYS

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Mol	Chain	Res	Type
2	B	1185	CYS
2	B	1193	GLN
2	B	1202	LEU
2	B	1214	PRO
2	B	1218	THR
2	B	1223	ASP
3	C	16	ASP
3	C	26	ASP
3	C	33	LEU
3	C	54	ASN
3	C	55	THR
3	C	56	THR
3	C	62	PHE
3	C	69	LEU
3	C	74	SER
3	C	77	ILE
3	C	83	SER
3	C	91	HIS
3	C	104	PHE
3	C	117	ASP
3	C	145	CYS
3	C	147	LEU
3	C	166	GLU
3	C	192	TRP
3	C	197	SER
3	C	202	PRO
3	C	217	ASP
3	C	238	ILE
3	C	240	VAL
3	C	245	VAL
3	C	259	LEU
3	C	262	LEU
3	C	266	ASP
4	D	11	ARG
4	D	14	ARG
4	D	15	LEU
4	D	16	LYS
4	D	17	LYS
4	D	21	GLU
4	D	22	GLU
4	D	23	ASN
4	D	29	LEU

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Mol	Chain	Res	Type
4	D	34	GLN
4	D	40	HIS
4	D	70	PHE
4	D	74	GLN
4	D	123	LEU
4	D	149	THR
4	D	155	ARG
4	D	159	THR
4	D	187	THR
4	D	200	ASN
4	D	213	GLU
4	D	214	LEU
4	D	219	THR
4	D	220	LEU
4	D	221	TYR
5	E	2	ASP
5	E	10	SER
5	E	31	THR
5	E	33	GLU
5	E	41	ASP
5	E	65	THR
5	E	66	GLU
5	E	72	PHE
5	E	74	ASP
5	E	78	LEU
5	E	92	THR
5	E	99	HIS
5	E	104	ASN
5	E	110	PHE
5	E	112	TYR
5	E	115	ASN
5	E	134	THR
5	E	171	LYS
5	E	191	LYS
5	E	212	ARG
6	F	72	LYS
6	F	79	ARG
6	F	84	TYR
6	F	90	ARG
6	F	111	LEU
6	F	112	GLU
6	F	119	ARG

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Mol	Chain	Res	Type
6	F	131	PRO
6	F	147	SER
6	F	153	VAL
7	G	1	MET
7	G	8	SER
7	G	13	LEU
7	G	21	ARG
7	G	31	LEU
7	G	51	TYR
7	G	74	TYR
7	G	101	VAL
7	G	118	ASP
7	G	126	ASN
7	G	168	LEU
8	H	11	GLN
8	H	26	ILE
8	H	27	GLU
8	H	36	CYS
8	H	46	LEU
8	H	53	ASP
8	H	61	SER
8	H	86	ASP
8	H	89	LEU
8	H	91	ASP
8	H	95	TYR
8	H	98	TYR
8	H	102	TYR
8	H	124	ARG
8	H	128	ASN
8	H	130	ARG
8	H	134	ASN
8	H	138	GLU
8	H	143	LEU
9	I	6	PHE
9	I	12	ASN
9	I	21	GLU
9	I	34	TYR
9	I	59	VAL
9	I	85	PHE
9	I	86	PHE
9	I	93	LYS
9	I	94	ASP

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Mol	Chain	Res	Type
9	I	101	PHE
9	I	110	PHE
9	I	114	GLN
10	J	2	ILE
10	J	13	VAL
10	J	25	LEU
10	J	43	ARG
10	J	48	ARG
10	J	53	HIS
11	K	25	THR
11	K	31	VAL
11	K	47	ARG
11	K	50	LEU
11	K	51	LEU
11	K	61	TYR
11	K	70	ARG
11	K	89	ASN
11	K	103	THR
11	K	107	THR
11	K	111	LEU
11	K	113	THR
11	K	114	LEU
12	L	27	LEU
12	L	38	LEU
12	L	55	ILE
12	L	65	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	71	GLN
1	A	75	ASN
1	A	169	ASN
1	A	171	GLN
1	A	213	HIS
1	A	225	ASN
1	A	253	ASN
1	A	282	ASN
1	A	299	HIS
1	A	339	ASN
1	A	390	GLN

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Mol	Chain	Res	Type
1	A	435	HIS
1	A	445	ASN
1	A	447	GLN
1	A	479	ASN
1	A	493	GLN
1	A	503	GLN
1	A	517	ASN
1	A	631	HIS
1	A	723	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	786	HIS
1	A	858	ASN
1	A	903	ASN
1	A	926	GLN
1	A	969	GLN
1	A	994	GLN
1	A	1048	ASN
1	A	1187	GLN
1	A	1203	ASN
1	A	1258	HIS
1	A	1312	ASN
1	A	1432	GLN
2	B	103	ASN
2	B	121	ASN
2	B	178	ASN
2	B	224	GLN
2	B	236	HIS
2	B	366	GLN
2	B	395	GLN
2	B	465	ASN
2	B	515	HIS
2	B	516	ASN
2	B	667	GLN
2	B	821	GLN
2	B	842	ASN
2	B	862	GLN
2	B	878	GLN
2	B	887	HIS
2	B	957	ASN
2	B	975	GLN

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Mol	Chain	Res	Type
2	B	1015	HIS
2	B	1062	HIS
2	B	1065	GLN
2	B	1076	HIS
2	B	1084	GLN
2	B	1117	GLN
2	B	1161	HIS
2	B	1179	GLN
2	B	1193	GLN
3	C	7	GLN
3	C	73	GLN
3	C	79	GLN
3	C	91	HIS
3	C	102	GLN
3	C	112	ASN
3	C	167	HIS
3	C	231	ASN
3	C	252	GLN
4	D	39	ASN
4	D	40	HIS
4	D	41	GLN
4	D	132	GLN
4	D	138	ASN
4	D	143	ASN
4	D	216	ASN
5	E	3	GLN
5	E	101	GLN
5	E	104	ASN
5	E	106	GLN
5	E	113	GLN
5	E	143	ASN
5	E	147	HIS
5	E	174	GLN
7	G	14	HIS
7	G	53	ASN
7	G	122	ASN
7	G	126	ASN
7	G	131	GLN
7	G	158	HIS
8	H	11	GLN
8	H	128	ASN
8	H	131	ASN

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Mol	Chain	Res	Type
8	H	133	ASN
9	I	12	ASN
9	I	46	HIS
9	I	87	GLN
9	I	108	HIS
10	J	53	HIS
11	K	65	HIS
11	K	89	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	3	10/18 (55%)	2 (20%)	1 (10%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	3	3	A
15	3	11	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	3	2	A

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
14	BRU	1	23	15,14	13,21,22	4.68	4 (30%)	16,30,33	4.09	3 (18%)

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
14	BRU	1	23	15,14	-	0/3/21/22	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	23	BRU	BR-C5	-15.06	1.50	1.90
14	1	23	BRU	C6-N1	3.19	1.39	1.35
14	1	23	BRU	C4-N3	3.53	1.39	1.33
14	1	23	BRU	C4-C5	5.75	1.45	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1	23	BRU	C5-C4-N3	-8.15	115.30	124.00
14	1	23	BRU	C5-C6-N1	2.03	123.78	119.79
14	1	23	BRU	C4-N3-C2	13.74	127.13	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	1	23	BRU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1416/1733 (81%)	-0.17	17 (1%) 81 69	15, 63, 100, 128	0
2	B	1112/1224 (90%)	-0.14	16 (1%) 78 65	15, 74, 111, 122	0
3	C	266/347 (76%)	-0.19	1 (0%) 93 88	31, 63, 93, 111	0
4	D	178/221 (80%)	-0.02	1 (0%) 90 83	40, 75, 106, 115	0
5	E	214/215 (99%)	0.13	1 (0%) 91 86	41, 87, 115, 124	0
6	F	87/155 (56%)	-0.48	0 100 100	17, 44, 73, 84	0
7	G	171/171 (100%)	-0.13	1 (0%) 90 83	44, 64, 92, 100	0
8	H	134/146 (91%)	0.40	1 (0%) 89 81	67, 95, 112, 117	0
9	I	114/122 (93%)	0.09	2 (1%) 71 58	62, 93, 109, 114	0
10	J	65/70 (92%)	-0.37	0 100 100	41, 60, 85, 92	0
11	K	114/120 (95%)	-0.14	0 100 100	28, 66, 83, 92	0
12	L	44/70 (62%)	0.14	0 100 100	42, 100, 111, 114	0
13	2	7/12 (58%)	1.47	1 (14%) 4 3	112, 116, 123, 124	0
14	1	18/26 (69%)	0.83	4 (22%) 1 1	68, 109, 126, 131	0
15	3	11/18 (61%)	0.48	1 (9%) 11 8	92, 97, 123, 126	0
All	All	3951/4650 (84%)	-0.11	46 (1%) 81 69	15, 70, 109, 131	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	253	ASN	3.9
1	A	1455	PRO	3.6
1	A	255	SER	3.5
1	A	149	GLU	3.2
15	3	1	C	3.2
1	A	256	GLN	3.1
2	B	709	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	251	SER	3.1
1	A	157	ASP	3.0
1	A	158	PRO	2.9
2	B	715	ALA	2.9
2	B	882	THR	2.9
2	B	505	ASP	2.9
1	A	155	GLU	2.8
7	G	122	ASN	2.8
2	B	883	LEU	2.8
2	B	919	SER	2.7
2	B	918	ILE	2.7
1	A	195	ASP	2.6
1	A	154	SER	2.6
1	A	44	THR	2.5
2	B	733	HIS	2.5
14	1	28	DA	2.5
2	B	431	TYR	2.4
1	A	156	ASP	2.4
9	I	76	PRO	2.4
2	B	250	PHE	2.4
2	B	435	THR	2.4
1	A	1124	HIS	2.3
14	1	12	DG	2.3
8	H	139	ASN	2.2
2	B	867	GLY	2.2
1	A	161	LEU	2.2
2	B	714	GLU	2.2
5	E	81	GLU	2.2
1	A	159	THR	2.1
9	I	74	GLU	2.1
14	1	15	DG	2.1
2	B	643	ASP	2.1
2	B	868	MET	2.1
13	2	1	DA	2.1
3	C	3	GLU	2.0
1	A	109	HIS	2.0
4	D	38	ILE	2.0
14	1	13	DT	2.0
2	B	722	ASP	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
14	BRU	1	23	20/21	0.80	0.26	-	81,90,95,98	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
16	ZN	A	2457	1/1	1.00	0.11	-1.45	35,35,35,35	0
17	MG	A	2458	1/1	0.96	0.13	-1.88	52,52,52,52	0
16	ZN	J	1066	1/1	0.99	0.17	-1.94	39,39,39,39	0
16	ZN	C	1269	1/1	1.00	0.07	-2.31	27,27,27,27	0
16	ZN	I	1121	1/1	0.99	0.09	-2.37	74,74,74,74	0
16	ZN	I	1122	1/1	0.97	0.11	-2.80	124,124,124,124	0
16	ZN	L	1071	1/1	0.97	0.07	-2.90	86,86,86,86	0
16	ZN	A	2456	1/1	0.96	0.06	-3.60	70,70,70,70	0
16	ZN	B	2225	1/1	0.99	0.16	-	32,32,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.