



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 06:45 am BST

PDB ID : 2JA5
Title : CPD lesion containing RNA Polymerase II elongation complex A
Authors : Brueckner, F.; Hennecke, U.; Carell, T.; Cramer, P.
Deposited on : 2006-11-23
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

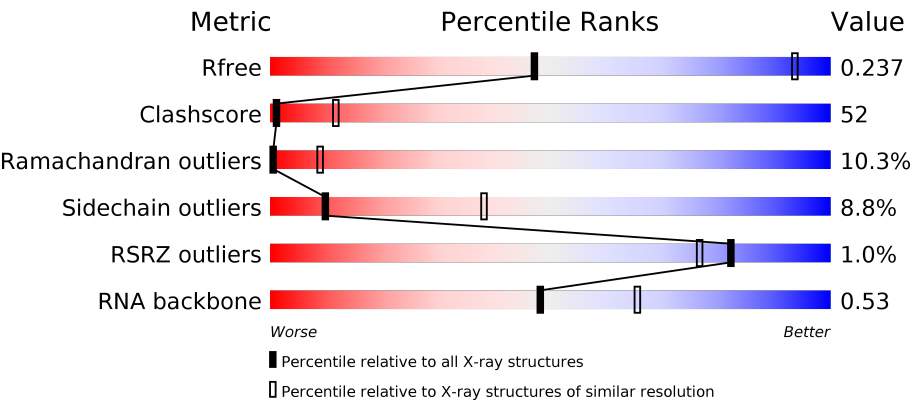
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1733	<div><div>%</div><div><div></div><div>26%</div><div>45%</div><div>10%</div><div>•</div><div>18%</div></div></div>
2	B	1224	<div><div>%</div><div><div></div><div>27%</div><div>52%</div><div>11%</div><div>•</div><div>9%</div></div></div>
3	C	318	<div><div></div><div><div></div><div>25%</div><div>49%</div><div>9%</div><div>•</div><div>16%</div></div></div>
4	D	221	<div><div></div><div><div></div><div>25%</div><div>41%</div><div>12%</div><div>•</div><div>20%</div></div></div>

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Mol	Chain	Length	Quality of chain
5	E	215	<div><div></div><div>46%49%5%</div></div>
6	F	155	<div><div></div><div>17%34%6%44%</div></div>
7	G	171	<div><div></div><div>%39%52%9%•</div></div>
8	H	146	<div><div></div><div>3%29%53%10%8%</div></div>
9	I	122	<div><div></div><div>%34%47%13%•5%</div></div>
10	J	70	<div><div></div><div>20%50%20%•7%</div></div>
11	K	120	<div><div></div><div>2%33%49%11%•5%</div></div>
12	L	70	<div><div></div><div>4%17%37%10%•34%</div></div>
13	P	11	<div><div></div><div>9%9%73%9%9%</div></div>
14	T	25	<div><div></div><div>36%8%56%</div></div>

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 31660 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	1421	Total	C	N	O	S	0	0	0
			11186	7048	1958	2118	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1115	Total	C	N	O	S	0	0	0
			8866	5614	1553	1644	55			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	177	Total	C	N	O	S	0	0	0
			1427	882	256	287	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	135	Total	C	N	O	S	0	0	0
			1084	683	183	214	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	116	Total	C	N	O	S	0	0	0
			944	581	172	181	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	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 13 is a RNA chain called 5'-R(*UP*UP*CP*GP*AP*CP*CP*AP*GP*GP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	P	10	Total	C	N	O	P	0	0	0
			212	96	41	66	9			

- Molecule 14 is a DNA chain called 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP *CP*

TP*TTP*TP*TP*CP*CP*BRUP*GP*GP*TP*CP*AP*TP*T)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
14	T	11	Total	Br	C	N	O	P	0	0	0
			219	1	106	34	68	10			

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

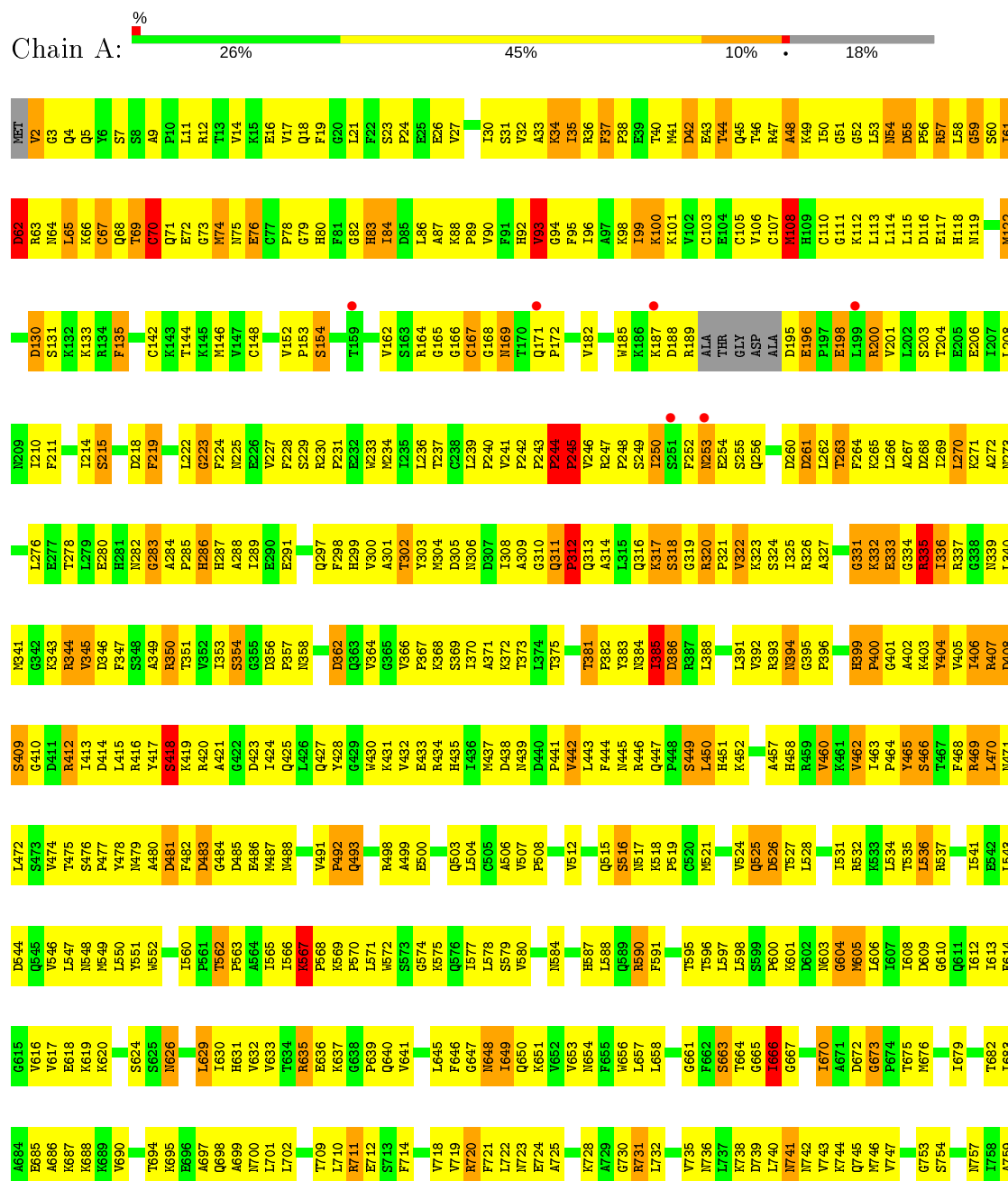
- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	8	Total	Zn	0	0
			8	8		

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

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

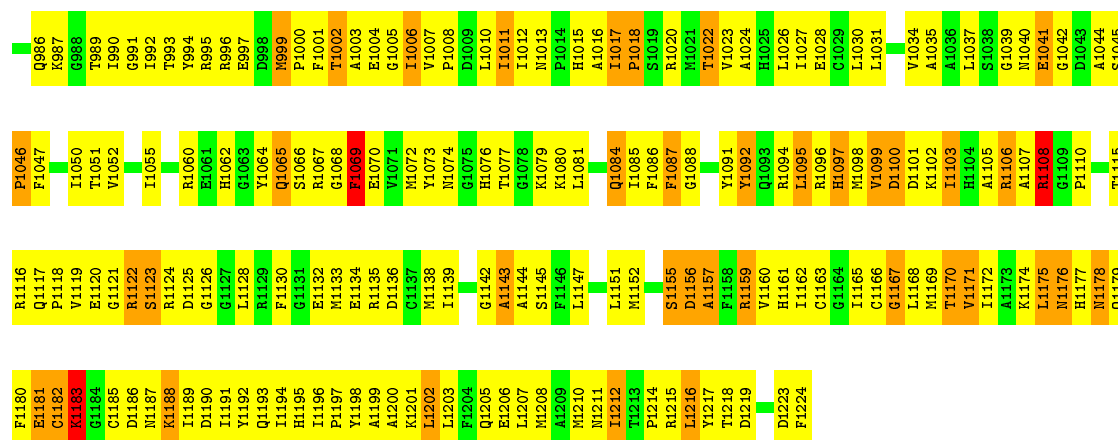


Q760	K895	Q968	L1037	N1106	LEU	LYS	V1316	L1381	V1443	ALA	TYR	SER
M761	K896	Q969	T1038	V1107	ASP	SER	M1317	L1382	M1444	MET	PRO	PRO
S762	K897	A1108	K1039	A1109	GLU	LEU	T1318	T1385	T1445	ALA	THR	THR
A763	K898	T970	Q1040	M1110	ALA	ALA	V1319	T1386	D1446	GLY	THR	THR
C764	V899	F971	D1043	N1111	ALA	ALA	P1320	H1387	E1447	PHE	PRO	PRO
V765	D900	D874	D1043	K1112	GLN	THR	D1323	H1388	E1448	THR	SER	THR
Q766	L901	H975	M1048	T1113	SER	GLU	P1324	F1389	S1449	ALA	TYR	TYR
Q767	L902	H976	I1049	P1114	PHE	GLU	T1325	M1390	V1450	ALA	TYR	TYR
Q768	N903	S979	Q1052	S1115	ASP	ASP	R1326	M1393	K1452	GLY	PRO	PRO
S769	T904	D980	F1053	L1116	ASP	E1255	I1327	T1394	R1453	GLY	THR	THR
V770	K838	R839	L1116	T1117	ASP	E1256	Y1328	G1395	M1454	ALA	PRO	PRO
E774	R840	R839	L1054	T1118	G1188	D1257	T1329	A1396	M1455	ASP	PRO	PRO
I775	L841	L841	R1055	Y1119	P1190	M1259	M1330	L1397		THR	TYR	TYR
	V842	V842	R1056	L1120	M1191	K1260	F1332	M1398		GLY	TYR	TYR
	K843	K843	V1057	L1121	L1192	K1261	L1333	R1399		GLN	TYR	TYR
	A844	A844	V1058	P1123	L1193	E1264	D1334	C1400		ILE	THR	THR
	L845	L845	H1059	H1124	L1197	N1265	I1335	S1401		GLU	SER	SER
D781	E846	E846	Q1061	E1127	D1198	T1266	M1336	F1402		ILE	PRO	PRO
R782	D847	D847	E1062	Q1130	M1202	L1268	V1337	E1403		GLY	PRO	PRO
T783	L848	L848	V1064	I1134	K1205	L1271	G1340	E1404		ALA	TYR	TYR
P785	Y852	Y852	L1067	R1135	D1206	R1274	I1341	V1405		GLY	PRO	PRO
H786	D853	D853	Q1070	I1138	T1207		E1342	E1407		GLY	SER	SER
F787	N854	N854	S1071	T1141	M1208		A1343	I1408		GLY	PRO	PRO
S788	R857	R857	I1072	T1141	M1209		R1345	L1409		VAL	THR	THR
K789	S859	S859	G1073	K1144	Q1211		V1212	F1411		THR	TYR	TYR
	L860	L860	E1074	S1145	G1213		L1348	A1412		PRO	PRO	PRO
	K861	K861	P1075	T1146	E1214		K1350	A1414		GLY	THR	THR
	N862	N862	I1007	V1146	E1215		R1352	S1415		PHE	SER	SER
	V863	V863	Q1008	A1149	T1216		V1352	E1417		GLY	PRO	PRO
	E801	E801	M1079	S1150	K1217		V1355	L1418		GLY	TYR	TYR
	I864	I864	T1080	E1151	Q1218		I1356	D1419		SER	SER	SER
	Q865	Q865	ASN	I1152	T1219			D1420		VAL	PRO	PRO
	F866	F866	THR	Y1153	F1220		D1359	C1421		GLY	THR	THR
	L867	L867	PHE	Y1154	K1221			R1422		PHE	SER	SER
	Y870	Y870	A1014	D1155	D1222			G1423		ALA	PRO	PRO
	D871	D871	V1015	P1156	D1223			V1424		ASP	PRO	PRO
	T809	T809	T1016	D1157	L1224			S1425		THR	TYR	TYR
	P810	P810	L1017	P1158	F1225			E1426		SER	SER	SER
	Q811	Q811	F1018	R1159	V1226			V1428		PRO	PRO	PRO
	E812	E812	VAL	S1160	W1228			L1430		THR	THR	THR
	F815	F815	ALA	K1092	D1233			G1431		TYR	THR	THR
	A876	A876	SER	V1093	L1236			M1432		LEU	PRO	PRO
	H877	H877	K1093	T1095	I1237			Q1432		MET	THR	THR
	A878	A878	V1094	E1163	L1238			A1434		THR	SER	SER
	I878	I878	T1095	P1164	I1239			M1435		SER	PRO	PRO
	Q881	Q881	S1096	D1166	R1239			T1372		ALA	PRO	PRO
	S882	S882	G1097	I1170	C1240			D1373		VAL	THR	THR
	R821	R821	V1098	Q1171	R1241			M1375		THR	PRO	PRO
	L884	L884	P1099	F1174	V1242			T1376		GLY	THR	THR
	G823	G823	R1100	L1176	V1243			Q1378		SER	PRO	PRO
	T824	T824	K1102		P1245			G1380		ASN	PRO	PRO
	I825	I825								ASP	THR	THR
	D826	D826										
	T827	T827										
	A828	A828										

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

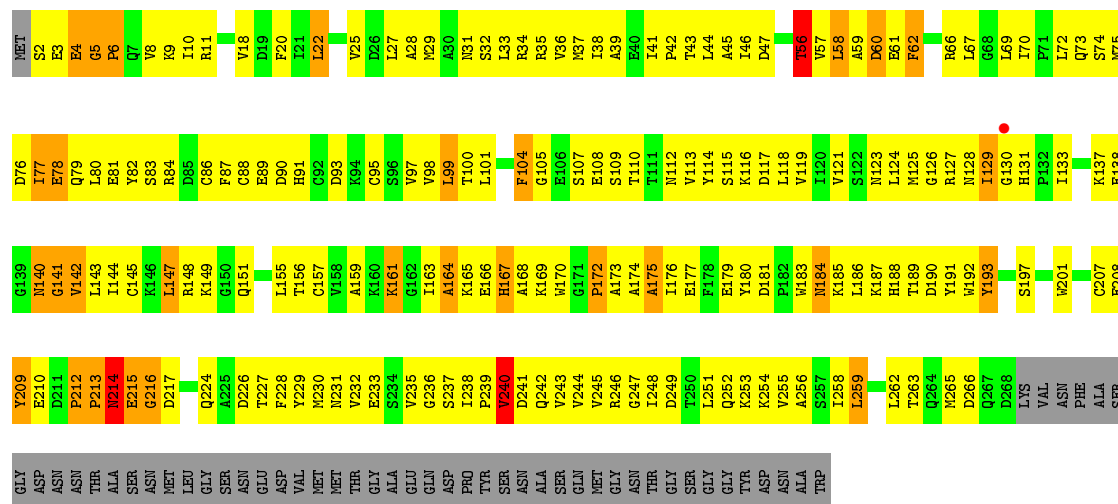






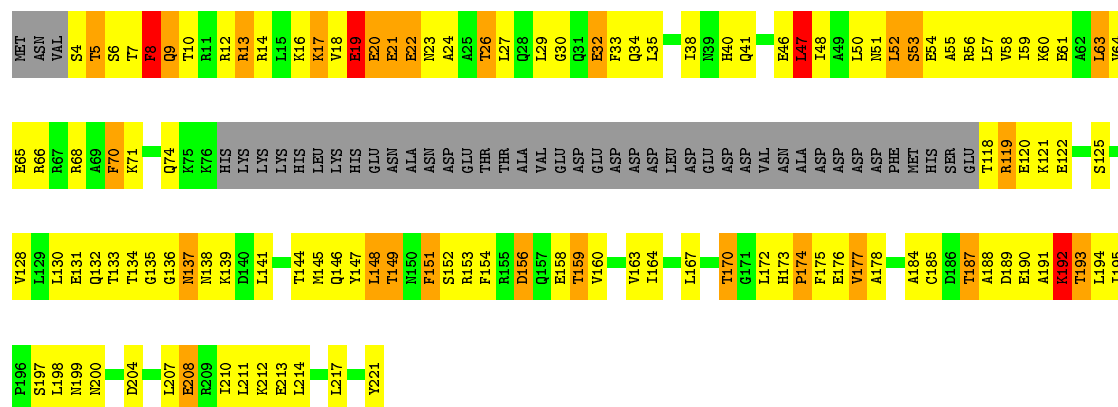
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 25% 49% 9% 16%



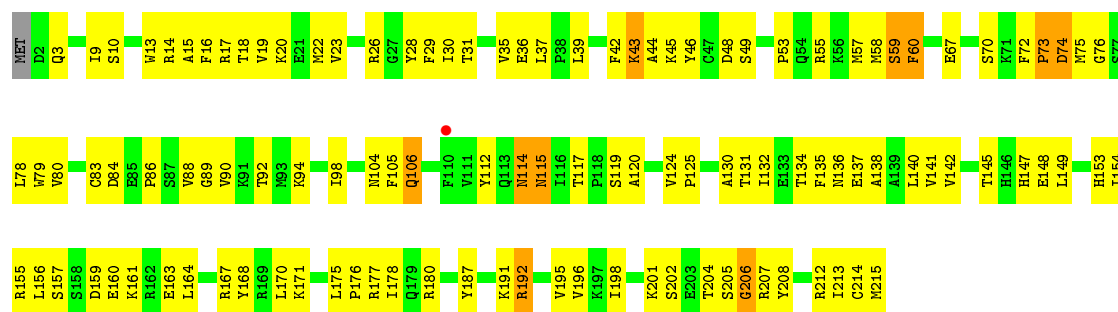
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D: 25% 41% 12% 20%



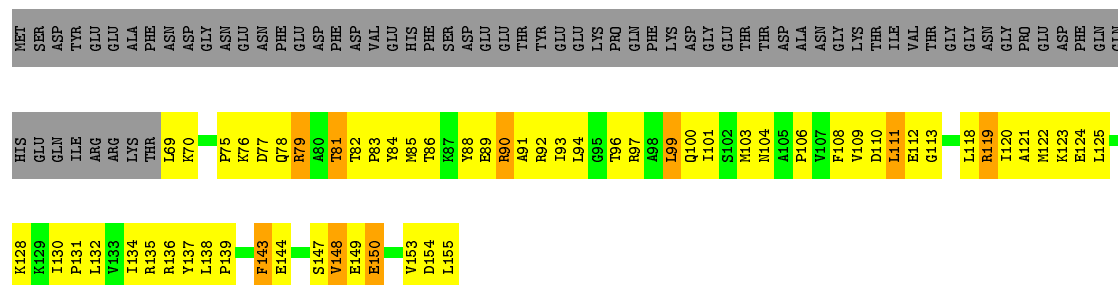
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 



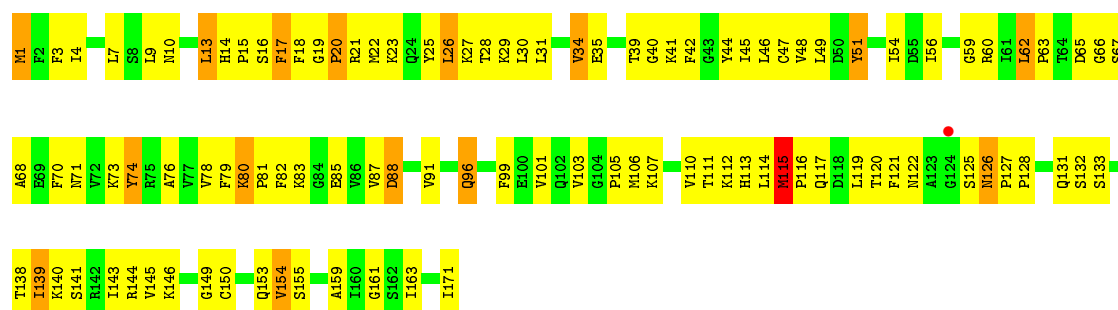
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 



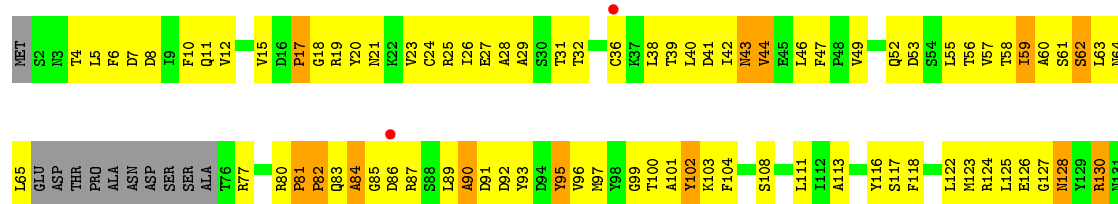
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

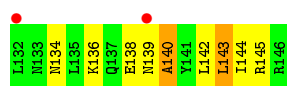
Chain G: 



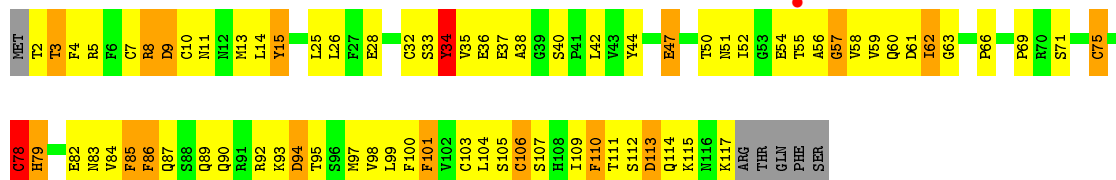
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 

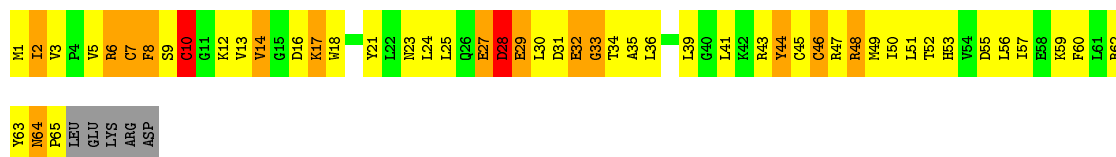
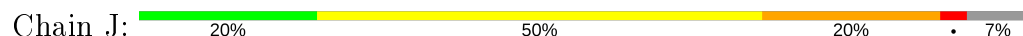




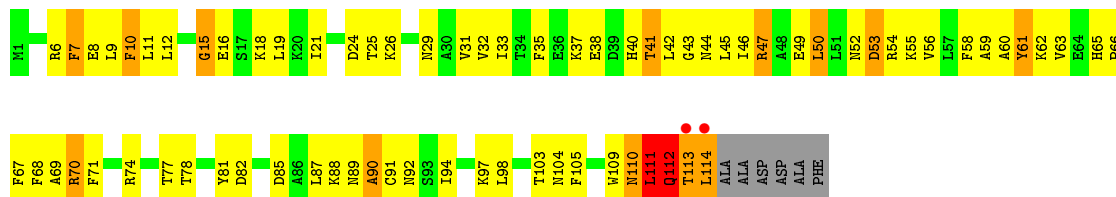
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



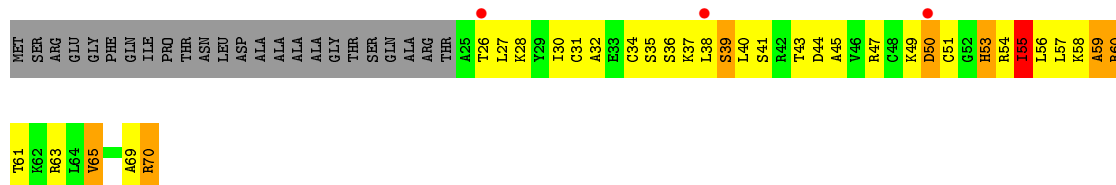
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



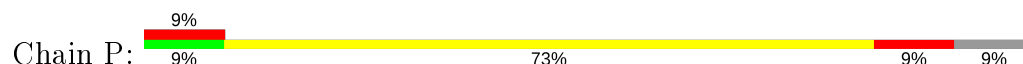
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11

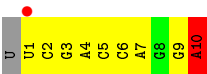


- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

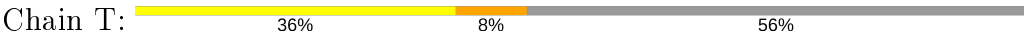


- Molecule 13: 5'-R(*UP*UP*CP*GP*AP*CP*CP*AP*GP*GP*AP)-3'





● Molecule 14: 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP *CP*TP*TTP*TP*TP*CP*CP *BRUP*GP*GP*TP*CP*AP*TP*T)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	222.21Å 392.21Å 284.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 48.98 – 3.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (50.00-3.80) 99.0 (48.98-3.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 3.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.270 , 0.280 0.217 , 0.237	Depositor DCC
R_{free} test set	4681 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	99.7	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 70.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.024 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.027 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	31660	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, 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	0.48	0/11385	0.73	1/15393 (0.0%)
2	B	0.46	0/9037	0.71	2/12181 (0.0%)
3	C	0.48	0/2138	0.72	0/2896
4	D	0.43	0/1437	0.68	1/1925 (0.1%)
5	E	0.43	0/1788	0.63	0/2406
6	F	0.55	0/716	0.77	0/964
7	G	0.48	0/1368	0.73	0/1844
8	H	0.40	0/1102	0.67	0/1492
9	I	0.41	0/962	0.68	0/1295
10	J	0.50	0/541	0.79	1/727 (0.1%)
11	K	0.90	6/937 (0.6%)	1.02	11/1265 (0.9%)
12	L	0.44	0/366	0.70	0/485
13	P	1.13	1/237 (0.4%)	1.22	2/368 (0.5%)
14	T	1.05	0/220	1.33	0/335
All	All	0.50	7/32234 (0.0%)	0.74	18/43576 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
14	T	0	2
All	All	0	4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	112	GLN	CA-C	9.87	1.78	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	113	THR	N-CA	9.16	1.64	1.46
11	K	112	GLN	CB-CG	9.05	1.76	1.52
11	K	112	GLN	N-CA	8.12	1.62	1.46
11	K	112	GLN	CG-CD	6.57	1.66	1.51
13	P	10	A	C5-C6	-6.52	1.35	1.41
11	K	113	THR	CA-C	6.38	1.69	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	113	THR	N-CA-C	9.53	136.74	111.00
13	P	1	U	N1-C1'-C2'	9.37	126.18	114.00
11	K	112	GLN	N-CA-C	8.61	134.26	111.00
11	K	114	LEU	CB-CG-CD1	8.38	125.24	111.00
11	K	114	LEU	N-CA-C	7.93	132.41	111.00
11	K	114	LEU	CA-C-O	-6.92	105.57	120.10
11	K	112	GLN	CA-C-N	6.13	130.69	117.20
11	K	114	LEU	CA-CB-CG	5.94	128.97	115.30
10	J	10	CYS	CA-CB-SG	5.84	124.51	114.00
11	K	111	LEU	N-CA-C	5.78	126.60	111.00
1	A	567	LYS	C-N-CD	5.61	140.19	128.40
11	K	113	THR	CB-CA-C	-5.60	96.48	111.60
2	B	111	ALA	N-CA-C	-5.53	96.06	111.00
11	K	111	LEU	CA-C-N	5.38	129.04	117.20
4	D	26	THR	N-CA-C	-5.29	96.72	111.00
11	K	112	GLN	N-CA-CB	-5.07	101.47	110.60
13	P	1	U	OP1-P-O3'	5.04	116.28	105.20
2	B	1185	CYS	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	TYR	Sidechain
2	B	486	TYR	Sidechain
14	T	19	DT	Sidechain
14	T	20	DC	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	11186	0	11266	1286	0
2	B	8866	0	8898	1020	0
3	C	2101	0	2055	267	0
4	D	1427	0	1451	141	0
5	E	1752	0	1776	127	0
6	F	705	0	730	84	0
7	G	1340	0	1357	161	0
8	H	1084	0	1057	123	0
9	I	944	0	899	101	0
10	J	532	0	542	98	0
11	K	919	0	929	109	0
12	L	364	0	386	43	0
13	P	212	0	109	20	0
14	T	219	0	125	31	0
15	A	1	0	0	0	0
16	A	8	0	0	0	0
All	All	31660	0	31580	3314	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 (3314) 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)
11:K:112:GLN:CB	11:K:112:GLN:CG	1.77	1.62
11:K:112:GLN:CA	11:K:112:GLN:C	1.78	1.51
2:B:343:ILE:HG23	2:B:347:LYS:HB2	1.18	1.17
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.26	1.17
1:A:1445:ILE:H	1:A:1445:ILE:HD12	1.12	1.15
2:B:336:ARG:HG2	2:B:348:ARG:HD3	1.28	1.13
1:A:53:LEU:HD23	1:A:54:ASN:N	1.64	1.11
5:E:22:MET:HE3	5:E:26:ARG:HH21	1.11	1.07
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.33	1.06
1:A:855:THR:HG21	1:A:857:ARG:HE	1.15	1.05
2:B:214:ALA:HB3	2:B:498:THR:HA	1.32	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.35	1.04
11:K:47:ARG:HH11	11:K:47:ARG:HB3	1.21	1.04
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.39	1.04
3:C:66:ARG:NH1	10:J:2:ILE:HG21	1.72	1.03
1:A:34:LYS:HD3	1:A:57:ARG:NH2	1.70	1.03
1:A:225:ASN:HD22	1:A:228:PHE:H	1.05	1.02
7:G:138:THR:HG22	7:G:139:ILE:H	1.23	1.02
2:B:502:ILE:HD12	2:B:502:ILE:H	1.21	1.02
14:T:26:DC:H2''	14:T:27:DA:O5'	1.60	1.02
1:A:53:LEU:CD2	1:A:54:ASN:H	1.72	1.01
2:B:336:ARG:HH22	2:B:345:LYS:HE2	1.25	1.00
7:G:13:LEU:HD21	7:G:17:PHE:HB2	1.39	1.00
3:C:101:LEU:HD13	3:C:118:LEU:HD23	1.43	0.99
3:C:43:THR:HG22	3:C:44:LEU:H	1.27	0.99
1:A:34:LYS:HD3	1:A:57:ARG:HH22	0.86	0.99
2:B:589:VAL:HG12	2:B:590:HIS:H	1.25	0.99
1:A:567:LYS:HB3	8:H:96:VAL:H	1.28	0.99
4:D:40:HIS:HB3	7:G:73:LYS:HZ3	1.24	0.99
1:A:524:VAL:HG12	1:A:525:GLN:H	1.25	0.98
14:T:26:DC:H2''	14:T:27:DA:C5'	1.93	0.98
2:B:1187:ASN:O	2:B:1188:LYS:HB2	1.63	0.98
2:B:65:GLU:HG3	2:B:66:ASP:H	1.29	0.97
1:A:567:LYS:CG	1:A:568:PRO:HD2	1.95	0.96
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.46	0.96
11:K:65:HIS:HD2	11:K:67:PHE:H	1.11	0.96
1:A:53:LEU:HD23	1:A:54:ASN:H	0.81	0.95
1:A:567:LYS:CD	1:A:568:PRO:HD2	1.96	0.95
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.46	0.95
3:C:166:GLU:HG3	11:K:10:PHE:HZ	1.31	0.95
1:A:1017:LEU:HB2	5:E:206:GLY:H	1.29	0.95
1:A:40:THR:HG22	1:A:41:MET:HG3	1.44	0.94
2:B:800:GLN:HB3	10:J:52:THR:HG21	1.49	0.94
2:B:516:ASN:N	2:B:516:ASN:HD22	1.63	0.94
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.50	0.94
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.31	0.94
4:D:144:THR:O	4:D:148:LEU:HB2	1.66	0.93
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.46	0.93
2:B:882:THR:HG22	2:B:884:ARG:H	1.29	0.93
1:A:754:SER:H	1:A:757:ASN:HD22	1.14	0.93
2:B:806:THR:HG22	2:B:808:ALA:H	1.31	0.93
2:B:510:LYS:HG2	2:B:511:PRO:HD3	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:14:HIS:CD2	7:G:16:SER:HB2	2.03	0.93
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.50	0.92
2:B:510:LYS:CG	2:B:511:PRO:HD3	1.98	0.92
3:C:6:PRO:HB3	3:C:25:VAL:CG1	1.99	0.92
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	1.70	0.92
1:A:709:THR:HG22	1:A:711:ARG:H	1.33	0.91
7:G:15:PRO:HA	7:G:18:PHE:CD1	2.04	0.91
10:J:1:MET:H1	10:J:57:ILE:H	1.02	0.91
2:B:168:GLY:H	2:B:450:ALA:HB1	1.35	0.91
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.51	0.91
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.51	0.91
2:B:770:GLN:OE1	2:B:983:ARG:HA	1.71	0.91
6:F:111:LEU:H	6:F:111:LEU:HD12	1.35	0.91
1:A:541:ILE:HD13	1:A:549:MET:HE1	1.51	0.91
2:B:336:ARG:HD3	2:B:348:ARG:HH11	1.36	0.91
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.52	0.90
9:I:85:PHE:H	9:I:85:PHE:HD2	1.18	0.90
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.51	0.90
11:K:65:HIS:CD2	11:K:67:PHE:H	1.89	0.90
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.51	0.90
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.50	0.90
10:J:1:MET:N	10:J:57:ILE:H	1.68	0.89
2:B:824:ILE:HG22	2:B:1087:PHE:HE2	1.37	0.89
2:B:393:LYS:HE3	2:B:393:LYS:HA	1.55	0.89
1:A:1424:VAL:HG13	1:A:1436:ILE:HD11	1.53	0.89
1:A:1094:VAL:HG12	1:A:1095:THR:H	1.33	0.89
7:G:81:PRO:HG3	7:G:106:MET:SD	2.12	0.89
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.55	0.89
2:B:879:ARG:HH11	2:B:883:LEU:HD22	1.39	0.88
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.02	0.88
2:B:98:THR:O	2:B:126:SER:HB2	1.72	0.88
4:D:40:HIS:HB3	7:G:73:LYS:NZ	1.86	0.88
9:I:8:ARG:HG3	9:I:34:TYR:HE1	1.36	0.88
2:B:1002:THR:HG21	2:B:1006:ILE:HD12	1.56	0.88
2:B:516:ASN:H	2:B:516:ASN:HD22	1.22	0.88
1:A:34:LYS:CD	1:A:57:ARG:HH22	1.81	0.88
2:B:343:ILE:CG2	2:B:348:ARG:HG3	2.03	0.88
1:A:58:LEU:HD21	1:A:243:PRO:HA	1.54	0.88
1:A:913:LEU:HD12	1:A:914:GLU:H	1.38	0.88
2:B:549:THR:HG22	2:B:550:ASP:H	1.38	0.87
7:G:34:VAL:HG12	7:G:45:ILE:HG21	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:36:CYS:HA	8:H:126:GLU:O	1.72	0.87
1:A:351:THR:HG22	2:B:1103:ILE:HA	1.56	0.87
2:B:1224:PHE:HE2	5:E:171:LYS:HG3	1.39	0.87
1:A:351:THR:HB	2:B:1103:ILE:HD12	1.57	0.87
1:A:382:PRO:HB3	1:A:428:TYR:HE2	1.40	0.87
10:J:1:MET:H1	10:J:57:ILE:N	1.73	0.87
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.57	0.86
1:A:58:LEU:CD1	1:A:59:GLY:H	1.88	0.86
1:A:1438:THR:HB	2:B:1144:ALA:HB3	1.53	0.86
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.56	0.86
5:E:19:VAL:O	5:E:23:VAL:HG23	1.75	0.86
2:B:340:ALA:HB2	2:B:343:ILE:HD12	1.57	0.86
1:A:1094:VAL:HG12	1:A:1095:THR:N	1.91	0.86
7:G:7:LEU:HB2	7:G:74:TYR:CE2	2.11	0.85
9:I:115:LYS:HD3	9:I:117:LYS:HE3	1.56	0.85
2:B:515:HIS:H	2:B:518:HIS:HD2	1.24	0.85
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.58	0.85
2:B:1197:PRO:HG2	2:B:1200:ALA:HB2	1.57	0.85
2:B:654:ARG:H	2:B:657:HIS:HD2	1.19	0.85
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.11	0.85
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.40	0.85
2:B:343:ILE:HG21	2:B:348:ARG:HG3	1.55	0.85
1:A:67:CYS:O	1:A:70:CYS:HB3	1.77	0.85
2:B:232:SER:HB3	2:B:261:ARG:HH21	1.41	0.85
7:G:80:LYS:HD3	7:G:80:LYS:N	1.92	0.84
1:A:709:THR:HG23	9:I:94:ASP:HA	1.58	0.84
5:E:22:MET:HE3	5:E:26:ARG:NH2	1.92	0.84
1:A:1394:THR:HG21	1:A:1398:MET:SD	2.18	0.84
2:B:46:GLN:HG3	2:B:47:GLN:H	1.39	0.84
2:B:842:ASN:ND2	2:B:845:SER:H	1.74	0.84
2:B:737:THR:HG21	9:I:66:PRO:HA	1.60	0.84
2:B:332:ASP:O	2:B:336:ARG:HG3	1.78	0.84
8:H:4:THR:HA	8:H:60:ALA:HB2	1.58	0.84
1:A:1329:THR:HG22	1:A:1331:SER:H	1.43	0.83
1:A:308:ILE:HG22	1:A:309:ALA:H	1.42	0.83
3:C:32:SER:O	3:C:36:VAL:HG23	1.77	0.83
1:A:58:LEU:HD12	1:A:59:GLY:H	1.44	0.83
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.08	0.83
6:F:82:THR:HG22	6:F:84:TYR:H	1.42	0.83
1:A:885:THR:O	1:A:940:ARG:HD2	1.78	0.83
2:B:465:ASN:HD22	2:B:465:ASN:N	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:847:ASP:HB3	3:C:167:HIS:NE2	1.91	0.83
8:H:100:THR:HG23	8:H:138:GLU:HA	1.57	0.83
1:A:741:ASN:HD22	1:A:744:LYS:H	1.27	0.83
6:F:86:THR:OG1	6:F:89:GLU:HG3	1.79	0.83
1:A:855:THR:HG21	1:A:857:ARG:NE	1.93	0.83
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.25	0.83
1:A:590:ARG:NH2	1:A:620:LYS:HB3	1.94	0.83
2:B:336:ARG:NH2	2:B:345:LYS:HG2	1.94	0.83
2:B:363:HIS:O	2:B:364:ILE:HB	1.76	0.83
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.60	0.83
1:A:34:LYS:H	1:A:57:ARG:NH2	1.77	0.82
1:A:427:GLN:HG3	1:A:430:TRP:CZ2	2.13	0.82
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.59	0.82
2:B:365:THR:HG23	2:B:367:LEU:H	1.42	0.82
2:B:955:THR:HG22	2:B:956:THR:H	1.44	0.82
14:T:21:DC:H2"	14:T:22:BRU:H5"	1.62	0.82
1:A:1116:LEU:N	1:A:1308:THR:HG22	1.94	0.82
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.60	0.82
7:G:14:HIS:ND1	7:G:15:PRO:HD2	1.95	0.82
1:A:866:PHE:C	1:A:867:ILE:HD12	1.99	0.82
13:P:3:G:H2'	13:P:4:A:C8	2.15	0.82
1:A:901:LEU:H	1:A:926:GLN:NE2	1.78	0.82
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.08	0.82
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.79	0.81
2:B:642:ASP:HA	2:B:649:LYS:HA	1.61	0.81
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.16	0.81
1:A:903:ASN:ND2	1:A:905:ASP:H	1.78	0.81
2:B:467:GLY:N	2:B:475:SER:HB3	1.95	0.81
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.10	0.81
8:H:81:PRO:HB2	8:H:82:PRO:HD2	1.62	0.81
1:A:1030:ARG:HG3	1:A:1034:GLU:OE2	1.81	0.81
2:B:343:ILE:HG21	2:B:348:ARG:N	1.95	0.81
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.61	0.81
3:C:239:PRO:HB2	3:C:241:ASP:OD1	1.81	0.81
10:J:64:ASN:HB3	10:J:65:PRO:CD	2.10	0.81
1:A:590:ARG:HH21	1:A:620:LYS:HB3	1.45	0.81
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.44	0.81
4:D:47:LEU:HD11	7:G:3:PHE:CD2	2.14	0.81
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.60	0.81
1:A:858:ASN:HD22	1:A:858:ASN:C	1.84	0.81
1:A:963:ILE:HD11	1:A:1048:ASN:HB3	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:59:ILE:HG22	8:H:60:ALA:N	1.94	0.81
1:A:321:PRO:O	1:A:322:VAL:HB	1.79	0.80
3:C:6:PRO:HB3	3:C:25:VAL:HG12	1.61	0.80
1:A:535:THR:HG21	1:A:616:VAL:HA	1.63	0.80
1:A:70:CYS:O	1:A:72:GLU:HG2	1.81	0.80
2:B:1095:LEU:HD12	2:B:1095:LEU:H	1.45	0.80
14:T:26:DC:H2''	14:T:27:DA:H5'	1.62	0.80
1:A:1171:GLN:HA	1:A:1174:PHE:CE1	2.17	0.80
1:A:1420:ASP:HB3	1:A:1422:ARG:HG3	1.64	0.80
1:A:779:PHE:HE1	1:A:785:PRO:HD3	1.47	0.80
3:C:167:HIS:HD2	3:C:168:ALA:H	1.30	0.80
3:C:47:ASP:HA	12:L:69:ALA:CB	2.12	0.80
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.65	0.79
1:A:886:ILE:HG22	1:A:887:GLY:N	1.96	0.79
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.64	0.79
9:I:105:SER:O	9:I:106:CYS:HB3	1.80	0.79
1:A:903:ASN:HD22	1:A:904:THR:N	1.79	0.79
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.62	0.79
2:B:613:VAL:HG13	2:B:627:PHE:O	1.83	0.79
4:D:47:LEU:HD13	4:D:48:ILE:H	1.47	0.79
10:J:48:ARG:HE	10:J:49:MET:HE2	1.48	0.79
14:T:25:DT:H2''	14:T:26:DC:O5'	1.82	0.79
1:A:1402:PHE:CE1	1:A:1403:GLU:HG3	2.18	0.79
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.18	0.79
1:A:450:LEU:H	1:A:450:LEU:HD12	1.48	0.79
7:G:80:LYS:HD3	7:G:80:LYS:H	1.47	0.79
9:I:55:THR:HG21	9:I:109:ILE:HD13	1.65	0.79
3:C:35:ARG:NH1	11:K:41:THR:H	1.80	0.78
3:C:73:GLN:HE21	3:C:75:MET:N	1.81	0.78
1:A:21:LEU:HD11	1:A:1414:ALA:HA	1.65	0.78
2:B:336:ARG:HD3	2:B:348:ARG:NH1	1.98	0.78
1:A:215:SER:HB3	1:A:218:ASP:OD2	1.84	0.78
2:B:171:PRO:HD2	2:B:457:LEU:HD13	1.65	0.78
2:B:244:LEU:HD21	2:B:366:GLN:NE2	1.98	0.78
2:B:975:GLN:O	2:B:990:ILE:HD12	1.83	0.78
1:A:472:LEU:O	1:A:475:THR:HB	1.83	0.78
2:B:336:ARG:CG	2:B:348:ARG:HD3	2.10	0.78
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.64	0.78
3:C:77:ILE:HG23	3:C:161:LYS:HE3	1.64	0.78
1:A:385:ILE:HG22	1:A:386:ASP:N	1.97	0.78
2:B:336:ARG:CD	2:B:348:ARG:HH11	1.96	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:708:GLU:O	2:B:710:LEU:N	2.17	0.78
1:A:84:ILE:HD11	1:A:270:LEU:HD13	1.65	0.78
1:A:768:GLN:CG	1:A:816:HIS:HA	2.13	0.78
1:A:14:VAL:HG21	2:B:1216:LEU:HD13	1.65	0.78
1:A:1036:ARG:HH11	1:A:1036:ARG:HG2	1.48	0.78
5:E:180:ARG:HH21	5:E:192:ARG:HB2	1.49	0.78
9:I:111:THR:HG22	9:I:112:SER:H	1.49	0.78
14:T:18:DT:H2''	14:T:19:DT:H5'	1.66	0.78
1:A:356:ASP:HB2	1:A:469:ARG:NH1	1.99	0.77
3:C:244:VAL:O	3:C:248:ILE:HG13	1.84	0.77
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.64	0.77
5:E:192:ARG:HH11	5:E:192:ARG:HG3	1.49	0.77
11:K:47:ARG:NH1	11:K:47:ARG:HB3	1.99	0.77
1:A:107:CYS:SG	1:A:171:GLN:HG2	2.25	0.77
1:A:1206:ASP:HB3	1:A:1274:ARG:HH12	1.49	0.77
2:B:189:LEU:HA	2:B:192:LEU:HD12	1.64	0.77
2:B:1162:ILE:HD11	2:B:1194:ILE:HD13	1.67	0.77
2:B:53:GLN:HG2	2:B:547:VAL:HG22	1.65	0.77
4:D:153:ARG:NH2	4:D:184:ALA:HA	1.99	0.77
6:F:69:LEU:HA	6:F:70:LYS:N	1.98	0.77
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.67	0.77
1:A:58:LEU:HD11	1:A:243:PRO:HB3	1.65	0.77
2:B:615:MET:C	2:B:616:ILE:HD12	2.05	0.77
3:C:70:ILE:HG12	3:C:142:VAL:HG11	1.67	0.77
7:G:59:GLY:HA3	7:G:70:PHE:CD2	2.20	0.77
1:A:1341:ILE:HG23	1:A:1342:GLU:N	1.99	0.77
2:B:359:GLU:O	2:B:362:PRO:HD3	1.84	0.77
8:H:56:THR:HB	8:H:145:ARG:HG2	1.65	0.77
1:A:567:LYS:HB3	8:H:96:VAL:N	1.99	0.76
3:C:212:PRO:HB3	3:C:213:PRO:HD2	1.67	0.76
3:C:43:THR:HG22	3:C:44:LEU:N	1.98	0.76
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.00	0.76
9:I:34:TYR:CD2	9:I:35:VAL:N	2.53	0.76
11:K:12:LEU:HD12	11:K:12:LEU:H	1.49	0.76
1:A:254:GLU:HB2	2:B:935:ARG:HH12	1.51	0.76
1:A:63:ARG:HA	1:A:74:MET:SD	2.25	0.76
1:A:798:GLY:HA2	1:A:815:PHE:CD1	2.19	0.76
1:A:896:ARG:HD3	1:A:897:TYR:HE1	1.50	0.76
2:B:798:TYR:HE2	3:C:62:PHE:CZ	2.03	0.76
1:A:269:ILE:HD13	1:A:300:VAL:HG22	1.68	0.76
1:A:58:LEU:CG	1:A:59:GLY:H	1.97	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:858:ASN:ND2	1:A:860:LEU:H	1.83	0.76
2:B:486:TYR:OH	2:B:1096:ARG:HB3	1.84	0.76
3:C:167:HIS:HD2	3:C:168:ALA:N	1.83	0.76
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.67	0.76
2:B:128:LEU:HB2	2:B:168:GLY:O	1.85	0.76
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.21	0.76
2:B:821:GLN:HE22	2:B:851:PHE:HA	1.49	0.76
2:B:879:ARG:NH1	2:B:883:LEU:HD22	2.00	0.76
1:A:903:ASN:C	1:A:903:ASN:HD22	1.89	0.76
4:D:47:LEU:HD11	7:G:3:PHE:HD2	1.50	0.76
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.65	0.76
2:B:1085:ILE:HD12	2:B:1085:ILE:N	2.00	0.76
3:C:2:SER:N	3:C:3:GLU:N	2.33	0.76
3:C:44:LEU:HB2	3:C:77:ILE:HD11	1.68	0.76
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.12	0.76
2:B:807:ARG:HG2	2:B:1045:SER:OG	1.86	0.76
7:G:23:LYS:HG3	7:G:56:ILE:CD1	2.16	0.76
9:I:103:CYS:HB3	9:I:106:CYS:SG	2.26	0.76
2:B:44:VAL:HG11	2:B:199:MET:HG2	1.67	0.76
8:H:130:ARG:H	8:H:130:ARG:HD2	1.48	0.76
1:A:1189:SER:O	1:A:1241:ARG:HD3	1.85	0.75
1:A:1244:ARG:HB3	1:A:1245:PRO:HD2	1.67	0.75
1:A:230:ARG:H	1:A:233:TRP:HE3	1.31	0.75
1:A:549:MET:SD	1:A:577:ILE:HD11	2.26	0.75
2:B:189:LEU:O	2:B:192:LEU:N	2.15	0.75
2:B:467:GLY:H	2:B:475:SER:HB3	1.51	0.75
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.68	0.75
1:A:646:PHE:O	1:A:650:GLN:HG3	1.87	0.75
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.20	0.75
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.67	0.75
2:B:112:LEU:HD12	2:B:113:TYR:H	1.51	0.75
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.49	0.75
1:A:35:ILE:HG22	1:A:35:ILE:O	1.86	0.75
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.21	0.75
2:B:217:ARG:HE	2:B:405:ARG:HB2	1.50	0.75
1:A:1312:ASN:O	1:A:1316:VAL:HG23	1.86	0.75
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.21	0.75
2:B:310:MET:HE3	2:B:387:LEU:HD12	1.69	0.75
1:A:1325:THR:O	5:E:148:GLU:HB2	1.86	0.75
2:B:1180:PHE:HB3	2:B:1191:ILE:CD1	2.16	0.75
3:C:164:ALA:HA	3:C:167:HIS:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:73:GLN:HE21	3:C:75:MET:H	1.33	0.75
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.67	0.74
8:H:61:SER:O	8:H:62:SER:HB3	1.85	0.74
11:K:112:GLN:HA	11:K:112:GLN:C	2.02	0.74
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.00	0.74
1:A:783:THR:HG21	1:A:815:PHE:CZ	2.23	0.74
2:B:1197:PRO:HG2	2:B:1200:ALA:CB	2.17	0.74
2:B:65:GLU:HG3	2:B:66:ASP:N	2.01	0.74
2:B:637:LEU:HD12	2:B:693:ILE:HD12	1.69	0.74
3:C:142:VAL:H	10:J:16:ASP:HB3	1.52	0.74
7:G:128:PRO:O	7:G:138:THR:HG23	1.87	0.74
1:A:714:PHE:O	1:A:718:VAL:HG23	1.87	0.74
4:D:153:ARG:HB3	4:D:154:PHE:CE1	2.23	0.74
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.28	0.74
1:A:512:VAL:HA	1:A:519:PRO:HA	1.68	0.74
1:A:534:LEU:O	1:A:574:GLY:HA3	1.85	0.74
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.69	0.74
2:B:35:SER:HA	2:B:811:TYR:HE2	1.52	0.74
2:B:859:TYR:OH	2:B:941:LEU:HD12	1.88	0.74
7:G:111:THR:HG22	7:G:113:HIS:H	1.51	0.74
1:A:567:LYS:HD3	8:H:95:TYR:CG	2.23	0.74
1:A:58:LEU:HD13	1:A:80:HIS:O	1.87	0.74
2:B:830:TYR:O	2:B:832:GLY:N	2.21	0.74
9:I:111:THR:HG22	9:I:112:SER:N	2.02	0.74
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.70	0.74
3:C:213:PRO:O	3:C:214:ASN:HB2	1.87	0.74
7:G:23:LYS:HG3	7:G:56:ILE:HD11	1.68	0.74
1:A:58:LEU:HD21	1:A:243:PRO:CA	2.17	0.74
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.70	0.74
8:H:59:ILE:HG22	8:H:60:ALA:H	1.53	0.74
2:B:839:MET:HE3	2:B:1010:LEU:HD21	1.69	0.74
2:B:336:ARG:HH22	2:B:345:LYS:CE	1.99	0.74
1:A:1444:MET:HG2	7:G:60:ARG:HA	1.68	0.74
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	2.03	0.74
2:B:515:HIS:HD2	2:B:517:THR:H	1.36	0.74
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.70	0.74
2:B:336:ARG:HG2	2:B:348:ARG:CD	2.14	0.73
2:B:516:ASN:ND2	2:B:516:ASN:N	2.36	0.73
3:C:67:LEU:HD11	3:C:155:LEU:CD1	2.18	0.73
6:F:103:MET:HE2	7:G:66:GLY:H	1.53	0.73
1:A:326:ARG:HH22	1:A:1407:GLU:HG3	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ARG:NH1	1:A:590:ARG:HG3	2.03	0.73
6:F:125:LEU:O	6:F:125:LEU:HG	1.88	0.73
9:I:34:TYR:HE2	9:I:36:GLU:HB3	1.53	0.73
1:A:225:ASN:ND2	1:A:228:PHE:H	1.84	0.73
1:A:518:LYS:HE2	1:A:624:SER:O	1.88	0.73
2:B:378:LEU:O	2:B:382:ILE:HG13	1.88	0.73
2:B:863:GLU:OE2	2:B:873:THR:HA	1.88	0.73
1:A:567:LYS:HD3	8:H:95:TYR:CD2	2.23	0.73
1:A:49:LYS:NZ	1:A:61:ILE:HG13	2.03	0.73
2:B:336:ARG:HH21	2:B:345:LYS:HG2	1.54	0.73
2:B:622:LYS:HE2	9:I:59:VAL:HG22	1.69	0.73
13:P:5:C:H2'	13:P:6:C:C6	2.23	0.73
13:P:5:C:H2'	13:P:6:C:H6	1.53	0.73
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.69	0.73
1:A:836:TYR:CD2	1:A:840:ARG:HD2	2.24	0.73
2:B:434:ARG:O	2:B:437:GLU:HB2	1.87	0.73
9:I:8:ARG:HG3	9:I:34:TYR:CE1	2.20	0.73
12:L:38:LEU:O	12:L:39:SER:HB3	1.89	0.73
1:A:325:ILE:HG21	2:B:1210:MET:HG3	1.70	0.73
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.70	0.73
1:A:1063:MET:CG	1:A:1436:ILE:HG23	2.19	0.73
1:A:982:THR:HB	1:A:985:ASP:H	1.53	0.73
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.70	0.73
1:A:1094:VAL:CG1	1:A:1095:THR:H	2.01	0.73
1:A:1424:VAL:HG13	1:A:1436:ILE:CD1	2.18	0.73
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.71	0.73
2:B:502:ILE:N	2:B:502:ILE:HD12	2.01	0.73
3:C:253:LYS:O	3:C:256:ALA:HB3	1.88	0.72
12:L:32:ALA:HB3	12:L:55:ILE:HD12	1.71	0.72
2:B:864:LYS:N	2:B:872:GLU:OE1	2.22	0.72
2:B:955:THR:HG22	2:B:956:THR:N	2.02	0.72
1:A:347:PHE:H	2:B:1107:ALA:HA	1.54	0.72
4:D:53:SER:HB3	4:D:152:SER:HB2	1.71	0.72
2:B:847:ASP:HB3	3:C:167:HIS:HE2	1.52	0.72
5:E:213:ILE:HG12	5:E:214:CYS:H	1.54	0.72
7:G:15:PRO:HA	7:G:18:PHE:CE1	2.24	0.72
1:A:92:HIS:O	1:A:94:GLY:N	2.21	0.72
3:C:147:LEU:HB2	3:C:151:GLN:HB2	1.69	0.72
1:A:106:VAL:HG13	1:A:112:LYS:O	1.88	0.72
2:B:280:ILE:HD13	2:B:334:ILE:HG12	1.70	0.72
1:A:960:ILE:O	1:A:963:ILE:HG22	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:616:ILE:N	2:B:616:ILE:HD12	2.04	0.72
1:A:382:PRO:HD3	1:A:428:TYR:CD2	2.25	0.72
2:B:1006:ILE:HD13	10:J:44:TYR:CE2	2.24	0.72
10:J:64:ASN:HD22	10:J:65:PRO:HD3	1.52	0.72
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.05	0.72
4:D:34:GLN:O	4:D:47:LEU:HD23	1.89	0.72
6:F:85:MET:HE1	6:F:93:ILE:HD12	1.71	0.72
1:A:794:PRO:HG2	1:A:795:GLU:OE2	1.90	0.71
7:G:47:CYS:O	7:G:76:ALA:HB1	1.90	0.71
2:B:1099:VAL:CG1	2:B:1100:ASP:N	2.53	0.71
11:K:31:VAL:HG12	11:K:32:VAL:N	2.04	0.71
1:A:1329:THR:HG22	1:A:1331:SER:N	2.05	0.71
1:A:58:LEU:HG	1:A:59:GLY:N	2.04	0.71
2:B:882:THR:HG22	2:B:884:ARG:N	2.04	0.71
1:A:58:LEU:HD21	1:A:244:PRO:HD2	1.73	0.71
1:A:855:THR:CG2	1:A:857:ARG:HE	1.99	0.71
11:K:65:HIS:HD2	11:K:67:PHE:N	1.88	0.71
1:A:1171:GLN:HA	1:A:1174:PHE:CD1	2.25	0.71
2:B:37:PHE:HE2	2:B:542:MET:HA	1.55	0.71
1:A:567:LYS:CB	8:H:95:TYR:HA	2.20	0.71
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.72	0.71
2:B:842:ASN:O	2:B:846:ILE:HG13	1.90	0.71
14:T:20:DC:H2''	14:T:21:DC:H5'	1.71	0.71
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.03	0.71
1:A:1313:LEU:HD23	1:A:1338:VAL:HG21	1.71	0.71
1:A:525:GLN:HG3	2:B:835:GLN:HG2	1.71	0.71
2:B:589:VAL:HG12	2:B:590:HIS:N	2.04	0.71
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.71	0.71
1:A:115:LEU:O	1:A:122:MET:HE2	1.90	0.71
1:A:754:SER:H	1:A:757:ASN:ND2	1.89	0.71
9:I:7:CYS:HB3	9:I:14:LEU:HD21	1.73	0.71
2:B:63:ILE:O	2:B:67:SER:HB3	1.90	0.71
3:C:174:ALA:HB2	3:C:235:VAL:HG22	1.73	0.71
3:C:133:ILE:HD11	3:C:237:SER:HA	1.73	0.71
4:D:7:THR:HB	7:G:42:PHE:CE2	2.26	0.71
1:A:832:ALA:HB2	14:T:18:DT:H71	1.72	0.71
14:T:24:DG:H2''	14:T:25:DT:H5'	1.72	0.71
1:A:335:ARG:NH1	2:B:1202:LEU:HD13	2.06	0.70
1:A:741:ASN:ND2	1:A:744:LYS:H	1.87	0.70
1:A:767:GLN:NE2	1:A:774:ARG:HB3	2.06	0.70
2:B:38:PHE:HD1	2:B:811:TYR:CD2	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:53:SER:HB3	4:D:152:SER:CB	2.21	0.70
2:B:95:ILE:HG13	2:B:129:PHE:O	1.90	0.70
4:D:56:ARG:HB2	4:D:148:LEU:HD22	1.72	0.70
10:J:64:ASN:ND2	10:J:65:PRO:HD3	2.06	0.70
6:F:111:LEU:N	6:F:111:LEU:HD12	2.06	0.70
1:A:58:LEU:HG	1:A:59:GLY:H	1.56	0.70
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.73	0.70
2:B:100:PRO:HD2	2:B:180:TYR:HE1	1.56	0.70
2:B:569:TYR:CE1	2:B:589:VAL:HG21	2.26	0.70
11:K:47:ARG:CB	11:K:47:ARG:HH11	2.02	0.70
11:K:6:ARG:O	11:K:9:LEU:HG	1.91	0.70
5:E:153:HIS:HB3	5:E:196:VAL:HG11	1.74	0.70
1:A:12:ARG:HD2	2:B:1218:THR:HB	1.73	0.70
1:A:1332:PHE:HD2	1:A:1332:PHE:H	1.39	0.70
1:A:254:GLU:O	1:A:256:GLN:N	2.24	0.70
1:A:444:PHE:CB	1:A:458:HIS:HD2	2.04	0.70
1:A:528:LEU:O	1:A:531:ILE:HG22	1.91	0.70
5:E:153:HIS:HB3	5:E:196:VAL:CG1	2.22	0.70
1:A:567:LYS:HE3	8:H:46:LEU:HB2	1.72	0.70
2:B:232:SER:CB	2:B:261:ARG:HH21	2.03	0.70
2:B:278:GLN:HG2	2:B:279:ASP:H	1.55	0.70
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.55	0.70
3:C:56:THR:HG22	3:C:57:VAL:H	1.55	0.70
2:B:942:ARG:NH2	14:T:24:DG:OP2	2.21	0.70
1:A:852:TYR:CD2	1:A:1060:PRO:HB2	2.27	0.70
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.74	0.70
7:G:14:HIS:HD2	7:G:16:SER:HB2	1.55	0.70
8:H:84:ALA:CA	8:H:87:ARG:HB2	2.21	0.70
14:T:18:DT:H2''	14:T:19:DT:C5'	2.21	0.70
5:E:202:SER:OG	5:E:204:THR:HG22	1.92	0.70
2:B:792:MET:HG3	2:B:855:PHE:HE1	1.57	0.69
4:D:176:GLU:C	4:D:178:ALA:H	1.96	0.69
4:D:22:GLU:H	4:D:22:GLU:CD	1.96	0.69
5:E:198:ILE:CD1	5:E:212:ARG:HG3	2.22	0.69
1:A:1005:GLU:O	1:A:1009:ASN:HB2	1.92	0.69
1:A:608:ILE:HB	1:A:613:ILE:HD11	1.73	0.69
1:A:351:THR:HB	2:B:1103:ILE:CD1	2.22	0.69
1:A:1341:ILE:HG23	1:A:1342:GLU:H	1.57	0.69
1:A:663:SER:OG	1:A:664:THR:N	2.25	0.69
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.72	0.69
2:B:899:ILE:HD12	2:B:911:ILE:HG23	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:TYR:HD1	2:B:180:TYR:H	1.40	0.69
2:B:579:ARG:HG2	2:B:579:ARG:HH11	1.56	0.69
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.74	0.69
2:B:860:MET:HG2	2:B:861:ASP:H	1.57	0.69
1:A:1436:ILE:O	1:A:1437:GLY:C	2.31	0.69
1:A:58:LEU:HD11	1:A:243:PRO:CB	2.22	0.69
1:A:886:ILE:HD11	1:A:943:LEU:HB3	1.74	0.69
2:B:295:GLY:H	2:B:298:LEU:HD23	1.56	0.69
2:B:603:LEU:HD13	2:B:608:ASP:HB2	1.73	0.69
2:B:745:PRO:O	2:B:748:ILE:HG12	1.92	0.69
1:A:1332:PHE:HD2	1:A:1332:PHE:N	1.90	0.69
1:A:61:ILE:HG22	1:A:62:ASP:H	1.57	0.69
1:A:637:LYS:HB3	1:A:641:VAL:HG11	1.72	0.69
1:A:913:LEU:HD12	1:A:914:GLU:N	2.07	0.69
1:A:596:THR:O	1:A:598:LEU:N	2.26	0.69
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.22	0.69
4:D:7:THR:HG21	4:D:32:GLU:CD	2.13	0.69
5:E:9:ILE:HD11	5:E:53:PRO:HD3	1.73	0.69
6:F:103:MET:O	6:F:104:ASN:HB2	1.91	0.69
2:B:953:LEU:O	2:B:953:LEU:HD23	1.92	0.69
4:D:134:THR:HG22	4:D:135:GLY:N	2.08	0.69
7:G:138:THR:HG22	7:G:139:ILE:N	2.04	0.69
11:K:111:LEU:C	11:K:112:GLN:HG2	2.13	0.69
1:A:1438:THR:HB	2:B:1144:ALA:CB	2.23	0.69
1:A:23:SER:HA	1:A:233:TRP:CD1	2.28	0.69
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.75	0.69
3:C:35:ARG:NH1	11:K:41:THR:N	2.40	0.69
14:T:21:DC:H2''	14:T:22:BRU:C5'	2.23	0.69
1:A:58:LEU:CG	1:A:59:GLY:N	2.55	0.69
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.21	0.69
2:B:36:ALA:HA	2:B:39:ARG:HD2	1.75	0.69
4:D:185:CYS:HB2	4:D:211:LEU:HD22	1.75	0.69
1:A:18:GLN:HB2	2:B:1215:ARG:HB2	1.75	0.69
8:H:102:TYR:OH	8:H:122:LEU:HD22	1.93	0.68
1:A:407:ARG:HB3	1:A:430:TRP:CE2	2.28	0.68
2:B:860:MET:HG2	2:B:861:ASP:N	2.08	0.68
3:C:167:HIS:CD2	3:C:168:ALA:N	2.61	0.68
5:E:135:PHE:HD2	5:E:140:LEU:HD21	1.56	0.68
12:L:30:ILE:O	12:L:56:LEU:HA	1.93	0.68
1:A:963:ILE:HD11	1:A:1048:ASN:CB	2.23	0.68
1:A:388:LEU:O	1:A:392:VAL:HG23	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASP:N	1:A:56:PRO:HD3	2.09	0.68
1:A:821:ARG:HB2	1:A:821:ARG:HH11	1.57	0.68
1:A:881:GLN:NE2	1:A:958:VAL:O	2.26	0.68
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.74	0.68
2:B:339:THR:HG22	2:B:339:THR:O	1.93	0.68
1:A:853:ASP:O	1:A:854:ASN:HB2	1.94	0.68
2:B:705:MET:H	2:B:710:LEU:HD12	1.58	0.68
1:A:35:ILE:HA	1:A:52:GLY:O	1.94	0.68
1:A:694:THR:O	1:A:698:GLN:HG3	1.94	0.68
2:B:1069:PHE:HD1	2:B:1069:PHE:H	1.41	0.68
2:B:1096:ARG:O	2:B:1097:HIS:HB2	1.94	0.68
2:B:411:PRO:O	2:B:414:ALA:HB3	1.94	0.68
1:A:1341:ILE:HD12	1:A:1379:GLY:O	1.94	0.68
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.75	0.68
3:C:90:ASP:O	3:C:91:HIS:HB3	1.93	0.68
1:A:441:PRO:HD2	1:A:498:ARG:NH2	2.09	0.68
1:A:567:LYS:NZ	8:H:46:LEU:HB2	2.09	0.68
1:A:590:ARG:HH11	1:A:590:ARG:HG3	1.58	0.68
1:A:68:GLN:C	1:A:70:CYS:H	1.94	0.68
2:B:114:PRO:HG2	2:B:115:GLN:H	1.56	0.68
1:A:269:ILE:HD11	1:A:300:VAL:HA	1.75	0.68
1:A:34:LYS:HE3	1:A:57:ARG:HH12	1.58	0.68
1:A:979:SER:OG	1:A:980:ASP:N	2.25	0.68
2:B:1106:ARG:NH1	2:B:1110:PRO:HG2	2.09	0.68
2:B:315:LYS:N	2:B:316:PRO:HD2	2.08	0.68
1:A:335:ARG:HA	1:A:339:ASN:HB2	1.76	0.68
1:A:57:ARG:O	1:A:68:GLN:HG3	1.94	0.68
2:B:1159:ARG:HD3	2:B:1193:GLN:CG	2.24	0.68
3:C:174:ALA:HB2	3:C:235:VAL:CG2	2.23	0.68
1:A:1445:ILE:H	1:A:1445:ILE:CD1	1.92	0.68
1:A:384:ASN:O	1:A:385:ILE:C	2.32	0.68
3:C:11:ARG:HD3	3:C:209:TYR:CE2	2.28	0.68
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.23	0.68
10:J:43:ARG:HG3	10:J:45:CYS:SG	2.33	0.68
1:A:372:LYS:HA	1:A:435:HIS:ND1	2.10	0.67
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.29	0.67
1:A:524:VAL:HG12	1:A:525:GLN:N	2.03	0.67
1:A:657:LEU:HD12	1:A:657:LEU:O	1.95	0.67
2:B:549:THR:H	2:B:628:THR:HG23	1.59	0.67
3:C:73:GLN:NE2	3:C:74:SER:H	1.92	0.67
1:A:1028:THR:O	1:A:1032:LEU:HD12	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:PHE:HB2	1:A:458:HIS:HD2	1.60	0.67
1:A:675:THR:O	1:A:679:ILE:HG13	1.93	0.67
4:D:189:ASP:O	4:D:193:THR:HB	1.93	0.67
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.75	0.67
2:B:516:ASN:ND2	2:B:516:ASN:H	1.85	0.67
3:C:147:LEU:N	3:C:147:LEU:HD23	2.09	0.67
4:D:63:LEU:HD13	4:D:133:THR:OG1	1.94	0.67
1:A:252:PHE:O	1:A:253:ASN:HB2	1.95	0.67
7:G:39:THR:HG22	7:G:41:LYS:H	1.60	0.67
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.76	0.67
1:A:414:ASP:OD1	1:A:416:ARG:HG2	1.95	0.67
4:D:52:LEU:HD21	4:D:147:TYR:HE2	1.59	0.67
1:A:1279:ILE:HD11	1:A:1316:VAL:HG21	1.75	0.67
1:A:33:ALA:HA	1:A:57:ARG:NH2	2.09	0.67
2:B:601:ARG:O	2:B:605:ARG:HG3	1.94	0.67
4:D:60:LYS:O	4:D:64:VAL:HG23	1.95	0.67
5:E:157:SER:OG	5:E:160:GLU:HG3	1.94	0.67
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.29	0.67
6:F:81:THR:HG23	6:F:144:GLU:OE2	1.95	0.67
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	1.95	0.67
1:A:265:LYS:HD2	1:A:265:LYS:N	2.09	0.67
2:B:1161:HIS:NE2	2:B:1175:LEU:HD21	2.10	0.67
2:B:351:TYR:O	2:B:355:ILE:HG13	1.95	0.67
2:B:794:ASN:O	2:B:795:ILE:HD12	1.94	0.67
5:E:198:ILE:HD11	5:E:212:ARG:HG3	1.75	0.67
9:I:34:TYR:HD2	9:I:35:VAL:N	1.92	0.67
3:C:35:ARG:HH12	11:K:41:THR:H	1.40	0.67
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.77	0.67
8:H:4:THR:HA	8:H:60:ALA:CB	2.25	0.67
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.29	0.66
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.59	0.66
2:B:603:LEU:HD12	2:B:609:ILE:HG13	1.76	0.66
3:C:147:LEU:HD12	3:C:151:GLN:O	1.95	0.66
1:A:699:ALA:HB1	1:A:701:LEU:HG	1.75	0.66
1:A:446:ARG:CD	1:A:480:ALA:HB2	2.26	0.66
2:B:953:LEU:CD2	2:B:965:LYS:HB2	2.24	0.66
7:G:79:PHE:HZ	7:G:106:MET:HE1	1.58	0.66
8:H:143:LEU:N	8:H:143:LEU:HD12	2.10	0.66
1:A:1289:ARG:HD2	1:A:1303:GLU:OE2	1.94	0.66
1:A:1445:ILE:N	1:A:1445:ILE:HD12	1.96	0.66
1:A:164:ARG:HG3	1:A:165:GLY:N	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:PRO:HD3	1:A:428:TYR:HD2	1.60	0.66
2:B:247:GLY:C	2:B:249:ARG:H	1.96	0.66
2:B:857:ARG:NH2	14:T:24:DG:OP1	2.29	0.66
5:E:192:ARG:NH1	5:E:192:ARG:HG3	2.11	0.66
10:J:14:VAL:HG12	10:J:14:VAL:O	1.95	0.66
1:A:1124:HIS:HB3	1:A:1130:GLN:HG2	1.78	0.66
1:A:856:THR:HB	1:A:865:GLN:HB2	1.77	0.66
7:G:13:LEU:CD2	7:G:17:PHE:HB2	2.20	0.66
1:A:1332:PHE:N	1:A:1332:PHE:CD2	2.62	0.66
1:A:1072:ILE:HD11	1:A:1368:MET:HA	1.77	0.66
1:A:986:ILE:HG22	1:A:987:VAL:N	2.09	0.66
2:B:1087:PHE:HD2	2:B:1088:GLY:N	1.94	0.66
12:L:47:ARG:HH21	12:L:54:ARG:HH21	1.42	0.66
1:A:1063:MET:HG3	1:A:1436:ILE:HG23	1.77	0.66
6:F:97:ARG:O	6:F:101:ILE:HG13	1.96	0.66
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.61	0.66
2:B:521:LEU:HB3	2:B:633:VAL:HG11	1.76	0.66
4:D:128:VAL:O	4:D:132:GLN:HG3	1.96	0.66
5:E:117:THR:HG22	5:E:119:SER:H	1.60	0.66
6:F:90:ARG:HD3	6:F:155:LEU:HD11	1.78	0.66
10:J:14:VAL:HG12	10:J:50:ILE:HD11	1.78	0.66
1:A:382:PRO:CB	1:A:428:TYR:HE2	2.08	0.66
1:A:438:ASP:OD1	1:A:462:VAL:HG23	1.96	0.66
2:B:1115:THR:O	2:B:1116:ARG:HB2	1.95	0.66
2:B:642:ASP:O	2:B:644:GLU:N	2.28	0.66
2:B:882:THR:HB	2:B:934:LYS:O	1.96	0.66
4:D:130:LEU:C	4:D:132:GLN:H	1.99	0.66
1:A:546:VAL:O	1:A:550:LEU:HG	1.95	0.65
1:A:869:GLY:O	5:E:204:THR:HG21	1.96	0.65
3:C:232:VAL:HG21	3:C:244:VAL:HG22	1.79	0.65
3:C:98:VAL:C	3:C:99:LEU:HD23	2.16	0.65
6:F:90:ARG:HG3	6:F:91:ALA:N	2.11	0.65
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.78	0.65
1:A:1035:TYR:O	1:A:1037:LEU:N	2.29	0.65
1:A:1039:LYS:HE3	1:A:1043:ASP:OD2	1.95	0.65
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.26	0.65
1:A:58:LEU:HD12	1:A:59:GLY:N	2.11	0.65
1:A:699:ALA:CB	1:A:701:LEU:HG	2.27	0.65
9:I:82:GLU:O	9:I:104:LEU:HG	1.96	0.65
10:J:1:MET:N	10:J:56:LEU:N	2.44	0.65
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:66:ARG:NH1	3:C:144:ILE:O	2.28	0.65
4:D:71:LYS:HA	4:D:74:GLN:HB2	1.77	0.65
8:H:81:PRO:CB	8:H:82:PRO:CD	2.74	0.65
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.12	0.65
1:A:1450:LEU:HG	1:A:1450:LEU:O	1.97	0.65
1:A:49:LYS:HE2	1:A:61:ILE:HD12	1.77	0.65
2:B:756:ILE:O	2:B:759:PRO:HD3	1.96	0.65
2:B:778:MET:HE3	2:B:1094:ARG:HD3	1.78	0.65
4:D:40:HIS:CE1	4:D:41:GLN:HG3	2.32	0.65
6:F:90:ARG:HD3	6:F:155:LEU:CD1	2.27	0.65
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.25	0.65
1:A:265:LYS:HD2	1:A:265:LYS:H	1.62	0.65
1:A:50:ILE:C	1:A:52:GLY:H	2.00	0.65
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.75	0.65
2:B:1065:GLN:HG3	2:B:1067:ARG:H	1.60	0.65
2:B:18:PHE:N	2:B:19:GLU:N	2.44	0.65
2:B:557:PHE:CD2	2:B:557:PHE:C	2.70	0.65
4:D:7:THR:HB	7:G:42:PHE:HE2	1.62	0.65
1:A:49:LYS:HZ1	1:A:61:ILE:HG13	1.62	0.65
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.78	0.65
2:B:1159:ARG:NH1	2:B:1159:ARG:HB3	2.11	0.65
3:C:123:ASN:HD22	3:C:125:MET:HG2	1.62	0.65
2:B:798:TYR:HE2	3:C:62:PHE:HZ	1.44	0.65
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.27	0.65
1:A:785:PRO:HG2	1:A:786:HIS:HD2	1.62	0.65
1:A:450:LEU:HB3	1:A:838:GLN:NE2	2.12	0.65
2:B:1169:MET:HE1	2:B:1201:LYS:HA	1.78	0.65
7:G:49:LEU:HG	7:G:76:ALA:HA	1.78	0.65
8:H:44:VAL:O	8:H:44:VAL:HG12	1.97	0.65
9:I:75:CYS:SG	9:I:79:HIS:N	2.69	0.65
1:A:1291:VAL:HG13	1:A:1292:PRO:HD2	1.78	0.65
1:A:588:LEU:O	1:A:606:LEU:HA	1.96	0.65
1:A:901:LEU:O	1:A:921:GLY:N	2.25	0.65
2:B:121:ASN:HA	2:B:207:GLY:HA2	1.79	0.65
2:B:57:TYR:HD1	2:B:57:TYR:N	1.95	0.65
2:B:850:LEU:HD12	2:B:851:PHE:N	2.11	0.65
1:A:450:LEU:N	1:A:450:LEU:HD12	2.12	0.64
1:A:899:VAL:HB	1:A:929:LEU:HD12	1.79	0.64
2:B:906:SER:O	2:B:941:LEU:HD23	1.97	0.64
1:A:567:LYS:CE	8:H:46:LEU:HB2	2.26	0.64
11:K:47:ARG:O	11:K:47:ARG:HD2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1029:ARG:HG3	1:A:1029:ARG:HH11	1.61	0.64
1:A:42:ASP:HB3	1:A:45:GLN:H	1.63	0.64
2:B:1172:ILE:O	2:B:1172:ILE:HG22	1.96	0.64
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.33	0.64
14:T:26:DC:C2'	14:T:27:DA:O5'	2.41	0.64
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.62	0.64
1:A:1100:ARG:NH2	1:A:1351:GLU:HG2	2.13	0.64
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.32	0.64
1:A:108:MET:N	1:A:108:MET:SD	2.70	0.64
1:A:626:ASN:O	1:A:631:HIS:CD2	2.50	0.64
2:B:336:ARG:NH2	2:B:345:LYS:HE2	2.06	0.64
2:B:57:TYR:CD1	2:B:57:TYR:N	2.66	0.64
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.28	0.64
4:D:48:ILE:HG21	7:G:4:ILE:HB	1.78	0.64
5:E:114:ASN:O	5:E:115:ASN:HB3	1.96	0.64
13:P:3:G:H2'	13:P:4:A:H8	1.58	0.64
1:A:23:SER:HA	1:A:233:TRP:NE1	2.13	0.64
1:A:244:PRO:O	1:A:246:VAL:N	2.30	0.64
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.30	0.64
2:B:1084:GLN:NE2	2:B:1084:GLN:N	2.45	0.64
2:B:824:ILE:CG2	2:B:1087:PHE:HE2	2.10	0.64
2:B:433:GLN:O	2:B:437:GLU:HG3	1.96	0.64
2:B:810:GLU:HB2	2:B:815:ARG:HH22	1.62	0.64
7:G:153:GLN:HG2	7:G:154:VAL:HG23	1.78	0.64
1:A:69:THR:O	1:A:71:GLN:N	2.30	0.64
2:B:654:ARG:H	2:B:657:HIS:CD2	2.10	0.64
4:D:40:HIS:CB	7:G:73:LYS:NZ	2.60	0.64
5:E:94:LYS:CE	5:E:98:ILE:HD11	2.26	0.64
4:D:40:HIS:CB	7:G:73:LYS:HZ3	2.04	0.64
1:A:598:LEU:HA	8:H:122:LEU:HD13	1.80	0.64
3:C:66:ARG:HH12	10:J:2:ILE:HG21	1.63	0.64
1:A:265:LYS:HE2	1:A:322:VAL:CG1	2.28	0.64
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.62	0.64
1:A:897:TYR:HD2	1:A:936:LEU:HD13	1.62	0.64
7:G:111:THR:HB	7:G:114:LEU:HB2	1.80	0.64
7:G:119:LEU:HD12	7:G:131:GLN:O	1.97	0.64
8:H:100:THR:OG1	8:H:138:GLU:HG3	1.98	0.64
9:I:34:TYR:CE2	9:I:36:GLU:HB3	2.33	0.64
1:A:984:LYS:O	1:A:988:LEU:HB2	1.98	0.64
2:B:232:SER:HB3	2:B:261:ARG:NH2	2.13	0.64
2:B:53:GLN:HG2	2:B:547:VAL:CG2	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:51:ASN:O	4:D:54:GLU:HB3	1.97	0.64
10:J:23:ASN:C	10:J:25:LEU:H	2.00	0.64
1:A:1348:LEU:HG	1:A:1372:VAL:CG2	2.28	0.64
1:A:58:LEU:CD2	1:A:244:PRO:HD2	2.27	0.64
1:A:666:ILE:HD12	1:A:667:GLY:H	1.63	0.64
7:G:145:VAL:HG12	7:G:146:LYS:N	2.12	0.64
10:J:48:ARG:HE	10:J:49:MET:CE	2.11	0.64
1:A:485:ASP:OD1	13:P:10:A:O2'	2.15	0.64
1:A:58:LEU:CD1	1:A:243:PRO:HB3	2.28	0.64
1:A:590:ARG:HB3	1:A:605:MET:N	2.12	0.64
2:B:35:SER:O	2:B:39:ARG:HG3	1.97	0.64
2:B:563:MET:HE3	2:B:580:VAL:HB	1.80	0.64
2:B:842:ASN:HB3	2:B:845:SER:OG	1.98	0.64
6:F:79:ARG:HG3	6:F:144:GLU:OE1	1.98	0.64
4:D:29:LEU:HD22	7:G:82:PHE:CE2	2.32	0.64
8:H:89:LEU:HB3	8:H:91:ASP:OD1	1.98	0.64
11:K:67:PHE:C	11:K:68:PHE:HD2	2.00	0.64
12:L:53:HIS:HB3	12:L:55:ILE:HD11	1.80	0.64
1:A:326:ARG:NH2	1:A:1407:GLU:HG3	2.13	0.63
1:A:591:PHE:HA	1:A:595:THR:HG21	1.80	0.63
1:A:728:LYS:O	1:A:732:LEU:HG	1.98	0.63
2:B:175:ARG:HH11	2:B:175:ARG:HG2	1.61	0.63
6:F:85:MET:CE	6:F:93:ILE:HD12	2.29	0.63
7:G:143:ILE:HG22	7:G:144:ARG:N	2.13	0.63
1:A:401:GLY:C	1:A:435:HIS:HD2	2.02	0.63
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.79	0.63
2:B:254:LEU:HD23	2:B:381:MET:CE	2.28	0.63
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.28	0.63
1:A:1445:ILE:HG12	7:G:18:PHE:CE2	2.32	0.63
1:A:19:PHE:O	1:A:1416:ALA:HA	1.98	0.63
2:B:839:MET:CE	2:B:1010:LEU:HD21	2.27	0.63
2:B:882:THR:CG2	2:B:884:ARG:HB2	2.29	0.63
8:H:116:TYR:HE2	8:H:140:ALA:HB1	1.63	0.63
12:L:70:ARG:HG2	12:L:70:ARG:HH11	1.63	0.63
1:A:356:ASP:HB2	1:A:469:ARG:HH11	1.64	0.63
2:B:1165:ILE:HG22	2:B:1166:CYS:N	2.12	0.63
2:B:806:THR:HG22	2:B:808:ALA:N	2.07	0.63
3:C:22:LEU:HD13	3:C:230:MET:CE	2.29	0.63
1:A:105:CYS:O	1:A:114:LEU:HG	1.98	0.63
1:A:1134:ILE:O	1:A:1138:ILE:HG13	1.99	0.63
1:A:743:VAL:O	1:A:747:VAL:HG23	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:589:VAL:CG1	2:B:590:HIS:H	2.08	0.63
3:C:167:HIS:CD2	3:C:168:ALA:H	2.16	0.63
3:C:214:ASN:HB3	3:C:217:ASP:OD2	1.98	0.63
4:D:8:PHE:CE2	4:D:40:HIS:HA	2.32	0.63
1:A:350:ARG:HH11	1:A:350:ARG:HG3	1.63	0.63
1:A:58:LEU:CD1	1:A:80:HIS:H	2.12	0.63
1:A:69:THR:C	1:A:71:GLN:H	2.01	0.63
3:C:189:THR:HG22	3:C:190:ASP:N	2.14	0.63
1:A:1329:THR:H	1:A:1335:ILE:HD11	1.63	0.63
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.33	0.63
1:A:463:ILE:HD12	1:A:469:ARG:HD2	1.80	0.63
2:B:1099:VAL:HG13	2:B:1100:ASP:N	2.14	0.63
2:B:825:VAL:CG1	2:B:826:ALA:N	2.62	0.63
2:B:918:ILE:HB	2:B:935:ARG:HD2	1.81	0.63
7:G:39:THR:HG22	7:G:40:GLY:N	2.13	0.63
1:A:1076:ALA:HA	1:A:1079:MET:CE	2.28	0.63
1:A:351:THR:HG21	2:B:1103:ILE:HG13	1.80	0.63
2:B:235:SER:HA	2:B:261:ARG:NH1	2.13	0.63
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.81	0.63
2:B:39:ARG:NH2	2:B:665:GLU:HG2	2.14	0.63
1:A:1214:GLU:O	1:A:1218:GLN:HG2	1.98	0.63
3:C:100:THR:OG1	3:C:121:VAL:HG21	1.99	0.63
4:D:51:ASN:O	4:D:52:LEU:O	2.17	0.63
11:K:61:TYR:C	11:K:61:TYR:CD2	2.72	0.63
1:A:475:THR:HG23	1:A:476:SER:N	2.13	0.62
2:B:431:TYR:CZ	2:B:447:ALA:HB2	2.34	0.62
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.28	0.62
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.81	0.62
7:G:1:MET:HG3	7:G:85:GLU:OE2	1.99	0.62
14:T:20:DC:H2''	14:T:21:DC:C5'	2.29	0.62
1:A:1187:GLN:O	1:A:1243:VAL:HG13	1.99	0.62
1:A:1372:VAL:O	1:A:1376:THR:HG22	1.99	0.62
1:A:34:LYS:CE	1:A:57:ARG:HH12	2.12	0.62
2:B:1084:GLN:NE2	2:B:1084:GLN:H	1.97	0.62
2:B:1223:ASP:O	2:B:1224:PHE:HB2	1.97	0.62
2:B:824:ILE:HG22	2:B:1087:PHE:CE2	2.28	0.62
2:B:880:THR:O	2:B:881:ASN:HB2	1.98	0.62
2:B:847:ASP:HB3	3:C:167:HIS:CD2	2.34	0.62
5:E:48:ASP:CG	5:E:49:SER:H	2.03	0.62
11:K:42:LEU:HD21	11:K:46:ILE:HD11	1.81	0.62
1:A:382:PRO:HB3	1:A:428:TYR:CE2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.33	0.62
3:C:124:LEU:O	3:C:127:ARG:HG2	1.99	0.62
9:I:50:THR:HG22	9:I:52:ILE:H	1.64	0.62
2:B:957:ASN:O	2:B:959:ASP:N	2.32	0.62
3:C:43:THR:CG2	3:C:44:LEU:H	2.08	0.62
3:C:69:LEU:HD12	3:C:69:LEU:N	2.15	0.62
2:B:1034:VAL:HG12	2:B:1035:ALA:N	2.15	0.62
2:B:515:HIS:H	2:B:518:HIS:CD2	2.10	0.62
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.81	0.62
5:E:157:SER:C	5:E:159:ASP:H	2.03	0.62
5:E:78:LEU:HD21	5:E:80:VAL:HG23	1.80	0.62
10:J:36:LEU:HD22	10:J:41:LEU:HD12	1.81	0.62
10:J:8:PHE:H	10:J:49:MET:HE1	1.63	0.62
1:A:253:ASN:HB3	2:B:935:ARG:CZ	2.29	0.62
6:F:118:LEU:O	6:F:122:MET:HG3	1.98	0.62
6:F:69:LEU:CA	6:F:70:LYS:N	2.62	0.62
1:A:1385:THR:O	1:A:1387:HIS:N	2.32	0.62
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.81	0.62
2:B:446:LEU:O	2:B:447:ALA:HB3	1.99	0.62
1:A:598:LEU:HD22	8:H:25:ARG:NH1	2.14	0.62
1:A:701:LEU:HA	9:I:115:LYS:HE3	1.81	0.62
3:C:66:ARG:NH2	10:J:3:VAL:O	2.32	0.62
1:A:63:ARG:HA	1:A:74:MET:CE	2.29	0.62
1:A:62:ASP:HB3	1:A:64:ASN:ND2	2.14	0.62
3:C:18:VAL:O	3:C:20:PHE:HD2	1.83	0.62
3:C:226:ASP:O	3:C:227:THR:HB	2.00	0.62
9:I:55:THR:HG22	9:I:58:VAL:HG21	1.80	0.62
3:C:167:HIS:HA	11:K:6:ARG:HH12	1.64	0.62
1:A:1006:ILE:HD12	5:E:163:GLU:HG3	1.80	0.62
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.30	0.62
2:B:782:LEU:HD12	2:B:788:ARG:HH11	1.64	0.62
2:B:916:THR:O	2:B:935:ARG:HG3	1.99	0.62
4:D:4:SER:O	4:D:5:THR:HB	1.98	0.62
10:J:16:ASP:OD1	10:J:17:LYS:HD2	2.00	0.62
12:L:58:LYS:O	12:L:58:LYS:HG2	2.00	0.62
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.80	0.62
2:B:1183:LYS:HE3	2:B:1183:LYS:N	2.14	0.62
2:B:185:THR:H	2:B:188:ASP:HB2	1.63	0.62
2:B:526:GLU:HG2	2:B:538:ASN:HD22	1.64	0.62
2:B:657:HIS:CE1	2:B:689:LEU:HD11	2.35	0.62
4:D:33:PHE:CE1	7:G:80:LYS:HE3	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:177:ARG:HD3	5:E:215:MET:HG3	1.82	0.62
2:B:902:GLY:O	12:L:65:VAL:HG11	2.00	0.62
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.30	0.61
1:A:69:THR:C	1:A:71:GLN:N	2.53	0.61
1:A:809:THR:OG1	1:A:812:GLU:HG3	2.00	0.61
11:K:63:VAL:HG23	11:K:63:VAL:O	2.00	0.61
1:A:108:MET:SD	1:A:210:ILE:HD13	2.41	0.61
1:A:84:ILE:HG22	1:A:239:LEU:HB3	1.82	0.61
1:A:399:HIS:O	1:A:401:GLY:N	2.33	0.61
1:A:475:THR:CG2	1:A:476:SER:N	2.63	0.61
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.36	0.61
3:C:208:GLU:O	3:C:210:GLU:N	2.33	0.61
4:D:4:SER:OG	4:D:5:THR:N	2.33	0.61
2:B:496:ARG:NH1	2:B:539:LEU:HB2	2.14	0.61
5:E:177:ARG:HD3	5:E:215:MET:CG	2.30	0.61
2:B:309:GLN:HG3	9:I:52:ILE:HD11	1.82	0.61
1:A:763:ALA:O	1:A:803:SER:HB3	1.99	0.61
1:A:765:VAL:HG23	1:A:802:ASN:O	2.00	0.61
2:B:859:TYR:CZ	2:B:941:LEU:HD12	2.35	0.61
4:D:130:LEU:O	4:D:132:GLN:N	2.33	0.61
1:A:1349:TYR:CA	1:A:1372:VAL:HG21	2.29	0.61
1:A:144:THR:O	1:A:146:MET:HG3	2.00	0.61
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.63	0.61
4:D:66:ARG:HD2	4:D:133:THR:HB	1.83	0.61
4:D:195:ILE:HG22	4:D:198:LEU:HG	1.82	0.61
6:F:76:LYS:O	6:F:79:ARG:HD3	2.01	0.61
8:H:63:LEU:HD22	8:H:90:ALA:HB3	1.82	0.61
10:J:36:LEU:HD12	10:J:47:ARG:NH1	2.15	0.61
10:J:48:ARG:HD2	10:J:49:MET:N	2.15	0.61
2:B:1159:ARG:HE	2:B:1193:GLN:HE21	1.47	0.61
2:B:622:LYS:CE	9:I:59:VAL:HG22	2.30	0.61
2:B:821:GLN:NE2	2:B:851:PHE:HA	2.14	0.61
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.25	0.61
1:A:844:ALA:C	1:A:845:LEU:HD23	2.21	0.61
2:B:882:THR:HG21	2:B:935:ARG:HA	1.82	0.61
4:D:134:THR:HG22	4:D:136:GLY:H	1.65	0.61
2:B:332:ASP:OD1	2:B:336:ARG:NE	2.34	0.61
2:B:344:LYS:O	2:B:345:LYS:HG3	2.01	0.61
2:B:464:GLY:HA2	2:B:479:VAL:O	2.01	0.61
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.81	0.61
5:E:15:ALA:O	5:E:19:VAL:HG23	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1120:LEU:HD12	1:A:1120:LEU:N	2.16	0.61
1:A:405:VAL:HG22	1:A:432:VAL:HG13	1.82	0.61
1:A:350:ARG:HA	1:A:468:PHE:HE1	1.66	0.61
2:B:281:PRO:O	2:B:283:VAL:N	2.34	0.61
2:B:620:ARG:NH2	9:I:89:GLN:NE2	2.48	0.61
2:B:975:GLN:HG2	2:B:976:ILE:H	1.64	0.61
3:C:179:GLU:HG2	3:C:180:TYR:N	2.16	0.61
7:G:34:VAL:CG1	7:G:45:ILE:HG21	2.30	0.61
2:B:185:THR:H	2:B:188:ASP:CB	2.13	0.61
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.30	0.61
3:C:73:GLN:HB3	3:C:131:HIS:H	1.66	0.61
8:H:116:TYR:HE2	8:H:140:ALA:CB	2.14	0.61
10:J:44:TYR:HA	10:J:47:ARG:CB	2.31	0.61
11:K:69:ALA:O	11:K:70:ARG:HB3	2.00	0.61
1:A:1341:ILE:CG2	1:A:1342:GLU:N	2.64	0.60
1:A:231:PRO:HA	1:A:234:MET:HE2	1.83	0.60
1:A:306:ASN:HB2	1:A:324:SER:HB3	1.83	0.60
1:A:58:LEU:HD11	1:A:80:HIS:H	1.65	0.60
2:B:176:SER:O	2:B:182:SER:HB3	2.01	0.60
2:B:842:ASN:HD22	2:B:845:SER:CB	2.14	0.60
4:D:17:LYS:HE3	4:D:17:LYS:CA	2.31	0.60
11:K:10:PHE:CD2	11:K:10:PHE:N	2.69	0.60
1:A:34:LYS:HB2	1:A:36:ARG:HH21	1.65	0.60
1:A:858:ASN:ND2	1:A:858:ASN:C	2.54	0.60
2:B:265:SER:O	2:B:266:ALA:HB3	2.01	0.60
2:B:510:LYS:HG3	2:B:511:PRO:HD3	1.84	0.60
2:B:525:ALA:O	2:B:768:THR:HA	2.02	0.60
4:D:52:LEU:O	4:D:54:GLU:N	2.34	0.60
1:A:33:ALA:O	1:A:83:HIS:HD2	1.84	0.60
1:A:742:ASN:O	1:A:745:GLN:HB2	2.01	0.60
1:A:1410:PHE:HA	2:B:1212:ILE:CD1	2.31	0.60
2:B:25:ILE:HD11	2:B:653:VAL:O	2.01	0.60
6:F:111:LEU:C	6:F:113:GLY:H	2.05	0.60
8:H:61:SER:HB2	8:H:139:ASN:HB3	1.82	0.60
10:J:44:TYR:HD2	10:J:44:TYR:H	1.47	0.60
12:L:53:HIS:HB3	12:L:55:ILE:CD1	2.30	0.60
2:B:1023:VAL:O	2:B:1026:LEU:HB2	2.01	0.60
2:B:1099:VAL:O	2:B:1101:ASP:N	2.35	0.60
2:B:278:GLN:HE22	2:B:337:ARG:HH21	1.46	0.60
12:L:32:ALA:HB3	12:L:55:ILE:CD1	2.31	0.60
1:A:55:ASP:C	1:A:57:ARG:H	2.04	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:CB	1:A:568:PRO:CD	2.79	0.60
2:B:465:ASN:ND2	2:B:465:ASN:N	2.47	0.60
2:B:801:LYS:O	10:J:52:THR:HG23	2.01	0.60
3:C:245:VAL:HA	3:C:248:ILE:HD12	1.84	0.60
1:A:1341:ILE:CG2	1:A:1342:GLU:H	2.14	0.60
1:A:709:THR:HB	1:A:712:GLU:HG3	1.84	0.60
1:A:78:PRO:HA	2:B:1201:LYS:NZ	2.17	0.60
13:P:9:G:C2'	13:P:10:A:H5'	2.31	0.60
1:A:416:ARG:O	1:A:417:TYR:HD2	1.84	0.60
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.83	0.60
5:E:105:PHE:O	5:E:106:GLN:HB2	2.01	0.60
1:A:537:ARG:HD2	8:H:20:TYR:HE1	1.67	0.60
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.84	0.60
1:A:1323:ASP:OD1	1:A:1325:THR:HB	2.01	0.60
1:A:311:GLN:O	1:A:312:PRO:C	2.40	0.60
1:A:47:ARG:HH12	1:A:254:GLU:HG2	1.67	0.60
2:B:563:MET:CE	2:B:580:VAL:HB	2.32	0.60
3:C:133:ILE:CD1	3:C:237:SER:HA	2.31	0.60
7:G:1:MET:O	7:G:3:PHE:CD1	2.55	0.60
1:A:392:VAL:HG13	1:A:415:LEU:CD1	2.29	0.60
1:A:590:ARG:HB2	1:A:605:MET:HB3	1.84	0.60
7:G:1:MET:SD	7:G:79:PHE:CD1	2.95	0.60
8:H:113:ALA:HB2	8:H:126:GLU:HG3	1.84	0.60
1:A:481:ASP:OD1	1:A:483:ASP:OD2	2.18	0.60
1:A:466:SER:O	2:B:1103:ILE:HD11	2.01	0.60
2:B:34:ILE:O	2:B:37:PHE:N	2.34	0.60
2:B:616:ILE:HG13	2:B:697:GLU:HA	1.83	0.60
2:B:753:ALA:O	2:B:756:ILE:HG13	2.02	0.60
6:F:93:ILE:HD11	6:F:134:ILE:CD1	2.27	0.60
1:A:1313:LEU:HD23	1:A:1338:VAL:CG2	2.31	0.59
1:A:154:SER:HB3	1:A:162:VAL:HG21	1.83	0.59
1:A:244:PRO:O	1:A:247:ARG:N	2.35	0.59
2:B:217:ARG:NE	2:B:405:ARG:HB2	2.15	0.59
2:B:308:TRP:HA	2:B:311:LEU:HD12	1.83	0.59
2:B:51:PHE:O	2:B:54:PHE:HB3	2.02	0.59
2:B:637:LEU:O	2:B:690:VAL:HG13	2.01	0.59
2:B:744:HIS:HD2	2:B:746:SER:OG	1.85	0.59
10:J:8:PHE:H	10:J:49:MET:CE	2.14	0.59
11:K:42:LEU:O	11:K:46:ILE:HG13	2.02	0.59
1:A:446:ARG:HB2	1:A:487:MET:SD	2.41	0.59
2:B:1001:PHE:CD2	3:C:34:ARG:NH2	2.71	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1180:PHE:HB3	2:B:1191:ILE:HD12	1.84	0.59
2:B:815:ARG:HD3	2:B:1041:GLU:OE2	2.02	0.59
2:B:822:ASN:O	10:J:48:ARG:NH1	2.35	0.59
2:B:843:GLN:O	2:B:846:ILE:N	2.35	0.59
2:B:980:PHE:HE1	2:B:990:ILE:HD11	1.67	0.59
3:C:242:GLN:HB3	3:C:246:ARG:HG3	1.84	0.59
1:A:1127:ASP:HB3	1:A:1130:GLN:CB	2.32	0.59
1:A:321:PRO:O	1:A:322:VAL:CB	2.49	0.59
1:A:427:GLN:HG3	1:A:430:TRP:CE2	2.37	0.59
1:A:534:LEU:HD13	1:A:656:TRP:CG	2.37	0.59
2:B:531:GLN:HG3	2:B:532:ALA:H	1.67	0.59
2:B:737:THR:CG2	9:I:66:PRO:HA	2.31	0.59
7:G:127:PRO:HG2	7:G:138:THR:HG21	1.84	0.59
1:A:164:ARG:HG3	1:A:165:GLY:H	1.65	0.59
1:A:547:LEU:HD22	11:K:58:PHE:CD1	2.37	0.59
2:B:910:VAL:HG12	2:B:912:ILE:H	1.67	0.59
4:D:52:LEU:C	4:D:54:GLU:H	2.04	0.59
4:D:66:ARG:O	4:D:70:PHE:HB2	2.03	0.59
7:G:7:LEU:HB2	7:G:74:TYR:HE2	1.62	0.59
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.41	0.59
9:I:86:PHE:CE1	9:I:100:PHE:HB2	2.37	0.59
1:A:1209:MET:SD	1:A:1236:LEU:HD22	2.42	0.59
1:A:471:ASN:OD1	1:A:472:LEU:N	2.35	0.59
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.33	0.59
2:B:33:VAL:HG21	2:B:638:PHE:HZ	1.67	0.59
8:H:81:PRO:HB2	8:H:82:PRO:CD	2.33	0.59
8:H:91:ASP:C	8:H:93:TYR:H	2.05	0.59
2:B:1007:VAL:CG2	2:B:1008:PRO:HD2	2.31	0.59
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.17	0.59
3:C:212:PRO:CB	3:C:213:PRO:HD2	2.33	0.59
3:C:241:ASP:O	3:C:245:VAL:HG23	2.03	0.59
3:C:66:ARG:NH1	10:J:2:ILE:CG2	2.59	0.59
6:F:111:LEU:H	6:F:111:LEU:CD1	2.12	0.59
1:A:1444:MET:CG	7:G:60:ARG:HA	2.33	0.59
1:A:1171:GLN:HA	1:A:1174:PHE:HE1	1.66	0.59
1:A:21:LEU:HG	1:A:1413:GLY:O	2.02	0.59
1:A:37:PHE:N	1:A:37:PHE:CD1	2.71	0.59
1:A:954:TRP:HB3	1:A:955:PRO:HD2	1.84	0.59
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.50	0.59
2:B:973:ILE:HG23	2:B:974:PRO:HD2	1.85	0.59
3:C:66:ARG:CZ	10:J:2:ILE:HG21	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1437:GLY:O	1:A:1439:GLY:N	2.36	0.59
1:A:87:ALA:CB	1:A:276:LEU:HD23	2.33	0.59
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	2.02	0.59
1:A:384:ASN:OD1	1:A:388:LEU:HD12	2.03	0.59
1:A:853:ASP:OD1	1:A:855:THR:HB	2.03	0.59
1:A:867:ILE:HG22	1:A:872:GLY:N	2.18	0.59
1:A:981:LEU:CD2	1:A:1039:LYS:HA	2.32	0.59
3:C:101:LEU:HD13	3:C:118:LEU:CD2	2.27	0.59
3:C:174:ALA:O	10:J:10:CYS:O	2.20	0.59
10:J:2:ILE:HG22	10:J:3:VAL:O	2.03	0.59
10:J:44:TYR:HA	10:J:47:ARG:HB3	1.85	0.59
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.67	0.59
1:A:504:LEU:HD12	1:A:504:LEU:N	2.17	0.59
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.68	0.59
4:D:27:LEU:HD22	4:D:173:HIS:CD2	2.38	0.59
7:G:3:PHE:CE1	7:G:80:LYS:HE2	2.38	0.59
8:H:93:TYR:HB3	8:H:144:ILE:O	2.03	0.59
1:A:107:CYS:N	1:A:114:LEU:HD21	2.18	0.59
1:A:399:HIS:HB3	1:A:400:PRO:CD	2.25	0.59
3:C:41:ILE:HD11	3:C:247:GLY:HA2	1.84	0.59
3:C:262:LEU:HD11	11:K:87:LEU:HD23	1.85	0.59
3:C:69:LEU:HD12	3:C:69:LEU:H	1.67	0.59
1:A:596:THR:C	1:A:598:LEU:H	2.03	0.58
2:B:343:ILE:CB	2:B:348:ARG:HG3	2.32	0.58
2:B:705:MET:H	2:B:710:LEU:CD1	2.16	0.58
10:J:64:ASN:CB	10:J:65:PRO:CD	2.80	0.58
1:A:1362:TYR:CD1	1:A:1363:VAL:N	2.72	0.58
1:A:816:HIS:CD2	2:B:764:SER:HB2	2.38	0.58
1:A:844:ALA:O	1:A:845:LEU:HD23	2.02	0.58
2:B:467:GLY:H	2:B:475:SER:CB	2.16	0.58
3:C:45:ALA:HA	3:C:72:LEU:CD1	2.33	0.58
4:D:47:LEU:HD13	4:D:48:ILE:N	2.16	0.58
7:G:1:MET:O	7:G:3:PHE:CE1	2.56	0.58
1:A:1279:ILE:O	1:A:1279:ILE:HG22	2.02	0.58
1:A:265:LYS:NZ	1:A:322:VAL:HG22	2.18	0.58
1:A:2:VAL:HG21	2:B:1157:ALA:C	2.23	0.58
1:A:606:LEU:HB3	1:A:614:PHE:CE2	2.39	0.58
2:B:401:PHE:HD2	2:B:521:LEU:HD12	1.68	0.58
2:B:778:MET:CE	2:B:1094:ARG:CD	2.80	0.58
7:G:51:TYR:C	7:G:51:TYR:CD2	2.77	0.58
1:A:997:LEU:HD13	1:A:1018:PHE:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1115:SER:HB3	1:A:1330:ASN:HD21	1.68	0.58
1:A:341:MET:HE1	1:A:843:LYS:HZ3	1.67	0.58
1:A:524:VAL:CG1	1:A:525:GLN:H	2.07	0.58
1:A:55:ASP:CG	1:A:55:ASP:O	2.39	0.58
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.34	0.58
6:F:138:LEU:HB3	6:F:139:PRO:HD2	1.85	0.58
7:G:88:ASP:OD2	7:G:88:ASP:N	2.36	0.58
8:H:26:ILE:CD1	8:H:49:VAL:HG11	2.33	0.58
9:I:103:CYS:CB	9:I:106:CYS:SG	2.92	0.58
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.18	0.58
1:A:17:VAL:HA	2:B:1215:ARG:O	2.04	0.58
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.69	0.58
2:B:401:PHE:HA	2:B:404:LYS:HG3	1.84	0.58
5:E:131:THR:HG21	5:E:191:LYS:NZ	2.17	0.58
11:K:53:ASP:OD1	11:K:55:LYS:HB2	2.04	0.58
1:A:1356:ILE:HD12	1:A:1368:MET:SD	2.43	0.58
1:A:224:PHE:HD2	1:A:229:SER:O	1.85	0.58
2:B:1045:SER:O	2:B:1046:PRO:O	2.22	0.58
3:C:166:GLU:HG3	11:K:10:PHE:CZ	2.23	0.58
3:C:186:LEU:HD21	3:C:224:GLN:O	2.03	0.58
5:E:124:VAL:HB	5:E:125:PRO:HD3	1.86	0.58
8:H:15:VAL:HG22	8:H:26:ILE:HG12	1.84	0.58
1:A:551:TYR:CE2	11:K:62:LYS:HE2	2.38	0.58
1:A:38:PRO:HA	1:A:270:LEU:HD23	1.85	0.58
2:B:168:GLY:N	2:B:450:ALA:HB1	2.15	0.58
7:G:39:THR:HG22	7:G:40:GLY:H	1.69	0.58
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.34	0.58
1:A:34:LYS:HB3	1:A:36:ARG:HE	1.69	0.58
1:A:401:GLY:C	1:A:435:HIS:CD2	2.76	0.58
1:A:58:LEU:HD21	1:A:243:PRO:CB	2.33	0.58
1:A:648:ASN:O	1:A:649:ILE:C	2.42	0.58
2:B:129:PHE:HE2	2:B:166:PHE:HD1	1.51	0.58
2:B:654:ARG:C	2:B:656:GLY:H	2.05	0.58
1:A:537:ARG:HD2	8:H:20:TYR:CE1	2.39	0.58
1:A:783:THR:HG22	1:A:784:LEU:HG	1.86	0.58
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.38	0.58
1:A:853:ASP:OD1	1:A:855:THR:N	2.36	0.58
1:A:997:LEU:HD13	1:A:1018:PHE:HE2	1.69	0.58
2:B:340:ALA:CB	2:B:343:ILE:HD12	2.31	0.58
6:F:77:ASP:C	6:F:79:ARG:H	2.07	0.58
6:F:99:LEU:HD12	6:F:99:LEU:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:62:ILE:HG12	9:I:62:ILE:O	2.04	0.58
11:K:15:GLY:O	11:K:16:GLU:HG3	2.04	0.58
1:A:760:GLN:HG2	1:A:765:VAL:O	2.04	0.58
1:A:341:MET:CE	1:A:843:LYS:HZ3	2.16	0.58
2:B:1079:LYS:HA	3:C:27:LEU:HD21	1.86	0.58
2:B:122:LEU:O	2:B:206:ASN:HA	2.04	0.58
2:B:223:VAL:HG21	2:B:380:TYR:HE2	1.69	0.58
2:B:843:GLN:O	2:B:846:ILE:HB	2.04	0.58
7:G:17:PHE:CD2	7:G:17:PHE:N	2.72	0.58
8:H:89:LEU:C	8:H:91:ASP:H	2.07	0.58
2:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.33	0.58
11:K:46:ILE:O	11:K:46:ILE:HG22	2.03	0.58
1:A:1191:TRP:CD1	1:A:1256:GLU:HB2	2.39	0.57
1:A:590:ARG:HH11	1:A:590:ARG:CG	2.17	0.57
1:A:68:GLN:O	1:A:70:CYS:N	2.36	0.57
2:B:466:TRP:O	2:B:468:GLU:N	2.37	0.57
1:A:782:ARG:NH2	2:B:699:GLU:O	2.36	0.57
4:D:57:LEU:O	4:D:61:GLU:HB2	2.04	0.57
7:G:35:GLU:OE2	7:G:48:VAL:HG23	2.04	0.57
9:I:2:THR:O	9:I:3:THR:C	2.41	0.57
1:A:547:LEU:HB3	11:K:58:PHE:CE1	2.39	0.57
14:T:19:DT:H2'	14:T:20:DC:C6	2.38	0.57
1:A:1333:ILE:O	1:A:1337:GLU:HG3	2.03	0.57
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.69	0.57
1:A:89:PRO:HB2	1:A:204:THR:HG22	1.86	0.57
2:B:515:HIS:CD2	2:B:517:THR:H	2.21	0.57
8:H:42:ILE:HG23	8:H:95:TYR:HE1	1.67	0.57
2:B:852:ARG:NH2	12:L:70:ARG:OXT	2.30	0.57
1:A:1313:LEU:O	1:A:1315:GLU:N	2.37	0.57
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.03	0.57
1:A:541:ILE:HD13	1:A:549:MET:CE	2.30	0.57
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.87	0.57
2:B:309:GLN:OE1	9:I:52:ILE:HD11	2.05	0.57
1:A:1175:SER:O	1:A:1176:LEU:HB2	2.04	0.57
1:A:629:LEU:O	1:A:633:VAL:HG23	2.05	0.57
2:B:192:LEU:O	2:B:193:LYS:HB2	2.05	0.57
2:B:583:ASN:HD21	2:B:628:THR:HB	1.68	0.57
2:B:871:THR:HG22	2:B:872:GLU:O	2.03	0.57
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.18	0.57
8:H:128:ASN:CG	8:H:128:ASN:O	2.42	0.57
1:A:364:VAL:O	1:A:364:VAL:HG13	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.85	0.57
2:B:1177:HIS:HB2	2:B:1179:GLN:HE21	1.69	0.57
2:B:278:GLN:NE2	2:B:337:ARG:HH21	2.02	0.57
5:E:175:LEU:HD23	5:E:176:PRO:HD2	1.85	0.57
8:H:123:MET:HG2	8:H:124:ARG:N	2.19	0.57
10:J:64:ASN:CB	10:J:65:PRO:HD3	2.34	0.57
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.86	0.57
2:B:51:PHE:CD2	2:B:173:MET:HB3	2.39	0.57
2:B:225:VAL:HA	2:B:237:VAL:O	2.05	0.57
2:B:38:PHE:CD1	2:B:811:TYR:CD2	2.92	0.57
3:C:129:ILE:HG23	3:C:130:GLY:N	2.18	0.57
3:C:174:ALA:O	3:C:175:ALA:HB2	2.05	0.57
1:A:1095:THR:O	1:A:1096:SER:HB2	2.03	0.57
1:A:1291:VAL:HG13	1:A:1292:PRO:CD	2.35	0.57
1:A:482:PHE:C	1:A:484:GLY:H	2.07	0.57
2:B:288:ALA:HA	2:B:331:LEU:HD12	1.87	0.57
2:B:635:ARG:NH2	2:B:742:GLU:OE2	2.35	0.57
2:B:776:GLN:O	2:B:1095:LEU:HA	2.04	0.57
3:C:175:ALA:HB3	10:J:43:ARG:NH2	2.20	0.57
6:F:130:ILE:O	6:F:148:VAL:HG21	2.05	0.57
7:G:79:PHE:CZ	7:G:106:MET:HE1	2.39	0.57
1:A:1001:ARG:O	1:A:1002:GLY:O	2.23	0.57
1:A:770:VAL:HA	1:A:822:GLU:OE1	2.05	0.57
2:B:125:SER:HA	2:B:171:PRO:HA	1.86	0.57
2:B:273:LEU:HD12	2:B:280:ILE:HD12	1.85	0.57
4:D:176:GLU:O	4:D:178:ALA:N	2.38	0.57
7:G:14:HIS:CE1	7:G:15:PRO:HD2	2.40	0.57
7:G:48:VAL:HA	7:G:76:ALA:HB2	1.86	0.57
14:T:25:DT:C2'	14:T:26:DC:O5'	2.53	0.57
1:A:785:PRO:HG2	1:A:786:HIS:CD2	2.40	0.57
2:B:1010:LEU:HD23	2:B:1092:TYR:CD1	2.40	0.57
1:A:343:LYS:HZ3	2:B:1197:PRO:HB3	1.70	0.57
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.86	0.57
2:B:792:MET:HG3	2:B:855:PHE:CE1	2.38	0.57
3:C:183:TRP:O	3:C:185:LYS:N	2.38	0.57
3:C:249:ASP:O	3:C:252:GLN:HB3	2.05	0.57
4:D:138:ASN:OD1	4:D:141:LEU:HB2	2.05	0.57
8:H:43:ASN:OD1	8:H:46:LEU:HG	2.05	0.57
11:K:47:ARG:C	11:K:47:ARG:HD2	2.25	0.57
1:A:130:ASP:O	1:A:133:LYS:N	2.36	0.57
1:A:1418:LEU:HD12	1:A:1419:ASP:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:SER:O	1:A:250:ILE:HG13	2.04	0.57
1:A:903:ASN:C	1:A:903:ASN:ND2	2.58	0.57
2:B:1084:GLN:HE21	2:B:1084:GLN:H	1.51	0.57
2:B:654:ARG:O	2:B:656:GLY:N	2.38	0.57
4:D:53:SER:HB3	4:D:152:SER:CA	2.35	0.57
5:E:112:TYR:CZ	5:E:136:ASN:HB2	2.39	0.57
8:H:127:GLY:O	8:H:128:ASN:HB2	2.05	0.57
8:H:23:VAL:HG22	8:H:43:ASN:HA	1.87	0.57
8:H:40:LEU:CD1	8:H:123:MET:HB2	2.34	0.57
1:A:381:THR:CG2	1:A:383:TYR:H	2.18	0.56
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.87	0.56
4:D:159:THR:O	4:D:163:VAL:HG23	2.05	0.56
8:H:11:GLN:HA	8:H:53:ASP:O	2.05	0.56
8:H:111:LEU:HD23	8:H:127:GLY:O	2.04	0.56
8:H:95:TYR:CE2	8:H:97:MET:HG3	2.40	0.56
1:A:1239:ARG:HB3	1:A:1239:ARG:NH1	2.19	0.56
3:C:35:ARG:HH11	11:K:41:THR:CA	2.18	0.56
4:D:18:VAL:O	4:D:18:VAL:HG13	2.05	0.56
6:F:75:PRO:O	6:F:77:ASP:O	2.24	0.56
7:G:143:ILE:CG2	7:G:144:ARG:N	2.68	0.56
4:D:47:LEU:HD11	7:G:3:PHE:CE2	2.40	0.56
8:H:84:ALA:CB	8:H:87:ARG:HB2	2.35	0.56
1:A:1152:ILE:HG13	9:I:44:TYR:HD2	1.71	0.56
10:J:12:LYS:O	10:J:14:VAL:HG23	2.05	0.56
1:A:438:ASP:O	1:A:439:ASN:HB2	2.06	0.56
2:B:611:PRO:HB3	2:B:685:LEU:HD11	1.86	0.56
2:B:745:PRO:O	2:B:747:MET:N	2.38	0.56
2:B:770:GLN:CD	2:B:983:ARG:HA	2.24	0.56
3:C:22:LEU:HD13	3:C:230:MET:HE1	1.87	0.56
3:C:41:ILE:HD11	3:C:247:GLY:CA	2.35	0.56
3:C:77:ILE:O	3:C:79:GLN:N	2.38	0.56
4:D:7:THR:O	4:D:9:GLN:N	2.38	0.56
11:K:110:ASN:O	11:K:111:LEU:HD23	2.05	0.56
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.37	0.56
1:A:1102:LYS:O	1:A:1106:ASN:ND2	2.38	0.56
1:A:406:ILE:HG13	1:A:431:LYS:HB2	1.87	0.56
1:A:392:VAL:HG22	1:A:432:VAL:HG11	1.87	0.56
1:A:42:ASP:HB3	1:A:45:GLN:HA	1.87	0.56
2:B:102:VAL:HG12	2:B:104:GLU:HG2	1.86	0.56
2:B:224:GLN:O	2:B:238:ALA:HA	2.06	0.56
5:E:94:LYS:HE2	5:E:98:ILE:CD1	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:75:PRO:HG2	6:F:78:GLN:HB2	1.86	0.56
7:G:99:PHE:CZ	7:G:143:ILE:HD13	2.40	0.56
10:J:27:GLU:O	10:J:29:GLU:N	2.34	0.56
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.88	0.56
1:A:56:PRO:O	1:A:57:ARG:HG3	2.06	0.56
1:A:920:LEU:HD23	1:A:921:GLY:N	2.21	0.56
7:G:1:MET:HE3	7:G:80:LYS:O	2.06	0.56
1:A:244:PRO:CB	1:A:245:PRO:HD3	2.32	0.56
1:A:798:GLY:HA2	1:A:815:PHE:HD1	1.67	0.56
1:A:853:ASP:OD1	1:A:855:THR:CB	2.54	0.56
2:B:879:ARG:HH11	2:B:883:LEU:CD2	2.14	0.56
3:C:104:PHE:HD2	3:C:105:GLY:N	2.03	0.56
5:E:31:THR:O	5:E:35:VAL:HG23	2.05	0.56
8:H:26:ILE:HD13	8:H:49:VAL:HG11	1.86	0.56
9:I:106:CYS:O	9:I:107:SER:HB2	2.06	0.56
1:A:1397:LEU:HB2	1:A:1426:GLU:OE1	2.05	0.56
1:A:590:ARG:HH21	1:A:620:LYS:CB	2.17	0.56
1:A:84:ILE:HG23	1:A:84:ILE:O	2.05	0.56
1:A:658:LEU:HD13	2:B:831:SER:N	2.21	0.56
5:E:157:SER:HG	5:E:160:GLU:HG3	1.69	0.56
9:I:112:SER:O	9:I:114:GLN:N	2.38	0.56
11:K:67:PHE:C	11:K:68:PHE:CD2	2.79	0.56
12:L:30:ILE:HD11	12:L:59:ALA:HB2	1.88	0.56
1:A:1420:ASP:O	1:A:1421:CYS:HB2	2.06	0.56
1:A:787:PHE:CE1	1:A:796:SER:HA	2.41	0.56
2:B:39:ARG:HH21	2:B:665:GLU:CD	2.07	0.56
2:B:797:TYR:HE1	2:B:854:LEU:HD23	1.70	0.56
3:C:243:VAL:HG12	3:C:243:VAL:O	2.05	0.56
6:F:103:MET:HE1	7:G:65:ASP:HB2	1.88	0.56
10:J:14:VAL:CG1	10:J:50:ILE:HD11	2.35	0.56
10:J:36:LEU:O	10:J:39:LEU:N	2.38	0.56
1:A:1166:ASP:OD2	1:A:1239:ARG:HD2	2.05	0.56
1:A:1341:ILE:O	1:A:1344:GLY:N	2.39	0.56
1:A:289:ILE:C	1:A:291:GLU:H	2.07	0.56
1:A:37:PHE:H	1:A:37:PHE:HD1	1.54	0.56
1:A:477:PRO:CG	1:A:521:MET:HG2	2.35	0.56
1:A:886:ILE:HG13	1:A:943:LEU:HD12	1.86	0.56
2:B:1020:ARG:HB2	2:B:1022:THR:HG22	1.88	0.56
2:B:466:TRP:CE3	2:B:466:TRP:HA	2.39	0.56
3:C:18:VAL:O	3:C:18:VAL:HG12	2.06	0.56
3:C:27:LEU:HD13	3:C:228:PHE:HE2	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:198:LEU:O	4:D:200:ASN:N	2.39	0.56
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.40	0.56
2:B:954:VAL:O	12:L:55:ILE:O	2.24	0.56
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.41	0.56
1:A:1447:GLU:OE2	7:G:23:LYS:HB2	2.06	0.56
1:A:720:ARG:O	1:A:724:GLU:HB2	2.06	0.56
2:B:1099:VAL:HG12	2:B:1100:ASP:H	1.71	0.56
5:E:207:ARG:HH11	5:E:207:ARG:CB	2.19	0.56
7:G:91:VAL:HB	7:G:139:ILE:O	2.06	0.56
10:J:7:CYS:CB	10:J:46:CYS:HB3	2.36	0.56
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.88	0.56
2:B:693:ILE:HD13	2:B:701:ILE:HD13	1.88	0.56
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.88	0.56
7:G:14:HIS:ND1	7:G:15:PRO:CD	2.69	0.56
13:P:4:A:H2'	13:P:5:C:H6	1.71	0.56
1:A:1057:VAL:HG12	1:A:1058:VAL:N	2.21	0.55
1:A:130:ASP:O	1:A:131:SER:C	2.45	0.55
1:A:1329:THR:CG2	1:A:1331:SER:H	2.16	0.55
2:B:842:ASN:ND2	2:B:845:SER:OG	2.32	0.55
3:C:31:ASN:O	3:C:34:ARG:HB3	2.06	0.55
3:C:66:ARG:NH2	10:J:5:VAL:HG23	2.20	0.55
5:E:145:THR:HG21	5:E:187:TYR:CD2	2.41	0.55
7:G:18:PHE:HA	7:G:22:MET:CE	2.36	0.55
1:A:547:LEU:HD22	11:K:58:PHE:HD1	1.70	0.55
1:A:834:THR:HG21	1:A:1077:THR:OG1	2.05	0.55
1:A:265:LYS:HZ3	1:A:322:VAL:HG13	1.70	0.55
1:A:404:TYR:HB2	1:A:433:GLU:HB2	1.88	0.55
1:A:639:PRO:HG2	1:A:640:GLN:H	1.70	0.55
1:A:829:VAL:C	1:A:831:THR:H	2.07	0.55
2:B:1023:VAL:O	2:B:1026:LEU:N	2.39	0.55
2:B:811:TYR:N	2:B:811:TYR:CD1	2.73	0.55
4:D:53:SER:CB	4:D:153:ARG:H	2.18	0.55
4:D:213:GLU:O	4:D:217:LEU:HG	2.06	0.55
5:E:177:ARG:C	5:E:212:ARG:HD3	2.26	0.55
9:I:15:TYR:CD1	9:I:15:TYR:N	2.74	0.55
1:A:166:GLY:O	1:A:167:CYS:SG	2.64	0.55
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.05	0.55
1:A:335:ARG:HH11	2:B:1202:LEU:HD13	1.69	0.55
4:D:176:GLU:HB3	4:D:198:LEU:HD21	1.88	0.55
4:D:192:LYS:HB3	4:D:192:LYS:HZ3	1.72	0.55
4:D:5:THR:O	4:D:5:THR:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:90:VAL:HA	5:E:120:ALA:HB2	1.88	0.55
8:H:102:TYR:N	8:H:102:TYR:CD2	2.73	0.55
8:H:41:ASP:O	8:H:42:ILE:HG13	2.06	0.55
1:A:262:LEU:O	1:A:264:PHE:N	2.40	0.55
1:A:284:ALA:O	1:A:286:HIS:N	2.33	0.55
1:A:385:ILE:CG2	1:A:386:ASP:N	2.66	0.55
1:A:90:VAL:HG13	1:A:297:GLN:HA	1.88	0.55
2:B:1107:ALA:O	2:B:1108:ARG:HG2	2.06	0.55
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.63	0.55
2:B:376:PHE:CE2	2:B:569:TYR:HD2	2.24	0.55
5:E:17:ARG:O	5:E:20:LYS:HB2	2.06	0.55
1:A:1153:TYR:CE1	9:I:42:LEU:HD13	2.42	0.55
1:A:1116:LEU:HB2	1:A:1329:THR:OG1	2.05	0.55
1:A:1261:LYS:O	1:A:1264:GLU:HB3	2.07	0.55
1:A:366:VAL:HG21	1:A:460:VAL:HG22	1.88	0.55
1:A:699:ALA:O	1:A:700:ASN:HB3	2.07	0.55
1:A:867:ILE:HG22	1:A:872:GLY:H	1.71	0.55
2:B:1183:LYS:N	2:B:1183:LYS:CE	2.70	0.55
1:A:1283:VAL:HG12	1:A:1284:MET:N	2.22	0.55
1:A:1120:LEU:O	1:A:1323:ASP:HB2	2.06	0.55
1:A:42:ASP:HB3	1:A:45:GLN:N	2.22	0.55
1:A:548:ASN:HA	11:K:60:ALA:HB1	1.88	0.55
2:B:521:LEU:HD13	2:B:633:VAL:HB	1.89	0.55
2:B:798:TYR:CE2	3:C:62:PHE:CZ	2.91	0.55
7:G:9:LEU:HD12	7:G:10:ASN:H	1.71	0.55
1:A:1116:LEU:HB3	1:A:1308:THR:HG21	1.89	0.55
1:A:34:LYS:H	1:A:57:ARG:HH22	1.54	0.55
1:A:914:GLU:HB2	1:A:979:SER:O	2.07	0.55
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.42	0.55
3:C:73:GLN:NE2	3:C:75:MET:N	2.53	0.55
3:C:165:LYS:O	11:K:6:ARG:NH1	2.40	0.55
1:A:1437:GLY:HA3	6:F:88:TYR:CD2	2.42	0.55
1:A:596:THR:C	1:A:598:LEU:N	2.59	0.55
1:A:805:LEU:HD11	2:B:1052:VAL:HG21	1.89	0.55
2:B:310:MET:CE	2:B:387:LEU:HD12	2.35	0.55
2:B:557:PHE:C	2:B:557:PHE:HD2	2.10	0.55
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.39	0.55
1:A:253:ASN:HB3	2:B:935:ARG:NH1	2.22	0.55
3:C:184:ASN:ND2	3:C:187:LYS:HA	2.21	0.55
10:J:32:GLU:CD	10:J:32:GLU:H	2.09	0.55
1:A:1107:VAL:HG12	1:A:1107:VAL:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1144:LYS:HB2	1:A:1268:LEU:O	2.07	0.55
1:A:211:PHE:HA	1:A:214:ILE:HG13	1.89	0.55
1:A:254:GLU:HB2	2:B:935:ARG:NH1	2.21	0.55
1:A:34:LYS:N	1:A:57:ARG:NH2	2.51	0.55
1:A:98:LYS:O	1:A:99:ILE:C	2.43	0.55
2:B:1106:ARG:HG3	2:B:1107:ALA:N	2.21	0.55
2:B:582:VAL:HG23	2:B:626:ILE:HB	1.88	0.55
2:B:658:ILE:HG22	2:B:659:ALA:N	2.21	0.55
2:B:996:ARG:NH2	3:C:175:ALA:HA	2.22	0.55
7:G:80:LYS:HG2	7:G:80:LYS:O	2.07	0.55
8:H:130:ARG:N	8:H:130:ARG:HD2	2.20	0.55
11:K:6:ARG:O	11:K:8:GLU:N	2.40	0.55
1:A:241:VAL:HG13	1:A:266:LEU:HD13	1.89	0.55
1:A:350:ARG:HB2	1:A:488:ASN:OD1	2.07	0.55
2:B:1069:PHE:HA	2:B:1085:ILE:O	2.06	0.55
2:B:705:MET:N	2:B:710:LEU:HD12	2.22	0.55
2:B:847:ASP:C	2:B:849:GLY:H	2.09	0.55
4:D:192:LYS:HE3	4:D:204:ASP:OD1	2.06	0.55
4:D:54:GLU:O	4:D:58:VAL:HG23	2.07	0.55
8:H:4:THR:O	8:H:5:LEU:HD23	2.07	0.55
10:J:44:TYR:N	10:J:44:TYR:CD2	2.75	0.55
14:T:27:DA:H2''	14:T:28:DT:O4'	2.07	0.55
1:A:1409:LEU:HD13	2:B:1207:LEU:HD11	1.89	0.54
1:A:88:LYS:HE3	1:A:280:GLU:OE2	2.07	0.54
1:A:42:ASP:HB3	1:A:45:GLN:CA	2.36	0.54
1:A:907:THR:CG2	1:A:908:LEU:N	2.70	0.54
1:A:966:ASN:O	1:A:967:ALA:C	2.46	0.54
2:B:1219:ASP:O	2:B:1219:ASP:OD1	2.25	0.54
2:B:579:ARG:HG2	2:B:579:ARG:NH1	2.19	0.54
4:D:134:THR:CG2	4:D:135:GLY:N	2.69	0.54
5:E:39:LEU:O	5:E:42:PHE:HB3	2.07	0.54
7:G:1:MET:O	7:G:1:MET:SD	2.65	0.54
1:A:1444:MET:HG2	7:G:60:ARG:CA	2.36	0.54
8:H:83:GLN:C	8:H:85:GLY:H	2.10	0.54
9:I:50:THR:CG2	9:I:52:ILE:HG12	2.37	0.54
5:E:147:HIS:CD2	5:E:149:LEU:H	2.25	0.54
13:P:4:A:H2'	13:P:5:C:C6	2.42	0.54
1:A:350:ARG:NH1	1:A:350:ARG:HG3	2.20	0.54
1:A:75:ASN:O	1:A:76:GLU:CB	2.54	0.54
1:A:828:ALA:HB1	2:B:530:GLY:HA2	1.86	0.54
1:A:965:GLN:O	1:A:968:GLN:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:653:VAL:HG22	2:B:689:LEU:HD13	1.89	0.54
8:H:82:PRO:C	8:H:84:ALA:H	2.10	0.54
11:K:31:VAL:CG1	11:K:32:VAL:N	2.69	0.54
12:L:55:ILE:O	12:L:56:LEU:HB2	2.06	0.54
1:A:1120:LEU:HD13	1:A:1304:TRP:O	2.08	0.54
1:A:317:LYS:O	1:A:318:SER:HB3	2.08	0.54
1:A:319:GLY:HA3	2:B:471:LYS:HA	1.89	0.54
1:A:381:THR:HG23	1:A:382:PRO:HD2	1.89	0.54
1:A:362:ASP:HB3	1:A:508:PRO:HG3	1.89	0.54
1:A:90:VAL:CG1	1:A:297:GLN:HA	2.37	0.54
2:B:1165:ILE:HG12	4:D:17:LYS:HD2	1.89	0.54
2:B:344:LYS:O	2:B:345:LYS:CB	2.55	0.54
2:B:797:TYR:HE1	2:B:854:LEU:CD2	2.19	0.54
5:E:78:LEU:C	5:E:78:LEU:HD23	2.27	0.54
7:G:48:VAL:HG13	7:G:74:TYR:HD1	1.72	0.54
9:I:55:THR:CG2	9:I:58:VAL:HG21	2.37	0.54
3:C:175:ALA:HB3	10:J:43:ARG:HH22	1.72	0.54
1:A:1076:ALA:HA	1:A:1079:MET:HE2	1.89	0.54
1:A:79:GLY:HA3	1:A:243:PRO:HG3	1.90	0.54
1:A:433:GLU:OE1	2:B:1108:ARG:NH1	2.41	0.54
1:A:666:ILE:N	1:A:666:ILE:HD12	2.22	0.54
1:A:866:PHE:O	1:A:867:ILE:HD12	2.06	0.54
2:B:172:ILE:HD13	2:B:178:ASN:CB	2.35	0.54
8:H:40:LEU:HD12	8:H:122:LEU:O	2.08	0.54
8:H:55:LEU:HD22	8:H:144:ILE:CG2	2.36	0.54
1:A:1036:ARG:HH11	1:A:1036:ARG:CG	2.19	0.54
1:A:222:LEU:O	1:A:224:PHE:N	2.41	0.54
2:B:778:MET:HE2	2:B:1094:ARG:HG2	1.88	0.54
2:B:360:PHE:CD2	2:B:360:PHE:C	2.80	0.54
2:B:594:ALA:HA	2:B:617:ARG:NH1	2.22	0.54
3:C:3:GLU:O	3:C:4:GLU:HG3	2.08	0.54
4:D:20:GLU:OE2	4:D:20:GLU:HA	2.08	0.54
5:E:9:ILE:CD1	5:E:53:PRO:HD3	2.37	0.54
5:E:78:LEU:HD23	5:E:79:TRP:N	2.22	0.54
1:A:1444:MET:HE2	6:F:135:ARG:HB2	1.88	0.54
12:L:31:CYS:SG	12:L:34:CYS:N	2.79	0.54
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.48	0.54
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.08	0.54
1:A:1349:TYR:HB2	1:A:1372:VAL:HG21	1.89	0.54
1:A:567:LYS:CG	1:A:568:PRO:CD	2.79	0.54
1:A:754:SER:N	1:A:757:ASN:HD22	1.96	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:MET:CE	1:A:843:LYS:NZ	2.70	0.54
2:B:1095:LEU:HD12	2:B:1095:LEU:N	2.20	0.54
2:B:343:ILE:CG2	2:B:347:LYS:HB2	2.12	0.54
2:B:386:LEU:O	2:B:388:CYS:N	2.41	0.54
2:B:63:ILE:HA	2:B:421:PHE:CE2	2.43	0.54
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.22	0.54
6:F:82:THR:HG22	6:F:84:TYR:N	2.16	0.54
8:H:47:PHE:CD2	8:H:95:TYR:HD1	2.26	0.54
9:I:25:LEU:HB3	9:I:38:ALA:HB2	1.89	0.54
1:A:1053:PHE:O	1:A:1055:ARG:N	2.40	0.54
1:A:786:HIS:CD2	1:A:786:HIS:N	2.75	0.54
1:A:869:GLY:O	1:A:870:GLU:HB2	2.08	0.54
2:B:1180:PHE:O	2:B:1181:GLU:O	2.26	0.54
2:B:680:THR:O	2:B:684:LEU:HD12	2.08	0.54
5:E:29:PHE:O	5:E:30:ILE:HG13	2.07	0.54
9:I:111:THR:CG2	9:I:112:SER:H	2.19	0.54
9:I:82:GLU:HB3	9:I:104:LEU:HD12	1.90	0.54
1:A:332:LYS:HG3	1:A:333:GLU:HG2	1.89	0.54
2:B:525:ALA:O	2:B:768:THR:HG23	2.07	0.54
3:C:179:GLU:HG2	3:C:180:TYR:H	1.73	0.54
7:G:34:VAL:HG11	7:G:74:TYR:HE1	1.73	0.54
1:A:1444:MET:CE	6:F:135:ARG:HB2	2.38	0.54
1:A:1444:MET:HE2	6:F:135:ARG:CB	2.38	0.54
1:A:89:PRO:HB2	1:A:204:THR:CG2	2.38	0.54
1:A:600:PRO:HG2	1:A:601:LYS:H	1.73	0.54
1:A:974:ASP:C	1:A:976:THR:H	2.12	0.54
2:B:1099:VAL:HG22	2:B:1103:ILE:CD1	2.38	0.54
1:A:18:GLN:CB	2:B:1215:ARG:HB2	2.38	0.54
9:I:101:PHE:HB2	9:I:110:PHE:CE2	2.43	0.54
1:A:590:ARG:O	1:A:591:PHE:HB2	2.08	0.53
1:A:552:TRP:HE3	1:A:651:LYS:HB3	1.73	0.53
1:A:665:GLY:O	1:A:667:GLY:N	2.41	0.53
2:B:1177:HIS:O	2:B:1179:GLN:N	2.41	0.53
2:B:1196:ILE:HB	2:B:1197:PRO:HD2	1.89	0.53
1:A:1410:PHE:HD2	2:B:1212:ILE:HD12	1.72	0.53
2:B:810:GLU:CB	2:B:815:ARG:HH22	2.20	0.53
7:G:7:LEU:CD1	7:G:45:ILE:HD11	2.38	0.53
1:A:1120:LEU:CD1	1:A:1120:LEU:N	2.72	0.53
1:A:12:ARG:O	2:B:1194:ILE:HG22	2.08	0.53
1:A:384:ASN:CG	1:A:388:LEU:HD12	2.28	0.53
1:A:34:LYS:NZ	1:A:57:ARG:NH1	2.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:746:SER:HB2	2:B:1046:PRO:HG2	1.90	0.53
2:B:310:MET:O	2:B:313:MET:HB2	2.09	0.53
3:C:112:ASN:HD22	3:C:112:ASN:N	2.05	0.53
4:D:194:LEU:C	4:D:195:ILE:HG13	2.28	0.53
6:F:69:LEU:N	6:F:70:LYS:CA	2.71	0.53
6:F:69:LEU:N	6:F:70:LYS:N	2.56	0.53
10:J:7:CYS:HB2	10:J:46:CYS:HB3	1.90	0.53
11:K:21:ILE:HG23	11:K:31:VAL:HG11	1.90	0.53
1:A:1323:ASP:C	1:A:1325:THR:H	2.12	0.53
2:B:1001:PHE:CE2	3:C:34:ARG:CZ	2.90	0.53
2:B:1017:ILE:HB	2:B:1018:PRO:CD	2.37	0.53
2:B:1174:LYS:O	2:B:1176:ASN:N	2.40	0.53
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.48	0.53
2:B:305:VAL:O	2:B:305:VAL:HG12	2.09	0.53
2:B:603:LEU:HB3	2:B:609:ILE:CD1	2.39	0.53
2:B:745:PRO:C	2:B:747:MET:H	2.12	0.53
2:B:830:TYR:O	2:B:831:SER:C	2.47	0.53
4:D:8:PHE:CZ	4:D:40:HIS:HA	2.42	0.53
6:F:69:LEU:N	6:F:70:LYS:HA	2.24	0.53
7:G:138:THR:HG22	7:G:139:ILE:HG13	1.89	0.53
9:I:98:VAL:HG11	9:I:113:ASP:OD1	2.07	0.53
9:I:115:LYS:CD	9:I:117:LYS:HE3	2.35	0.53
1:A:340:LEU:HD21	2:B:1200:ALA:N	2.22	0.53
1:A:53:LEU:HD22	1:A:54:ASN:HD22	1.73	0.53
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.39	0.53
2:B:27:ALA:O	2:B:29:ASP:N	2.42	0.53
2:B:797:TYR:HB2	2:B:852:ARG:O	2.09	0.53
5:E:213:ILE:HG12	5:E:214:CYS:N	2.23	0.53
7:G:122:ASN:ND2	7:G:125:SER:HB3	2.24	0.53
9:I:13:MET:HG3	9:I:14:LEU:N	2.23	0.53
2:B:130:VAL:HB	2:B:167:ILE:CD1	2.39	0.53
2:B:293:PRO:HG2	2:B:296:GLU:CB	2.39	0.53
2:B:343:ILE:HG22	2:B:345:LYS:H	1.72	0.53
2:B:37:PHE:CD1	2:B:41:LYS:HG3	2.44	0.53
2:B:580:VAL:HG22	2:B:624:LEU:HB3	1.90	0.53
5:E:157:SER:C	5:E:159:ASP:N	2.60	0.53
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.39	0.53
1:A:632:VAL:O	1:A:633:VAL:C	2.47	0.53
1:A:783:THR:HG21	1:A:815:PHE:CE2	2.42	0.53
2:B:1163:CYS:SG	2:B:1165:ILE:HB	2.49	0.53
2:B:1182:CYS:SG	2:B:1182:CYS:O	2.67	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:VAL:O	2:B:45:SER:C	2.46	0.53
2:B:911:ILE:HG22	2:B:911:ILE:O	2.08	0.53
4:D:208:GLU:O	4:D:212:LYS:HG3	2.08	0.53
6:F:109:VAL:HG12	6:F:110:ASP:N	2.23	0.53
9:I:14:LEU:HA	9:I:28:GLU:O	2.08	0.53
10:J:27:GLU:C	10:J:29:GLU:H	2.10	0.53
1:A:929:LEU:HD23	1:A:983:ILE:HG21	1.90	0.53
2:B:1013:ASN:OD1	2:B:1015:HIS:N	2.38	0.53
2:B:408:LEU:HG	2:B:409:ALA:H	1.74	0.53
2:B:616:ILE:N	2:B:616:ILE:CD1	2.71	0.53
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.90	0.53
10:J:44:TYR:HD2	10:J:44:TYR:N	2.07	0.53
1:A:1209:MET:CE	1:A:1236:LEU:HB3	2.39	0.53
1:A:1206:ASP:CB	1:A:1274:ARG:HH12	2.22	0.53
1:A:1369:ALA:O	1:A:1370:LEU:C	2.47	0.53
1:A:316:GLN:O	1:A:317:LYS:C	2.45	0.53
1:A:349:ALA:C	2:B:1128:LEU:HD11	2.29	0.53
1:A:722:LEU:HD22	1:A:799:PHE:CD1	2.44	0.53
2:B:449:ASN:C	2:B:451:LYS:H	2.12	0.53
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.91	0.53
1:A:1441:PHE:HZ	6:F:89:GLU:HA	1.72	0.53
7:G:154:VAL:HG12	7:G:155:SER:N	2.24	0.53
8:H:100:THR:HG22	8:H:101:ALA:N	2.22	0.53
11:K:109:TRP:O	11:K:111:LEU:N	2.36	0.53
11:K:112:GLN:CB	11:K:112:GLN:C	2.74	0.53
1:A:547:LEU:HB3	11:K:58:PHE:HE1	1.74	0.53
12:L:28:LYS:HB2	12:L:39:SER:HA	1.91	0.53
1:A:1332:PHE:CE1	1:A:1348:LEU:HD13	2.44	0.53
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.09	0.53
1:A:71:GLN:O	1:A:73:GLY:N	2.37	0.53
1:A:768:GLN:HG2	1:A:816:HIS:CA	2.38	0.53
2:B:1065:GLN:NE2	2:B:1067:ARG:H	2.00	0.53
2:B:496:ARG:HH12	2:B:539:LEU:HB2	1.73	0.53
2:B:640:VAL:O	2:B:641:GLU:C	2.48	0.53
2:B:955:THR:CG2	2:B:956:THR:H	2.17	0.53
3:C:35:ARG:HH11	11:K:41:THR:N	2.06	0.53
8:H:99:GLY:HA3	8:H:118:PHE:HA	1.91	0.53
2:B:365:THR:HG23	2:B:367:LEU:HG	1.90	0.53
2:B:515:HIS:O	2:B:518:HIS:HB2	2.08	0.53
2:B:758:PHE:N	2:B:759:PRO:CD	2.72	0.53
3:C:104:PHE:HD2	3:C:105:GLY:H	1.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:73:GLN:NE2	3:C:74:SER:N	2.57	0.53
13:P:6:C:H2'	13:P:7:A:H8	1.73	0.53
1:A:1334:ASP:O	1:A:1336:MET:N	2.42	0.52
1:A:269:ILE:CD1	1:A:300:VAL:HA	2.37	0.52
1:A:34:LYS:CB	1:A:36:ARG:HE	2.20	0.52
1:A:626:ASN:O	1:A:631:HIS:HD2	1.90	0.52
1:A:527:THR:CG2	1:A:650:GLN:HA	2.40	0.52
1:A:527:THR:HG23	1:A:650:GLN:HA	1.91	0.52
2:B:114:PRO:O	2:B:116:GLU:N	2.42	0.52
2:B:1162:ILE:HD11	2:B:1194:ILE:CD1	2.38	0.52
2:B:863:GLU:OE1	2:B:962:LYS:HB2	2.09	0.52
3:C:263:THR:C	3:C:265:MET:H	2.12	0.52
1:A:1151:GLU:HA	9:I:44:TYR:O	2.09	0.52
10:J:43:ARG:O	10:J:47:ARG:HB2	2.09	0.52
1:A:282:ASN:O	1:A:284:ALA:N	2.43	0.52
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.43	0.52
1:A:982:THR:N	1:A:985:ASP:HB2	2.24	0.52
2:B:1142:GLY:HA3	6:F:88:TYR:HE2	1.74	0.52
2:B:309:GLN:CD	9:I:52:ILE:HD11	2.29	0.52
2:B:337:ARG:C	2:B:338:GLY:N	2.62	0.52
3:C:112:ASN:HB2	3:C:114:TYR:CE1	2.44	0.52
11:K:55:LYS:HB2	11:K:81:TYR:HE1	1.75	0.52
1:A:442:VAL:O	1:A:457:ALA:HA	2.09	0.52
1:A:730:GLY:O	1:A:732:LEU:N	2.42	0.52
1:A:845:LEU:HB3	1:A:848:ILE:HD12	1.91	0.52
1:A:979:SER:OG	1:A:981:LEU:HG	2.09	0.52
2:B:121:ASN:HA	2:B:207:GLY:CA	2.39	0.52
3:C:161:LYS:O	3:C:170:TRP:NE1	2.43	0.52
3:C:242:GLN:HA	3:C:245:VAL:HG23	1.92	0.52
1:A:971:PHE:CE2	1:A:1040:GLN:HG2	2.44	0.52
1:A:1279:ILE:CD1	1:A:1316:VAL:HG21	2.38	0.52
1:A:601:LYS:HB2	1:A:603:ASN:ND2	2.24	0.52
1:A:968:GLN:O	1:A:970:THR:N	2.43	0.52
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.92	0.52
2:B:54:PHE:O	2:B:58:THR:HB	2.09	0.52
2:B:798:TYR:HE2	3:C:62:PHE:CE2	2.26	0.52
2:B:843:GLN:O	2:B:844:SER:C	2.48	0.52
7:G:96:GLN:HB3	7:G:121:PHE:CE2	2.45	0.52
1:A:1424:VAL:CG1	1:A:1436:ILE:HD11	2.33	0.52
1:A:528:LEU:HD12	1:A:528:LEU:C	2.30	0.52
1:A:687:LYS:O	1:A:690:VAL:HB	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:ILE:CG2	1:A:872:GLY:N	2.72	0.52
1:A:901:LEU:H	1:A:926:GLN:HE21	1.55	0.52
1:A:666:ILE:HD11	2:B:1067:ARG:O	2.10	0.52
2:B:981:ALA:CB	2:B:987:LYS:HA	2.39	0.52
3:C:88:CYS:SG	3:C:91:HIS:HA	2.50	0.52
6:F:96:THR:O	6:F:100:GLN:HG3	2.09	0.52
8:H:64:ASN:O	8:H:65:LEU:HB2	2.08	0.52
2:B:1039:GLY:HA2	10:J:51:LEU:HD22	1.90	0.52
12:L:70:ARG:HG2	12:L:70:ARG:NH1	2.24	0.52
1:A:1373:ASP:HA	1:A:1376:THR:CG2	2.40	0.52
1:A:1424:VAL:HG11	2:B:1139:ILE:CD1	2.35	0.52
1:A:90:VAL:HG13	1:A:297:GLN:CD	2.30	0.52
2:B:979:LYS:HG2	2:B:1095:LEU:HD13	1.92	0.52
2:B:1134:GLU:CD	2:B:1134:GLU:H	2.13	0.52
1:A:500:GLU:OE2	2:B:1145:SER:HB2	2.09	0.52
2:B:167:ILE:HG22	2:B:453:ILE:HD12	1.90	0.52
2:B:197:PHE:HZ	2:B:816:GLU:HG2	1.75	0.52
2:B:357:GLN:O	2:B:366:GLN:HA	2.09	0.52
3:C:76:ASP:OD2	3:C:128:ASN:N	2.41	0.52
13:P:6:C:O2'	13:P:7:A:H5'	2.10	0.52
1:A:1389:PHE:CD1	1:A:1389:PHE:C	2.82	0.52
1:A:444:PHE:CB	1:A:458:HIS:CD2	2.91	0.52
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.92	0.52
2:B:1180:PHE:HB3	2:B:1191:ILE:HD13	1.90	0.52
2:B:1202:LEU:HD22	2:B:1206:GLU:CD	2.31	0.52
2:B:343:ILE:CG2	2:B:348:ARG:N	2.68	0.52
2:B:542:MET:HG2	2:B:747:MET:HB3	1.91	0.52
3:C:235:VAL:HG13	10:J:13:VAL:CG2	2.38	0.52
9:I:69:PRO:HB2	9:I:85:PHE:CE2	2.45	0.52
12:L:32:ALA:CB	12:L:55:ILE:HD12	2.40	0.52
1:A:42:ASP:HA	1:A:46:THR:O	2.10	0.52
1:A:58:LEU:CD1	1:A:59:GLY:N	2.68	0.52
1:A:982:THR:H	1:A:985:ASP:HB2	1.74	0.52
1:A:982:THR:O	1:A:985:ASP:HB2	2.09	0.52
2:B:1182:CYS:O	2:B:1183:LYS:O	2.28	0.52
2:B:217:ARG:C	2:B:217:ARG:HD2	2.30	0.52
2:B:825:VAL:HG12	2:B:826:ALA:N	2.24	0.52
4:D:50:LEU:HD13	4:D:55:ALA:HA	1.91	0.52
5:E:84:ASP:O	5:E:86:PRO:HD3	2.10	0.52
7:G:59:GLY:CA	7:G:70:PHE:CD2	2.92	0.52
1:A:1004:ASN:O	1:A:1008:GLN:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1348:LEU:HG	1:A:1372:VAL:HG23	1.91	0.52
1:A:474:VAL:C	1:A:477:PRO:HD2	2.31	0.52
1:A:485:ASP:OD1	13:P:10:A:H4'	2.10	0.52
1:A:34:LYS:HZ1	1:A:57:ARG:NH1	2.08	0.52
1:A:942:PHE:HD2	1:A:943:LEU:HD23	1.75	0.52
1:A:947:PHE:CD2	1:A:954:TRP:CE2	2.97	0.52
2:B:1034:VAL:O	2:B:1037:LEU:N	2.39	0.52
2:B:778:MET:HE2	2:B:1094:ARG:CD	2.39	0.52
2:B:549:THR:HG22	2:B:550:ASP:N	2.17	0.52
2:B:770:GLN:HG2	2:B:983:ARG:O	2.09	0.52
2:B:899:ILE:CG2	2:B:949:VAL:HG21	2.40	0.52
2:B:863:GLU:O	2:B:961:LEU:HD22	2.10	0.52
3:C:38:ILE:HA	3:C:173:ALA:HB2	1.92	0.52
10:J:23:ASN:C	10:J:25:LEU:N	2.61	0.52
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.57	0.52
1:A:244:PRO:HB2	1:A:245:PRO:CD	2.38	0.52
1:A:34:LYS:HG2	1:A:36:ARG:NH2	2.25	0.52
1:A:840:ARG:O	1:A:841:LEU:C	2.48	0.52
1:A:857:ARG:HD3	1:A:861:GLY:O	2.10	0.52
2:B:1065:GLN:NE2	2:B:1066:SER:N	2.58	0.52
2:B:731:VAL:HG12	2:B:732:SER:N	2.24	0.52
3:C:100:THR:HG22	3:C:101:LEU:N	2.24	0.52
3:C:76:ASP:O	3:C:79:GLN:HG2	2.11	0.52
13:P:4:A:O2'	13:P:5:C:H5'	2.10	0.52
1:A:1006:ILE:CD1	5:E:163:GLU:HG3	2.40	0.51
2:B:1099:VAL:HG22	2:B:1103:ILE:HD13	1.90	0.51
2:B:1147:LEU:CD2	2:B:1151:LEU:HD22	2.40	0.51
3:C:140:ASN:O	3:C:141:GLY:O	2.27	0.51
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.90	0.51
2:B:798:TYR:CE2	3:C:62:PHE:CE2	2.98	0.51
5:E:178:ILE:HG22	5:E:213:ILE:O	2.10	0.51
6:F:103:MET:CE	7:G:66:GLY:H	2.21	0.51
1:A:551:TYR:CZ	11:K:62:LYS:HE2	2.45	0.51
1:A:873:MET:C	1:A:1058:VAL:HG23	2.31	0.51
1:A:1095:THR:O	1:A:1096:SER:CB	2.58	0.51
1:A:608:ILE:C	1:A:610:GLY:N	2.64	0.51
1:A:584:ASN:O	1:A:637:LYS:HE3	2.11	0.51
2:B:37:PHE:CE1	2:B:41:LYS:HG3	2.46	0.51
5:E:112:TYR:OH	5:E:136:ASN:HB2	2.11	0.51
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.91	0.51
11:K:46:ILE:O	11:K:50:LEU:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1333:ILE:HG22	1:A:1334:ASP:N	2.25	0.51
1:A:317:LYS:O	1:A:318:SER:CB	2.59	0.51
2:B:1121:GLY:C	2:B:1123:SER:N	2.62	0.51
2:B:343:ILE:HB	2:B:348:ARG:HE	1.75	0.51
2:B:498:THR:HB	2:B:537:LYS:O	2.10	0.51
6:F:135:ARG:HG2	6:F:137:TYR:CE1	2.45	0.51
3:C:29:MET:HE1	11:K:98:LEU:HG	1.91	0.51
1:A:1118:VAL:HG12	1:A:1327:ILE:HG13	1.92	0.51
1:A:34:LYS:CE	1:A:57:ARG:NH1	2.74	0.51
1:A:670:ILE:HG23	1:A:805:LEU:HD21	1.92	0.51
2:B:39:ARG:HG2	2:B:39:ARG:HH11	1.75	0.51
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.91	0.51
4:D:53:SER:HB3	4:D:153:ARG:H	1.75	0.51
4:D:176:GLU:C	4:D:178:ALA:N	2.63	0.51
6:F:99:LEU:O	6:F:103:MET:HG2	2.09	0.51
8:H:84:ALA:HA	8:H:87:ARG:CB	2.35	0.51
9:I:101:PHE:N	9:I:101:PHE:CD1	2.78	0.51
2:B:797:TYR:O	10:J:1:MET:HG2	2.10	0.51
1:A:606:LEU:HB3	1:A:614:PHE:CD2	2.45	0.51
1:A:683:ILE:HD13	1:A:801:GLU:HG3	1.92	0.51
1:A:699:ALA:O	1:A:700:ASN:CB	2.58	0.51
1:A:870:GLU:HG2	5:E:208:TYR:CD1	2.46	0.51
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.43	0.51
2:B:112:LEU:HD12	2:B:113:TYR:N	2.24	0.51
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.92	0.51
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.92	0.51
2:B:213:ILE:O	2:B:215:GLN:HG2	2.10	0.51
2:B:220:GLY:O	2:B:222:ILE:HG13	2.11	0.51
6:F:89:GLU:HB3	6:F:134:ILE:CD1	2.40	0.51
4:D:48:ILE:CG2	7:G:4:ILE:HB	2.40	0.51
9:I:111:THR:CG2	9:I:112:SER:N	2.71	0.51
11:K:19:LEU:HD22	11:K:33:ILE:CG2	2.40	0.51
1:A:264:PHE:O	1:A:267:ALA:HB3	2.11	0.51
1:A:265:LYS:HZ3	1:A:322:VAL:HG22	1.75	0.51
1:A:587:HIS:ND1	1:A:965:GLN:OE1	2.44	0.51
1:A:767:GLN:HE21	1:A:774:ARG:HB3	1.75	0.51
2:B:1138:MET:HE2	2:B:1143:ALA:HB3	1.92	0.51
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.14	0.51
2:B:498:THR:CG2	2:B:499:ASN:N	2.74	0.51
3:C:213:PRO:HG2	3:C:214:ASN:H	1.76	0.51
4:D:17:LYS:HE3	4:D:17:LYS:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:99:LEU:C	6:F:99:LEU:HD12	2.31	0.51
7:G:115:MET:CB	7:G:116:PRO:HD2	2.40	0.51
7:G:139:ILE:HG22	7:G:140:LYS:N	2.24	0.51
1:A:107:CYS:H	1:A:114:LEU:HD21	1.75	0.51
1:A:384:ASN:O	1:A:386:ASP:N	2.43	0.51
1:A:399:HIS:CB	1:A:400:PRO:CD	2.85	0.51
1:A:41:MET:HB3	1:A:48:ALA:O	2.11	0.51
1:A:549:MET:SD	1:A:577:ILE:CD1	2.98	0.51
1:A:832:ALA:HB2	14:T:18:DT:C7	2.41	0.51
1:A:947:PHE:CD2	1:A:954:TRP:CZ2	2.99	0.51
2:B:1017:ILE:CB	2:B:1018:PRO:HD3	2.39	0.51
2:B:46:GLN:HG3	2:B:47:GLN:N	2.16	0.51
2:B:731:VAL:HG12	2:B:732:SER:H	1.76	0.51
2:B:745:PRO:C	2:B:747:MET:N	2.64	0.51
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.93	0.51
7:G:145:VAL:CG1	7:G:146:LYS:N	2.73	0.51
8:H:4:THR:CA	8:H:60:ALA:HB2	2.35	0.51
2:B:309:GLN:CG	9:I:52:ILE:HD11	2.39	0.51
11:K:40:HIS:O	11:K:43:GLY:N	2.44	0.51
12:L:58:LYS:O	12:L:59:ALA:O	2.29	0.51
14:T:18:DT:H2''	14:T:19:DT:O5'	2.11	0.51
1:A:381:THR:HG21	1:A:383:TYR:CD1	2.46	0.51
1:A:40:THR:HG22	1:A:41:MET:CG	2.29	0.51
2:B:309:GLN:HG3	9:I:52:ILE:CD1	2.40	0.51
2:B:882:THR:O	2:B:883:LEU:HB2	2.11	0.51
5:E:180:ARG:NH2	5:E:192:ARG:HB2	2.22	0.51
1:A:1376:THR:O	1:A:1377:THR:C	2.48	0.51
1:A:1412:ALA:HA	1:A:1417:GLU:OE2	2.10	0.51
1:A:563:PRO:HG3	1:A:572:TRP:CE2	2.46	0.51
1:A:913:LEU:HD23	1:A:919:ILE:HD12	1.92	0.51
2:B:999:MET:HE2	2:B:1000:PRO:HD2	1.93	0.51
4:D:118:THR:HB	4:D:121:LYS:HB2	1.93	0.51
7:G:26:LEU:O	7:G:27:LYS:C	2.48	0.51
1:A:499:ALA:O	1:A:503:GLN:HG2	2.11	0.51
1:A:577:ILE:O	1:A:580:VAL:HG23	2.12	0.51
1:A:61:ILE:O	1:A:63:ARG:N	2.44	0.51
1:A:730:GLY:C	1:A:732:LEU:H	2.14	0.51
1:A:882:SER:HB3	1:A:953:ASN:OD1	2.10	0.51
2:B:1121:GLY:O	2:B:1123:SER:N	2.43	0.51
2:B:1138:MET:CE	2:B:1138:MET:HA	2.40	0.51
2:B:1155:SER:OG	2:B:1156:ASP:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1152:MET:HE1	2:B:1157:ALA:HA	1.91	0.51
2:B:226:PHE:CD1	2:B:398:ARG:NH2	2.79	0.51
2:B:542:MET:HB3	2:B:636:PRO:HD2	1.92	0.51
2:B:859:TYR:OH	2:B:941:LEU:CD1	2.58	0.51
3:C:189:THR:HG22	3:C:190:ASP:H	1.76	0.51
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.45	0.51
5:E:145:THR:HG21	5:E:187:TYR:CE2	2.46	0.51
1:A:963:ILE:HD13	1:A:1049:ILE:HG13	1.92	0.50
1:A:1114:PRO:O	1:A:1115:SER:O	2.28	0.50
1:A:567:LYS:HD2	1:A:568:PRO:CD	2.32	0.50
2:B:999:MET:HG2	2:B:1007:VAL:HG22	1.92	0.50
1:A:805:LEU:CD1	2:B:1052:VAL:HG21	2.41	0.50
2:B:274:PRO:O	2:B:275:TYR:HB2	2.12	0.50
2:B:364:ILE:HG12	2:B:585:VAL:CG1	2.33	0.50
2:B:758:PHE:O	2:B:760:ASP:N	2.44	0.50
2:B:841:MET:SD	2:B:846:ILE:HD11	2.50	0.50
1:A:254:GLU:CB	2:B:935:ARG:HH12	2.20	0.50
3:C:8:VAL:HG12	3:C:9:LYS:H	1.75	0.50
7:G:117:GLN:C	7:G:119:LEU:H	2.14	0.50
7:G:112:LYS:NZ	7:G:120:THR:HA	2.27	0.50
11:K:45:LEU:HG	11:K:94:ILE:CD1	2.39	0.50
1:A:1036:ARG:NH1	1:A:1036:ARG:HG2	2.23	0.50
1:A:1057:VAL:HG12	1:A:1058:VAL:H	1.76	0.50
1:A:535:THR:CG2	1:A:616:VAL:HA	2.38	0.50
1:A:718:VAL:O	1:A:721:PHE:HB2	2.11	0.50
2:B:687:GLU:O	2:B:689:LEU:HG	2.12	0.50
7:G:44:TYR:CD2	7:G:105:PRO:HB2	2.46	0.50
8:H:58:THR:HG22	8:H:59:ILE:H	1.77	0.50
12:L:38:LEU:HD11	12:L:49:LYS:HE2	1.93	0.50
1:A:44:THR:O	1:A:45:GLN:HB2	2.12	0.50
2:B:841:MET:O	2:B:993:THR:HA	2.11	0.50
2:B:971:THR:OG1	3:C:61:GLU:HG3	2.10	0.50
8:H:39:THR:O	8:H:123:MET:HA	2.11	0.50
1:A:472:LEU:O	1:A:475:THR:CB	2.58	0.50
1:A:492:PRO:O	1:A:493:GLN:NE2	2.44	0.50
2:B:486:TYR:CE1	2:B:1096:ARG:HD3	2.45	0.50
2:B:597:MET:O	2:B:599:THR:N	2.44	0.50
2:B:787:VAL:O	2:B:787:VAL:HG12	2.10	0.50
3:C:58:LEU:HD22	3:C:58:LEU:N	2.26	0.50
9:I:86:PHE:HE1	9:I:100:PHE:HB2	1.76	0.50
12:L:38:LEU:O	12:L:39:SER:CB	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:39:SER:O	12:L:40:LEU:HG	2.10	0.50
1:A:1097:GLY:C	1:A:1099:PRO:HD2	2.31	0.50
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.76	0.50
2:B:97:VAL:HG12	2:B:178:ASN:HD21	1.77	0.50
2:B:310:MET:HE3	2:B:387:LEU:CD1	2.40	0.50
2:B:376:PHE:HE2	2:B:569:TYR:HD2	1.58	0.50
3:C:6:PRO:HB3	3:C:25:VAL:HG13	1.88	0.50
5:E:168:TYR:CB	5:E:170:LEU:HG	2.42	0.50
8:H:142:LEU:C	8:H:143:LEU:HD12	2.32	0.50
8:H:25:ARG:HA	8:H:41:ASP:HA	1.93	0.50
9:I:61:ASP:C	9:I:63:GLY:H	2.15	0.50
1:A:447:GLN:NE2	14:T:20:DC:H4'	2.26	0.50
1:A:1213:GLY:O	1:A:1214:GLU:C	2.50	0.50
1:A:195:ASP:O	1:A:196:GLU:HB3	2.12	0.50
1:A:49:LYS:HZ1	1:A:61:ILE:N	2.09	0.50
1:A:566:ILE:O	1:A:567:LYS:O	2.30	0.50
1:A:75:ASN:O	1:A:76:GLU:HB2	2.12	0.50
2:B:343:ILE:HB	2:B:348:ARG:HG3	1.92	0.50
2:B:531:GLN:CG	2:B:532:ALA:H	2.20	0.50
2:B:850:LEU:HD12	2:B:851:PHE:H	1.76	0.50
5:E:13:TRP:O	5:E:16:PHE:HB3	2.11	0.50
5:E:35:VAL:C	5:E:37:LEU:H	2.13	0.50
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.46	0.50
13:P:9:G:H2'	13:P:10:A:H5'	1.93	0.50
1:A:1162:VAL:HG12	1:A:1162:VAL:O	2.12	0.50
1:A:1280:GLU:O	1:A:1281:ARG:O	2.30	0.50
1:A:1308:THR:HG23	1:A:1309:ASP:N	2.26	0.50
1:A:1111:MET:HE1	1:A:1330:ASN:OD1	2.12	0.50
1:A:1373:ASP:HA	1:A:1376:THR:HG22	1.94	0.50
1:A:187:LYS:HE3	1:A:198:GLU:OE2	2.12	0.50
1:A:108:MET:HB3	1:A:210:ILE:CD1	2.41	0.50
1:A:265:LYS:HE2	1:A:322:VAL:HG11	1.93	0.50
1:A:344:ARG:HB3	2:B:1118:PRO:HB2	1.94	0.50
1:A:42:ASP:C	1:A:44:THR:H	2.13	0.50
1:A:4:GLN:O	1:A:5:GLN:HB2	2.11	0.50
2:B:827:ILE:O	2:B:1085:ILE:HG23	2.12	0.50
2:B:579:ARG:CB	2:B:586:TRP:HE1	2.24	0.50
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.93	0.50
2:B:841:MET:HE1	2:B:980:PHE:CE1	2.47	0.50
3:C:46:ILE:HG13	3:C:72:LEU:HD11	1.92	0.50
4:D:19:GLU:O	4:D:21:GLU:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:55:ARG:C	5:E:57:MET:N	2.65	0.50
6:F:143:PHE:C	6:F:143:PHE:CD1	2.84	0.50
9:I:32:CYS:SG	9:I:33:SER:N	2.85	0.50
9:I:26:LEU:CD2	9:I:37:GLU:HA	2.38	0.50
10:J:28:ASP:O	10:J:30:LEU:HG	2.12	0.50
13:P:10:A:C8	13:P:10:A:H3'	2.46	0.50
1:A:1053:PHE:O	1:A:1056:SER:N	2.42	0.50
2:B:102:VAL:O	2:B:109:THR:HA	2.11	0.50
2:B:1085:ILE:CD1	2:B:1085:ILE:N	2.70	0.50
1:A:1410:PHE:HA	2:B:1212:ILE:HD11	1.92	0.50
2:B:327:ARG:O	2:B:331:LEU:HD13	2.12	0.50
2:B:770:GLN:C	2:B:772:ALA:H	2.14	0.50
7:G:111:THR:HG22	7:G:113:HIS:N	2.25	0.50
2:B:193:LYS:NZ	12:L:32:ALA:HB1	2.25	0.50
1:A:1029:ARG:HG3	1:A:1029:ARG:NH1	2.27	0.50
1:A:1149:ALA:CB	9:I:47:GLU:HA	2.41	0.50
1:A:630:ILE:HD13	1:A:646:PHE:CZ	2.47	0.50
1:A:817:ALA:O	1:A:820:GLY:N	2.45	0.50
1:A:913:LEU:HD21	1:A:915:SER:OG	2.12	0.50
2:B:1102:LYS:O	2:B:1103:ILE:C	2.49	0.50
2:B:616:ILE:CG1	2:B:697:GLU:HA	2.42	0.50
3:C:58:LEU:HD21	10:J:57:ILE:HD12	1.94	0.50
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.93	0.49
1:A:18:GLN:HB3	2:B:1215:ARG:HG3	1.94	0.49
1:A:449:SER:O	2:B:1133:MET:HB3	2.11	0.49
1:A:506:ALA:C	1:A:508:PRO:HD2	2.32	0.49
1:A:341:MET:CE	2:B:1135:ARG:NH1	2.75	0.49
2:B:39:ARG:HG2	2:B:39:ARG:NH1	2.27	0.49
2:B:831:SER:HB3	2:B:994:TYR:OH	2.12	0.49
8:H:116:TYR:HB2	8:H:123:MET:HB3	1.94	0.49
9:I:92:ARG:HB3	9:I:95:THR:OG1	2.11	0.49
1:A:500:GLU:OE1	2:B:1143:ALA:C	2.50	0.49
1:A:774:ARG:O	1:A:775:ILE:C	2.49	0.49
1:A:412:ARG:NH2	2:B:1108:ARG:NH1	2.60	0.49
2:B:185:THR:O	2:B:188:ASP:HB2	2.12	0.49
3:C:236:GLY:O	3:C:237:SER:C	2.51	0.49
5:E:67:GLU:O	5:E:70:SER:HB3	2.11	0.49
8:H:38:LEU:HD13	8:H:125:LEU:HD13	1.94	0.49
1:A:1076:ALA:HA	1:A:1079:MET:HE3	1.93	0.49
1:A:1116:LEU:HD11	1:A:1118:VAL:HG13	1.94	0.49
1:A:1332:PHE:O	1:A:1333:ILE:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:PRO:HA	2:B:1201:LYS:HZ2	1.77	0.49
2:B:34:ILE:O	2:B:35:SER:C	2.50	0.49
2:B:382:ILE:O	2:B:386:LEU:HG	2.12	0.49
2:B:654:ARG:N	2:B:657:HIS:HD2	1.98	0.49
2:B:990:ILE:HG22	2:B:991:GLY:N	2.27	0.49
7:G:1:MET:SD	7:G:79:PHE:HD1	2.35	0.49
9:I:110:PHE:H	9:I:110:PHE:HD2	1.59	0.49
9:I:99:LEU:O	9:I:111:THR:HG23	2.12	0.49
1:A:1094:VAL:CG1	1:A:1095:THR:N	2.60	0.49
1:A:166:GLY:O	1:A:167:CYS:CB	2.60	0.49
1:A:203:SER:OG	1:A:206:GLU:HB2	2.13	0.49
1:A:71:GLN:C	1:A:73:GLY:H	2.14	0.49
1:A:832:ALA:CB	14:T:18:DT:H71	2.41	0.49
2:B:1181:GLU:O	2:B:1182:CYS:HB2	2.12	0.49
2:B:126:SER:O	2:B:169:ARG:HA	2.13	0.49
2:B:247:GLY:C	2:B:249:ARG:N	2.65	0.49
2:B:337:ARG:C	2:B:338:GLY:CA	2.81	0.49
2:B:558:LEU:O	2:B:561:TRP:N	2.45	0.49
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.93	0.49
7:G:34:VAL:HG11	7:G:74:TYR:CE1	2.48	0.49
9:I:85:PHE:N	9:I:85:PHE:CD2	2.65	0.49
1:A:1096:SER:O	1:A:1100:ARG:HB3	2.11	0.49
1:A:182:VAL:HG22	1:A:201:VAL:HA	1.94	0.49
1:A:208:LEU:HD23	1:A:208:LEU:O	2.13	0.49
1:A:567:LYS:HB3	8:H:95:TYR:CA	2.39	0.49
1:A:606:LEU:CB	1:A:614:PHE:CE2	2.95	0.49
2:B:120:ARG:O	2:B:121:ASN:HB2	2.13	0.49
2:B:223:VAL:CG1	2:B:381:MET:HG2	2.43	0.49
2:B:696:GLU:O	2:B:699:GLU:HB2	2.11	0.49
2:B:197:PHE:CZ	2:B:816:GLU:HG2	2.47	0.49
10:J:56:LEU:O	10:J:59:LYS:N	2.45	0.49
13:P:10:A:C8	13:P:10:A:C3'	2.95	0.49
1:A:1299:VAL:CG1	1:A:1300:LYS:N	2.75	0.49
1:A:1434:ALA:HB3	1:A:1436:ILE:HD12	1.94	0.49
2:B:365:THR:HG23	2:B:367:LEU:N	2.21	0.49
2:B:372:SER:O	2:B:376:PHE:HD1	1.96	0.49
2:B:459:TYR:CD2	2:B:459:TYR:C	2.86	0.49
2:B:579:ARG:N	2:B:589:VAL:HG13	2.28	0.49
2:B:839:MET:HE3	2:B:1010:LEU:CD2	2.42	0.49
2:B:992:ILE:HG12	2:B:993:THR:N	2.27	0.49
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:177:VAL:O	4:D:177:VAL:HG12	2.11	0.49
5:E:23:VAL:O	5:E:28:TYR:HB2	2.13	0.49
7:G:34:VAL:HG12	7:G:45:ILE:CG2	2.38	0.49
11:K:31:VAL:HG12	11:K:32:VAL:H	1.75	0.49
14:T:23:DG:H2'	14:T:24:DG:C8	2.48	0.49
1:A:116:ASP:C	1:A:118:HIS:N	2.66	0.49
1:A:1225:PHE:CE2	1:A:1227:ILE:HD11	2.47	0.49
1:A:1111:MET:CE	1:A:1330:ASN:OD1	2.60	0.49
1:A:1334:ASP:O	1:A:1337:GLU:N	2.45	0.49
1:A:418:SER:O	1:A:420:ARG:N	2.46	0.49
1:A:402:ALA:CB	1:A:434:ARG:HA	2.43	0.49
1:A:647:GLY:O	1:A:651:LYS:HG3	2.12	0.49
2:B:1084:GLN:C	2:B:1085:ILE:HD12	2.32	0.49
2:B:486:TYR:CZ	2:B:1096:ARG:HB3	2.47	0.49
1:A:351:THR:CB	2:B:1103:ILE:HD12	2.36	0.49
2:B:1142:GLY:O	2:B:1144:ALA:N	2.45	0.49
2:B:1156:ASP:O	2:B:1157:ALA:O	2.31	0.49
2:B:429:PHE:HA	2:B:432:MET:HE3	1.95	0.49
2:B:785:TYR:CD1	2:B:785:TYR:C	2.86	0.49
2:B:792:MET:HA	2:B:856:PHE:O	2.13	0.49
1:A:526:ASP:OD1	2:B:1013:ASN:ND2	2.46	0.49
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.95	0.49
2:B:223:VAL:HG21	2:B:380:TYR:CE2	2.47	0.49
2:B:797:TYR:O	2:B:799:PRO:HD3	2.13	0.49
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.33	0.49
1:A:278:THR:O	1:A:278:THR:HG22	2.12	0.49
1:A:500:GLU:O	1:A:504:LEU:HD13	2.13	0.49
1:A:863:VAL:HG11	1:A:866:PHE:CD2	2.47	0.49
1:A:883:LEU:CD2	1:A:1021:LEU:HB2	2.43	0.49
2:B:181:LEU:HD22	2:B:189:LEU:CD2	2.42	0.49
2:B:370:PHE:HE2	2:B:373:ARG:HH11	1.61	0.49
2:B:597:MET:O	2:B:600:LEU:N	2.43	0.49
2:B:909:ASP:N	2:B:909:ASP:OD1	2.41	0.49
2:B:872:GLU:CD	2:B:914:LYS:HE2	2.33	0.49
3:C:113:VAL:CG2	3:C:147:LEU:HD21	2.43	0.49
5:E:161:LYS:HD2	5:E:195:VAL:HG23	1.95	0.49
5:E:195:VAL:HG22	5:E:213:ILE:HG13	1.94	0.49
1:A:504:LEU:HD11	6:F:91:ALA:HB1	1.95	0.49
11:K:21:ILE:HG23	11:K:31:VAL:CG1	2.43	0.49
11:K:55:LYS:CB	11:K:81:TYR:CE1	2.96	0.49
1:A:1453:TYR:O	1:A:1454:MET:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LYS:HE2	1:A:322:VAL:HG13	1.94	0.49
1:A:34:LYS:NZ	1:A:57:ARG:CZ	2.76	0.49
1:A:606:LEU:HD23	1:A:614:PHE:HE2	1.78	0.49
1:A:49:LYS:HZ3	1:A:61:ILE:HG13	1.74	0.49
1:A:666:ILE:CD1	1:A:667:GLY:H	2.26	0.49
2:B:827:ILE:HD12	2:B:1086:PHE:CD2	2.48	0.49
2:B:293:PRO:HG2	2:B:296:GLU:HB3	1.94	0.49
2:B:683:SER:O	2:B:687:GLU:HB2	2.13	0.49
3:C:254:LYS:C	3:C:256:ALA:N	2.66	0.49
10:J:1:MET:H3	10:J:56:LEU:N	2.11	0.49
1:A:1385:THR:C	1:A:1387:HIS:N	2.67	0.48
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.94	0.48
1:A:829:VAL:C	1:A:831:THR:N	2.67	0.48
2:B:233:PRO:HG2	2:B:234:ILE:HD12	1.95	0.48
2:B:467:GLY:N	2:B:475:SER:CB	2.71	0.48
2:B:770:GLN:OE1	2:B:983:ARG:CA	2.54	0.48
2:B:979:LYS:HG2	2:B:1095:LEU:CD1	2.43	0.48
3:C:27:LEU:HD13	3:C:228:PHE:CE2	2.47	0.48
4:D:51:ASN:ND2	4:D:54:GLU:OE2	2.46	0.48
4:D:59:ILE:O	4:D:60:LYS:C	2.50	0.48
5:E:55:ARG:C	5:E:57:MET:H	2.15	0.48
5:E:90:VAL:HG22	5:E:90:VAL:O	2.13	0.48
7:G:91:VAL:HA	7:G:101:VAL:HA	1.96	0.48
7:G:1:MET:O	7:G:1:MET:CE	2.61	0.48
7:G:23:LYS:HG3	7:G:56:ILE:HD12	1.92	0.48
2:B:1077:THR:HG22	11:K:44:ASN:HD21	1.77	0.48
1:A:1224:LEU:HD12	1:A:1241:ARG:O	2.13	0.48
1:A:168:GLY:O	1:A:169:ASN:C	2.49	0.48
1:A:32:VAL:HG23	1:A:32:VAL:O	2.13	0.48
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.95	0.48
1:A:50:ILE:O	1:A:52:GLY:N	2.44	0.48
1:A:958:VAL:HG22	1:A:1052:GLN:HB3	1.95	0.48
1:A:982:THR:HG22	1:A:984:LYS:H	1.76	0.48
2:B:1010:LEU:HD23	2:B:1092:TYR:CE1	2.49	0.48
2:B:1121:GLY:O	2:B:1124:ARG:N	2.41	0.48
2:B:785:TYR:CD1	2:B:786:ASN:N	2.81	0.48
2:B:950:ASP:O	2:B:951:GLN:HB2	2.13	0.48
3:C:39:ALA:CA	3:C:164:ALA:HB3	2.44	0.48
5:E:124:VAL:HG13	5:E:132:ILE:CB	2.41	0.48
6:F:132:LEU:O	6:F:148:VAL:HG22	2.13	0.48
6:F:75:PRO:HG3	6:F:78:GLN:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:149:GLY:O	7:G:159:ALA:HB1	2.13	0.48
7:G:51:TYR:O	7:G:51:TYR:CD2	2.65	0.48
8:H:103:LYS:HG2	8:H:104:PHE:N	2.29	0.48
9:I:84:VAL:O	9:I:84:VAL:HG13	2.13	0.48
12:L:34:CYS:O	12:L:36:SER:N	2.46	0.48
1:A:1389:PHE:CD1	1:A:1390:ASN:N	2.82	0.48
1:A:236:LEU:HD11	1:A:304:MET:HE1	1.95	0.48
1:A:241:VAL:O	1:A:242:PRO:C	2.51	0.48
1:A:242:PRO:HA	1:A:243:PRO:HD2	1.68	0.48
1:A:262:LEU:C	1:A:264:PHE:N	2.66	0.48
1:A:90:VAL:HG13	1:A:297:GLN:OE1	2.12	0.48
1:A:298:PHE:O	1:A:301:ALA:HB3	2.13	0.48
2:B:229:ALA:CB	2:B:231:PRO:HD2	2.43	0.48
2:B:388:CYS:C	2:B:390:LEU:H	2.15	0.48
5:E:124:VAL:HA	5:E:132:ILE:HD12	1.95	0.48
1:A:852:TYR:CD1	6:F:136:ARG:HB3	2.48	0.48
10:J:57:ILE:HA	10:J:60:PHE:CD2	2.47	0.48
11:K:68:PHE:CD2	11:K:68:PHE:N	2.78	0.48
2:B:900:ALA:HB3	12:L:61:THR:OG1	2.13	0.48
1:A:1036:ARG:NH1	1:A:1036:ARG:CG	2.77	0.48
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.95	0.48
1:A:577:ILE:HG13	1:A:578:LEU:N	2.27	0.48
1:A:666:ILE:HD11	2:B:1086:PHE:HE1	1.77	0.48
1:A:886:ILE:HD11	1:A:943:LEU:CB	2.43	0.48
2:B:1002:THR:HG21	2:B:1006:ILE:CD1	2.37	0.48
2:B:1099:VAL:CG1	2:B:1100:ASP:H	2.20	0.48
3:C:173:ALA:O	3:C:174:ALA:HB3	2.13	0.48
3:C:56:THR:HG22	3:C:57:VAL:N	2.27	0.48
4:D:52:LEU:CD2	4:D:147:TYR:HE2	2.26	0.48
5:E:14:ARG:HH21	5:E:141:VAL:CG1	2.26	0.48
6:F:130:ILE:O	6:F:148:VAL:CG2	2.61	0.48
9:I:112:SER:O	9:I:114:GLN:HG3	2.12	0.48
9:I:52:ILE:HG13	9:I:52:ILE:O	2.13	0.48
1:A:368:LYS:O	1:A:369:SER:C	2.52	0.48
2:B:118:ARG:HG2	2:B:204:ILE:HD13	1.95	0.48
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.13	0.48
3:C:97:VAL:HG12	3:C:99:LEU:CD2	2.43	0.48
1:A:1118:VAL:HG12	1:A:1327:ILE:CD1	2.44	0.48
1:A:34:LYS:H	1:A:57:ARG:HH21	1.55	0.48
1:A:532:ARG:O	1:A:535:THR:HB	2.14	0.48
1:A:663:SER:HB2	2:B:827:ILE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:958:VAL:HG12	1:A:958:VAL:O	2.13	0.48
2:B:1068:GLY:O	2:B:1069:PHE:O	2.31	0.48
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.94	0.48
2:B:236:HIS:CE1	2:B:389:ALA:HA	2.48	0.48
2:B:794:ASN:C	2:B:795:ILE:HD12	2.34	0.48
4:D:13:ARG:HB2	4:D:17:LYS:HZ2	1.77	0.48
9:I:33:SER:O	9:I:35:VAL:HG23	2.13	0.48
1:A:135:PHE:HB2	1:A:223:GLY:H	1.79	0.48
1:A:244:PRO:CB	1:A:245:PRO:CD	2.91	0.48
1:A:335:ARG:O	1:A:336:ILE:C	2.52	0.48
1:A:67:CYS:O	1:A:68:GLN:HB2	2.14	0.48
1:A:853:ASP:OD1	1:A:855:THR:CG2	2.61	0.48
2:B:1006:ILE:HD13	10:J:44:TYR:HE2	1.73	0.48
2:B:496:ARG:HB3	2:B:496:ARG:HH11	1.78	0.48
2:B:758:PHE:N	2:B:759:PRO:HD2	2.29	0.48
2:B:814:PHE:C	2:B:816:GLU:H	2.16	0.48
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.96	0.48
4:D:24:ALA:C	4:D:26:THR:H	2.16	0.48
7:G:25:TYR:O	7:G:28:THR:HB	2.14	0.48
8:H:89:LEU:O	8:H:91:ASP:N	2.47	0.48
12:L:47:ARG:HH21	12:L:54:ARG:NH2	2.11	0.48
1:A:1289:ARG:NH1	1:A:1326:ARG:NH1	2.62	0.48
1:A:1364:ASN:O	1:A:1365:TYR:C	2.52	0.48
1:A:95:PHE:CZ	1:A:1414:ALA:HB2	2.48	0.48
1:A:475:THR:CG2	1:A:476:SER:H	2.26	0.48
2:B:95:ILE:CG1	2:B:130:VAL:HG22	2.44	0.48
3:C:114:TYR:CD2	3:C:140:ASN:HB2	2.49	0.48
3:C:60:ASP:OD2	12:L:60:ARG:NH2	2.47	0.48
4:D:130:LEU:C	4:D:132:GLN:N	2.67	0.48
1:A:1450:LEU:HD11	6:F:108:PHE:CZ	2.48	0.48
9:I:60:GLN:NE2	9:I:107:SER:OG	2.47	0.48
9:I:71:SER:OG	9:I:83:ASN:HB2	2.13	0.48
1:A:1130:GLN:O	1:A:1134:ILE:HG13	2.14	0.48
1:A:1293:SER:OG	1:A:1294:PRO:HD2	2.13	0.48
1:A:1398:MET:HB2	1:A:1426:GLU:OE2	2.14	0.48
1:A:1446:ASP:HB3	1:A:1449:SER:OG	2.14	0.48
1:A:21:LEU:HD12	1:A:229:SER:HB2	1.96	0.48
1:A:300:VAL:O	1:A:300:VAL:HG12	2.13	0.48
1:A:470:LEU:HD22	1:A:487:MET:CE	2.43	0.48
1:A:50:ILE:C	1:A:52:GLY:N	2.66	0.48
1:A:528:LEU:O	1:A:528:LEU:HD12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:728:LYS:HA	1:A:731:ARG:HB2	1.95	0.48
1:A:79:GLY:H	2:B:1205:GLN:HE22	1.61	0.48
1:A:341:MET:HE1	1:A:843:LYS:NZ	2.27	0.48
1:A:852:TYR:HA	1:A:1060:PRO:HB3	1.96	0.48
2:B:363:HIS:O	2:B:364:ILE:CB	2.54	0.48
2:B:388:CYS:O	2:B:390:LEU:N	2.47	0.48
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.29	0.48
2:B:857:ARG:HD2	2:B:945:GLU:OE1	2.13	0.48
10:J:7:CYS:SG	10:J:49:MET:HE3	2.54	0.48
14:T:18:DT:C2'	14:T:19:DT:O5'	2.62	0.48
1:A:1141:THR:OG1	1:A:1205:LYS:HD3	2.13	0.48
1:A:23:SER:CB	1:A:233:TRP:NE1	2.77	0.48
1:A:347:PHE:HE2	1:A:375:THR:HG23	1.78	0.48
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.95	0.48
1:A:915:SER:O	1:A:919:ILE:HG13	2.14	0.48
2:B:1001:PHE:CE2	3:C:34:ARG:NE	2.81	0.48
2:B:1182:CYS:O	2:B:1183:LYS:C	2.52	0.48
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.14	0.48
2:B:582:VAL:HG12	2:B:587:HIS:NE2	2.29	0.48
2:B:24:PRO:O	2:B:655:LYS:HB2	2.14	0.48
2:B:799:PRO:HB3	2:B:818:PRO:HG2	1.96	0.48
2:B:910:VAL:HG12	2:B:911:ILE:N	2.29	0.48
3:C:213:PRO:O	3:C:214:ASN:CB	2.61	0.48
5:E:163:GLU:O	5:E:164:LEU:C	2.53	0.48
6:F:109:VAL:HG11	6:F:123:LYS:HD3	1.95	0.48
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.14	0.47
1:A:339:ASN:O	1:A:343:LYS:HG2	2.13	0.47
1:A:393:ARG:O	1:A:395:GLY:N	2.47	0.47
2:B:1110:PRO:HB2	2:B:1119:VAL:HG21	1.96	0.47
2:B:1208:MET:O	2:B:1211:ASN:N	2.46	0.47
2:B:344:LYS:O	2:B:345:LYS:HB2	2.13	0.47
2:B:502:ILE:H	2:B:502:ILE:CD1	2.01	0.47
2:B:642:ASP:CA	2:B:649:LYS:HA	2.40	0.47
2:B:762:ASN:OD1	2:B:1024:ALA:HB3	2.14	0.47
2:B:874:PHE:HA	2:B:913:GLY:O	2.14	0.47
3:C:123:ASN:ND2	3:C:125:MET:CG	2.77	0.47
3:C:254:LYS:C	3:C:256:ALA:H	2.16	0.47
3:C:99:LEU:HD23	3:C:99:LEU:N	2.28	0.47
4:D:170:THR:CG2	4:D:172:LEU:HG	2.43	0.47
7:G:7:LEU:HD11	7:G:45:ILE:HD11	1.96	0.47
8:H:62:SER:C	8:H:64:ASN:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1226:VAL:HG13	1:A:1240:CYS:HB3	1.96	0.47
1:A:1265:ASN:C	1:A:1267:MET:N	2.66	0.47
1:A:1377:THR:O	1:A:1379:GLY:N	2.47	0.47
1:A:26:GLU:O	1:A:27:VAL:C	2.52	0.47
1:A:817:ALA:O	1:A:818:MET:C	2.53	0.47
1:A:886:ILE:HG13	1:A:943:LEU:CD1	2.43	0.47
5:E:10:SER:O	5:E:14:ARG:HG3	2.14	0.47
5:E:30:ILE:HG22	5:E:31:THR:N	2.27	0.47
6:F:89:GLU:OE2	6:F:134:ILE:HG21	2.14	0.47
7:G:106:MET:HG2	7:G:107:LYS:N	2.28	0.47
1:A:19:PHE:HE1	1:A:1396:ALA:HB3	1.79	0.47
1:A:1445:ILE:HD12	7:G:59:GLY:O	2.13	0.47
1:A:332:LYS:C	1:A:334:GLY:H	2.17	0.47
1:A:603:ASN:O	1:A:604:GLY:C	2.52	0.47
1:A:466:SER:HB3	2:B:1103:ILE:HG12	1.96	0.47
2:B:424:LEU:HD22	2:B:453:ILE:HD11	1.97	0.47
2:B:854:LEU:HB3	2:B:856:PHE:HE1	1.79	0.47
2:B:1005:GLY:HA2	3:C:176:ILE:O	2.13	0.47
3:C:22:LEU:HD13	3:C:230:MET:HE3	1.95	0.47
3:C:36:VAL:HG11	3:C:251:LEU:HB2	1.95	0.47
4:D:167:LEU:HB3	4:D:177:VAL:HG13	1.96	0.47
6:F:94:LEU:HD21	6:F:122:MET:HA	1.95	0.47
7:G:18:PHE:HA	7:G:22:MET:HE2	1.96	0.47
8:H:38:LEU:HD12	8:H:124:ARG:O	2.14	0.47
3:C:66:ARG:HH21	10:J:5:VAL:HG23	1.79	0.47
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.95	0.47
1:A:47:ARG:HH12	1:A:254:GLU:CG	2.26	0.47
1:A:335:ARG:N	1:A:339:ASN:HD22	2.12	0.47
1:A:60:SER:C	1:A:61:ILE:HG13	2.34	0.47
1:A:608:ILE:HD12	1:A:613:ILE:CD1	2.45	0.47
1:A:639:PRO:HG2	1:A:640:GLN:N	2.29	0.47
1:A:809:THR:H	1:A:812:GLU:HB2	1.80	0.47
1:A:98:LYS:O	1:A:100:LYS:N	2.47	0.47
2:B:329:THR:O	2:B:332:ASP:HB3	2.15	0.47
2:B:521:LEU:HB3	2:B:633:VAL:CG1	2.43	0.47
2:B:53:GLN:O	2:B:53:GLN:HG3	2.15	0.47
2:B:658:ILE:O	2:B:661:LEU:HB2	2.14	0.47
3:C:18:VAL:O	3:C:20:PHE:CD2	2.65	0.47
3:C:254:LYS:O	3:C:256:ALA:N	2.47	0.47
3:C:58:LEU:CD2	3:C:58:LEU:N	2.77	0.47
4:D:156:ASP:C	4:D:158:GLU:H	2.16	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1441:PHE:CE2	6:F:89:GLU:HG2	2.49	0.47
7:G:1:MET:HE1	7:G:80:LYS:H	1.79	0.47
9:I:51:ASN:O	9:I:54:GLU:HG3	2.15	0.47
9:I:55:THR:O	9:I:55:THR:HG22	2.14	0.47
11:K:40:HIS:O	11:K:41:THR:C	2.52	0.47
1:A:1219:THR:HG21	1:A:1271:ILE:CD1	2.44	0.47
1:A:1405:THR:HB	1:A:1406:VAL:H	1.50	0.47
1:A:268:ASP:HB3	1:A:299:HIS:ND1	2.29	0.47
1:A:92:HIS:HD2	1:A:304:MET:CE	2.27	0.47
1:A:444:PHE:HB3	1:A:458:HIS:CD2	2.49	0.47
1:A:98:LYS:O	1:A:101:LYS:N	2.47	0.47
2:B:123:THR:O	2:B:125:SER:N	2.47	0.47
2:B:25:ILE:HD11	2:B:653:VAL:C	2.35	0.47
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.14	0.47
3:C:22:LEU:HD23	3:C:25:VAL:HG21	1.95	0.47
8:H:102:TYR:CE2	8:H:117:SER:HB2	2.49	0.47
8:H:104:PHE:CZ	8:H:136:LYS:HA	2.50	0.47
9:I:101:PHE:CE1	9:I:112:SER:HB2	2.49	0.47
1:A:1074:GLU:C	1:A:1076:ALA:H	2.18	0.47
1:A:248:PRO:O	1:A:260:ASP:HB2	2.14	0.47
1:A:332:LYS:O	1:A:334:GLY:N	2.48	0.47
1:A:68:GLN:C	1:A:70:CYS:N	2.65	0.47
1:A:877:HIS:O	1:A:878:ILE:HG12	2.14	0.47
1:A:947:PHE:HD2	1:A:954:TRP:CZ2	2.32	0.47
2:B:1084:GLN:HE21	2:B:1084:GLN:N	2.10	0.47
2:B:190:TYR:CE1	2:B:196:PRO:HG3	2.49	0.47
2:B:259:TYR:HB2	2:B:268:THR:HG23	1.96	0.47
2:B:412:LEU:HB3	2:B:466:TRP:CZ2	2.49	0.47
2:B:936:ASP:OD1	2:B:938:SER:N	2.42	0.47
2:B:953:LEU:HD21	2:B:965:LYS:HB2	1.96	0.47
3:C:168:ALA:O	3:C:170:TRP:N	2.48	0.47
6:F:119:ARG:HG3	6:F:119:ARG:HH11	1.80	0.47
9:I:50:THR:HG22	9:I:51:ASN:N	2.28	0.47
10:J:7:CYS:SG	10:J:8:PHE:N	2.87	0.47
11:K:24:ASP:OD1	11:K:26:LYS:N	2.48	0.47
3:C:47:ASP:CA	12:L:69:ALA:CB	2.90	0.47
1:A:1290:LYS:O	1:A:1291:VAL:HG23	2.14	0.47
1:A:1100:ARG:NH2	1:A:1351:GLU:CG	2.71	0.47
1:A:302:THR:HA	1:A:305:ASP:O	2.14	0.47
1:A:415:LEU:HA	1:A:415:LEU:HD23	1.64	0.47
2:B:729:ILE:O	2:B:729:ILE:HG22	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:59:ALA:O	3:C:60:ASP:C	2.53	0.47
11:K:52:ASN:O	11:K:54:ARG:N	2.47	0.47
13:P:2:C:C2'	13:P:3:G:H5'	2.44	0.47
1:A:1243:VAL:HG12	1:A:1244:ARG:N	2.28	0.47
1:A:1404:GLU:O	1:A:1407:GLU:HB2	2.15	0.47
1:A:308:ILE:HG22	1:A:309:ALA:N	2.19	0.47
1:A:381:THR:HG23	1:A:383:TYR:H	1.80	0.47
1:A:53:LEU:O	1:A:54:ASN:C	2.51	0.47
1:A:857:ARG:HG2	1:A:863:VAL:HA	1.96	0.47
2:B:757:PRO:HG3	2:B:1028:GLU:OE2	2.15	0.47
2:B:1106:ARG:HH11	2:B:1110:PRO:HG2	1.80	0.47
2:B:590:HIS:HD2	2:B:593:PRO:HB3	1.79	0.47
2:B:814:PHE:C	2:B:816:GLU:N	2.68	0.47
2:B:827:ILE:HD12	2:B:1086:PHE:HD2	1.79	0.47
3:C:215:GLU:O	3:C:216:GLY:C	2.53	0.47
3:C:36:VAL:HG21	3:C:251:LEU:HD22	1.96	0.47
7:G:79:PHE:CE2	7:G:105:PRO:HG2	2.50	0.47
8:H:123:MET:HE3	8:H:142:LEU:CD2	2.45	0.47
8:H:18:GLY:O	8:H:19:ARG:HB2	2.14	0.47
9:I:5:ARG:HD3	9:I:36:GLU:OE2	2.15	0.47
9:I:59:VAL:C	9:I:61:ASP:H	2.17	0.47
9:I:69:PRO:HG2	9:I:85:PHE:CD2	2.50	0.47
10:J:31:ASP:O	10:J:32:GLU:C	2.53	0.47
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.95	0.47
1:A:1437:GLY:O	1:A:1438:THR:C	2.53	0.47
1:A:381:THR:HG23	1:A:382:PRO:CD	2.44	0.47
1:A:403:LYS:O	1:A:404:TYR:CG	2.67	0.47
1:A:414:ASP:C	1:A:414:ASP:OD1	2.53	0.47
1:A:3:GLY:O	1:A:4:GLN:HB2	2.15	0.47
1:A:844:ALA:HB2	1:A:1389:PHE:CE2	2.50	0.47
2:B:165:VAL:HG11	2:B:448:ILE:CD1	2.44	0.47
2:B:343:ILE:HG23	2:B:347:LYS:CB	2.13	0.47
2:B:210:LYS:HG3	2:B:461:LEU:O	2.14	0.47
3:C:99:LEU:HA	3:C:119:VAL:O	2.14	0.47
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.49	0.47
6:F:86:THR:HG23	6:F:89:GLU:OE1	2.15	0.47
11:K:67:PHE:O	11:K:68:PHE:HD2	1.98	0.47
13:P:10:A:H8	13:P:10:A:H3'	1.80	0.47
1:A:1097:GLY:O	1:A:1100:ARG:N	2.46	0.47
1:A:230:ARG:N	1:A:233:TRP:CE3	2.64	0.47
1:A:243:PRO:O	1:A:244:PRO:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:PHE:HB2	1:A:256:GLN:NE2	2.30	0.47
1:A:72:GLU:OE2	2:B:1175:LEU:HB2	2.15	0.47
1:A:780:VAL:O	1:A:782:ARG:HG2	2.15	0.47
2:B:1162:ILE:HG22	2:B:1163:CYS:H	1.80	0.47
2:B:1166:CYS:O	2:B:1168:LEU:N	2.48	0.47
2:B:547:VAL:HG12	2:B:612:GLU:OE2	2.15	0.47
2:B:763:GLN:O	2:B:765:PRO:N	2.48	0.47
2:B:955:THR:CG2	2:B:956:THR:N	2.72	0.47
3:C:167:HIS:CD2	3:C:169:LYS:H	2.33	0.47
7:G:138:THR:CG2	7:G:139:ILE:H	2.02	0.47
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.15	0.47
1:A:326:ARG:HG2	1:A:327:ALA:N	2.29	0.47
1:A:418:SER:C	1:A:420:ARG:N	2.68	0.47
1:A:43:GLU:O	1:A:44:THR:CB	2.63	0.47
1:A:767:GLN:HA	1:A:799:PHE:HA	1.97	0.47
2:B:1077:THR:HG22	11:K:44:ASN:ND2	2.30	0.47
2:B:1223:ASP:HB3	2:B:1224:PHE:H	1.56	0.47
2:B:171:PRO:HD2	2:B:457:LEU:CD1	2.42	0.47
2:B:244:LEU:C	2:B:246:LYS:N	2.68	0.47
2:B:446:LEU:O	2:B:447:ALA:CB	2.63	0.47
2:B:710:LEU:O	2:B:711:GLU:HG2	2.15	0.47
2:B:824:ILE:HG12	10:J:48:ARG:HH12	1.79	0.47
5:E:124:VAL:HB	5:E:125:PRO:CD	2.45	0.47
5:E:147:HIS:HD2	5:E:149:LEU:H	1.62	0.47
7:G:117:GLN:C	7:G:119:LEU:N	2.69	0.47
10:J:16:ASP:O	10:J:18:TRP:N	2.48	0.47
11:K:111:LEU:C	11:K:112:GLN:CG	2.83	0.47
1:A:474:VAL:HG22	1:A:474:VAL:O	2.15	0.46
1:A:595:THR:O	1:A:596:THR:HG23	2.14	0.46
1:A:920:LEU:HD23	1:A:920:LEU:C	2.35	0.46
2:B:653:VAL:HG23	2:B:689:LEU:HB3	1.96	0.46
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.50	0.46
1:A:667:GLY:HA3	3:C:192:TRP:CH2	2.49	0.46
3:C:239:PRO:O	3:C:241:ASP:N	2.48	0.46
6:F:108:PHE:HE1	6:F:131:PRO:HG3	1.80	0.46
8:H:7:ASP:O	8:H:8:ASP:HB2	2.14	0.46
11:K:6:ARG:C	11:K:8:GLU:H	2.18	0.46
1:A:899:VAL:CG2	1:A:1029:ARG:HG2	2.46	0.46
1:A:874:ASP:CA	1:A:1058:VAL:HG22	2.45	0.46
1:A:1226:VAL:HG22	1:A:1240:CYS:HB3	1.96	0.46
1:A:1342:GLU:OE2	5:E:212:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:PRO:HB3	1:A:237:THR:HB	1.97	0.46
1:A:722:LEU:O	1:A:725:ALA:HB3	2.15	0.46
1:A:92:HIS:O	1:A:95:PHE:N	2.40	0.46
2:B:826:ALA:HB2	2:B:1008:PRO:HB3	1.97	0.46
2:B:1064:TYR:O	2:B:1065:GLN:C	2.54	0.46
2:B:1151:LEU:CD1	2:B:1151:LEU:N	2.78	0.46
2:B:259:TYR:H	2:B:259:TYR:HD1	1.62	0.46
2:B:654:ARG:C	2:B:656:GLY:N	2.68	0.46
3:C:143:LEU:C	3:C:143:LEU:HD12	2.35	0.46
4:D:56:ARG:HD3	4:D:149:THR:HA	1.98	0.46
5:E:13:TRP:CE3	5:E:39:LEU:HD13	2.50	0.46
7:G:1:MET:C	7:G:1:MET:SD	2.93	0.46
7:G:20:PRO:HG2	7:G:21:ARG:H	1.79	0.46
1:A:1161:THR:HG22	1:A:1163:ILE:HG13	1.97	0.46
1:A:265:LYS:NZ	1:A:322:VAL:HG13	2.30	0.46
1:A:567:LYS:HE3	8:H:46:LEU:CB	2.45	0.46
1:A:7:SER:C	1:A:9:ALA:H	2.19	0.46
1:A:450:LEU:HB3	1:A:838:GLN:HE21	1.78	0.46
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.96	0.46
4:D:52:LEU:C	4:D:54:GLU:N	2.68	0.46
1:A:1324:PRO:HB2	5:E:142:VAL:HG11	1.96	0.46
6:F:123:LYS:O	6:F:124:GLU:C	2.54	0.46
7:G:29:LYS:O	7:G:30:LEU:C	2.54	0.46
7:G:13:LEU:O	7:G:67:SER:HA	2.16	0.46
8:H:10:PHE:CE1	8:H:57:VAL:HB	2.50	0.46
8:H:10:PHE:HA	8:H:29:ALA:O	2.15	0.46
9:I:99:LEU:HB2	9:I:101:PHE:CE1	2.50	0.46
3:C:169:LYS:NZ	12:L:69:ALA:HB3	2.31	0.46
1:A:1211:GLN:O	1:A:1212:VAL:C	2.53	0.46
1:A:1239:ARG:HH11	1:A:1239:ARG:CB	2.28	0.46
1:A:565:ILE:O	1:A:570:PRO:HA	2.15	0.46
2:B:1017:ILE:HG22	2:B:1018:PRO:N	2.30	0.46
2:B:1023:VAL:O	2:B:1024:ALA:C	2.54	0.46
2:B:113:TYR:CD2	2:B:192:LEU:HD22	2.50	0.46
2:B:640:VAL:O	2:B:640:VAL:HG12	2.16	0.46
2:B:96:TYR:HB2	2:B:129:PHE:HB2	1.98	0.46
3:C:11:ARG:HD3	3:C:209:TYR:CZ	2.51	0.46
3:C:73:GLN:HE21	3:C:74:SER:N	2.14	0.46
5:E:134:THR:C	5:E:135:PHE:HD1	2.17	0.46
7:G:91:VAL:HG23	7:G:141:SER:O	2.16	0.46
1:A:975:HIS:HA	1:A:1036:ARG:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:LEU:HD13	1:A:656:TRP:CD2	2.50	0.46
1:A:56:PRO:O	1:A:57:ARG:CG	2.64	0.46
1:A:84:ILE:O	1:A:84:ILE:CG2	2.63	0.46
1:A:862:ASN:O	1:A:864:ILE:HG13	2.15	0.46
1:A:929:LEU:CD2	1:A:983:ILE:HG21	2.46	0.46
2:B:361:LEU:N	2:B:362:PRO:CD	2.78	0.46
2:B:434:ARG:HA	2:B:437:GLU:CD	2.35	0.46
2:B:510:LYS:CG	2:B:511:PRO:CD	2.85	0.46
2:B:899:ILE:HG22	2:B:900:ALA:N	2.30	0.46
2:B:957:ASN:O	2:B:960:GLY:N	2.47	0.46
3:C:77:ILE:HG22	3:C:78:GLU:N	2.31	0.46
4:D:53:SER:CB	4:D:152:SER:HB2	2.44	0.46
4:D:51:ASN:C	4:D:52:LEU:O	2.53	0.46
5:E:136:ASN:OD1	5:E:138:ALA:N	2.49	0.46
6:F:101:ILE:HD13	6:F:120:ILE:CG2	2.45	0.46
8:H:58:THR:HG22	8:H:59:ILE:N	2.31	0.46
8:H:93:TYR:CD1	8:H:93:TYR:N	2.82	0.46
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.98	0.46
11:K:55:LYS:CB	11:K:81:TYR:HE1	2.28	0.46
1:A:1224:LEU:HD11	1:A:1240:CYS:HB2	1.96	0.46
1:A:1349:TYR:CB	1:A:1372:VAL:HG21	2.46	0.46
1:A:24:PRO:HD2	1:A:233:TRP:CD1	2.51	0.46
1:A:265:LYS:CE	1:A:322:VAL:HG13	2.45	0.46
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.97	0.46
1:A:353:ILE:HB	1:A:470:LEU:CD2	2.44	0.46
1:A:370:ILE:O	1:A:372:LYS:N	2.48	0.46
1:A:735:VAL:O	1:A:735:VAL:HG12	2.14	0.46
2:B:118:ARG:HH11	2:B:204:ILE:HD11	1.81	0.46
2:B:291:ILE:HD13	2:B:300:HIS:CD2	2.51	0.46
2:B:479:VAL:O	2:B:480:SER:HB3	2.14	0.46
2:B:801:LYS:O	10:J:52:THR:CG2	2.63	0.46
3:C:184:ASN:HD21	3:C:187:LYS:HA	1.80	0.46
3:C:82:TYR:O	3:C:83:SER:C	2.53	0.46
1:A:896:ARG:NH2	1:A:1030:ARG:HH21	2.13	0.46
1:A:1120:LEU:CD1	1:A:1120:LEU:H	2.29	0.46
1:A:1161:THR:CG2	1:A:1163:ILE:HG13	2.45	0.46
1:A:1325:THR:CG2	1:A:1325:THR:O	2.63	0.46
1:A:230:ARG:HG3	1:A:233:TRP:CZ3	2.49	0.46
1:A:471:ASN:O	1:A:474:VAL:HG12	2.15	0.46
1:A:53:LEU:CD2	1:A:54:ASN:N	2.52	0.46
1:A:843:LYS:HD3	1:A:846:GLU:OE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:981:LEU:HD21	1:A:1039:LYS:HA	1.97	0.46
1:A:996:ASN:O	1:A:998:LEU:HD12	2.15	0.46
2:B:1095:LEU:H	2:B:1095:LEU:CD1	2.16	0.46
2:B:1099:VAL:C	2:B:1101:ASP:H	2.19	0.46
3:C:34:ARG:O	3:C:38:ILE:HG13	2.16	0.46
3:C:70:ILE:HD11	3:C:144:ILE:CG1	2.45	0.46
11:K:42:LEU:HD21	11:K:46:ILE:CD1	2.45	0.46
1:A:185:TRP:CZ3	1:A:200:ARG:HG2	2.50	0.46
1:A:356:ASP:O	1:A:358:ASN:N	2.49	0.46
1:A:637:LYS:CB	1:A:641:VAL:HG11	2.45	0.46
1:A:672:ASP:HB2	1:A:736:ASN:OD1	2.14	0.46
1:A:768:GLN:HG3	1:A:816:HIS:HA	1.97	0.46
1:A:946:VAL:HG22	5:E:201:LYS:HD2	1.98	0.46
2:B:1017:ILE:CB	2:B:1018:PRO:CD	2.94	0.46
2:B:227:LYS:HB2	2:B:395:GLN:OE1	2.15	0.46
2:B:658:ILE:O	2:B:661:LEU:N	2.38	0.46
2:B:766:ARG:HD3	2:B:766:ARG:HA	1.79	0.46
2:B:861:ASP:OD1	2:B:862:GLN:N	2.49	0.46
3:C:137:LYS:HB3	3:C:138:GLU:OE1	2.16	0.46
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.51	0.46
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.97	0.46
2:B:798:TYR:CE2	3:C:62:PHE:HZ	2.29	0.46
4:D:151:PHE:N	4:D:151:PHE:CD1	2.84	0.46
4:D:68:ARG:C	4:D:70:PHE:H	2.19	0.46
1:A:1259:MET:C	1:A:1261:LYS:H	2.18	0.46
1:A:261:ASP:O	1:A:264:PHE:HB2	2.16	0.46
1:A:356:ASP:C	1:A:358:ASN:H	2.19	0.46
1:A:399:HIS:CG	1:A:400:PRO:N	2.83	0.46
1:A:64:ASN:O	1:A:65:LEU:C	2.54	0.46
1:A:785:PRO:HG2	2:B:703:ILE:HD12	1.97	0.46
1:A:841:LEU:O	1:A:845:LEU:HG	2.15	0.46
2:B:1060:ARG:HA	2:B:1060:ARG:HD2	1.60	0.46
2:B:1070:GLU:OE1	10:J:44:TYR:OH	2.29	0.46
2:B:1176:ASN:C	2:B:1178:ASN:H	2.17	0.46
2:B:898:LEU:CD2	2:B:964:VAL:HG11	2.46	0.46
2:B:911:ILE:CG2	2:B:966:VAL:HG11	2.46	0.46
2:B:995:ARG:HH12	3:C:165:LYS:HG2	1.81	0.46
4:D:27:LEU:HD22	4:D:173:HIS:HD2	1.79	0.46
9:I:54:GLU:HB3	9:I:100:PHE:CE2	2.51	0.46
1:A:548:ASN:OD1	11:K:60:ALA:HB1	2.15	0.46
1:A:1030:ARG:NH1	1:A:1035:TYR:OH	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ILE:HG13	1:A:482:PHE:HD2	1.80	0.46
1:A:341:MET:HE3	2:B:1135:ARG:NH1	2.31	0.46
2:B:410:GLY:O	2:B:412:LEU:N	2.49	0.46
2:B:212:LEU:HD23	2:B:480:SER:HB2	1.98	0.46
2:B:530:GLY:O	2:B:531:GLN:HG3	2.16	0.46
3:C:123:ASN:ND2	3:C:125:MET:SD	2.88	0.46
3:C:166:GLU:O	3:C:167:HIS:HB2	2.16	0.46
5:E:46:TYR:CD2	5:E:58:MET:HG2	2.51	0.46
6:F:77:ASP:C	6:F:79:ARG:N	2.69	0.46
7:G:99:PHE:CD1	7:G:99:PHE:C	2.89	0.46
1:A:503:GLN:C	1:A:504:LEU:HD12	2.35	0.45
1:A:608:ILE:O	1:A:610:GLY:N	2.50	0.45
1:A:89:PRO:HB3	1:A:208:LEU:HD12	1.99	0.45
2:B:1065:GLN:NE2	2:B:1067:ARG:HG2	2.31	0.45
1:A:373:THR:HG21	2:B:1105:ALA:HB3	1.98	0.45
2:B:190:TYR:CE2	10:J:62:ARG:HB3	2.51	0.45
2:B:449:ASN:O	2:B:451:LYS:N	2.49	0.45
2:B:53:GLN:CB	2:B:547:VAL:HG21	2.45	0.45
2:B:591:ARG:O	2:B:593:PRO:HD3	2.15	0.45
2:B:704:ALA:HB2	2:B:738:PHE:CD2	2.51	0.45
3:C:89:GLU:O	3:C:90:ASP:HB3	2.15	0.45
4:D:51:ASN:O	4:D:52:LEU:C	2.55	0.45
4:D:7:THR:HG23	4:D:7:THR:O	2.15	0.45
5:E:55:ARG:O	5:E:57:MET:N	2.49	0.45
1:A:567:LYS:HE3	8:H:46:LEU:HD12	1.98	0.45
8:H:59:ILE:CG2	8:H:60:ALA:H	2.23	0.45
9:I:56:ALA:O	9:I:57:GLY:O	2.33	0.45
1:A:1164:PRO:HG2	1:A:1165:GLU:H	1.82	0.45
1:A:117:GLU:H	1:A:117:GLU:CD	2.20	0.45
1:A:1423:GLY:O	1:A:1424:VAL:C	2.55	0.45
1:A:230:ARG:HB2	1:A:233:TRP:CE3	2.51	0.45
1:A:58:LEU:HD21	1:A:243:PRO:HB3	1.97	0.45
1:A:71:GLN:C	1:A:73:GLY:N	2.70	0.45
1:A:852:TYR:CD2	1:A:1060:PRO:CB	2.97	0.45
2:B:189:LEU:O	2:B:192:LEU:HB2	2.16	0.45
2:B:237:VAL:HG12	2:B:238:ALA:N	2.31	0.45
2:B:303:TYR:N	2:B:303:TYR:CD2	2.82	0.45
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.52	0.45
2:B:757:PRO:HD3	2:B:983:ARG:NH2	2.31	0.45
3:C:168:ALA:C	3:C:170:TRP:N	2.69	0.45
3:C:33:LEU:O	3:C:34:ARG:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:17:LYS:HE3	4:D:17:LYS:N	2.31	0.45
7:G:10:ASN:OD1	7:G:71:ASN:HA	2.16	0.45
8:H:61:SER:O	8:H:62:SER:CB	2.58	0.45
9:I:15:TYR:HD1	9:I:15:TYR:N	2.13	0.45
2:B:833:TYR:CZ	11:K:66:PRO:HG3	2.51	0.45
13:P:6:C:H2'	13:P:7:A:C8	2.51	0.45
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.80	0.45
1:A:115:LEU:HB2	1:A:122:MET:CE	2.46	0.45
1:A:675:THR:OG1	1:A:736:ASN:ND2	2.50	0.45
1:A:874:ASP:HA	1:A:1058:VAL:HG22	1.97	0.45
2:B:1138:MET:HA	2:B:1138:MET:HE3	1.99	0.45
1:A:1438:THR:CB	2:B:1144:ALA:HB3	2.38	0.45
2:B:294:ASP:O	2:B:296:GLU:N	2.46	0.45
2:B:210:LYS:HA	2:B:481:GLN:O	2.17	0.45
2:B:597:MET:C	2:B:599:THR:N	2.70	0.45
2:B:860:MET:CG	2:B:861:ASP:N	2.78	0.45
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.41	0.45
3:C:8:VAL:HG12	3:C:9:LYS:N	2.31	0.45
4:D:195:ILE:O	4:D:195:ILE:HG22	2.17	0.45
7:G:79:PHE:HZ	7:G:106:MET:CE	2.25	0.45
10:J:23:ASN:O	10:J:25:LEU:N	2.49	0.45
11:K:31:VAL:CG1	11:K:32:VAL:H	2.29	0.45
11:K:65:HIS:CD2	11:K:65:HIS:C	2.89	0.45
1:A:331:GLY:O	1:A:332:LYS:HB3	2.16	0.45
1:A:909:ASP:C	1:A:911:SER:H	2.20	0.45
2:B:199:MET:N	2:B:199:MET:SD	2.86	0.45
2:B:234:ILE:O	2:B:261:ARG:NH2	2.48	0.45
2:B:37:PHE:HD2	2:B:542:MET:SD	2.39	0.45
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.16	0.45
2:B:583:ASN:OD1	2:B:628:THR:N	2.43	0.45
3:C:31:ASN:O	3:C:32:SER:C	2.53	0.45
4:D:9:GLN:OE1	4:D:38:ILE:HD12	2.16	0.45
4:D:64:VAL:C	4:D:66:ARG:H	2.19	0.45
5:E:177:ARG:HG2	5:E:213:ILE:HG22	1.99	0.45
6:F:111:LEU:O	6:F:113:GLY:N	2.47	0.45
14:T:24:DG:H2''	14:T:25:DT:C5'	2.42	0.45
1:A:30:ILE:HG23	2:B:1170:THR:HG23	1.98	0.45
1:A:477:PRO:HG3	1:A:521:MET:HG2	1.97	0.45
1:A:535:THR:HG21	1:A:617:VAL:H	1.80	0.45
1:A:527:THR:HG21	1:A:650:GLN:HG2	1.99	0.45
1:A:832:ALA:HA	14:T:18:DT:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1065:GLN:NE2	2:B:1066:SER:H	2.14	0.45
2:B:226:PHE:HA	2:B:395:GLN:CG	2.45	0.45
2:B:295:GLY:N	2:B:298:LEU:HD23	2.28	0.45
2:B:280:ILE:CD1	2:B:334:ILE:HG12	2.43	0.45
2:B:681:TRP:O	2:B:684:LEU:N	2.50	0.45
2:B:899:ILE:HD13	2:B:905:VAL:HG11	1.97	0.45
4:D:173:HIS:ND1	4:D:174:PRO:HD2	2.32	0.45
4:D:187:THR:HG22	4:D:188:ALA:H	1.82	0.45
5:E:72:PHE:CE2	5:E:155:ARG:NH2	2.84	0.45
5:E:156:LEU:HD12	5:E:195:VAL:HB	1.98	0.45
7:G:106:MET:HB3	7:G:106:MET:HE2	1.74	0.45
9:I:115:LYS:HD3	9:I:117:LYS:CE	2.39	0.45
1:A:1451:VAL:O	1:A:1454:MET:HG2	2.16	0.45
1:A:152:VAL:HG12	1:A:153:PRO:HD2	1.98	0.45
1:A:427:GLN:O	1:A:428:TYR:C	2.53	0.45
1:A:673:GLY:O	1:A:676:MET:HB2	2.17	0.45
1:A:95:PHE:O	1:A:96:ILE:C	2.54	0.45
2:B:1162:ILE:HG22	2:B:1163:CYS:N	2.31	0.45
2:B:519:TRP:C	2:B:519:TRP:CD1	2.90	0.45
1:A:472:LEU:CD2	2:B:836:GLU:HG3	2.46	0.45
2:B:913:GLY:HA2	2:B:938:SER:OG	2.17	0.45
5:E:16:PHE:HZ	5:E:20:LYS:HE2	1.76	0.45
8:H:10:PHE:HE1	8:H:57:VAL:HB	1.81	0.45
8:H:58:THR:HB	8:H:143:LEU:HD13	1.99	0.45
8:H:91:ASP:O	8:H:93:TYR:N	2.49	0.45
9:I:8:ARG:CG	9:I:34:TYR:HE1	2.18	0.45
12:L:49:LYS:O	12:L:50:ASP:CB	2.63	0.45
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.44	0.45
1:A:341:MET:HE2	1:A:843:LYS:NZ	2.31	0.45
1:A:43:GLU:O	1:A:44:THR:HB	2.16	0.45
1:A:818:MET:HA	2:B:514:LEU:HB3	1.98	0.45
1:A:87:ALA:HB1	1:A:276:LEU:HD23	1.99	0.45
2:B:1187:ASN:OD1	2:B:1190:ASP:N	2.49	0.45
2:B:1202:LEU:O	2:B:1203:LEU:C	2.54	0.45
2:B:19:GLU:O	2:B:20:ASP:C	2.55	0.45
2:B:838:SER:HA	2:B:989:THR:O	2.16	0.45
2:B:866:TYR:HD1	2:B:870:ILE:O	1.99	0.45
2:B:903:VAL:HG12	2:B:904:ARG:N	2.32	0.45
2:B:999:MET:HA	2:B:999:MET:CE	2.47	0.45
3:C:172:PRO:O	3:C:235:VAL:HG23	2.17	0.45
3:C:208:GLU:C	3:C:210:GLU:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:236:GLY:C	3:C:238:ILE:N	2.69	0.45
3:C:34:ARG:HA	3:C:37:MET:HE2	1.99	0.45
3:C:69:LEU:O	10:J:6:ARG:HD2	2.16	0.45
1:A:1339:LEU:HD13	5:E:147:HIS:CD2	2.52	0.45
8:H:31:THR:O	8:H:31:THR:HG22	2.16	0.45
9:I:8:ARG:O	9:I:10:CYS:N	2.50	0.45
10:J:32:GLU:O	10:J:33:GLY:C	2.54	0.45
11:K:55:LYS:HB3	11:K:81:TYR:CE1	2.52	0.45
1:A:219:PHE:O	1:A:222:LEU:O	2.34	0.45
1:A:313:GLN:O	1:A:314:ALA:HB3	2.17	0.45
1:A:821:ARG:HB2	1:A:821:ARG:NH1	2.27	0.45
1:A:821:ARG:O	1:A:825:ILE:HG13	2.16	0.45
1:A:901:LEU:HD22	1:A:919:ILE:CG2	2.47	0.45
2:B:1177:HIS:C	2:B:1179:GLN:H	2.19	0.45
2:B:388:CYS:C	2:B:390:LEU:N	2.69	0.45
2:B:847:ASP:C	2:B:849:GLY:N	2.70	0.45
3:C:251:LEU:HD12	3:C:251:LEU:O	2.16	0.45
3:C:67:LEU:HD11	3:C:155:LEU:HD13	1.98	0.45
3:C:77:ILE:C	3:C:79:GLN:H	2.19	0.45
4:D:191:ALA:C	4:D:193:THR:H	2.20	0.45
4:D:29:LEU:HD13	7:G:82:PHE:CZ	2.52	0.45
5:E:29:PHE:C	5:E:30:ILE:HG13	2.37	0.45
11:K:59:ALA:HA	11:K:74:ARG:O	2.17	0.45
1:A:1409:LEU:O	1:A:1412:ALA:HB3	2.17	0.45
1:A:1418:LEU:HD12	1:A:1419:ASP:H	1.81	0.45
1:A:230:ARG:N	1:A:233:TRP:HE3	2.07	0.45
1:A:666:ILE:HG12	2:B:1030:LEU:HD22	1.99	0.45
1:A:842:VAL:HG11	2:B:1136:ASP:OD2	2.17	0.45
2:B:180:TYR:CD1	2:B:180:TYR:N	2.78	0.45
2:B:244:LEU:O	2:B:246:LYS:N	2.50	0.45
2:B:487:THR:O	2:B:490:SER:HB3	2.17	0.45
2:B:558:LEU:O	2:B:560:GLU:N	2.49	0.45
4:D:192:LYS:HG2	4:D:207:LEU:CD2	2.47	0.45
5:E:161:LYS:C	5:E:163:GLU:N	2.69	0.45
7:G:14:HIS:CD2	7:G:16:SER:CB	2.90	0.45
8:H:40:LEU:HD22	8:H:123:MET:CE	2.46	0.45
1:A:698:GLN:HA	9:I:97:MET:O	2.16	0.45
10:J:41:LEU:HD11	10:J:50:ILE:HG13	1.99	0.45
1:A:1102:LYS:HG2	1:A:1106:ASN:HD21	1.82	0.45
1:A:110:CYS:HB3	1:A:167:CYS:SG	2.57	0.45
1:A:1400:CYS:O	1:A:1405:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:SER:O	1:A:24:PRO:C	2.54	0.45
1:A:285:PRO:O	1:A:287:HIS:N	2.49	0.45
1:A:534:LEU:O	1:A:534:LEU:HG	2.15	0.45
1:A:730:GLY:C	1:A:732:LEU:N	2.69	0.45
1:A:920:LEU:CD2	1:A:920:LEU:C	2.86	0.45
1:A:92:HIS:O	1:A:93:VAL:C	2.54	0.45
2:B:315:LYS:N	2:B:316:PRO:CD	2.79	0.45
2:B:614:SER:C	2:B:615:MET:HG3	2.37	0.45
2:B:638:PHE:HB3	2:B:651:LEU:HD22	1.99	0.45
3:C:209:TYR:H	3:C:209:TYR:HD1	1.63	0.45
3:C:44:LEU:HD21	3:C:159:ALA:HB1	1.98	0.45
4:D:59:ILE:HG21	4:D:145:MET:SD	2.57	0.45
6:F:97:ARG:NH2	6:F:106:PRO:O	2.50	0.45
7:G:18:PHE:HA	7:G:22:MET:HE3	1.98	0.45
9:I:4:PHE:C	9:I:4:PHE:CD1	2.89	0.45
2:B:1039:GLY:HA2	10:J:51:LEU:HD21	1.97	0.45
11:K:35:PHE:CD1	11:K:71:PHE:CE1	3.04	0.45
1:A:547:LEU:HD13	11:K:58:PHE:CD1	2.52	0.45
1:A:1192:LEU:HG	1:A:1193:LEU:N	2.32	0.44
1:A:577:ILE:O	1:A:578:LEU:C	2.52	0.44
1:A:58:LEU:HD11	1:A:243:PRO:HB2	1.99	0.44
1:A:32:VAL:HG21	1:A:68:GLN:NE2	2.33	0.44
1:A:697:ALA:HB2	1:A:702:LEU:HD12	1.99	0.44
2:B:531:GLN:HG3	2:B:532:ALA:N	2.30	0.44
2:B:893:LEU:HD22	2:B:897:GLY:C	2.37	0.44
3:C:47:ASP:HA	3:C:169:LYS:NZ	2.32	0.44
4:D:10:THR:O	4:D:10:THR:HG23	2.17	0.44
4:D:14:ARG:N	4:D:17:LYS:HZ3	2.15	0.44
7:G:31:LEU:CD2	7:G:48:VAL:HG21	2.46	0.44
7:G:3:PHE:CD1	7:G:80:LYS:NZ	2.83	0.44
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.98	0.44
8:H:95:TYR:HE2	8:H:97:MET:CG	2.30	0.44
1:A:1319:VAL:HG13	1:A:1320:PRO:HD2	1.98	0.44
1:A:1384:VAL:HG12	1:A:1384:VAL:O	2.18	0.44
1:A:219:PHE:CE2	1:A:231:PRO:HD2	2.53	0.44
1:A:871:ASP:OD2	1:A:873:MET:HB2	2.17	0.44
2:B:1002:THR:O	2:B:1004:GLU:N	2.50	0.44
2:B:129:PHE:CE2	2:B:166:PHE:HD1	2.34	0.44
2:B:603:LEU:HB3	2:B:609:ILE:HG13	1.98	0.44
2:B:730:ARG:O	2:B:731:VAL:O	2.35	0.44
2:B:744:HIS:HD2	2:B:746:SER:CB	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:763:GLN:O	2:B:764:SER:C	2.55	0.44
10:J:21:TYR:HB2	10:J:39:LEU:HD13	1.98	0.44
2:B:1006:ILE:HG22	10:J:45:CYS:HB3	1.98	0.44
12:L:40:LEU:HB3	12:L:41:SER:H	1.69	0.44
12:L:61:THR:HG22	12:L:63:ARG:HG2	1.99	0.44
1:A:1013:ASP:O	1:A:1015:VAL:N	2.51	0.44
1:A:1206:ASP:O	1:A:1274:ARG:NH1	2.51	0.44
1:A:418:SER:C	1:A:420:ARG:H	2.21	0.44
1:A:382:PRO:HD3	1:A:428:TYR:CE2	2.51	0.44
1:A:59:GLY:HA2	1:A:67:CYS:SG	2.56	0.44
1:A:774:ARG:NH2	1:A:797:LYS:HB2	2.32	0.44
1:A:806:ARG:HH12	2:B:729:ILE:CD1	2.31	0.44
2:B:258:LEU:O	2:B:258:LEU:HG	2.17	0.44
2:B:259:TYR:N	2:B:259:TYR:CD1	2.85	0.44
2:B:281:PRO:O	2:B:282:ILE:C	2.56	0.44
2:B:806:THR:CG2	2:B:808:ALA:HB3	2.47	0.44
7:G:115:MET:HB3	7:G:163:ILE:HD11	1.99	0.44
2:B:1076:HIS:CD2	11:K:40:HIS:CE1	3.05	0.44
11:K:89:ASN:O	11:K:92:ASN:N	2.50	0.44
1:A:1197:LEU:HD12	1:A:1209:MET:HE1	1.98	0.44
1:A:1208:THR:O	1:A:1209:MET:C	2.55	0.44
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.33	0.44
1:A:1291:VAL:HG13	1:A:1292:PRO:N	2.33	0.44
1:A:577:ILE:C	1:A:579:SER:N	2.68	0.44
1:A:61:ILE:HG22	1:A:62:ASP:N	2.28	0.44
1:A:821:ARG:HD2	1:A:825:ILE:HD11	1.98	0.44
2:B:1016:ALA:O	2:B:1020:ARG:HG3	2.18	0.44
4:D:35:LEU:HD13	4:D:173:HIS:ND1	2.33	0.44
11:K:103:THR:O	11:K:105:PHE:N	2.51	0.44
11:K:49:GLU:OE2	11:K:97:LYS:HE3	2.18	0.44
1:A:1265:ASN:C	1:A:1267:MET:H	2.21	0.44
1:A:12:ARG:NE	2:B:1192:TYR:HE2	2.14	0.44
1:A:335:ARG:CA	1:A:339:ASN:HD22	2.31	0.44
2:B:184:ALA:HB1	2:B:188:ASP:HB3	1.98	0.44
2:B:189:LEU:O	2:B:190:TYR:C	2.55	0.44
2:B:265:SER:O	2:B:266:ALA:CB	2.65	0.44
2:B:336:ARG:NH2	2:B:345:LYS:CG	2.73	0.44
2:B:343:ILE:HG21	2:B:348:ARG:CA	2.46	0.44
2:B:344:LYS:O	2:B:345:LYS:CG	2.65	0.44
2:B:549:THR:N	2:B:628:THR:HG23	2.31	0.44
2:B:899:ILE:O	2:B:952:VAL:HG21	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:167:HIS:HA	11:K:6:ARG:NH1	2.32	0.44
4:D:71:LYS:HA	4:D:74:GLN:CB	2.44	0.44
5:E:207:ARG:HB3	5:E:207:ARG:HH11	1.83	0.44
5:E:55:ARG:HD2	5:E:83:CYS:O	2.18	0.44
8:H:56:THR:HB	8:H:145:ARG:CG	2.42	0.44
11:K:89:ASN:O	11:K:91:CYS:N	2.51	0.44
2:B:230:ALA:N	2:B:231:PRO:CD	2.80	0.44
3:C:189:THR:CG2	3:C:190:ASP:N	2.80	0.44
3:C:177:GLU:HG3	3:C:231:ASN:HD22	1.82	0.44
8:H:138:GLU:O	8:H:139:ASN:C	2.55	0.44
1:A:371:ALA:O	1:A:435:HIS:HB3	2.18	0.44
1:A:601:LYS:HB2	1:A:603:ASN:HD21	1.83	0.44
1:A:936:LEU:O	1:A:939:ASP:HB2	2.17	0.44
2:B:1110:PRO:HG3	2:B:1125:ASP:HB3	2.00	0.44
2:B:185:THR:N	2:B:188:ASP:HB2	2.29	0.44
2:B:903:VAL:CG1	2:B:904:ARG:N	2.81	0.44
4:D:156:ASP:C	4:D:158:GLU:N	2.71	0.44
5:E:205:SER:O	5:E:206:GLY:C	2.56	0.44
5:E:207:ARG:CB	5:E:207:ARG:NH1	2.81	0.44
6:F:111:LEU:C	6:F:113:GLY:N	2.70	0.44
7:G:83:LYS:HE2	7:G:150:CYS:H	1.83	0.44
7:G:9:LEU:HD12	7:G:10:ASN:N	2.32	0.44
10:J:13:VAL:C	10:J:14:VAL:HG23	2.38	0.44
1:A:1118:VAL:O	1:A:1118:VAL:HG23	2.18	0.44
1:A:1219:THR:HG21	1:A:1271:ILE:HG13	1.99	0.44
1:A:1396:ALA:O	1:A:1398:MET:N	2.51	0.44
1:A:225:ASN:ND2	1:A:227:VAL:H	2.16	0.44
1:A:252:PHE:HB2	1:A:256:GLN:CD	2.38	0.44
1:A:417:TYR:O	1:A:418:SER:C	2.55	0.44
1:A:42:ASP:C	1:A:44:THR:N	2.70	0.44
1:A:606:LEU:HD23	1:A:614:PHE:CE2	2.52	0.44
1:A:697:ALA:C	1:A:699:ALA:H	2.21	0.44
1:A:779:PHE:O	1:A:780:VAL:C	2.55	0.44
1:A:846:GLU:OE1	1:A:1425:SER:OG	2.33	0.44
2:B:1121:GLY:C	2:B:1123:SER:H	2.21	0.44
2:B:287:ARG:NH1	2:B:324:ILE:O	2.51	0.44
1:A:785:PRO:CG	2:B:703:ILE:HD12	2.48	0.44
2:B:711:GLU:H	2:B:712:PRO:HD2	1.82	0.44
2:B:871:THR:HG22	2:B:872:GLU:N	2.32	0.44
2:B:977:GLY:HA3	2:B:1099:VAL:HB	2.00	0.44
2:B:986:GLN:HA	2:B:986:GLN:OE1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:235:VAL:HG13	10:J:13:VAL:HG23	1.99	0.44
3:C:255:VAL:HG12	11:K:91:CYS:HB3	2.00	0.44
4:D:29:LEU:HD22	7:G:82:PHE:CD2	2.53	0.44
4:D:64:VAL:O	4:D:66:ARG:N	2.51	0.44
7:G:115:MET:CB	7:G:116:PRO:CD	2.96	0.44
10:J:32:GLU:O	10:J:35:ALA:N	2.51	0.44
11:K:56:VAL:HG22	11:K:77:THR:HG22	2.00	0.44
1:A:1222:ASN:O	1:A:1223:ASP:HB3	2.17	0.44
1:A:349:ALA:HB2	2:B:1105:ALA:HA	1.98	0.44
1:A:367:PRO:O	1:A:368:LYS:C	2.57	0.44
1:A:809:THR:O	1:A:810:PRO:C	2.56	0.44
1:A:960:ILE:O	1:A:961:ARG:C	2.55	0.44
2:B:1010:LEU:HA	2:B:1010:LEU:HD12	1.81	0.44
2:B:1152:MET:CE	2:B:1157:ALA:HA	2.47	0.44
2:B:247:GLY:O	2:B:249:ARG:N	2.50	0.44
2:B:337:ARG:C	2:B:338:GLY:HA2	2.39	0.44
2:B:472:ALA:C	2:B:474:SER:H	2.19	0.44
2:B:591:ARG:O	2:B:592:ASN:C	2.56	0.44
2:B:710:LEU:O	2:B:711:GLU:OE2	2.35	0.44
2:B:806:THR:HG22	2:B:808:ALA:HB3	1.99	0.44
3:C:86:CYS:O	3:C:88:CYS:N	2.51	0.44
5:E:73:PRO:O	5:E:75:MET:N	2.46	0.44
8:H:26:ILE:CG2	8:H:27:GLU:N	2.81	0.44
8:H:59:ILE:CG2	8:H:60:ALA:N	2.66	0.44
1:A:1116:LEU:N	1:A:1308:THR:CG2	2.74	0.43
1:A:1313:LEU:HB3	1:A:1338:VAL:HG21	1.99	0.43
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.98	0.43
1:A:442:VAL:CG2	1:A:460:VAL:HG23	2.48	0.43
1:A:853:ASP:O	1:A:854:ASN:CB	2.65	0.43
1:A:976:THR:HG23	8:H:136:LYS:NZ	2.33	0.43
2:B:1030:LEU:HA	2:B:1030:LEU:HD12	1.88	0.43
2:B:167:ILE:HG22	2:B:453:ILE:CD1	2.47	0.43
2:B:276:ILE:HD13	2:B:334:ILE:HG23	2.00	0.43
2:B:388:CYS:O	2:B:391:ASP:N	2.42	0.43
2:B:412:LEU:HB3	2:B:466:TRP:HZ2	1.83	0.43
2:B:575:PRO:HG2	2:B:576:ASP:H	1.83	0.43
2:B:707:PRO:O	2:B:711:GLU:HG3	2.17	0.43
2:B:97:VAL:HG12	2:B:178:ASN:ND2	2.33	0.43
3:C:256:ALA:O	3:C:259:LEU:N	2.51	0.43
2:B:1001:PHE:HD2	3:C:34:ARG:NH2	2.15	0.43
1:A:1305:VAL:HG12	1:A:1306:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.54	0.43
1:A:353:ILE:CD1	1:A:487:MET:HE2	2.48	0.43
1:A:463:ILE:HB	1:A:464:PRO:CD	2.46	0.43
1:A:57:ARG:O	1:A:68:GLN:CG	2.64	0.43
1:A:763:ALA:C	1:A:803:SER:HB3	2.39	0.43
1:A:845:LEU:O	1:A:846:GLU:C	2.55	0.43
1:A:886:ILE:CG2	1:A:887:GLY:N	2.67	0.43
2:B:1162:ILE:C	2:B:1171:VAL:HG21	2.38	0.43
2:B:469:GLN:HB2	2:B:470:LYS:H	1.41	0.43
2:B:996:ARG:HH21	3:C:175:ALA:HA	1.82	0.43
3:C:20:PHE:HE1	3:C:22:LEU:HD12	1.83	0.43
9:I:85:PHE:N	9:I:85:PHE:HD2	1.99	0.43
11:K:82:ASP:O	11:K:85:ASP:HB2	2.18	0.43
1:A:1329:THR:CG2	1:A:1331:SER:HB3	2.48	0.43
1:A:289:ILE:C	1:A:291:GLU:N	2.71	0.43
1:A:35:ILE:HB	1:A:83:HIS:O	2.18	0.43
1:A:49:LYS:NZ	1:A:61:ILE:CG1	2.76	0.43
1:A:567:LYS:HG3	1:A:568:PRO:CD	2.45	0.43
1:A:569:LYS:O	1:A:571:LEU:HD13	2.17	0.43
1:A:738:LYS:HB2	1:A:740:LEU:HG	1.99	0.43
1:A:874:ASP:O	1:A:876:ALA:N	2.52	0.43
2:B:1151:LEU:N	2:B:1151:LEU:HD12	2.33	0.43
2:B:426:LYS:O	2:B:426:LYS:HG3	2.18	0.43
2:B:376:PHE:O	2:B:586:TRP:HZ3	2.00	0.43
3:C:141:GLY:HA2	10:J:16:ASP:HB3	2.00	0.43
3:C:45:ALA:O	3:C:159:ALA:HA	2.18	0.43
5:E:48:ASP:CG	5:E:49:SER:N	2.70	0.43
1:A:358:ASN:HD22	11:K:66:PRO:HD2	1.83	0.43
12:L:55:ILE:HG12	12:L:55:ILE:H	1.35	0.43
1:A:106:VAL:HA	1:A:114:LEU:HD21	2.01	0.43
1:A:116:ASP:C	1:A:118:HIS:H	2.22	0.43
1:A:1209:MET:HE1	1:A:1236:LEU:HB3	2.00	0.43
1:A:188:ASP:OD1	1:A:189:ARG:N	2.51	0.43
1:A:283:GLY:O	1:A:285:PRO:CD	2.66	0.43
1:A:2:VAL:HG13	2:B:1195:HIS:CE1	2.53	0.43
1:A:420:ARG:O	1:A:421:ALA:C	2.56	0.43
1:A:608:ILE:HG13	1:A:613:ILE:HD12	1.99	0.43
1:A:723:ASN:C	1:A:725:ALA:N	2.72	0.43
1:A:967:ALA:O	1:A:968:GLN:O	2.37	0.43
2:B:1031:LEU:HD13	2:B:1055:ILE:HD11	2.01	0.43
2:B:1189:ILE:HG22	2:B:1190:ASP:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:434:ARG:HA	2:B:437:GLU:OE2	2.18	0.43
2:B:582:VAL:HA	2:B:626:ILE:O	2.18	0.43
2:B:969:ARG:HD2	3:C:61:GLU:OE2	2.18	0.43
3:C:66:ARG:CZ	10:J:2:ILE:CG2	2.95	0.43
4:D:137:ASN:C	4:D:137:ASN:HD22	2.21	0.43
6:F:89:GLU:HB3	6:F:134:ILE:HD13	2.01	0.43
7:G:13:LEU:HD22	7:G:14:HIS:O	2.18	0.43
7:G:18:PHE:HZ	7:G:68:ALA:HB2	1.83	0.43
1:A:1067:LEU:CD1	1:A:1067:LEU:C	2.87	0.43
1:A:1073:GLY:O	1:A:1076:ALA:HB3	2.19	0.43
1:A:1114:PRO:HB2	1:A:1311:VAL:HG23	1.99	0.43
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.18	0.43
1:A:408:ASP:C	1:A:410:GLY:H	2.22	0.43
1:A:441:PRO:HD2	1:A:498:ARG:CZ	2.48	0.43
1:A:575:LYS:HB3	1:A:612:ILE:CG2	2.48	0.43
2:B:1040:ASN:O	2:B:1041:GLU:C	2.55	0.43
2:B:221:ASN:OD1	2:B:242:SER:HA	2.17	0.43
2:B:361:LEU:HD21	2:B:377:PHE:HD2	1.76	0.43
2:B:386:LEU:O	2:B:387:LEU:C	2.57	0.43
3:C:70:ILE:O	3:C:70:ILE:HG22	2.18	0.43
4:D:134:THR:CG2	4:D:135:GLY:H	2.30	0.43
5:E:23:VAL:HG13	5:E:78:LEU:HD13	2.00	0.43
1:A:1215:ARG:HA	1:A:1215:ARG:HD2	1.69	0.43
1:A:34:LYS:N	1:A:34:LYS:HD3	2.33	0.43
1:A:478:TYR:O	1:A:479:ASN:HB3	2.19	0.43
1:A:645:LEU:O	1:A:646:PHE:C	2.54	0.43
1:A:709:THR:HG21	9:I:93:LYS:O	2.18	0.43
2:B:766:ARG:HH22	2:B:1020:ARG:HH11	1.67	0.43
2:B:1130:PHE:HZ	2:B:1138:MET:HG2	1.82	0.43
2:B:642:ASP:HB3	2:B:649:LYS:CE	2.48	0.43
2:B:843:GLN:NE2	2:B:847:ASP:OD1	2.49	0.43
2:B:911:ILE:CD1	2:B:941:LEU:HD13	2.40	0.43
3:C:242:GLN:C	3:C:244:VAL:H	2.20	0.43
3:C:74:SER:HB2	3:C:77:ILE:CG1	2.48	0.43
3:C:80:LEU:O	3:C:80:LEU:HG	2.17	0.43
4:D:119:ARG:HG2	4:D:120:GLU:N	2.33	0.43
7:G:106:MET:CG	7:G:107:LYS:N	2.80	0.43
7:G:62:LEU:HA	7:G:62:LEU:HD23	1.83	0.43
8:H:95:TYR:CE2	8:H:97:MET:CG	3.02	0.43
11:K:65:HIS:NE2	11:K:67:PHE:CG	2.86	0.43
14:T:25:DT:H2''	14:T:26:DC:C5'	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:885:THR:O	1:A:885:THR:HG22	2.18	0.43
2:B:839:MET:HB3	2:B:1012:ILE:HG22	2.00	0.43
2:B:778:MET:HE2	2:B:1094:ARG:CG	2.48	0.43
2:B:1162:ILE:HG23	2:B:1168:LEU:O	2.18	0.43
2:B:224:GLN:HA	2:B:396:ASP:OD2	2.18	0.43
2:B:400:HIS:O	2:B:402:GLY:N	2.52	0.43
2:B:560:GLU:O	2:B:561:TRP:CD1	2.72	0.43
2:B:604:ARG:NH2	2:B:613:VAL:O	2.52	0.43
3:C:179:GLU:O	3:C:180:TYR:HB3	2.19	0.43
3:C:238:ILE:HG22	3:C:243:VAL:HG23	2.01	0.43
3:C:259:LEU:CD1	11:K:91:CYS:HB2	2.49	0.43
4:D:47:LEU:CD1	4:D:48:ILE:N	2.81	0.43
5:E:153:HIS:O	5:E:154:ILE:CG1	2.67	0.43
7:G:126:ASN:HA	7:G:126:ASN:HD22	1.64	0.43
7:G:15:PRO:O	7:G:16:SER:C	2.56	0.43
11:K:103:THR:C	11:K:105:PHE:H	2.20	0.43
11:K:18:LYS:NZ	11:K:38:GLU:HG2	2.33	0.43
1:A:1362:TYR:HD1	1:A:1363:VAL:N	2.16	0.43
1:A:1428:VAL:HG13	2:B:1151:LEU:CD2	2.49	0.43
1:A:381:THR:HG22	1:A:383:TYR:H	1.83	0.43
1:A:47:ARG:O	1:A:48:ALA:HB2	2.19	0.43
1:A:574:GLY:O	1:A:575:LYS:C	2.57	0.43
1:A:590:ARG:NH2	1:A:620:LYS:CB	2.73	0.43
2:B:1007:VAL:HG22	2:B:1008:PRO:CD	2.45	0.43
2:B:129:PHE:HA	2:B:165:VAL:O	2.19	0.43
2:B:552:MET:C	2:B:554:ILE:H	2.21	0.43
2:B:95:ILE:HG13	2:B:130:VAL:HG22	2.01	0.43
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.99	0.43
3:C:41:ILE:HA	3:C:42:PRO:HD3	1.73	0.43
4:D:122:GLU:HA	4:D:125:SER:OG	2.18	0.43
4:D:35:LEU:HD13	4:D:174:PRO:HD2	2.01	0.43
6:F:143:PHE:HD1	6:F:143:PHE:C	2.21	0.43
11:K:31:VAL:O	11:K:74:ARG:HA	2.19	0.43
12:L:30:ILE:HG22	12:L:31:CYS:N	2.33	0.43
12:L:31:CYS:HB3	12:L:34:CYS:C	2.39	0.43
13:P:9:G:C2	14:T:21:DC:O2	2.72	0.43
1:A:1121:GLU:O	1:A:1122:PRO:C	2.56	0.43
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.99	0.43
1:A:262:LEU:C	1:A:264:PHE:H	2.21	0.43
1:A:320:ARG:HH21	1:A:323:LYS:NZ	2.17	0.43
1:A:49:LYS:HZ1	1:A:61:ILE:CG1	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:PRO:HG2	1:A:521:MET:HG2	1.99	0.43
2:B:175:ARG:NH1	2:B:175:ARG:HG2	2.31	0.43
2:B:311:LEU:O	2:B:312:GLU:C	2.57	0.43
2:B:337:ARG:HA	2:B:337:ARG:HD2	1.80	0.43
2:B:343:ILE:CG2	2:B:348:ARG:H	2.32	0.43
2:B:370:PHE:HE2	2:B:373:ARG:NH1	2.17	0.43
2:B:383:ASN:O	2:B:384:ARG:C	2.57	0.43
3:C:124:LEU:CD2	3:C:129:ILE:HG22	2.48	0.43
3:C:20:PHE:CE1	3:C:22:LEU:HD12	2.54	0.43
3:C:229:TYR:CD1	3:C:229:TYR:N	2.86	0.43
4:D:141:LEU:HA	4:D:141:LEU:HD12	1.76	0.43
4:D:46:GLU:C	4:D:47:LEU:O	2.57	0.43
7:G:132:SER:OG	7:G:133:SER:N	2.51	0.43
7:G:26:LEU:O	7:G:29:LYS:N	2.52	0.43
4:D:23:ASN:O	7:G:83:LYS:HB2	2.19	0.43
1:A:1394:THR:CG2	1:A:1398:MET:SD	3.00	0.43
1:A:1450:LEU:O	1:A:1450:LEU:CG	2.65	0.43
1:A:481:ASP:OD1	1:A:483:ASP:CG	2.57	0.43
2:B:1115:THR:HG22	2:B:1117:GLN:N	2.34	0.43
2:B:1156:ASP:HB3	2:B:1197:PRO:HA	1.99	0.43
2:B:1198:TYR:CD2	2:B:1198:TYR:C	2.92	0.43
2:B:642:ASP:HB3	2:B:649:LYS:HE3	2.00	0.43
2:B:683:SER:C	2:B:685:LEU:N	2.72	0.43
6:F:82:THR:HA	6:F:83:PRO:HD3	1.80	0.43
9:I:58:VAL:HG12	9:I:58:VAL:O	2.18	0.43
1:A:873:MET:C	1:A:1058:VAL:CG2	2.88	0.42
1:A:1225:PHE:HE2	1:A:1227:ILE:HD11	1.84	0.42
1:A:1323:ASP:O	1:A:1325:THR:N	2.52	0.42
1:A:172:PRO:HD3	1:A:185:TRP:NE1	2.34	0.42
1:A:452:LYS:HB3	1:A:452:LYS:HE2	1.77	0.42
1:A:685:GLU:HG3	1:A:686:ALA:N	2.33	0.42
1:A:804:TYR:HH	1:A:816:HIS:HE2	1.65	0.42
1:A:867:ILE:N	1:A:867:ILE:HD12	2.34	0.42
1:A:901:LEU:HD22	1:A:919:ILE:HG22	2.01	0.42
1:A:901:LEU:CG	1:A:926:GLN:HE21	2.25	0.42
2:B:899:ILE:CG2	2:B:903:VAL:HB	2.49	0.42
2:B:980:PHE:HD2	2:B:1094:ARG:HA	1.83	0.42
3:C:3:GLU:O	3:C:4:GLU:CG	2.67	0.42
7:G:80:LYS:O	7:G:82:PHE:CE1	2.72	0.42
10:J:34:THR:O	10:J:35:ALA:C	2.57	0.42
12:L:27:LEU:HD23	12:L:27:LEU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:THR:HA	1:A:563:PRO:HD3	1.87	0.42
1:A:826:ASP:HB2	1:A:830:LYS:HD3	2.00	0.42
1:A:89:PRO:C	1:A:204:THR:HG21	2.39	0.42
1:A:919:ILE:O	1:A:920:LEU:C	2.57	0.42
2:B:1060:ARG:C	2:B:1062:HIS:H	2.21	0.42
2:B:234:ILE:O	2:B:261:ARG:CZ	2.67	0.42
2:B:446:LEU:N	2:B:446:LEU:HD23	2.34	0.42
5:E:14:ARG:O	5:E:17:ARG:HB3	2.19	0.42
4:D:47:LEU:CD1	7:G:3:PHE:HD2	2.27	0.42
7:G:4:ILE:HG22	7:G:4:ILE:O	2.20	0.42
8:H:11:GLN:O	8:H:28:ALA:HB1	2.18	0.42
9:I:61:ASP:C	9:I:63:GLY:N	2.71	0.42
10:J:36:LEU:HA	10:J:39:LEU:HD12	2.01	0.42
1:A:1010:ALA:O	1:A:1013:ASP:HB2	2.19	0.42
1:A:1013:ASP:C	1:A:1015:VAL:H	2.22	0.42
1:A:1146:VAL:HG11	1:A:1207:LEU:HD12	2.01	0.42
1:A:1385:THR:C	1:A:1387:HIS:H	2.22	0.42
1:A:224:PHE:CD2	1:A:231:PRO:HG3	2.53	0.42
1:A:325:ILE:O	1:A:326:ARG:C	2.57	0.42
1:A:381:THR:HG22	1:A:383:TYR:N	2.34	0.42
1:A:603:ASN:O	1:A:604:GLY:O	2.37	0.42
1:A:49:LYS:HZ2	1:A:60:SER:HA	1.84	0.42
1:A:639:PRO:CG	1:A:640:GLN:H	2.32	0.42
1:A:646:PHE:O	1:A:647:GLY:C	2.57	0.42
1:A:932:GLU:O	1:A:935:GLN:HB3	2.19	0.42
2:B:1159:ARG:HD2	2:B:1159:ARG:C	2.39	0.42
2:B:1177:HIS:CB	2:B:1179:GLN:HE21	2.32	0.42
2:B:1197:PRO:O	2:B:1200:ALA:N	2.52	0.42
2:B:1216:LEU:N	2:B:1216:LEU:HD23	2.34	0.42
2:B:498:THR:HG23	2:B:499:ASN:N	2.33	0.42
2:B:55:VAL:O	2:B:56:ASP:C	2.58	0.42
3:C:74:SER:HB2	3:C:77:ILE:HG12	2.00	0.42
4:D:153:ARG:C	4:D:154:PHE:CD1	2.92	0.42
9:I:100:PHE:N	9:I:100:PHE:CD1	2.86	0.42
9:I:34:TYR:C	9:I:34:TYR:CD2	2.91	0.42
13:P:5:C:O2'	13:P:6:C:H5'	2.19	0.42
1:A:1074:GLU:C	1:A:1076:ALA:N	2.72	0.42
1:A:1450:LEU:HD21	7:G:18:PHE:O	2.19	0.42
1:A:224:PHE:CE2	1:A:231:PRO:HA	2.54	0.42
1:A:325:ILE:HG21	2:B:1210:MET:CG	2.45	0.42
1:A:388:LEU:HD22	1:A:432:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:THR:HG23	1:A:728:LYS:HE3	2.00	0.42
1:A:7:SER:OG	2:B:1193:GLN:NE2	2.53	0.42
1:A:913:LEU:HG	1:A:915:SER:N	2.34	0.42
1:A:921:GLY:O	1:A:922:ASP:C	2.58	0.42
1:A:902:LEU:CG	1:A:926:GLN:HG3	2.48	0.42
2:B:1085:ILE:HG22	2:B:1086:PHE:N	2.34	0.42
2:B:240:ILE:HG22	2:B:254:LEU:HB3	1.99	0.42
2:B:331:LEU:N	2:B:331:LEU:HD12	2.35	0.42
2:B:39:ARG:CZ	2:B:665:GLU:HG2	2.49	0.42
2:B:983:ARG:HD2	2:B:1091:TYR:CD2	2.50	0.42
3:C:99:LEU:HD12	3:C:118:LEU:HD13	2.01	0.42
7:G:1:MET:HG2	7:G:85:GLU:CD	2.40	0.42
9:I:7:CYS:SG	9:I:8:ARG:O	2.77	0.42
11:K:89:ASN:O	11:K:90:ALA:C	2.57	0.42
1:A:130:ASP:HB3	1:A:133:LYS:HB2	2.00	0.42
1:A:1385:THR:O	1:A:1388:GLY:N	2.51	0.42
1:A:93:VAL:CG1	1:A:301:ALA:HB1	2.39	0.42
1:A:304:MET:SD	2:B:1210:MET:HA	2.60	0.42
1:A:608:ILE:C	1:A:610:GLY:H	2.21	0.42
1:A:61:ILE:CG2	1:A:62:ASP:H	2.24	0.42
1:A:683:ILE:O	1:A:686:ALA:N	2.52	0.42
1:A:901:LEU:N	1:A:926:GLN:NE2	2.57	0.42
2:B:558:LEU:C	2:B:560:GLU:N	2.72	0.42
2:B:750:GLY:O	2:B:751:VAL:C	2.58	0.42
3:C:44:LEU:HD21	3:C:159:ALA:CB	2.50	0.42
8:H:143:LEU:N	8:H:143:LEU:CD1	2.81	0.42
1:A:1115:SER:OG	1:A:1116:LEU:N	2.52	0.42
1:A:1443:VAL:O	1:A:1444:MET:HG3	2.20	0.42
1:A:409:SER:O	1:A:410:GLY:C	2.58	0.42
1:A:442:VAL:HG21	1:A:460:VAL:HG23	2.02	0.42
1:A:444:PHE:HB3	1:A:458:HIS:HD2	1.79	0.42
1:A:516:SER:O	1:A:518:LYS:N	2.53	0.42
1:A:901:LEU:HA	1:A:907:THR:OG1	2.20	0.42
1:A:964:ILE:O	1:A:967:ALA:N	2.53	0.42
2:B:294:ASP:C	2:B:296:GLU:H	2.22	0.42
2:B:597:MET:C	2:B:599:THR:H	2.21	0.42
3:C:46:ILE:HG23	3:C:157:CYS:HB3	2.01	0.42
3:C:191:TYR:CD2	3:C:201:TRP:CD1	3.07	0.42
3:C:236:GLY:O	3:C:238:ILE:N	2.52	0.42
12:L:43:THR:C	12:L:45:ALA:H	2.23	0.42
1:A:1402:PHE:CD1	1:A:1403:GLU:HG3	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1430:LEU:HB2	1:A:1432:GLN:HG3	2.02	0.42
1:A:172:PRO:HG3	1:A:185:TRP:CZ2	2.54	0.42
1:A:347:PHE:CE2	1:A:493:GLN:OE1	2.72	0.42
2:B:1167:GLY:H	2:B:1217:TYR:HE1	1.68	0.42
2:B:43:LEU:HD13	2:B:812:LEU:HD23	2.02	0.42
2:B:460:ALA:HB1	2:B:466:TRP:CZ3	2.55	0.42
2:B:820:GLY:N	2:B:1091:TYR:OH	2.52	0.42
3:C:259:LEU:HD13	11:K:91:CYS:HB2	2.02	0.42
4:D:7:THR:HB	7:G:42:PHE:CZ	2.55	0.42
5:E:136:ASN:OD1	5:E:137:GLU:N	2.53	0.42
1:A:857:ARG:NH1	6:F:139:PRO:HB2	2.35	0.42
8:H:4:THR:HG22	8:H:5:LEU:H	1.85	0.42
9:I:56:ALA:O	9:I:57:GLY:C	2.57	0.42
1:A:1009:ASN:O	1:A:1013:ASP:OD2	2.38	0.42
1:A:1157:ASP:C	1:A:1159:ARG:H	2.23	0.42
1:A:54:ASN:HB3	1:A:247:ARG:HH22	1.85	0.42
1:A:606:LEU:CD2	1:A:614:PHE:HE2	2.32	0.42
1:A:863:VAL:HG11	1:A:866:PHE:CE2	2.55	0.42
2:B:996:ARG:HG2	2:B:1007:VAL:HG11	2.01	0.42
2:B:1178:ASN:O	2:B:1180:PHE:CD1	2.73	0.42
2:B:263:GLY:O	2:B:264:SER:C	2.57	0.42
2:B:33:VAL:O	2:B:36:ALA:HB3	2.20	0.42
2:B:45:SER:O	2:B:46:GLN:C	2.57	0.42
2:B:37:PHE:CD2	2:B:542:MET:SD	3.12	0.42
2:B:763:GLN:O	2:B:766:ARG:N	2.51	0.42
2:B:885:MET:HB3	2:B:886:LYS:H	1.67	0.42
3:C:88:CYS:SG	3:C:91:HIS:CA	3.07	0.42
5:E:88:VAL:HG12	5:E:89:GLY:N	2.34	0.42
1:A:1027:ALA:O	1:A:1028:THR:C	2.58	0.42
1:A:860:LEU:HD11	1:A:1393:ASN:HB2	2.01	0.42
1:A:224:PHE:CE2	1:A:231:PRO:HG3	2.54	0.42
1:A:399:HIS:O	1:A:400:PRO:C	2.56	0.42
2:B:710:LEU:C	2:B:711:GLU:HG2	2.40	0.42
2:B:945:GLU:O	2:B:946:ASN:HB3	2.19	0.42
3:C:112:ASN:CB	3:C:114:TYR:CE1	3.03	0.42
4:D:118:THR:O	4:D:118:THR:HG22	2.20	0.42
5:E:168:TYR:HB3	5:E:170:LEU:HG	2.00	0.42
5:E:207:ARG:HB2	5:E:207:ARG:NH1	2.34	0.42
5:E:35:VAL:O	5:E:37:LEU:N	2.52	0.42
1:A:1134:ILE:HB	1:A:1306:LEU:HD11	2.01	0.42
1:A:35:ILE:HD12	1:A:241:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ARG:HG2	1:A:430:TRP:CZ3	2.55	0.42
1:A:416:ARG:O	1:A:417:TYR:CD2	2.69	0.42
1:A:507:VAL:N	1:A:508:PRO:CD	2.82	0.42
1:A:761:MET:HA	1:A:804:TYR:HB2	2.01	0.42
2:B:1074:ASN:HB2	2:B:1081:LEU:HD21	2.01	0.42
2:B:118:ARG:CG	2:B:204:ILE:HD13	2.50	0.42
2:B:230:ALA:N	2:B:231:PRO:HD2	2.34	0.42
2:B:603:LEU:HA	2:B:603:LEU:HD22	1.89	0.42
2:B:765:PRO:O	2:B:768:THR:N	2.53	0.42
2:B:846:ILE:HG23	2:B:974:PRO:HG2	2.01	0.42
3:C:193:TYR:HD2	3:C:197:SER:HB3	1.85	0.42
4:D:33:PHE:CZ	7:G:80:LYS:HE3	2.55	0.42
7:G:1:MET:HE3	7:G:80:LYS:C	2.40	0.42
3:C:35:ARG:NH1	11:K:41:THR:OG1	2.53	0.42
1:A:1070:GLN:O	1:A:1071:SER:C	2.56	0.41
1:A:250:ILE:HG22	1:A:250:ILE:O	2.19	0.41
1:A:42:ASP:OD1	1:A:45:GLN:O	2.38	0.41
1:A:464:PRO:O	1:A:465:TYR:O	2.38	0.41
1:A:816:HIS:CD2	2:B:764:SER:H	2.37	0.41
1:A:341:MET:HE1	2:B:1135:ARG:NH1	2.34	0.41
2:B:223:VAL:HG12	2:B:381:MET:HG2	2.02	0.41
4:D:190:GLU:O	4:D:194:LEU:HG	2.21	0.41
5:E:153:HIS:C	5:E:154:ILE:HG13	2.40	0.41
6:F:90:ARG:HD3	6:F:155:LEU:HD12	2.02	0.41
7:G:73:LYS:HE2	7:G:74:TYR:O	2.20	0.41
8:H:99:GLY:HA3	8:H:117:SER:O	2.20	0.41
3:C:84:ARG:NE	11:K:11:LEU:HD11	2.35	0.41
14:T:19:DT:H2'	14:T:20:DC:H6	1.81	0.41
1:A:1205:LYS:O	1:A:1206:ASP:C	2.57	0.41
1:A:1299:VAL:HG12	1:A:1300:LYS:H	1.84	0.41
1:A:299:HIS:C	1:A:301:ALA:H	2.24	0.41
1:A:33:ALA:HA	1:A:57:ARG:HH21	1.85	0.41
1:A:351:THR:O	1:A:486:GLU:HA	2.21	0.41
1:A:358:ASN:ND2	11:K:66:PRO:HD2	2.35	0.41
1:A:391:LEU:O	1:A:394:ASN:HB2	2.19	0.41
1:A:416:ARG:C	1:A:417:TYR:CD2	2.94	0.41
1:A:469:ARG:NH2	2:B:991:GLY:O	2.53	0.41
1:A:842:VAL:HG12	1:A:843:LYS:N	2.34	0.41
2:B:283:VAL:O	2:B:286:PHE:N	2.54	0.41
2:B:431:TYR:CE2	2:B:447:ALA:HB2	2.54	0.41
2:B:641:GLU:OE1	2:B:641:GLU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:859:TYR:CD1	2:B:859:TYR:N	2.89	0.41
2:B:889:THR:HG22	2:B:891:ASP:HB2	2.02	0.41
3:C:116:LYS:HD3	3:C:140:ASN:HB3	2.01	0.41
3:C:124:LEU:HD22	3:C:129:ILE:HG22	2.01	0.41
4:D:63:LEU:HA	4:D:63:LEU:HD22	1.77	0.41
6:F:147:SER:OG	6:F:150:GLU:HG3	2.20	0.41
6:F:88:TYR:N	6:F:88:TYR:CD1	2.88	0.41
7:G:13:LEU:HD21	7:G:17:PHE:CB	2.28	0.41
8:H:89:LEU:C	8:H:91:ASP:N	2.73	0.41
12:L:43:THR:O	12:L:43:THR:HG22	2.20	0.41
1:A:1096:SER:O	1:A:1100:ARG:CB	2.68	0.41
1:A:119:ASN:O	1:A:122:MET:HB3	2.19	0.41
1:A:1260:LEU:O	1:A:1260:LEU:HG	2.20	0.41
1:A:1336:MET:CE	1:A:1381:LEU:HG	2.50	0.41
1:A:23:SER:HB2	1:A:233:TRP:HE1	1.85	0.41
1:A:270:LEU:O	1:A:271:LYS:C	2.58	0.41
1:A:695:LYS:C	1:A:697:ALA:H	2.22	0.41
2:B:1202:LEU:HD23	2:B:1206:GLU:HG3	2.02	0.41
2:B:336:ARG:CD	2:B:348:ARG:HD3	2.50	0.41
2:B:552:MET:O	2:B:554:ILE:N	2.53	0.41
2:B:635:ARG:HG3	2:B:635:ARG:NH1	2.35	0.41
3:C:263:THR:C	3:C:265:MET:N	2.74	0.41
5:E:114:ASN:HD22	5:E:114:ASN:HA	1.66	0.41
5:E:42:PHE:O	5:E:43:LYS:C	2.58	0.41
5:E:58:MET:O	5:E:59:SER:O	2.38	0.41
11:K:52:ASN:O	11:K:53:ASP:C	2.58	0.41
14:T:21:DC:C5	14:T:22:BRU:BR	3.28	0.41
1:A:1409:LEU:HA	1:A:1409:LEU:HD23	1.93	0.41
1:A:1447:GLU:OE1	1:A:1447:GLU:C	2.59	0.41
1:A:344:ARG:C	1:A:345:VAL:CG1	2.89	0.41
1:A:536:LEU:O	1:A:537:ARG:C	2.57	0.41
1:A:570:PRO:C	1:A:571:LEU:HD12	2.40	0.41
1:A:672:ASP:O	1:A:673:GLY:C	2.59	0.41
2:B:1197:PRO:O	2:B:1200:ALA:HB3	2.21	0.41
2:B:294:ASP:N	2:B:294:ASP:OD2	2.51	0.41
2:B:510:LYS:HG3	2:B:511:PRO:CD	2.50	0.41
5:E:60:PHE:CE2	5:E:80:VAL:HB	2.55	0.41
7:G:88:ASP:HB3	7:G:144:ARG:HA	2.03	0.41
7:G:87:VAL:HG23	7:G:103:VAL:HG21	2.02	0.41
1:A:1280:GLU:O	1:A:1281:ARG:C	2.58	0.41
1:A:1445:ILE:HG12	7:G:18:PHE:HE2	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:LYS:HB3	1:A:612:ILE:HG21	2.02	0.41
1:A:683:ILE:O	1:A:686:ALA:HB3	2.20	0.41
1:A:711:ARG:NH2	9:I:87:GLN:OE1	2.53	0.41
1:A:839:ARG:O	1:A:842:VAL:HB	2.19	0.41
2:B:758:PHE:HZ	2:B:1031:LEU:HD22	1.86	0.41
2:B:978:ASP:OD2	2:B:1098:MET:HG2	2.20	0.41
2:B:1115:THR:CG2	2:B:1117:GLN:HG3	2.51	0.41
2:B:890:TYR:OH	2:B:936:ASP:OD2	2.33	0.41
3:C:168:ALA:O	3:C:169:LYS:C	2.58	0.41
4:D:167:LEU:O	4:D:170:THR:OG1	2.29	0.41
4:D:191:ALA:O	4:D:193:THR:N	2.54	0.41
4:D:40:HIS:CG	4:D:41:GLN:N	2.89	0.41
4:D:56:ARG:NH2	4:D:57:LEU:HD21	2.36	0.41
5:E:180:ARG:NH2	5:E:192:ARG:HD2	2.35	0.41
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.82	0.41
1:A:1011:GLN:HE22	1:A:1015:VAL:HG21	1.79	0.41
1:A:1243:VAL:CG1	1:A:1244:ARG:N	2.82	0.41
1:A:172:PRO:HB3	1:A:185:TRP:CD2	2.56	0.41
1:A:320:ARG:HA	1:A:321:PRO:HD3	1.89	0.41
2:B:222:ILE:O	2:B:240:ILE:HA	2.20	0.41
2:B:221:ASN:N	2:B:241:ARG:O	2.35	0.41
2:B:382:ILE:HG13	2:B:382:ILE:H	1.67	0.41
2:B:95:ILE:HB	2:B:130:VAL:HG22	2.02	0.41
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.56	0.41
3:C:115:SER:HB3	3:C:142:VAL:HB	2.01	0.41
3:C:31:ASN:O	3:C:34:ARG:N	2.53	0.41
3:C:67:LEU:HD21	3:C:144:ILE:HD13	2.03	0.41
4:D:4:SER:O	4:D:5:THR:CB	2.68	0.41
8:H:12:VAL:HA	8:H:28:ALA:HB2	2.03	0.41
8:H:91:ASP:C	8:H:93:TYR:N	2.71	0.41
10:J:28:ASP:O	10:J:29:GLU:C	2.59	0.41
1:A:1134:ILE:O	1:A:1135:ARG:C	2.58	0.41
1:A:1437:GLY:CA	6:F:88:TYR:CD2	3.03	0.41
1:A:146:MET:HA	1:A:171:GLN:HB2	2.02	0.41
1:A:283:GLY:O	1:A:285:PRO:HD3	2.20	0.41
1:A:310:GLY:O	1:A:312:PRO:HD2	2.21	0.41
1:A:709:THR:HG22	1:A:710:LEU:N	2.35	0.41
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.85	0.41
2:B:1002:THR:HG23	2:B:1006:ILE:HG13	2.02	0.41
2:B:1031:LEU:O	2:B:1034:VAL:HB	2.20	0.41
2:B:185:THR:O	2:B:188:ASP:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:467:GLY:CA	2:B:475:SER:HB3	2.49	0.41
2:B:604:ARG:O	2:B:606:LYS:N	2.53	0.41
2:B:604:ARG:C	2:B:606:LYS:H	2.24	0.41
2:B:618:ASP:O	2:B:619:ILE:C	2.58	0.41
2:B:642:ASP:HB3	2:B:649:LYS:CG	2.51	0.41
2:B:806:THR:C	2:B:808:ALA:N	2.74	0.41
2:B:865:LYS:C	2:B:866:TYR:CD1	2.94	0.41
4:D:210:ILE:O	4:D:214:LEU:HG	2.20	0.41
6:F:128:LYS:HD3	6:F:149:GLU:O	2.20	0.41
7:G:110:VAL:HG22	7:G:161:GLY:O	2.20	0.41
11:K:69:ALA:O	11:K:70:ARG:CB	2.63	0.41
1:A:1151:GLU:HB3	1:A:1153:TYR:HE1	1.86	0.41
1:A:167:CYS:O	1:A:167:CYS:SG	2.78	0.41
1:A:270:LEU:O	1:A:273:ASN:HB3	2.20	0.41
1:A:403:LYS:O	1:A:404:TYR:CD2	2.74	0.41
1:A:630:ILE:O	1:A:631:HIS:C	2.57	0.41
1:A:710:LEU:H	1:A:710:LEU:HD12	1.86	0.41
1:A:711:ARG:O	1:A:714:PHE:N	2.50	0.41
1:A:746:MET:HE3	2:B:1018:PRO:HG2	2.03	0.41
2:B:751:VAL:HG13	2:B:812:LEU:HD22	2.03	0.41
2:B:764:SER:HB3	2:B:765:PRO:CD	2.50	0.41
2:B:865:LYS:HE2	2:B:871:THR:OG1	2.21	0.41
3:C:242:GLN:C	3:C:244:VAL:N	2.74	0.41
3:C:258:ILE:N	3:C:258:ILE:HD12	2.36	0.41
4:D:146:GLN:O	4:D:149:THR:HG22	2.20	0.41
4:D:192:LYS:HB3	4:D:192:LYS:NZ	2.35	0.41
5:E:14:ARG:HH21	5:E:141:VAL:HG12	1.85	0.41
6:F:121:ALA:O	6:F:122:MET:C	2.59	0.41
7:G:35:GLU:CG	7:G:48:VAL:HG23	2.50	0.41
10:J:1:MET:H3	10:J:56:LEU:H	1.67	0.41
12:L:36:SER:O	12:L:37:LYS:C	2.58	0.41
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.42	0.41
1:A:1244:ARG:O	1:A:1245:PRO:O	2.39	0.41
1:A:437:MET:O	1:A:438:ASP:C	2.58	0.41
1:A:354:SER:HA	1:A:482:PHE:CD2	2.55	0.41
1:A:524:VAL:O	1:A:525:GLN:C	2.59	0.41
1:A:58:LEU:CD1	1:A:80:HIS:HB2	2.50	0.41
2:B:95:ILE:CB	2:B:130:VAL:HG22	2.51	0.41
2:B:100:PRO:HD3	2:B:172:ILE:HD12	2.03	0.41
2:B:300:HIS:CE1	2:B:376:PHE:CE1	3.08	0.41
2:B:386:LEU:C	2:B:388:CYS:N	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:814:PHE:O	2:B:816:GLU:N	2.54	0.41
2:B:828:ALA:HB2	2:B:1085:ILE:CG2	2.51	0.41
2:B:948:ILE:HG22	2:B:949:VAL:O	2.20	0.41
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.54	0.41
3:C:265:MET:O	3:C:265:MET:HG2	2.20	0.41
3:C:31:ASN:O	3:C:35:ARG:HG3	2.20	0.41
5:E:114:ASN:O	5:E:115:ASN:CB	2.64	0.41
5:E:153:HIS:O	5:E:154:ILE:HG13	2.20	0.41
5:E:22:MET:CE	5:E:26:ARG:HH21	2.02	0.41
5:E:92:THR:HG22	5:E:92:THR:O	2.20	0.41
6:F:77:ASP:O	6:F:78:GLN:HB2	2.19	0.41
7:G:88:ASP:HA	7:G:144:ARG:HA	2.02	0.41
10:J:52:THR:O	10:J:53:HIS:C	2.58	0.41
11:K:18:LYS:NZ	11:K:37:LYS:O	2.54	0.41
1:A:1064:VAL:HG12	1:A:1064:VAL:O	2.21	0.41
1:A:1265:ASN:O	1:A:1268:LEU:N	2.51	0.41
1:A:1063:MET:SD	1:A:1436:ILE:HG23	2.61	0.41
1:A:370:ILE:O	1:A:371:ALA:C	2.55	0.41
1:A:356:ASP:CB	1:A:469:ARG:NH1	2.80	0.41
1:A:482:PHE:C	1:A:484:GLY:N	2.73	0.41
1:A:719:VAL:O	1:A:721:PHE:N	2.54	0.41
1:A:897:TYR:CD1	1:A:897:TYR:N	2.89	0.41
1:A:343:LYS:NZ	2:B:1151:LEU:O	2.42	0.41
2:B:29:ASP:O	2:B:30:SER:C	2.59	0.41
2:B:314:LEU:O	2:B:317:CYS:HB3	2.20	0.41
2:B:999:MET:HB3	2:B:1007:VAL:HG21	2.02	0.41
5:E:131:THR:HG21	5:E:191:LYS:HZ1	1.85	0.41
5:E:161:LYS:C	5:E:163:GLU:H	2.23	0.41
5:E:167:ARG:HD3	5:E:167:ARG:HA	1.72	0.41
7:G:80:LYS:CD	7:G:80:LYS:N	2.72	0.41
8:H:80:ARG:HA	8:H:81:PRO:HD3	1.68	0.41
9:I:61:ASP:O	9:I:63:GLY:N	2.54	0.41
11:K:63:VAL:O	11:K:63:VAL:CG2	2.68	0.41
14:T:19:DT:H2''	14:T:20:DC:C5'	2.51	0.41
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.20	0.41
1:A:1095:THR:OG1	1:A:1113:THR:HB	2.21	0.41
1:A:282:ASN:HB3	1:A:283:GLY:H	1.78	0.41
1:A:535:THR:HG22	1:A:536:LEU:N	2.34	0.41
1:A:535:THR:HG23	1:A:575:LYS:HE2	2.03	0.41
1:A:666:ILE:HD11	2:B:1086:PHE:CE1	2.56	0.41
1:A:898:ARG:O	1:A:1029:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1124:ARG:C	2:B:1126:GLY:N	2.74	0.41
2:B:96:TYR:HE1	2:B:131:ASP:OD2	2.03	0.41
2:B:213:ILE:HD12	2:B:497:ARG:HB3	2.03	0.41
2:B:39:ARG:NH2	2:B:665:GLU:CG	2.82	0.41
3:C:9:LYS:O	3:C:10:ILE:C	2.59	0.41
4:D:56:ARG:HA	4:D:148:LEU:HD13	2.03	0.41
6:F:92:ARG:O	6:F:93:ILE:C	2.58	0.41
8:H:56:THR:HG21	8:H:145:ARG:HE	1.85	0.41
8:H:15:VAL:HG22	8:H:26:ILE:CG1	2.48	0.41
8:H:6:PHE:O	8:H:58:THR:HA	2.20	0.41
9:I:78:CYS:HB3	9:I:106:CYS:SG	2.60	0.41
9:I:69:PRO:O	9:I:84:VAL:HA	2.21	0.41
10:J:13:VAL:O	10:J:14:VAL:CG2	2.69	0.41
12:L:38:LEU:CD1	12:L:49:LYS:HE2	2.50	0.41
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.51	0.40
1:A:1074:GLU:N	1:A:1075:PRO:HD2	2.36	0.40
1:A:1362:TYR:C	1:A:1362:TYR:CD1	2.92	0.40
1:A:406:ILE:HG13	1:A:431:LYS:CB	2.51	0.40
1:A:416:ARG:HG3	1:A:417:TYR:CE2	2.56	0.40
1:A:653:VAL:O	1:A:654:ASN:C	2.59	0.40
1:A:688:LYS:C	1:A:690:VAL:H	2.24	0.40
1:A:968:GLN:C	1:A:970:THR:H	2.24	0.40
2:B:1040:ASN:O	2:B:1042:GLY:N	2.54	0.40
2:B:1117:GLN:HE21	2:B:1199:ALA:HB2	1.86	0.40
2:B:799:PRO:CB	2:B:818:PRO:HG2	2.51	0.40
4:D:27:LEU:HG	4:D:197:SER:HB2	2.03	0.40
5:E:112:TYR:CE1	5:E:136:ASN:HB2	2.56	0.40
5:E:18:THR:O	5:E:19:VAL:C	2.58	0.40
7:G:20:PRO:HG2	7:G:21:ARG:N	2.36	0.40
8:H:83:GLN:C	8:H:85:GLY:N	2.75	0.40
9:I:90:GLN:HE21	9:I:92:ARG:HD2	1.86	0.40
1:A:1011:GLN:NE2	1:A:1015:VAL:CG2	2.81	0.40
1:A:103:CYS:O	1:A:106:VAL:O	2.39	0.40
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.57	0.40
1:A:70:CYS:SG	1:A:70:CYS:O	2.80	0.40
1:A:73:GLY:O	1:A:75:ASN:N	2.54	0.40
1:A:824:LEU:HD23	1:A:824:LEU:HA	1.88	0.40
2:B:240:ILE:HG21	2:B:381:MET:HE1	2.03	0.40
2:B:419:THR:O	2:B:419:THR:HG22	2.21	0.40
2:B:707:PRO:HG2	2:B:708:GLU:H	1.84	0.40
2:B:911:ILE:O	2:B:912:ILE:CG1	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1065:GLN:HB2	3:C:201:TRP:CZ3	2.55	0.40
3:C:27:LEU:O	3:C:28:ALA:C	2.59	0.40
3:C:5:GLY:HA3	3:C:6:PRO:HD2	1.76	0.40
7:G:1:MET:SD	7:G:79:PHE:CE1	3.14	0.40
7:G:9:LEU:HD23	7:G:30:LEU:HD12	2.03	0.40
1:A:971:PHE:HE2	1:A:1040:GLN:HG2	1.86	0.40
1:A:1213:GLY:O	1:A:1216:ILE:N	2.55	0.40
1:A:23:SER:CA	1:A:233:TRP:NE1	2.84	0.40
1:A:33:ALA:O	1:A:83:HIS:CD2	2.71	0.40
1:A:491:VAL:O	1:A:493:GLN:NE2	2.55	0.40
1:A:50:ILE:HG22	1:A:51:GLY:N	2.36	0.40
1:A:578:LEU:HD23	1:A:612:ILE:CD1	2.51	0.40
1:A:635:ARG:HH11	1:A:635:ARG:HA	1.87	0.40
1:A:78:PRO:HA	2:B:1201:LYS:HZ1	1.85	0.40
1:A:823:GLY:O	1:A:824:LEU:C	2.60	0.40
1:A:898:ARG:HB2	1:A:933:TYR:CE1	2.57	0.40
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.56	0.40
2:B:1050:ILE:HG22	2:B:1051:THR:N	2.36	0.40
2:B:254:LEU:HD23	2:B:381:MET:HE3	2.02	0.40
2:B:368:GLU:O	2:B:370:PHE:N	2.52	0.40
2:B:376:PHE:CE2	2:B:569:TYR:CD2	3.07	0.40
2:B:458:LYS:O	2:B:459:TYR:C	2.59	0.40
2:B:753:ALA:HA	2:B:756:ILE:CD1	2.51	0.40
2:B:763:GLN:C	2:B:765:PRO:HD2	2.41	0.40
3:C:107:SER:C	3:C:109:SER:H	2.24	0.40
4:D:160:VAL:O	4:D:164:ILE:HG13	2.20	0.40
5:E:156:LEU:HD12	5:E:195:VAL:CG1	2.51	0.40
7:G:39:THR:CG2	7:G:40:GLY:N	2.82	0.40
8:H:83:GLN:O	8:H:85:GLY:N	2.53	0.40
12:L:40:LEU:HD22	12:L:44:ASP:CB	2.52	0.40
1:A:1254:ALA:O	1:A:1255:GLU:HB2	2.21	0.40
1:A:1260:LEU:CG	1:A:1260:LEU:O	2.70	0.40
1:A:24:PRO:HD2	1:A:233:TRP:NE1	2.37	0.40
1:A:263:THR:HG22	1:A:263:THR:O	2.20	0.40
1:A:362:ASP:HB3	1:A:508:PRO:CG	2.51	0.40
2:B:1006:ILE:HD13	10:J:44:TYR:CZ	2.55	0.40
1:A:14:VAL:CG2	2:B:1216:LEU:HD13	2.42	0.40
2:B:603:LEU:HD12	2:B:609:ILE:CG1	2.47	0.40
2:B:806:THR:HG22	2:B:808:ALA:CB	2.51	0.40
3:C:262:LEU:HD23	3:C:262:LEU:HA	1.88	0.40
5:E:177:ARG:HG2	5:E:213:ILE:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:85:MET:HE1	6:F:148:VAL:HG12	2.02	0.40
6:F:89:GLU:O	6:F:93:ILE:HG13	2.21	0.40
8:H:99:GLY:N	8:H:118:PHE:CD2	2.90	0.40
8:H:55:LEU:HD22	8:H:144:ILE:HG21	2.01	0.40
9:I:13:MET:O	9:I:14:LEU:HD23	2.21	0.40
11:K:65:HIS:NE2	11:K:67:PHE:CD2	2.85	0.40
1:A:1170:ILE:HG13	1:A:1170:ILE:H	1.53	0.40
1:A:356:ASP:OD1	1:A:358:ASN:HB2	2.21	0.40
1:A:388:LEU:CD2	1:A:432:VAL:HB	2.52	0.40
1:A:396:PRO:HG3	1:A:416:ARG:HB3	2.03	0.40
1:A:41:MET:HB2	1:A:42:ASP:H	1.49	0.40
1:A:688:LYS:C	1:A:690:VAL:N	2.75	0.40
1:A:31:SER:OG	1:A:82:GLY:HA2	2.21	0.40
2:B:552:MET:HA	2:B:555:ILE:HB	2.03	0.40
2:B:693:ILE:HD11	2:B:740:HIS:CD2	2.56	0.40
2:B:744:HIS:CD2	2:B:746:SER:OG	2.69	0.40
2:B:485:ARG:NH2	2:B:782:LEU:HD11	2.37	0.40
2:B:825:VAL:HG21	2:B:1092:TYR:HE1	1.86	0.40
3:C:254:LYS:O	3:C:258:ILE:HD13	2.22	0.40
3:C:80:LEU:HD11	3:C:95:CYS:CA	2.50	0.40
6:F:93:ILE:HD13	6:F:148:VAL:CG1	2.50	0.40
7:G:35:GLU:OE2	7:G:47:CYS:HA	2.21	0.40
9:I:34:TYR:O	9:I:35:VAL:CG2	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1410/1733 (81%)	975 (69%)	289 (20%)	146 (10%)	0	9
2	B	1096/1224 (90%)	781 (71%)	200 (18%)	115 (10%)	0	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	264/318 (83%)	171 (65%)	65 (25%)	28 (11%)	0	8
4	D	173/221 (78%)	124 (72%)	31 (18%)	18 (10%)	0	9
5	E	212/215 (99%)	154 (73%)	44 (21%)	14 (7%)	1	19
6	F	84/155 (54%)	69 (82%)	11 (13%)	4 (5%)	2	24
7	G	169/171 (99%)	131 (78%)	28 (17%)	10 (6%)	1	21
8	H	131/146 (90%)	82 (63%)	32 (24%)	17 (13%)	0	5
9	I	114/122 (93%)	80 (70%)	23 (20%)	11 (10%)	0	10
10	J	63/70 (90%)	37 (59%)	12 (19%)	14 (22%)	0	1
11	K	112/120 (93%)	85 (76%)	16 (14%)	11 (10%)	0	10
12	L	44/70 (63%)	18 (41%)	17 (39%)	9 (20%)	0	2
All	All	3872/4565 (85%)	2707 (70%)	768 (20%)	397 (10%)	0	9

All (397) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	THR
1	A	48	ALA
1	A	57	ARG
1	A	62	ASP
1	A	65	LEU
1	A	74	MET
1	A	93	VAL
1	A	167	CYS
1	A	223	GLY
1	A	255	SER
1	A	286	HIS
1	A	311	GLN
1	A	312	PRO
1	A	318	SER
1	A	322	VAL
1	A	335	ARG
1	A	385	ILE
1	A	423	ASP
1	A	517	ASN
1	A	536	LEU
1	A	567	LYS
1	A	597	LEU
1	A	666	ILE

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Mol	Chain	Res	Type
1	A	789	LYS
1	A	968	GLN
1	A	969	GLN
1	A	986	ILE
1	A	1002	GLY
1	A	1014	ALA
1	A	1036	ARG
1	A	1096	SER
1	A	1115	SER
1	A	1122	PRO
1	A	1223	ASP
1	A	1281	ARG
1	A	1314	SER
1	A	1341	ILE
1	A	1365	TYR
1	A	1378	GLN
1	A	1405	THR
1	A	1438	THR
2	B	45	SER
2	B	46	GLN
2	B	108	VAL
2	B	258	LEU
2	B	282	ILE
2	B	367	LEU
2	B	450	ALA
2	B	466	TRP
2	B	467	GLY
2	B	474	SER
2	B	643	ASP
2	B	708	GLU
2	B	709	ASP
2	B	727	LYS
2	B	731	VAL
2	B	751	VAL
2	B	831	SER
2	B	881	ASN
2	B	943	SER
2	B	958	GLN
2	B	1046	PRO
2	B	1069	PHE
2	B	1097	HIS
2	B	1156	ASP

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Mol	Chain	Res	Type
2	B	1157	ALA
2	B	1167	GLY
2	B	1171	VAL
2	B	1175	LEU
2	B	1178	ASN
2	B	1181	GLU
2	B	1182	CYS
2	B	1183	LYS
2	B	1186	ASP
2	B	1188	LYS
3	C	6	PRO
3	C	78	GLU
3	C	87	PHE
3	C	141	GLY
3	C	149	LYS
3	C	156	THR
3	C	161	LYS
3	C	184	ASN
3	C	209	TYR
3	C	214	ASN
3	C	215	GLU
4	D	5	THR
4	D	8	PHE
4	D	19	GLU
4	D	20	GLU
4	D	52	LEU
4	D	177	VAL
4	D	199	ASN
5	E	3	GLN
5	E	59	SER
5	E	73	PRO
5	E	74	ASP
5	E	106	GLN
5	E	130	ALA
5	E	206	GLY
7	G	63	PRO
7	G	139	ILE
8	H	62	SER
8	H	81	PRO
8	H	82	PRO
8	H	108	SER
8	H	128	ASN

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Mol	Chain	Res	Type
9	I	3	THR
9	I	9	ASP
9	I	11	ASN
9	I	57	GLY
9	I	79	HIS
9	I	106	CYS
10	J	2	ILE
10	J	6	ARG
10	J	27	GLU
10	J	28	ASP
10	J	29	GLU
10	J	32	GLU
10	J	55	ASP
10	J	64	ASN
11	K	7	PHE
11	K	110	ASN
12	L	35	SER
12	L	50	ASP
12	L	59	ALA
12	L	60	ARG
1	A	42	ASP
1	A	54	ASN
1	A	59	GLY
1	A	61	ILE
1	A	66	LYS
1	A	70	CYS
1	A	76	GLU
1	A	154	SER
1	A	219	PHE
1	A	244	PRO
1	A	250	ILE
1	A	253	ASN
1	A	263	THR
1	A	283	GLY
1	A	336	ILE
1	A	394	ASN
1	A	465	TYR
1	A	543	LEU
1	A	604	GLY
1	A	626	ASN
1	A	649	ILE
1	A	661	GLY

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Mol	Chain	Res	Type
1	A	753	GLY
1	A	780	VAL
1	A	825	ILE
1	A	847	ASP
1	A	875	ALA
1	A	1054	LEU
1	A	1114	PRO
1	A	1116	LEU
1	A	1212	VAL
1	A	1335	ILE
1	A	1366	ARG
1	A	1377	THR
1	A	1386	ARG
1	A	1389	PHE
1	A	1397	LEU
2	B	28	GLU
2	B	48	LEU
2	B	115	GLN
2	B	186	GLU
2	B	260	GLY
2	B	266	ALA
2	B	322	PHE
2	B	345	LYS
2	B	369	GLY
2	B	387	LEU
2	B	401	PHE
2	B	513	GLN
2	B	591	ARG
2	B	605	ARG
2	B	619	ILE
2	B	641	GLU
2	B	655	LYS
2	B	764	SER
2	B	792	MET
2	B	869	SER
2	B	907	GLY
2	B	909	ASP
2	B	1017	ILE
2	B	1018	PRO
2	B	1065	GLN
2	B	1100	ASP
2	B	1108	ARG

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Mol	Chain	Res	Type
2	B	1155	SER
3	C	4	GLU
3	C	81	GLU
3	C	110	THR
3	C	175	ALA
3	C	213	PRO
3	C	216	GLY
4	D	21	GLU
4	D	53	SER
4	D	131	GLU
4	D	192	LYS
5	E	36	GLU
8	H	17	PRO
8	H	21	ASN
8	H	32	THR
8	H	59	ILE
8	H	77	ARG
8	H	84	ALA
9	I	47	GLU
9	I	113	ASP
10	J	14	VAL
10	J	17	LYS
10	J	33	GLY
11	K	15	GLY
11	K	53	ASP
11	K	70	ARG
11	K	112	GLN
12	L	26	THR
12	L	53	HIS
12	L	55	ILE
1	A	69	THR
1	A	111	GLY
1	A	135	PHE
1	A	245	PRO
1	A	317	LYS
1	A	386	ASP
1	A	399	HIS
1	A	409	SER
1	A	418	SER
1	A	483	ASP
1	A	492	PRO
1	A	525	GLN

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Mol	Chain	Res	Type
1	A	544	ASP
1	A	619	LYS
1	A	648	ASN
1	A	731	ARG
1	A	846	GLU
1	A	871	ASP
1	A	979	SER
1	A	1120	LEU
1	A	1124	HIS
1	A	1221	LYS
1	A	1280	GLU
2	B	56	ASP
2	B	65	GLU
2	B	94	LYS
2	B	229	ALA
2	B	259	TYR
2	B	264	SER
2	B	283	VAL
2	B	559	SER
2	B	613	VAL
2	B	711	GLU
2	B	746	SER
2	B	884	ARG
2	B	891	ASP
2	B	945	GLU
2	B	1003	ALA
2	B	1041	GLU
2	B	1143	ALA
3	C	60	ASP
3	C	148	ARG
3	C	240	VAL
4	D	12	ARG
4	D	47	LEU
4	D	65	GLU
5	E	44	ALA
5	E	45	LYS
5	E	115	ASN
5	E	192	ARG
6	F	154	ASP
8	H	44	VAL
8	H	90	ALA
8	H	92	ASP

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Mol	Chain	Res	Type
8	H	140	ALA
9	I	34	TYR
9	I	78	CYS
11	K	88	LYS
11	K	90	ALA
11	K	104	ASN
1	A	113	LEU
1	A	148	CYS
1	A	272	ALA
1	A	331	GLY
1	A	332	LYS
1	A	333	GLU
1	A	526	ASP
1	A	609	ASP
1	A	636	GLU
1	A	759	ALA
1	A	817	ALA
1	A	1165	GLU
1	A	1233	ASP
1	A	1402	PHE
2	B	61	ASP
2	B	206	ASN
2	B	328	GLU
2	B	365	THR
2	B	389	ALA
2	B	531	GLN
2	B	540	SER
2	B	598	GLU
2	B	629	ASP
2	B	752	ALA
2	B	758	PHE
2	B	818	PRO
2	B	951	GLN
2	B	982	SER
2	B	1011	ILE
3	C	56	THR
3	C	167	HIS
4	D	9	GLN
4	D	30	GLY
6	F	112	GLU
6	F	150	GLU
7	G	17	PHE

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Mol	Chain	Res	Type
7	G	154	VAL
8	H	52	GLN
10	J	8	PHE
10	J	63	TYR
11	K	29	ASN
11	K	41	THR
1	A	55	ASP
1	A	86	LEU
1	A	99	ILE
1	A	108	MET
1	A	169	ASN
1	A	400	PRO
1	A	419	LYS
1	A	424	ILE
1	A	516	SER
1	A	605	MET
1	A	854	ASN
1	A	895	LYS
1	A	958	VAL
1	A	975	HIS
1	A	1127	ASP
1	A	1454	MET
2	B	58	THR
2	B	114	PRO
2	B	124	TYR
2	B	571	PRO
2	B	867	GLY
2	B	878	GLN
2	B	894	ASP
2	B	901	PRO
3	C	117	ASP
3	C	142	VAL
3	C	164	ALA
3	C	212	PRO
4	D	119	ARG
5	E	43	LYS
6	F	81	THR
7	G	20	PRO
8	H	43	ASN
10	J	24	LEU
12	L	39	SER
12	L	57	LEU

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Mol	Chain	Res	Type
1	A	362	ASP
1	A	720	ARG
1	A	1098	VAL
1	A	1318	THR
1	A	1324	PRO
2	B	470	LYS
2	B	728	ARG
2	B	734	HIS
2	B	797	TYR
2	B	880	THR
4	D	6	SER
7	G	26	LEU
7	G	115	MET
1	A	84	ILE
1	A	673	GLY
1	A	1158	PRO
2	B	712	PRO
2	B	1214	PRO
5	E	76	GLY
7	G	62	LEU
1	A	196	GLU
1	A	1437	GLY
2	B	364	ILE
2	B	759	PRO
9	I	62	ILE
1	A	842	VAL
1	A	1164	PRO
3	C	5	GLY
3	C	126	GLY
7	G	19	GLY
7	G	34	VAL
1	A	35	ILE
1	A	357	PRO
1	A	775	ILE
2	B	231	PRO
2	B	411	PRO
2	B	1103	ILE
2	B	824	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1244/1520 (82%)	1129 (91%)	115 (9%)	9	35
2	B	967/1061 (91%)	884 (91%)	83 (9%)	10	40
3	C	235/274 (86%)	214 (91%)	21 (9%)	9	38
4	D	159/200 (80%)	135 (85%)	24 (15%)	3	18
5	E	196/197 (100%)	192 (98%)	4 (2%)	55	75
6	F	77/137 (56%)	69 (90%)	8 (10%)	7	30
7	G	152/152 (100%)	141 (93%)	11 (7%)	14	45
8	H	119/128 (93%)	113 (95%)	6 (5%)	24	55
9	I	110/116 (95%)	98 (89%)	12 (11%)	6	29
10	J	60/65 (92%)	53 (88%)	7 (12%)	5	27
11	K	99/102 (97%)	89 (90%)	10 (10%)	7	32
12	L	40/57 (70%)	36 (90%)	4 (10%)	7	32
All	All	3458/4009 (86%)	3153 (91%)	305 (9%)	10	38

All (305) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	11	LEU
1	A	34	LYS
1	A	37	PHE
1	A	62	ASP
1	A	67	CYS
1	A	70	CYS
1	A	83	HIS
1	A	93	VAL
1	A	100	LYS
1	A	108	MET
1	A	122	MET
1	A	130	ASP
1	A	142	CYS

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Mol	Chain	Res	Type
1	A	198	GLU
1	A	200	ARG
1	A	215	SER
1	A	244	PRO
1	A	245	PRO
1	A	261	ASP
1	A	270	LEU
1	A	302	THR
1	A	312	PRO
1	A	320	ARG
1	A	335	ARG
1	A	344	ARG
1	A	345	VAL
1	A	350	ARG
1	A	354	SER
1	A	381	THR
1	A	385	ILE
1	A	404	TYR
1	A	406	ILE
1	A	407	ARG
1	A	408	ASP
1	A	412	ARG
1	A	418	SER
1	A	425	GLN
1	A	442	VAL
1	A	443	LEU
1	A	445	ASN
1	A	449	SER
1	A	450	LEU
1	A	451	HIS
1	A	460	VAL
1	A	462	VAL
1	A	466	SER
1	A	469	ARG
1	A	470	LEU
1	A	481	ASP
1	A	493	GLN
1	A	515	GLN
1	A	560	ILE
1	A	562	THR
1	A	590	ARG
1	A	618	GLU

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Mol	Chain	Res	Type
1	A	629	LEU
1	A	635	ARG
1	A	663	SER
1	A	666	ILE
1	A	670	ILE
1	A	711	ARG
1	A	739	ASP
1	A	741	ASN
1	A	768	GLN
1	A	774	ARG
1	A	779	PHE
1	A	821	ARG
1	A	827	THR
1	A	845	LEU
1	A	858	ASN
1	A	859	SER
1	A	886	ILE
1	A	890	ASP
1	A	903	ASN
1	A	906	HIS
1	A	929	LEU
1	A	940	ARG
1	A	969	GLN
1	A	992	ASP
1	A	1009	ASN
1	A	1029	ARG
1	A	1030	ARG
1	A	1035	TYR
1	A	1052	GLN
1	A	1067	LEU
1	A	1110	ASN
1	A	1116	LEU
1	A	1122	PRO
1	A	1127	ASP
1	A	1170	ILE
1	A	1187	GLN
1	A	1206	ASP
1	A	1264	GLU
1	A	1267	MET
1	A	1271	ILE
1	A	1291	VAL
1	A	1295	THR

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Mol	Chain	Res	Type
1	A	1297	GLU
1	A	1309	ASP
1	A	1332	PHE
1	A	1333	ILE
1	A	1359	ASP
1	A	1364	ASN
1	A	1372	VAL
1	A	1376	THR
1	A	1385	THR
1	A	1386	ARG
1	A	1389	PHE
1	A	1405	THR
1	A	1432	GLN
1	A	1442	ASP
1	A	1443	VAL
1	A	1445	ILE
1	A	1447	GLU
2	B	30	SER
2	B	35	SER
2	B	57	TYR
2	B	106	ASP
2	B	128	LEU
2	B	175	ARG
2	B	180	TYR
2	B	188	ASP
2	B	194	GLU
2	B	199	MET
2	B	217	ARG
2	B	223	VAL
2	B	268	THR
2	B	294	ASP
2	B	298	LEU
2	B	365	THR
2	B	371	GLU
2	B	393	LYS
2	B	396	ASP
2	B	399	ASP
2	B	401	PHE
2	B	427	ASP
2	B	429	PHE
2	B	463	THR
2	B	465	ASN

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Mol	Chain	Res	Type
2	B	466	TRP
2	B	485	ARG
2	B	496	ARG
2	B	498	THR
2	B	502	ILE
2	B	516	ASN
2	B	557	PHE
2	B	582	VAL
2	B	593	PRO
2	B	603	LEU
2	B	615	MET
2	B	628	THR
2	B	635	ARG
2	B	644	GLU
2	B	682	SER
2	B	684	LEU
2	B	724	ASP
2	B	737	THR
2	B	742	GLU
2	B	785	TYR
2	B	790	ASP
2	B	811	TYR
2	B	830	TYR
2	B	835	GLN
2	B	837	ASP
2	B	839	MET
2	B	844	SER
2	B	858	SER
2	B	878	GLN
2	B	901	PRO
2	B	909	ASP
2	B	935	ARG
2	B	939	THR
2	B	953	LEU
2	B	999	MET
2	B	1002	THR
2	B	1006	ILE
2	B	1022	THR
2	B	1047	PHE
2	B	1069	PHE
2	B	1084	GLN
2	B	1087	PHE

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Mol	Chain	Res	Type
2	B	1092	TYR
2	B	1095	LEU
2	B	1099	VAL
2	B	1106	ARG
2	B	1108	ARG
2	B	1120	GLU
2	B	1122	ARG
2	B	1123	SER
2	B	1159	ARG
2	B	1160	VAL
2	B	1170	THR
2	B	1176	ASN
2	B	1183	LYS
2	B	1202	LEU
2	B	1212	ILE
2	B	1216	LEU
3	C	22	LEU
3	C	56	THR
3	C	58	LEU
3	C	62	PHE
3	C	77	ILE
3	C	93	ASP
3	C	99	LEU
3	C	104	PHE
3	C	108	GLU
3	C	129	ILE
3	C	140	ASN
3	C	145	CYS
3	C	147	LEU
3	C	163	ILE
3	C	172	PRO
3	C	193	TYR
3	C	214	ASN
3	C	233	GLU
3	C	240	VAL
3	C	259	LEU
3	C	266	ASP
4	D	8	PHE
4	D	13	ARG
4	D	16	LYS
4	D	17	LYS
4	D	19	GLU

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Mol	Chain	Res	Type
4	D	22	GLU
4	D	32	GLU
4	D	47	LEU
4	D	63	LEU
4	D	70	PHE
4	D	137	ASN
4	D	139	LYS
4	D	148	LEU
4	D	149	THR
4	D	151	PHE
4	D	156	ASP
4	D	159	THR
4	D	170	THR
4	D	174	PRO
4	D	187	THR
4	D	192	LYS
4	D	193	THR
4	D	208	GLU
4	D	221	TYR
5	E	60	PHE
5	E	74	ASP
5	E	104	ASN
5	E	114	ASN
6	F	79	ARG
6	F	90	ARG
6	F	99	LEU
6	F	111	LEU
6	F	119	ARG
6	F	143	PHE
6	F	148	VAL
6	F	153	VAL
7	G	1	MET
7	G	13	LEU
7	G	51	TYR
7	G	74	TYR
7	G	78	VAL
7	G	80	LYS
7	G	88	ASP
7	G	96	GLN
7	G	115	MET
7	G	126	ASN
7	G	171	ILE

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Mol	Chain	Res	Type
8	H	86	ASP
8	H	95	TYR
8	H	102	TYR
8	H	130	ARG
8	H	134	ASN
8	H	143	LEU
9	I	8	ARG
9	I	9	ASP
9	I	15	TYR
9	I	34	TYR
9	I	40	SER
9	I	75	CYS
9	I	78	CYS
9	I	85	PHE
9	I	86	PHE
9	I	94	ASP
9	I	101	PHE
9	I	110	PHE
10	J	7	CYS
10	J	9	SER
10	J	10	CYS
10	J	28	ASP
10	J	44	TYR
10	J	46	CYS
10	J	48	ARG
11	K	10	PHE
11	K	25	THR
11	K	47	ARG
11	K	50	LEU
11	K	61	TYR
11	K	78	THR
11	K	111	LEU
11	K	112	GLN
11	K	113	THR
11	K	114	LEU
12	L	51	CYS
12	L	55	ILE
12	L	65	VAL
12	L	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	64	ASN
1	A	68	GLN
1	A	83	HIS
1	A	92	HIS
1	A	118	HIS
1	A	225	ASN
1	A	339	ASN
1	A	358	ASN
1	A	435	HIS
1	A	479	ASN
1	A	631	HIS
1	A	654	ASN
1	A	741	ASN
1	A	757	ASN
1	A	768	GLN
1	A	786	HIS
1	A	858	ASN
1	A	903	ASN
1	A	926	GLN
1	A	1140	HIS
1	A	1218	GLN
1	A	1364	ASN
1	A	1432	GLN
2	B	46	GLN
2	B	178	ASN
2	B	215	GLN
2	B	236	HIS
2	B	300	HIS
2	B	363	HIS
2	B	366	GLN
2	B	449	ASN
2	B	465	ASN
2	B	499	ASN
2	B	513	GLN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	657	HIS
2	B	734	HIS
2	B	744	HIS
2	B	794	ASN

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Mol	Chain	Res	Type
2	B	821	GLN
2	B	842	ASN
2	B	975	GLN
2	B	1015	HIS
2	B	1025	HIS
2	B	1065	GLN
2	B	1076	HIS
2	B	1084	GLN
2	B	1117	GLN
2	B	1179	GLN
2	B	1193	GLN
3	C	73	GLN
3	C	112	ASN
3	C	123	ASN
3	C	167	HIS
3	C	231	ASN
3	C	252	GLN
4	D	39	ASN
4	D	40	HIS
4	D	137	ASN
4	D	179	GLN
5	E	8	ASN
5	E	101	GLN
5	E	104	ASN
5	E	114	ASN
5	E	147	HIS
7	G	53	ASN
7	G	97	HIS
7	G	122	ASN
7	G	126	ASN
9	I	12	ASN
9	I	90	GLN
10	J	64	ASN
11	K	44	ASN
11	K	65	HIS
11	K	76	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	P	9/11 (81%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	P	10	A

There are no RNA pucker outliers to report.

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	T	22	13,14	15,21,22	1.87	3 (20%)	17,30,33	3.96	3 (17%)

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	T	22	13,14	-	0/4/21/22	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	22	BRU	C4-C5	5.50	1.45	1.38
14	T	22	BRU	C4-N3	3.45	1.39	1.33
14	T	22	BRU	C6-C5	-2.07	1.34	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	22	BRU	C4-N3-C2	14.02	126.98	115.14
14	T	22	BRU	C5-C4-N3	-6.79	115.51	123.64
14	T	22	BRU	C5-C6-N1	2.93	123.75	119.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	22	BRU	3	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2
1	A	1
3	C	1
6	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	2:SER	C	3:GLU	N	4.08
1	B	18:PHE	C	19:GLU	N	3.80
1	F	69:LEU	C	70:LYS	N	3.44
1	A	1175:SER	C	1176:LEU	N	3.41
1	B	337:ARG	C	338:GLY	N	2.62

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1421/1733 (81%)	-0.34	10 (0%) 87 83	12, 73, 146, 189	0
2	B	1115/1224 (91%)	-0.25	17 (1%) 73 66	12, 83, 154, 191	0
3	C	267/318 (83%)	-0.39	1 (0%) 92 89	30, 69, 125, 150	0
4	D	177/221 (80%)	-0.18	0 100 100	53, 104, 145, 162	0
5	E	214/215 (99%)	-0.19	1 (0%) 91 87	45, 126, 174, 178	0
6	F	87/155 (56%)	-0.54	0 100 100	17, 49, 91, 119	0
7	G	171/171 (100%)	-0.26	1 (0%) 89 85	53, 77, 115, 126	0
8	H	135/146 (92%)	0.20	4 (2%) 50 40	87, 128, 162, 171	0
9	I	116/122 (95%)	-0.05	1 (0%) 84 79	69, 122, 151, 173	0
10	J	65/70 (92%)	-0.63	0 100 100	35, 66, 109, 118	0
11	K	114/120 (95%)	-0.33	2 (1%) 68 61	33, 73, 102, 140	0
12	L	46/70 (65%)	0.33	3 (6%) 18 14	69, 141, 161, 169	0
13	P	10/11 (90%)	-0.05	1 (10%) 7 6	71, 85, 160, 163	0
14	T	10/25 (40%)	-0.36	0 100 100	72, 96, 137, 158	0
All	All	3948/4601 (85%)	-0.27	41 (1%) 82 76	12, 82, 154, 191	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	114	LEU	6.4
11	K	113	THR	6.4
2	B	882	THR	5.4
2	B	471	LYS	3.8
8	H	139	ASN	3.6
1	A	1257	ASP	3.4
2	B	713	ALA	3.3
1	A	159	THR	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	709	ASP	3.1
2	B	334	ILE	2.9
12	L	50	ASP	2.9
8	H	132	LEU	2.8
2	B	733	HIS	2.8
2	B	883	LEU	2.7
2	B	432	MET	2.7
3	C	130	GLY	2.7
2	B	666	TYR	2.6
2	B	734	HIS	2.6
1	A	1256	GLU	2.6
7	G	124	GLY	2.6
2	B	868	MET	2.5
1	A	253	ASN	2.5
5	E	110	PHE	2.5
1	A	251	SER	2.5
2	B	714	GLU	2.4
1	A	1455	PRO	2.3
13	P	1	U	2.3
12	L	26	THR	2.3
2	B	428	ILE	2.2
2	B	448	ILE	2.2
2	B	133	LYS	2.2
12	L	38	LEU	2.2
1	A	171	GLN	2.2
2	B	732	SER	2.2
8	H	86	ASP	2.1
1	A	187	LYS	2.1
9	I	55	THR	2.1
2	B	715	ALA	2.1
8	H	36	CYS	2.0
1	A	199	LEU	2.0
1	A	1109	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	BRU	T	22	20/21	0.87	0.18	59,61,68,69	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
16	ZN	A	2464	1/1	0.98	0.07	82,82,82,82	0
16	ZN	A	2461	1/1	0.98	0.08	163,163,163,163	0
16	ZN	A	2462	1/1	0.99	0.07	23,23,23,23	0
16	ZN	A	2459	1/1	0.99	0.04	115,115,115,115	0
16	ZN	A	2463	1/1	0.99	0.13	42,42,42,42	0
16	ZN	A	2460	1/1	0.99	0.14	69,69,69,69	0
16	ZN	A	2465	1/1	0.99	0.07	31,31,31,31	0
15	MG	A	2457	1/1	1.00	0.15	21,21,21,21	0
16	ZN	A	2458	1/1	1.00	0.14	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.