



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 20, 2018 – 09:44 pm GMT

PDB ID : 6C3O
EMDB ID: : EMD-7338
Title : Cryo-EM structure of human KATP bound to ATP and ADP in quatrefoil form
Authors : Lee, K.P.K.; Chen, J.; MacKinnon, R.
Deposited on : 2018-01-10
Resolution : 3.90 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

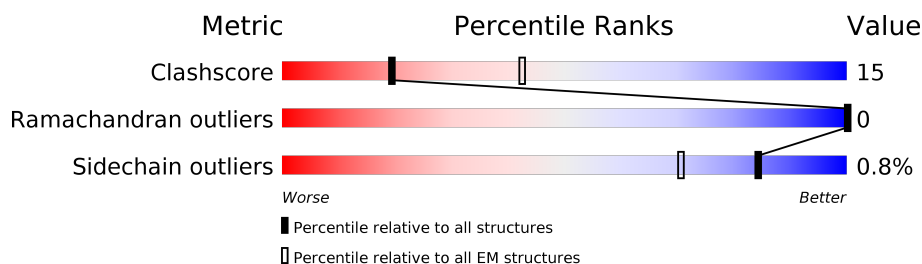
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	51% 29% 19%
1	B	406	50% 31% 19%
1	C	406	50% 31% 19%
1	D	406	50% 31% 19%
2	E	1581	56% 25% 18%
2	F	1581	56% 26% 18%
2	G	1581	55% 26% 18%
2	H	1581	56% 26% 18%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 49055 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
			2501	1616	427	441	17		
1	C	328	Total	C	N	O	S	0	0
			2501	1616	427	441	17		
1	B	328	Total	C	N	O	S	0	0
			2501	1616	427	441	17		
1	D	328	Total	C	N	O	S	0	0
			2501	1616	427	441	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
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

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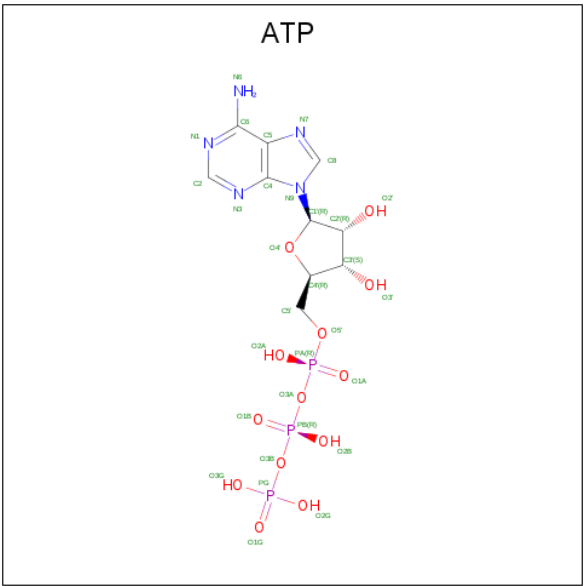
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Chain	Residue	Modelled	Actual	Comment	Reference
C	391	SER	-	expression tag	UNP Q14654
C	392	ASN	-	expression tag	UNP Q14654
C	393	SER	-	expression tag	UNP Q14654
C	394	LEU	-	expression tag	UNP Q14654
C	395	GLU	-	expression tag	UNP Q14654
C	396	VAL	-	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
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
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
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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	1290	Total	C	N	O	S	0	0
			9671	6307	1626	1687	51		
2	H	1290	Total	C	N	O	S	0	0
			9671	6307	1626	1687	51		
2	G	1290	Total	C	N	O	S	0	0
			9671	6307	1626	1687	51		
2	F	1290	Total	C	N	O	S	0	0
			9671	6307	1626	1687	51		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



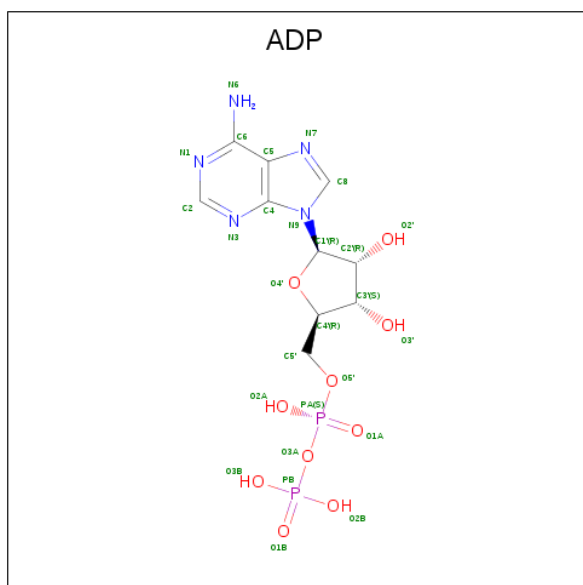
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Mol	Chain	Residues	Atoms					AltConf
3	G	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
4	A	3	Total	K	0
			3	3	

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

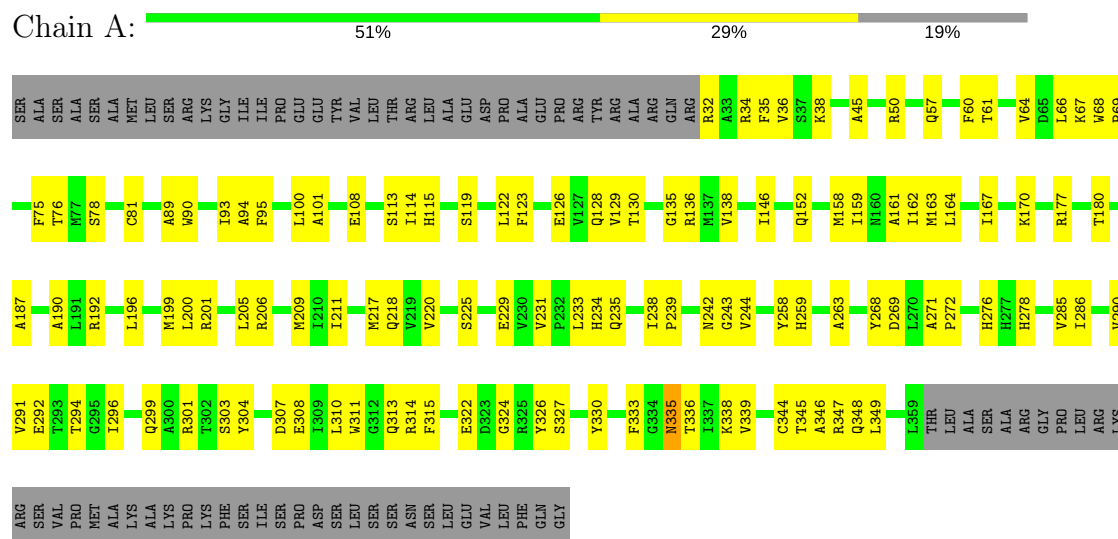


Mol	Chain	Residues	Atoms		AltConf
6	H	2	Total 2	Mg 2	0
6	G	2	Total 2	Mg 2	0
6	F	2	Total 2	Mg 2	0
6	E	2	Total 2	Mg 2	0

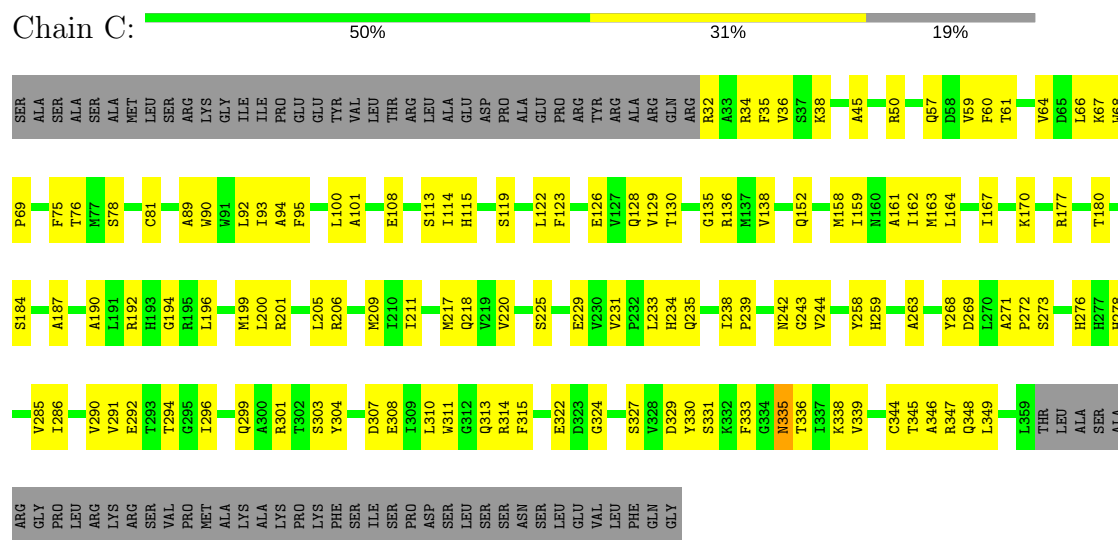
3 Residue-property plots

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

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

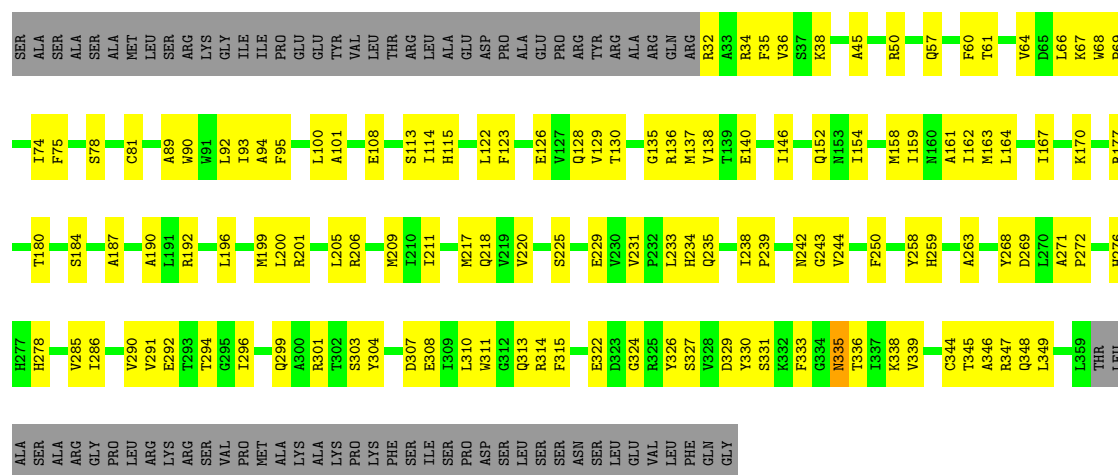


- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



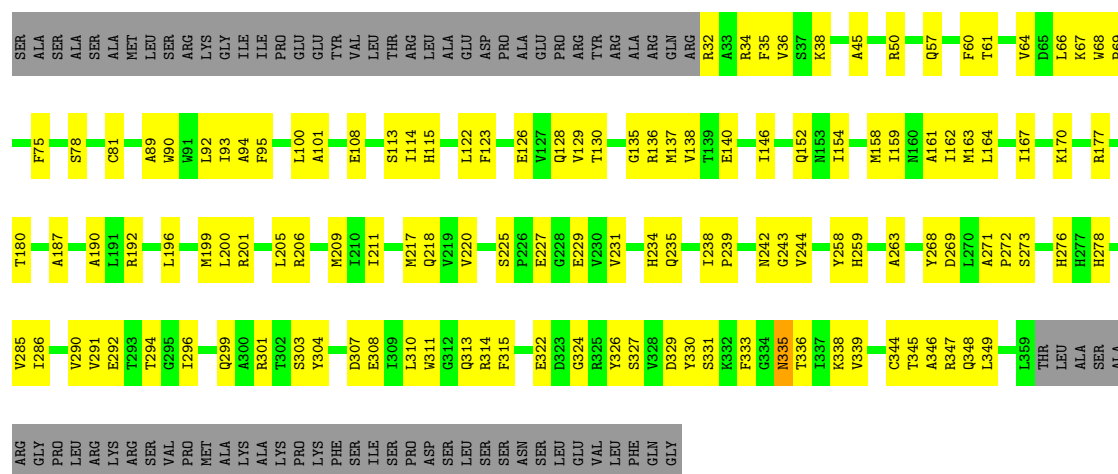
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11





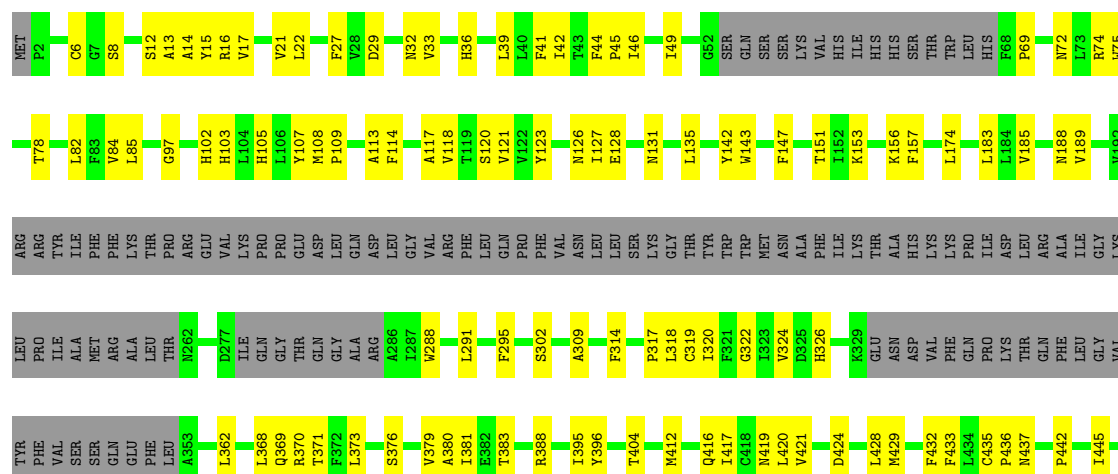
• Molecule 1: ATP-sensitive inward rectifier potassium channel 11

Chain D: 50% 31% 19%



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

Chain E: 56% 25% 18%





Category	Percentage
Very good	56%
Good	26%
Not good	18%



I1549	C1445	A1310	T1194	L1073	HIS	L930	P809	L723	ALA	I567	L451	VAL	TYR	ILE
D1560	S1446	R1313	H1202	I1075	GLN	MET	D810	L727	VAL	V563	L452	PRO	PHE	GLY
K1561	I1562	I1314	H1202	W1087	ARG	ASN	I811	L733	LEU	SER	L453	LEU	VAL	LYS
					E994	GLN	H816		ARG	PHE	Y454	VAL	SER	ILE
	E1455	Y1325	T1212	L1090	Y1003	GLN	T820		VAL	PHE	I455	VAL	GLN	ILE
R1568			I1213	K1091	L1004	GLN	Q821		VAL	LYS	L456	VAL	GLN	ILE
K1569	L1459	I1346	R1214	V1092	L1011	LEU	G823		ASN	GLU	G457	ASN	GLU	MET
D1570	K1460	N1348	F1216	F1216	L1012	GLU	S823		ARG	ALA	V458	ARG	PHE	ARG
S1571						LYS			LYS	ASP	L461	LEU	LEU	ALA
K1581	K1464	S1350	Y1218	N1102	L1012	GLU	L829		ARG	PHE	L461	PRO	ARG	THR
		V1351		F1124	H1023	THR			ALA	SER		ALA	THR	THR
	D1471		L1226		H1024	VAL	Q833		ASP	V573	A465	ASP	THR	V262
	A1472	S1355	D1231	D1127	V1025	THR	R834		SER	S574		GLU	THR	D277
	I1473	S1356	D1231	C1128	L1026	GLU	Q835		GLU	V575	I468	ASP	GLN	ILE
	I1474		S1232	N1129	V1027	ARG	R836		ILE	F577		CYS	GLY	GLN
		L1361	N1233	T1130	A1028	LYS			GLY		A471	ARG	THR	GLY
E1479		K1362	W1234	I1131	I1029	ALA	R841		GLU	L582	P472	GLY	THR	THR
M1480	H1363	H1363	I1235	D1132	D1030	THR	H846		ASP	F583	V477	LEU	GLN	GLN
F1481	V1364	V1364	I1235	Q1133	Y1031	GLU			PRO			THR	GLY	GLY
S1482		M1244	N1244	H1135	W1032	PRO	H849		PRO	V587	K480	GLY	ARG	GLY
	Q1372	R1245	W1246	I1135	K1035	GLN	V849		GLU	L590	S487	LEU	ALA	ALA
Q1485			H1246			GLY	F851		ARG	F591	E490	GLN	I381	A286
R1486	G1375	G1375	L1247	S1137	D1038	LEU	D865		THR	L592		SER	E582	I287
Q1487	I1376	I1376	E1248	T1138		SER			GLU	L593		LEU	T383	W288
L1488		L1139		L1139	ALA	ARG			VAL			VAL	R388	
	R1379	M1251		L1142	LEU	ALA	G871		THR	S595	E494	PRO	I395	L291
L1491				S1143	THR	MET			ASP	V596	L496	PRO	I396	F295
A1492	K1384	I1254	G1255	R1144	LEU	SER	L875		LEU	V597	K497	ASP	Y396	
R1493					THR	SER			ILE	S599	Q498	GLY	T404	A309
	F1392				PRO	ARG	D878		ASP	T600	N500	ASP	F314	
I1501			V1259	S1151	ALA	GLY	R881		LYS			ASP	M412	
F1502				A1152	ASN	LEU			ASP	L604	R504	ASP		P317
I1503	F1398	L1153	A1263	A1152	ASN	LEU	V886		ASN	V605		Q416	L318	L318
M1504	E1399	A1154		L1153	CYS	GLN	T887		C677	S606	K510	1417	C319	C319
D1505	G1400	I1267	I1267	V1155	SER	ASP	H888		A770	V607		C418	I320	I320
E1506	L1401	S1268	N1269	I1156	LEU	GLU	K889		V679		R519	N419	F321	F321
A1507	I1402	I1270	S1270	S1157	SER	GLU	L890		Q680	R620	T520	L420	G322	G322
T1508		L1271	R1271	V1162	GLN	GLU	Q891		I681	GLU	R521	V421	I323	I323
A1509			H1272	F1163	GLU	GLU	Y892			GLU		V324	L324	L324
S1510			R1273	L1164	GLU	GLU	L893		Y685	GLN	A537	D424	V324	V324
I1511	L1417	L1417	E1274	V1165	CYS	GLU	L893			GLN	I538	D325	H326	H326
D1512	R1418		L1275	A1166	THR	GLU	P894		I701	CYS	L538	L428	H326	H326
M1513		S1422	S1276	L1167	LEU	GLU	H895		R702	ALA	T540	M429		
A1514		I1423	A1277	L1168	ASP	ALA	A896		I703	PRO				
T1515		I1423			GLN	ALA	D897			HIS				K329
E1516	I1424		L1284	P1169	GLN	ALA	W898			GLU				GLU
		V1429	T1285	L1170	T1061	GLU	W898			GLU	S543	F432	ASN	ASN
R1530	L1430		T1286	A1171	Y1062	SER	I899			THR		F433	ASP	ASP
T1531	F1431		A1287	I1172	Y1063	GLU	I900		L708	PRO	N547	L434	VAL	VAL
					A1064	GLU			I710	PRO	T548	C435	PHE	PHE
	I1535			I1177	M1065	ASP	G905		V712	GLN	A549	P436	GLN	GLN
	R1436		N1292		V1066	ASP	T906			GLY	I550	M437	PRO	PRO
F1437					F1067	ASN	I907		G713	THR	P551		LYS	LYS
R1538			F1293	Y1180	T1068	LEU			Q714	PRO	I552	P442	THR	THR
	N1438		N1295	F1181	V1069	SER	R918		V715	ALA	A553		PHE	PHE
T1541				R1182	L1070	SER			G716	SER	A554	I445	LEU	LEU
	D1440			V1183	L1070	MET			C717	TYR	V555		GLY	GLY
L1547	F1441		M1300		C1071	LEU	Q822			GLN				
V1549				L1191	S1072	LEU								

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

Chain G:

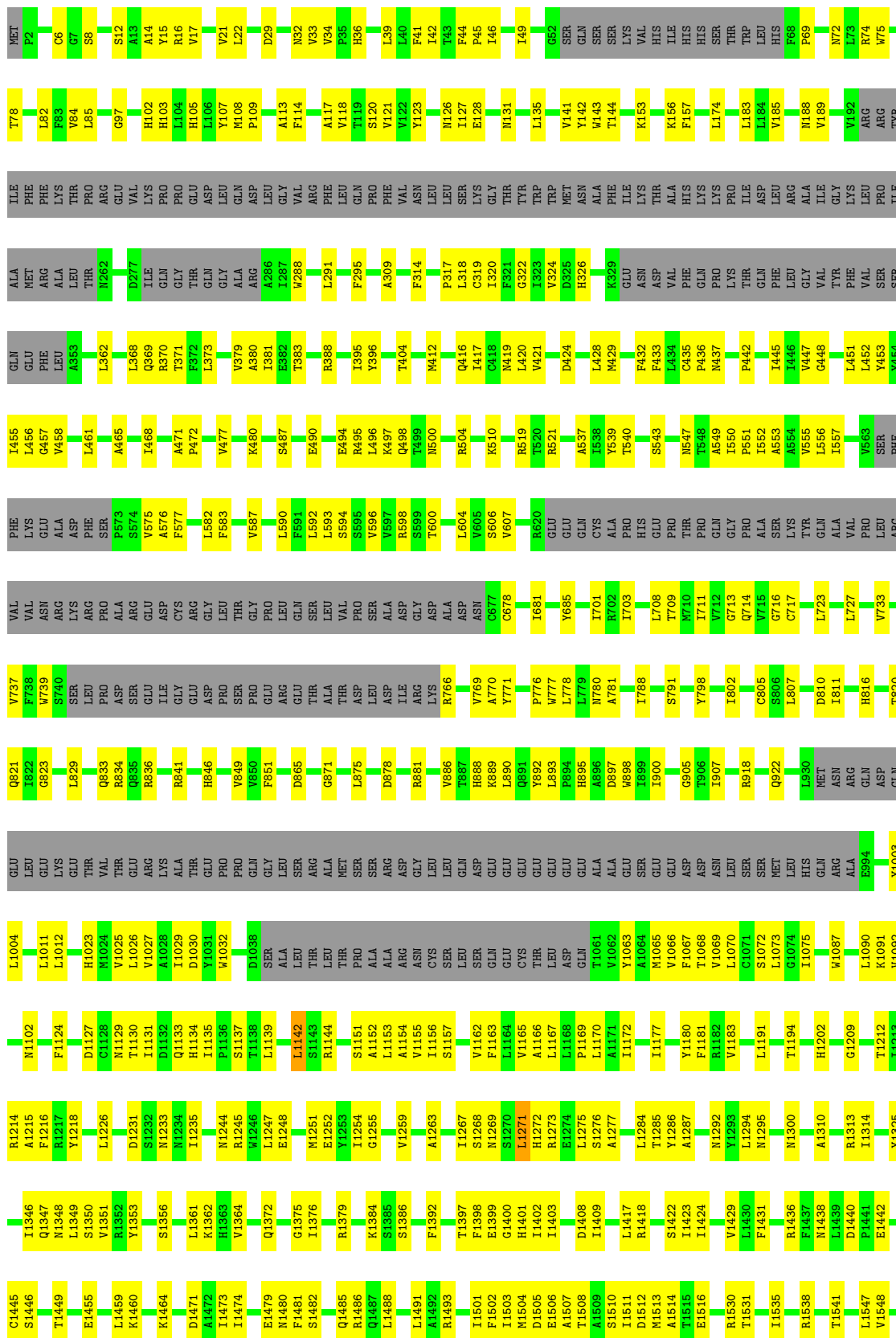


MET	F2	C6	G7	S8	S12	A13	A14	Y15	R16	V17	V21	L22	F27	V28	D29	N32	V33	V34	P35	H36	L39	L40	F41	I42	F44	P45	I46	I49	G52	SER	GLN	SER	SER	LYS	VAL	HIS	ILE	HIS	HIS	SER	THR	TRP	HIS	F68	P69	N72	L73	R74
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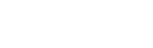
N1438	R1313	H1202	W1087	ALA	ARG	D810	L727	ALA	I557	L451	TYR	GLY	V192	W75
L1439	I1314	G1209	L1090	E994	GLN	I811	L727	VAL	V553	L452	PHE	LYS	ARG	T78
P1441	Y1003	T1212	K1091	Y1003	ASP	H816	V733	PRO	PHE	Y453	VAL	LEU	ARG	L82
E1442	L1004	I1213	V1092	L1004	GLU	T820	V737	ARG	PHE	Y454	GLN	ILE	TYR	F83
C1445	L1011	R1214	N1102	L1011	LEU	Q821	F738	VAL	PHE	Y455	ALA	ALA	ILE	V84
S1446	Q1347	A1215	N1102	L1012	GLU	I822	F739	ASN	GLY	L456	GLU	MET	PHE	L85
T1449	L1349	F1216	F1124	L1012	LYS	G823	W740	ARG	ALA	G457	PHE	ALA	PHE	G97
E1455	S1350	Y1218	F1124	M1024	GLU	L829	SER	LYS	ASP	A353	LEU	LEU	THR	
L1459	R1352	L1226	D1127	M1024	THR	L829	PRO	ARG	PHE	L461	THR	N262	PRO	
K1460	Y1353	D1231	C8128	V1025	GLU	Q833	ASP	ALA	SER	A465	L362	H103	ARG	H102
K1464	D1354	S1232	N1129	L1026	ARG	R834	SER	ARG	S573	A468	L368	L104	VAL	H103
K1471	S1355	N1233	I1131	A1028	LYS	Q836	ILE	GLU	V575	I469	Q369	H105	LYS	L104
D1471	S1356	N1234	D1132	I1029	ALA	R836	GLY	CYS	A576	A471	R370	L106	PRO	H105
A1472	L1361	I1235	Q1133	Y1030	THR	R841	GLU	ARG	F577	P472	F372	Y107	PRO	Y107
I1473	K1362	N1244	H1134	W1032	PRO	H846	ASP	GLY	L582	V477	L373	M108	GLU	Y108
I1474	H1363	R1245	P1136	W1032	PRO	H846	PRO	LEU	F583		Q374	P109	ASP	P109
E1479	G1372	L1247	S1137	D1038	GLN	V849	SER	THR	V587	K480	V379	A113	GLN	A113
N1480	I1376	E1248	T1138	SER	LEU	F851	PRO	GLY	F587	S487	A380	F114	LEU	F114
F1481	G1375	M1251	L1142	ALA	ALA	D865	THR	SER	L592	E490	F382	A117	GLY	A117
S1482	I1376	I1254	S1143	LEU	THR	G871	ALA	LEU	S594	E494	T383	V118	VAL	V118
Q1485	R1379	G1255	S1144	THR	LEU	G871	THR	ALA	S595	R495	R388	S120	PHE	S120
Q1487	R1486	I1259	S1151	THR	GLY	L875	ASP	VAL	V596	L496	I395	V122	GLN	V122
L1488	K1384	V1259	A1152	PRO	SER	D878	LEU	PRO	V597	K497	Y396	Y123	PRO	Y123
A1491	S1385	A1263	A1153	ALA	ASP	R881	ILE	ASP	V598	Q498	T404	N126	PHE	N126
L1492	S1386	I1267	I1155	ARG	GLY	R881	GLY	ASP	S599	T499	M412	I127	ASN	I127
R1493	F1392	I1267	I1156	ASN	LEU	V886	LYS	ALA	T600	N500	P317	E128	LEU	E128
I1501	T1397	S1268	S1157	SER	ASP	T887	R766	ASN	L604	R504	Q416	N131	LYS	N131
F1502	F1398	N1269	V1162	LEU	GLU	H888	V769	GLN	V605	R510	L318	L135	LYS	L135
I1503	E1399	S1270	F1163	SER	GLU	K889	A770	ASN	S606	K510	C319		GLY	
M1504	G1400	L1271	L1164	GLN	GLU	L890	Y771	C877	V607	R519	I417		THR	
D1505	H1401	I1272	V1165	THR	GLU	Q891	P776	C878	R620	T520	C418	Y142	TYR	Y142
E1506	I1402	R1273	A1166	CYS	GLU	Y892	W777	Q880	GLU	T521	L420	W143	TRP	W143
A1507	I1403	E1274	L1167	THR	GLU	L893	W778	I681	GLN	R521	V421	F147	TRP	F147
T1508	D1408	L1275	L1168	ASP	ALA	P894	L779	Y685	GLU	A537	D424	I148	MET	I148
A1509	I1409	S1276	P1169	GLN	ALA	H895	N780	T701	CYS	T538			ASN	
S1510	T1409	A1277	L1170	T1061	GLU	A896	A781	R702	ALA	Y639	L428	T151	ALA	T151
I1511	L1417	L1284	A1171	V1062	SER	D897	I788	I703	PRO	T540	M429	I152	ILE	I152
D1512	R1418	T1285	I1172	Y1063	GLU	W898	I788	I703	HIS	S543	F432	K153	LYS	K153
M1513	S1422	Y1286	I1177	A1064	ASP	I899	S791	L708	PRO	R547	F433	K156	THR	K156
A1514	I1423	A1287	Y1180	V1066	ASP	I900	Y798	T709	THR	R547	L434	F157	ALA	F157
E1516	I1424	N1292	F1181	V1067	ASN	I907	Y798	T709	PRO	T548	C435		LYS	
R1530	V1429	L1294	R1182	V1069	LEU	R918	I802	I711	GLN	A549	P436	L174	PRO	L174
T1531	L1430	N1295	V1183	V1069	SER	Q822	I802	I712	GLY	P551	N437	L183	LYS	L183
I1535	F1431	N1300	L1191	C1071	MET	L930	C805	G713	ALA	T552	P442	V185	ILE	V185
R1538	R1436	A1310	T1194	S1072	LEU	MET	S886	G715	SER	A553	I445	N188	ASP	N188
	F1437			L1074	HIS	Q808	L807	G716	TYR	A554	I445	V189	LEU	V189
				I1075	GLN	ASN	P809	L723	GLN	L556	G448		ALA	
					ARG								ILE	

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

Chain F:



D1560				
K1561				
P1562				
R1568				
S1571				
K1581				



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	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: ATP, K, MG, 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	0.38	0/2557	0.47	0/3482
1	B	0.38	0/2557	0.47	0/3482
1	C	0.38	0/2557	0.47	0/3482
1	D	0.38	0/2557	0.47	0/3482
2	E	0.33	0/9862	0.48	0/13439
2	F	0.33	0/9862	0.48	0/13439
2	G	0.33	0/9862	0.48	0/13439
2	H	0.33	0/9862	0.48	0/13439
All	All	0.34	0/49676	0.48	0/67684

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2501	0	2491	98	0
1	B	2501	0	2491	102	0
1	C	2501	0	2491	115	0
1	D	2501	0	2491	110	0
2	E	9671	0	9660	277	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	9671	0	9660	283	0
2	G	9671	0	9660	297	0
2	H	9671	0	9660	293	0
3	A	31	0	12	1	0
3	B	31	0	12	1	0
3	C	31	0	12	1	0
3	D	31	0	12	1	0
3	E	31	0	12	3	0
3	F	31	0	12	3	0
3	G	31	0	12	3	0
3	H	31	0	12	3	0
4	A	3	0	0	0	0
5	E	27	0	12	0	0
5	F	27	0	12	0	0
5	G	27	0	12	0	0
5	H	27	0	12	0	0
6	E	2	0	0	0	0
6	F	2	0	0	0	0
6	G	2	0	0	0	0
6	H	2	0	0	0	0
All	All	49055	0	48748	1483	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 15.

All (1483) 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:888:HIS:ND1	2:G:1512:ASP:OD1	1.66	1.28
2:F:888:HIS:ND1	2:F:1512:ASP:OD1	1.66	1.25
2:H:888:HIS:ND1	2:H:1512:ASP:OD1	1.66	1.24
2:E:888:HIS:ND1	2:E:1512:ASP:OD1	1.66	1.24
1:C:276:HIS:CD2	2:G:1355:SER:HB2	1.89	1.06
1:C:276:HIS:HD2	2:G:1355:SER:HB2	1.20	0.98
1:D:101:ALA:HB2	2:H:16:ARG:HB2	1.51	0.92
2:G:888:HIS:CE1	2:G:1512:ASP:OD1	2.23	0.92
2:F:888:HIS:CE1	2:F:1512:ASP:OD1	2.23	0.91
2:H:888:HIS:CE1	2:H:1512:ASP:OD1	2.23	0.91
2:E:888:HIS:CE1	2:E:1512:ASP:OD1	2.23	0.91
1:D:278:HIS:CG	2:H:1356:SER:OG	2.24	0.91
1:A:81:CYS:HB2	2:E:41:PHE:HB3	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:309:ALA:O	2:H:369:GLN:NE2	2.08	0.87
1:C:273:SER:OG	2:G:1398:PHE:CD2	2.27	0.87
2:F:309:ALA:O	2:F:369:GLN:NE2	2.08	0.87
1:C:81:CYS:HB2	2:G:41:PHE:HB3	1.56	0.86
1:A:67:LYS:HG2	1:A:69:PRO:HD2	1.58	0.86
1:B:67:LYS:HG2	1:B:69:PRO:HD2	1.58	0.86
2:E:309:ALA:O	2:E:369:GLN:NE2	2.08	0.86
2:G:309:ALA:O	2:G:369:GLN:NE2	2.08	0.86
1:C:67:LYS:HG2	1:C:69:PRO:HD2	1.58	0.85
1:B:101:ALA:HB2	2:F:16:ARG:HB2	1.58	0.85
2:F:723:LEU:HB3	2:F:851:PHE:HZ	1.41	0.85
1:D:67:LYS:HG2	1:D:69:PRO:HD2	1.58	0.84
1:D:278:HIS:CD2	2:H:1356:SER:OG	2.30	0.84
2:H:496:LEU:HD13	2:H:500:ASN:HD21	1.43	0.84
2:H:723:LEU:HB3	2:H:851:PHE:HZ	1.41	0.83
2:E:723:LEU:HB3	2:E:851:PHE:HZ	1.41	0.83
2:F:496:LEU:HD13	2:F:500:ASN:HD21	1.43	0.82
2:E:496:LEU:HD13	2:E:500:ASN:HD21	1.43	0.82
2:G:723:LEU:HB3	2:G:851:PHE:HZ	1.41	0.82
2:G:496:LEU:HD13	2:G:500:ASN:HD21	1.43	0.82
2:G:1510:SER:C	2:G:1511:ILE:HD13	2.03	0.80
1:D:81:CYS:HB2	2:H:41:PHE:HB3	1.62	0.80
2:H:424:ASP:OD1	2:H:606:SER:OG	2.01	0.79
2:E:1510:SER:C	2:E:1511:ILE:HD13	2.03	0.79
2:F:1510:SER:C	2:F:1511:ILE:HD13	2.03	0.79
2:H:1510:SER:C	2:H:1511:ILE:HD13	2.03	0.78
2:E:424:ASP:OD1	2:E:606:SER:OG	2.01	0.78
2:F:1459:LEU:HD21	2:F:1488:LEU:HB3	1.66	0.78
2:H:1025:VAL:HG11	2:H:1073:LEU:HD22	1.66	0.78
2:H:1508:THR:HA	2:H:1511:ILE:HG12	1.65	0.78
2:H:1459:LEU:HD21	2:H:1488:LEU:HB3	1.66	0.78
2:E:1459:LEU:HD21	2:E:1488:LEU:HB3	1.66	0.78
2:E:1025:VAL:HG11	2:E:1073:LEU:HD22	1.66	0.77
2:F:424:ASP:OD1	2:F:606:SER:OG	2.01	0.77
2:G:1459:LEU:HD21	2:G:1488:LEU:HB3	1.66	0.77
2:G:424:ASP:OD1	2:G:606:SER:OG	2.01	0.77
2:F:547:ASN:HD22	2:F:594:SER:HB2	1.50	0.77
2:G:1508:THR:HA	2:G:1511:ILE:HG12	1.66	0.77
2:G:97:GLY:HA2	2:G:1268:SER:HB2	1.67	0.77
1:B:278:HIS:CG	2:F:1356:SER:OG	2.38	0.77
2:H:97:GLY:HA2	2:H:1268:SER:HB2	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:97:GLY:HA2	2:F:1268:SER:HB2	1.67	0.76
2:F:1508:THR:HA	2:F:1511:ILE:HG12	1.65	0.76
1:C:101:ALA:HB2	2:G:16:ARG:HB2	1.67	0.76
2:H:547:ASN:HD22	2:H:594:SER:HB2	1.50	0.76
2:F:1025:VAL:HG11	2:F:1073:LEU:HD22	1.66	0.76
2:E:1508:THR:HA	2:E:1511:ILE:HG12	1.66	0.76
1:B:81:CYS:HB2	2:F:41:PHE:HB3	1.68	0.76
2:G:1025:VAL:HG11	2:G:1073:LEU:HD22	1.65	0.76
2:E:97:GLY:HA2	2:E:1268:SER:HB2	1.67	0.76
2:G:547:ASN:HD22	2:G:594:SER:HB2	1.50	0.76
2:E:1170:LEU:HD21	2:E:1254:ILE:HG23	1.68	0.75
2:H:1216:PHE:HB3	2:H:1218:TYR:HD2	1.51	0.75
2:E:1429:VAL:O	2:E:1493:ARG:NH1	2.18	0.75
2:E:1445:CYS:HG	2:E:1449:THR:HG1	1.30	0.75
2:F:1170:LEU:HD21	2:F:1254:ILE:HG23	1.68	0.74
2:G:598:ARG:NH1	2:G:1137:SER:OG	2.20	0.74
2:E:547:ASN:HD22	2:E:594:SER:HB2	1.50	0.74
2:H:1429:VAL:O	2:H:1493:ARG:NH1	2.17	0.74
2:H:1170:LEU:HD21	2:H:1254:ILE:HG23	1.68	0.74
1:A:136:ARG:NH2	1:B:138:VAL:O	2.18	0.74
2:E:1216:PHE:HB3	2:E:1218:TYR:HD2	1.51	0.74
2:F:29:ASP:OD2	2:F:105:HIS:ND1	2.17	0.74
2:G:1216:PHE:HB3	2:G:1218:TYR:HD2	1.51	0.74
2:F:556:LEU:HD11	2:F:1068:THR:HG22	1.69	0.74
2:H:598:ARG:NH1	2:H:1137:SER:OG	2.20	0.74
2:E:598:ARG:NH1	2:E:1137:SER:OG	2.20	0.74
2:G:1170:LEU:HD21	2:G:1254:ILE:HG23	1.68	0.74
2:G:1429:VAL:O	2:G:1493:ARG:NH1	2.17	0.74
2:F:598:ARG:NH1	2:F:1137:SER:OG	2.20	0.73
2:G:6:CYS:HA	2:G:103:HIS:HB2	1.70	0.73
2:F:1216:PHE:HB3	2:F:1218:TYR:HD2	1.51	0.73
2:G:556:LEU:HD11	2:G:1068:THR:HG22	1.69	0.73
2:H:6:CYS:HA	2:H:103:HIS:HB2	1.70	0.73
2:F:1501:ILE:HG22	2:F:1531:THR:HB	1.70	0.73
2:G:711:ILE:HB	2:G:886:VAL:HG12	1.71	0.73
2:E:6:CYS:HA	2:E:103:HIS:HB2	1.70	0.73
2:H:1501:ILE:HG22	2:H:1531:THR:HB	1.70	0.73
2:H:711:ILE:HB	2:H:886:VAL:HG12	1.71	0.73
2:E:1511:ILE:HD13	2:E:1511:ILE:N	2.04	0.72
2:E:437:ASN:HD22	2:E:592:LEU:HD23	1.54	0.72
2:F:437:ASN:HD22	2:F:592:LEU:HD23	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:556:LEU:HD11	2:E:1068:THR:HG22	1.69	0.72
2:F:6:CYS:HA	2:F:103:HIS:HB2	1.70	0.72
2:H:437:ASN:HD22	2:H:592:LEU:HD23	1.55	0.72
1:B:34:ARG:HH12	1:B:38:LYS:HG2	1.54	0.72
1:D:92:LEU:HD22	2:H:34:VAL:HG21	1.72	0.72
2:G:29:ASP:OD2	2:G:105:HIS:ND1	2.17	0.72
1:C:34:ARG:HH12	1:C:38:LYS:HG2	1.54	0.72
2:E:1501:ILE:HG22	2:E:1531:THR:HB	1.70	0.72
2:E:711:ILE:HB	2:E:886:VAL:HG12	1.71	0.72
2:H:556:LEU:HD11	2:H:1068:THR:HG22	1.69	0.72
2:F:711:ILE:HB	2:F:886:VAL:HG12	1.71	0.71
2:H:1511:ILE:HD13	2:H:1511:ILE:N	2.04	0.71
1:C:136:ARG:NH2	1:D:138:VAL:O	2.21	0.71
2:F:714:GLN:C	2:F:1512:ASP:OD2	2.29	0.71
2:G:714:GLN:C	2:G:1512:ASP:OD2	2.29	0.71
2:G:1501:ILE:HG22	2:G:1531:THR:HB	1.70	0.71
2:G:437:ASN:HD22	2:G:592:LEU:HD23	1.54	0.71
2:H:714:GLN:C	2:H:1512:ASP:OD2	2.29	0.71
2:E:714:GLN:C	2:E:1512:ASP:OD2	2.29	0.71
2:E:29:ASP:OD2	2:E:105:HIS:ND1	2.17	0.71
2:F:1511:ILE:HD13	2:F:1511:ILE:N	2.04	0.71
1:C:278:HIS:CG	2:G:1356:SER:OG	2.44	0.71
2:G:1511:ILE:HD13	2:G:1511:ILE:N	2.04	0.71
1:B:278:HIS:CD2	2:F:1356:SER:OG	2.43	0.71
2:G:739:TRP:HE3	2:G:766:ARG:HA	1.55	0.71
2:G:587:VAL:HA	2:G:590:LEU:HD12	1.72	0.70
2:H:29:ASP:OD2	2:H:105:HIS:ND1	2.17	0.70
2:F:1429:VAL:O	2:F:1493:ARG:NH1	2.17	0.70
2:H:1029:ILE:HD12	2:H:1070:LEU:HB3	1.74	0.70
2:E:739:TRP:HE3	2:E:766:ARG:HA	1.55	0.70
2:G:1029:ILE:HD12	2:G:1070:LEU:HB3	1.74	0.70
2:E:1029:ILE:HD12	2:E:1070:LEU:HB3	1.74	0.70
2:F:739:TRP:HE3	2:F:766:ARG:HA	1.55	0.70
2:F:587:VAL:HA	2:F:590:LEU:HD12	1.72	0.70
1:A:34:ARG:HH12	1:A:38:LYS:HG2	1.54	0.70
2:E:587:VAL:HA	2:E:590:LEU:HD12	1.72	0.70
2:H:739:TRP:HE3	2:H:766:ARG:HA	1.56	0.69
1:B:66:LEU:O	1:B:170:LYS:NZ	2.26	0.69
1:D:34:ARG:HH12	1:D:38:LYS:HG2	1.54	0.69
1:D:66:LEU:O	1:D:170:LYS:NZ	2.26	0.69
1:A:66:LEU:O	1:A:170:LYS:NZ	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:865:ASP:OD1	2:E:892:TYR:OH	2.11	0.69
2:F:1029:ILE:HD12	2:F:1070:LEU:HB3	1.74	0.69
2:F:118:VAL:HG11	2:F:1172:ILE:HG21	1.75	0.69
2:H:118:VAL:HG11	2:H:1172:ILE:HG21	1.75	0.69
2:H:587:VAL:HA	2:H:590:LEU:HD12	1.72	0.69
1:B:192:ARG:NH2	1:B:199:MET:SD	2.66	0.69
1:D:192:ARG:NH2	1:D:199:MET:SD	2.66	0.69
2:G:118:VAL:HG11	2:G:1172:ILE:HG21	1.75	0.69
2:G:865:ASP:OD1	2:G:892:TYR:OH	2.11	0.68
1:B:113:SER:OG	1:B:135:GLY:O	2.12	0.68
1:C:66:LEU:O	1:C:170:LYS:NZ	2.26	0.68
1:C:177:ARG:HH12	1:C:206:ARG:HB2	1.59	0.68
1:A:192:ARG:NH2	1:A:199:MET:SD	2.66	0.68
1:C:192:ARG:NH2	1:C:199:MET:SD	2.66	0.68
1:C:273:SER:OG	2:G:1398:PHE:HD2	1.75	0.68
2:E:118:VAL:HG11	2:E:1172:ILE:HG21	1.75	0.68
1:B:177:ARG:HH12	1:B:206:ARG:HB2	1.58	0.68
2:F:865:ASP:OD1	2:F:892:TYR:OH	2.11	0.68
2:H:1479:GLU:HA	2:H:1486:ARG:HH11	1.59	0.68
1:A:113:SER:OG	1:A:135:GLY:O	2.12	0.68
2:F:1479:GLU:HA	2:F:1486:ARG:HH11	1.59	0.68
1:C:278:HIS:CD2	2:G:1356:SER:OG	2.47	0.68
1:C:113:SER:OG	1:C:135:GLY:O	2.12	0.68
2:F:547:ASN:OD1	2:F:590:LEU:HB3	1.94	0.68
1:D:276:HIS:HD2	2:H:1355:SER:HB2	1.59	0.67
2:H:1259:VAL:HA	2:H:1287:ALA:HB1	1.76	0.67
2:H:322:GLY:O	2:H:326:HIS:ND1	2.22	0.67
2:E:1259:VAL:HA	2:E:1287:ALA:HB1	1.76	0.67
2:G:547:ASN:OD1	2:G:590:LEU:HB3	1.94	0.67
2:E:547:ASN:OD1	2:E:590:LEU:HB3	1.94	0.67
1:D:177:ARG:HH12	1:D:206:ARG:HB2	1.59	0.67
2:F:322:GLY:O	2:F:326:HIS:ND1	2.22	0.67
2:H:865:ASP:OD1	2:H:892:TYR:OH	2.11	0.67
2:F:1259:VAL:HA	2:F:1287:ALA:HB1	1.76	0.66
2:G:1259:VAL:HA	2:G:1287:ALA:HB1	1.76	0.66
2:E:1479:GLU:HA	2:E:1486:ARG:HH11	1.59	0.66
2:H:547:ASN:OD1	2:H:590:LEU:HB3	1.94	0.66
1:A:177:ARG:HH12	1:A:206:ARG:HB2	1.59	0.66
1:C:220:VAL:HG22	1:C:235:GLN:HG2	1.77	0.66
2:E:370:ARG:HD3	2:E:373:LEU:HD12	1.77	0.66
2:G:1479:GLU:HA	2:G:1486:ARG:HH11	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:HIS:CD2	2:H:1355:SER:HB2	2.30	0.66
1:B:272:PRO:HG3	1:B:311:TRP:CE2	2.31	0.66
1:A:272:PRO:HG3	1:A:311:TRP:CE2	2.31	0.66
2:F:370:ARG:HD3	2:F:373:LEU:HD12	1.77	0.66
2:H:889:LYS:HB3	2:H:1538:ARG:HH22	1.61	0.66
1:B:220:VAL:HG22	1:B:235:GLN:HG2	1.77	0.66
1:C:239:PRO:O	1:C:259:HIS:ND1	2.25	0.66
1:D:278:HIS:CD2	2:H:1356:SER:HG	2.12	0.66
1:A:220:VAL:HG22	1:A:235:GLN:HG2	1.77	0.66
2:G:889:LYS:HB3	2:G:1538:ARG:HH22	1.61	0.66
2:E:322:GLY:O	2:E:326:HIS:ND1	2.22	0.65
1:C:272:PRO:HG3	1:C:311:TRP:CE2	2.31	0.65
1:D:272:PRO:HG3	1:D:311:TRP:CE2	2.31	0.65
1:C:273:SER:HG	2:G:1398:PHE:HD2	1.39	0.65
1:D:113:SER:OG	1:D:135:GLY:O	2.12	0.65
2:E:889:LYS:HB3	2:E:1538:ARG:HH22	1.61	0.65
2:F:889:LYS:HB3	2:F:1538:ARG:HH22	1.61	0.65
1:D:220:VAL:HG22	1:D:235:GLN:HG2	1.77	0.65
2:G:370:ARG:HD3	2:G:373:LEU:HD12	1.77	0.65
2:F:1127:ASP:HB3	2:F:1314:ILE:HD11	1.79	0.65
2:G:1127:ASP:HB3	2:G:1314:ILE:HD11	1.79	0.65
2:H:370:ARG:HD3	2:H:373:LEU:HD12	1.77	0.65
1:A:167:ILE:HG21	1:B:161:ALA:HB1	1.78	0.65
1:B:239:PRO:O	1:B:259:HIS:ND1	2.25	0.65
2:G:322:GLY:O	2:G:326:HIS:ND1	2.22	0.65
2:E:1424:ILE:HD12	2:E:1504:MET:HG2	1.79	0.65
1:C:278:HIS:ND1	2:G:1355:SER:OG	2.27	0.64
2:E:1127:ASP:HB3	2:E:1314:ILE:HD11	1.79	0.64
2:G:1011:LEU:HD21	2:G:1087:TRP:CE3	2.33	0.64
2:G:314:PHE:CZ	2:G:448:GLY:HA2	2.33	0.64
2:H:1011:LEU:HD21	2:H:1087:TRP:CE3	2.33	0.64
2:H:314:PHE:CZ	2:H:448:GLY:HA2	2.33	0.64
2:F:1011:LEU:HD21	2:F:1087:TRP:CE3	2.33	0.64
2:E:1011:LEU:HD21	2:E:1087:TRP:CE3	2.33	0.64
2:E:69:PRO:HD2	2:E:189:VAL:HG12	1.80	0.64
2:H:69:PRO:HD2	2:H:189:VAL:HG12	1.80	0.64
2:E:314:PHE:CZ	2:E:448:GLY:HA2	2.33	0.63
2:H:1127:ASP:HB3	2:H:1314:ILE:HD11	1.79	0.63
2:F:314:PHE:CZ	2:F:448:GLY:HA2	2.33	0.63
2:F:1424:ILE:HD12	2:F:1504:MET:HG2	1.79	0.63
1:B:92:LEU:HD22	2:F:34:VAL:HG21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1424:ILE:HD12	2:G:1504:MET:HG2	1.79	0.63
1:C:273:SER:HB2	2:G:1399:GLU:OE2	1.99	0.63
2:F:510:LYS:NZ	2:F:1325:TYR:OH	2.31	0.63
2:H:510:LYS:NZ	2:H:1325:TYR:OH	2.31	0.63
2:G:510:LYS:NZ	2:G:1325:TYR:OH	2.31	0.63
2:G:1409:ILE:HG13	2:G:1417:LEU:HD11	1.81	0.62
2:H:1424:ILE:HD12	2:H:1504:MET:HG2	1.79	0.62
2:F:295:PHE:CZ	2:F:383:THR:HB	2.34	0.62
2:G:69:PRO:HD2	2:G:189:VAL:HG12	1.80	0.62
1:A:101:ALA:HB2	2:E:16:ARG:HB2	1.81	0.62
2:E:510:LYS:NZ	2:E:1325:TYR:OH	2.31	0.62
2:E:723:LEU:HB3	2:E:851:PHE:CZ	2.31	0.62
2:G:1424:ILE:HD13	2:G:1491:LEU:HG	1.82	0.62
2:G:295:PHE:CZ	2:G:383:THR:HB	2.34	0.62
2:G:420:LEU:O	2:G:424:ASP:HB3	2.00	0.62
2:H:380:ALA:O	2:H:383:THR:OG1	2.18	0.62
1:B:95:PHE:HD1	1:B:100:LEU:HD12	1.65	0.62
2:F:69:PRO:HD2	2:F:189:VAL:HG12	1.80	0.62
1:D:313:GLN:HG2	1:D:338:LYS:HA	1.82	0.62
2:H:829:LEU:HD13	2:H:833:GLN:HB2	1.82	0.62
2:E:420:LEU:O	2:E:424:ASP:HB3	2.00	0.62
2:H:1424:ILE:HD13	2:H:1491:LEU:HG	1.82	0.61
1:A:313:GLN:HG2	1:A:338:LYS:HA	1.82	0.61
1:C:167:ILE:HG21	1:D:161:ALA:HB1	1.81	0.61
2:E:36:HIS:CE1	2:E:113:ALA:HB2	2.35	0.61
2:G:36:HIS:CE1	2:G:113:ALA:HB2	2.35	0.61
1:A:239:PRO:O	1:A:259:HIS:ND1	2.25	0.61
1:B:313:GLN:HG2	1:B:338:LYS:HA	1.82	0.61
2:E:1409:ILE:HG13	2:E:1417:LEU:HD11	1.81	0.61
2:E:295:PHE:CZ	2:E:383:THR:HB	2.34	0.61
2:F:420:LEU:O	2:F:424:ASP:HB3	2.00	0.61
2:H:295:PHE:CZ	2:H:383:THR:HB	2.34	0.61
2:E:380:ALA:O	2:E:383:THR:OG1	2.18	0.61
2:F:1409:ILE:HG13	2:F:1417:LEU:HD11	1.81	0.61
2:H:1409:ILE:HG13	2:H:1417:LEU:HD11	1.81	0.61
2:F:74:ARG:HH21	2:F:185:VAL:HG12	1.66	0.61
1:C:95:PHE:HD1	1:C:100:LEU:HD12	1.65	0.61
1:C:278:HIS:HB2	2:G:1355:SER:HG	1.66	0.61
2:H:420:LEU:O	2:H:424:ASP:HB3	2.00	0.61
2:H:723:LEU:HB3	2:H:851:PHE:CZ	2.31	0.61
2:E:1560:ASP:OD1	2:E:1561:LYS:N	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:74:ARG:HH21	2:E:185:VAL:HG12	1.66	0.61
2:E:829:LEU:HD13	2:E:833:GLN:HB2	1.82	0.61
2:F:1482:SER:OG	3:F:2004:ATP:O3A	2.19	0.61
2:G:829:LEU:HD13	2:G:833:GLN:HB2	1.82	0.61
2:E:78:THR:HG21	2:E:121:VAL:HG21	1.82	0.61
2:F:829:LEU:HD13	2:F:833:GLN:HB2	1.82	0.61
1:C:61:THR:HA	1:C:64:VAL:HG12	1.82	0.60
1:D:95:PHE:HD1	1:D:100:LEU:HD12	1.65	0.60
2:F:36:HIS:CE1	2:F:113:ALA:HB2	2.35	0.60
2:F:380:ALA:O	2:F:383:THR:OG1	2.18	0.60
2:G:74:ARG:HH21	2:G:185:VAL:HG12	1.66	0.60
1:C:92:LEU:HD22	2:G:34:VAL:HG21	1.83	0.60
2:H:36:HIS:CE1	2:H:113:ALA:HB2	2.35	0.60
2:E:1482:SER:OG	3:E:2004:ATP:O3A	2.19	0.60
2:G:412:MET:HA	2:G:416:GLN:HE21	1.66	0.60
1:B:61:THR:HA	1:B:64:VAL:HG12	1.82	0.60
2:F:810:ASP:OD2	2:F:836:ARG:NH2	2.35	0.60
2:G:1473:ILE:O	2:G:1480:ASN:ND2	2.34	0.60
1:A:95:PHE:HD1	1:A:100:LEU:HD12	1.65	0.60
1:C:313:GLN:HG2	1:C:338:LYS:HA	1.82	0.60
1:D:239:PRO:O	1:D:259:HIS:ND1	2.25	0.60
2:F:1424:ILE:HD13	2:F:1491:LEU:HG	1.82	0.60
2:F:412:MET:HA	2:F:416:GLN:HE21	1.66	0.60
2:F:78:THR:HG21	2:F:121:VAL:HG21	1.82	0.60
1:A:61:THR:HA	1:A:64:VAL:HG12	1.82	0.60
1:D:314:ARG:HE	1:D:339:VAL:HG21	1.66	0.60
2:E:8:SER:H	2:E:12:SER:CB	2.14	0.60
2:E:1424:ILE:HD13	2:E:1491:LEU:HG	1.82	0.60
2:F:1263:ALA:O	2:F:1267:ILE:HG12	2.02	0.60
2:G:78:THR:HG21	2:G:121:VAL:HG21	1.82	0.60
2:H:1473:ILE:O	2:H:1480:ASN:ND2	2.34	0.60
2:H:412:MET:HA	2:H:416:GLN:HE21	1.66	0.60
2:F:452:LEU:HB3	2:F:461:LEU:HD22	1.84	0.60
2:F:770:ALA:HA	2:F:1216:PHE:HE1	1.67	0.60
2:G:8:SER:H	2:G:12:SER:CB	2.14	0.60
2:H:78:THR:HG21	2:H:121:VAL:HG21	1.82	0.60
2:H:810:ASP:OD2	2:H:836:ARG:NH2	2.35	0.60
1:D:61:THR:HA	1:D:64:VAL:HG12	1.82	0.60
2:F:8:SER:H	2:F:12:SER:CB	2.14	0.60
2:G:1350:SER:HB2	2:G:1399:GLU:HB2	1.84	0.60
2:H:74:ARG:HH21	2:H:185:VAL:HG12	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:ARG:HE	1:C:339:VAL:HG21	1.66	0.60
2:E:1263:ALA:O	2:E:1267:ILE:HG12	2.02	0.60
2:E:1350:SER:HB2	2:E:1399:GLU:HB2	1.84	0.60
2:G:288:TRP:HE1	2:G:607:VAL:HG21	1.67	0.60
2:G:810:ASP:OD2	2:G:836:ARG:NH2	2.35	0.60
1:B:218:GLN:HE21	1:B:235:GLN:HB3	1.67	0.60
2:F:1473:ILE:O	2:F:1480:ASN:ND2	2.34	0.60
1:C:273:SER:OG	2:G:1398:PHE:CE2	2.51	0.60
2:H:770:ALA:HA	2:H:1216:PHE:HE1	1.67	0.60
1:C:218:GLN:HE21	1:C:235:GLN:HB3	1.67	0.60
3:C:501:ATP:N1	1:D:50:ARG:N	2.47	0.60
2:G:452:LEU:HB3	2:G:461:LEU:HD22	1.84	0.60
1:B:238:ILE:HD11	1:B:259:HIS:CD2	2.37	0.59
2:G:778:LEU:HA	2:G:841:ARG:HH12	1.67	0.59
1:D:238:ILE:HD11	1:D:259:HIS:CD2	2.37	0.59
2:H:1263:ALA:O	2:H:1267:ILE:HG12	2.02	0.59
2:H:1350:SER:HB2	2:H:1399:GLU:HB2	1.84	0.59
2:E:1473:ILE:O	2:E:1480:ASN:ND2	2.34	0.59
2:E:288:TRP:HE1	2:E:607:VAL:HG21	1.67	0.59
2:E:412:MET:HA	2:E:416:GLN:HE21	1.66	0.59
2:E:452:LEU:HB3	2:E:461:LEU:HD22	1.84	0.59
2:F:114:PHE:CE2	2:F:1169:PRO:HB3	2.37	0.59
2:F:778:LEU:HA	2:F:841:ARG:HH12	1.67	0.59
2:H:1027:VAL:HG21	2:H:1151:SER:HB2	1.84	0.59
2:H:288:TRP:HE1	2:H:607:VAL:HG21	1.67	0.59
1:A:95:PHE:HE1	2:E:16:ARG:HG2	1.67	0.59
2:F:1027:VAL:HG21	2:F:1151:SER:HB2	1.84	0.59
2:F:319:CYS:SG	2:F:362:LEU:HB2	2.42	0.59
2:G:1263:ALA:O	2:G:1267:ILE:HG12	2.02	0.59
2:G:1482:SER:OG	3:G:2004:ATP:O3A	2.19	0.59
2:H:452:LEU:HB3	2:H:461:LEU:HD22	1.84	0.59
1:A:218:GLN:HE21	1:A:235:GLN:HB3	1.67	0.59
1:D:218:GLN:HE21	1:D:235:GLN:HB3	1.67	0.59
2:E:1216:PHE:HB3	2:E:1218:TYR:CD2	2.37	0.59
2:E:810:ASP:OD2	2:E:836:ARG:NH2	2.35	0.59
2:G:114:PHE:CE2	2:G:1169:PRO:HB3	2.37	0.59
2:G:319:CYS:SG	2:G:362:LEU:HB2	2.42	0.59
2:H:1216:PHE:HB3	2:H:1218:TYR:CD2	2.37	0.59
2:H:8:SER:H	2:H:12:SER:CB	2.14	0.59
2:G:1560:ASP:OD1	2:G:1561:LYS:N	2.32	0.59
1:A:314:ARG:HE	1:A:339:VAL:HG21	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:ILE:HD11	1:C:259:HIS:CD2	2.37	0.59
2:E:1027:VAL:HG21	2:E:1151:SER:HB2	1.85	0.59
2:H:114:PHE:CE2	2:H:1169:PRO:HB3	2.38	0.59
1:B:314:ARG:HE	1:B:339:VAL:HG21	1.66	0.59
1:D:217:MET:HG2	1:D:285:VAL:HG22	1.84	0.59
2:E:770:ALA:HA	2:E:1216:PHE:HE1	1.67	0.59
2:F:1350:SER:HB2	2:F:1399:GLU:HB2	1.84	0.59
2:F:496:LEU:HD13	2:F:500:ASN:ND2	2.16	0.59
2:G:1027:VAL:HG21	2:G:1151:SER:HB2	1.84	0.59
2:G:496:LEU:HD13	2:G:500:ASN:ND2	2.16	0.59
1:B:217:MET:HG2	1:B:285:VAL:HG22	1.84	0.59
2:E:320:ILE:HG12	2:E:1284:LEU:HD13	1.85	0.59
2:E:778:LEU:HA	2:E:841:ARG:HH12	1.67	0.59
2:G:320:ILE:HG12	2:G:1284:LEU:HD13	1.85	0.59
2:H:1560:ASP:OD1	2:H:1561:LYS:N	2.33	0.59
1:A:238:ILE:HD11	1:A:259:HIS:CD2	2.37	0.59
2:E:319:CYS:SG	2:E:362:LEU:HB2	2.42	0.59
1:C:217:MET:HG2	1:C:285:VAL:HG22	1.84	0.58
2:F:918:ARG:NH2	2:F:922:GLN:OE1	2.36	0.58
2:F:320:ILE:HG12	2:F:1284:LEU:HD13	1.85	0.58
2:G:770:ALA:HA	2:G:1216:PHE:HE1	1.67	0.58
2:H:319:CYS:SG	2:H:362:LEU:HB2	2.42	0.58
1:B:276:HIS:NE2	1:B:278:HIS:O	2.37	0.58
1:A:50:ARG:N	3:D:501:ATP:N1	2.45	0.58
2:E:114:PHE:CE2	2:E:1169:PRO:HB3	2.37	0.58
2:E:477:VAL:HG11	2:E:543:SER:HB2	1.85	0.58
2:F:288:TRP:HE1	2:F:607:VAL:HG21	1.67	0.58
2:G:380:ALA:O	2:G:383:THR:OG1	2.18	0.58
2:F:477:VAL:HG11	2:F:543:SER:HB2	1.85	0.58
2:H:320:ILE:HG12	2:H:1284:LEU:HD13	1.85	0.58
1:D:273:SER:OG	2:H:1398:PHE:CE2	2.56	0.58
2:H:1482:SER:OG	3:H:2004:ATP:O3A	2.19	0.58
1:A:276:HIS:NE2	1:A:278:HIS:O	2.37	0.58
1:C:276:HIS:NE2	1:C:278:HIS:O	2.37	0.58
2:F:723:LEU:HB3	2:F:851:PHE:CZ	2.31	0.58
2:G:309:ALA:C	2:G:369:GLN:HE22	2.04	0.58
2:G:477:VAL:HG11	2:G:543:SER:HB2	1.85	0.58
1:A:239:PRO:HB3	1:D:244:VAL:HG22	1.86	0.58
2:E:918:ARG:NH2	2:E:922:GLN:OE1	2.36	0.58
2:G:918:ARG:NH2	2:G:922:GLN:OE1	2.36	0.58
2:H:318:LEU:HD21	2:H:451:LEU:HD21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:477:VAL:HG11	2:H:543:SER:HB2	1.85	0.58
2:H:555:VAL:HG12	2:H:583:PHE:HD2	1.69	0.58
2:H:778:LEU:HA	2:H:841:ARG:HH12	1.67	0.58
1:A:217:MET:HG2	1:A:285:VAL:HG22	1.85	0.57
1:C:75:PHE:O	1:C:78:SER:OG	2.19	0.57
1:D:276:HIS:NE2	1:D:278:HIS:O	2.37	0.57
2:F:776:PRO:O	2:F:834:ARG:NH2	2.37	0.57
2:G:1436:ARG:NH2	2:G:1471:ASP:OD1	2.37	0.57
2:G:318:LEU:HD21	2:G:451:LEU:HD21	1.86	0.57
2:H:1436:ARG:NH2	2:H:1471:ASP:OD1	2.37	0.57
2:H:455:ILE:HG23	2:H:456:LEU:HG	1.86	0.57
2:F:1351:VAL:HG22	2:F:1361:LEU:HB3	1.87	0.57
2:F:318:LEU:HD21	2:F:451:LEU:HD21	1.87	0.57
2:H:496:LEU:HD13	2:H:500:ASN:ND2	2.16	0.57
2:H:918:ARG:NH2	2:H:922:GLN:OE1	2.36	0.57
2:F:1153:LEU:HD11	2:F:1167:LEU:HG	1.87	0.57
2:H:1153:LEU:HD11	2:H:1167:LEU:HG	1.87	0.57
2:F:309:ALA:C	2:F:369:GLN:HE22	2.04	0.57
2:G:723:LEU:HB3	2:G:851:PHE:CZ	2.31	0.57
2:F:456:LEU:HD22	2:F:575:VAL:HA	1.87	0.57
2:E:1351:VAL:HG22	2:E:1361:LEU:HB3	1.87	0.57
2:E:318:LEU:HD21	2:E:451:LEU:HD21	1.86	0.57
2:E:309:ALA:C	2:E:369:GLN:HE22	2.04	0.57
2:E:776:PRO:O	2:E:834:ARG:NH2	2.37	0.57
2:F:1436:ARG:NH2	2:F:1471:ASP:OD1	2.37	0.57
2:G:1153:LEU:HD11	2:G:1167:LEU:HG	1.87	0.57
1:C:239:PRO:HB3	1:B:244:VAL:HG22	1.85	0.57
2:E:1436:ARG:NH2	2:E:1471:ASP:OD1	2.37	0.57
2:E:455:ILE:HG23	2:E:456:LEU:HG	1.86	0.57
2:G:455:ILE:HG23	2:G:456:LEU:HG	1.86	0.57
2:H:776:PRO:O	2:H:834:ARG:NH2	2.38	0.57
2:G:555:VAL:HG12	2:G:583:PHE:HD2	1.69	0.56
2:E:117:ALA:O	2:E:120:SER:OG	2.17	0.56
2:G:1351:VAL:HG22	2:G:1361:LEU:HB3	1.87	0.56
1:C:122:LEU:HD21	1:D:146:ILE:HG12	1.87	0.56
2:E:1153:LEU:HD11	2:E:1167:LEU:HG	1.87	0.56
2:E:555:VAL:HG12	2:E:583:PHE:HD2	1.69	0.56
2:E:456:LEU:HD22	2:E:575:VAL:HA	1.87	0.56
2:G:776:PRO:O	2:G:834:ARG:NH2	2.37	0.56
2:F:1560:ASP:OD1	2:F:1561:LYS:N	2.33	0.56
2:F:455:ILE:HG23	2:F:456:LEU:HG	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:496:LEU:HD13	2:E:500:ASN:ND2	2.16	0.56
2:E:711:ILE:HG13	2:E:900:ILE:HB	1.87	0.56
1:B:211:ILE:HB	1:B:290:VAL:HB	1.88	0.56
1:C:211:ILE:HB	1:C:290:VAL:HB	1.87	0.56
2:G:498:GLN:HE22	2:G:521:ARG:NH1	2.04	0.56
2:H:498:GLN:HE22	2:H:521:ARG:NH1	2.04	0.56
2:F:498:GLN:HE22	2:F:521:ARG:NH1	2.04	0.56
2:G:1191:LEU:HA	2:G:1194:THR:HG22	1.88	0.56
2:H:1191:LEU:HA	2:H:1194:THR:HG22	1.88	0.56
2:F:555:VAL:HG12	2:F:583:PHE:HD2	1.69	0.56
2:G:711:ILE:HG13	2:G:900:ILE:HB	1.87	0.55
2:F:1191:LEU:HA	2:F:1194:THR:HG22	1.88	0.55
2:H:1351:VAL:HG22	2:H:1361:LEU:HB3	1.87	0.55
2:E:498:GLN:HE22	2:E:521:ARG:NH1	2.04	0.55
1:A:161:ALA:HB1	1:D:167:ILE:HG21	1.87	0.55
2:E:1191:LEU:HA	2:E:1194:THR:HG22	1.88	0.55
2:H:117:ALA:O	2:H:120:SER:OG	2.17	0.55
2:H:309:ALA:C	2:H:369:GLN:HE22	2.04	0.55
2:H:711:ILE:HG13	2:H:900:ILE:HB	1.87	0.55
2:H:456:LEU:HD22	2:H:575:VAL:HA	1.87	0.55
2:F:14:ALA:HA	2:F:17:VAL:HG13	1.89	0.55
2:F:381:ILE:HG13	2:F:433:PHE:CE1	2.42	0.55
2:F:455:ILE:O	2:F:457:GLY:N	2.40	0.55
2:F:711:ILE:HG13	2:F:900:ILE:HB	1.87	0.55
1:D:269:ASP:OD1	1:D:347:ARG:NE	2.33	0.55
1:A:211:ILE:HB	1:A:290:VAL:HB	1.88	0.55
1:D:75:PHE:O	1:D:78:SER:OG	2.19	0.55
2:E:1506:GLU:H	2:E:1535:ILE:HB	1.72	0.55
2:E:295:PHE:HZ	2:E:383:THR:HB	1.72	0.55
2:G:14:ALA:HA	2:G:17:VAL:HG13	1.89	0.55
1:A:138:VAL:O	1:D:136:ARG:NH2	2.32	0.54
2:E:388:ARG:NH1	2:E:429:MET:SD	2.80	0.54
2:E:455:ILE:O	2:E:457:GLY:N	2.40	0.54
2:G:388:ARG:NH1	2:G:429:MET:SD	2.81	0.54
2:G:455:ILE:O	2:G:457:GLY:N	2.40	0.54
2:H:388:ARG:NH1	2:H:429:MET:SD	2.80	0.54
2:E:14:ALA:HA	2:E:17:VAL:HG13	1.89	0.54
2:F:1506:GLU:H	2:F:1535:ILE:HB	1.72	0.54
2:F:404:THR:OG1	2:F:1214:ARG:NH2	2.41	0.54
2:G:456:LEU:HD22	2:G:575:VAL:HA	1.87	0.54
2:F:388:ARG:NH1	2:F:429:MET:SD	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:455:ILE:O	2:H:457:GLY:N	2.40	0.54
2:E:708:LEU:O	2:E:897:ASP:N	2.40	0.54
2:G:1506:GLU:H	2:G:1535:ILE:HB	1.72	0.54
2:H:1506:GLU:H	2:H:1535:ILE:HB	1.72	0.54
2:H:14:ALA:HA	2:H:17:VAL:HG13	1.89	0.54
2:E:381:ILE:HG13	2:E:433:PHE:CE1	2.42	0.54
2:G:381:ILE:HG13	2:G:433:PHE:CE1	2.42	0.54
2:H:33:VAL:HG22	2:H:109:PRO:HB3	1.89	0.54
1:C:129:VAL:O	1:C:130:THR:OG1	2.23	0.54
1:D:211:ILE:HB	1:D:290:VAL:HB	1.88	0.54
2:E:102:HIS:HD2	2:E:1273:ARG:HH11	1.56	0.54
2:G:480:LYS:HG3	2:G:539:TYR:CE2	2.43	0.54
2:H:1177:ILE:HD11	2:H:1251:MET:SD	2.48	0.54
2:H:295:PHE:HZ	2:H:383:THR:HB	1.73	0.54
2:F:708:LEU:O	2:F:897:ASP:N	2.41	0.54
2:G:404:THR:OG1	2:G:1214:ARG:NH2	2.41	0.54
2:H:102:HIS:HD2	2:H:1273:ARG:HH11	1.56	0.54
1:A:129:VAL:O	1:A:130:THR:OG1	2.23	0.54
2:F:1216:PHE:HB3	2:F:1218:TYR:CD2	2.37	0.54
2:H:381:ILE:HG13	2:H:433:PHE:CE1	2.42	0.54
2:F:1177:ILE:HD11	2:F:1251:MET:SD	2.48	0.54
2:G:1177:ILE:HD11	2:G:1251:MET:SD	2.48	0.54
2:G:6:CYS:H	2:G:16:ARG:NH1	2.06	0.54
2:G:708:LEU:O	2:G:897:ASP:N	2.41	0.54
2:E:1177:ILE:HD11	2:E:1251:MET:SD	2.48	0.53
2:E:33:VAL:HG22	2:E:109:PRO:HB3	1.89	0.53
2:H:404:THR:OG1	2:H:1214:ARG:NH2	2.40	0.53
2:G:102:HIS:HD2	2:G:1273:ARG:HH11	1.56	0.53
2:G:495:ARG:NH1	2:G:1124:PHE:O	2.38	0.53
2:G:727:LEU:HD21	2:G:1215:ALA:HB2	1.90	0.53
2:E:1066:VAL:HA	2:E:1069:VAL:HG12	1.90	0.53
2:E:404:THR:OG1	2:E:1214:ARG:NH2	2.41	0.53
2:E:575:VAL:HG23	2:E:576:ALA:H	1.74	0.53
1:D:95:PHE:CD2	2:H:27:PHE:HD1	2.26	0.53
2:E:6:CYS:H	2:E:16:ARG:NH1	2.06	0.53
2:F:1066:VAL:HA	2:F:1069:VAL:HG12	1.90	0.53
2:G:33:VAL:HG22	2:G:109:PRO:HB3	1.89	0.53
2:H:480:LYS:HG3	2:H:539:TYR:CE2	2.43	0.53
1:C:269:ASP:OD1	1:C:347:ARG:NE	2.33	0.53
2:F:33:VAL:HG22	2:F:109:PRO:HB3	1.89	0.53
2:H:6:CYS:H	2:H:16:ARG:NH1	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:802:ILE:HG23	2:H:807:LEU:HB3	1.91	0.53
2:G:1216:PHE:HB3	2:G:1218:TYR:CD2	2.37	0.53
2:E:727:LEU:HD21	2:E:1215:ALA:HB2	1.90	0.53
1:C:95:PHE:HE2	2:G:27:PHE:HB2	1.72	0.53
2:G:74:ARG:HH22	2:G:189:VAL:HG21	1.74	0.53
2:E:495:ARG:NH1	2:E:1124:PHE:O	2.38	0.53
2:E:74:ARG:HH22	2:E:189:VAL:HG21	1.74	0.53
1:A:34:ARG:NH1	1:A:38:LYS:HG2	2.24	0.53
1:C:34:ARG:NH1	1:C:38:LYS:HG2	2.24	0.53
2:F:295:PHE:HZ	2:F:383:THR:HB	1.73	0.53
1:A:95:PHE:HE2	2:E:27:PHE:HB2	1.73	0.53
1:C:161:ALA:HB1	1:B:167:ILE:HG21	1.90	0.53
2:F:1032:TRP:HZ2	2:F:1063:TYR:HD1	1.57	0.53
2:G:1032:TRP:HZ2	2:G:1063:TYR:HD1	1.57	0.53
2:G:1353:TYR:OH	2:G:1386:SER:OG	2.21	0.53
1:A:122:LEU:HD21	1:B:146:ILE:HG12	1.90	0.52
2:E:480:LYS:HG3	2:E:539:TYR:CE2	2.43	0.52
2:F:102:HIS:HD2	2:F:1273:ARG:HH11	1.56	0.52
2:F:74:ARG:HH22	2:F:189:VAL:HG21	1.74	0.52
2:F:480:LYS:HG3	2:F:539:TYR:CE2	2.43	0.52
2:F:727:LEU:HD21	2:F:1215:ALA:HB2	1.90	0.52
2:H:727:LEU:HD21	2:H:1215:ALA:HB2	1.90	0.52
1:A:34:ARG:NH2	1:A:303:SER:OG	2.35	0.52
1:C:327:SER:HA	1:D:45:ALA:HB3	1.90	0.52
1:D:32:ARG:CZ	1:D:278:HIS:HA	2.39	0.52
2:E:802:ILE:HG23	2:E:807:LEU:HB3	1.91	0.52
2:F:1129:ASN:OD1	2:F:1133:GLN:NE2	2.43	0.52
2:F:6:CYS:H	2:F:16:ARG:NH1	2.06	0.52
2:H:575:VAL:HG23	2:H:576:ALA:H	1.74	0.52
1:C:276:HIS:HD2	2:G:1355:SER:CB	2.06	0.52
1:D:273:SER:OG	2:H:1398:PHE:CD2	2.59	0.52
2:H:74:ARG:HH22	2:H:189:VAL:HG21	1.74	0.52
1:C:45:ALA:HB3	1:B:327:SER:HA	1.92	0.52
1:C:138:VAL:O	1:B:136:ARG:NH2	2.34	0.52
2:F:575:VAL:HG23	2:F:576:ALA:H	1.74	0.52
2:G:1066:VAL:HA	2:G:1069:VAL:HG12	1.90	0.52
2:G:802:ILE:HG23	2:G:807:LEU:HB3	1.91	0.52
1:A:187:ALA:O	1:A:310:LEU:N	2.43	0.52
1:A:32:ARG:CZ	1:A:278:HIS:HA	2.40	0.52
1:C:50:ARG:N	3:B:501:ATP:N1	2.51	0.52
2:H:1066:VAL:HA	2:H:1069:VAL:HG12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1129:ASN:OD1	2:H:1133:GLN:NE2	2.43	0.52
2:H:593:LEU:HA	2:H:596:VAL:HB	1.92	0.52
1:A:75:PHE:O	1:A:78:SER:OG	2.19	0.52
2:G:1129:ASN:OD1	2:G:1133:GLN:NE2	2.43	0.52
2:H:1032:TRP:HZ3	2:H:1067:PHE:HB2	1.74	0.52
2:H:708:LEU:O	2:H:897:ASP:N	2.40	0.52
1:D:129:VAL:O	1:D:130:THR:OG1	2.23	0.52
1:D:187:ALA:O	1:D:310:LEU:N	2.43	0.52
2:F:802:ILE:HG23	2:F:807:LEU:HB3	1.91	0.52
2:F:495:ARG:NH1	2:F:1124:PHE:O	2.38	0.52
2:G:295:PHE:HZ	2:G:383:THR:HB	1.73	0.52
2:G:593:LEU:HA	2:G:596:VAL:HB	1.92	0.52
2:E:1129:ASN:OD1	2:E:1133:GLN:NE2	2.43	0.51
2:G:487:SER:HA	2:G:490:GLU:HG2	1.92	0.51
2:G:575:VAL:HG23	2:G:576:ALA:H	1.74	0.51
1:C:32:ARG:CZ	1:C:278:HIS:HA	2.39	0.51
2:F:1353:TYR:OH	2:F:1386:SER:OG	2.22	0.51
2:G:412:MET:HA	2:G:416:GLN:NE2	2.26	0.51
2:G:465:ALA:HA	2:G:468:ILE:HD12	1.93	0.51
1:A:327:SER:HA	1:B:45:ALA:HB3	1.92	0.51
1:B:187:ALA:O	1:B:310:LEU:N	2.43	0.51
2:E:1032:TRP:HZ3	2:E:1067:PHE:HB2	1.75	0.51
2:E:465:ALA:HA	2:E:468:ILE:HD12	1.93	0.51
2:F:487:SER:HA	2:F:490:GLU:HG2	1.92	0.51
2:F:739:TRP:CE3	2:F:766:ARG:HA	2.42	0.51
2:G:1269:ASN:O	2:G:1273:ARG:N	2.29	0.51
2:H:846:HIS:ND1	2:H:846:HIS:O	2.44	0.51
1:C:187:ALA:O	1:C:310:LEU:N	2.43	0.51
2:E:846:HIS:ND1	2:E:846:HIS:O	2.44	0.51
1:A:271:ALA:HB2	1:A:345:THR:HG22	1.93	0.51
1:C:34:ARG:NH2	1:C:303:SER:OG	2.35	0.51
2:E:451:LEU:O	2:E:455:ILE:HG22	2.11	0.51
2:F:1032:TRP:HZ3	2:F:1067:PHE:HB2	1.75	0.51
2:H:1032:TRP:HZ2	2:H:1063:TYR:HD1	1.57	0.51
1:A:177:ARG:HG2	1:A:291:VAL:HG22	1.93	0.51
1:B:32:ARG:CZ	1:B:278:HIS:HA	2.39	0.51
2:E:1032:TRP:HZ2	2:E:1063:TYR:HD1	1.57	0.51
2:E:678:CYS:HB2	2:E:703:ILE:O	2.11	0.51
2:F:593:LEU:HA	2:F:596:VAL:HB	1.92	0.51
2:G:500:ASN:O	2:G:504:ARG:HG2	2.11	0.51
2:H:549:ALA:HB1	2:H:1075:ILE:HG13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:ARG:NH1	1:D:38:LYS:HG2	2.24	0.51
2:E:487:SER:HA	2:E:490:GLU:HG2	1.92	0.51
2:F:537:ALA:HA	2:F:540:THR:HG22	1.93	0.51
2:G:1011:LEU:HD11	2:G:1091:LYS:HD3	1.93	0.51
2:G:678:CYS:HB2	2:G:703:ILE:O	2.11	0.51
2:H:465:ALA:HA	2:H:468:ILE:HD12	1.93	0.51
2:H:487:SER:HA	2:H:490:GLU:HG2	1.92	0.51
2:E:14:ALA:O	2:E:17:VAL:HG22	2.11	0.51
2:E:412:MET:HA	2:E:416:GLN:NE2	2.26	0.51
2:F:1011:LEU:HD11	2:F:1091:LYS:HD3	1.93	0.51
2:F:871:GLY:O	2:F:875:LEU:HG	2.11	0.51
2:G:451:LEU:O	2:G:455:ILE:HG22	2.11	0.51
2:H:1011:LEU:HD11	2:H:1091:LYS:HD3	1.93	0.51
2:H:1445:CYS:SG	2:H:1449:THR:OG1	2.54	0.51
2:H:14:ALA:O	2:H:17:VAL:HG22	2.11	0.51
2:H:412:MET:HA	2:H:416:GLN:NE2	2.26	0.51
1:B:271:ALA:HB2	1:B:345:THR:HG22	1.93	0.51
2:E:500:ASN:O	2:E:504:ARG:HG2	2.11	0.51
2:G:1032:TRP:HZ3	2:G:1067:PHE:HB2	1.75	0.51
2:G:871:GLY:O	2:G:875:LEU:HG	2.11	0.51
2:H:451:LEU:O	2:H:455:ILE:HG22	2.11	0.51
1:B:177:ARG:HG2	1:B:291:VAL:HG22	1.93	0.51
1:D:314:ARG:NE	1:D:339:VAL:HG21	2.26	0.51
2:E:442:PRO:HA	2:E:445:ILE:HG22	1.93	0.51
2:F:451:LEU:O	2:F:455:ILE:HG22	2.11	0.51
2:G:537:ALA:HA	2:G:540:THR:HG22	1.93	0.51
2:H:678:CYS:HB2	2:H:703:ILE:O	2.11	0.51
2:H:871:GLY:O	2:H:875:LEU:HG	2.11	0.51
1:B:209:MET:O	1:B:292:GLU:HB2	2.11	0.50
1:C:231:VAL:HB	1:C:234:HIS:HB2	1.94	0.50
1:D:177:ARG:HG2	1:D:291:VAL:HG22	1.93	0.50
2:E:1011:LEU:HD11	2:E:1091:LYS:HD3	1.93	0.50
2:E:600:THR:O	2:E:604:LEU:HD23	2.12	0.50
2:E:871:GLY:O	2:E:875:LEU:HG	2.11	0.50
2:F:465:ALA:HA	2:F:468:ILE:HD12	1.93	0.50
2:F:500:ASN:O	2:F:504:ARG:HG2	2.11	0.50
1:C:209:MET:O	1:C:292:GLU:HB2	2.11	0.50
2:E:593:LEU:HA	2:E:596:VAL:HB	1.92	0.50
2:F:1445:CYS:SG	2:F:1449:THR:OG1	2.54	0.50
2:F:678:CYS:HB2	2:F:703:ILE:O	2.11	0.50
2:G:14:ALA:O	2:G:17:VAL:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:442:PRO:HA	2:G:445:ILE:HG22	1.94	0.50
2:G:519:ARG:HD2	2:G:1102:ASN:OD1	2.12	0.50
2:H:21:VAL:HG23	2:H:22:LEU:HD12	1.93	0.50
1:B:231:VAL:HB	1:B:234:HIS:HB2	1.94	0.50
1:D:271:ALA:HB2	1:D:345:THR:HG22	1.93	0.50
2:F:442:PRO:HA	2:F:445:ILE:HG22	1.94	0.50
2:F:497:LYS:HA	2:F:500:ASN:HD22	1.76	0.50
2:G:846:HIS:O	2:G:846:HIS:ND1	2.44	0.50
2:H:547:ASN:ND2	2:H:590:LEU:O	2.29	0.50
2:H:600:THR:O	2:H:604:LEU:HD23	2.12	0.50
1:A:209:MET:O	1:A:292:GLU:HB2	2.11	0.50
1:A:314:ARG:NE	1:A:339:VAL:HG21	2.26	0.50
1:C:322:GLU:O	1:C:324:GLY:N	2.44	0.50
2:E:1131:ILE:HA	2:E:1135:ILE:HD12	1.93	0.50
2:F:1202:HIS:HD2	2:F:1226:LEU:HD12	1.77	0.50
2:F:1422:SER:HB2	2:F:1502:PHE:CB	2.42	0.50
2:F:600:THR:O	2:F:604:LEU:HD23	2.12	0.50
2:G:600:THR:O	2:G:604:LEU:HD23	2.12	0.50
2:H:1375:GLY:N	2:H:1547:LEU:O	2.45	0.50
2:E:549:ALA:HB1	2:E:1075:ILE:HG13	1.93	0.50
2:E:739:TRP:CE3	2:E:766:ARG:HA	2.42	0.50
2:F:412:MET:HA	2:F:416:GLN:NE2	2.26	0.50
2:F:846:HIS:O	2:F:846:HIS:ND1	2.44	0.50
2:G:497:LYS:HA	2:G:500:ASN:HD22	1.76	0.50
1:C:177:ARG:HG2	1:C:291:VAL:HG22	1.93	0.50
1:D:209:MET:O	1:D:292:GLU:HB2	2.11	0.50
1:D:335:ASN:HD22	1:D:336:THR:N	2.10	0.50
2:F:6:CYS:HB3	2:F:105:HIS:CD2	2.47	0.50
2:F:1482:SER:HG	3:F:2004:ATP:PB	2.34	0.50
2:H:442:PRO:HA	2:H:445:ILE:HG22	1.94	0.50
2:H:500:ASN:O	2:H:504:ARG:HG2	2.11	0.50
2:H:537:ALA:HA	2:H:540:THR:HG22	1.93	0.50
2:H:739:TRP:CE3	2:H:766:ARG:HA	2.43	0.50
1:B:335:ASN:HD22	1:B:336:THR:N	2.10	0.50
1:C:314:ARG:NE	1:C:339:VAL:HG21	2.26	0.50
1:D:95:PHE:HE2	2:H:27:PHE:HB2	1.76	0.50
2:E:1026:LEU:O	2:E:1029:ILE:HG22	2.12	0.50
2:E:1422:SER:HB2	2:E:1502:PHE:CB	2.42	0.50
2:F:549:ALA:HB1	2:F:1075:ILE:HG13	1.93	0.50
2:G:1422:SER:HB2	2:G:1502:PHE:CB	2.42	0.50
2:H:780:ASN:HA	2:H:823:GLY:HA3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:VAL:HB	2:G:49:ILE:HD12	1.93	0.50
1:D:113:SER:HA	1:D:115:HIS:CE1	2.47	0.50
2:G:1375:GLY:N	2:G:1547:LEU:O	2.45	0.50
2:G:549:ALA:HB1	2:G:1075:ILE:HG13	1.93	0.50
2:H:495:ARG:NH1	2:H:1124:PHE:O	2.38	0.50
2:H:1202:HIS:HD2	2:H:1226:LEU:HD12	1.77	0.50
1:C:225:SER:OG	1:C:229:GLU:N	2.45	0.50
2:E:781:ALA:HA	2:E:821:GLN:HE22	1.77	0.50
2:G:117:ALA:O	2:G:120:SER:OG	2.17	0.50
2:H:1131:ILE:HA	2:H:1135:ILE:HD12	1.93	0.50
2:H:1392:PHE:HD1	2:H:1418:ARG:HG2	1.77	0.50
1:A:231:VAL:HB	1:A:234:HIS:HB2	1.94	0.49
1:C:335:ASN:HD22	1:C:336:THR:N	2.10	0.49
2:E:1202:HIS:HD2	2:E:1226:LEU:HD12	1.77	0.49
1:A:101:ALA:HB1	2:E:13:ALA:O	2.12	0.49
2:E:537:ALA:HA	2:E:540:THR:HG22	1.93	0.49
2:F:1026:LEU:O	2:F:1029:ILE:HG22	2.12	0.49
2:F:14:ALA:O	2:F:17:VAL:HG22	2.11	0.49
2:F:519:ARG:HD2	2:F:1102:ASN:OD1	2.12	0.49
2:H:519:ARG:HD2	2:H:1102:ASN:OD1	2.12	0.49
1:C:271:ALA:HB2	1:C:345:THR:HG22	1.93	0.49
1:D:225:SER:OG	1:D:229:GLU:N	2.45	0.49
1:D:322:GLU:O	1:D:324:GLY:N	2.44	0.49
2:E:452:LEU:HD21	2:E:582:LEU:HD22	1.95	0.49
1:A:225:SER:OG	1:A:229:GLU:N	2.45	0.49
2:E:497:LYS:HA	2:E:500:ASN:HD22	1.76	0.49
2:F:1131:ILE:HA	2:F:1135:ILE:HD12	1.93	0.49
2:G:1131:ILE:HA	2:G:1135:ILE:HD12	1.93	0.49
2:G:396:TYR:CD1	2:G:1226:LEU:HD13	2.48	0.49
2:G:781:ALA:HA	2:G:821:GLN:HE22	1.77	0.49
1:A:322:GLU:O	1:A:324:GLY:N	2.45	0.49
1:D:177:ARG:NH1	1:D:206:ARG:HB2	2.26	0.49
2:F:780:ASN:HA	2:F:823:GLY:HA3	1.94	0.49
2:F:781:ALA:HA	2:F:821:GLN:HE22	1.77	0.49
2:H:1026:LEU:O	2:H:1029:ILE:HG22	2.12	0.49
2:H:396:TYR:CD1	2:H:1226:LEU:HD13	2.48	0.49
2:H:781:ALA:HA	2:H:821:GLN:HE22	1.77	0.49
1:B:322:GLU:O	1:B:324:GLY:N	2.45	0.49
1:B:75:PHE:O	1:B:78:SER:OG	2.19	0.49
1:C:113:SER:HA	1:C:115:HIS:CE1	2.47	0.49
1:D:231:VAL:HB	1:D:234:HIS:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1392:PHE:HD1	2:E:1418:ARG:HG2	1.77	0.49
2:E:21:VAL:HG23	2:E:22:LEU:HD12	1.93	0.49
2:G:1026:LEU:O	2:G:1029:ILE:HG22	2.12	0.49
2:G:1202:HIS:HD2	2:G:1226:LEU:HD12	1.77	0.49
1:B:314:ARG:NE	1:B:339:VAL:HG21	2.26	0.49
1:D:273:SER:HG	2:H:1398:PHE:HD2	1.51	0.49
2:E:519:ARG:HD2	2:E:1102:ASN:OD1	2.12	0.49
2:F:396:TYR:CD1	2:F:1226:LEU:HD13	2.48	0.49
2:F:1375:GLY:N	2:F:1547:LEU:O	2.45	0.49
2:F:21:VAL:HG23	2:F:22:LEU:HD12	1.93	0.49
2:F:452:LEU:HD21	2:F:582:LEU:HD22	1.94	0.49
2:H:452:LEU:HD21	2:H:582:LEU:HD22	1.94	0.49
1:A:113:SER:HA	1:A:115:HIS:CE1	2.47	0.49
1:A:335:ASN:HD22	1:A:336:THR:N	2.10	0.49
1:B:113:SER:HA	1:B:115:HIS:CE1	2.47	0.49
1:B:34:ARG:NH2	1:B:303:SER:OG	2.35	0.49
2:E:780:ASN:HA	2:E:823:GLY:HA3	1.94	0.49
2:G:1392:PHE:HD1	2:G:1418:ARG:HG2	1.77	0.49
2:G:428:LEU:O	2:G:432:PHE:HD2	1.96	0.49
2:G:780:ASN:HA	2:G:823:GLY:HA3	1.94	0.49
2:H:1422:SER:HB2	2:H:1502:PHE:CB	2.42	0.49
1:A:177:ARG:NH1	1:A:206:ARG:HB2	2.26	0.49
1:A:45:ALA:HB3	1:D:327:SER:HA	1.94	0.49
2:E:396:TYR:CD1	2:E:1226:LEU:HD13	2.48	0.49
2:G:6:CYS:HB3	2:G:105:HIS:CD2	2.47	0.49
2:G:21:VAL:HG23	2:G:22:LEU:HD12	1.93	0.49
2:H:428:LEU:O	2:H:432:PHE:HD2	1.96	0.49
1:B:225:SER:OG	1:B:229:GLU:N	2.45	0.49
1:B:278:HIS:CD2	2:F:1356:SER:HG	2.29	0.49
2:E:6:CYS:HB3	2:E:105:HIS:CD2	2.47	0.49
2:F:713:GLY:O	2:F:1512:ASP:OD2	2.31	0.49
2:E:428:LEU:O	2:E:432:PHE:HD2	1.96	0.49
2:F:547:ASN:ND2	2:F:590:LEU:O	2.29	0.49
2:H:6:CYS:HB3	2:H:105:HIS:CD2	2.47	0.49
2:E:1423:ILE:HG13	2:E:1503:ILE:HG23	1.94	0.48
2:G:739:TRP:CE3	2:G:766:ARG:HA	2.43	0.48
2:H:1516:GLU:OE2	2:H:1541:THR:OG1	2.21	0.48
2:E:547:ASN:ND2	2:E:594:SER:HB2	2.26	0.48
2:F:1269:ASN:O	2:F:1273:ARG:N	2.29	0.48
1:A:344:CYS:SG	1:A:349:LEU:HD22	2.53	0.48
2:E:1032:TRP:HH2	2:E:1063:TYR:O	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:547:ASN:ND2	2:F:594:SER:HB2	2.25	0.48
2:H:1153:LEU:HD12	2:H:1156:ILE:HD11	1.96	0.48
1:A:95:PHE:CE1	2:E:16:ARG:HG2	2.49	0.48
1:B:344:CYS:SG	1:B:349:LEU:HD22	2.53	0.48
2:F:1032:TRP:HH2	2:F:1063:TYR:O	1.96	0.48
2:H:1423:ILE:HG13	2:H:1503:ILE:HG23	1.94	0.48
1:C:344:CYS:SG	1:C:349:LEU:HD22	2.53	0.48
2:E:713:GLY:O	2:E:1512:ASP:OD2	2.31	0.48
2:F:1423:ILE:HG13	2:F:1503:ILE:HG23	1.94	0.48
2:F:428:LEU:O	2:F:432:PHE:HD2	1.96	0.48
2:G:452:LEU:HD21	2:G:582:LEU:HD22	1.94	0.48
2:H:1275:LEU:HD12	2:H:1276:SER:N	2.29	0.48
2:H:497:LYS:HA	2:H:500:ASN:HD22	1.76	0.48
1:D:66:LEU:HD23	1:D:67:LYS:N	2.29	0.48
2:E:143:TRP:HB2	2:E:183:LEU:HD23	1.96	0.48
2:H:713:GLY:O	2:H:1512:ASP:OD2	2.31	0.48
1:A:244:VAL:HG22	1:B:239:PRO:HB3	1.95	0.48
1:B:129:VAL:O	1:B:130:THR:OG1	2.23	0.48
1:D:344:CYS:SG	1:D:349:LEU:HD22	2.53	0.48
2:E:453:TYR:O	2:E:458:VAL:HA	2.14	0.48
2:F:1392:PHE:HD1	2:F:1418:ARG:HG2	1.77	0.48
2:G:1032:TRP:HH2	2:G:1063:TYR:O	1.96	0.48
2:H:1375:GLY:O	2:H:1549:ILE:N	2.40	0.48
2:H:143:TRP:HB2	2:H:183:LEU:HD23	1.96	0.48
1:D:34:ARG:NH2	1:D:303:SER:OG	2.35	0.48
2:E:135:LEU:O	2:E:135:LEU:HD13	2.14	0.48
2:F:1275:LEU:HD12	2:F:1276:SER:N	2.29	0.48
2:G:1153:LEU:HD12	2:G:1156:ILE:HD11	1.96	0.48
2:G:453:TYR:O	2:G:458:VAL:HA	2.14	0.48
1:A:307:ASP:OD1	1:A:308:GLU:N	2.47	0.48
1:C:159:ILE:O	1:C:163:MET:HG2	2.14	0.48
2:F:816:HIS:HB2	2:F:820:THR:HA	1.96	0.48
2:G:429:MET:HG2	2:G:433:PHE:CZ	2.49	0.48
2:H:135:LEU:O	2:H:135:LEU:HD13	2.14	0.48
2:H:453:TYR:O	2:H:458:VAL:HA	2.14	0.48
1:C:263:ALA:HA	1:C:268:TYR:CG	2.49	0.48
1:D:263:ALA:HA	1:D:268:TYR:CG	2.49	0.48
1:D:307:ASP:OD1	1:D:308:GLU:N	2.47	0.48
2:G:713:GLY:O	2:G:1512:ASP:OD2	2.31	0.48
2:G:547:ASN:ND2	2:G:590:LEU:O	2.30	0.48
1:B:307:ASP:OD1	1:B:308:GLU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1139:LEU:O	2:F:1142:LEU:HD23	2.14	0.47
2:F:143:TRP:HB2	2:F:183:LEU:HD23	1.96	0.47
2:F:453:TYR:O	2:F:458:VAL:HA	2.14	0.47
2:G:1275:LEU:HD12	2:G:1276:SER:N	2.29	0.47
2:G:1445:CYS:SG	2:G:1449:THR:OG1	2.54	0.47
2:H:1032:TRP:HH2	2:H:1063:TYR:O	1.96	0.47
2:H:429:MET:HG2	2:H:433:PHE:CZ	2.49	0.47
1:B:94:ALA:HB2	1:B:114:ILE:HD11	1.96	0.47
1:B:330:TYR:O	1:B:333:PHE:HB2	2.14	0.47
2:E:1087:TRP:HA	2:E:1090:LEU:HD12	1.96	0.47
2:G:1154:ALA:O	2:G:1157:SER:OG	2.26	0.47
2:G:135:LEU:O	2:G:135:LEU:HD13	2.14	0.47
2:G:816:HIS:HB2	2:G:820:THR:HA	1.96	0.47
1:B:66:LEU:HD23	1:B:67:LYS:N	2.29	0.47
1:C:57:GLN:O	1:C:60:PHE:HB3	2.15	0.47
1:D:94:ALA:HB2	1:D:114:ILE:HD11	1.96	0.47
2:E:1275:LEU:HD12	2:E:1276:SER:N	2.29	0.47
2:G:1423:ILE:HG13	2:G:1503:ILE:HG23	1.94	0.47
2:G:143:TRP:HB2	2:G:183:LEU:HD23	1.96	0.47
2:H:1032:TRP:CZ3	2:H:1067:PHE:HB2	2.49	0.47
1:A:263:ALA:HA	1:A:268:TYR:CG	2.49	0.47
3:A:501:ATP:N1	1:B:50:ARG:N	2.57	0.47
1:A:76:THR:HG22	1:B:154:ILE:HG21	1.97	0.47
1:B:159:ILE:O	1:B:163:MET:HG2	2.14	0.47
1:B:57:GLN:O	1:B:60:PHE:HB3	2.14	0.47
1:C:330:TYR:O	1:C:333:PHE:HB2	2.14	0.47
2:E:429:MET:HG2	2:E:433:PHE:CZ	2.49	0.47
2:F:1153:LEU:HD12	2:F:1156:ILE:HD11	1.96	0.47
2:G:1032:TRP:CZ3	2:G:1067:PHE:HB2	2.49	0.47
2:H:816:HIS:HB2	2:H:820:THR:HA	1.96	0.47
1:A:330:TYR:O	1:A:333:PHE:HB2	2.14	0.47
1:B:35:PHE:CD2	1:B:36:VAL:HG23	2.50	0.47
1:B:34:ARG:NH1	1:B:38:LYS:HG2	2.24	0.47
1:C:94:ALA:HB2	1:C:114:ILE:HD11	1.97	0.47
1:C:307:ASP:OD1	1:C:308:GLU:N	2.47	0.47
1:C:35:PHE:CD2	1:C:36:VAL:HG23	2.50	0.47
2:E:547:ASN:ND2	2:E:590:LEU:O	2.29	0.47
2:E:816:HIS:HB2	2:E:820:THR:HA	1.96	0.47
2:G:1548:VAL:HG23	2:G:1562:PRO:HG3	1.97	0.47
2:H:1139:LEU:O	2:H:1142:LEU:HD23	2.14	0.47
2:H:1245:ARG:NH2	2:H:1248:GLU:OE1	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ALA:O	1:A:93:ILE:HG12	2.15	0.47
1:C:66:LEU:HD23	1:C:67:LYS:N	2.29	0.47
1:D:330:TYR:O	1:D:333:PHE:HB2	2.14	0.47
2:E:1375:GLY:O	2:E:1549:ILE:N	2.40	0.47
2:E:550:ILE:HD11	2:E:590:LEU:HD13	1.97	0.47
2:F:1032:TRP:CZ3	2:F:1067:PHE:HB2	2.49	0.47
2:F:1087:TRP:HA	2:F:1090:LEU:HD12	1.97	0.47
1:C:177:ARG:NH1	1:C:206:ARG:HB2	2.26	0.47
2:E:1139:LEU:O	2:E:1142:LEU:HD23	2.14	0.47
2:F:82:LEU:HG	2:F:114:PHE:CE1	2.50	0.47
2:G:577:PHE:HE2	2:G:1285:THR:HG1	1.63	0.47
2:H:550:ILE:HD11	2:H:590:LEU:HD13	1.97	0.47
1:A:94:ALA:HB2	1:A:114:ILE:HD11	1.97	0.47
1:A:159:ILE:O	1:A:163:MET:HG2	2.14	0.47
2:E:1032:TRP:CZ3	2:E:1067:PHE:HB2	2.49	0.47
2:E:798:TYR:CZ	2:E:802:ILE:HD11	2.50	0.47
2:F:1481:PHE:HB3	2:F:1485:GLN:HB2	1.97	0.47
2:F:429:MET:HG2	2:F:433:PHE:CZ	2.49	0.47
1:C:95:PHE:CD2	2:G:27:PHE:HD1	2.32	0.47
2:H:1269:ASN:O	2:H:1273:ARG:N	2.29	0.47
2:H:1284:LEU:HD12	2:H:1285:THR:N	2.30	0.47
2:H:798:TYR:CZ	2:H:802:ILE:HD11	2.50	0.47
1:A:66:LEU:HD23	1:A:67:LYS:N	2.29	0.47
1:D:201:ARG:HD2	1:D:315:PHE:HB3	1.97	0.47
2:E:324:VAL:HG13	2:E:1277:ALA:HB1	1.97	0.47
2:F:1422:SER:HB2	2:F:1502:PHE:HB3	1.96	0.47
2:H:82:LEU:HG	2:H:114:PHE:CE1	2.50	0.47
1:D:278:HIS:ND1	2:H:1355:SER:OG	2.34	0.47
2:H:701:ILE:HD11	2:H:907:ILE:HG21	1.97	0.47
1:B:263:ALA:HA	1:B:268:TYR:CG	2.49	0.47
2:E:1153:LEU:HD12	2:E:1156:ILE:HD11	1.96	0.47
2:E:1398:PHE:CD2	2:E:1399:GLU:HG2	2.50	0.47
2:E:1481:PHE:HB3	2:E:1485:GLN:HB2	1.97	0.47
2:F:135:LEU:HD13	2:F:135:LEU:O	2.14	0.47
2:H:85:LEU:HD11	2:H:113:ALA:HB3	1.97	0.47
1:C:89:ALA:O	1:C:93:ILE:HG12	2.15	0.47
1:D:57:GLN:O	1:D:60:PHE:HB3	2.14	0.47
2:E:1422:SER:HB2	2:E:1502:PHE:HB3	1.96	0.47
2:F:1398:PHE:CD2	2:F:1399:GLU:HG2	2.50	0.47
2:F:798:TYR:CZ	2:F:802:ILE:HD11	2.50	0.47
2:G:547:ASN:ND2	2:G:594:SER:HB2	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1422:SER:HB2	2:H:1502:PHE:HB3	1.96	0.47
1:A:136:ARG:HH12	1:B:137:MET:CG	2.28	0.46
1:A:201:ARG:HD2	1:A:315:PHE:HB3	1.97	0.46
1:A:95:PHE:HE1	2:E:16:ARG:CG	2.27	0.46
1:B:177:ARG:NH1	1:B:206:ARG:HB2	2.26	0.46
1:B:201:ARG:HD2	1:B:315:PHE:HB3	1.97	0.46
2:E:82:LEU:HG	2:E:114:PHE:CE1	2.50	0.46
2:E:1181:PHE:CG	2:E:1247:LEU:HD22	2.51	0.46
2:E:1284:LEU:HD12	2:E:1285:THR:N	2.30	0.46
2:E:1446:SER:O	2:E:1449:THR:OG1	2.34	0.46
2:E:701:ILE:HD11	2:E:907:ILE:HG21	1.97	0.46
2:F:324:VAL:HG13	2:F:1277:ALA:HB1	1.97	0.46
2:F:1516:GLU:OE2	2:F:1541:THR:OG1	2.21	0.46
2:G:1181:PHE:CG	2:G:1247:LEU:HD22	2.51	0.46
2:G:1284:LEU:HD12	2:G:1285:THR:N	2.30	0.46
2:G:1516:GLU:OE2	2:G:1541:THR:OG1	2.21	0.46
2:G:701:ILE:HD11	2:G:907:ILE:HG21	1.97	0.46
2:E:1349:LEU:HB3	2:E:1364:VAL:HG13	1.97	0.46
2:F:1446:SER:O	2:F:1449:THR:OG1	2.33	0.46
2:F:701:ILE:HD11	2:F:907:ILE:HG21	1.97	0.46
2:G:1481:PHE:HB3	2:G:1485:GLN:HB2	1.97	0.46
2:H:1181:PHE:CG	2:H:1247:LEU:HD22	2.51	0.46
2:H:46:ILE:HD12	2:H:123:TYR:OH	2.16	0.46
1:A:344:CYS:HB2	1:A:348:GLN:OE1	2.16	0.46
1:A:57:GLN:O	1:A:60:PHE:HB3	2.15	0.46
1:D:159:ILE:O	1:D:163:MET:HG2	2.14	0.46
1:D:89:ALA:O	1:D:93:ILE:HG12	2.15	0.46
2:E:1269:ASN:O	2:E:1273:ARG:N	2.29	0.46
2:G:1139:LEU:O	2:G:1142:LEU:HD23	2.14	0.46
2:G:85:LEU:HD11	2:G:113:ALA:HB3	1.97	0.46
2:G:550:ILE:HD11	2:G:590:LEU:HD13	1.97	0.46
2:G:798:TYR:CZ	2:G:802:ILE:HD11	2.50	0.46
2:H:1087:TRP:HA	2:H:1090:LEU:HD12	1.97	0.46
2:H:770:ALA:HA	2:H:1216:PHE:CE1	2.50	0.46
1:B:344:CYS:HB2	1:B:348:GLN:OE1	2.16	0.46
1:D:344:CYS:HB2	1:D:348:GLN:OE1	2.16	0.46
2:E:1548:VAL:HG23	2:E:1562:PRO:HG3	1.97	0.46
2:F:1548:VAL:HG23	2:F:1562:PRO:HG3	1.97	0.46
2:G:770:ALA:HA	2:G:1216:PHE:CE1	2.49	0.46
2:G:82:LEU:HG	2:G:114:PHE:CE1	2.50	0.46
2:H:1481:PHE:HB3	2:H:1485:GLN:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:VAL:HG22	1:D:239:PRO:HB3	1.98	0.46
1:D:35:PHE:CD2	1:D:36:VAL:HG23	2.50	0.46
2:F:379:VAL:O	2:F:383:THR:HG23	2.16	0.46
2:F:550:ILE:HD11	2:F:590:LEU:HD13	1.97	0.46
2:G:1349:LEU:HB3	2:G:1364:VAL:HG13	1.97	0.46
2:G:1375:GLY:O	2:G:1549:ILE:N	2.40	0.46
2:H:1398:PHE:CD2	2:H:1399:GLU:HG2	2.50	0.46
1:C:201:ARG:HD2	1:C:315:PHE:HB3	1.97	0.46
2:F:1003:TYR:CE1	2:F:1092:VAL:HG11	2.51	0.46
2:F:577:PHE:HE2	2:F:1285:THR:HG1	1.61	0.46
2:G:1087:TRP:HA	2:G:1090:LEU:HD12	1.96	0.46
2:G:153:LYS:O	2:G:157:PHE:HB2	2.16	0.46
2:G:324:VAL:HG13	2:G:1277:ALA:HB1	1.97	0.46
2:H:1548:VAL:HG23	2:H:1562:PRO:HG3	1.97	0.46
1:A:35:PHE:CD2	1:A:36:VAL:HG23	2.50	0.46
1:C:329:ASP:OD1	1:C:331:SER:OG	2.31	0.46
1:A:233:LEU:HD21	1:D:326:TYR:CZ	2.51	0.46
2:E:577:PHE:HE2	2:E:1285:THR:HG1	1.63	0.46
2:F:1284:LEU:HD12	2:F:1285:THR:N	2.30	0.46
2:G:1003:TYR:CE1	2:G:1092:VAL:HG11	2.51	0.46
2:G:1152:ALA:O	2:G:1156:ILE:HG12	2.16	0.46
2:G:1398:PHE:CD2	2:G:1399:GLU:HG2	2.50	0.46
1:B:89:ALA:O	1:B:93:ILE:HG12	2.15	0.46
1:C:218:GLN:NE2	1:C:235:GLN:OE1	2.49	0.46
2:E:1030:ASP:OD2	2:E:1286:TYR:OH	2.32	0.46
2:E:1375:GLY:N	2:E:1547:LEU:O	2.45	0.46
2:E:379:VAL:O	2:E:383:THR:HG23	2.16	0.46
2:E:46:ILE:HD12	2:E:123:TYR:OH	2.16	0.46
2:F:108:MET:N	2:F:109:PRO:HD2	2.31	0.46
2:F:1181:PHE:CG	2:F:1247:LEU:HD22	2.50	0.46
2:F:494:GLU:O	2:F:498:GLN:HG2	2.16	0.46
2:G:127:ILE:O	2:G:131:ASN:N	2.45	0.46
2:G:1379:ARG:O	2:G:1384:LYS:NZ	2.49	0.46
2:H:1349:LEU:HB3	2:H:1364:VAL:HG13	1.97	0.46
2:H:1446:SER:O	2:H:1449:THR:OG1	2.34	0.46
2:H:379:VAL:O	2:H:383:THR:HG23	2.16	0.46
1:A:218:GLN:NE2	1:A:235:GLN:OE1	2.49	0.46
2:E:1231:ASP:O	2:E:1235:ILE:HG12	2.16	0.46
2:F:45:PRO:O	2:F:49:ILE:HG23	2.16	0.46
2:G:1231:ASP:O	2:G:1235:ILE:HG12	2.16	0.46
2:G:379:VAL:O	2:G:383:THR:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:324:VAL:HG13	2:H:1277:ALA:HB1	1.97	0.46
2:H:461:LEU:O	2:H:461:LEU:HD12	2.16	0.46
2:H:494:GLU:O	2:H:498:GLN:HG2	2.16	0.46
2:H:547:ASN:ND2	2:H:594:SER:HB2	2.26	0.46
1:C:344:CYS:HB2	1:C:348:GLN:OE1	2.16	0.46
2:E:85:LEU:HD11	2:E:113:ALA:HB3	1.97	0.46
2:G:108:MET:N	2:G:109:PRO:HD2	2.31	0.46
2:H:1152:ALA:O	2:H:1156:ILE:HG12	2.16	0.46
2:H:45:PRO:O	2:H:49:ILE:HG23	2.16	0.46
1:B:218:GLN:NE2	1:B:235:GLN:OE1	2.49	0.45
1:C:200:LEU:HD21	1:C:285:VAL:HG21	1.98	0.45
1:C:194:GLY:N	1:D:227:GLU:OE2	2.24	0.45
2:E:45:PRO:O	2:E:49:ILE:HG23	2.16	0.45
2:F:681:ILE:HG12	2:F:737:VAL:HG22	1.98	0.45
2:G:1431:PHE:HB2	2:G:1438:ASN:ND2	2.31	0.45
2:G:1422:SER:HB2	2:G:1502:PHE:HB3	1.96	0.45
2:H:681:ILE:HG12	2:H:737:VAL:HG22	1.98	0.45
2:E:108:MET:N	2:E:109:PRO:HD2	2.31	0.45
2:F:1231:ASP:O	2:F:1235:ILE:HG12	2.16	0.45
2:F:1379:ARG:O	2:F:1384:LYS:NZ	2.49	0.45
2:F:153:LYS:O	2:F:157:PHE:HB2	2.16	0.45
2:F:46:ILE:HD12	2:F:123:TYR:OH	2.16	0.45
2:F:85:LEU:HD11	2:F:113:ALA:HB3	1.97	0.45
2:G:45:PRO:O	2:G:49:ILE:HG23	2.16	0.45
2:H:108:MET:N	2:H:109:PRO:HD2	2.31	0.45
2:H:1431:PHE:HB2	2:H:1438:ASN:ND2	2.31	0.45
2:H:1372:GLN:HA	2:H:1530:ARG:O	2.17	0.45
1:B:200:LEU:HD21	1:B:285:VAL:HG21	1.98	0.45
2:E:1152:ALA:O	2:E:1156:ILE:HG12	2.16	0.45
2:E:153:LYS:O	2:E:157:PHE:HB2	2.16	0.45
2:G:1482:SER:HG	3:G:2004:ATP:PB	2.40	0.45
1:D:218:GLN:NE2	1:D:235:GLN:OE1	2.49	0.45
2:E:1003:TYR:CE1	2:E:1092:VAL:HG11	2.51	0.45
2:F:1152:ALA:O	2:F:1156:ILE:HG12	2.16	0.45
2:F:1431:PHE:HB2	2:F:1438:ASN:ND2	2.31	0.45
2:G:1446:SER:O	2:G:1449:THR:OG1	2.34	0.45
2:G:461:LEU:O	2:G:461:LEU:HD12	2.16	0.45
2:H:1231:ASP:O	2:H:1235:ILE:HG12	2.16	0.45
1:C:233:LEU:HD21	1:B:326:TYR:CZ	2.51	0.45
1:C:199:MET:HG2	1:C:258:TYR:HB3	1.99	0.45
1:C:299:GLN:NE2	1:C:301:ARG:HD2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1431:PHE:HB2	2:E:1438:ASN:ND2	2.31	0.45
2:H:455:ILE:C	2:H:457:GLY:H	2.20	0.45
2:E:1151:SER:O	2:E:1155:VAL:HG23	2.17	0.45
2:E:32:ASN:ND2	2:E:153:LYS:HD2	2.32	0.45
2:F:1072:SER:O	2:F:1075:ILE:HG22	2.17	0.45
2:F:117:ALA:O	2:F:120:SER:OG	2.17	0.45
2:F:1181:PHE:CD2	2:F:1247:LEU:HD22	2.52	0.45
2:F:455:ILE:C	2:F:457:GLY:H	2.20	0.45
2:F:788:ILE:HG22	2:F:791:SER:H	1.82	0.45
2:G:32:ASN:ND2	2:G:153:LYS:HD2	2.32	0.45
2:G:46:ILE:HD12	2:G:123:TYR:OH	2.16	0.45
2:G:681:ILE:HG12	2:G:737:VAL:HG22	1.98	0.45
2:H:1003:TYR:CE1	2:H:1092:VAL:HG11	2.51	0.45
2:H:1023:HIS:HE1	2:H:1144:ARG:HA	1.82	0.45
2:H:153:LYS:O	2:H:157:PHE:HB2	2.16	0.45
1:A:299:GLN:NE2	1:A:301:ARG:HD2	2.32	0.45
1:B:346:ALA:HA	1:B:349:LEU:HB2	1.99	0.45
1:D:199:MET:HG2	1:D:258:TYR:HB3	1.99	0.45
2:E:455:ILE:C	2:E:457:GLY:H	2.20	0.45
2:E:788:ILE:HG22	2:E:791:SER:H	1.82	0.45
2:G:716:GLY:N	3:G:2004:ATP:O2G	2.34	0.45
1:B:299:GLN:NE2	1:B:301:ARG:HD2	2.32	0.45
1:C:346:ALA:HA	1:C:349:LEU:HB2	1.99	0.45
1:D:128:GLN:HB2	1:D:152:GLN:HE21	1.82	0.45
1:D:68:TRP:CD2	1:D:170:LYS:HE3	2.52	0.45
2:F:291:LEU:O	2:F:295:PHE:HB3	2.16	0.45
2:G:1023:HIS:HE1	2:G:1144:ARG:HA	1.82	0.45
2:H:1030:ASP:OD2	2:H:1286:TYR:OH	2.32	0.45
2:H:1151:SER:O	2:H:1155:VAL:HG23	2.17	0.45
2:H:893:LEU:C	2:H:895:HIS:H	2.20	0.45
2:E:461:LEU:O	2:E:461:LEU:HD12	2.16	0.45
2:E:494:GLU:O	2:E:498:GLN:HG2	2.16	0.45
2:F:1349:LEU:HB3	2:F:1364:VAL:HG13	1.97	0.45
2:G:1245:ARG:NH2	2:G:1248:GLU:OE1	2.42	0.45
2:G:807:LEU:HG	2:G:811:ILE:HG13	1.99	0.45
2:H:1310:ALA:HA	2:H:1313:ARG:NH2	2.32	0.45
1:A:269:ASP:OD1	1:A:347:ARG:NE	2.33	0.45
1:A:90:TRP:CE2	1:A:123:PHE:HE2	2.35	0.45
1:C:268:TYR:CZ	1:C:347:ARG:HA	2.52	0.45
1:D:200:LEU:HD21	1:D:285:VAL:HG21	1.98	0.45
1:D:294:THR:OG1	1:D:296:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1023:HIS:HE1	2:E:1144:ARG:HA	1.82	0.45
2:E:1372:GLN:HA	2:E:1530:ARG:O	2.17	0.45
2:F:1151:SER:O	2:F:1155:VAL:HG23	2.17	0.45
2:G:1181:PHE:CD2	2:G:1247:LEU:HD22	2.52	0.45
2:H:1181:PHE:CD2	2:H:1247:LEU:HD22	2.52	0.45
2:H:1379:ARG:O	2:H:1384:LYS:NZ	2.49	0.45
1:A:68:TRP:CD2	1:A:170:LYS:HE3	2.52	0.44
1:B:294:THR:OG1	1:B:296:ILE:HG12	2.17	0.44
1:B:268:TYR:CZ	1:B:347:ARG:HA	2.52	0.44
1:D:90:TRP:CE2	1:D:123:PHE:HE2	2.36	0.44
2:E:1072:SER:O	2:E:1075:ILE:HG22	2.17	0.44
2:F:1271:LEU:HG	2:F:1272:HIS:CD2	2.52	0.44
2:G:771:TYR:HD2	2:G:1212:THR:HG22	1.82	0.44
2:G:1351:VAL:HG12	2:G:1397:THR:HA	1.99	0.44
2:G:1372:GLN:HA	2:G:1530:ARG:O	2.17	0.44
2:H:1072:SER:O	2:H:1075:ILE:HG22	2.17	0.44
2:H:1154:ALA:O	2:H:1157:SER:OG	2.26	0.44
1:A:200:LEU:HD21	1:A:285:VAL:HG21	1.98	0.44
1:D:268:TYR:CZ	1:D:347:ARG:HA	2.52	0.44
1:D:95:PHE:HD2	2:H:27:PHE:HD1	1.65	0.44
2:E:1271:LEU:HG	2:E:1272:HIS:CD2	2.52	0.44
2:E:1516:GLU:OE2	2:E:1541:THR:OG1	2.21	0.44
2:E:291:LEU:O	2:E:295:PHE:HB3	2.17	0.44
2:F:1310:ALA:HA	2:F:1313:ARG:NH2	2.32	0.44
2:F:381:ILE:HG13	2:F:433:PHE:CZ	2.53	0.44
2:F:417:ILE:O	2:F:420:LEU:HG	2.18	0.44
2:F:461:LEU:HD12	2:F:461:LEU:O	2.16	0.44
2:G:36:HIS:HD2	2:G:142:TYR:HE1	1.66	0.44
2:G:291:LEU:O	2:G:295:PHE:HB3	2.16	0.44
2:G:455:ILE:C	2:G:457:GLY:H	2.20	0.44
2:G:494:GLU:O	2:G:498:GLN:HG2	2.16	0.44
2:G:788:ILE:HG22	2:G:791:SER:H	1.82	0.44
2:H:1351:VAL:HG12	2:H:1397:THR:HA	2.00	0.44
1:A:268:TYR:CZ	1:A:347:ARG:HA	2.52	0.44
1:B:286:ILE:HG23	1:B:299:GLN:HE21	1.83	0.44
1:D:299:GLN:NE2	1:D:301:ARG:HD2	2.32	0.44
2:E:1181:PHE:CD2	2:E:1247:LEU:HD22	2.52	0.44
2:E:893:LEU:C	2:E:895:HIS:H	2.20	0.44
2:F:1023:HIS:HE1	2:F:1144:ARG:HA	1.82	0.44
2:F:771:TYR:HD2	2:F:1212:THR:HG22	1.82	0.44
2:G:1151:SER:O	2:G:1155:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:32:ASN:HD21	2:G:153:LYS:HD2	1.83	0.44
1:B:128:GLN:HB2	1:B:152:GLN:HE21	1.82	0.44
1:B:68:TRP:CD2	1:B:170:LYS:HE3	2.52	0.44
1:C:294:THR:OG1	1:C:296:ILE:HG12	2.17	0.44
1:C:76:THR:HG22	1:D:154:ILE:HG21	1.99	0.44
1:A:278:HIS:ND1	2:E:1355:SER:OG	2.47	0.44
2:E:417:ILE:O	2:E:420:LEU:HG	2.18	0.44
2:E:807:LEU:HG	2:E:811:ILE:HG13	1.99	0.44
2:F:1245:ARG:NH2	2:F:1248:GLU:OE1	2.42	0.44
2:F:1348:ASN:O	2:F:1350:SER:N	2.49	0.44
2:F:1372:GLN:HA	2:F:1530:ARG:O	2.17	0.44
2:F:36:HIS:HD2	2:F:142:TYR:HE1	1.66	0.44
2:F:889:LYS:NZ	2:F:892:TYR:HE2	2.16	0.44
2:G:1310:ALA:HA	2:G:1313:ARG:NH2	2.32	0.44
2:G:381:ILE:HG13	2:G:433:PHE:CZ	2.53	0.44
2:G:889:LYS:NZ	2:G:892:TYR:HE2	2.16	0.44
2:H:291:LEU:O	2:H:295:PHE:HB3	2.17	0.44
1:A:199:MET:HG2	1:A:258:TYR:HB3	1.99	0.44
1:A:164:LEU:HD11	1:B:164:LEU:HD13	1.99	0.44
1:C:68:TRP:CD2	1:C:170:LYS:HE3	2.52	0.44
1:D:286:ILE:HG23	1:D:299:GLN:HE21	1.82	0.44
2:E:1348:ASN:O	2:E:1350:SER:N	2.49	0.44
2:E:36:HIS:HD2	2:E:142:TYR:HE1	1.66	0.44
2:E:471:ALA:HB3	2:E:472:PRO:HD3	2.00	0.44
2:E:889:LYS:NZ	2:E:892:TYR:HE2	2.16	0.44
2:F:32:ASN:ND2	2:F:153:LYS:HD2	2.32	0.44
2:F:770:ALA:HA	2:F:1216:PHE:CE1	2.50	0.44
2:G:1455:GLU:OE1	2:G:1460:LYS:HB3	2.18	0.44
2:G:417:ILE:O	2:G:420:LEU:HG	2.18	0.44
2:G:893:LEU:C	2:G:895:HIS:H	2.20	0.44
2:H:771:TYR:HD2	2:H:1212:THR:HG22	1.82	0.44
1:A:294:THR:OG1	1:A:296:ILE:HG12	2.17	0.44
1:B:329:ASP:OD1	1:B:331:SER:OG	2.31	0.44
2:E:1066:VAL:O	2:E:1069:VAL:HG12	2.18	0.44
2:E:32:ASN:HD21	2:E:153:LYS:HD2	1.83	0.44
2:E:681:ILE:HG12	2:E:737:VAL:HG22	1.98	0.44
2:F:1455:GLU:OE1	2:F:1460:LYS:HB3	2.18	0.44
2:G:1348:ASN:O	2:G:1350:SER:N	2.49	0.44
2:H:1376:ILE:HB	2:H:1535:ILE:HD13	2.00	0.44
2:H:36:HIS:HD2	2:H:142:TYR:HE1	1.66	0.44
2:H:471:ALA:HB3	2:H:472:PRO:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:788:ILE:HG22	2:H:791:SER:H	1.82	0.44
1:A:128:GLN:HB2	1:A:152:GLN:HE21	1.82	0.44
2:E:1455:GLU:OE1	2:E:1460:LYS:HB3	2.18	0.44
2:F:32:ASN:HD21	2:F:153:LYS:HD2	1.83	0.44
2:F:893:LEU:C	2:F:895:HIS:H	2.20	0.44
2:H:1066:VAL:O	2:H:1069:VAL:HG12	2.18	0.44
1:A:346:ALA:HA	1:A:349:LEU:HB2	1.99	0.44
1:B:199:MET:HG2	1:B:258:TYR:HB3	1.99	0.44
1:C:286:ILE:HG23	1:C:299:GLN:HE21	1.82	0.44
1:C:90:TRP:CE2	1:C:123:PHE:HE2	2.36	0.44
1:D:199:MET:HG2	1:D:258:TYR:CB	2.48	0.44
2:G:437:ASN:ND2	2:G:592:LEU:HD23	2.29	0.44
2:H:32:ASN:ND2	2:H:153:LYS:HD2	2.32	0.44
2:H:435:CYS:N	2:H:436:PRO:HD2	2.33	0.44
2:H:807:LEU:HG	2:H:811:ILE:HG13	1.99	0.44
1:A:286:ILE:HG23	1:A:299:GLN:HE21	1.82	0.44
1:C:126:GLU:OE2	1:C:136:ARG:NH1	2.51	0.44
1:C:229:GLU:HB3	1:B:314:ARG:CZ	2.48	0.44
2:E:127:ILE:O	2:E:131:ASN:N	2.45	0.44
2:E:381:ILE:HG13	2:E:433:PHE:CZ	2.53	0.44
2:F:1460:LYS:O	2:F:1464:LYS:HG2	2.18	0.44
2:G:1066:VAL:O	2:G:1069:VAL:HG12	2.18	0.44
2:G:127:ILE:HG23	2:G:128:GLU:N	2.33	0.44
2:H:32:ASN:HD21	2:H:153:LYS:HD2	1.83	0.44
1:D:126:GLU:OE2	1:D:136:ARG:NH1	2.51	0.43
2:E:1379:ARG:O	2:E:1384:LYS:NZ	2.49	0.43
2:F:807:LEU:HG	2:F:811:ILE:HG13	1.99	0.43
2:G:1251:MET:HE3	2:G:1294:LEU:HD11	1.99	0.43
2:G:1271:LEU:HG	2:G:1272:HIS:CD2	2.52	0.43
2:H:127:ILE:HG23	2:H:128:GLU:N	2.33	0.43
2:H:127:ILE:O	2:H:131:ASN:N	2.45	0.43
2:H:141:VAL:O	2:H:144:THR:OG1	2.32	0.43
1:A:119:SER:OG	1:B:140:GLU:OE2	2.17	0.43
1:B:269:ASP:OD1	1:B:347:ARG:NE	2.33	0.43
1:C:190:ALA:O	1:C:196:LEU:HD12	2.18	0.43
1:C:199:MET:HG2	1:C:258:TYR:CB	2.48	0.43
1:D:346:ALA:HA	1:D:349:LEU:HB2	1.99	0.43
2:F:1030:ASP:OD2	2:F:1286:TYR:OH	2.32	0.43
2:G:1460:LYS:O	2:G:1464:LYS:HG2	2.19	0.43
2:G:1376:ILE:HB	2:G:1535:ILE:HD13	2.00	0.43
2:H:1251:MET:HE3	2:H:1294:LEU:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:ALA:O	1:B:196:LEU:HD12	2.18	0.43
1:B:199:MET:HG2	1:B:258:TYR:CB	2.48	0.43
2:E:1310:ALA:HA	2:E:1313:ARG:NH2	2.32	0.43
2:F:1251:MET:HE3	2:F:1294:LEU:HD11	1.99	0.43
2:F:1351:VAL:HG12	2:F:1397:THR:HA	1.99	0.43
2:G:1180:TYR:O	2:G:1183:VAL:HG12	2.19	0.43
2:H:1180:TYR:O	2:H:1183:VAL:HG12	2.19	0.43
2:H:417:ILE:O	2:H:420:LEU:HG	2.18	0.43
1:A:199:MET:HG2	1:A:258:TYR:CB	2.48	0.43
1:D:122:LEU:O	1:D:126:GLU:HG3	2.19	0.43
1:D:190:ALA:O	1:D:196:LEU:HD12	2.18	0.43
2:E:1351:VAL:HG12	2:E:1397:THR:HA	1.99	0.43
2:E:1376:ILE:HB	2:E:1535:ILE:HD13	2.00	0.43
2:F:1130:THR:O	2:F:1134:HIS:HB2	2.19	0.43
2:G:1072:SER:O	2:G:1075:ILE:HG22	2.17	0.43
2:G:1491:LEU:HD11	2:G:1507:ALA:HB1	2.00	0.43
2:G:471:ALA:HB3	2:G:472:PRO:HD3	2.00	0.43
2:H:1271:LEU:HG	2:H:1272:HIS:CD2	2.52	0.43
2:H:1460:LYS:O	2:H:1464:LYS:HG2	2.18	0.43
2:H:309:ALA:HB1	2:H:369:GLN:OE1	2.19	0.43
1:B:90:TRP:CE2	1:B:123:PHE:HE2	2.36	0.43
1:B:184:SER:O	1:B:304:TYR:OH	2.32	0.43
1:D:200:LEU:HD22	1:D:304:TYR:CE2	2.54	0.43
2:F:1154:ALA:O	2:F:1157:SER:OG	2.26	0.43
2:F:309:ALA:HB1	2:F:369:GLN:OE1	2.19	0.43
2:F:314:PHE:HZ	2:F:448:GLY:HA2	1.83	0.43
2:G:39:LEU:HA	2:G:42:ILE:HG22	2.01	0.43
2:H:381:ILE:HG13	2:H:433:PHE:CZ	2.53	0.43
1:A:126:GLU:OE2	1:A:136:ARG:NH1	2.51	0.43
1:B:126:GLU:OE2	1:B:136:ARG:NH1	2.51	0.43
1:C:128:GLN:HB2	1:C:152:GLN:HE21	1.82	0.43
2:E:552:ILE:HA	2:E:555:VAL:HG22	2.01	0.43
2:F:1066:VAL:O	2:F:1069:VAL:HG12	2.18	0.43
2:F:127:ILE:O	2:F:131:ASN:N	2.45	0.43
2:F:1491:LEU:HD11	2:F:1507:ALA:HB1	1.99	0.43
2:F:435:CYS:N	2:F:436:PRO:HD2	2.33	0.43
2:G:771:TYR:HD1	2:G:851:PHE:HD2	1.66	0.43
2:H:1482:SER:HG	3:H:2004:ATP:PB	2.41	0.43
1:A:122:LEU:O	1:A:126:GLU:HG3	2.19	0.43
2:E:1130:THR:O	2:E:1134:HIS:HB2	2.19	0.43
2:E:127:ILE:HG23	2:E:128:GLU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1491:LEU:HD11	2:E:1507:ALA:HB1	1.99	0.43
2:F:471:ALA:HB3	2:F:472:PRO:HD3	2.00	0.43
2:H:1130:THR:O	2:H:1134:HIS:HB2	2.19	0.43
2:H:1491:LEU:HD11	2:H:1507:ALA:HB1	1.99	0.43
2:H:889:LYS:NZ	2:H:892:TYR:HE2	2.16	0.43
1:A:108:GLU:N	1:A:108:GLU:OE1	2.52	0.43
1:A:190:ALA:O	1:A:196:LEU:HD12	2.18	0.43
1:C:108:GLU:OE1	1:C:108:GLU:N	2.52	0.43
1:C:200:LEU:HD22	1:C:304:TYR:CE2	2.54	0.43
2:E:39:LEU:HA	2:E:42:ILE:HG22	2.01	0.43
2:E:771:TYR:HD1	2:E:851:PHE:HD2	1.66	0.43
2:H:395:ILE:HG21	2:H:421:VAL:HG12	2.01	0.43
2:H:39:LEU:HA	2:H:42:ILE:HG22	2.01	0.43
2:H:890:LEU:O	2:H:893:LEU:HG	2.19	0.43
1:B:242:ASN:OD1	1:B:243:GLY:N	2.52	0.43
1:B:34:ARG:HH21	1:B:303:SER:HG	1.61	0.43
1:C:286:ILE:HD13	1:B:250:PHE:CD1	2.54	0.43
2:E:771:TYR:HD2	2:E:1212:THR:HG22	1.82	0.43
2:E:1251:MET:HE3	2:E:1294:LEU:HD11	2.00	0.43
2:E:309:ALA:HB1	2:E:369:GLN:OE1	2.19	0.43
2:F:1180:TYR:O	2:F:1183:VAL:HG12	2.19	0.43
2:H:552:ILE:HA	2:H:555:VAL:HG22	2.01	0.43
2:E:1460:LYS:O	2:E:1464:LYS:HG2	2.19	0.43
2:F:685:TYR:O	2:F:733:VAL:N	2.52	0.43
2:H:368:LEU:O	2:H:371:THR:HG22	2.19	0.43
2:H:771:TYR:HD1	2:H:851:PHE:HD2	1.66	0.43
1:C:158:MET:O	1:C:162:ILE:HG12	2.19	0.42
1:D:108:GLU:OE1	1:D:108:GLU:N	2.52	0.42
2:E:1180:TYR:O	2:E:1183:VAL:HG12	2.19	0.42
2:E:435:CYS:N	2:E:436:PRO:HD2	2.33	0.42
2:F:1065:MET:O	2:F:1068:THR:OG1	2.33	0.42
2:F:141:VAL:O	2:F:144:THR:OG1	2.32	0.42
2:F:395:ILE:HG21	2:F:421:VAL:HG12	2.00	0.42
2:G:1440:ASP:HB3	2:G:1442:GLU:O	2.19	0.42
2:G:714:GLN:HE22	2:G:1514:ALA:HB3	1.84	0.42
2:G:890:LEU:O	2:G:893:LEU:HG	2.19	0.42
2:H:1455:GLU:OE1	2:H:1460:LYS:HB3	2.18	0.42
1:A:200:LEU:HD22	1:A:304:TYR:CE2	2.54	0.42
1:A:242:ASN:OD1	1:A:243:GLY:N	2.52	0.42
1:B:200:LEU:HD22	1:B:304:TYR:CE2	2.54	0.42
1:C:122:LEU:O	1:C:126:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:127:ILE:HG23	2:F:128:GLU:N	2.33	0.42
2:F:1440:ASP:HB3	2:F:1442:GLU:O	2.19	0.42
2:G:309:ALA:HB1	2:G:369:GLN:OE1	2.19	0.42
1:B:122:LEU:O	1:B:126:GLU:HG3	2.19	0.42
2:E:395:ILE:HG21	2:E:421:VAL:HG12	2.01	0.42
2:F:1438:ASN:OD1	2:F:1474:ILE:HD12	2.19	0.42
2:F:368:LEU:O	2:F:371:THR:HG22	2.19	0.42
2:F:714:GLN:HE22	2:F:1514:ALA:HB3	1.84	0.42
2:G:368:LEU:O	2:G:371:THR:HG22	2.19	0.42
2:G:552:ILE:HA	2:G:555:VAL:HG22	2.01	0.42
1:A:158:MET:O	1:A:162:ILE:HG12	2.19	0.42
2:F:1376:ILE:HB	2:F:1535:ILE:HD13	2.00	0.42
2:F:552:ILE:HA	2:F:555:VAL:HG22	2.01	0.42
2:G:435:CYS:N	2:G:436:PRO:HD2	2.33	0.42
2:G:685:TYR:O	2:G:733:VAL:N	2.52	0.42
2:H:107:TYR:CD2	2:H:1165:VAL:HG21	2.55	0.42
2:H:1348:ASN:O	2:H:1350:SER:N	2.49	0.42
2:H:685:TYR:O	2:H:733:VAL:N	2.52	0.42
1:C:36:VAL:HB	1:C:303:SER:HB3	2.01	0.42
2:E:1245:ARG:NH2	2:E:1248:GLU:OE1	2.42	0.42
2:E:1438:ASN:OD1	2:E:1474:ILE:HD12	2.19	0.42
2:E:685:TYR:O	2:E:733:VAL:N	2.52	0.42
2:G:1438:ASN:OD1	2:G:1474:ILE:HD12	2.19	0.42
2:G:395:ILE:HG21	2:G:421:VAL:HG12	2.01	0.42
2:H:1142:LEU:HB3	2:H:1300:ASN:HB3	2.01	0.42
2:H:1162:VAL:O	2:H:1165:VAL:HG22	2.20	0.42
2:H:1440:ASP:HB3	2:H:1442:GLU:O	2.19	0.42
1:B:158:MET:O	1:B:162:ILE:HG12	2.19	0.42
1:C:233:LEU:HD21	1:B:326:TYR:CE1	2.54	0.42
2:E:1350:SER:HA	2:E:1362:LYS:HA	2.02	0.42
2:E:890:LEU:O	2:E:893:LEU:HG	2.19	0.42
2:G:1130:THR:O	2:G:1134:HIS:HB2	2.19	0.42
2:H:1350:SER:HA	2:H:1362:LYS:HA	2.02	0.42
1:C:34:ARG:HH21	1:C:303:SER:HG	1.62	0.42
2:E:1440:ASP:HB3	2:E:1442:GLU:O	2.19	0.42
2:F:44:PHE:HB2	2:F:45:PRO:HD3	2.02	0.42
2:G:1162:VAL:O	2:G:1165:VAL:HG22	2.20	0.42
2:G:12:SER:C	2:G:15:TYR:H	2.22	0.42
2:G:314:PHE:HZ	2:G:448:GLY:HA2	1.83	0.42
1:A:180:THR:OG1	1:A:205:LEU:HB2	2.20	0.42
1:A:263:ALA:HA	1:A:268:TYR:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:VAL:HB	1:B:303:SER:HB3	2.01	0.42
2:E:317:PRO:HA	2:E:320:ILE:HD12	2.02	0.42
2:E:770:ALA:HA	2:E:1216:PHE:CE1	2.50	0.42
2:F:890:LEU:O	2:F:893:LEU:HG	2.19	0.42
2:G:1166:ALA:C	2:G:1169:PRO:HD2	2.40	0.42
2:G:1350:SER:HA	2:G:1362:LYS:HA	2.02	0.42
2:G:317:PRO:HA	2:G:320:ILE:HD12	2.02	0.42
2:H:716:GLY:N	3:H:2004:ATP:O2G	2.34	0.42
2:H:44:PHE:HB2	2:H:45:PRO:HD3	2.02	0.42
1:C:233:LEU:HD11	1:B:326:TYR:CG	2.55	0.42
1:D:95:PHE:HE2	2:H:27:PHE:CB	2.32	0.42
2:E:368:LEU:O	2:E:371:THR:HG22	2.19	0.42
2:E:44:PHE:HB2	2:E:45:PRO:HD3	2.02	0.42
2:F:39:LEU:HA	2:F:42:ILE:HG22	2.01	0.42
2:G:1251:MET:HB2	2:G:1295:ASN:HD21	1.84	0.42
2:G:878:ASP:OD2	2:G:881:ARG:HB2	2.20	0.42
1:B:108:GLU:N	1:B:108:GLU:OE1	2.52	0.42
1:C:180:THR:OG1	1:C:205:LEU:HB2	2.20	0.42
2:E:1166:ALA:C	2:E:1169:PRO:HD2	2.40	0.42
2:E:714:GLN:HE22	2:E:1514:ALA:HB3	1.84	0.42
2:F:12:SER:C	2:F:15:TYR:H	2.22	0.42
2:F:553:ALA:O	2:F:557:ILE:HG12	2.20	0.42
2:G:1142:LEU:HB3	2:G:1300:ASN:HB3	2.01	0.42
2:G:107:TYR:CD2	2:G:1165:VAL:HG21	2.55	0.42
2:G:553:ALA:O	2:G:557:ILE:HG12	2.20	0.42
2:H:1348:ASN:O	2:H:1400:GLY:HA3	2.20	0.42
2:H:1488:LEU:HD13	2:H:1488:LEU:HA	1.89	0.42
2:H:22:LEU:HB3	2:H:156:LYS:HE3	2.02	0.42
1:A:229:GLU:HB3	1:D:314:ARG:CZ	2.50	0.41
1:A:136:ARG:NH1	1:B:137:MET:SD	2.93	0.41
1:B:180:THR:OG1	1:B:205:LEU:HB2	2.20	0.41
2:E:1163:PHE:CE2	2:E:1167:LEU:HB2	2.55	0.41
2:E:716:GLY:N	3:E:2004:ATP:O2G	2.34	0.41
2:E:769:VAL:HG13	2:E:849:VAL:O	2.20	0.41
2:F:1162:VAL:O	2:F:1165:VAL:HG22	2.20	0.41
2:F:1347:GLN:HE21	2:F:1401:HIS:CE1	2.38	0.41
2:F:317:PRO:HA	2:F:320:ILE:HD12	2.02	0.41
2:F:771:TYR:HD1	2:F:851:PHE:HD2	1.66	0.41
2:G:44:PHE:HB2	2:G:45:PRO:HD3	2.02	0.41
2:H:714:GLN:HE22	2:H:1514:ALA:HB3	1.84	0.41
2:H:317:PRO:HA	2:H:320:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ALA:HA	1:B:268:TYR:CD1	2.55	0.41
1:D:263:ALA:HA	1:D:268:TYR:CD1	2.55	0.41
1:D:36:VAL:HB	1:D:303:SER:HB3	2.01	0.41
2:E:1004:LEU:HB2	2:E:1012:LEU:HD21	2.03	0.41
2:H:396:TYR:CG	2:H:1226:LEU:HD13	2.55	0.41
2:H:1438:ASN:OD1	2:H:1474:ILE:HD12	2.19	0.41
2:H:547:ASN:HD21	2:H:590:LEU:C	2.19	0.41
1:D:180:THR:OG1	1:D:205:LEU:HB2	2.20	0.41
2:E:107:TYR:CD2	2:E:1165:VAL:HG21	2.55	0.41
2:E:1142:LEU:HB3	2:E:1300:ASN:HB3	2.02	0.41
2:E:1348:ASN:O	2:E:1400:GLY:HA3	2.20	0.41
2:E:1482:SER:HG	3:E:2004:ATP:PB	2.43	0.41
2:E:22:LEU:HB3	2:E:156:LYS:HE3	2.02	0.41
2:F:107:TYR:CD2	2:F:1165:VAL:HG21	2.55	0.41
2:F:1403:ILE:HD13	2:F:1408:ASP:HA	2.02	0.41
2:F:22:LEU:HB3	2:F:156:LYS:HE3	2.02	0.41
2:F:878:ASP:OD2	2:F:881:ARG:HB2	2.20	0.41
2:G:1403:ILE:HD13	2:G:1408:ASP:HA	2.02	0.41
2:H:1166:ALA:C	2:H:1169:PRO:HD2	2.40	0.41
2:H:1568:ARG:HH21	2:H:1571:SER:HA	1.85	0.41
2:H:314:PHE:HZ	2:H:448:GLY:HA2	1.83	0.41
1:A:233:LEU:HD11	1:D:326:TYR:CG	2.56	0.41
1:C:263:ALA:HA	1:C:268:TYR:CD1	2.55	0.41
1:D:158:MET:O	1:D:162:ILE:HG12	2.19	0.41
1:C:164:LEU:HD11	1:D:164:LEU:HD13	2.02	0.41
1:D:273:SER:HG	2:H:1398:PHE:HE2	1.58	0.41
2:F:1142:LEU:HB3	2:F:1300:ASN:HB3	2.02	0.41
2:F:1251:MET:HB2	2:F:1295:ASN:HD21	1.84	0.41
2:F:1350:SER:HA	2:F:1362:LYS:HA	2.02	0.41
2:G:22:LEU:HB3	2:G:156:LYS:HE3	2.02	0.41
2:H:1251:MET:HB2	2:H:1295:ASN:HD21	1.84	0.41
2:H:769:VAL:HG13	2:H:849:VAL:O	2.20	0.41
2:H:878:ASP:OD2	2:H:881:ARG:HB2	2.20	0.41
2:E:1023:HIS:CE1	2:E:1144:ARG:HA	2.56	0.41
2:E:553:ALA:O	2:E:557:ILE:HG12	2.20	0.41
2:E:437:ASN:ND2	2:E:592:LEU:HD23	2.29	0.41
2:E:878:ASP:OD2	2:E:881:ARG:HB2	2.20	0.41
2:F:1163:PHE:CE2	2:F:1167:LEU:HB2	2.56	0.41
2:F:1568:ARG:HH21	2:F:1571:SER:HA	1.85	0.41
2:F:84:VAL:HG11	2:F:174:LEU:HD12	2.03	0.41
2:F:6:CYS:H	2:F:16:ARG:HH11	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:805:CYS:O	2:F:836:ARG:HD2	2.20	0.41
2:G:1347:GLN:HE21	2:G:1401:HIS:CE1	2.38	0.41
2:H:1004:LEU:HB2	2:H:1012:LEU:HD21	2.03	0.41
2:H:12:SER:C	2:H:15:TYR:H	2.22	0.41
2:H:1346:ILE:HG22	2:H:1402:ILE:HG13	2.02	0.41
2:H:550:ILE:N	2:H:551:PRO:HD2	2.36	0.41
2:H:72:ASN:HA	2:H:75:TRP:HD1	1.85	0.41
1:C:218:GLN:NE2	1:C:235:GLN:HB3	2.35	0.41
2:E:1162:VAL:O	2:E:1165:VAL:HG22	2.20	0.41
2:E:1251:MET:HB2	2:E:1295:ASN:HD21	1.84	0.41
2:E:1346:ILE:HG22	2:E:1402:ILE:HG13	2.02	0.41
2:F:1346:ILE:HG22	2:F:1402:ILE:HG13	2.02	0.41
2:F:716:GLY:N	3:F:2004:ATP:O2G	2.34	0.41
2:H:1163:PHE:CE2	2:H:1167:LEU:HB2	2.56	0.41
1:C:314:ARG:CZ	1:D:229:GLU:HB3	2.51	0.41
1:C:119:SER:OG	1:D:140:GLU:OE2	2.23	0.41
2:E:6:CYS:H	2:E:16:ARG:HH11	1.68	0.41
2:F:1255:GLY:O	2:F:1259:VAL:HG23	2.21	0.41
2:G:1023:HIS:CE1	2:G:1144:ARG:HA	2.56	0.41
2:G:1348:ASN:O	2:G:1400:GLY:HA3	2.20	0.41
2:G:396:TYR:CG	2:G:1226:LEU:HD13	2.55	0.41
2:H:320:ILE:HG23	2:H:1284:LEU:HD11	2.03	0.41
2:H:428:LEU:HA	2:H:428:LEU:HD23	1.91	0.41
2:H:553:ALA:O	2:H:557:ILE:HG12	2.20	0.41
2:H:84:VAL:HG11	2:H:174:LEU:HD12	2.03	0.41
1:A:36:VAL:HB	1:A:303:SER:HB3	2.01	0.41
1:A:38:LYS:NZ	1:A:308:GLU:OE1	2.53	0.41
2:E:12:SER:C	2:E:15:TYR:H	2.22	0.41
2:E:709:THR:HA	2:E:898:TRP:O	2.21	0.41
2:E:72:ASN:HA	2:E:75:TRP:HD1	1.85	0.41
2:F:1023:HIS:CE1	2:F:1144:ARG:HA	2.56	0.41
2:F:547:ASN:HD21	2:F:590:LEU:C	2.19	0.41
2:G:1568:ARG:HH21	2:G:1571:SER:HA	1.85	0.41
2:G:769:VAL:HG13	2:G:849:VAL:O	2.21	0.41
2:G:84:VAL:HG11	2:G:174:LEU:HD12	2.03	0.41
2:H:1255:GLY:O	2:H:1259:VAL:HG23	2.21	0.41
2:H:147:PHE:O	2:H:151:THR:HG23	2.21	0.41
1:B:335:ASN:HD22	1:B:336:THR:H	1.69	0.41
1:C:242:ASN:OD1	1:C:243:GLY:N	2.52	0.41
2:E:550:ILE:N	2:E:551:PRO:HD2	2.36	0.41
2:E:709:THR:HB	2:E:898:TRP:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:314:PHE:CE2	2:F:447:VAL:HG12	2.56	0.41
2:F:396:TYR:CG	2:F:1226:LEU:HD13	2.55	0.41
2:F:550:ILE:N	2:F:551:PRO:HD2	2.35	0.41
2:F:72:ASN:HA	2:F:75:TRP:HD1	1.85	0.41
2:G:1255:GLY:O	2:G:1259:VAL:HG23	2.21	0.41
2:G:147:PHE:O	2:G:151:THR:HG23	2.21	0.41
2:G:72:ASN:HA	2:G:75:TRP:HD1	1.85	0.41
1:B:74:ILE:HD13	2:F:49:ILE:HG22	2.03	0.41
1:C:184:SER:O	1:C:304:TYR:OH	2.32	0.41
1:C:95:PHE:HE2	2:G:27:PHE:CB	2.34	0.41
1:C:314:ARG:HD2	1:D:229:GLU:OE1	2.21	0.41
2:E:396:TYR:CG	2:E:1226:LEU:HD13	2.56	0.41
2:E:1255:GLY:O	2:E:1259:VAL:HG23	2.21	0.41
2:E:302:SER:OG	2:E:376:SER:O	2.31	0.41
2:F:320:ILE:HG23	2:F:1284:LEU:HD11	2.03	0.41
2:F:322:GLY:C	2:F:326:HIS:HD1	2.18	0.41
2:G:455:ILE:C	2:G:456:LEU:HG	2.41	0.41
2:G:777:TRP:CZ3	2:G:1209:GLY:HA3	2.56	0.41
2:H:455:ILE:C	2:H:456:LEU:HG	2.41	0.41
1:D:242:ASN:OD1	1:D:243:GLY:N	2.52	0.41
2:E:1347:GLN:HE21	2:E:1401:HIS:CE1	2.38	0.41
2:E:1568:ARG:HH21	2:E:1571:SER:HA	1.85	0.41
2:E:889:LYS:HZ2	2:E:892:TYR:HE2	1.67	0.41
2:F:1166:ALA:C	2:F:1169:PRO:HD2	2.40	0.41
2:G:1131:ILE:HA	2:G:1135:ILE:CD1	2.51	0.41
2:G:547:ASN:HD21	2:G:590:LEU:C	2.19	0.41
2:G:679:VAL:HA	2:G:738:PHE:O	2.21	0.41
2:G:709:THR:HA	2:G:898:TRP:O	2.21	0.41
2:H:1568:ARG:C	2:H:1570:ASP:H	2.24	0.41
1:D:329:ASP:OD1	1:D:331:SER:OG	2.31	0.40
2:E:84:VAL:HG11	2:E:174:LEU:HD12	2.03	0.40
2:E:455:ILE:C	2:E:456:LEU:HG	2.41	0.40
2:E:805:CYS:O	2:E:836:ARG:HD2	2.20	0.40
2:F:1004:LEU:HB2	2:F:1012:LEU:HD21	2.03	0.40
2:F:709:THR:HA	2:F:898:TRP:O	2.21	0.40
2:G:1346:ILE:HG22	2:G:1402:ILE:HG13	2.02	0.40
2:G:805:CYS:O	2:G:836:ARG:HD2	2.20	0.40
2:F:777:TRP:CZ3	2:F:1209:GLY:HA3	2.56	0.40
2:F:1348:ASN:O	2:F:1400:GLY:HA3	2.20	0.40
2:G:36:HIS:HD2	2:G:142:TYR:CE1	2.40	0.40
2:G:374:GLN:NE2	2:G:1245:ARG:HE	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:808:GLN:HB2	2:G:809:PRO:HD3	2.03	0.40
2:H:1065:MET:O	2:H:1068:THR:OG1	2.33	0.40
2:H:709:THR:HA	2:H:898:TRP:O	2.21	0.40
2:H:679:VAL:HA	2:H:738:PHE:O	2.21	0.40
1:A:146:ILE:HG12	1:D:122:LEU:HD21	2.02	0.40
1:D:218:GLN:NE2	1:D:235:GLN:HB3	2.35	0.40
1:D:335:ASN:HD22	1:D:336:THR:H	1.69	0.40
2:E:147:PHE:O	2:E:151:THR:HG23	2.21	0.40
2:F:370:ARG:HB3	2:F:1252:GLU:HG2	2.04	0.40
2:F:1505:ASP:HA	2:F:1535:ILE:HB	2.03	0.40
2:G:1004:LEU:HB2	2:G:1012:LEU:HD21	2.03	0.40
2:G:1065:MET:O	2:G:1068:THR:OG1	2.33	0.40
2:G:320:ILE:HG23	2:G:1284:LEU:HD11	2.03	0.40
2:H:1131:ILE:HA	2:H:1135:ILE:CD1	2.51	0.40
2:H:1347:GLN:HE21	2:H:1401:HIS:CE1	2.38	0.40
2:H:805:CYS:O	2:H:836:ARG:HD2	2.20	0.40
2:E:370:ARG:HB3	2:E:1252:GLU:HG2	2.04	0.40
2:F:717:CYS:O	2:F:905:GLY:N	2.54	0.40
2:G:1163:PHE:CE2	2:G:1167:LEU:HB2	2.55	0.40
2:H:1031:TYR:CE2	2:H:1035:LYS:HD2	2.57	0.40
2:H:577:PHE:HE2	2:H:1285:THR:HG1	1.63	0.40
2:H:717:CYS:O	2:H:905:GLY:N	2.54	0.40
1:A:326:TYR:CZ	1:B:233:LEU:HD21	2.57	0.40
1:C:229:GLU:OE1	1:B:314:ARG:HD2	2.22	0.40
1:C:136:ARG:HH12	1:D:137:MET:CG	2.34	0.40
2:E:808:GLN:HB2	2:E:809:PRO:HD3	2.03	0.40
2:F:455:ILE:C	2:F:456:LEU:HG	2.41	0.40
2:F:769:VAL:HG13	2:F:849:VAL:O	2.21	0.40
2:F:709:THR:HB	2:F:898:TRP:HB3	2.03	0.40
2:G:1031:TYR:CE2	2:G:1035:LYS:HD2	2.57	0.40
2:G:148:ILE:O	2:G:151:THR:OG1	2.34	0.40
2:G:1505:ASP:HA	2:G:1535:ILE:HB	2.03	0.40
2:G:550:ILE:N	2:G:551:PRO:HD2	2.35	0.40
2:H:808:GLN:HB2	2:H:809:PRO:HD3	2.03	0.40
2:H:709:THR:HB	2:H:898:TRP:HB3	2.03	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%)	301 (92%)	25 (8%)	0	100	100
1	B	326/406 (80%)	302 (93%)	24 (7%)	0	100	100
1	C	326/406 (80%)	303 (93%)	23 (7%)	0	100	100
1	D	326/406 (80%)	303 (93%)	23 (7%)	0	100	100
2	E	1270/1581 (80%)	1175 (92%)	95 (8%)	0	100	100
2	F	1270/1581 (80%)	1175 (92%)	95 (8%)	0	100	100
2	G	1270/1581 (80%)	1175 (92%)	95 (8%)	0	100	100
2	H	1270/1581 (80%)	1175 (92%)	95 (8%)	0	100	100
All	All	6384/7948 (80%)	5909 (93%)	475 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	264/348 (76%)	263 (100%)	1 (0%)	92	96
1	B	264/348 (76%)	263 (100%)	1 (0%)	92	96
1	C	264/348 (76%)	263 (100%)	1 (0%)	92	96
1	D	264/348 (76%)	263 (100%)	1 (0%)	92	96
2	E	987/1368 (72%)	978 (99%)	9 (1%)	81	90
2	F	987/1368 (72%)	978 (99%)	9 (1%)	81	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	987/1368 (72%)	978 (99%)	9 (1%)	81	90
2	H	987/1368 (72%)	978 (99%)	9 (1%)	81	90
All	All	5004/6864 (73%)	4964 (99%)	40 (1%)	84	91

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	335	ASN
1	C	335	ASN
1	B	335	ASN
1	D	335	ASN
2	E	126	ASN
2	E	188	ASN
2	E	419	ASN
2	E	1142	LEU
2	E	1233	ASN
2	E	1244	ASN
2	E	1271	LEU
2	E	1292	ASN
2	E	1513	MET
2	H	126	ASN
2	H	188	ASN
2	H	419	ASN
2	H	1142	LEU
2	H	1233	ASN
2	H	1244	ASN
2	H	1271	LEU
2	H	1292	ASN
2	H	1513	MET
2	G	126	ASN
2	G	188	ASN
2	G	419	ASN
2	G	1142	LEU
2	G	1233	ASN
2	G	1244	ASN
2	G	1271	LEU
2	G	1292	ASN
2	G	1513	MET
2	F	126	ASN
2	F	188	ASN
2	F	419	ASN

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Mol	Chain	Res	Type
2	F	1142	LEU
2	F	1233	ASN
2	F	1244	ASN
2	F	1271	LEU
2	F	1292	ASN
2	F	1513	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	HIS
1	A	193	HIS
1	A	218	GLN
1	A	235	GLN
1	A	277	HIS
1	A	335	ASN
1	C	115	HIS
1	C	193	HIS
1	C	218	GLN
1	C	235	GLN
1	C	277	HIS
1	C	335	ASN
1	B	115	HIS
1	B	193	HIS
1	B	218	GLN
1	B	235	GLN
1	B	277	HIS
1	B	335	ASN
1	D	115	HIS
1	D	193	HIS
1	D	218	GLN
1	D	235	GLN
1	D	277	HIS
1	D	335	ASN
2	E	36	HIS
2	E	102	HIS
2	E	126	ASN
2	E	188	ASN
2	E	416	GLN
2	E	419	ASN
2	E	437	ASN
2	E	498	GLN

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Mol	Chain	Res	Type
2	E	500	ASN
2	E	707	GLN
2	E	714	GLN
2	E	821	GLN
2	E	1129	ASN
2	E	1133	GLN
2	E	1202	HIS
2	E	1244	ASN
2	E	1272	HIS
2	H	36	HIS
2	H	102	HIS
2	H	126	ASN
2	H	188	ASN
2	H	416	GLN
2	H	419	ASN
2	H	437	ASN
2	H	498	GLN
2	H	500	ASN
2	H	707	GLN
2	H	714	GLN
2	H	821	GLN
2	H	1129	ASN
2	H	1133	GLN
2	H	1202	HIS
2	H	1244	ASN
2	H	1272	HIS
2	G	36	HIS
2	G	102	HIS
2	G	126	ASN
2	G	188	ASN
2	G	416	GLN
2	G	419	ASN
2	G	437	ASN
2	G	498	GLN
2	G	500	ASN
2	G	707	GLN
2	G	714	GLN
2	G	821	GLN
2	G	1129	ASN
2	G	1133	GLN
2	G	1202	HIS
2	G	1244	ASN

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Mol	Chain	Res	Type
2	G	1272	HIS
2	F	36	HIS
2	F	102	HIS
2	F	126	ASN
2	F	188	ASN
2	F	416	GLN
2	F	419	ASN
2	F	437	ASN
2	F	498	GLN
2	F	500	ASN
2	F	707	GLN
2	F	714	GLN
2	F	821	GLN
2	F	1129	ASN
2	F	1133	GLN
2	F	1202	HIS
2	F	1244	ASN
2	F	1272	HIS

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 23 ligands modelled in this entry, 11 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	B	501	-	27,33,33	0.96	1 (3%)	27,52,52	1.94	4 (14%)
3	ATP	C	501	-	27,33,33	0.96	2 (7%)	27,52,52	1.96	4 (14%)
3	ATP	D	501	-	27,33,33	0.94	1 (3%)	27,52,52	2.03	4 (14%)
5	ADP	E	2001	6	25,29,29	1.00	1 (4%)	25,45,45	1.79	3 (12%)
3	ATP	E	2004	6	27,33,33	0.98	2 (7%)	27,52,52	1.82	5 (18%)
5	ADP	F	2001	6	25,29,29	1.00	1 (4%)	25,45,45	1.79	3 (12%)
3	ATP	F	2004	6	27,33,33	0.97	1 (3%)	27,52,52	1.82	4 (14%)
5	ADP	G	2001	6	25,29,29	0.99	1 (4%)	25,45,45	1.80	3 (12%)
3	ATP	G	2004	6	27,33,33	0.97	2 (7%)	27,52,52	1.81	5 (18%)
5	ADP	H	2001	6	25,29,29	0.99	1 (4%)	25,45,45	1.79	3 (12%)
3	ATP	H	2004	6	27,33,33	0.97	2 (7%)	27,52,52	1.82	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	B	501	-	-	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
5	ADP	E	2001	6	-	0/12/32/32	0/3/3/3
3	ATP	E	2004	6	-	0/18/38/38	0/3/3/3
5	ADP	F	2001	6	-	0/12/32/32	0/3/3/3
3	ATP	F	2004	6	-	0/18/38/38	0/3/3/3
5	ADP	G	2001	6	-	0/12/32/32	0/3/3/3
3	ATP	G	2004	6	-	0/18/38/38	0/3/3/3
5	ADP	H	2001	6	-	0/12/32/32	0/3/3/3
3	ATP	H	2004	6	-	0/18/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2004	ATP	C8-N9	-2.11	1.34	1.36
3	E	2004	ATP	C8-N9	-2.09	1.34	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	2004	ATP	C8-N9	-2.06	1.34	1.36
3	C	501	ATP	C8-N9	-2.00	1.34	1.36
3	D	501	ATP	C5-C4	2.78	1.46	1.40
3	G	2004	ATP	C5-C4	2.82	1.46	1.40
3	H	2004	ATP	C5-C4	2.82	1.46	1.40
3	A	501	ATP	C5-C4	2.85	1.46	1.40
5	H	2001	ADP	C5-C4	2.86	1.47	1.40
3	C	501	ATP	C5-C4	2.87	1.47	1.40
3	E	2004	ATP	C5-C4	2.89	1.47	1.40
3	B	501	ATP	C5-C4	2.90	1.47	1.40
5	E	2001	ADP	C5-C4	2.91	1.47	1.40
3	F	2004	ATP	C5-C4	2.91	1.47	1.40
5	G	2001	ADP	C5-C4	2.91	1.47	1.40
5	F	2001	ADP	C5-C4	2.92	1.47	1.40

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	ATP	N3-C2-N1	-6.03	123.70	128.86
5	G	2001	ADP	N3-C2-N1	-5.95	123.77	128.86
3	A	501	ATP	N3-C2-N1	-5.95	123.78	128.86
3	B	501	ATP	N3-C2-N1	-5.92	123.79	128.86
3	C	501	ATP	N3-C2-N1	-5.92	123.80	128.86
5	E	2001	ADP	N3-C2-N1	-5.89	123.82	128.86
5	F	2001	ADP	N3-C2-N1	-5.89	123.82	128.86
5	H	2001	ADP	N3-C2-N1	-5.87	123.84	128.86
3	F	2004	ATP	N3-C2-N1	-5.63	124.04	128.86
3	E	2004	ATP	N3-C2-N1	-5.61	124.06	128.86
3	H	2004	ATP	N3-C2-N1	-5.59	124.08	128.86
3	G	2004	ATP	N3-C2-N1	-5.57	124.09	128.86
3	A	501	ATP	PA-O3A-PB	-4.90	116.17	132.63
3	D	501	ATP	PA-O3A-PB	-4.64	117.04	132.63
3	C	501	ATP	PA-O3A-PB	-4.30	118.19	132.63
3	B	501	ATP	PA-O3A-PB	-4.06	118.97	132.63
3	D	501	ATP	PB-O3B-PG	-4.06	118.98	132.63
3	C	501	ATP	PB-O3B-PG	-3.92	119.46	132.63
3	B	501	ATP	PB-O3B-PG	-3.91	119.48	132.63
5	G	2001	ADP	PA-O3A-PB	-3.91	119.49	132.63
5	E	2001	ADP	PA-O3A-PB	-3.90	119.51	132.63
5	H	2001	ADP	PA-O3A-PB	-3.90	119.53	132.63
5	F	2001	ADP	PA-O3A-PB	-3.88	119.60	132.63
3	A	501	ATP	PB-O3B-PG	-3.84	119.73	132.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2004	ATP	PA-O3A-PB	-3.35	121.36	132.63
3	H	2004	ATP	PA-O3A-PB	-3.34	121.42	132.63
3	E	2004	ATP	PA-O3A-PB	-3.33	121.43	132.63
3	G	2004	ATP	PA-O3A-PB	-3.33	121.43	132.63
3	F	2004	ATP	C4-C5-N7	-2.88	106.63	109.41
3	H	2004	ATP	C4-C5-N7	-2.88	106.63	109.41
3	G	2004	ATP	PB-O3B-PG	-2.84	123.08	132.63
3	F	2004	ATP	PB-O3B-PG	-2.83	123.11	132.63
3	E	2004	ATP	PB-O3B-PG	-2.83	123.11	132.63
3	E	2004	ATP	C4-C5-N7	-2.83	106.68	109.41
3	H	2004	ATP	PB-O3B-PG	-2.82	123.16	132.63
3	G	2004	ATP	C4-C5-N7	-2.79	106.71	109.41
3	B	501	ATP	C4-C5-N7	-2.78	106.72	109.41
3	C	501	ATP	C4-C5-N7	-2.75	106.75	109.41
3	D	501	ATP	C4-C5-N7	-2.74	106.76	109.41
5	H	2001	ADP	C4-C5-N7	-2.73	106.77	109.41
3	A	501	ATP	C4-C5-N7	-2.72	106.79	109.41
5	E	2001	ADP	C4-C5-N7	-2.70	106.81	109.41
5	G	2001	ADP	C4-C5-N7	-2.69	106.81	109.41
5	F	2001	ADP	C4-C5-N7	-2.68	106.82	109.41
3	E	2004	ATP	C2'-C3'-C4'	2.01	106.47	102.62
3	H	2004	ATP	C2'-C3'-C4'	2.02	106.50	102.62
3	G	2004	ATP	C2'-C3'-C4'	2.03	106.52	102.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	ATP	1	0
3	B	501	ATP	1	0
3	C	501	ATP	1	0
3	D	501	ATP	1	0
3	E	2004	ATP	3	0
3	F	2004	ATP	3	0
3	G	2004	ATP	3	0
3	H	2004	ATP	3	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.