



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 20, 2018 – 08:32 pm GMT

PDB ID : 6C3P
EMDB ID: : EMD-7339
Title : Cryo-EM structure of human KATP bound to ATP and ADP in propeller form
Authors : Lee, K.P.K.; Chen, J.; MacKinnon, R.
Deposited on : 2018-01-10
Resolution : 5.60 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

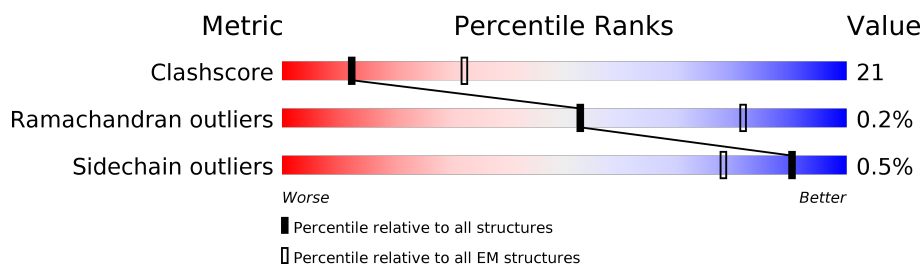
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136279	1886
Ramachandran outliers	132675	1663
Sidechain outliers	132484	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	406	47% 34% 19%
1	B	406	45% 36% 19%
1	C	406	47% 34% 19%
1	D	406	47% 34% 19%
2	E	1581	53% 33% 14%
2	F	1581	53% 32% 14%
2	G	1581	53% 32% 14%
2	H	1581	53% 32% 14%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 50696 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 ATP-sensitive inward rectifier potassium channel 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	328	Total	C	N	O	S	0	0
			2506	1619	428	442	17		
1	D	328	Total	C	N	O	S	0	0
			2506	1619	428	442	17		
1	B	328	Total	C	N	O	S	0	0
			2506	1619	428	442	17		
1	C	328	Total	C	N	O	S	0	0
			2506	1619	428	442	17		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	SER	-	expression tag	UNP Q14654
A	-4	ALA	-	expression tag	UNP Q14654
A	-3	SER	-	expression tag	UNP Q14654
A	-2	ALA	-	expression tag	UNP Q14654
A	-1	SER	-	expression tag	UNP Q14654
A	0	ALA	-	expression tag	UNP Q14654
A	391	SER	-	expression tag	UNP Q14654
A	392	ASN	-	expression tag	UNP Q14654
A	393	SER	-	expression tag	UNP Q14654
A	394	LEU	-	expression tag	UNP Q14654
A	395	GLU	-	expression tag	UNP Q14654
A	396	VAL	-	expression tag	UNP Q14654
A	397	LEU	-	expression tag	UNP Q14654
A	398	PHE	-	expression tag	UNP Q14654
A	399	GLN	-	expression tag	UNP Q14654
A	400	GLY	-	expression tag	UNP Q14654
D	-5	SER	-	expression tag	UNP Q14654
D	-4	ALA	-	expression tag	UNP Q14654
D	-3	SER	-	expression tag	UNP Q14654
D	-2	ALA	-	expression tag	UNP Q14654
D	-1	SER	-	expression tag	UNP Q14654
D	0	ALA	-	expression tag	UNP Q14654

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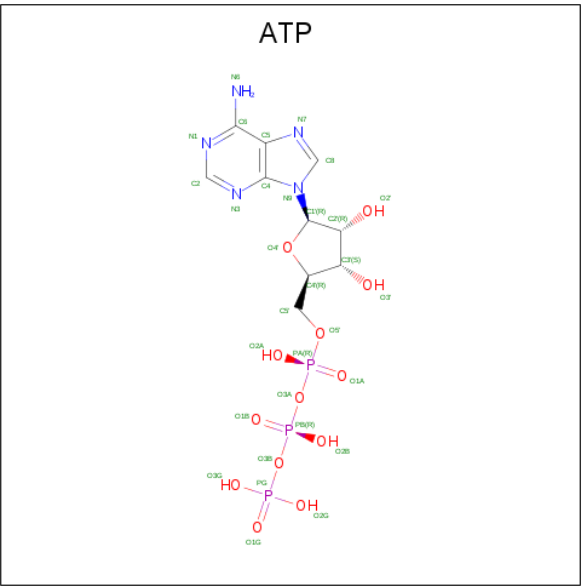
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Chain	Residue	Modelled	Actual	Comment	Reference
D	391	SER	-	expression tag	UNP Q14654
D	392	ASN	-	expression tag	UNP Q14654
D	393	SER	-	expression tag	UNP Q14654
D	394	LEU	-	expression tag	UNP Q14654
D	395	GLU	-	expression tag	UNP Q14654
D	396	VAL	-	expression tag	UNP Q14654
D	397	LEU	-	expression tag	UNP Q14654
D	398	PHE	-	expression tag	UNP Q14654
D	399	GLN	-	expression tag	UNP Q14654
D	400	GLY	-	expression tag	UNP Q14654
B	-5	SER	-	expression tag	UNP Q14654
B	-4	ALA	-	expression tag	UNP Q14654
B	-3	SER	-	expression tag	UNP Q14654
B	-2	ALA	-	expression tag	UNP Q14654
B	-1	SER	-	expression tag	UNP Q14654
B	0	ALA	-	expression tag	UNP Q14654
B	391	SER	-	expression tag	UNP Q14654
B	392	ASN	-	expression tag	UNP Q14654
B	393	SER	-	expression tag	UNP Q14654
B	394	LEU	-	expression tag	UNP Q14654
B	395	GLU	-	expression tag	UNP Q14654
B	396	VAL	-	expression tag	UNP Q14654
B	397	LEU	-	expression tag	UNP Q14654
B	398	PHE	-	expression tag	UNP Q14654
B	399	GLN	-	expression tag	UNP Q14654
B	400	GLY	-	expression tag	UNP Q14654
C	-5	SER	-	expression tag	UNP Q14654
C	-4	ALA	-	expression tag	UNP Q14654
C	-3	SER	-	expression tag	UNP Q14654
C	-2	ALA	-	expression tag	UNP Q14654
C	-1	SER	-	expression tag	UNP Q14654
C	0	ALA	-	expression tag	UNP Q14654
C	391	SER	-	expression tag	UNP Q14654
C	392	ASN	-	expression tag	UNP Q14654
C	393	SER	-	expression tag	UNP Q14654
C	394	LEU	-	expression tag	UNP Q14654
C	395	GLU	-	expression tag	UNP Q14654
C	396	VAL	-	expression tag	UNP Q14654
C	397	LEU	-	expression tag	UNP Q14654
C	398	PHE	-	expression tag	UNP Q14654
C	399	GLN	-	expression tag	UNP Q14654
C	400	GLY	-	expression tag	UNP Q14654

- Molecule 2 is a protein called ATP-binding cassette sub-family C member 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	1359	Total	C	N	O	S	0	0
			10077	6567	1699	1760	51		
2	H	1359	Total	C	N	O	S	0	0
			10077	6567	1699	1760	51		
2	G	1359	Total	C	N	O	S	0	0
			10077	6567	1699	1760	51		
2	F	1359	Total	C	N	O	S	0	0
			10077	6567	1699	1760	51		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



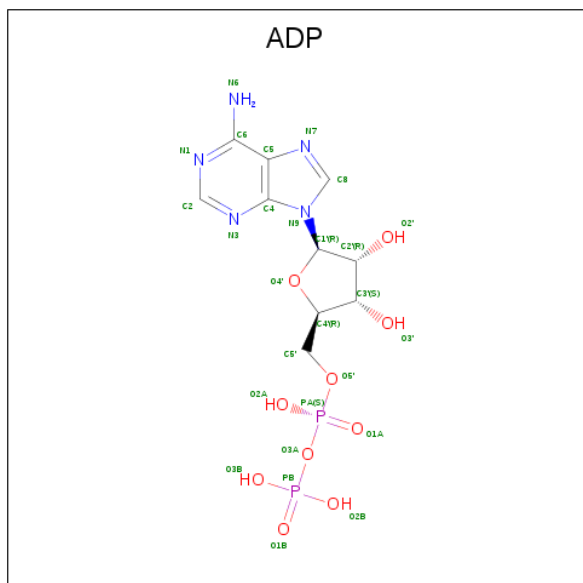
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	A	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	H	1	Total	C	N	O	P	0
			31	10	5	13	3	

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Mol	Chain	Residues	Atoms					AltConf
3	G	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
4	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

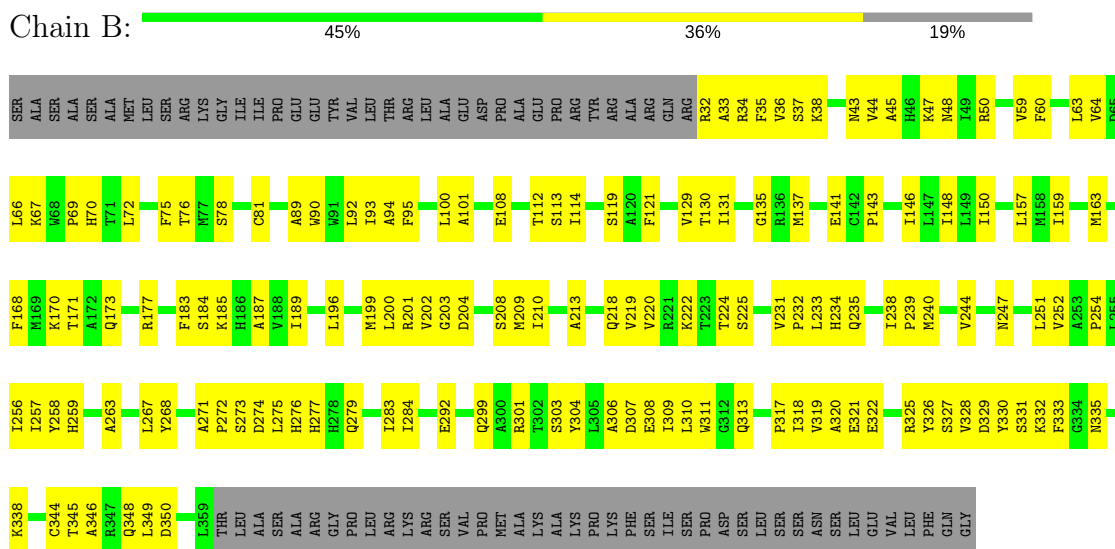
Mol	Chain	Residues	Atoms		AltConf
5	H	2	Total	Mg	0
			2	2	
5	G	2	Total	Mg	0
			2	2	
5	F	2	Total	Mg	0
			2	2	

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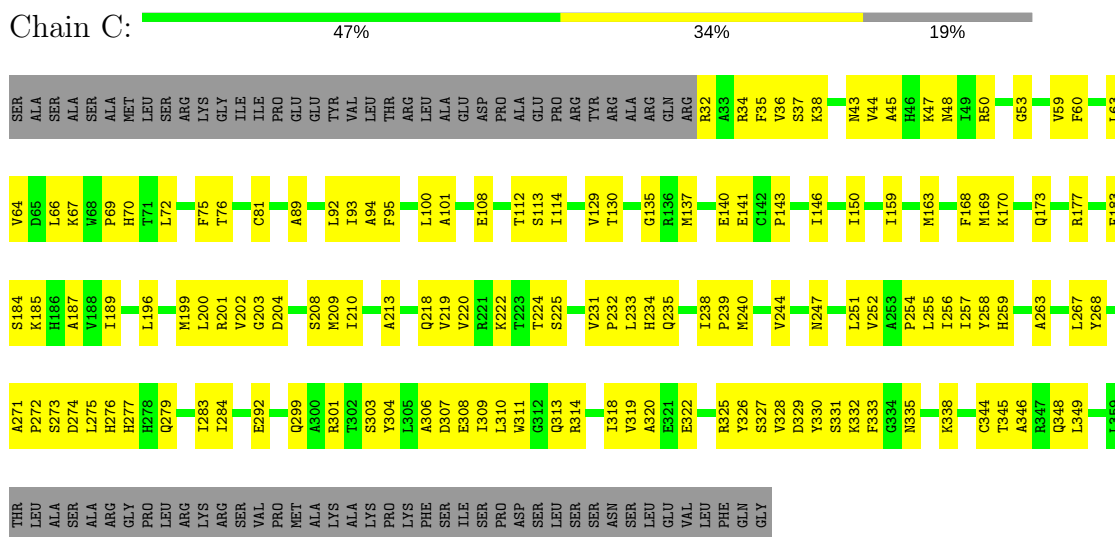
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	E	2	2	2	0

Chain B:



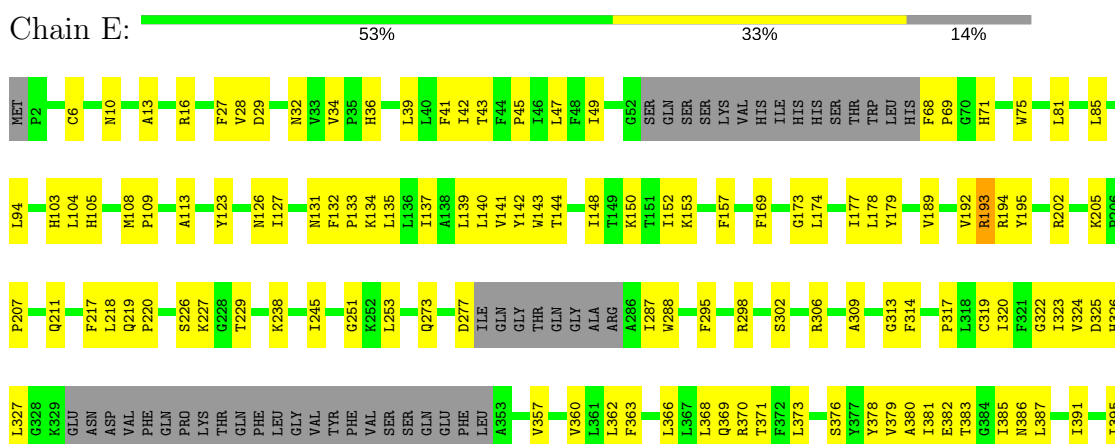
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

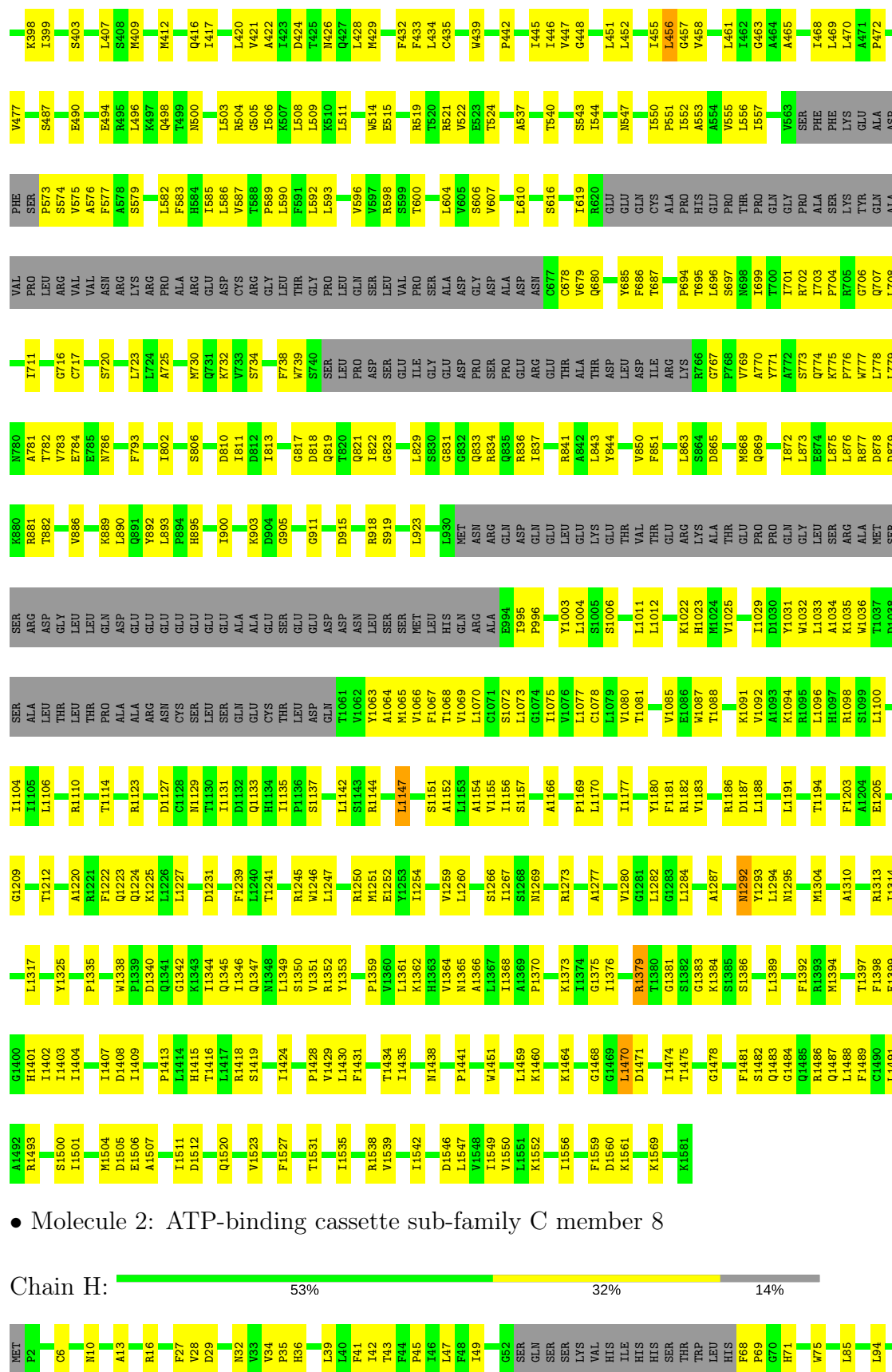
Chain C:



- Molecule 2: ATP-binding cassette sub-family C member 8

Chain E:





• Molecule 2: ATP-binding cassette sub-family C member 8




● Molecule 2: ATP-binding cassette sub-family C member 8

Chain G:

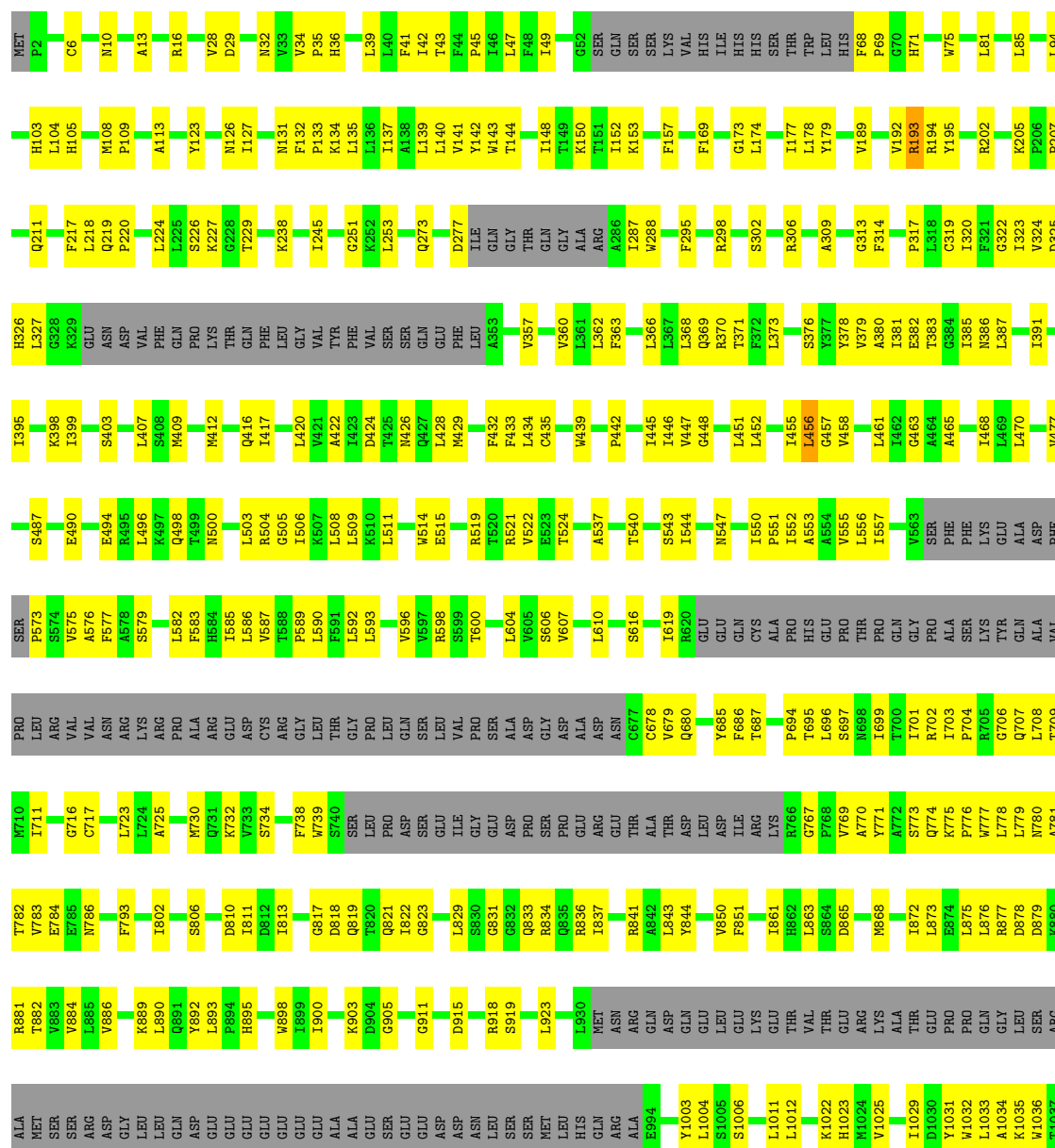


Q1224	T1114	THR	LEU	K889	N786	C717	VAL	A576	E490	T395	H526	Q211	H103	NET
L1225	R1123	PRO	GLN	K890	F793	S720	ASN	F577	E490	K398	G328	F217	L104	P2
L1227		ALA	GLU	K891			ARG	A578	E494	L399	L329	L218	H105	C6
D1231	D1127	ARG	GLU	K892	I802	L723	PRO	L582	L496	S403	ASN	Q219	M108	N10
F1239	G1128	CYS	GLU	K893	S806	A725	ALA	F583	K497		ASP	P220	P109	
L1240	N1129	SER	GLU	H895			ARG	H584	Q498	L407	VAL		A113	A13
L1241	T1130	LEU	GLU	I900	D810	M730	GLU	L585	T499	S408	PHE	L224	A113	
A1242	D1132	GLN	ALA	I903	D812	Q731	ASP	L586	N500	M409	GLN	L225		R16
A1243	Q1133	GLU	ALA	K903	I813	K732	CYS	V587			PRO	S226	Y123	
N1244	H1134	CYS	GLU	D904	G817	S734	ARG	T588	L503	M412	LYS	K227		V28
R1245	I1135	THR	SER	G905	D818	W739	LEU	L590	R504	Q416	THR	G228	N126	D29
L1246	P1136	LEU	GLU	G911	Q819	SER	THR	F591	L506	1417	GLN	T229	I127	
L1247	S1137	GLN	GLU	G911	T820	S740	PRO	V587	L592		LEU	K238		N32
R1250	L1142	ASP	ASP	D915	Q821	LEU	LEU	L593	L508	L420	GLY	L245		V34
M1251	S1143	ASN	ASN	R918	I822	PRO	GLN	V596	K510	V431	VAL	I245		P35
E1252	R1144	LEU	LEU	S919	G823	ASP	SER	V597	L511	A422	THR	G251	L135	H36
I1253		SER	SER			SER	LEU	R598		D424	VAL	L253		
L1254	L1147	MET	MET	L923	L829	GLU	VAL	S599	W514	T425	SER	L253	L136	L39
V1259	S1151	LEU	LEU		S830	ILE	PRO	T600	E515	M426	GLN		A138	F41
L1260		HIS	HIS	L930	G832	GLY	SER	L604	R521	Q427	GLN	Q273	L139	I42
S1266	A1154	ARG	ARG	MET	I833	ASP	ASP	W605	V522	M429	GLU	D277	L140	I42
L1267	I1156	GLN	GLN	ASN	R834	PRO	GLY	S606	E523		PHE	ILE	V141	T43
S1268	S1157	GLN	F994	ARG	Q835	SER	ASP	V607	T524	F432	ALA	GLN	W142	P45
N1269		ASP	ASP	ASP	R836	PRO	ALA			F433	GLY	GLY	W143	I46
	A1166	GLN	P996	GLN	I837	GLU	ASP	L610	A837	L434	THR	THR	T144	L47
R1273		GLU	GLU	GLU	R841	ARG	ASN	S616	T540	C435	GLN	THR	T148	F46
A1277	P1169	LEU	Y1003	LEU	A842	THR	C677				V360	GLN	T149	L49
V1280	L1170	LYS	S1005	LYS	Y844	ALA	C678	1619	S543	P442	L362	ALA	K150	G52
G1281	I1177	GLU	S1006	GLU		ASP	Q680	GLU	I544	I445	F363	ARG	T151	SER
L1282		THR	THR	THR	V850	LEU	Y685	GLU	N547	L446	L366	I287	K153	SER
G1283		VAL	L1011	VAL	F851	ASP	F686	GLN	GLU	G448	L367	W288	K153	SER
L1284		THR	L1012	THR		ILE	T687	CYS	I550	L451	L368	F295	F157	LYS
T1285		GLU	K1022	GLU	L863	ARG	P694	ALA	P551	L451	Q369	R298	F169	VAL
Y1286		ARG	H1023	ARG	D865	LYS	T695	PRO	I552	L452	R370			ILE
A1287		LYS	H1024	LYS			L696	HIS	A553		G370		G173	HIS
L1288		ALA	M1025	ALA	D865	R766	L697	GLU	A554	F372	F372	S302	L174	HIS
M1289		THR	V1025	THR	M868	V769	N698	PRO	V555	L456	G457	R306	I177	SER
		GLU	I1029	GLU	I872	A770	I699	THR	L556	V458			L178	THR
L1191		PRO	D1030	PRO	L873	Y771	T700	GLN	I557		S376	A309	Y179	LEU
N1292		ASN	H1030	ASN	L873	A772	I701	GLY	V653	L461	V378			HIS
Y1293		GLN	Y1031	GLN	S874	S773	R702	PRO	SER	L462	V379	G313	V189	F68
L1294		GLY	W1032	GLY	L875	Q774	I703	THR	PHE	G463	P314			P69
N1295		LEU	L1033	LEU	L876	K775	T703	ALA	PHE	A464	I381		V192	G70
		SER	A1034	SER	R877	P776	P704	SER	LYS	A465	T381	P317	R193	H71
M1304		ARG	K1035	ARG	D878	W777	R705	LYS	GLU	E382	T383	L318	R194	
		ALA	W1036	ALA	D879	L778	Q706	TVR	ALA	GLU	G384	C319	Y195	W75
A1310		MET	T1037	MET	K880	L779	Q707	GLN	ALA	I468	G384	I320	Y195	
		SER	D1038	SER	R881	N780	L708	ALA	ASP	L469	I385			
R1313		THR	ALA	THR	R881	A781	T709	VAL	PHE	L470	N386	F321	R202	L81
I1314		ARG	ALA	ARG	T882	W782	W710	PRO	SER	L387	I323		K205	L85
F1222	R1221	ASP	LEU	ASP	V884	T783	I711	LEU	P573	V477	I323		K205	L85
L1317		THR	THR	THR	L885	E784	T711	ARG	S574		V324	P206	P207	L94
		LEU	LEU	LEU	V886	E785	T716	VAL	V575	S487	D325			



• Molecule 2: ATP-binding cassette sub-family C member 8

Chain F: 53% 32% 14%



D1038	SER	I1104	T1212	L1317	I1402	S1500
	ALA	I1105	A1220	Y1325	I1403	I1501
	LEU	L1106	R1221	F1222	I1404	F1502
	THR		Q1223	P1335	I1407	I1503
	LEU	R1110	Q1224	W1338	D1408	M1504
	THR	T1114	K1225	P1339	I1409	D1505
	PRO		L1226	D1340	P1413	E1506
	ALA	R1123	L1227	Q1341	T1416	A1507
	ARG	D1127	D1231	G1342	R1417	I1511
	ASN	G1128		A1343	L1418	D1512
CYS	M1129	F1239	I1344	I1423	Q1520	
LEU	T1130	L1240	Q1345	I1424	V1523	
SER	I1131	T1241	I1346			
GLN	D1132		Q1347	V1429	F1527	
GLU	Q1133	R1245	W1348	L1430		
CYS	H1134	W1246	L1349	F1431	T1531	
THR	I1135	L1247	S1350			
LEU	P1136		V1351	T1434	I1535	
ASP	S1137	R1250	R1352	I1435		
GLN		M1251	Y1353			
T1061	L1142	E1252	P1359	M1438	R1538	
Y1062	S1143	I1254	L1361		V1539	
A1064	R1144	V1254	K1362	P1441	I1542	
M1065	L1147	V1259	H1363	W1451	D1546	
V1066		L1260	V1364		L1547	
F1067	S1151		S1365	L1459	Y1548	
T1068	A1154	I1267	A1366	K1460	I1549	
V1069	V1155	S1268	L1367		V1550	
L1070	I1156	M1269	L1368	K1464		
G1071	S1157			A1465	I1556	
S1072		R1273	K1373	L1466		
L1073	A1166		I1374	P1467	F1559	
G1074	P1169	A1277	G1375	G1468	D1560	
I1075	L1170		I1376	G1469	K1561	
L1077		V1280	R1379	L1470		
C1078	I1177	G1281	T1380	D1471	K1581	
L1079		L1282	G1381			
V1080	Y1180	L1284	G1383	T1474		
T1081	F1181		K1384	T1475		
	R1182	A1287	S1385	G1478		
V1085	V1183	L1288	S1386			
E1086		M1289		F1481		
W1087	R1186		L1389	S1482		
T1088	D1187	M1292		Q1483		
	L1188	Y1293		G1484		
K1091		L1294	F1392	Q1485		
V1092	L1191	M1295	A1393	R1486		
A1093			M1394	G1487		
K1094	T1194	M1304		L1488		
R1095	E1205	A1310	T1397	F1489		
L1096			F1398	C1490		
R1097			E1399	L1491		
S1098	G1209	R1313	W1401	A1492		
T1099		L1314	H1402	P1493		

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	47282	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.18	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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 >2	RMSZ	# Z >2
1	A	0.36	0/2563	0.51	0/3490
1	B	0.36	0/2563	0.51	0/3490
1	C	0.36	0/2563	0.51	0/3490
1	D	0.36	0/2563	0.51	0/3490
2	E	0.32	0/10282	0.50	2/14031 (0.0%)
2	F	0.32	0/10282	0.50	2/14031 (0.0%)
2	G	0.32	0/10282	0.50	2/14031 (0.0%)
2	H	0.32	0/10282	0.50	2/14031 (0.0%)
All	All	0.33	0/51380	0.50	8/70084 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	2
2	F	0	2
2	G	0	2
2	H	0	2
All	All	0	8

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1294	LEU	CA-CB-CG	5.39	127.69	115.30
2	G	1294	LEU	CA-CB-CG	5.37	127.64	115.30
2	F	1294	LEU	CA-CB-CG	5.37	127.64	115.30
2	E	1294	LEU	CA-CB-CG	5.35	127.61	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1470	LEU	CA-CB-CG	5.18	127.21	115.30
2	E	1470	LEU	CA-CB-CG	5.17	127.20	115.30
2	F	1470	LEU	CA-CB-CG	5.17	127.19	115.30
2	H	1470	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	193	ARG	Peptide
2	E	202	ARG	Peptide
2	F	193	ARG	Peptide
2	F	202	ARG	Peptide
2	G	193	ARG	Peptide
2	G	202	ARG	Peptide
2	H	193	ARG	Peptide
2	H	202	ARG	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2506	0	2494	129	0
1	B	2506	0	2494	130	0
1	C	2506	0	2494	120	0
1	D	2506	0	2494	122	0
2	E	10077	0	9922	408	0
2	F	10077	0	9922	407	0
2	G	10077	0	9922	406	0
2	H	10077	0	9922	404	0
3	A	62	0	24	8	0
3	C	31	0	12	3	0
3	D	31	0	12	4	0
3	E	31	0	12	5	0
3	F	31	0	12	2	0
3	G	31	0	12	4	0
3	H	31	0	12	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	27	0	12	2	0
4	F	27	0	12	2	0
4	G	27	0	12	2	0
4	H	27	0	12	2	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
5	G	2	0	0	0	0
5	H	2	0	0	0	0
All	All	50696	0	49808	2070	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 21.

All (2070) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1501:ILE:HG22	2:G:1531:THR:HB	1.55	0.88
2:H:1501:ILE:HG22	2:H:1531:THR:HB	1.55	0.88
2:F:1501:ILE:HG22	2:F:1531:THR:HB	1.55	0.87
2:H:1459:LEU:HD21	2:H:1488:LEU:HB3	1.58	0.86
2:E:1501:ILE:HG22	2:E:1531:THR:HB	1.55	0.85
2:E:1459:LEU:HD21	2:E:1488:LEU:HB3	1.58	0.85
2:F:1459:LEU:HD21	2:F:1488:LEU:HB3	1.58	0.85
2:H:1350:SER:HB2	2:H:1399:GLU:HB2	1.58	0.84
2:H:193:ARG:O	2:H:195:TYR:N	2.11	0.84
2:E:193:ARG:O	2:E:195:TYR:N	2.10	0.84
2:F:1350:SER:HB2	2:F:1399:GLU:HB2	1.58	0.84
2:E:1350:SER:HB2	2:E:1399:GLU:HB2	1.58	0.83
2:G:1459:LEU:HD21	2:G:1488:LEU:HB3	1.58	0.83
2:G:1350:SER:HB2	2:G:1399:GLU:HB2	1.58	0.83
1:A:67:LYS:HG2	1:A:69:PRO:HD2	1.61	0.83
1:D:67:LYS:HG2	1:D:69:PRO:HD2	1.61	0.82
2:F:193:ARG:O	2:F:195:TYR:N	2.10	0.82
2:G:193:ARG:O	2:G:195:TYR:N	2.11	0.82
1:B:67:LYS:HG2	1:B:69:PRO:HD2	1.61	0.82
1:C:81:CYS:HB2	2:G:41:PHE:HB3	1.60	0.82
1:A:101:ALA:HB2	2:E:16:ARG:HB2	1.60	0.82
1:C:67:LYS:HG2	1:C:69:PRO:HD2	1.61	0.81
2:H:424:ASP:OD1	2:H:606:SER:OG	2.00	0.79
2:E:424:ASP:OD1	2:E:606:SER:OG	2.00	0.79
2:G:424:ASP:OD1	2:G:606:SER:OG	2.00	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:810:ASP:OD2	2:G:836:ARG:NH2	2.16	0.79
2:E:810:ASP:OD2	2:E:836:ARG:NH2	2.16	0.78
2:F:424:ASP:OD1	2:F:606:SER:OG	2.00	0.78
1:A:81:CYS:HB2	2:E:41:PHE:HB3	1.65	0.78
2:E:309:ALA:O	2:E:369:GLN:NE2	2.17	0.78
2:E:218:LEU:HD23	2:E:219:GLN:H	1.48	0.77
2:H:810:ASP:OD2	2:H:836:ARG:NH2	2.16	0.77
2:E:412:MET:HA	2:E:416:GLN:HE21	1.49	0.77
2:G:412:MET:HA	2:G:416:GLN:HE21	1.49	0.77
2:F:810:ASP:OD2	2:F:836:ARG:NH2	2.16	0.77
2:F:865:ASP:OD1	2:F:892:TYR:OH	2.03	0.77
2:G:218:LEU:HD23	2:G:219:GLN:H	1.48	0.77
2:G:309:ALA:O	2:G:369:GLN:NE2	2.18	0.77
2:H:412:MET:HA	2:H:416:GLN:HE21	1.50	0.77
2:F:218:LEU:HD23	2:F:219:GLN:H	1.48	0.76
2:H:218:LEU:HD23	2:H:219:GLN:H	1.48	0.76
2:F:380:ALA:O	2:F:383:THR:OG1	2.03	0.76
2:G:380:ALA:O	2:G:383:THR:OG1	2.03	0.76
2:H:380:ALA:O	2:H:383:THR:OG1	2.03	0.76
2:F:309:ALA:O	2:F:369:GLN:NE2	2.18	0.76
2:H:865:ASP:OD1	2:H:892:TYR:OH	2.03	0.76
2:E:380:ALA:O	2:E:383:THR:OG1	2.03	0.75
2:H:309:ALA:O	2:H:369:GLN:NE2	2.18	0.75
1:A:44:VAL:HG22	1:D:326:TYR:HB2	1.67	0.75
2:F:412:MET:HA	2:F:416:GLN:HE21	1.49	0.75
2:H:432:PHE:HA	2:H:435:CYS:HB2	1.69	0.75
2:G:432:PHE:HA	2:G:435:CYS:HB2	1.69	0.75
2:E:711:ILE:HB	2:E:886:VAL:HG12	1.69	0.75
2:E:865:ASP:OD1	2:E:892:TYR:OH	2.03	0.74
1:D:44:VAL:HG22	1:C:326:TYR:HB2	1.68	0.74
2:F:711:ILE:HB	2:F:886:VAL:HG12	1.69	0.74
2:E:773:SER:OG	2:E:775:LYS:O	2.06	0.74
2:G:456:LEU:HD11	2:G:579:SER:HB2	1.70	0.74
2:G:773:SER:OG	2:G:775:LYS:O	2.06	0.74
2:G:865:ASP:OD1	2:G:892:TYR:OH	2.03	0.74
1:C:218:GLN:HE21	1:C:235:GLN:HB3	1.54	0.73
2:E:432:PHE:HA	2:E:435:CYS:HB2	1.69	0.73
2:F:432:PHE:HA	2:F:435:CYS:HB2	1.69	0.73
1:D:218:GLN:HE21	1:D:235:GLN:HB3	1.54	0.73
2:G:711:ILE:HB	2:G:886:VAL:HG12	1.69	0.73
2:H:711:ILE:HB	2:H:886:VAL:HG12	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:GLN:HE21	1:B:235:GLN:HB3	1.54	0.72
3:A:502:ATP:N6	1:D:330:TYR:O	2.23	0.72
2:F:456:LEU:HD11	2:F:579:SER:HB2	1.70	0.72
1:D:81:CYS:HB2	2:H:41:PHE:HB3	1.69	0.72
2:H:456:LEU:HD11	2:H:579:SER:HB2	1.70	0.72
1:D:101:ALA:HB2	2:H:16:ARG:HB2	1.71	0.72
2:G:1031:TYR:HA	2:G:1282:LEU:HD11	1.71	0.71
2:G:1259:VAL:HA	2:G:1287:ALA:HB1	1.72	0.71
2:F:1259:VAL:HA	2:F:1287:ALA:HB1	1.72	0.71
2:F:773:SER:OG	2:F:775:LYS:O	2.06	0.71
2:H:1031:TYR:HA	2:H:1282:LEU:HD11	1.71	0.71
2:H:773:SER:OG	2:H:775:LYS:O	2.06	0.71
1:A:218:GLN:HE21	1:A:235:GLN:HB3	1.54	0.71
2:E:1031:TYR:HA	2:E:1282:LEU:HD11	1.71	0.71
2:E:456:LEU:HD11	2:E:579:SER:HB2	1.70	0.71
2:E:1259:VAL:HA	2:E:1287:ALA:HB1	1.72	0.70
2:E:420:LEU:O	2:E:424:ASP:HB3	1.92	0.70
2:F:1031:TYR:HA	2:F:1282:LEU:HD11	1.71	0.70
2:E:370:ARG:HG3	2:E:373:LEU:HD12	1.73	0.70
2:F:370:ARG:HG3	2:F:373:LEU:HD12	1.74	0.70
2:H:1259:VAL:HA	2:H:1287:ALA:HB1	1.72	0.70
2:H:219:GLN:HB3	2:H:227:LYS:HG2	1.73	0.70
2:H:370:ARG:HG3	2:H:373:LEU:HD12	1.73	0.70
2:G:420:LEU:O	2:G:424:ASP:HB3	1.92	0.70
2:H:420:LEU:O	2:H:424:ASP:HB3	1.92	0.70
2:G:452:LEU:HB3	2:G:461:LEU:HD22	1.75	0.69
2:E:132:PHE:O	2:E:135:LEU:N	2.23	0.69
2:H:29:ASP:OD2	2:H:105:HIS:ND1	2.20	0.69
2:E:193:ARG:O	2:E:195:TYR:HD1	1.75	0.69
2:F:420:LEU:O	2:F:424:ASP:HB3	1.92	0.69
2:F:193:ARG:O	2:F:195:TYR:HD1	1.75	0.69
2:G:1491:LEU:HD11	2:G:1507:ALA:HB1	1.74	0.69
2:F:1481:PHE:O	2:F:1486:ARG:NH2	2.26	0.69
2:F:219:GLN:HB3	2:F:227:LYS:HG2	1.73	0.69
2:E:29:ASP:OD2	2:E:105:HIS:ND1	2.21	0.69
2:H:10:ASN:HA	2:H:13:ALA:HB3	1.74	0.69
2:G:193:ARG:O	2:G:195:TYR:HD1	1.75	0.69
2:H:193:ARG:O	2:H:195:TYR:HD1	1.75	0.69
1:B:32:ARG:NE	1:B:277:HIS:O	2.26	0.69
2:E:1491:LEU:HD11	2:E:1507:ALA:HB1	1.74	0.69
2:G:370:ARG:HG3	2:G:373:LEU:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1491:LEU:HD11	2:H:1507:ALA:HB1	1.74	0.69
2:E:1389:LEU:HB3	2:E:1394:MET:HB2	1.74	0.69
1:D:276:HIS:CE1	1:D:279:GLN:HB2	2.28	0.68
2:E:1481:PHE:O	2:E:1486:ARG:NH2	2.26	0.68
2:G:1389:LEU:HB3	2:G:1394:MET:HB2	1.74	0.68
1:A:32:ARG:NE	1:A:277:HIS:O	2.26	0.68
1:B:313:GLN:HG2	1:B:338:LYS:HA	1.75	0.68
1:C:276:HIS:CE1	1:C:279:GLN:HB2	2.29	0.68
1:C:32:ARG:NE	1:C:277:HIS:O	2.26	0.68
2:G:1353:TYR:HH	2:G:1386:SER:HG	1.41	0.68
1:A:313:GLN:HG2	1:A:338:LYS:HA	1.75	0.68
1:B:326:TYR:HB2	1:C:44:VAL:HG22	1.75	0.68
1:C:313:GLN:HG2	1:C:338:LYS:HA	1.75	0.68
2:F:10:ASN:HA	2:F:13:ALA:HB3	1.75	0.68
2:G:1481:PHE:O	2:G:1486:ARG:NH2	2.26	0.68
2:H:1481:PHE:O	2:H:1486:ARG:NH2	2.26	0.68
2:F:1389:LEU:HB3	2:F:1394:MET:HB2	1.74	0.68
2:G:219:GLN:HB3	2:G:227:LYS:HG2	1.74	0.68
2:H:456:LEU:HD22	2:H:575:VAL:HA	1.76	0.68
1:B:276:HIS:CE1	1:B:279:GLN:HB2	2.28	0.68
1:D:32:ARG:NE	1:D:277:HIS:O	2.26	0.68
2:E:10:ASN:HA	2:E:13:ALA:HB3	1.75	0.68
2:E:219:GLN:HB3	2:E:227:LYS:HG2	1.74	0.68
2:G:456:LEU:HD22	2:G:575:VAL:HA	1.76	0.68
2:F:1491:LEU:HD11	2:F:1507:ALA:HB1	1.74	0.68
1:A:276:HIS:CE1	1:A:279:GLN:HB2	2.28	0.68
2:G:29:ASP:OD2	2:G:105:HIS:ND1	2.21	0.68
1:C:201:ARG:HA	1:C:256:ILE:HA	1.76	0.68
2:F:452:LEU:HB3	2:F:461:LEU:HD22	1.75	0.68
2:G:1376:ILE:HG12	2:G:1549:ILE:HB	1.76	0.68
2:H:132:PHE:O	2:H:135:LEU:N	2.23	0.68
2:H:1376:ILE:HG12	2:H:1549:ILE:HB	1.76	0.68
2:E:498:GLN:HB3	2:E:522:VAL:HG22	1.76	0.67
2:G:498:GLN:HB3	2:G:522:VAL:HG22	1.76	0.67
2:E:452:LEU:HB3	2:E:461:LEU:HD22	1.75	0.67
2:F:498:GLN:HB3	2:F:522:VAL:HG22	1.76	0.67
2:G:302:SER:OG	2:G:376:SER:O	2.12	0.67
1:B:201:ARG:HA	1:B:256:ILE:HA	1.77	0.67
2:G:10:ASN:HA	2:G:13:ALA:HB3	1.74	0.67
2:H:452:LEU:HB3	2:H:461:LEU:HD22	1.75	0.67
2:E:434:LEU:HD13	2:E:596:VAL:HA	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:829:LEU:HD13	2:E:833:GLN:HB2	1.77	0.67
2:H:1389:LEU:HB3	2:H:1394:MET:HB2	1.74	0.67
2:E:456:LEU:HD22	2:E:575:VAL:HA	1.76	0.67
2:F:1004:LEU:HB2	2:F:1012:LEU:HD21	1.77	0.67
2:F:434:LEU:HD13	2:F:596:VAL:HA	1.77	0.67
2:G:132:PHE:O	2:G:135:LEU:N	2.23	0.67
2:G:320:ILE:HG23	2:G:1284:LEU:HD11	1.77	0.67
3:D:501:ATP:N6	1:C:330:TYR:O	2.27	0.67
1:D:313:GLN:HG2	1:D:338:LYS:HA	1.74	0.67
2:F:132:PHE:O	2:F:135:LEU:N	2.23	0.67
2:G:1004:LEU:HB2	2:G:1012:LEU:HD21	1.77	0.67
2:H:829:LEU:HD13	2:H:833:GLN:HB2	1.77	0.67
2:G:455:ILE:HG13	2:G:456:LEU:H	1.60	0.66
2:E:1004:LEU:HB2	2:E:1012:LEU:HD21	1.77	0.66
2:E:1376:ILE:HG12	2:E:1549:ILE:HB	1.76	0.66
2:E:1353:TYR:HH	2:E:1386:SER:HG	1.42	0.66
2:H:1011:LEU:HD11	2:H:1091:LYS:HD3	1.78	0.66
2:H:704:PRO:HB2	2:H:707:GLN:HG3	1.78	0.66
1:D:184:SER:O	1:D:304:TYR:OH	2.09	0.66
2:F:302:SER:OG	2:F:376:SER:O	2.12	0.66
2:F:456:LEU:HD22	2:F:575:VAL:HA	1.76	0.66
2:H:498:GLN:HB3	2:H:522:VAL:HG22	1.77	0.66
2:E:1131:ILE:HA	2:E:1135:ILE:HG12	1.77	0.66
2:F:29:ASP:OD2	2:F:105:HIS:ND1	2.20	0.66
2:G:1131:ILE:HA	2:G:1135:ILE:HG12	1.77	0.66
2:H:434:LEU:HD13	2:H:596:VAL:HA	1.77	0.66
1:A:201:ARG:HA	1:A:256:ILE:HA	1.76	0.66
1:D:201:ARG:HA	1:D:256:ILE:HA	1.76	0.66
2:H:320:ILE:HG23	2:H:1284:LEU:HD11	1.77	0.66
1:D:50:ARG:HB2	3:D:501:ATP:C6	2.30	0.66
2:E:302:SER:OG	2:E:376:SER:O	2.12	0.66
2:F:1011:LEU:HD11	2:F:1091:LYS:HD3	1.78	0.66
2:G:704:PRO:HB2	2:G:707:GLN:HG3	1.78	0.66
2:F:829:LEU:HD13	2:F:833:GLN:HB2	1.77	0.66
2:H:302:SER:OG	2:H:376:SER:O	2.12	0.66
2:H:717:CYS:O	2:H:905:GLY:N	2.28	0.66
1:B:274:ASP:OD1	1:B:279:GLN:NE2	2.29	0.65
1:C:274:ASP:OD1	1:C:279:GLN:NE2	2.29	0.65
2:F:320:ILE:HG23	2:F:1284:LEU:HD11	1.77	0.65
2:G:717:CYS:O	2:G:905:GLY:N	2.28	0.65
2:H:1004:LEU:HB2	2:H:1012:LEU:HD21	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1376:ILE:HG12	2:F:1549:ILE:HB	1.76	0.65
1:A:274:ASP:OD1	1:A:279:GLN:NE2	2.29	0.65
1:D:274:ASP:OD1	1:D:279:GLN:NE2	2.29	0.65
2:F:1131:ILE:HA	2:F:1135:ILE:HG12	1.77	0.65
2:G:1011:LEU:HD11	2:G:1091:LYS:HD3	1.78	0.65
2:G:829:LEU:HD13	2:G:833:GLN:HB2	1.77	0.65
2:F:455:ILE:HG13	2:F:456:LEU:H	1.60	0.65
2:G:434:LEU:HD13	2:G:596:VAL:HA	1.77	0.65
2:H:1131:ILE:HA	2:H:1135:ILE:HG12	1.77	0.65
1:C:184:SER:O	1:C:304:TYR:OH	2.09	0.65
2:E:309:ALA:C	2:E:369:GLN:HE22	2.00	0.65
3:A:501:ATP:C6	1:B:50:ARG:HB2	2.32	0.65
2:E:1011:LEU:HD11	2:E:1091:LYS:HD3	1.78	0.65
2:F:309:ALA:C	2:F:369:GLN:HE22	2.00	0.65
2:E:320:ILE:HG23	2:E:1284:LEU:HD11	1.77	0.65
2:E:455:ILE:HG13	2:E:456:LEU:H	1.61	0.65
2:E:577:PHE:CZ	2:E:1282:LEU:HA	2.32	0.65
2:G:1389:LEU:HD22	2:G:1394:MET:HG3	1.79	0.65
2:H:1389:LEU:HD22	2:H:1394:MET:HG3	1.79	0.65
2:H:455:ILE:HG13	2:H:456:LEU:H	1.61	0.64
2:F:577:PHE:CZ	2:F:1282:LEU:HA	2.32	0.64
2:H:577:PHE:CZ	2:H:1282:LEU:HA	2.32	0.64
2:G:226:SER:HA	2:G:229:THR:HG22	1.79	0.64
2:E:1389:LEU:HD22	2:E:1394:MET:HG3	1.79	0.64
2:E:704:PRO:HB2	2:E:707:GLN:HG3	1.78	0.64
2:F:226:SER:HA	2:F:229:THR:HG22	1.79	0.64
1:A:184:SER:O	1:A:304:TYR:OH	2.09	0.64
1:B:177:ARG:NH2	1:B:208:SER:O	2.31	0.64
1:B:244:VAL:HG22	1:C:239:PRO:HB3	1.79	0.64
2:F:717:CYS:O	2:F:905:GLY:N	2.28	0.64
2:G:577:PHE:CZ	2:G:1282:LEU:HA	2.32	0.64
2:F:1389:LEU:HD22	2:F:1394:MET:HG3	1.79	0.64
2:F:704:PRO:HB2	2:F:707:GLN:HG3	1.78	0.64
1:A:177:ARG:NH2	1:A:208:SER:O	2.31	0.63
1:D:177:ARG:NH2	1:D:208:SER:O	2.31	0.63
1:D:218:GLN:O	1:D:284:ILE:N	2.24	0.63
2:F:94:LEU:HD11	2:F:357:VAL:HG21	1.80	0.63
2:H:309:ALA:C	2:H:369:GLN:HE22	2.00	0.63
1:D:38:LYS:HZ3	1:D:185:LYS:HG3	1.62	0.63
1:B:200:LEU:O	1:B:257:ILE:N	2.31	0.63
1:A:50:ARG:HB2	3:A:502:ATP:C6	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:LYS:HZ3	1:C:185:LYS:HG3	1.62	0.63
2:E:226:SER:HA	2:E:229:THR:HG22	1.79	0.63
2:F:686:PHE:HB2	2:F:696:LEU:HB2	1.81	0.63
2:F:452:LEU:HA	2:F:455:ILE:HG22	1.81	0.63
2:G:1424:ILE:HD12	2:G:1504:MET:HG2	1.81	0.63
2:H:452:LEU:HA	2:H:455:ILE:HG22	1.81	0.63
2:E:94:LEU:HD11	2:E:357:VAL:HG21	1.80	0.63
2:G:309:ALA:C	2:G:369:GLN:HE22	2.00	0.63
2:H:850:VAL:HG21	2:H:881:ARG:HE	1.64	0.63
2:E:686:PHE:HB2	2:E:696:LEU:HB2	1.81	0.63
2:H:1342:GLY:HA3	2:H:1501:ILE:HG21	1.81	0.63
2:H:226:SER:HA	2:H:229:THR:HG22	1.79	0.63
1:A:33:ALA:O	1:D:326:TYR:OH	2.06	0.62
2:G:94:LEU:HD11	2:G:357:VAL:HG21	1.80	0.62
1:A:227:GLU:OE2	1:D:194:GLY:N	2.31	0.62
1:C:200:LEU:O	1:C:257:ILE:N	2.31	0.62
1:B:81:CYS:HB2	2:F:41:PHE:HB3	1.80	0.62
2:G:1023:HIS:HB2	2:G:1147:LEU:HD12	1.81	0.62
2:G:1342:GLY:HA3	2:G:1501:ILE:HG21	1.81	0.62
2:G:1379:ARG:O	2:G:1384:LYS:NZ	2.32	0.62
2:H:1424:ILE:HD12	2:H:1504:MET:HG2	1.81	0.62
2:E:850:VAL:HG21	2:E:881:ARG:HE	1.64	0.62
2:E:1342:GLY:HA3	2:E:1501:ILE:HG21	1.81	0.62
2:F:295:PHE:CZ	2:F:383:THR:HB	2.35	0.62
1:A:34:ARG:NH2	1:A:303:SER:OG	2.32	0.62
2:E:717:CYS:O	2:E:905:GLY:N	2.28	0.62
2:F:1023:HIS:HB2	2:F:1147:LEU:HD12	1.81	0.62
2:G:850:VAL:HG21	2:G:881:ARG:HE	1.64	0.62
2:H:1379:ARG:O	2:H:1384:LYS:NZ	2.32	0.62
2:E:295:PHE:CZ	2:E:383:THR:HB	2.34	0.62
2:E:452:LEU:HA	2:E:455:ILE:HG22	1.81	0.62
2:E:1023:HIS:HB2	2:E:1147:LEU:HD12	1.81	0.62
2:F:1379:ARG:O	2:F:1384:LYS:NZ	2.32	0.62
2:F:295:PHE:HZ	2:F:383:THR:HB	1.65	0.62
2:G:295:PHE:CZ	2:G:383:THR:HB	2.35	0.62
1:A:94:ALA:HB2	1:A:114:ILE:HD11	1.82	0.62
2:G:573:PRO:HG2	2:G:575:VAL:HG22	1.82	0.62
2:H:295:PHE:CZ	2:H:383:THR:HB	2.35	0.62
1:B:94:ALA:HB2	1:B:114:ILE:HD11	1.82	0.62
2:F:379:VAL:O	2:F:383:THR:HG23	1.99	0.62
1:C:201:ARG:NH1	1:C:333:PHE:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:295:PHE:HZ	2:E:383:THR:HB	1.65	0.62
2:G:686:PHE:HB2	2:G:696:LEU:HB2	1.81	0.62
2:H:379:VAL:O	2:H:383:THR:HG23	1.99	0.62
2:H:573:PRO:HG2	2:H:575:VAL:HG22	1.82	0.62
2:H:686:PHE:HB2	2:H:696:LEU:HB2	1.81	0.62
1:A:251:LEU:HD11	1:A:254:PRO:HA	1.82	0.61
1:C:251:LEU:HD11	1:C:254:PRO:HA	1.82	0.61
2:E:573:PRO:HG2	2:E:575:VAL:HG22	1.82	0.61
2:G:379:VAL:O	2:G:383:THR:HG23	1.99	0.61
2:G:600:THR:O	2:G:604:LEU:HG	2.00	0.61
1:B:251:LEU:HD11	1:B:254:PRO:HA	1.82	0.61
2:E:1424:ILE:HD12	2:E:1504:MET:HG2	1.81	0.61
2:E:379:VAL:O	2:E:383:THR:HG23	1.99	0.61
2:F:1342:GLY:HA3	2:F:1501:ILE:HG21	1.81	0.61
2:F:1424:ILE:HD12	2:F:1504:MET:HG2	1.81	0.61
1:B:201:ARG:NH1	1:B:333:PHE:O	2.33	0.61
1:C:50:ARG:HB2	3:C:501:ATP:C6	2.34	0.61
2:H:1023:HIS:HB2	2:H:1147:LEU:HD12	1.81	0.61
2:H:600:THR:O	2:H:604:LEU:HG	2.00	0.61
1:A:329:ASP:OD1	1:A:331:SER:OG	2.14	0.61
2:E:1379:ARG:O	2:E:1384:LYS:NZ	2.32	0.61
2:E:774:GLN:HG2	2:E:1483:GLN:HG3	1.83	0.61
2:E:403:SER:HA	2:E:619:ILE:HG12	1.83	0.61
2:H:723:LEU:HB3	2:H:851:PHE:CZ	2.36	0.61
2:H:94:LEU:HD11	2:H:357:VAL:HG21	1.80	0.61
1:A:200:LEU:O	1:A:257:ILE:N	2.31	0.61
1:D:177:ARG:NH1	1:D:208:SER:OG	2.34	0.61
2:F:403:SER:HA	2:F:619:ILE:HG12	1.83	0.61
1:A:219:VAL:HA	1:A:283:ILE:HA	1.83	0.61
2:F:1403:ILE:HD13	2:F:1408:ASP:HA	1.82	0.61
2:F:723:LEU:HB3	2:F:851:PHE:CZ	2.36	0.61
2:G:1430:LEU:HD23	2:G:1474:ILE:HD13	1.83	0.61
2:G:403:SER:HA	2:G:619:ILE:HG12	1.83	0.61
2:H:774:GLN:HG2	2:H:1483:GLN:HG3	1.83	0.61
2:H:403:SER:HA	2:H:619:ILE:HG12	1.83	0.61
1:B:177:ARG:NH1	1:B:208:SER:OG	2.34	0.61
1:D:201:ARG:NH1	1:D:333:PHE:O	2.33	0.61
1:D:200:LEU:O	1:D:257:ILE:N	2.31	0.61
2:F:850:VAL:HG21	2:F:881:ARG:HE	1.64	0.61
2:G:774:GLN:HG2	2:G:1483:GLN:HG3	1.83	0.61
1:C:177:ARG:NH2	1:C:208:SER:O	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:600:THR:O	2:E:604:LEU:HG	2.00	0.60
1:A:330:TYR:O	3:A:501:ATP:N6	2.34	0.60
2:E:723:LEU:HB3	2:E:851:PHE:CZ	2.36	0.60
2:F:1110:ARG:HE	2:F:1114:THR:HG1	1.47	0.60
1:A:229:GLU:HB3	1:D:314:ARG:HH11	1.67	0.60
2:F:1430:LEU:HD23	2:F:1474:ILE:HD13	1.83	0.60
2:F:573:PRO:HG2	2:F:575:VAL:HG22	1.82	0.60
2:F:600:THR:O	2:F:604:LEU:HG	2.00	0.60
1:D:251:LEU:HD11	1:D:254:PRO:HA	1.82	0.60
2:H:295:PHE:HZ	2:H:383:THR:HB	1.65	0.60
1:A:177:ARG:NH1	1:A:208:SER:OG	2.34	0.60
1:B:219:VAL:HA	1:B:283:ILE:HA	1.83	0.60
1:B:34:ARG:NH2	1:B:303:SER:OG	2.32	0.60
1:A:326:TYR:HB2	1:B:44:VAL:HG22	1.81	0.60
1:C:94:ALA:HB2	1:C:114:ILE:HD11	1.82	0.60
1:C:177:ARG:NH1	1:C:208:SER:OG	2.34	0.60
1:C:34:ARG:NH2	1:C:303:SER:OG	2.32	0.60
1:B:101:ALA:HB2	2:F:16:ARG:HB2	1.83	0.60
2:F:322:GLY:O	2:F:326:HIS:ND1	2.30	0.60
2:G:452:LEU:HA	2:G:455:ILE:HG22	1.81	0.60
2:G:521:ARG:O	2:G:524:THR:OG1	2.17	0.60
1:A:203:GLY:HA2	1:A:254:PRO:HB3	1.84	0.60
1:B:38:LYS:HZ3	1:B:185:LYS:HG3	1.65	0.60
1:D:94:ALA:HB2	1:D:114:ILE:HD11	1.82	0.60
2:E:1110:ARG:HE	2:E:1114:THR:HG1	1.47	0.60
1:B:203:GLY:HA2	1:B:254:PRO:HB3	1.84	0.60
1:C:101:ALA:HB2	2:G:16:ARG:HB2	1.83	0.60
2:E:1403:ILE:HD13	2:E:1408:ASP:HA	1.83	0.60
2:E:314:PHE:CZ	2:E:448:GLY:HA2	2.37	0.60
2:F:774:GLN:HG2	2:F:1483:GLN:HG3	1.83	0.60
2:G:1110:ARG:HE	2:G:1114:THR:HG1	1.48	0.60
2:G:295:PHE:HZ	2:G:383:THR:HB	1.65	0.60
2:H:314:PHE:CZ	2:H:448:GLY:HA2	2.37	0.60
2:F:133:PRO:HB2	2:F:195:TYR:CZ	2.36	0.60
2:H:1403:ILE:HD13	2:H:1408:ASP:HA	1.82	0.60
2:H:1430:LEU:HD23	2:H:1474:ILE:HD13	1.83	0.60
2:H:133:PRO:HB2	2:H:195:TYR:CZ	2.36	0.60
1:C:219:VAL:HA	1:C:283:ILE:HA	1.83	0.60
2:E:133:PRO:HB2	2:E:195:TYR:CZ	2.36	0.60
2:F:1424:ILE:HD13	2:F:1491:LEU:HG	1.84	0.60
2:G:314:PHE:CZ	2:G:448:GLY:HA2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:521:ARG:O	2:F:524:THR:OG1	2.17	0.60
2:F:1154:ALA:O	2:F:1157:SER:OG	2.19	0.59
2:H:508:LEU:HD22	2:H:1431:PHE:HZ	1.67	0.59
1:A:38:LYS:HZ3	1:A:185:LYS:HG3	1.66	0.59
2:E:1424:ILE:HD13	2:E:1491:LEU:HG	1.84	0.59
2:F:1500:SER:O	2:F:1531:THR:N	2.28	0.59
1:C:203:GLY:HA2	1:C:254:PRO:HB3	1.84	0.59
1:D:203:GLY:HA2	1:D:254:PRO:HB3	1.84	0.59
2:G:133:PRO:HB2	2:G:195:TYR:CZ	2.36	0.59
2:G:723:LEU:HB3	2:G:851:PHE:CZ	2.36	0.59
2:H:494:GLU:O	2:H:498:GLN:HG2	2.02	0.59
1:C:231:VAL:HG23	1:C:234:HIS:HB2	1.84	0.59
2:F:314:PHE:CZ	2:F:448:GLY:HA2	2.37	0.59
2:F:422:ALA:O	2:F:426:ASN:ND2	2.36	0.59
2:G:508:LEU:HD22	2:G:1431:PHE:HZ	1.67	0.59
2:H:422:ALA:O	2:H:426:ASN:ND2	2.36	0.59
1:B:59:VAL:O	1:B:63:LEU:HB2	2.02	0.59
2:E:521:ARG:O	2:E:524:THR:OG1	2.17	0.59
2:F:442:PRO:HA	2:F:445:ILE:HG22	1.84	0.59
2:F:494:GLU:O	2:F:498:GLN:HG2	2.02	0.59
2:G:1269:ASN:O	2:G:1273:ARG:N	2.28	0.59
2:G:1403:ILE:HD13	2:G:1408:ASP:HA	1.82	0.59
2:H:1154:ALA:O	2:H:1157:SER:OG	2.19	0.59
1:B:231:VAL:HG23	1:B:234:HIS:HB2	1.84	0.59
2:E:1430:LEU:HD23	2:E:1474:ILE:HD13	1.83	0.59
1:C:238:ILE:HD11	1:C:259:HIS:CD2	2.38	0.59
1:A:201:ARG:NH1	1:A:333:PHE:O	2.33	0.59
1:A:59:VAL:O	1:A:63:LEU:HB2	2.02	0.59
1:D:231:VAL:HG23	1:D:234:HIS:HB2	1.84	0.59
1:D:219:VAL:HA	1:D:283:ILE:HA	1.83	0.59
2:E:322:GLY:O	2:E:326:HIS:ND1	2.30	0.59
2:E:494:GLU:O	2:E:498:GLN:HG2	2.02	0.59
2:G:422:ALA:O	2:G:426:ASN:ND2	2.35	0.59
1:B:307:ASP:OD1	1:B:308:GLU:N	2.36	0.59
2:G:1424:ILE:HD13	2:G:1491:LEU:HG	1.84	0.59
2:H:1375:GLY:N	2:H:1547:LEU:O	2.32	0.59
1:C:59:VAL:O	1:C:63:LEU:HB2	2.02	0.59
2:E:323:ILE:HG23	2:E:1267:ILE:HD11	1.85	0.59
2:F:508:LEU:HD22	2:F:1431:PHE:HZ	1.67	0.59
1:A:66:LEU:O	1:A:170:LYS:NZ	2.32	0.58
1:C:307:ASP:OD1	1:C:308:GLU:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:ASP:OD1	1:D:308:GLU:N	2.36	0.58
1:D:59:VAL:O	1:D:63:LEU:HB2	2.02	0.58
2:E:442:PRO:HA	2:E:445:ILE:HG22	1.84	0.58
2:G:494:GLU:O	2:G:498:GLN:HG2	2.02	0.58
2:H:1424:ILE:HD13	2:H:1491:LEU:HG	1.84	0.58
2:H:1500:SER:O	2:H:1531:THR:N	2.28	0.58
2:E:422:ALA:O	2:E:426:ASN:ND2	2.36	0.58
2:H:1501:ILE:HA	2:H:1531:THR:O	2.03	0.58
1:B:32:ARG:NH2	1:B:279:GLN:O	2.30	0.58
2:F:555:VAL:HG12	2:F:583:PHE:HD2	1.69	0.58
2:H:878:ASP:OD1	2:H:879:ASP:N	2.36	0.58
2:E:1501:ILE:HA	2:E:1531:THR:O	2.04	0.58
2:E:890:LEU:HA	2:E:893:LEU:HD23	1.84	0.58
2:F:878:ASP:OD1	2:F:879:ASP:N	2.36	0.58
2:G:442:PRO:HA	2:G:445:ILE:HG22	1.84	0.58
2:H:711:ILE:HG13	2:H:900:ILE:HB	1.86	0.58
1:D:329:ASP:OD1	1:D:331:SER:OG	2.14	0.58
2:F:1501:ILE:HA	2:F:1531:THR:O	2.04	0.58
2:F:786:ASN:ND2	2:F:822:ILE:HD11	2.19	0.58
2:F:711:ILE:HG13	2:F:900:ILE:HB	1.86	0.58
2:G:890:LEU:HA	2:G:893:LEU:HD23	1.85	0.58
2:H:322:GLY:O	2:H:326:HIS:ND1	2.30	0.58
1:A:218:GLN:O	1:A:284:ILE:N	2.24	0.58
1:A:231:VAL:HG23	1:A:234:HIS:HB2	1.84	0.58
1:D:238:ILE:HD11	1:D:259:HIS:CD2	2.38	0.58
1:D:34:ARG:NH2	1:D:303:SER:OG	2.32	0.58
2:E:598:ARG:NH1	2:E:1137:SER:OG	2.37	0.58
2:E:508:LEU:HD22	2:E:1431:PHE:HZ	1.67	0.58
2:F:1032:TRP:CH2	2:F:1066:VAL:HG13	2.39	0.58
2:H:1110:ARG:HE	2:H:1114:THR:HG1	1.49	0.58
2:H:1032:TRP:CH2	2:H:1066:VAL:HG13	2.39	0.58
2:H:442:PRO:HA	2:H:445:ILE:HG22	1.84	0.58
1:A:346:ALA:HA	1:A:349:LEU:HB2	1.86	0.58
1:B:238:ILE:HD11	1:B:259:HIS:CD2	2.38	0.58
2:E:555:VAL:HG12	2:E:583:PHE:HD2	1.69	0.58
2:F:323:ILE:HG23	2:F:1267:ILE:HD11	1.85	0.58
2:F:1353:TYR:HH	2:F:1386:SER:HG	1.48	0.58
2:G:323:ILE:HG23	2:G:1267:ILE:HD11	1.85	0.58
2:G:555:VAL:HG12	2:G:583:PHE:HD2	1.69	0.58
2:G:711:ILE:HG13	2:G:900:ILE:HB	1.86	0.58
1:C:346:ALA:HA	1:C:349:LEU:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:LEU:O	1:D:170:LYS:NZ	2.32	0.58
2:F:509:LEU:HB3	2:F:515:GLU:HG2	1.86	0.58
2:F:890:LEU:HA	2:F:893:LEU:HD23	1.84	0.58
2:G:598:ARG:NH1	2:G:1137:SER:OG	2.37	0.58
1:A:238:ILE:HD11	1:A:259:HIS:CD2	2.38	0.57
1:B:184:SER:O	1:B:304:TYR:OH	2.09	0.57
2:E:786:ASN:ND2	2:E:822:ILE:HD11	2.19	0.57
2:G:1032:TRP:CH2	2:G:1066:VAL:HG13	2.39	0.57
2:H:786:ASN:ND2	2:H:822:ILE:HD11	2.19	0.57
1:A:307:ASP:OD1	1:A:308:GLU:N	2.36	0.57
2:E:1032:TRP:CH2	2:E:1066:VAL:HG13	2.39	0.57
2:G:1154:ALA:O	2:G:1157:SER:OG	2.19	0.57
2:G:878:ASP:OD1	2:G:879:ASP:N	2.36	0.57
2:H:890:LEU:HA	2:H:893:LEU:HD23	1.84	0.57
1:A:229:GLU:HB3	1:D:314:ARG:NH1	2.18	0.57
1:B:346:ALA:HA	1:B:349:LEU:HB2	1.86	0.57
2:F:836:ARG:HD3	2:F:863:LEU:HD23	1.87	0.57
2:G:412:MET:HA	2:G:416:GLN:NE2	2.19	0.57
2:H:521:ARG:O	2:H:524:THR:OG1	2.17	0.57
1:B:218:GLN:O	1:B:284:ILE:N	2.24	0.57
1:A:189:ILE:HD11	1:A:309:ILE:HG22	1.87	0.57
2:G:1500:SER:O	2:G:1531:THR:N	2.28	0.57
2:G:1501:ILE:HA	2:G:1531:THR:O	2.04	0.57
2:F:378:TYR:HA	2:F:381:ILE:HG22	1.87	0.57
2:G:381:ILE:HG13	2:G:433:PHE:CE1	2.40	0.57
1:A:121:PHE:HE2	1:B:150:ILE:HD11	1.70	0.57
1:B:330:TYR:O	3:C:501:ATP:N6	2.38	0.57
1:D:346:ALA:HA	1:D:349:LEU:HB2	1.86	0.57
2:E:711:ILE:HG13	2:E:900:ILE:HB	1.86	0.57
2:H:1269:ASN:O	2:H:1273:ARG:N	2.28	0.57
1:B:329:ASP:OD1	1:B:331:SER:OG	2.14	0.57
2:E:1065:MET:O	2:E:1068:THR:OG1	2.20	0.57
2:E:836:ARG:HD3	2:E:863:LEU:HD23	1.87	0.57
2:E:878:ASP:OD1	2:E:879:ASP:N	2.36	0.57
2:G:786:ASN:ND2	2:G:822:ILE:HD11	2.19	0.57
1:D:189:ILE:HD11	1:D:309:ILE:HG22	1.87	0.57
2:G:378:TYR:HA	2:G:381:ILE:HG22	1.87	0.57
2:G:679:VAL:HG22	2:G:739:TRP:CD1	2.40	0.57
2:H:323:ILE:HG23	2:H:1267:ILE:HD11	1.85	0.57
2:H:555:VAL:HG12	2:H:583:PHE:HD2	1.69	0.57
1:A:218:GLN:NE2	1:A:235:GLN:HB3	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ILE:O	1:B:163:MET:HG2	2.05	0.57
1:C:329:ASP:OD1	1:C:331:SER:OG	2.14	0.57
2:E:1123:ARG:HA	2:E:1127:ASP:HB2	1.87	0.57
2:E:412:MET:HA	2:E:416:GLN:NE2	2.19	0.57
2:E:509:LEU:HB3	2:E:515:GLU:HG2	1.86	0.57
2:F:381:ILE:HG13	2:F:433:PHE:CE1	2.40	0.57
2:G:509:LEU:HB3	2:G:515:GLU:HG2	1.86	0.57
2:H:412:MET:HA	2:H:416:GLN:NE2	2.19	0.57
1:A:92:LEU:HD22	2:E:34:VAL:HG21	1.87	0.56
2:F:775:LYS:HB3	2:F:1483:GLN:HE22	1.70	0.56
2:H:381:ILE:HG13	2:H:433:PHE:CE1	2.40	0.56
1:D:159:ILE:O	1:D:163:MET:HG2	2.05	0.56
2:F:598:ARG:NH1	2:F:1137:SER:OG	2.37	0.56
2:G:1182:ARG:HH22	2:G:1186:ARG:HH21	1.53	0.56
2:H:378:TYR:HA	2:H:381:ILE:HG22	1.87	0.56
1:A:95:PHE:HE2	2:E:27:PHE:HA	1.70	0.56
2:F:1065:MET:O	2:F:1068:THR:OG1	2.20	0.56
1:B:189:ILE:HD11	1:B:309:ILE:HG22	1.87	0.56
2:F:1123:ARG:HA	2:F:1127:ASP:HB2	1.87	0.56
2:F:1338:TRP:O	2:F:1340:ASP:N	2.39	0.56
2:F:1431:PHE:HB2	2:F:1438:ASN:HD22	1.70	0.56
2:G:1431:PHE:HB2	2:G:1438:ASN:HD22	1.70	0.56
2:H:1415:HIS:O	2:H:1419:SER:OG	2.18	0.56
2:H:775:LYS:HB3	2:H:1483:GLN:HE22	1.71	0.56
2:H:679:VAL:HG22	2:H:739:TRP:CD1	2.40	0.56
2:E:378:TYR:HA	2:E:381:ILE:HG22	1.87	0.56
2:G:322:GLY:O	2:G:326:HIS:ND1	2.30	0.56
2:H:509:LEU:HB3	2:H:515:GLU:HG2	1.86	0.56
1:C:177:ARG:NH2	1:C:204:ASP:OD2	2.38	0.56
2:F:1182:ARG:HH22	2:F:1186:ARG:HH21	1.53	0.56
2:H:598:ARG:NH1	2:H:1137:SER:OG	2.37	0.56
2:H:1431:PHE:HB2	2:H:1438:ASN:HD22	1.70	0.56
1:B:218:GLN:NE2	1:B:235:GLN:HB3	2.20	0.56
1:C:218:GLN:O	1:C:284:ILE:N	2.24	0.56
2:E:775:LYS:HB3	2:E:1483:GLN:HE22	1.70	0.56
1:B:171:THR:HG23	1:C:169:MET:HE1	1.88	0.56
2:E:217:PHE:HB2	2:E:251:GLY:HA3	1.88	0.56
2:E:319:CYS:SG	2:E:362:LEU:HB2	2.46	0.56
2:E:381:ILE:HG13	2:E:433:PHE:CE1	2.40	0.56
2:G:1506:GLU:H	2:G:1535:ILE:HB	1.71	0.56
1:B:177:ARG:NH2	1:B:204:ASP:OD2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:MET:HE1	1:B:252:VAL:HG22	1.88	0.56
2:E:1338:TRP:O	2:E:1340:ASP:N	2.39	0.56
2:E:679:VAL:HG22	2:E:739:TRP:CD1	2.40	0.56
2:F:319:CYS:SG	2:F:362:LEU:HB2	2.46	0.56
2:G:1065:MET:O	2:G:1068:THR:OG1	2.20	0.56
2:G:775:LYS:HB3	2:G:1483:GLN:HE22	1.71	0.56
2:H:1506:GLU:H	2:H:1535:ILE:HB	1.71	0.56
1:A:159:ILE:O	1:A:163:MET:HG2	2.05	0.56
1:D:218:GLN:NE2	1:D:235:GLN:HB3	2.20	0.56
2:F:217:PHE:HB2	2:F:251:GLY:HA3	1.88	0.56
2:G:1123:ARG:HA	2:G:1127:ASP:HB2	1.87	0.56
2:H:319:CYS:SG	2:H:362:LEU:HB2	2.46	0.56
1:A:244:VAL:HG22	1:B:239:PRO:HB3	1.88	0.56
1:C:159:ILE:O	1:C:163:MET:HG2	2.05	0.56
2:G:706:GLY:N	2:G:882:THR:OG1	2.38	0.56
1:D:92:LEU:HD22	2:H:34:VAL:HG21	1.88	0.55
2:F:429:MET:HG2	2:F:433:PHE:CZ	2.41	0.55
2:H:429:MET:HG2	2:H:433:PHE:CZ	2.42	0.55
2:H:836:ARG:HD3	2:H:863:LEU:HD23	1.87	0.55
2:E:1032:TRP:HH2	2:E:1066:VAL:HG13	1.72	0.55
2:F:679:VAL:HG22	2:F:739:TRP:CD1	2.40	0.55
2:H:831:GLY:HA2	2:H:834:ARG:HD3	1.89	0.55
1:C:189:ILE:HD11	1:C:309:ILE:HG22	1.87	0.55
1:D:177:ARG:NH2	1:D:204:ASP:OD2	2.38	0.55
1:D:32:ARG:NH2	1:D:279:GLN:O	2.30	0.55
2:F:775:LYS:HB3	2:F:1483:GLN:NE2	2.21	0.55
2:G:429:MET:HG2	2:G:433:PHE:CZ	2.41	0.55
2:H:1246:TRP:HE1	2:H:1250:ARG:NH2	2.04	0.55
2:E:412:MET:HB2	2:E:417:ILE:HD11	1.89	0.55
2:F:412:MET:HB2	2:F:417:ILE:HD11	1.89	0.55
2:G:1351:VAL:HA	2:G:1397:THR:HA	1.89	0.55
2:G:686:PHE:HB3	2:G:730:MET:SD	2.47	0.55
2:H:1123:ARG:HA	2:H:1127:ASP:HB2	1.87	0.55
2:H:217:PHE:HB2	2:H:251:GLY:HA3	1.88	0.55
1:A:177:ARG:NH2	1:A:204:ASP:OD2	2.38	0.55
1:A:32:ARG:NH2	1:A:279:GLN:O	2.30	0.55
1:A:35:PHE:CD2	1:A:36:VAL:HG23	2.42	0.55
1:C:218:GLN:NE2	1:C:235:GLN:HB3	2.20	0.55
2:E:1431:PHE:HB2	2:E:1438:ASN:HD22	1.70	0.55
2:E:775:LYS:HB3	2:E:1483:GLN:NE2	2.21	0.55
2:F:1351:VAL:HA	2:F:1397:THR:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:141:VAL:O	2:G:144:THR:OG1	2.21	0.55
2:G:319:CYS:SG	2:G:362:LEU:HB2	2.46	0.55
2:G:1246:TRP:HE1	2:G:1250:ARG:NH2	2.04	0.55
2:G:1338:TRP:O	2:G:1340:ASP:N	2.39	0.55
2:H:1182:ARG:HH22	2:H:1186:ARG:HH21	1.53	0.55
2:H:1338:TRP:O	2:H:1340:ASP:N	2.38	0.55
2:H:686:PHE:HB3	2:H:730:MET:SD	2.47	0.55
2:E:1154:ALA:O	2:E:1157:SER:OG	2.19	0.55
2:E:1246:TRP:HE1	2:E:1250:ARG:NH2	2.04	0.55
2:E:313:GLY:H	2:E:369:GLN:NE2	2.05	0.55
2:F:686:PHE:HB3	2:F:730:MET:SD	2.47	0.55
2:H:1032:TRP:HH2	2:H:1066:VAL:HG13	1.72	0.55
2:E:429:MET:HG2	2:E:433:PHE:CZ	2.41	0.55
2:F:313:GLY:H	2:F:369:GLN:NE2	2.05	0.55
2:H:133:PRO:HB2	2:H:195:TYR:CE1	2.42	0.55
2:H:412:MET:HB2	2:H:417:ILE:HD11	1.89	0.55
2:H:775:LYS:HB3	2:H:1483:GLN:NE2	2.21	0.55
2:E:1182:ARG:HH22	2:E:1186:ARG:HH21	1.53	0.55
2:E:141:VAL:O	2:E:144:THR:OG1	2.21	0.55
2:E:1560:ASP:OD1	2:E:1561:LYS:N	2.39	0.55
2:E:686:PHE:HB3	2:E:730:MET:SD	2.47	0.55
2:F:1269:ASN:O	2:F:1273:ARG:N	2.28	0.55
2:G:1560:ASP:OD1	2:G:1561:LYS:N	2.39	0.55
2:G:836:ARG:HD3	2:G:863:LEU:HD23	1.87	0.55
1:B:35:PHE:CD2	1:B:36:VAL:HG23	2.42	0.54
1:D:129:VAL:O	1:D:130:THR:OG1	2.23	0.54
2:F:509:LEU:HB3	2:F:515:GLU:CG	2.38	0.54
2:G:775:LYS:HB3	2:G:1483:GLN:NE2	2.21	0.54
2:G:217:PHE:HB2	2:G:251:GLY:HA3	1.88	0.54
2:F:1032:TRP:HH2	2:F:1066:VAL:HG13	1.72	0.54
2:G:1180:TYR:O	2:G:1183:VAL:HG12	2.08	0.54
1:C:35:PHE:CD2	1:C:36:VAL:HG23	2.42	0.54
2:F:782:THR:HG22	2:F:784:GLU:H	1.73	0.54
2:G:137:ILE:HG23	2:G:195:TYR:OH	2.08	0.54
2:G:509:LEU:HB3	2:G:515:GLU:CG	2.38	0.54
2:G:723:LEU:HB3	2:G:851:PHE:HZ	1.73	0.54
2:H:313:GLY:H	2:H:369:GLN:NE2	2.05	0.54
2:H:782:THR:HG23	2:H:819:GLN:HA	1.89	0.54
2:E:716:GLY:N	3:E:2004:ATP:O3G	2.34	0.54
2:G:831:GLY:HA2	2:G:834:ARG:HD3	1.89	0.54
2:H:1180:TYR:O	2:H:1183:VAL:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1351:VAL:HA	2:H:1397:THR:HA	1.89	0.54
2:H:723:LEU:HB3	2:H:851:PHE:HZ	1.72	0.54
2:E:1351:VAL:HA	2:E:1397:THR:HA	1.89	0.54
2:E:133:PRO:HB2	2:E:195:TYR:CE1	2.42	0.54
2:F:141:VAL:O	2:F:144:THR:OG1	2.21	0.54
2:G:514:TRP:CD2	2:G:1441:PRO:HG2	2.42	0.54
2:E:370:ARG:HG2	2:E:1252:GLU:CD	2.28	0.54
2:E:514:TRP:CD2	2:E:1441:PRO:HG2	2.42	0.54
2:F:412:MET:HA	2:F:416:GLN:NE2	2.19	0.54
2:G:782:THR:HG23	2:G:819:GLN:HA	1.89	0.54
2:F:1180:TYR:O	2:F:1183:VAL:HG12	2.08	0.54
2:G:1032:TRP:HH2	2:G:1066:VAL:HG13	1.72	0.54
2:G:47:LEU:HD21	2:G:126:ASN:HD22	1.73	0.54
2:H:514:TRP:CD2	2:H:1441:PRO:HG2	2.42	0.54
1:C:129:VAL:O	1:C:130:THR:OG1	2.23	0.54
1:A:46:HIS:O	1:D:330:TYR:HD2	1.91	0.54
1:D:35:PHE:CD2	1:D:36:VAL:HG23	2.42	0.54
2:E:47:LEU:HD21	2:E:126:ASN:HD22	1.73	0.54
2:F:1506:GLU:H	2:F:1535:ILE:HB	1.71	0.54
2:F:514:TRP:CD2	2:F:1441:PRO:HG2	2.42	0.54
2:G:412:MET:HB2	2:G:417:ILE:HD11	1.89	0.54
2:H:1129:ASN:OD1	2:H:1133:GLN:NE2	2.41	0.54
2:H:137:ILE:HG23	2:H:195:TYR:OH	2.08	0.54
2:H:782:THR:HG22	2:H:784:GLU:H	1.73	0.54
2:E:1011:LEU:HD22	2:E:1088:THR:HB	1.90	0.54
2:E:509:LEU:HB3	2:E:515:GLU:CG	2.38	0.54
2:F:1246:TRP:HE1	2:F:1250:ARG:NH2	2.04	0.54
2:G:1431:PHE:O	2:G:1438:ASN:ND2	2.34	0.54
2:G:1129:ASN:OD1	2:G:1133:GLN:NE2	2.41	0.54
2:G:586:LEU:O	2:G:589:PRO:HD2	2.08	0.54
2:H:1011:LEU:HD22	2:H:1088:THR:HB	1.90	0.54
2:H:47:LEU:HD21	2:H:126:ASN:HD22	1.73	0.54
2:H:509:LEU:HB3	2:H:515:GLU:CG	2.38	0.54
1:B:317:PRO:HB3	1:C:232:PRO:HD3	1.89	0.53
1:C:32:ARG:NH2	1:C:279:GLN:O	2.30	0.53
2:E:706:GLY:N	2:E:882:THR:OG1	2.38	0.53
2:F:1129:ASN:OD1	2:F:1133:GLN:NE2	2.41	0.53
2:F:370:ARG:HG2	2:F:1252:GLU:CD	2.29	0.53
2:F:137:ILE:HG23	2:F:195:TYR:OH	2.08	0.53
2:F:586:LEU:O	2:F:589:PRO:HD2	2.08	0.53
2:H:1431:PHE:O	2:H:1438:ASN:ND2	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1180:TYR:O	2:E:1183:VAL:HG12	2.08	0.53
2:E:1500:SER:O	2:E:1531:THR:N	2.28	0.53
2:F:47:LEU:HD21	2:F:126:ASN:HD22	1.73	0.53
2:F:831:GLY:HA2	2:F:834:ARG:HD3	1.89	0.53
2:G:133:PRO:HB2	2:G:195:TYR:CE1	2.42	0.53
2:G:313:GLY:H	2:G:369:GLN:NE2	2.05	0.53
1:A:112:THR:OG1	1:A:137:MET:N	2.42	0.53
2:E:1269:ASN:O	2:E:1273:ARG:N	2.28	0.53
2:E:782:THR:HG23	2:E:819:GLN:HA	1.89	0.53
2:F:133:PRO:HB2	2:F:195:TYR:CE1	2.42	0.53
2:F:782:THR:HG23	2:F:819:GLN:HA	1.89	0.53
2:G:1398:PHE:CD2	2:G:1399:GLU:HG2	2.44	0.53
2:H:1344:ILE:O	2:H:1368:ILE:N	2.29	0.53
2:H:451:LEU:O	2:H:455:ILE:N	2.42	0.53
2:H:586:LEU:O	2:H:589:PRO:HD2	2.08	0.53
1:B:275:LEU:HD21	1:B:311:TRP:HB2	1.91	0.53
2:E:137:ILE:HG23	2:E:195:TYR:OH	2.08	0.53
2:E:1460:LYS:HG2	2:E:1464:LYS:HZ2	1.74	0.53
2:E:1506:GLU:H	2:E:1535:ILE:HB	1.71	0.53
2:H:370:ARG:HG2	2:H:1252:GLU:CD	2.29	0.53
1:A:275:LEU:HD21	1:A:311:TRP:HB2	1.91	0.53
2:E:1129:ASN:OD1	2:E:1133:GLN:NE2	2.41	0.53
2:E:1383:GLY:HA2	4:E:2001:ADP:H5'1	1.91	0.53
2:E:451:LEU:O	2:E:455:ILE:N	2.41	0.53
2:E:831:GLY:HA2	2:E:834:ARG:HD3	1.89	0.53
2:F:723:LEU:HB3	2:F:851:PHE:HZ	1.72	0.53
2:G:1011:LEU:HD22	2:G:1088:THR:HB	1.90	0.53
2:H:1398:PHE:CD2	2:H:1399:GLU:HG2	2.44	0.53
2:E:1398:PHE:CD2	2:E:1399:GLU:HG2	2.44	0.53
2:F:1011:LEU:HD22	2:F:1088:THR:HB	1.91	0.53
2:G:193:ARG:O	2:G:195:TYR:CD1	2.59	0.53
2:H:71:HIS:O	2:H:75:TRP:HD1	1.92	0.53
2:E:586:LEU:O	2:E:589:PRO:HD2	2.08	0.53
2:E:779:LEU:HA	2:E:1205:GLU:OE1	2.09	0.53
2:F:71:HIS:O	2:F:75:TRP:HD1	1.92	0.53
2:G:1383:GLY:HA2	4:G:2001:ADP:H5'1	1.91	0.53
2:G:782:THR:HG22	2:G:784:GLU:H	1.73	0.53
2:H:500:ASN:O	2:H:504:ARG:HG2	2.09	0.53
1:B:199:MET:HG2	1:B:258:TYR:CB	2.39	0.53
1:D:199:MET:HG2	1:D:258:TYR:CB	2.39	0.53
2:E:500:ASN:O	2:E:504:ARG:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:193:ARG:O	2:F:195:TYR:CD1	2.59	0.53
2:G:1375:GLY:N	2:G:1547:LEU:O	2.32	0.53
2:E:782:THR:HG22	2:E:784:GLU:H	1.73	0.53
2:F:1383:GLY:HA2	4:F:2001:ADP:H5'1	1.91	0.53
2:G:500:ASN:O	2:G:504:ARG:HG2	2.09	0.53
2:H:1383:GLY:HA2	4:H:2001:ADP:H5'1	1.91	0.53
2:H:706:GLY:N	2:H:882:THR:OG1	2.38	0.53
2:H:686:PHE:HA	2:H:732:LYS:HA	1.91	0.52
1:A:199:MET:HG2	1:A:258:TYR:CB	2.39	0.52
2:E:1344:ILE:O	2:E:1368:ILE:N	2.29	0.52
2:E:71:HIS:O	2:E:75:TRP:HD1	1.92	0.52
2:F:1398:PHE:CD2	2:F:1399:GLU:HG2	2.44	0.52
2:F:369:GLN:HG3	2:F:370:ARG:HD2	1.92	0.52
2:F:451:LEU:O	2:F:455:ILE:N	2.42	0.52
2:F:500:ASN:O	2:F:504:ARG:HG2	2.09	0.52
2:G:317:PRO:HA	2:G:320:ILE:HD12	1.92	0.52
2:G:451:LEU:O	2:G:455:ILE:N	2.41	0.52
2:G:71:HIS:O	2:G:75:TRP:HD1	1.92	0.52
2:H:317:PRO:HA	2:H:320:ILE:HD12	1.92	0.52
1:C:199:MET:HG2	1:C:258:TYR:CB	2.39	0.52
2:E:723:LEU:HB3	2:E:851:PHE:HZ	1.73	0.52
2:F:779:LEU:HA	2:F:1205:GLU:OE1	2.09	0.52
2:F:395:ILE:O	2:F:399:ILE:HG12	2.09	0.52
2:G:868:MET:O	2:G:872:ILE:HB	2.10	0.52
1:B:199:MET:HG2	1:B:258:TYR:HB2	1.92	0.52
2:E:1370:PRO:O	2:E:1531:THR:OG1	2.16	0.52
2:F:139:LEU:HD12	2:F:143:TRP:HE1	1.74	0.52
2:G:1351:VAL:HG22	2:G:1361:LEU:HB3	1.91	0.52
2:E:193:ARG:O	2:E:195:TYR:CD1	2.60	0.52
2:H:779:LEU:HA	2:H:1205:GLU:OE1	2.09	0.52
2:H:369:GLN:HG3	2:H:370:ARG:HD2	1.92	0.52
1:A:199:MET:HG2	1:A:258:TYR:HB2	1.92	0.52
1:D:275:LEU:HD21	1:D:311:TRP:HB2	1.91	0.52
2:E:139:LEU:HD12	2:E:143:TRP:HE1	1.74	0.52
2:E:369:GLN:HG3	2:E:370:ARG:HD2	1.92	0.52
2:F:686:PHE:HA	2:F:732:LYS:HA	1.91	0.52
2:G:779:LEU:HA	2:G:1205:GLU:OE1	2.09	0.52
2:G:370:ARG:HG2	2:G:1252:GLU:CD	2.29	0.52
2:G:1556:ILE:HG21	2:G:1559:PHE:HB3	1.91	0.52
2:G:369:GLN:HG3	2:G:370:ARG:HD2	1.92	0.52
2:E:1556:ILE:HG21	2:E:1559:PHE:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:686:PHE:HA	2:E:732:LYS:HA	1.91	0.52
2:G:1408:ASP:OD1	2:G:1409:ILE:N	2.40	0.52
2:H:395:ILE:O	2:H:399:ILE:HG12	2.09	0.52
2:F:771:TYR:HD2	2:F:1212:THR:HG22	1.75	0.52
2:G:395:ILE:O	2:G:399:ILE:HG12	2.09	0.52
1:C:275:LEU:HD21	1:C:311:TRP:HB2	1.91	0.52
2:E:1351:VAL:HG22	2:E:1361:LEU:HB3	1.91	0.52
2:E:1431:PHE:O	2:E:1438:ASN:ND2	2.35	0.52
2:E:317:PRO:HA	2:E:320:ILE:HD12	1.92	0.52
2:F:1310:ALA:HA	2:F:1313:ARG:NH2	2.25	0.52
2:F:1375:GLY:O	2:F:1549:ILE:N	2.43	0.52
2:F:587:VAL:HA	2:F:590:LEU:HD12	1.92	0.52
2:H:1310:ALA:HA	2:H:1313:ARG:NH2	2.25	0.52
2:H:868:MET:O	2:H:872:ILE:HB	2.10	0.52
1:B:121:PHE:HE2	1:C:150:ILE:HD11	1.75	0.52
1:C:199:MET:HG2	1:C:258:TYR:HB2	1.92	0.52
2:E:587:VAL:HA	2:E:590:LEU:HD12	1.92	0.52
2:G:1004:LEU:HD22	2:G:1012:LEU:HD11	1.92	0.52
1:D:112:THR:OG1	1:D:137:MET:N	2.41	0.51
2:E:1375:GLY:N	2:E:1547:LEU:O	2.32	0.51
2:G:1310:ALA:HA	2:G:1313:ARG:NH2	2.25	0.51
2:F:1351:VAL:HG22	2:F:1361:LEU:HB3	1.91	0.51
2:F:1375:GLY:N	2:F:1547:LEU:O	2.32	0.51
2:H:139:LEU:HD12	2:H:143:TRP:HE1	1.74	0.51
2:H:382:GLU:OE2	2:H:386:ASN:ND2	2.37	0.51
2:E:395:ILE:O	2:E:399:ILE:HG12	2.09	0.51
2:E:42:ILE:HG23	2:E:43:THR:HG23	1.92	0.51
2:E:868:MET:O	2:E:872:ILE:HB	2.10	0.51
2:F:1004:LEU:HD22	2:F:1012:LEU:HD11	1.92	0.51
2:F:317:PRO:HA	2:F:320:ILE:HD12	1.92	0.51
2:F:706:GLY:N	2:F:882:THR:OG1	2.38	0.51
2:G:139:LEU:HD12	2:G:143:TRP:HE1	1.74	0.51
2:H:42:ILE:HG23	2:H:43:THR:HG23	1.92	0.51
2:H:587:VAL:HA	2:H:590:LEU:HD12	1.92	0.51
1:A:95:PHE:HD1	1:A:100:LEU:HD12	1.75	0.51
1:A:272:PRO:HD3	1:A:311:TRP:CZ2	2.46	0.51
2:E:1310:ALA:HA	2:E:1313:ARG:NH2	2.25	0.51
2:H:1375:GLY:O	2:H:1549:ILE:N	2.43	0.51
2:H:1560:ASP:OD1	2:H:1561:LYS:N	2.39	0.51
1:D:272:PRO:HD3	1:D:311:TRP:CZ2	2.46	0.51
2:E:1004:LEU:HD22	2:E:1012:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1375:GLY:O	2:E:1549:ILE:N	2.43	0.51
2:E:771:TYR:HD2	2:E:1212:THR:HG22	1.75	0.51
2:G:686:PHE:HA	2:G:732:LYS:HA	1.91	0.51
2:H:1004:LEU:HD22	2:H:1012:LEU:HD11	1.93	0.51
2:H:1065:MET:O	2:H:1068:THR:OG1	2.20	0.51
1:B:272:PRO:HD3	1:B:311:TRP:CZ2	2.46	0.51
1:C:112:THR:OG1	1:C:137:MET:N	2.42	0.51
2:F:868:MET:O	2:F:872:ILE:HB	2.10	0.51
2:H:253:LEU:HD11	2:H:1231:ASP:HB3	1.93	0.51
2:H:1408:ASP:OD1	2:H:1409:ILE:N	2.40	0.51
1:A:47:LYS:HE3	1:D:327:SER:HB2	1.93	0.51
1:B:275:LEU:HA	1:B:306:ALA:HB1	1.93	0.51
1:D:199:MET:HG2	1:D:258:TYR:HB2	1.92	0.51
2:F:1560:ASP:OD1	2:F:1561:LYS:N	2.39	0.51
2:F:218:LEU:HD23	2:F:219:GLN:N	2.23	0.51
2:F:598:ARG:HH12	2:F:1137:SER:HG	1.56	0.51
2:G:273:GLN:O	2:G:277:ASP:N	2.39	0.51
2:G:587:VAL:HA	2:G:590:LEU:HD12	1.92	0.51
2:G:771:TYR:HD2	2:G:1212:THR:HG22	1.75	0.51
2:H:193:ARG:O	2:H:195:TYR:CD1	2.59	0.51
2:H:777:TRP:CZ3	2:H:1209:GLY:HA3	2.46	0.51
1:A:46:HIS:HD2	1:D:330:TYR:CZ	2.29	0.51
2:G:1375:GLY:O	2:G:1549:ILE:N	2.43	0.51
2:G:39:LEU:HD22	2:G:142:TYR:CE2	2.46	0.51
2:H:716:GLY:N	3:H:2004:ATP:O3G	2.34	0.51
1:A:209:MET:HE1	1:A:252:VAL:HG22	1.92	0.51
1:B:108:GLU:HB2	1:B:141:GLU:HG3	1.93	0.51
1:C:108:GLU:HB2	1:C:141:GLU:HG3	1.93	0.51
1:D:344:CYS:SG	1:D:349:LEU:HD22	2.51	0.51
2:E:253:LEU:HD11	2:E:1231:ASP:HB3	1.93	0.51
2:E:1451:TRP:CE3	2:E:1460:LYS:HG3	2.46	0.51
2:G:777:TRP:CZ3	2:G:1209:GLY:HA3	2.46	0.51
2:H:704:PRO:HB2	2:H:707:GLN:CG	2.41	0.51
2:H:771:TYR:HD2	2:H:1212:THR:HG22	1.75	0.51
1:B:95:PHE:HD1	1:B:100:LEU:HD12	1.75	0.50
1:C:272:PRO:HD3	1:C:311:TRP:CZ2	2.46	0.50
2:E:1482:SER:OG	3:E:2004:ATP:O3A	2.26	0.50
2:F:1451:TRP:CE3	2:F:1460:LYS:HG3	2.46	0.50
2:F:1556:ILE:HG21	2:F:1559:PHE:HB3	1.91	0.50
2:F:42:ILE:HG23	2:F:43:THR:HG23	1.92	0.50
2:G:104:LEU:H	2:G:104:LEU:HD23	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1351:VAL:HG22	2:H:1361:LEU:HB3	1.91	0.50
2:H:1478:GLY:HA3	2:H:1486:ARG:HD3	1.94	0.50
1:C:66:LEU:O	1:C:170:LYS:NZ	2.32	0.50
2:G:777:TRP:CH2	2:G:1209:GLY:HA3	2.46	0.50
2:H:1556:ILE:HG21	2:H:1559:PHE:HB3	1.91	0.50
2:H:511:LEU:HD22	2:H:1392:PHE:HD2	1.76	0.50
1:A:344:CYS:SG	1:A:349:LEU:HD22	2.51	0.50
1:C:95:PHE:HD1	1:C:100:LEU:HD12	1.75	0.50
2:E:1064:ALA:O	2:E:1068:THR:HG23	2.12	0.50
2:F:357:VAL:HA	2:F:360:VAL:HG12	1.94	0.50
2:G:1478:GLY:HA3	2:G:1486:ARG:HD3	1.94	0.50
2:G:452:LEU:HD21	2:G:582:LEU:HD22	1.93	0.50
2:H:1460:LYS:HG2	2:H:1464:LYS:HZ2	1.76	0.50
1:D:238:ILE:HD12	1:D:267:LEU:HD13	1.93	0.50
2:E:39:LEU:HD22	2:E:142:TYR:CE2	2.46	0.50
2:E:777:TRP:CZ3	2:E:1209:GLY:HA3	2.46	0.50
2:F:1344:ILE:O	2:F:1368:ILE:N	2.29	0.50
2:F:253:LEU:HD11	2:F:1231:ASP:HB3	1.93	0.50
2:G:704:PRO:HB2	2:G:707:GLN:CG	2.41	0.50
1:B:344:CYS:SG	1:B:349:LEU:HD22	2.51	0.50
1:C:275:LEU:HA	1:C:306:ALA:HB1	1.94	0.50
2:E:777:TRP:CH2	2:E:1209:GLY:HA3	2.47	0.50
2:F:1353:TYR:OH	2:F:1386:SER:OG	2.23	0.50
2:G:511:LEU:HD22	2:G:1392:PHE:HD2	1.76	0.50
2:H:1451:TRP:CE3	2:H:1460:LYS:HG3	2.47	0.50
2:H:452:LEU:HD21	2:H:582:LEU:HD22	1.93	0.50
2:E:1408:ASP:OD1	2:E:1409:ILE:N	2.40	0.50
2:E:287:ILE:HD11	2:E:607:VAL:HG13	1.94	0.50
2:E:452:LEU:HD21	2:E:582:LEU:HD22	1.92	0.50
2:F:1408:ASP:OD1	2:F:1409:ILE:N	2.40	0.50
2:F:39:LEU:HD22	2:F:142:TYR:CE2	2.46	0.50
2:H:287:ILE:HD11	2:H:607:VAL:HG13	1.94	0.50
1:A:108:GLU:HB2	1:A:141:GLU:HG3	1.93	0.50
1:A:275:LEU:HA	1:A:306:ALA:HB1	1.94	0.50
1:C:209:MET:O	1:C:292:GLU:HB2	2.12	0.50
1:D:108:GLU:HB2	1:D:141:GLU:HG3	1.93	0.50
2:E:1478:GLY:HA3	2:E:1486:ARG:HD3	1.94	0.50
2:E:357:VAL:HA	2:E:360:VAL:HG12	1.94	0.50
2:E:39:LEU:HA	2:E:42:ILE:HG22	1.94	0.50
2:F:777:TRP:CZ3	2:F:1209:GLY:HA3	2.46	0.50
2:G:1100:LEU:HD22	2:G:1314:ILE:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:253:LEU:HD11	2:G:1231:ASP:HB3	1.93	0.50
2:H:363:PHE:CD1	2:H:1260:LEU:HB2	2.47	0.50
2:H:777:TRP:CH2	2:H:1209:GLY:HA3	2.47	0.50
1:A:238:ILE:HD12	1:A:267:LEU:HD13	1.93	0.50
1:B:66:LEU:O	1:B:170:LYS:NZ	2.32	0.50
1:D:95:PHE:HD1	1:D:100:LEU:HD12	1.76	0.50
2:E:382:GLU:OE2	2:E:386:ASN:ND2	2.37	0.50
2:E:704:PRO:HB2	2:E:707:GLN:CG	2.41	0.50
2:F:1064:ALA:O	2:F:1068:THR:HG23	2.12	0.50
2:F:39:LEU:HA	2:F:42:ILE:HG22	1.94	0.50
2:G:357:VAL:HA	2:G:360:VAL:HG12	1.93	0.50
1:A:187:ALA:O	1:A:310:LEU:N	2.45	0.50
2:F:1478:GLY:HA3	2:F:1486:ARG:HD3	1.94	0.50
2:F:687:THR:HB	2:F:694:PRO:HA	1.94	0.50
2:G:317:PRO:HG3	2:G:585:ILE:HD12	1.94	0.50
2:G:42:ILE:HG23	2:G:43:THR:HG23	1.92	0.50
2:G:552:ILE:HA	2:G:555:VAL:HG22	1.94	0.50
2:H:1346:ILE:HD11	2:H:1364:VAL:HG22	1.94	0.50
2:H:141:VAL:O	2:H:144:THR:OG1	2.21	0.50
2:H:686:PHE:HE2	2:H:699:ILE:HD11	1.77	0.50
1:C:344:CYS:SG	1:C:349:LEU:HD22	2.51	0.49
1:D:60:PHE:O	1:D:64:VAL:HG23	2.12	0.49
2:E:1346:ILE:HD11	2:E:1364:VAL:HG22	1.93	0.49
2:F:716:GLY:N	3:F:2004:ATP:O3G	2.33	0.49
2:F:287:ILE:HD11	2:F:607:VAL:HG13	1.94	0.49
2:F:452:LEU:HD21	2:F:582:LEU:HD22	1.93	0.49
2:F:704:PRO:HB2	2:F:707:GLN:CG	2.41	0.49
2:G:1064:ALA:O	2:G:1068:THR:HG23	2.12	0.49
1:B:72:LEU:O	1:B:76:THR:HG23	2.13	0.49
1:C:220:VAL:HG12	1:C:235:GLN:HG2	1.94	0.49
1:C:239:PRO:O	1:C:259:HIS:ND1	2.34	0.49
1:C:60:PHE:O	1:C:64:VAL:HG23	2.12	0.49
1:D:220:VAL:HG12	1:D:235:GLN:HG2	1.94	0.49
1:D:275:LEU:HA	1:D:306:ALA:HB1	1.93	0.49
2:F:104:LEU:HD23	2:F:104:LEU:H	1.77	0.49
2:G:1451:TRP:CE3	2:G:1460:LYS:HG3	2.46	0.49
2:G:686:PHE:HE2	2:G:699:ILE:HD11	1.77	0.49
2:G:687:THR:HB	2:G:694:PRO:HA	1.95	0.49
2:H:1100:LEU:HD22	2:H:1314:ILE:HG23	1.94	0.49
2:H:39:LEU:HA	2:H:42:ILE:HG22	1.94	0.49
2:H:39:LEU:HD22	2:H:142:TYR:CE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ALA:HB3	1:A:47:LYS:HZ2	1.76	0.49
1:C:238:ILE:HD12	1:C:267:LEU:HD13	1.93	0.49
2:E:1539:VAL:O	2:E:1542:ILE:HG22	2.13	0.49
2:E:686:PHE:HE2	2:E:699:ILE:HD11	1.77	0.49
2:H:1064:ALA:O	2:H:1068:THR:HG23	2.12	0.49
2:H:317:PRO:HG3	2:H:585:ILE:HD12	1.94	0.49
1:D:187:ALA:O	1:D:310:LEU:N	2.45	0.49
2:E:363:PHE:CD1	2:E:1260:LEU:HB2	2.47	0.49
2:F:317:PRO:HG3	2:F:585:ILE:HD12	1.94	0.49
2:F:777:TRP:CH2	2:F:1209:GLY:HA3	2.47	0.49
2:G:1415:HIS:O	2:G:1419:SER:OG	2.18	0.49
2:H:104:LEU:H	2:H:104:LEU:HD23	1.77	0.49
1:A:60:PHE:O	1:A:64:VAL:HG23	2.12	0.49
1:C:322:GLU:N	1:C:325:ARG:O	2.46	0.49
2:F:1100:LEU:HD22	2:F:1314:ILE:HG23	1.94	0.49
2:F:1539:VAL:O	2:F:1542:ILE:HG22	2.13	0.49
2:F:511:LEU:HD22	2:F:1392:PHE:HD2	1.76	0.49
2:H:1151:SER:O	2:H:1155:VAL:HG23	2.13	0.49
1:A:220:VAL:HG12	1:A:235:GLN:HG2	1.94	0.49
1:A:319:VAL:HB	1:B:232:PRO:HG2	1.95	0.49
1:A:322:GLU:N	1:A:325:ARG:O	2.46	0.49
1:B:209:MET:O	1:B:292:GLU:HB2	2.12	0.49
1:C:72:LEU:O	1:C:76:THR:HG23	2.13	0.49
2:E:317:PRO:HG3	2:E:585:ILE:HD12	1.94	0.49
2:E:511:LEU:HD22	2:E:1392:PHE:HD2	1.76	0.49
2:E:778:LEU:HA	2:E:841:ARG:NH1	2.28	0.49
2:H:381:ILE:HG21	2:H:1241:THR:HG21	1.95	0.49
1:B:238:ILE:HD12	1:B:267:LEU:HD13	1.93	0.49
1:B:187:ALA:O	1:B:310:LEU:N	2.45	0.49
1:C:272:PRO:O	1:C:273:SER:OG	2.27	0.49
1:D:322:GLU:N	1:D:325:ARG:O	2.46	0.49
2:E:1003:TYR:CE1	2:E:1092:VAL:HG11	2.48	0.49
2:E:1100:LEU:HD22	2:E:1314:ILE:HG23	1.94	0.49
2:E:1373:LYS:O	2:E:1546:ASP:N	2.31	0.49
2:F:1066:VAL:O	2:F:1069:VAL:HG12	2.13	0.49
2:F:363:PHE:CD1	2:F:1260:LEU:HB2	2.47	0.49
2:F:461:LEU:O	2:F:463:GLY:N	2.46	0.49
2:G:363:PHE:CD1	2:G:1260:LEU:HB2	2.47	0.49
2:G:686:PHE:O	2:G:695:THR:N	2.46	0.49
1:C:113:SER:OG	1:C:135:GLY:O	2.29	0.49
1:C:209:MET:HE1	1:C:252:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1151:SER:O	2:E:1155:VAL:HG23	2.13	0.49
2:E:1392:PHE:HB3	2:E:1418:ARG:NE	2.28	0.49
2:E:771:TYR:CD2	2:E:1212:THR:HG22	2.48	0.49
2:F:552:ILE:HA	2:F:555:VAL:HG22	1.94	0.49
2:G:1151:SER:O	2:G:1155:VAL:HG23	2.13	0.49
2:G:381:ILE:HG21	2:G:1241:THR:HG21	1.95	0.49
2:G:1460:LYS:HG2	2:G:1464:LYS:NZ	2.28	0.49
2:G:1381:GLY:HA2	4:G:2001:ADP:H5'2	1.94	0.49
2:H:1381:GLY:HA2	4:H:2001:ADP:H5'2	1.94	0.49
1:A:72:LEU:O	1:A:76:THR:HG23	2.13	0.49
1:B:112:THR:OG1	1:B:137:MET:N	2.42	0.49
1:C:318:ILE:O	1:C:329:ASP:N	2.45	0.49
1:C:320:ALA:O	1:C:327:SER:OG	2.31	0.49
2:E:1478:GLY:O	2:E:1486:ARG:NH2	2.46	0.49
2:E:552:ILE:HA	2:E:555:VAL:HG22	1.94	0.49
2:F:1003:TYR:CE1	2:F:1092:VAL:HG11	2.48	0.49
2:F:1550:VAL:O	2:F:1556:ILE:HA	2.13	0.49
2:F:382:GLU:OE2	2:F:386:ASN:ND2	2.37	0.49
2:G:1460:LYS:HG2	2:G:1464:LYS:HZ2	1.77	0.49
2:G:461:LEU:O	2:G:463:GLY:N	2.46	0.49
2:G:778:LEU:HD13	2:G:823:GLY:HA2	1.95	0.49
2:H:1550:VAL:O	2:H:1556:ILE:HA	2.13	0.49
1:A:209:MET:O	1:A:292:GLU:HB2	2.12	0.49
1:B:60:PHE:O	1:B:64:VAL:HG23	2.12	0.49
1:D:209:MET:O	1:D:292:GLU:HB2	2.12	0.49
2:E:1381:GLY:HA2	4:E:2001:ADP:H5'2	1.94	0.49
2:E:686:PHE:O	2:E:695:THR:N	2.46	0.49
2:E:778:LEU:HD13	2:E:823:GLY:HA2	1.95	0.49
2:F:381:ILE:HG21	2:F:1241:THR:HG21	1.95	0.49
2:F:1451:TRP:HE3	2:F:1460:LYS:HG3	1.78	0.49
2:G:1066:VAL:O	2:G:1069:VAL:HG12	2.13	0.49
2:G:778:LEU:HA	2:G:841:ARG:NH1	2.28	0.49
2:H:1003:TYR:CE1	2:H:1092:VAL:HG11	2.48	0.49
2:E:381:ILE:HG21	2:E:1241:THR:HG21	1.95	0.48
2:F:320:ILE:O	2:F:324:VAL:HG23	2.13	0.48
2:F:417:ILE:O	2:F:420:LEU:HG	2.13	0.48
2:G:1266:SER:HB3	2:G:1280:VAL:HG13	1.95	0.48
2:G:1484:GLY:O	2:G:1488:LEU:HD23	2.13	0.48
2:G:287:ILE:HD11	2:G:607:VAL:HG13	1.94	0.48
2:H:1392:PHE:HB3	2:H:1418:ARG:NE	2.28	0.48
2:H:357:VAL:HA	2:H:360:VAL:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:461:LEU:O	2:H:463:GLY:N	2.46	0.48
2:H:679:VAL:HG13	2:H:739:TRP:CD1	2.48	0.48
1:A:129:VAL:O	1:A:130:THR:OG1	2.23	0.48
1:B:220:VAL:HG12	1:B:235:GLN:HG2	1.94	0.48
1:B:322:GLU:N	1:B:325:ARG:O	2.46	0.48
1:C:187:ALA:O	1:C:310:LEU:N	2.45	0.48
2:F:1003:TYR:CZ	2:F:1135:ILE:HG21	2.49	0.48
2:F:1151:SER:O	2:F:1155:VAL:HG23	2.13	0.48
2:F:1346:ILE:HD11	2:F:1364:VAL:HG22	1.93	0.48
2:F:686:PHE:O	2:F:695:THR:N	2.46	0.48
2:F:679:VAL:HG13	2:F:739:TRP:CD1	2.48	0.48
2:H:1003:TYR:CZ	2:H:1135:ILE:HG21	2.48	0.48
2:H:1451:TRP:HE3	2:H:1460:LYS:HG3	1.78	0.48
2:H:774:GLN:NE2	3:H:2004:ATP:O2G	2.47	0.48
2:E:1451:TRP:HE3	2:E:1460:LYS:HG3	1.78	0.48
2:E:1460:LYS:HG2	2:E:1464:LYS:NZ	2.28	0.48
2:E:774:GLN:NE2	3:E:2004:ATP:O2G	2.47	0.48
2:F:1029:ILE:HD12	2:F:1070:LEU:HB3	1.95	0.48
2:G:1003:TYR:CE1	2:G:1092:VAL:HG11	2.48	0.48
2:G:1550:VAL:O	2:G:1556:ILE:HA	2.13	0.48
2:G:774:GLN:NE2	3:G:2004:ATP:O2G	2.46	0.48
2:G:39:LEU:HA	2:G:42:ILE:HG22	1.94	0.48
2:E:104:LEU:H	2:E:104:LEU:HD23	1.77	0.48
2:E:1029:ILE:HD12	2:E:1070:LEU:HB3	1.95	0.48
2:E:461:LEU:O	2:E:463:GLY:N	2.46	0.48
2:E:679:VAL:HG13	2:E:739:TRP:CD1	2.48	0.48
2:E:687:THR:HB	2:E:694:PRO:HA	1.95	0.48
2:F:778:LEU:HA	2:F:841:ARG:NH1	2.28	0.48
2:G:1451:TRP:HE3	2:G:1460:LYS:HG3	1.78	0.48
2:G:771:TYR:CD2	2:G:1212:THR:HG22	2.48	0.48
2:H:1094:LYS:HE2	2:H:1098:ARG:HH22	1.79	0.48
1:A:326:TYR:OH	1:B:33:ALA:O	2.22	0.48
1:D:72:LEU:O	1:D:76:THR:HG23	2.13	0.48
2:F:1392:PHE:HB3	2:F:1418:ARG:NE	2.28	0.48
2:F:686:PHE:HE2	2:F:699:ILE:HD11	1.77	0.48
2:G:1346:ILE:HD11	2:G:1364:VAL:HG22	1.93	0.48
2:H:1373:LYS:O	2:H:1546:ASP:N	2.31	0.48
2:H:1478:GLY:O	2:H:1486:ARG:NH2	2.46	0.48
2:H:314:PHE:CE2	2:H:447:VAL:HG12	2.49	0.48
2:H:687:THR:HB	2:H:694:PRO:HA	1.95	0.48
2:H:771:TYR:CD2	2:H:1212:THR:HG22	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:PRO:O	1:B:259:HIS:ND1	2.34	0.48
2:E:1066:VAL:O	2:E:1069:VAL:HG12	2.13	0.48
2:E:1468:GLY:O	2:E:1471:ASP:HB2	2.14	0.48
2:E:218:LEU:HD23	2:E:219:GLN:N	2.23	0.48
2:E:417:ILE:O	2:E:420:LEU:HG	2.13	0.48
2:F:1460:LYS:HG2	2:F:1464:LYS:NZ	2.28	0.48
2:F:771:TYR:CD2	2:F:1212:THR:HG22	2.48	0.48
2:G:1392:PHE:HB3	2:G:1418:ARG:NE	2.28	0.48
2:G:716:GLY:N	3:G:2004:ATP:O3G	2.33	0.48
2:G:314:PHE:CE2	2:G:447:VAL:HG12	2.49	0.48
2:H:1468:GLY:O	2:H:1471:ASP:HB2	2.14	0.48
2:H:782:THR:OG1	2:H:821:GLN:OE1	2.16	0.48
2:H:889:LYS:HB3	2:H:1538:ARG:HH12	1.78	0.48
1:D:318:ILE:O	1:D:329:ASP:N	2.45	0.48
2:E:1292:ASN:HB3	2:E:1293:TYR:CD2	2.49	0.48
2:H:1222:PHE:HD1	2:H:1225:LYS:HD3	1.79	0.48
2:H:1266:SER:HB3	2:H:1280:VAL:HG13	1.95	0.48
2:H:1539:VAL:O	2:H:1542:ILE:HG22	2.13	0.48
1:A:46:HIS:O	1:D:328:VAL:O	2.32	0.48
2:E:1003:TYR:CZ	2:E:1135:ILE:HG21	2.49	0.48
2:E:1415:HIS:O	2:E:1419:SER:OG	2.18	0.48
2:E:1550:VAL:O	2:E:1556:ILE:HA	2.13	0.48
2:E:320:ILE:O	2:E:324:VAL:HG23	2.13	0.48
2:F:1381:GLY:HA2	4:F:2001:ADP:H5'2	1.94	0.48
2:G:1003:TYR:CZ	2:G:1135:ILE:HG21	2.48	0.48
2:G:1182:ARG:NH2	2:G:1186:ARG:HH21	2.12	0.48
2:G:1468:GLY:O	2:G:1471:ASP:HB2	2.14	0.48
2:H:598:ARG:HH12	2:H:1137:SER:HG	1.61	0.48
2:H:686:PHE:O	2:H:695:THR:N	2.46	0.48
2:E:1484:GLY:O	2:E:1488:LEU:HD23	2.14	0.48
2:E:680:GLN:HB2	2:E:701:ILE:O	2.14	0.48
2:F:1478:GLY:O	2:F:1486:ARG:NH2	2.47	0.48
2:G:1344:ILE:O	2:G:1368:ILE:N	2.29	0.48
2:G:1539:VAL:O	2:G:1542:ILE:HG22	2.12	0.48
2:G:417:ILE:O	2:G:420:LEU:HG	2.13	0.48
2:G:505:GLY:HA3	2:G:1429:VAL:HG11	1.96	0.48
2:H:552:ILE:HA	2:H:555:VAL:HG22	1.94	0.48
1:A:38:LYS:NZ	1:A:185:LYS:HG3	2.29	0.48
1:B:38:LYS:NZ	1:B:185:LYS:HG3	2.29	0.48
2:G:1222:PHE:HD1	2:G:1225:LYS:HD3	1.79	0.48
2:G:32:ASN:ND2	2:G:153:LYS:HD2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1292:ASN:HB3	2:H:1293:TYR:CD2	2.49	0.48
2:H:1460:LYS:HG2	2:H:1464:LYS:NZ	2.28	0.48
2:H:273:GLN:O	2:H:277:ASP:N	2.39	0.48
2:H:320:ILE:O	2:H:324:VAL:HG23	2.13	0.48
1:B:171:THR:HG23	1:C:169:MET:CE	2.44	0.47
1:D:240:MET:HG2	1:D:247:ASN:HD22	1.79	0.47
2:F:1032:TRP:CZ2	2:F:1063:TYR:HD1	2.32	0.47
2:F:1346:ILE:HG13	2:F:1365:ASN:HA	1.96	0.47
2:F:1468:GLY:O	2:F:1471:ASP:HB2	2.13	0.47
2:G:1006:SER:HB2	2:G:1092:VAL:HG13	1.96	0.47
2:G:1292:ASN:HB3	2:G:1293:TYR:CD2	2.49	0.47
1:C:272:PRO:HB3	1:C:311:TRP:CE2	2.49	0.47
1:D:272:PRO:HB3	1:D:311:TRP:CE2	2.49	0.47
2:E:1094:LYS:HE2	2:E:1098:ARG:HH22	1.79	0.47
2:E:1266:SER:HB3	2:E:1280:VAL:HG13	1.95	0.47
2:E:1346:ILE:HG13	2:E:1365:ASN:HA	1.96	0.47
2:F:1036:TRP:CZ3	2:F:1063:TYR:HB2	2.49	0.47
2:F:1182:ARG:NH2	2:F:1186:ARG:HH21	2.12	0.47
2:F:1222:PHE:HD1	2:F:1225:LYS:HD3	1.79	0.47
2:F:778:LEU:HD13	2:F:823:GLY:HA2	1.95	0.47
2:G:1036:TRP:HZ3	2:G:1063:TYR:HB2	1.80	0.47
2:G:1094:LYS:HE2	2:G:1098:ARG:HH22	1.79	0.47
2:G:1478:GLY:O	2:G:1486:ARG:NH2	2.46	0.47
2:G:320:ILE:O	2:G:324:VAL:HG23	2.13	0.47
2:H:1032:TRP:CZ2	2:H:1063:TYR:HD1	2.32	0.47
2:H:455:ILE:O	2:H:457:GLY:N	2.47	0.47
2:H:680:GLN:HB2	2:H:701:ILE:O	2.14	0.47
1:A:122:LEU:HD21	1:B:146:ILE:HG12	1.97	0.47
1:B:272:PRO:HB3	1:B:311:TRP:CE2	2.49	0.47
1:C:170:LYS:O	1:C:173:GLN:HB2	2.15	0.47
1:D:209:MET:HE1	1:D:252:VAL:HG22	1.96	0.47
2:E:1100:LEU:O	2:E:1104:ILE:HG12	2.15	0.47
2:E:455:ILE:O	2:E:457:GLY:N	2.48	0.47
2:F:1031:TYR:O	2:F:1034:ALA:HB3	2.14	0.47
2:F:1266:SER:HB3	2:F:1280:VAL:HG13	1.95	0.47
2:G:1029:ILE:HD12	2:G:1070:LEU:HB3	1.95	0.47
2:G:1036:TRP:CZ3	2:G:1063:TYR:HB2	2.49	0.47
2:G:455:ILE:O	2:G:457:GLY:N	2.48	0.47
2:G:679:VAL:HG13	2:G:739:TRP:CD1	2.48	0.47
2:H:1031:TYR:O	2:H:1034:ALA:HB3	2.14	0.47
2:H:1100:LEU:O	2:H:1104:ILE:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1484:GLY:O	2:H:1488:LEU:HD23	2.13	0.47
2:H:32:ASN:ND2	2:H:153:LYS:HD2	2.29	0.47
2:H:417:ILE:O	2:H:420:LEU:HG	2.13	0.47
2:H:778:LEU:HA	2:H:841:ARG:NH1	2.28	0.47
2:E:1511:ILE:HG22	2:E:1512:ASP:O	2.15	0.47
2:E:889:LYS:HB3	2:E:1538:ARG:HH22	1.80	0.47
2:E:314:PHE:CE2	2:E:447:VAL:HG12	2.49	0.47
2:F:1292:ASN:HB3	2:F:1293:TYR:CD2	2.49	0.47
2:H:505:GLY:HA3	2:H:1429:VAL:HG11	1.96	0.47
1:C:196:LEU:HD21	1:C:311:TRP:CH2	2.50	0.47
2:E:1031:TYR:O	2:E:1034:ALA:HB3	2.15	0.47
2:F:1094:LYS:HE2	2:F:1098:ARG:HH22	1.79	0.47
2:F:1484:GLY:O	2:F:1488:LEU:HD23	2.14	0.47
2:F:314:PHE:CE2	2:F:447:VAL:HG12	2.49	0.47
2:F:32:ASN:ND2	2:F:153:LYS:HD2	2.29	0.47
2:G:1170:LEU:HD12	2:G:1254:ILE:HG23	1.97	0.47
2:G:889:LYS:HB3	2:G:1538:ARG:HH12	1.79	0.47
2:G:1482:SER:OG	3:G:2004:ATP:O3A	2.26	0.47
2:H:1170:LEU:HD12	2:H:1254:ILE:HG23	1.97	0.47
1:B:196:LEU:HD21	1:B:311:TRP:CH2	2.50	0.47
1:D:38:LYS:NZ	1:D:185:LYS:HG3	2.29	0.47
2:E:1006:SER:HB2	2:E:1092:VAL:HG13	1.97	0.47
2:E:1036:TRP:CZ3	2:E:1063:TYR:HB2	2.49	0.47
2:F:774:GLN:NE2	3:F:2004:ATP:O2G	2.47	0.47
2:G:850:VAL:CG2	2:G:881:ARG:HE	2.28	0.47
2:H:1006:SER:HB2	2:H:1092:VAL:HG13	1.97	0.47
2:H:1346:ILE:HG22	2:H:1402:ILE:HG13	1.97	0.47
2:H:1511:ILE:HG22	2:H:1512:ASP:O	2.14	0.47
1:C:38:LYS:NZ	1:C:185:LYS:HG3	2.29	0.47
1:C:240:MET:HG2	1:C:247:ASN:HD22	1.79	0.47
2:F:1511:ILE:HG22	2:F:1512:ASP:O	2.14	0.47
2:F:455:ILE:O	2:F:458:VAL:N	2.48	0.47
2:F:496:LEU:O	2:F:500:ASN:ND2	2.48	0.47
2:F:850:VAL:CG2	2:F:881:ARG:HE	2.28	0.47
2:G:1031:TYR:O	2:G:1034:ALA:HB3	2.15	0.47
2:G:1032:TRP:CZ2	2:G:1063:TYR:HD1	2.32	0.47
2:G:680:GLN:HB2	2:G:701:ILE:O	2.14	0.47
2:H:1066:VAL:O	2:H:1069:VAL:HG12	2.13	0.47
2:H:455:ILE:O	2:H:458:VAL:N	2.48	0.47
2:H:786:ASN:HB2	2:H:841:ARG:HH11	1.79	0.47
1:A:121:PHE:CE2	1:B:150:ILE:HD11	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:PRO:HB3	1:A:311:TRP:CE2	2.49	0.47
1:A:50:ARG:NH1	3:A:502:ATP:H2'	2.30	0.47
1:B:170:LYS:O	1:B:173:GLN:HB2	2.15	0.47
1:B:319:VAL:HB	1:C:232:PRO:HG2	1.97	0.47
1:D:320:ALA:O	1:D:327:SER:OG	2.31	0.47
2:F:273:GLN:O	2:F:277:ASP:N	2.39	0.47
1:C:53:GLY:C	2:G:132:PHE:HZ	2.18	0.47
2:G:150:LYS:HG3	2:G:179:TYR:HE2	1.80	0.47
2:G:218:LEU:HD22	2:G:220:PRO:HD3	1.97	0.47
2:H:1036:TRP:CZ3	2:H:1063:TYR:HB2	2.49	0.47
2:H:1182:ARG:NH2	2:H:1186:ARG:HH21	2.12	0.47
2:H:778:LEU:HD13	2:H:823:GLY:HA2	1.95	0.47
2:E:1032:TRP:CZ2	2:E:1063:TYR:HD1	2.32	0.47
2:E:1188:LEU:HD21	2:E:1239:PHE:HB3	1.96	0.47
2:E:889:LYS:HB3	2:E:1538:ARG:HH12	1.79	0.47
2:F:1036:TRP:HZ3	2:F:1063:TYR:HB2	1.79	0.47
2:F:1100:LEU:O	2:F:1104:ILE:HG12	2.15	0.47
2:H:1029:ILE:HD12	2:H:1070:LEU:HB3	1.95	0.47
1:A:165:GLY:HA2	1:D:168:PHE:HD1	1.79	0.47
1:A:240:MET:HG2	1:A:247:ASN:HD22	1.79	0.47
2:E:32:ASN:ND2	2:E:153:LYS:HD2	2.29	0.47
2:E:69:PRO:HG3	2:E:192:VAL:HG11	1.97	0.47
2:E:786:ASN:HB2	2:E:841:ARG:HH11	1.79	0.47
2:G:1011:LEU:HD21	2:G:1087:TRP:CE3	2.50	0.47
2:H:1036:TRP:HZ3	2:H:1063:TYR:HB2	1.80	0.47
2:H:218:LEU:HD22	2:H:220:PRO:HD3	1.97	0.47
2:H:537:ALA:HA	2:H:540:THR:HG22	1.97	0.47
1:D:170:LYS:O	1:D:173:GLN:HB2	2.15	0.47
2:F:218:LEU:HD22	2:F:220:PRO:HD3	1.97	0.47
2:G:434:LEU:HD22	2:G:596:VAL:HG22	1.97	0.47
2:G:786:ASN:HB2	2:G:841:ARG:HH11	1.79	0.47
2:H:1188:LEU:HD21	2:H:1239:PHE:HB3	1.96	0.47
2:H:850:VAL:CG2	2:H:881:ARG:HE	2.28	0.47
1:A:277:HIS:ND1	1:A:277:HIS:O	2.49	0.46
1:A:317:PRO:HB3	1:B:232:PRO:HD3	1.97	0.46
1:B:45:ALA:HB3	1:B:47:LYS:NZ	2.31	0.46
1:D:196:LEU:HD21	1:D:311:TRP:CH2	2.49	0.46
2:E:1170:LEU:HD12	2:E:1254:ILE:HG23	1.97	0.46
2:E:782:THR:HG22	2:E:784:GLU:N	2.30	0.46
2:F:1006:SER:HB2	2:F:1092:VAL:HG13	1.97	0.46
2:F:69:PRO:HD2	2:F:189:VAL:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:680:GLN:HB2	2:F:701:ILE:O	2.14	0.46
2:G:1188:LEU:HD21	2:G:1239:PHE:HB3	1.96	0.46
2:G:150:LYS:HG3	2:G:179:TYR:CE2	2.51	0.46
2:H:496:LEU:O	2:H:500:ASN:ND2	2.48	0.46
2:E:505:GLY:HA3	2:E:1429:VAL:HG11	1.96	0.46
2:E:218:LEU:HD22	2:E:220:PRO:HD3	1.97	0.46
2:E:850:VAL:CG2	2:E:881:ARG:HE	2.28	0.46
2:F:69:PRO:HG3	2:F:192:VAL:HG11	1.97	0.46
2:F:723:LEU:HD22	2:F:851:PHE:HE1	1.80	0.46
2:G:288:TRP:NE1	2:G:607:VAL:HG11	2.31	0.46
2:H:288:TRP:NE1	2:H:607:VAL:HG11	2.31	0.46
2:H:434:LEU:HD22	2:H:596:VAL:HG22	1.98	0.46
1:A:170:LYS:O	1:A:173:GLN:HB2	2.15	0.46
1:B:240:MET:HG2	1:B:247:ASN:HD22	1.79	0.46
1:D:45:ALA:HB3	1:D:47:LYS:NZ	2.30	0.46
2:F:1181:PHE:CD2	2:F:1247:LEU:HD22	2.50	0.46
2:F:434:LEU:HD22	2:F:596:VAL:HG22	1.98	0.46
2:F:455:ILE:O	2:F:457:GLY:N	2.48	0.46
2:F:786:ASN:HB2	2:F:841:ARG:HH11	1.79	0.46
2:G:782:THR:HG22	2:G:784:GLU:N	2.30	0.46
1:B:277:HIS:ND1	1:B:277:HIS:O	2.49	0.46
1:B:37:SER:HB2	1:B:43:ASN:HD21	1.81	0.46
1:C:45:ALA:HB3	1:C:47:LYS:NZ	2.30	0.46
2:E:1222:PHE:HD1	2:E:1225:LYS:HD3	1.79	0.46
2:E:496:LEU:O	2:E:500:ASN:ND2	2.48	0.46
2:E:537:ALA:HA	2:E:540:THR:HG22	1.97	0.46
2:E:723:LEU:HD22	2:E:851:PHE:HE1	1.81	0.46
2:F:150:LYS:HG3	2:F:179:TYR:HE2	1.80	0.46
2:G:1100:LEU:O	2:G:1104:ILE:HG12	2.15	0.46
2:G:1346:ILE:HG13	2:G:1365:ASN:HA	1.96	0.46
2:G:69:PRO:HD2	2:G:189:VAL:HG23	1.98	0.46
2:G:409:MET:O	2:G:1475:THR:HG21	2.16	0.46
2:G:45:PRO:O	2:G:49:ILE:HG23	2.16	0.46
2:H:1338:TRP:HH2	2:H:1404:ILE:HB	1.81	0.46
2:H:723:LEU:HD22	2:H:851:PHE:HE1	1.81	0.46
1:A:196:LEU:HD21	1:A:311:TRP:CH2	2.50	0.46
1:D:95:PHE:HE2	2:H:27:PHE:HA	1.80	0.46
2:E:1072:SER:O	2:E:1075:ILE:HG22	2.16	0.46
2:E:1338:TRP:HH2	2:E:1404:ILE:HB	1.81	0.46
2:E:1346:ILE:HG22	2:E:1402:ILE:HG13	1.97	0.46
2:E:679:VAL:HG22	2:E:739:TRP:HD1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1147:LEU:HD22	2:F:1147:LEU:HA	1.83	0.46
2:F:1188:LEU:HD21	2:F:1239:PHE:HB3	1.96	0.46
2:G:833:GLN:HG2	2:G:836:ARG:NH2	2.31	0.46
2:H:1066:VAL:HA	2:H:1069:VAL:HG12	1.98	0.46
2:H:1181:PHE:CD2	2:H:1247:LEU:HD22	2.51	0.46
2:H:409:MET:O	2:H:1475:THR:HG21	2.16	0.46
2:H:218:LEU:HD23	2:H:219:GLN:N	2.23	0.46
2:E:1142:LEU:HD13	2:E:1304:MET:SD	2.56	0.46
2:E:1182:ARG:NH2	2:E:1186:ARG:HH21	2.12	0.46
2:E:843:LEU:O	2:E:881:ARG:NH2	2.41	0.46
2:F:1072:SER:O	2:F:1075:ILE:HG22	2.16	0.46
2:F:889:LYS:HB3	2:F:1538:ARG:HH22	1.80	0.46
2:F:889:LYS:HB3	2:F:1538:ARG:HH12	1.78	0.46
2:G:1403:ILE:HA	2:G:1407:ILE:O	2.16	0.46
2:G:1430:LEU:HD23	2:G:1474:ILE:HG21	1.98	0.46
2:G:1511:ILE:HG22	2:G:1512:ASP:O	2.15	0.46
2:G:889:LYS:HB3	2:G:1538:ARG:HH22	1.80	0.46
2:H:1142:LEU:HD13	2:H:1304:MET:SD	2.56	0.46
2:H:1346:ILE:HG13	2:H:1365:ASN:HA	1.96	0.46
2:H:1403:ILE:HA	2:H:1407:ILE:O	2.16	0.46
2:H:150:LYS:HG3	2:H:179:TYR:HE2	1.80	0.46
2:H:889:LYS:HB3	2:H:1538:ARG:HH22	1.80	0.46
2:H:679:VAL:HG22	2:H:739:TRP:HD1	1.81	0.46
2:H:782:THR:HG22	2:H:784:GLU:N	2.30	0.46
2:F:1011:LEU:HD21	2:F:1087:TRP:CE3	2.50	0.46
2:F:1170:LEU:HD12	2:F:1254:ILE:HG23	1.97	0.46
2:F:288:TRP:NE1	2:F:607:VAL:HG11	2.31	0.46
2:F:717:CYS:HB2	2:F:903:LYS:HA	1.98	0.46
2:G:455:ILE:O	2:G:458:VAL:N	2.48	0.46
2:G:678:CYS:HB2	2:G:703:ILE:O	2.16	0.46
2:H:45:PRO:O	2:H:49:ILE:HG23	2.16	0.46
2:H:833:GLN:HG2	2:H:836:ARG:NH2	2.31	0.46
1:D:37:SER:HB2	1:D:43:ASN:HD21	1.81	0.46
2:E:1022:LYS:HE2	2:E:1078:CYS:HA	1.97	0.46
2:E:150:LYS:HG3	2:E:179:TYR:HE2	1.80	0.46
2:E:455:ILE:O	2:E:458:VAL:N	2.48	0.46
2:E:45:PRO:O	2:E:49:ILE:HG23	2.16	0.46
2:E:782:THR:OG1	2:E:821:GLN:OE1	2.16	0.46
2:F:1142:LEU:HD13	2:F:1304:MET:SD	2.56	0.46
2:G:496:LEU:O	2:G:500:ASN:ND2	2.48	0.46
2:G:717:CYS:HB2	2:G:903:LYS:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:717:CYS:HB2	2:H:903:LYS:HA	1.98	0.46
1:B:318:ILE:O	1:B:329:ASP:N	2.45	0.46
1:C:277:HIS:ND1	1:C:277:HIS:O	2.49	0.46
1:C:37:SER:HB2	1:C:43:ASN:HD21	1.81	0.46
1:C:92:LEU:HD22	2:G:34:VAL:HG21	1.98	0.46
2:E:69:PRO:HD2	2:E:189:VAL:HG23	1.97	0.46
2:E:434:LEU:HD22	2:E:596:VAL:HG22	1.98	0.46
2:E:833:GLN:HG2	2:E:836:ARG:NH2	2.31	0.46
2:F:505:GLY:HA3	2:F:1429:VAL:HG11	1.96	0.46
2:F:843:LEU:O	2:F:881:ARG:NH2	2.41	0.46
2:H:1430:LEU:HD23	2:H:1474:ILE:HG21	1.98	0.46
2:E:1011:LEU:HD21	2:E:1087:TRP:CE3	2.50	0.46
2:E:1181:PHE:CD2	2:E:1247:LEU:HD22	2.51	0.46
2:E:1349:LEU:HB3	2:E:1364:VAL:HG13	1.98	0.46
2:E:1345:GLN:HA	2:E:1366:ALA:O	2.16	0.46
2:E:555:VAL:HG12	2:E:583:PHE:CD2	2.50	0.46
2:E:717:CYS:HB2	2:E:903:LYS:HA	1.98	0.46
2:F:1346:ILE:HG22	2:F:1402:ILE:HG13	1.97	0.46
2:F:150:LYS:HG3	2:F:179:TYR:CE2	2.51	0.46
2:F:782:THR:HG22	2:F:784:GLU:N	2.30	0.46
2:F:85:LEU:HA	2:F:85:LEU:HD13	1.82	0.46
2:G:1072:SER:O	2:G:1075:ILE:HG22	2.16	0.46
2:G:1181:PHE:CD2	2:G:1247:LEU:HD22	2.50	0.46
2:G:537:ALA:HA	2:G:540:THR:HG22	1.97	0.46
2:H:1022:LYS:HE2	2:H:1078:CYS:HA	1.97	0.46
2:H:150:LYS:HG3	2:H:179:TYR:CE2	2.51	0.46
1:B:119:SER:OG	1:C:140:GLU:OE2	2.27	0.45
1:C:143:PRO:HA	1:C:146:ILE:HD12	1.98	0.45
1:C:263:ALA:HA	1:C:268:TYR:CG	2.51	0.45
1:C:272:PRO:HB3	1:C:311:TRP:CD1	2.52	0.45
1:D:277:HIS:ND1	1:D:277:HIS:O	2.49	0.45
1:A:232:PRO:HD3	1:D:317:PRO:HB3	1.98	0.45
2:F:1338:TRP:HH2	2:F:1404:ILE:HB	1.81	0.45
2:F:679:VAL:HG22	2:F:739:TRP:HD1	1.81	0.45
2:G:1335:PRO:HD2	2:G:1338:TRP:CD1	2.52	0.45
2:H:1011:LEU:HD21	2:H:1087:TRP:CE3	2.50	0.45
2:H:1335:PRO:HD2	2:H:1338:TRP:CD1	2.52	0.45
1:A:318:ILE:O	1:A:329:ASP:N	2.45	0.45
1:A:318:ILE:HA	1:A:332:LYS:HZ1	1.80	0.45
1:A:89:ALA:O	1:A:93:ILE:HG12	2.17	0.45
1:D:272:PRO:HB3	1:D:311:TRP:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:273:GLN:O	2:E:277:ASP:N	2.39	0.45
2:G:69:PRO:HG3	2:G:192:VAL:HG11	1.97	0.45
2:G:382:GLU:OE2	2:G:386:ASN:ND2	2.37	0.45
2:G:723:LEU:HD22	2:G:851:PHE:HE1	1.81	0.45
1:A:332:LYS:HA	1:A:335:ASN:OD1	2.16	0.45
1:A:45:ALA:HB3	1:A:47:LYS:NZ	2.31	0.45
1:D:229:GLU:HB3	1:C:314:ARG:NH1	2.31	0.45
1:D:263:ALA:HA	1:D:268:TYR:CG	2.51	0.45
2:F:1347:GLN:HE21	2:F:1401:HIS:CE1	2.35	0.45
2:F:1403:ILE:HA	2:F:1407:ILE:O	2.16	0.45
2:F:409:MET:O	2:F:1475:THR:HG21	2.16	0.45
2:F:45:PRO:O	2:F:49:ILE:HG23	2.16	0.45
2:F:678:CYS:HB2	2:F:703:ILE:O	2.16	0.45
2:F:833:GLN:HG2	2:F:836:ARG:NH2	2.31	0.45
2:H:1072:SER:O	2:H:1075:ILE:HG22	2.16	0.45
2:H:1345:GLN:HA	2:H:1366:ALA:O	2.17	0.45
1:A:183:PHE:CE1	1:A:202:VAL:HG23	2.52	0.45
2:E:1435:ILE:HB	2:E:1470:LEU:HB2	1.99	0.45
2:E:1430:LEU:HD23	2:E:1474:ILE:HG21	1.98	0.45
2:F:1335:PRO:HD2	2:F:1338:TRP:CD1	2.52	0.45
2:F:1430:LEU:HD23	2:F:1474:ILE:HG21	1.98	0.45
2:F:28:VAL:O	2:F:32:ASN:ND2	2.50	0.45
2:F:465:ALA:HA	2:F:468:ILE:HD12	1.98	0.45
2:G:1066:VAL:HA	2:G:1069:VAL:HG12	1.98	0.45
2:G:1346:ILE:HG22	2:G:1402:ILE:HG13	1.97	0.45
2:H:1482:SER:OG	3:H:2004:ATP:O3A	2.26	0.45
1:B:272:PRO:HB3	1:B:311:TRP:CD1	2.52	0.45
1:D:239:PRO:HB3	1:C:244:VAL:HG22	1.98	0.45
1:D:200:LEU:N	1:D:257:ILE:O	2.47	0.45
2:E:1036:TRP:HZ3	2:E:1063:TYR:HB2	1.80	0.45
2:E:1347:GLN:HE21	2:E:1401:HIS:CE1	2.35	0.45
2:E:150:LYS:HG3	2:E:179:TYR:CE2	2.51	0.45
2:E:686:PHE:CD1	2:E:725:ALA:HB1	2.52	0.45
2:E:837:ILE:HG22	2:E:841:ARG:NH2	2.32	0.45
2:F:1431:PHE:O	2:F:1438:ASN:ND2	2.35	0.45
2:G:1022:LYS:HE2	2:G:1078:CYS:HA	1.97	0.45
2:G:1142:LEU:HD13	2:G:1304:MET:SD	2.56	0.45
2:G:680:GLN:OE1	2:G:702:ARG:NE	2.50	0.45
2:G:837:ILE:HG22	2:G:841:ARG:NH2	2.32	0.45
2:H:69:PRO:HD2	2:H:189:VAL:HG23	1.98	0.45
1:A:263:ALA:HA	1:A:268:TYR:CG	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:LYS:HA	1:D:335:ASN:OD1	2.17	0.45
2:E:678:CYS:HB2	2:E:703:ILE:O	2.16	0.45
2:F:1349:LEU:HB3	2:F:1364:VAL:HG13	1.98	0.45
2:G:555:VAL:HG12	2:G:583:PHE:CD2	2.50	0.45
2:H:28:VAL:O	2:H:32:ASN:ND2	2.50	0.45
2:H:678:CYS:HB2	2:H:703:ILE:O	2.16	0.45
1:B:263:ALA:HA	1:B:268:TYR:CG	2.51	0.45
1:B:332:LYS:HA	1:B:335:ASN:OD1	2.17	0.45
1:B:89:ALA:O	1:B:93:ILE:HG12	2.17	0.45
1:D:183:PHE:CE1	1:D:202:VAL:HG23	2.52	0.45
2:E:1359:PRO:HB3	2:E:1398:PHE:CZ	2.52	0.45
2:F:298:ARG:HD2	2:F:383:THR:HG22	1.99	0.45
2:F:442:PRO:O	2:F:446:ILE:HG12	2.17	0.45
2:H:720:SER:N	3:H:2004:ATP:O2B	2.35	0.45
1:A:272:PRO:HB3	1:A:311:TRP:CD1	2.51	0.45
1:A:37:SER:HB2	1:A:43:ASN:HD21	1.81	0.45
3:A:501:ATP:H2'	1:B:50:ARG:NH1	2.31	0.45
1:C:332:LYS:HA	1:C:335:ASN:OD1	2.17	0.45
1:C:89:ALA:O	1:C:93:ILE:HG12	2.17	0.45
1:A:47:LYS:NZ	1:D:327:SER:HA	2.32	0.45
1:D:89:ALA:O	1:D:93:ILE:HG12	2.17	0.45
2:E:1335:PRO:HD2	2:E:1338:TRP:CD1	2.52	0.45
2:E:288:TRP:NE1	2:E:607:VAL:HG11	2.31	0.45
2:F:537:ALA:HA	2:F:540:THR:HG22	1.97	0.45
2:F:686:PHE:CD1	2:F:725:ALA:HB1	2.52	0.45
2:H:1359:PRO:HB3	2:H:1398:PHE:CZ	2.52	0.45
2:H:686:PHE:CD1	2:H:725:ALA:HB1	2.52	0.45
1:B:92:LEU:HD22	2:F:34:VAL:HG21	1.99	0.45
2:E:409:MET:O	2:E:1475:THR:HG21	2.16	0.45
2:E:680:GLN:OE1	2:E:702:ARG:NE	2.50	0.45
2:F:1022:LYS:HE2	2:F:1078:CYS:HA	1.98	0.45
2:F:1066:VAL:HA	2:F:1069:VAL:HG12	1.98	0.45
2:F:1345:GLN:HA	2:F:1366:ALA:O	2.17	0.45
2:G:1335:PRO:HD2	2:G:1338:TRP:HD1	1.82	0.45
2:G:1338:TRP:HH2	2:G:1404:ILE:HB	1.81	0.45
2:G:1345:GLN:HA	2:G:1366:ALA:O	2.16	0.45
2:G:218:LEU:HD23	2:G:219:GLN:N	2.23	0.45
2:G:28:VAL:O	2:G:32:ASN:ND2	2.50	0.45
2:G:298:ARG:HD2	2:G:383:THR:HG22	1.98	0.45
2:H:1335:PRO:HD2	2:H:1338:TRP:HD1	1.82	0.45
2:H:69:PRO:HG3	2:H:192:VAL:HG11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:442:PRO:O	2:H:446:ILE:HG12	2.17	0.45
1:B:143:PRO:HA	1:B:146:ILE:HD12	1.98	0.45
1:B:183:PHE:CE1	1:B:202:VAL:HG23	2.52	0.45
1:B:200:LEU:N	1:B:257:ILE:O	2.47	0.45
2:E:28:VAL:O	2:E:32:ASN:ND2	2.50	0.45
2:G:1269:ASN:OD1	2:G:1273:ARG:HB3	2.17	0.45
2:G:1347:GLN:HE21	2:G:1401:HIS:CE1	2.35	0.45
2:H:1106:LEU:HG	2:H:1325:TYR:CE2	2.52	0.45
2:H:465:ALA:HA	2:H:468:ILE:HD12	1.99	0.45
2:H:428:LEU:HD11	2:H:610:LEU:HD11	1.99	0.45
2:H:680:GLN:OE1	2:H:702:ARG:NE	2.50	0.45
1:A:143:PRO:HA	1:A:146:ILE:HD12	1.99	0.44
1:D:67:LYS:HD3	1:D:70:HIS:CE1	2.52	0.44
2:E:1403:ILE:HA	2:E:1407:ILE:O	2.16	0.44
2:E:1486:ARG:HA	2:E:1489:PHE:HD2	1.82	0.44
2:E:919:SER:O	2:E:923:LEU:HB2	2.18	0.44
2:F:1222:PHE:CD1	2:F:1225:LYS:HD3	2.53	0.44
2:F:889:LYS:HB3	2:F:1538:ARG:NH1	2.32	0.44
2:G:131:ASN:O	2:G:133:PRO:HD3	2.17	0.44
2:G:593:LEU:HA	2:G:596:VAL:HB	1.99	0.44
2:H:457:GLY:O	2:H:461:LEU:HD23	2.17	0.44
2:H:777:TRP:CG	2:H:778:LEU:N	2.86	0.44
1:B:218:GLN:N	1:B:284:ILE:O	2.51	0.44
1:B:67:LYS:HD3	1:B:70:HIS:CE1	2.52	0.44
2:E:1222:PHE:CD1	2:E:1225:LYS:HD3	2.52	0.44
2:E:1335:PRO:HD2	2:E:1338:TRP:HD1	1.83	0.44
2:E:298:ARG:HD2	2:E:383:THR:HG22	1.98	0.44
2:E:556:LEU:HD11	2:E:1068:THR:HG22	1.99	0.44
2:E:592:LEU:O	2:E:596:VAL:HG23	2.18	0.44
2:F:1486:ARG:HA	2:F:1489:PHE:HD2	1.82	0.44
2:F:435:CYS:HG	2:F:439:TRP:HZ3	1.64	0.44
2:G:1106:LEU:HG	2:G:1325:TYR:CE2	2.52	0.44
2:G:442:PRO:O	2:G:446:ILE:HG12	2.17	0.44
2:G:457:GLY:O	2:G:461:LEU:HD23	2.17	0.44
2:G:777:TRP:CG	2:G:778:LEU:N	2.85	0.44
2:G:85:LEU:HA	2:G:85:LEU:HD13	1.82	0.44
1:A:67:LYS:HD3	1:A:70:HIS:CE1	2.52	0.44
1:D:143:PRO:HA	1:D:146:ILE:HD12	1.98	0.44
1:D:319:VAL:HG22	1:D:328:VAL:HG22	1.99	0.44
2:E:123:TYR:O	2:E:127:ILE:HG12	2.17	0.44
2:F:131:ASN:O	2:F:133:PRO:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:556:LEU:HD11	2:F:1068:THR:HG22	1.99	0.44
2:G:1359:PRO:HB3	2:G:1398:PHE:CZ	2.52	0.44
2:G:428:LEU:HD11	2:G:610:LEU:HD11	2.00	0.44
2:G:810:ASP:O	2:G:813:ILE:HG22	2.18	0.44
2:H:123:TYR:O	2:H:127:ILE:HG12	2.17	0.44
2:H:503:LEU:HD23	2:H:506:ILE:HD13	1.99	0.44
1:C:183:PHE:CE1	1:C:202:VAL:HG23	2.52	0.44
1:C:45:ALA:HB3	1:C:47:LYS:HZ2	1.83	0.44
1:D:276:HIS:O	1:D:306:ALA:HB3	2.18	0.44
1:D:318:ILE:HB	1:D:329:ASP:O	2.18	0.44
2:F:123:TYR:O	2:F:127:ILE:HG12	2.17	0.44
2:F:1269:ASN:OD1	2:F:1273:ARG:HB3	2.17	0.44
2:F:1373:LYS:O	2:F:1546:ASP:N	2.31	0.44
2:F:593:LEU:HA	2:F:596:VAL:HB	1.99	0.44
2:F:777:TRP:CG	2:F:778:LEU:N	2.85	0.44
2:G:1349:LEU:HB3	2:G:1364:VAL:HG13	1.98	0.44
2:H:1222:PHE:CD1	2:H:1225:LYS:HD3	2.52	0.44
2:H:306:ARG:HB2	2:H:376:SER:OG	2.18	0.44
2:H:776:PRO:HG2	2:H:834:ARG:NH1	2.32	0.44
1:C:67:LYS:HD3	1:C:70:HIS:CE1	2.52	0.44
2:E:1087:TRP:CE2	2:E:1091:LYS:HD2	2.53	0.44
2:E:1106:LEU:HG	2:E:1325:TYR:CE2	2.52	0.44
2:E:131:ASN:O	2:E:133:PRO:HD3	2.17	0.44
2:E:140:LEU:O	2:E:144:THR:HG23	2.18	0.44
2:E:306:ARG:HB2	2:E:376:SER:OG	2.18	0.44
2:E:810:ASP:O	2:E:813:ILE:HG22	2.18	0.44
2:E:889:LYS:HB3	2:E:1538:ARG:NH1	2.33	0.44
2:F:1106:LEU:HG	2:F:1325:TYR:CE2	2.52	0.44
2:F:457:GLY:O	2:F:461:LEU:HD23	2.17	0.44
2:F:776:PRO:HG2	2:F:834:ARG:NH1	2.32	0.44
2:F:837:ILE:HG22	2:F:841:ARG:NH2	2.32	0.44
2:H:1347:GLN:HE21	2:H:1401:HIS:CE1	2.35	0.44
2:H:810:ASP:O	2:H:813:ILE:HG22	2.18	0.44
2:F:1335:PRO:HD2	2:F:1338:TRP:HD1	1.82	0.44
2:G:1087:TRP:CE2	2:G:1091:LYS:HD2	2.53	0.44
2:G:889:LYS:HB3	2:G:1538:ARG:NH1	2.33	0.44
2:G:782:THR:OG1	2:G:821:GLN:OE1	2.15	0.44
2:G:776:PRO:HG2	2:G:834:ARG:NH1	2.32	0.44
1:A:276:HIS:O	1:A:306:ALA:HB3	2.18	0.44
1:B:129:VAL:O	1:B:130:THR:OG1	2.23	0.44
1:D:272:PRO:O	1:D:273:SER:OG	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:132:PHE:O	2:E:134:LYS:N	2.51	0.44
2:E:428:LEU:HD11	2:E:610:LEU:HD11	1.99	0.44
2:E:777:TRP:CG	2:E:778:LEU:N	2.86	0.44
2:F:592:LEU:O	2:F:596:VAL:HG23	2.18	0.44
2:G:1123:ARG:HG2	2:G:1317:LEU:HD12	2.00	0.44
2:G:514:TRP:CZ3	2:G:1493:ARG:HD2	2.53	0.44
2:G:148:ILE:O	2:G:152:ILE:HG12	2.18	0.44
2:H:1191:LEU:HA	2:H:1194:THR:HG22	2.00	0.44
2:H:370:ARG:CB	2:H:1252:GLU:HG2	2.48	0.44
2:H:1486:ARG:HA	2:H:1489:PHE:HD2	1.82	0.44
2:H:837:ILE:HG22	2:H:841:ARG:NH2	2.32	0.44
1:A:113:SER:OG	1:A:135:GLY:O	2.30	0.44
2:E:544:ILE:HG23	2:E:1144:ARG:HH22	1.83	0.44
2:E:1191:LEU:HA	2:E:1194:THR:HG22	2.00	0.44
2:E:1269:ASN:OD1	2:E:1273:ARG:HB3	2.17	0.44
2:E:573:PRO:HB2	2:E:574:SER:H	1.64	0.44
2:F:1177:ILE:HD11	2:F:1251:MET:SD	2.58	0.44
2:F:1191:LEU:HA	2:F:1194:THR:HG22	2.00	0.44
2:F:1434:THR:O	2:F:1438:ASN:N	2.39	0.44
2:F:555:VAL:HG12	2:F:583:PHE:CD2	2.50	0.44
2:G:556:LEU:HD11	2:G:1068:THR:HG22	1.99	0.44
2:G:1222:PHE:CD1	2:G:1225:LYS:HD3	2.53	0.44
2:G:140:LEU:O	2:G:144:THR:HG23	2.18	0.44
2:G:465:ALA:HA	2:G:468:ILE:HD12	1.99	0.44
2:G:679:VAL:HG22	2:G:739:TRP:HD1	1.81	0.44
2:H:1123:ARG:HG2	2:H:1317:LEU:HD12	2.00	0.44
2:H:132:PHE:O	2:H:134:LYS:N	2.51	0.44
2:H:1435:ILE:HB	2:H:1470:LEU:HB2	1.99	0.44
2:H:544:ILE:HG23	2:H:1144:ARG:HH22	1.83	0.44
1:B:113:SER:OG	1:B:135:GLY:O	2.30	0.44
1:C:276:HIS:O	1:C:306:ALA:HB3	2.18	0.44
1:D:66:LEU:HD21	1:D:70:HIS:HB2	2.00	0.44
2:E:720:SER:N	3:E:2004:ATP:O2B	2.35	0.44
2:E:776:PRO:HG2	2:E:834:ARG:NH1	2.32	0.44
2:F:1081:THR:O	2:F:1085:VAL:HG23	2.18	0.44
2:F:1123:ARG:HG2	2:F:1317:LEU:HD12	2.00	0.44
2:F:132:PHE:O	2:F:134:LYS:N	2.51	0.44
2:F:306:ARG:HB2	2:F:376:SER:OG	2.18	0.44
2:F:680:GLN:OE1	2:F:702:ARG:NE	2.50	0.44
2:G:1191:LEU:HA	2:G:1194:THR:HG22	2.00	0.44
2:G:370:ARG:CB	2:G:1252:GLU:HG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:123:TYR:O	2:G:127:ILE:HG12	2.17	0.44
2:G:1435:ILE:HB	2:G:1470:LEU:HB2	1.99	0.44
2:G:783:VAL:HB	2:G:818:ASP:O	2.18	0.44
2:H:148:ILE:O	2:H:152:ILE:HG12	2.18	0.44
2:H:555:VAL:HG12	2:H:583:PHE:CD2	2.50	0.44
1:B:222:LYS:HG3	1:B:232:PRO:HA	2.00	0.43
1:B:121:PHE:CE2	1:C:150:ILE:HD11	2.52	0.43
1:C:318:ILE:HB	1:C:329:ASP:O	2.18	0.43
2:E:1066:VAL:HA	2:E:1069:VAL:HG12	1.98	0.43
2:E:370:ARG:CB	2:E:1252:GLU:HG2	2.48	0.43
2:E:1123:ARG:HG2	2:E:1317:LEU:HD12	2.00	0.43
2:E:514:TRP:CZ3	2:E:1493:ARG:HD2	2.53	0.43
2:E:465:ALA:HA	2:E:468:ILE:HD12	1.99	0.43
2:E:6:CYS:HA	2:E:103:HIS:HB2	2.00	0.43
2:F:1087:TRP:CE2	2:F:1091:LYS:HD2	2.53	0.43
2:F:1359:PRO:HB3	2:F:1398:PHE:CZ	2.52	0.43
2:F:140:LEU:O	2:F:144:THR:HG23	2.18	0.43
2:F:148:ILE:O	2:F:152:ILE:HG12	2.18	0.43
2:F:428:LEU:HD11	2:F:610:LEU:HD11	2.00	0.43
2:F:783:VAL:HB	2:F:818:ASP:O	2.18	0.43
2:G:1081:THR:O	2:G:1085:VAL:HG23	2.18	0.43
2:H:550:ILE:N	2:H:551:PRO:HD2	2.33	0.43
2:H:593:LEU:HA	2:H:596:VAL:HB	1.99	0.43
1:B:94:ALA:CB	1:B:114:ILE:HD11	2.48	0.43
1:B:319:VAL:HG22	1:B:328:VAL:HG22	1.99	0.43
1:C:318:ILE:HA	1:C:332:LYS:HZ2	1.84	0.43
1:D:218:GLN:N	1:D:284:ILE:O	2.50	0.43
1:D:318:ILE:HA	1:D:332:LYS:HZ1	1.83	0.43
2:G:1031:TYR:HA	2:G:1282:LEU:CD1	2.45	0.43
2:G:1177:ILE:HD11	2:G:1251:MET:SD	2.58	0.43
2:G:306:ARG:HB2	2:G:376:SER:OG	2.18	0.43
2:G:592:LEU:O	2:G:596:VAL:HG23	2.17	0.43
2:G:686:PHE:CD1	2:G:725:ALA:HB1	2.52	0.43
2:G:6:CYS:HA	2:G:103:HIS:HB2	2.01	0.43
2:H:1087:TRP:CE2	2:H:1091:LYS:HD2	2.53	0.43
2:H:327:LEU:HD22	2:H:1277:ALA:HB2	2.01	0.43
2:H:556:LEU:HD11	2:H:1068:THR:HG22	1.99	0.43
2:H:919:SER:O	2:H:923:LEU:HB2	2.18	0.43
1:A:94:ALA:CB	1:A:114:ILE:HD11	2.49	0.43
1:A:177:ARG:HH21	1:A:204:ASP:CG	2.22	0.43
1:A:318:ILE:HB	1:A:329:ASP:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:ILE:HG12	1:C:130:THR:HA	2.01	0.43
2:E:148:ILE:O	2:E:152:ILE:HG12	2.18	0.43
2:E:550:ILE:N	2:E:551:PRO:HD2	2.33	0.43
2:E:593:LEU:HA	2:E:596:VAL:HB	1.99	0.43
2:F:919:SER:O	2:F:923:LEU:HB2	2.18	0.43
2:G:132:PHE:O	2:G:134:LYS:N	2.51	0.43
2:G:1413:PRO:HB2	2:G:1416:THR:HG23	2.01	0.43
2:G:309:ALA:HB1	2:G:369:GLN:OE1	2.18	0.43
2:H:1081:THR:O	2:H:1085:VAL:HG23	2.18	0.43
2:H:1177:ILE:HD11	2:H:1251:MET:SD	2.58	0.43
2:H:1269:ASN:OD1	2:H:1273:ARG:HB3	2.17	0.43
2:H:131:ASN:O	2:H:133:PRO:HD3	2.17	0.43
1:A:222:LYS:HG3	1:A:232:PRO:HA	2.00	0.43
1:A:319:VAL:HG22	1:A:328:VAL:HG22	2.00	0.43
1:B:177:ARG:HH21	1:B:204:ASP:CG	2.22	0.43
1:C:66:LEU:HD21	1:C:70:HIS:HB2	2.00	0.43
2:E:1081:THR:O	2:E:1085:VAL:HG23	2.18	0.43
2:E:108:MET:N	2:E:109:PRO:HD2	2.33	0.43
2:E:1177:ILE:HD11	2:E:1251:MET:SD	2.58	0.43
2:E:1350:SER:HA	2:E:1361:LEU:O	2.19	0.43
2:E:783:VAL:HB	2:E:818:ASP:O	2.18	0.43
2:F:544:ILE:HG23	2:F:1144:ARG:HH22	1.83	0.43
2:F:873:LEU:O	2:F:877:ARG:HB2	2.18	0.43
2:H:368:LEU:HA	2:H:371:THR:HG22	2.01	0.43
2:H:508:LEU:HD22	2:H:1431:PHE:CZ	2.51	0.43
1:A:239:PRO:O	1:A:259:HIS:ND1	2.34	0.43
1:A:320:ALA:O	1:A:327:SER:OG	2.31	0.43
1:B:272:PRO:O	1:B:273:SER:OG	2.27	0.43
1:C:94:ALA:CB	1:C:114:ILE:HD11	2.48	0.43
2:E:327:LEU:O	2:E:327:LEU:HD23	2.19	0.43
2:E:309:ALA:HB1	2:E:369:GLN:OE1	2.19	0.43
2:E:442:PRO:O	2:E:446:ILE:HG12	2.17	0.43
2:F:6:CYS:HA	2:F:103:HIS:HB2	2.01	0.43
2:F:108:MET:N	2:F:109:PRO:HD2	2.33	0.43
2:F:1350:SER:HA	2:F:1361:LEU:O	2.19	0.43
2:F:889:LYS:HB3	2:F:1538:ARG:NH2	2.34	0.43
2:F:503:LEU:HD23	2:F:506:ILE:HD13	1.99	0.43
2:F:802:ILE:O	2:F:806:SER:N	2.52	0.43
2:F:708:LEU:HB2	2:F:876:LEU:HD21	2.01	0.43
2:G:1223:GLN:O	2:G:1227:LEU:HD13	2.19	0.43
2:G:1486:ARG:HA	2:G:1489:PHE:HD2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:708:LEU:HB2	2:G:876:LEU:HD21	2.01	0.43
2:H:140:LEU:O	2:H:144:THR:HG23	2.18	0.43
1:A:50:ARG:NH1	3:A:502:ATP:O2B	2.48	0.43
1:A:50:ARG:HB2	3:A:502:ATP:C5	2.53	0.43
1:A:66:LEU:HD21	1:A:70:HIS:HB2	2.00	0.43
1:C:177:ARG:HH21	1:C:204:ASP:CG	2.22	0.43
2:E:1223:GLN:O	2:E:1227:LEU:HD13	2.19	0.43
2:E:368:LEU:HA	2:E:371:THR:HG22	2.01	0.43
2:E:802:ILE:O	2:E:806:SER:N	2.52	0.43
2:H:1223:GLN:O	2:H:1227:LEU:HD13	2.19	0.43
2:H:1349:LEU:HB3	2:H:1364:VAL:HG13	1.99	0.43
2:H:139:LEU:O	2:H:143:TRP:HD1	2.02	0.43
2:H:514:TRP:CZ3	2:H:1493:ARG:HD2	2.53	0.43
2:H:298:ARG:HD2	2:H:383:THR:HG22	1.98	0.43
2:H:573:PRO:HB2	2:H:574:SER:H	1.64	0.43
2:H:592:LEU:O	2:H:596:VAL:HG23	2.18	0.43
2:H:6:CYS:HA	2:H:103:HIS:HB2	2.00	0.43
2:H:783:VAL:HB	2:H:818:ASP:O	2.18	0.43
1:A:299:GLN:O	1:A:301:ARG:NH1	2.52	0.43
1:B:276:HIS:O	1:B:306:ALA:HB3	2.18	0.43
1:D:224:THR:HG22	1:D:225:SER:O	2.19	0.43
2:E:327:LEU:HD22	2:E:1277:ALA:HB2	2.01	0.43
2:E:575:VAL:HG23	2:E:576:ALA:N	2.34	0.43
2:E:868:MET:HG3	2:E:872:ILE:HG13	2.01	0.43
2:F:1223:GLN:O	2:F:1227:LEU:HD13	2.18	0.43
2:F:370:ARG:CB	2:F:1252:GLU:HG2	2.48	0.43
2:F:810:ASP:O	2:F:813:ILE:HG22	2.18	0.43
2:G:1064:ALA:O	2:G:1067:PHE:HB3	2.19	0.43
2:G:553:ALA:O	2:G:557:ILE:HG12	2.19	0.43
2:G:575:VAL:HG23	2:G:576:ALA:N	2.34	0.43
1:B:168:PHE:CZ	1:C:168:PHE:CD2	3.07	0.43
1:C:319:VAL:HG22	1:C:328:VAL:HG22	2.00	0.43
1:C:35:PHE:CE1	1:C:233:LEU:HD13	2.54	0.43
2:E:1166:ALA:O	2:E:1169:PRO:HD2	2.19	0.43
2:E:139:LEU:O	2:E:143:TRP:HD1	2.02	0.43
2:E:173:GLY:O	2:E:177:ILE:HG12	2.19	0.43
2:E:457:GLY:O	2:E:461:LEU:HD23	2.18	0.43
2:E:470:LEU:HD13	2:E:550:ILE:HG21	2.01	0.43
2:E:68:PHE:N	2:E:69:PRO:CD	2.82	0.43
2:F:1166:ALA:O	2:F:1169:PRO:HD2	2.19	0.43
2:F:309:ALA:HB1	2:F:369:GLN:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:514:TRP:CZ3	2:F:1493:ARG:HD2	2.53	0.43
2:G:108:MET:N	2:G:109:PRO:HD2	2.33	0.43
2:G:544:ILE:HG23	2:G:1144:ARG:HH22	1.83	0.43
2:G:327:LEU:O	2:G:327:LEU:HD23	2.19	0.43
2:H:108:MET:N	2:H:109:PRO:HD2	2.33	0.43
2:H:238:LYS:HA	2:H:1180:TYR:OH	2.19	0.43
2:H:1245:ARG:HA	2:H:1245:ARG:NE	2.34	0.43
2:H:366:LEU:HA	2:H:369:GLN:HB3	2.00	0.43
2:H:553:ALA:O	2:H:557:ILE:HG12	2.19	0.43
1:B:157:LEU:HD23	1:B:157:LEU:HA	1.85	0.43
1:B:224:THR:HG22	1:B:225:SER:O	2.19	0.43
1:B:318:ILE:HB	1:B:329:ASP:O	2.18	0.43
1:C:224:THR:HG22	1:C:225:SER:O	2.19	0.43
1:D:239:PRO:O	1:D:259:HIS:ND1	2.34	0.43
2:E:708:LEU:HB2	2:E:876:LEU:HD21	2.01	0.43
2:F:253:LEU:HD21	2:F:1231:ASP:CG	2.39	0.43
2:F:550:ILE:N	2:F:551:PRO:HD2	2.33	0.43
2:F:892:TYR:HD1	2:F:895:HIS:ND1	2.17	0.43
2:G:1092:VAL:O	2:G:1096:LEU:HG	2.19	0.43
2:G:245:ILE:N	2:G:1187:ASP:OD2	2.52	0.43
2:G:720:SER:N	3:G:2004:ATP:O2B	2.35	0.43
2:G:253:LEU:HD21	2:G:1231:ASP:CG	2.39	0.43
2:G:802:ILE:O	2:G:806:SER:N	2.52	0.43
2:G:873:LEU:O	2:G:877:ARG:HB2	2.18	0.43
2:G:919:SER:O	2:G:923:LEU:HB2	2.17	0.43
2:H:327:LEU:HD23	2:H:327:LEU:O	2.19	0.43
2:H:889:LYS:HB3	2:H:1538:ARG:NH1	2.33	0.43
1:D:35:PHE:CE1	1:D:233:LEU:HD13	2.54	0.43
1:D:299:GLN:O	1:D:301:ARG:NH1	2.52	0.43
2:E:553:ALA:O	2:E:557:ILE:HG12	2.19	0.43
2:E:911:GLY:HA3	2:E:915:ASP:OD2	2.19	0.43
2:F:1032:TRP:CD1	2:F:1035:LYS:HD3	2.54	0.43
2:F:1123:ARG:HE	2:F:1317:LEU:HD11	1.84	0.43
2:F:139:LEU:O	2:F:143:TRP:HD1	2.02	0.43
2:F:366:LEU:HA	2:F:369:GLN:HB3	2.00	0.43
2:F:508:LEU:HD22	2:F:1431:PHE:CZ	2.51	0.43
2:F:553:ALA:O	2:F:557:ILE:HG12	2.19	0.43
2:G:1123:ARG:HE	2:G:1317:LEU:HD11	1.84	0.43
2:G:327:LEU:HD22	2:G:1277:ALA:HB2	2.01	0.43
2:G:1350:SER:HA	2:G:1361:LEU:O	2.19	0.43
2:G:366:LEU:HA	2:G:369:GLN:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:487:SER:HA	2:G:490:GLU:HG2	2.01	0.43
2:G:892:TYR:HD1	2:G:895:HIS:ND1	2.17	0.43
2:H:1032:TRP:CD1	2:H:1035:LYS:HD3	2.54	0.43
2:H:174:LEU:HD13	2:H:178:LEU:HD13	2.01	0.43
2:H:575:VAL:HG23	2:H:576:ALA:N	2.34	0.43
2:H:802:ILE:O	2:H:806:SER:N	2.52	0.43
2:H:892:TYR:HD1	2:H:895:HIS:ND1	2.17	0.43
1:A:218:GLN:N	1:A:284:ILE:O	2.51	0.42
1:A:65:ASP:HB2	1:D:293:THR:HG22	2.00	0.42
1:B:35:PHE:CE1	1:B:233:LEU:HD13	2.54	0.42
1:D:268:TYR:OH	1:D:350:ASP:OD2	2.22	0.42
2:E:1092:VAL:O	2:E:1096:LEU:HG	2.19	0.42
2:E:1350:SER:HA	2:E:1362:LYS:HA	2.01	0.42
2:E:205:LYS:O	2:E:207:PRO:HD3	2.19	0.42
2:F:1245:ARG:HA	2:F:1245:ARG:NE	2.34	0.42
2:F:470:LEU:HD13	2:F:550:ILE:HG21	2.01	0.42
2:F:685:TYR:CD1	2:F:697:SER:HA	2.55	0.42
2:G:1166:ALA:O	2:G:1169:PRO:HD2	2.19	0.42
2:G:174:LEU:HD13	2:G:178:LEU:HD13	2.01	0.42
2:G:868:MET:HG3	2:G:872:ILE:HG13	2.01	0.42
2:H:1166:ALA:O	2:H:1169:PRO:HD2	2.19	0.42
2:H:1413:PRO:HB2	2:H:1416:THR:HG23	2.01	0.42
2:H:309:ALA:HB1	2:H:369:GLN:OE1	2.18	0.42
2:E:1031:TYR:HA	2:E:1282:LEU:CD1	2.45	0.42
2:E:253:LEU:HD21	2:E:1231:ASP:CG	2.39	0.42
2:E:1123:ARG:HE	2:E:1317:LEU:HD11	1.84	0.42
2:E:174:LEU:HD13	2:E:178:LEU:HD13	2.01	0.42
2:E:892:TYR:HD1	2:E:895:HIS:ND1	2.17	0.42
2:F:1106:LEU:HG	2:F:1325:TYR:HE2	1.85	0.42
2:F:238:LYS:HA	2:F:1180:TYR:OH	2.19	0.42
2:F:205:LYS:O	2:F:207:PRO:HD3	2.19	0.42
2:F:487:SER:HA	2:F:490:GLU:HG2	2.01	0.42
2:G:1032:TRP:CD1	2:G:1035:LYS:HD3	2.54	0.42
2:G:1106:LEU:HG	2:G:1325:TYR:HE2	1.85	0.42
2:G:1245:ARG:HA	2:G:1245:ARG:NE	2.34	0.42
2:G:889:LYS:HB3	2:G:1538:ARG:NH2	2.34	0.42
2:G:173:GLY:O	2:G:177:ILE:HG12	2.19	0.42
2:H:1092:VAL:O	2:H:1096:LEU:HG	2.19	0.42
2:H:889:LYS:HB3	2:H:1538:ARG:NH2	2.34	0.42
2:H:173:GLY:O	2:H:177:ILE:HG12	2.19	0.42
1:B:35:PHE:CD1	1:B:233:LEU:HD13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:LEU:HD21	1:B:70:HIS:HB2	2.00	0.42
1:C:222:LYS:HG3	1:C:232:PRO:HA	2.00	0.42
1:D:113:SER:OG	1:D:135:GLY:O	2.30	0.42
2:E:685:TYR:CD1	2:E:697:SER:HA	2.55	0.42
2:F:1092:VAL:O	2:F:1096:LEU:HG	2.19	0.42
2:F:1435:ILE:HB	2:F:1470:LEU:HB2	1.99	0.42
2:F:327:LEU:HD22	2:F:1277:ALA:HB2	2.01	0.42
2:F:575:VAL:HG23	2:F:576:ALA:N	2.34	0.42
2:F:850:VAL:HG21	2:F:881:ARG:NE	2.32	0.42
2:G:503:LEU:HD23	2:G:506:ILE:HD13	2.00	0.42
2:H:1064:ALA:O	2:H:1067:PHE:HB3	2.19	0.42
1:A:267:LEU:HD21	1:A:283:ILE:HD11	2.01	0.42
1:A:344:CYS:HB2	1:A:348:GLN:OE1	2.20	0.42
1:A:63:LEU:HD11	1:A:75:PHE:CZ	2.55	0.42
1:C:200:LEU:N	1:C:257:ILE:O	2.47	0.42
2:E:1064:ALA:O	2:E:1067:PHE:HB3	2.19	0.42
2:E:889:LYS:HB3	2:E:1538:ARG:NH2	2.34	0.42
2:F:1064:ALA:O	2:F:1067:PHE:HB3	2.19	0.42
2:F:1413:PRO:HB2	2:F:1416:THR:HG23	2.01	0.42
2:F:398:LYS:NZ	2:F:616:SER:HB2	2.35	0.42
2:F:868:MET:HG3	2:F:872:ILE:HG13	2.01	0.42
2:G:1460:LYS:O	2:G:1464:LYS:HG3	2.20	0.42
2:G:238:LYS:HA	2:G:1180:TYR:OH	2.19	0.42
2:G:325:ASP:OD1	2:G:326:HIS:N	2.53	0.42
2:G:550:ILE:N	2:G:551:PRO:HD2	2.34	0.42
2:G:911:GLY:HA3	2:G:915:ASP:OD2	2.20	0.42
2:H:708:LEU:HB2	2:H:876:LEU:HD21	2.01	0.42
1:A:35:PHE:CE1	1:A:233:LEU:HD13	2.54	0.42
1:B:272:PRO:C	1:B:274:ASP:H	2.23	0.42
1:C:35:PHE:CD1	1:C:233:LEU:HD13	2.54	0.42
1:D:177:ARG:HH21	1:D:204:ASP:CG	2.22	0.42
1:D:222:LYS:HG3	1:D:232:PRO:HA	2.00	0.42
2:E:1147:LEU:HA	2:E:1147:LEU:HD22	1.83	0.42
2:E:238:LYS:HA	2:E:1180:TYR:OH	2.19	0.42
2:E:207:PRO:HA	2:E:211:GLN:H	1.85	0.42
2:E:366:LEU:HA	2:E:369:GLN:HB3	2.00	0.42
2:E:503:LEU:HD23	2:E:506:ILE:HD13	2.00	0.42
2:E:873:LEU:O	2:E:877:ARG:HB2	2.18	0.42
2:F:911:GLY:HA3	2:F:915:ASP:OD2	2.19	0.42
2:G:68:PHE:N	2:G:69:PRO:CD	2.82	0.42
2:H:1033:LEU:HD12	2:H:1036:TRP:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1350:SER:HA	2:H:1361:LEU:O	2.19	0.42
2:H:68:PHE:N	2:H:69:PRO:CD	2.82	0.42
1:A:35:PHE:CD1	1:A:233:LEU:HD13	2.54	0.42
1:C:344:CYS:HB2	1:C:348:GLN:OE1	2.20	0.42
2:E:1352:ARG:HB3	2:E:1359:PRO:HA	2.02	0.42
2:F:1466:LEU:HA	2:F:1467:PRO:HD3	1.95	0.42
2:F:477:VAL:HG11	2:F:543:SER:HB2	2.02	0.42
2:F:68:PHE:N	2:F:69:PRO:CD	2.82	0.42
2:G:1033:LEU:HD12	2:G:1036:TRP:HB3	2.02	0.42
2:H:36:HIS:CE1	2:H:113:ALA:HB2	2.55	0.42
2:H:253:LEU:HD21	2:H:1231:ASP:CG	2.39	0.42
2:H:85:LEU:HD13	2:H:85:LEU:HA	1.82	0.42
1:B:299:GLN:O	1:B:301:ARG:NH1	2.52	0.42
1:C:218:GLN:N	1:C:284:ILE:O	2.50	0.42
1:D:63:LEU:HD11	1:D:75:PHE:CZ	2.55	0.42
2:E:1032:TRP:CD1	2:E:1035:LYS:HD3	2.54	0.42
2:E:36:HIS:CE1	2:E:113:ALA:HB2	2.55	0.42
2:E:1413:PRO:HB2	2:E:1416:THR:HG23	2.01	0.42
2:E:508:LEU:HD22	2:E:1431:PHE:CZ	2.51	0.42
2:E:477:VAL:HG11	2:E:543:SER:HB2	2.02	0.42
2:F:245:ILE:N	2:F:1187:ASP:OD2	2.52	0.42
2:F:1352:ARG:HB3	2:F:1359:PRO:HA	2.02	0.42
2:G:1147:LEU:HD22	2:G:1147:LEU:HA	1.83	0.42
2:G:1347:GLN:HA	2:G:1365:ASN:HB3	2.02	0.42
2:G:36:HIS:CE1	2:G:113:ALA:HB2	2.55	0.42
2:H:205:LYS:O	2:H:207:PRO:HD3	2.19	0.42
2:H:207:PRO:HA	2:H:211:GLN:H	1.85	0.42
1:A:224:THR:HG22	1:A:225:SER:O	2.19	0.42
1:A:239:PRO:HB3	1:D:244:VAL:HG22	2.02	0.42
1:B:330:TYR:O	1:B:333:PHE:HB2	2.20	0.42
1:B:268:TYR:OH	1:B:350:ASP:OD2	2.22	0.42
2:E:1106:LEU:HG	2:E:1325:TYR:HE2	1.84	0.42
2:E:1220:ALA:O	2:E:1224:GLN:HG2	2.20	0.42
2:E:325:ASP:OD1	2:E:326:HIS:N	2.53	0.42
2:F:1031:TYR:HA	2:F:1282:LEU:CD1	2.46	0.42
2:F:368:LEU:HA	2:F:371:THR:HG22	2.01	0.42
2:G:1220:ALA:O	2:G:1224:GLN:HG2	2.20	0.42
2:G:1373:LYS:O	2:G:1546:ASP:N	2.31	0.42
2:G:1392:PHE:O	2:G:1418:ARG:NH1	2.47	0.42
2:G:205:LYS:O	2:G:207:PRO:HD3	2.19	0.42
2:H:1077:LEU:HA	2:H:1080:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1349:LEU:HB3	2:H:1364:VAL:CG1	2.50	0.42
2:H:477:VAL:HG11	2:H:543:SER:HB2	2.02	0.42
1:A:95:PHE:CD1	1:A:100:LEU:HD12	2.54	0.42
1:A:272:PRO:C	1:A:274:ASP:H	2.23	0.42
1:C:330:TYR:O	1:C:333:PHE:HB2	2.20	0.42
1:D:35:PHE:CD1	1:D:233:LEU:HD13	2.54	0.42
2:E:1520:GLN:HA	2:E:1523:VAL:HG12	2.02	0.42
2:E:685:TYR:CD2	2:E:734:SER:HB3	2.55	0.42
2:G:850:VAL:HG21	2:G:881:ARG:NE	2.32	0.42
2:H:1520:GLN:HA	2:H:1523:VAL:HG12	2.02	0.42
2:H:381:ILE:O	2:H:385:ILE:HG12	2.20	0.42
1:B:183:PHE:O	3:C:501:ATP:H5'1	2.20	0.42
1:B:321:GLU:OE2	1:C:32:ARG:N	2.53	0.42
1:B:63:LEU:HD11	1:B:75:PHE:CZ	2.55	0.42
1:C:299:GLN:O	1:C:301:ARG:NH1	2.52	0.42
2:E:85:LEU:HD13	2:E:85:LEU:HA	1.82	0.42
2:F:1033:LEU:HD12	2:F:1036:TRP:HB3	2.02	0.42
2:F:1505:ASP:HA	2:F:1535:ILE:HB	2.02	0.42
2:F:174:LEU:HD13	2:F:178:LEU:HD13	2.01	0.42
2:F:872:ILE:HD13	2:F:875:LEU:HD12	2.02	0.42
2:G:1352:ARG:HB3	2:G:1359:PRO:HA	2.02	0.42
2:G:139:LEU:O	2:G:143:TRP:HD1	2.02	0.42
2:H:1123:ARG:HE	2:H:1317:LEU:HD11	1.84	0.42
2:H:1350:SER:HA	2:H:1362:LYS:HA	2.01	0.42
2:H:1523:VAL:O	2:H:1527:PHE:HB2	2.20	0.42
1:B:344:CYS:HB2	1:B:348:GLN:OE1	2.20	0.41
1:D:344:CYS:HB2	1:D:348:GLN:OE1	2.20	0.41
2:E:1245:ARG:HA	2:E:1245:ARG:NE	2.34	0.41
2:E:1460:LYS:O	2:E:1464:LYS:HG3	2.20	0.41
2:F:1032:TRP:HD1	2:F:1035:LYS:HD3	1.85	0.41
2:F:1350:SER:HA	2:F:1362:LYS:HA	2.01	0.41
2:F:173:GLY:O	2:F:177:ILE:HG12	2.19	0.41
2:F:322:GLY:C	2:F:326:HIS:HD1	2.21	0.41
2:F:327:LEU:O	2:F:327:LEU:HD23	2.19	0.41
2:G:470:LEU:HD13	2:G:550:ILE:HG21	2.01	0.41
2:G:685:TYR:CD2	2:G:734:SER:HB3	2.55	0.41
2:H:1220:ALA:O	2:H:1224:GLN:HG2	2.20	0.41
2:H:1352:ARG:HB3	2:H:1359:PRO:HA	2.02	0.41
2:H:245:ILE:N	2:H:1187:ASP:OD2	2.52	0.41
2:H:470:LEU:HD13	2:H:550:ILE:HG21	2.01	0.41
2:H:685:TYR:CD2	2:H:734:SER:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:911:GLY:HA3	2:H:915:ASP:OD2	2.19	0.41
1:B:95:PHE:CD1	1:B:100:LEU:HD12	2.54	0.41
2:E:1033:LEU:HD12	2:E:1036:TRP:HB3	2.02	0.41
2:E:398:LYS:NZ	2:E:616:SER:HB2	2.35	0.41
2:F:1077:LEU:HA	2:F:1080:VAL:HG12	2.02	0.41
2:F:387:LEU:O	2:F:391:ILE:HG12	2.20	0.41
2:F:781:ALA:HA	2:F:821:GLN:HE22	1.85	0.41
2:G:1032:TRP:HD1	2:G:1035:LYS:HD3	1.86	0.41
2:G:1077:LEU:HA	2:G:1080:VAL:HG12	2.02	0.41
2:G:685:TYR:CD1	2:G:697:SER:HA	2.55	0.41
2:G:781:ALA:HA	2:G:821:GLN:HE22	1.86	0.41
2:H:1434:THR:O	2:H:1438:ASN:N	2.39	0.41
2:H:325:ASP:OD1	2:H:326:HIS:N	2.53	0.41
2:H:381:ILE:HD13	2:H:1241:THR:HG23	2.02	0.41
2:H:685:TYR:CD1	2:H:697:SER:HA	2.55	0.41
2:H:873:LEU:O	2:H:877:ARG:HB2	2.19	0.41
1:A:254:PRO:HD2	1:A:328:VAL:HG11	2.03	0.41
1:A:299:GLN:NE2	1:A:301:ARG:HD2	2.36	0.41
1:B:313:GLN:HE21	1:B:338:LYS:HG2	1.86	0.41
1:C:202:VAL:N	1:C:255:LEU:O	2.40	0.41
1:C:63:LEU:HD11	1:C:75:PHE:CZ	2.55	0.41
1:D:267:LEU:HD21	1:D:283:ILE:HD11	2.01	0.41
2:E:1434:THR:O	2:E:1438:ASN:N	2.39	0.41
2:E:387:LEU:O	2:E:391:ILE:HG12	2.20	0.41
2:E:850:VAL:HG21	2:E:881:ARG:NE	2.32	0.41
2:F:381:ILE:O	2:F:385:ILE:HG12	2.20	0.41
2:F:451:LEU:HD13	2:F:455:ILE:HB	2.03	0.41
2:G:1520:GLN:HA	2:G:1523:VAL:HG12	2.02	0.41
2:G:1523:VAL:O	2:G:1527:PHE:HB2	2.21	0.41
2:H:1147:LEU:HD22	2:H:1147:LEU:HA	1.83	0.41
1:C:299:GLN:NE2	1:C:301:ARG:HD2	2.36	0.41
1:D:229:GLU:HB3	1:C:314:ARG:HH11	1.86	0.41
1:D:50:ARG:NH1	3:D:501:ATP:H2'	2.36	0.41
2:E:245:ILE:N	2:E:1187:ASP:OD2	2.52	0.41
2:E:157:PHE:HE2	2:E:169:PHE:HB2	1.85	0.41
2:E:381:ILE:O	2:E:385:ILE:HG12	2.20	0.41
2:E:407:LEU:HD12	2:E:412:MET:O	2.21	0.41
2:E:781:ALA:HA	2:E:821:GLN:HE22	1.86	0.41
2:F:1025:VAL:HG21	2:F:1073:LEU:HD22	2.03	0.41
2:F:1317:LEU:HA	2:F:1317:LEU:HD23	1.85	0.41
2:F:325:ASP:OD1	2:F:326:HIS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:407:LEU:HD12	2:F:412:MET:O	2.20	0.41
2:F:767:GLY:O	2:F:769:VAL:N	2.52	0.41
2:G:477:VAL:HG11	2:G:543:SER:HB2	2.02	0.41
2:H:157:PHE:HE2	2:H:169:PHE:HB2	1.85	0.41
2:H:407:LEU:HD12	2:H:412:MET:O	2.21	0.41
1:B:299:GLN:NE2	1:B:301:ARG:HD2	2.36	0.41
1:B:320:ALA:O	1:B:327:SER:OG	2.31	0.41
1:D:299:GLN:NE2	1:D:301:ARG:HD2	2.36	0.41
1:A:46:HIS:CD2	1:D:330:TYR:CE2	3.09	0.41
2:E:1379:ARG:NE	2:E:1552:LYS:O	2.47	0.41
2:E:487:SER:HA	2:E:490:GLU:HG2	2.01	0.41
2:F:207:PRO:HA	2:F:211:GLN:H	1.85	0.41
2:F:36:HIS:CE1	2:F:113:ALA:HB2	2.55	0.41
2:F:679:VAL:HA	2:F:738:PHE:O	2.21	0.41
2:G:1088:THR:O	2:G:1092:VAL:HG23	2.20	0.41
2:G:1349:LEU:HB3	2:G:1364:VAL:CG1	2.50	0.41
2:G:207:PRO:HA	2:G:211:GLN:H	1.85	0.41
2:G:322:GLY:C	2:G:326:HIS:HD1	2.21	0.41
2:H:1031:TYR:HA	2:H:1282:LEU:CD1	2.46	0.41
2:H:387:LEU:O	2:H:391:ILE:HG12	2.20	0.41
2:H:487:SER:HA	2:H:490:GLU:HG2	2.02	0.41
2:H:398:LYS:NZ	2:H:616:SER:HB2	2.35	0.41
2:H:781:ALA:HA	2:H:821:GLN:HE22	1.86	0.41
1:A:313:GLN:HE21	1:A:338:LYS:HG2	1.86	0.41
1:B:267:LEU:HD21	1:B:283:ILE:HD11	2.01	0.41
1:B:271:ALA:HB2	1:B:345:THR:HG22	2.02	0.41
1:D:95:PHE:CD1	1:D:100:LEU:HD12	2.54	0.41
1:D:272:PRO:C	1:D:274:ASP:H	2.23	0.41
2:E:811:ILE:O	2:E:817:GLY:HA2	2.21	0.41
2:F:1088:THR:O	2:F:1092:VAL:HG23	2.20	0.41
2:F:1347:GLN:HA	2:F:1365:ASN:HB3	2.02	0.41
2:F:685:TYR:CD2	2:F:734:SER:HB3	2.55	0.41
2:G:1033:LEU:O	2:G:1036:TRP:HB3	2.21	0.41
2:G:1505:ASP:HA	2:G:1535:ILE:HB	2.02	0.41
2:G:157:PHE:HE2	2:G:169:PHE:HB2	1.85	0.41
2:G:381:ILE:O	2:G:385:ILE:HG12	2.20	0.41
2:G:398:LYS:NZ	2:G:616:SER:HB2	2.35	0.41
2:H:1025:VAL:HG21	2:H:1073:LEU:HD22	2.03	0.41
2:H:868:MET:HG3	2:H:872:ILE:HG13	2.01	0.41
1:A:240:MET:HG2	1:A:247:ASN:ND2	2.36	0.41
1:A:330:TYR:O	1:A:333:PHE:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:PRO:HD2	1:B:328:VAL:HG11	2.03	0.41
1:B:75:PHE:O	1:B:78:SER:OG	2.27	0.41
1:C:254:PRO:HD2	1:C:328:VAL:HG11	2.02	0.41
1:D:50:ARG:HB2	3:D:501:ATP:C5	2.56	0.41
2:E:1349:LEU:HB3	2:E:1364:VAL:CG1	2.50	0.41
2:E:1402:ILE:HG23	2:E:1409:ILE:HB	2.03	0.41
2:E:1523:VAL:O	2:E:1527:PHE:HB2	2.20	0.41
2:F:1392:PHE:O	2:F:1418:ARG:NH1	2.47	0.41
2:F:1460:LYS:O	2:F:1464:LYS:HG3	2.20	0.41
2:G:368:LEU:HA	2:G:371:THR:HG22	2.01	0.41
2:G:811:ILE:O	2:G:817:GLY:HA2	2.21	0.41
2:G:793:PHE:HA	2:G:844:TYR:OH	2.21	0.41
2:H:575:VAL:HG23	2:H:576:ALA:H	1.86	0.41
2:H:679:VAL:HA	2:H:738:PHE:O	2.21	0.41
2:H:811:ILE:O	2:H:817:GLY:HA2	2.21	0.41
2:H:850:VAL:HG21	2:H:881:ARG:NE	2.32	0.41
1:B:240:MET:HG2	1:B:247:ASN:ND2	2.36	0.41
1:C:271:ALA:HB2	1:C:345:THR:HG22	2.02	0.41
1:D:165:GLY:HA2	1:C:168:PHE:HD1	1.85	0.41
1:D:254:PRO:HD2	1:D:328:VAL:HG11	2.02	0.41
1:D:330:TYR:O	1:D:333:PHE:HB2	2.20	0.41
2:E:769:VAL:HG12	2:E:770:ALA:O	2.21	0.41
2:F:224:LEU:HA	2:F:227:LYS:HB2	2.03	0.41
2:F:769:VAL:HG12	2:F:770:ALA:O	2.21	0.41
2:F:811:ILE:O	2:F:817:GLY:HA2	2.21	0.41
2:G:1350:SER:HA	2:G:1362:LYS:HA	2.01	0.41
2:G:872:ILE:HD13	2:G:875:LEU:HD12	2.02	0.41
2:H:137:ILE:O	2:H:140:LEU:HB3	2.21	0.41
2:H:793:PHE:HA	2:H:844:TYR:OH	2.21	0.41
1:A:200:LEU:N	1:A:257:ILE:O	2.47	0.41
1:B:45:ALA:HB3	1:B:47:LYS:HZ2	1.85	0.41
1:C:313:GLN:HE21	1:C:338:LYS:HG2	1.86	0.41
1:D:210:ILE:HG23	1:D:213:ALA:HB2	2.03	0.41
2:E:1428:PRO:HB3	2:E:1487:GLN:HA	2.03	0.41
2:E:1505:ASP:HA	2:E:1535:ILE:HB	2.02	0.41
2:E:774:GLN:HE22	3:E:2004:ATP:PG	2.44	0.41
2:E:424:ASP:OD2	2:E:610:LEU:HD21	2.21	0.41
2:E:435:CYS:HG	2:E:439:TRP:HZ3	1.67	0.41
2:F:1349:LEU:HB3	2:F:1364:VAL:CG1	2.50	0.41
2:F:1520:GLN:HA	2:F:1523:VAL:HG12	2.02	0.41
2:F:157:PHE:HE2	2:F:169:PHE:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:709:THR:HG22	2:F:884:VAL:HG22	2.03	0.41
2:F:781:ALA:HA	2:F:821:GLN:NE2	2.36	0.41
2:G:387:LEU:O	2:G:391:ILE:HG12	2.20	0.41
2:H:1106:LEU:HG	2:H:1325:TYR:HE2	1.84	0.41
2:H:511:LEU:O	2:H:1418:ARG:HB3	2.21	0.41
1:D:240:MET:HG2	1:D:247:ASN:ND2	2.36	0.41
2:E:1025:VAL:HG21	2:E:1073:LEU:HD22	2.03	0.41
2:E:1569:LYS:O	2:E:1569:LYS:HD2	2.21	0.41
2:E:381:ILE:HD13	2:E:1241:THR:HG23	2.02	0.41
2:E:451:LEU:HD13	2:E:455:ILE:HB	2.03	0.41
2:F:381:ILE:HD13	2:F:1241:THR:HG23	2.02	0.41
2:F:782:THR:OG1	2:F:821:GLN:OE1	2.16	0.41
2:G:780:ASN:ND2	2:G:1205:GLU:OE2	2.54	0.41
2:G:137:ILE:O	2:G:140:LEU:HB3	2.21	0.41
2:G:424:ASP:OD2	2:G:610:LEU:HD21	2.21	0.41
2:G:709:THR:HG22	2:G:884:VAL:HG22	2.03	0.41
2:H:1033:LEU:O	2:H:1036:TRP:HB3	2.21	0.41
2:H:769:VAL:HG12	2:H:770:ALA:O	2.21	0.41
1:B:210:ILE:HG23	1:B:213:ALA:HB2	2.03	0.41
1:C:240:MET:HG2	1:C:247:ASN:ND2	2.36	0.41
2:E:1033:LEU:O	2:E:1036:TRP:HB3	2.21	0.41
2:E:1088:THR:O	2:E:1092:VAL:HG23	2.20	0.41
2:E:1317:LEU:HD23	2:E:1317:LEU:HA	1.85	0.41
2:E:137:ILE:O	2:E:140:LEU:HB3	2.21	0.41
2:E:81:LEU:HD11	2:E:179:TYR:HE1	1.86	0.41
2:E:679:VAL:HA	2:E:738:PHE:O	2.21	0.41
2:F:575:VAL:HG23	2:F:576:ALA:H	1.86	0.41
2:G:368:LEU:O	2:G:371:THR:HG22	2.21	0.41
2:G:843:LEU:O	2:G:881:ARG:NH2	2.41	0.41
2:H:1428:PRO:HB3	2:H:1487:GLN:HA	2.03	0.41
2:H:1569:LYS:HD2	2:H:1569:LYS:O	2.21	0.41
2:H:224:LEU:HA	2:H:227:LYS:HB2	2.03	0.41
2:H:424:ASP:OD2	2:H:610:LEU:HD21	2.21	0.41
1:A:95:PHE:CD2	2:E:27:PHE:HD1	2.39	0.40
1:C:210:ILE:HG23	1:C:213:ALA:HB2	2.03	0.40
1:C:267:LEU:HD21	1:C:283:ILE:HD11	2.01	0.40
1:C:272:PRO:C	1:C:274:ASP:H	2.23	0.40
2:F:29:ASP:OD1	2:F:109:PRO:HG3	2.21	0.40
2:F:1438:ASN:OD1	2:F:1474:ILE:HD12	2.21	0.40
2:F:1423:ILE:HG13	2:F:1503:ILE:HG23	2.03	0.40
2:F:81:LEU:HD11	2:F:179:TYR:HE1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:424:ASP:OD2	2:F:610:LEU:HD21	2.21	0.40
2:G:35:PRO:O	2:G:142:TYR:HE1	2.05	0.40
2:G:1438:ASN:OD1	2:G:1474:ILE:HD12	2.22	0.40
2:G:451:LEU:HD13	2:G:455:ILE:HB	2.03	0.40
2:H:1032:TRP:HD1	2:H:1035:LYS:HD3	1.86	0.40
2:H:774:GLN:HE22	3:H:2004:ATP:PG	2.44	0.40
1:A:90:TRP:CZ2	1:A:148:ILE:HG22	2.56	0.40
1:B:275:LEU:HB2	1:B:306:ALA:O	2.22	0.40
1:B:90:TRP:CZ2	1:B:148:ILE:HG22	2.56	0.40
2:E:515:GLU:O	2:E:519:ARG:CB	2.70	0.40
2:E:767:GLY:O	2:E:769:VAL:N	2.52	0.40
2:E:872:ILE:HD13	2:E:875:LEU:HD12	2.02	0.40
2:F:1033:LEU:O	2:F:1036:TRP:HB3	2.21	0.40
2:F:1220:ALA:O	2:F:1224:GLN:HG2	2.20	0.40
2:F:1523:VAL:O	2:F:1527:PHE:HB2	2.20	0.40
2:F:368:LEU:O	2:F:371:THR:HG22	2.22	0.40
2:F:793:PHE:HA	2:F:844:TYR:OH	2.21	0.40
2:F:861:ILE:HG13	2:F:861:ILE:H	1.72	0.40
2:G:1181:PHE:HE1	2:G:1243:ALA:HB1	1.86	0.40
2:G:1369:ALA:HB1	2:G:1370:PRO:HD2	2.04	0.40
2:G:1402:ILE:HG23	2:G:1409:ILE:HB	2.03	0.40
2:G:381:ILE:HD13	2:G:1241:THR:HG23	2.03	0.40
2:G:575:VAL:HG23	2:G:576:ALA:H	1.86	0.40
2:H:1155:VAL:HG11	2:H:1286:TYR:CE2	2.57	0.40
2:H:368:LEU:O	2:H:371:THR:HG22	2.21	0.40
2:H:786:ASN:OD1	2:H:787:ILE:N	2.54	0.40
2:H:872:ILE:HD13	2:H:875:LEU:HD12	2.02	0.40
1:A:210:ILE:HG23	1:A:213:ALA:HB2	2.03	0.40
1:B:318:ILE:HA	1:B:332:LYS:HZ2	1.86	0.40
2:E:469:LEU:O	2:E:472:PRO:HD2	2.21	0.40
2:E:575:VAL:HG23	2:E:576:ALA:H	1.86	0.40
2:E:770:ALA:HB3	2:E:850:VAL:HA	2.04	0.40
2:F:780:ASN:ND2	2:F:1205:GLU:OE2	2.54	0.40
2:F:515:GLU:O	2:F:519:ARG:CB	2.69	0.40
2:G:1289:MET:O	2:G:1293:TYR:HD2	2.05	0.40
2:G:1431:PHE:HB2	2:G:1438:ASN:ND2	2.36	0.40
2:G:511:LEU:O	2:G:1418:ARG:HB3	2.21	0.40
2:G:573:PRO:HB2	2:G:574:SER:H	1.64	0.40
2:G:769:VAL:HG12	2:G:770:ALA:O	2.21	0.40
2:H:1088:THR:O	2:H:1092:VAL:HG23	2.20	0.40
2:H:1392:PHE:O	2:H:1418:ARG:NH1	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:35:PRO:O	2:H:142:TYR:HE1	2.05	0.40
2:H:1505:ASP:HA	2:H:1535:ILE:HB	2.03	0.40
2:H:781:ALA:HA	2:H:821:GLN:NE2	2.36	0.40
2:H:843:LEU:O	2:H:881:ARG:NH2	2.41	0.40
2:H:770:ALA:HB3	2:H:850:VAL:HA	2.04	0.40
2:H:995:ILE:N	2:H:996:PRO:HD2	2.36	0.40
2:E:1032:TRP:HD1	2:E:1035:LYS:HD3	1.86	0.40
2:E:1077:LEU:HA	2:E:1080:VAL:HG12	2.02	0.40
2:E:1392:PHE:O	2:E:1418:ARG:NH1	2.47	0.40
2:E:793:PHE:HA	2:E:844:TYR:OH	2.21	0.40
2:E:995:ILE:N	2:E:996:PRO:HD2	2.36	0.40
2:F:137:ILE:O	2:F:140:LEU:HB3	2.21	0.40
2:F:35:PRO:O	2:F:142:TYR:HE1	2.05	0.40
2:G:1012:LEU:HD13	2:G:1012:LEU:HA	1.95	0.40
2:G:1428:PRO:HB3	2:G:1487:GLN:HA	2.03	0.40
2:G:81:LEU:HD11	2:G:179:TYR:HE1	1.86	0.40
2:G:224:LEU:HA	2:G:227:LYS:HB2	2.03	0.40
2:G:685:TYR:HB2	2:G:734:SER:N	2.36	0.40
2:H:1152:ALA:O	2:H:1156:ILE:HG12	2.21	0.40
1:B:271:ALA:HB2	1:B:345:THR:CG2	2.52	0.40
2:E:1152:ALA:O	2:E:1156:ILE:HG12	2.21	0.40
2:E:421:VAL:HG11	2:E:1203:PHE:CD2	2.57	0.40
2:E:781:ALA:HA	2:E:821:GLN:NE2	2.36	0.40
2:E:869:GLN:O	2:E:873:LEU:HB3	2.22	0.40
2:F:1289:MET:O	2:F:1293:TYR:HD2	2.05	0.40
2:F:370:ARG:HB3	2:F:1252:GLU:HG2	2.03	0.40
2:F:457:GLY:O	2:F:461:LEU:HB3	2.22	0.40
2:F:709:THR:HA	2:F:898:TRP:O	2.22	0.40
2:G:1025:VAL:HG21	2:G:1073:LEU:HD22	2.03	0.40
2:G:1155:VAL:HG11	2:G:1286:TYR:CE2	2.57	0.40
2:G:407:LEU:HD12	2:G:412:MET:O	2.21	0.40
2:G:995:ILE:N	2:G:996:PRO:HD2	2.36	0.40
2:H:1347:GLN:HA	2:H:1365:ASN:HB3	2.02	0.40
2:H:1402:ILE:HG23	2:H:1409:ILE:HB	2.03	0.40
2:H:1438:ASN:OD1	2:H:1474:ILE:HD12	2.21	0.40
2:H:1460:LYS:O	2:H:1464:LYS:HG3	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	326/406 (80%)	293 (90%)	32 (10%)	1 (0%)	43	81
1	B	326/406 (80%)	293 (90%)	32 (10%)	1 (0%)	43	81
1	C	326/406 (80%)	293 (90%)	32 (10%)	1 (0%)	43	81
1	D	326/406 (80%)	292 (90%)	33 (10%)	1 (0%)	43	81
2	E	1341/1581 (85%)	1242 (93%)	97 (7%)	2 (0%)	53	88
2	F	1341/1581 (85%)	1241 (92%)	98 (7%)	2 (0%)	53	88
2	G	1341/1581 (85%)	1240 (92%)	99 (7%)	2 (0%)	53	88
2	H	1341/1581 (85%)	1241 (92%)	98 (7%)	2 (0%)	53	88
All	All	6668/7948 (84%)	6135 (92%)	521 (8%)	12 (0%)	53	85

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	194	ARG
2	H	194	ARG
2	G	194	ARG
2	F	194	ARG
1	A	48	ASN
1	D	48	ASN
1	B	48	ASN
1	C	48	ASN
2	E	456	LEU
2	H	456	LEU
2	G	456	LEU
2	F	456	LEU

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 PDB entries followed by that with respect to all EM

entries.

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	265/348 (76%)	265 (100%)	0	100	100
1	B	265/348 (76%)	265 (100%)	0	100	100
1	C	265/348 (76%)	265 (100%)	0	100	100
1	D	265/348 (76%)	265 (100%)	0	100	100
2	E	1004/1368 (73%)	998 (99%)	6 (1%)	87	93
2	F	1004/1368 (73%)	998 (99%)	6 (1%)	87	93
2	G	1004/1368 (73%)	998 (99%)	6 (1%)	87	93
2	H	1004/1368 (73%)	998 (99%)	6 (1%)	87	93
All	All	5076/6864 (74%)	5052 (100%)	24 (0%)	90	94

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	547	ASN
2	E	918	ARG
2	E	1147	LEU
2	E	1292	ASN
2	E	1295	ASN
2	E	1379	ARG
2	H	547	ASN
2	H	918	ARG
2	H	1147	LEU
2	H	1292	ASN
2	H	1295	ASN
2	H	1379	ARG
2	G	547	ASN
2	G	918	ARG
2	G	1147	LEU
2	G	1292	ASN
2	G	1295	ASN
2	G	1379	ARG
2	F	547	ASN
2	F	918	ARG
2	F	1147	LEU
2	F	1292	ASN
2	F	1295	ASN

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Mol	Chain	Res	Type
2	F	1379	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	46	HIS
1	A	193	HIS
1	A	247	ASN
1	A	276	HIS
1	A	278	HIS
1	A	279	GLN
1	D	43	ASN
1	D	46	HIS
1	D	193	HIS
1	D	247	ASN
1	D	276	HIS
1	D	278	HIS
1	D	279	GLN
1	B	43	ASN
1	B	46	HIS
1	B	247	ASN
1	B	276	HIS
1	B	278	HIS
1	B	279	GLN
1	C	43	ASN
1	C	46	HIS
1	C	247	ASN
1	C	276	HIS
1	C	278	HIS
1	C	279	GLN
2	E	36	HIS
2	E	103	HIS
2	E	126	ASN
2	E	188	ASN
2	E	416	GLN
2	E	426	ASN
2	E	474	GLN
2	E	498	GLN
2	E	926	HIS
2	E	1129	ASN
2	E	1133	GLN

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Mol	Chain	Res	Type
2	E	1272	HIS
2	E	1292	ASN
2	E	1483	GLN
2	H	32	ASN
2	H	36	HIS
2	H	103	HIS
2	H	126	ASN
2	H	188	ASN
2	H	416	GLN
2	H	426	ASN
2	H	474	GLN
2	H	498	GLN
2	H	926	HIS
2	H	1129	ASN
2	H	1133	GLN
2	H	1272	HIS
2	H	1292	ASN
2	H	1483	GLN
2	G	32	ASN
2	G	36	HIS
2	G	103	HIS
2	G	126	ASN
2	G	188	ASN
2	G	416	GLN
2	G	426	ASN
2	G	474	GLN
2	G	498	GLN
2	G	926	HIS
2	G	1102	ASN
2	G	1129	ASN
2	G	1133	GLN
2	G	1272	HIS
2	G	1292	ASN
2	G	1483	GLN
2	F	36	HIS
2	F	103	HIS
2	F	126	ASN
2	F	188	ASN
2	F	416	GLN
2	F	426	ASN
2	F	474	GLN
2	F	498	GLN

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Mol	Chain	Res	Type
2	F	926	HIS
2	F	1102	ASN
2	F	1129	ASN
2	F	1133	GLN
2	F	1272	HIS
2	F	1292	ASN
2	F	1483	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

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	$\# Z > 2$
3	ATP	A	501	-	27,33,33	0.96	1 (3%)	27,52,52	2.01	4 (14%)
3	ATP	A	502	-	27,33,33	0.94	1 (3%)	27,52,52	2.04	4 (14%)
3	ATP	C	501	-	27,33,33	0.96	1 (3%)	27,52,52	2.02	4 (14%)
3	ATP	D	501	-	27,33,33	0.95	1 (3%)	27,52,52	2.01	4 (14%)
4	ADP	E	2001	5	25,29,29	0.98	1 (4%)	25,45,45	1.83	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	E	2004	5	27,33,33	0.97	1 (3%)	27,52,52	1.96	5 (18%)
4	ADP	F	2001	5	25,29,29	1.00	1 (4%)	25,45,45	1.83	3 (12%)
3	ATP	F	2004	5	27,33,33	1.00	1 (3%)	27,52,52	1.95	5 (18%)
4	ADP	G	2001	5	25,29,29	0.99	1 (4%)	25,45,45	1.82	3 (12%)
3	ATP	G	2004	5	27,33,33	0.97	1 (3%)	27,52,52	1.95	5 (18%)
4	ADP	H	2001	5	25,29,29	0.99	1 (4%)	25,45,45	1.83	3 (12%)
3	ATP	H	2004	5	27,33,33	0.98	1 (3%)	27,52,52	1.95	5 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	501	-	-	0/18/38/38	0/3/3/3
3	ATP	A	502	-	-	0/18/38/38	0/3/3/3
3	ATP	C	501	-	-	0/18/38/38	0/3/3/3
3	ATP	D	501	-	-	0/18/38/38	0/3/3/3
4	ADP	E	2001	5	-	0/12/32/32	0/3/3/3
3	ATP	E	2004	5	-	0/18/38/38	0/3/3/3
4	ADP	F	2001	5	-	0/12/32/32	0/3/3/3
3	ATP	F	2004	5	-	0/18/38/38	0/3/3/3
4	ADP	G	2001	5	-	0/12/32/32	0/3/3/3
3	ATP	G	2004	5	-	0/18/38/38	0/3/3/3
4	ADP	H	2001	5	-	0/12/32/32	0/3/3/3
3	ATP	H	2004	5	-	0/18/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2004	ATP	C5-C4	2.90	1.47	1.40
3	E	2004	ATP	C5-C4	2.92	1.47	1.40
3	D	501	ATP	C5-C4	2.95	1.47	1.40
3	H	2004	ATP	C5-C4	2.95	1.47	1.40
4	G	2001	ADP	C5-C4	2.96	1.47	1.40
4	E	2001	ADP	C5-C4	2.96	1.47	1.40
3	F	2004	ATP	C5-C4	2.97	1.47	1.40
3	A	502	ATP	C5-C4	2.98	1.47	1.40
3	A	501	ATP	C5-C4	2.98	1.47	1.40
4	H	2001	ADP	C5-C4	2.99	1.47	1.40
3	C	501	ATP	C5-C4	3.01	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	2001	ADP	C5-C4	3.04	1.47	1.40

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	2001	ADP	N3-C2-N1	-6.27	123.49	128.86
4	E	2001	ADP	N3-C2-N1	-6.26	123.51	128.86
4	F	2001	ADP	N3-C2-N1	-6.23	123.53	128.86
4	G	2001	ADP	N3-C2-N1	-6.20	123.56	128.86
3	C	501	ATP	N3-C2-N1	-5.85	123.85	128.86
3	E	2004	ATP	N3-C2-N1	-5.78	123.91	128.86
3	A	502	ATP	N3-C2-N1	-5.77	123.92	128.86
3	G	2004	ATP	N3-C2-N1	-5.76	123.93	128.86
3	F	2004	ATP	N3-C2-N1	-5.75	123.94	128.86
3	H	2004	ATP	N3-C2-N1	-5.74	123.95	128.86
3	A	501	ATP	N3-C2-N1	-5.72	123.97	128.86
3	D	501	ATP	N3-C2-N1	-5.66	124.02	128.86
3	A	502	ATP	PA-O3A-PB	-4.72	116.77	132.63
3	D	501	ATP	PA-O3A-PB	-4.70	116.85	132.63
3	C	501	ATP	PA-O3A-PB	-4.63	117.08	132.63
3	A	501	ATP	PA-O3A-PB	-4.61	117.14	132.63
3	D	501	ATP	PB-O3B-PG	-4.26	118.31	132.63
3	F	2004	ATP	PB-O3B-PG	-4.26	118.32	132.63
3	A	502	ATP	PB-O3B-PG	-4.25	118.35	132.63
3	H	2004	ATP	PB-O3B-PG	-4.25	118.36	132.63
3	G	2004	ATP	PB-O3B-PG	-4.24	118.37	132.63
3	E	2004	ATP	PB-O3B-PG	-4.24	118.37	132.63
3	C	501	ATP	PB-O3B-PG	-4.17	118.61	132.63
3	A	501	ATP	PB-O3B-PG	-4.15	118.69	132.63
3	H	2004	ATP	PA-O3A-PB	-4.07	118.95	132.63
3	E	2004	ATP	PA-O3A-PB	-4.05	119.01	132.63
3	F	2004	ATP	PA-O3A-PB	-4.04	119.03	132.63
3	G	2004	ATP	PA-O3A-PB	-4.04	119.06	132.63
4	G	2001	ADP	PA-O3A-PB	-3.74	120.07	132.63
4	H	2001	ADP	PA-O3A-PB	-3.73	120.09	132.63
4	E	2001	ADP	PA-O3A-PB	-3.72	120.14	132.63
4	F	2001	ADP	PA-O3A-PB	-3.71	120.15	132.63
3	C	501	ATP	C4-C5-N7	-3.08	106.44	109.41
3	A	501	ATP	C4-C5-N7	-3.05	106.47	109.41
3	A	502	ATP	C4-C5-N7	-2.99	106.53	109.41
3	D	501	ATP	C4-C5-N7	-2.90	106.61	109.41
4	F	2001	ADP	C4-C5-N7	-2.82	106.68	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2001	ADP	C4-C5-N7	-2.75	106.75	109.41
4	H	2001	ADP	C4-C5-N7	-2.74	106.76	109.41
4	E	2001	ADP	C4-C5-N7	-2.74	106.77	109.41
3	E	2004	ATP	C4-C5-N7	-2.67	106.83	109.41
3	F	2004	ATP	C4-C5-N7	-2.66	106.84	109.41
3	H	2004	ATP	C4-C5-N7	-2.66	106.84	109.41
3	G	2004	ATP	C4-C5-N7	-2.59	106.91	109.41
3	G	2004	ATP	C2'-C3'-C4'	2.08	106.62	102.62
3	F	2004	ATP	C2'-C3'-C4'	2.09	106.64	102.62
3	E	2004	ATP	C2'-C3'-C4'	2.10	106.66	102.62
3	H	2004	ATP	C2'-C3'-C4'	2.11	106.66	102.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	ATP	3	0
3	A	502	ATP	5	0
3	C	501	ATP	3	0
3	D	501	ATP	4	0
4	E	2001	ADP	2	0
3	E	2004	ATP	5	0
4	F	2001	ADP	2	0
3	F	2004	ATP	2	0
4	G	2001	ADP	2	0
3	G	2004	ATP	4	0
4	H	2001	ADP	2	0
3	H	2004	ATP	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.