



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:00 PM UTC

PDB ID : 6CUX / pdb_00006cux
Title : Escherichia coli RpoB S531L mutant RNA polymerase holoenzyme in complex with Kanglemycin A
Authors : Molodtsov, V.; Murakami, K.S.
Deposited on : 2018-03-26
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

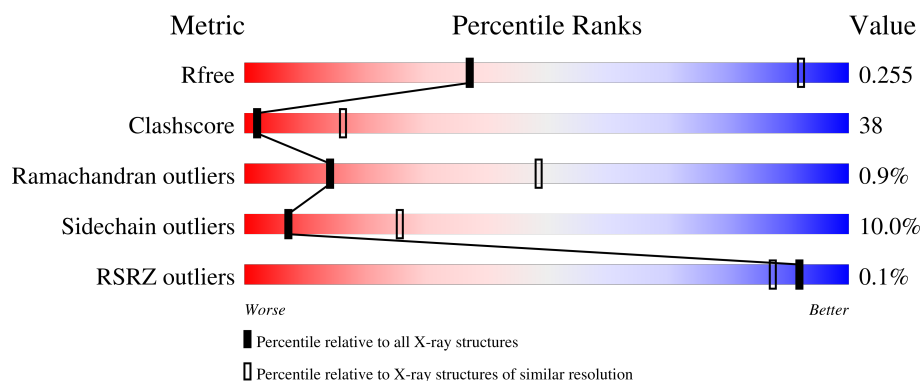
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 Å.

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



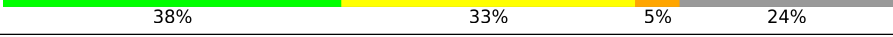
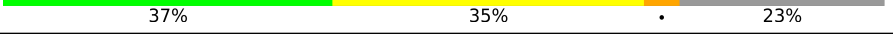
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)

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

Mol	Chain	Length	Quality of chain
1	A	329	33% 31% 6% 31%
1	B	329	24% 37% . 35%
1	G	329	28% 35% 5% 32%
1	H	329	% 28% 34% . 35%
2	C	1342	44% 49% 6%

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Mol	Chain	Length	Quality of chain
2	I	1342	
3	D	1407	
3	J	1407	
4	E	91	
4	K	91	
5	F	613	
5	L	613	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	ZN	J	1502	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 55005 atoms, of which 62 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1753	1091	311	345	6			
1	B	214	Total	C	N	O	S	0	0	0
			1649	1029	290	324	6			
1	G	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	H	215	Total	C	N	O	S	0	0	0
			1659	1037	291	325	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1339	Total	C	N	O	S	0	0	0
			10548	6620	1834	2050	44			
2	I	1328	Total	C	N	O	S	0	0	0
			10486	6583	1822	2038	43			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	531	LEU	SER	conflict	UNP P0A8V2
I	531	LEU	SER	conflict	UNP P0A8V2

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1166	Total	C	N	O	S	0	0	0
			9089	5714	1627	1702	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9001	5659	1612	1684	46			

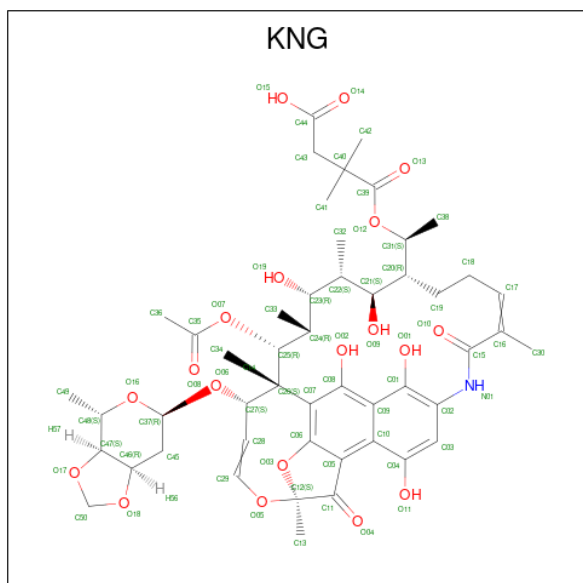
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	468	Total	C	N	O	S	0	0	0
			3813	2389	678	723	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

- Molecule 6 is Kanglemycin A (CCD ID: KNG) (formula: $C_{50}H_{67}NO_{19}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	H	N	O	0	0
			132	50	62	1	19		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Mg	0	0
			1	1		
7	J	1	Total	Mg	0	0
			1	1		

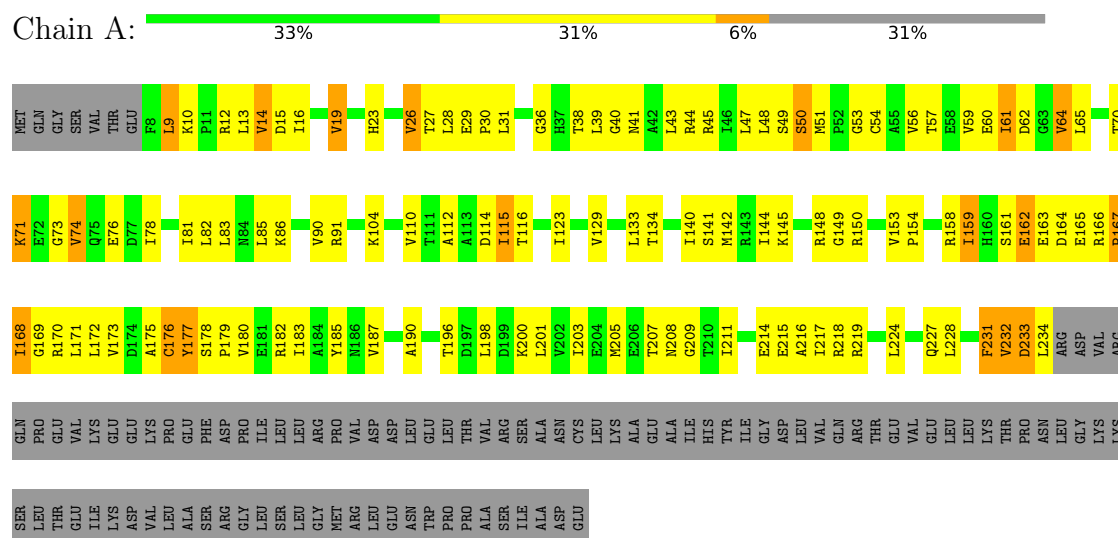
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total 2	Zn 2	0	0
8	J	2	Total 2	Zn 2	0	0

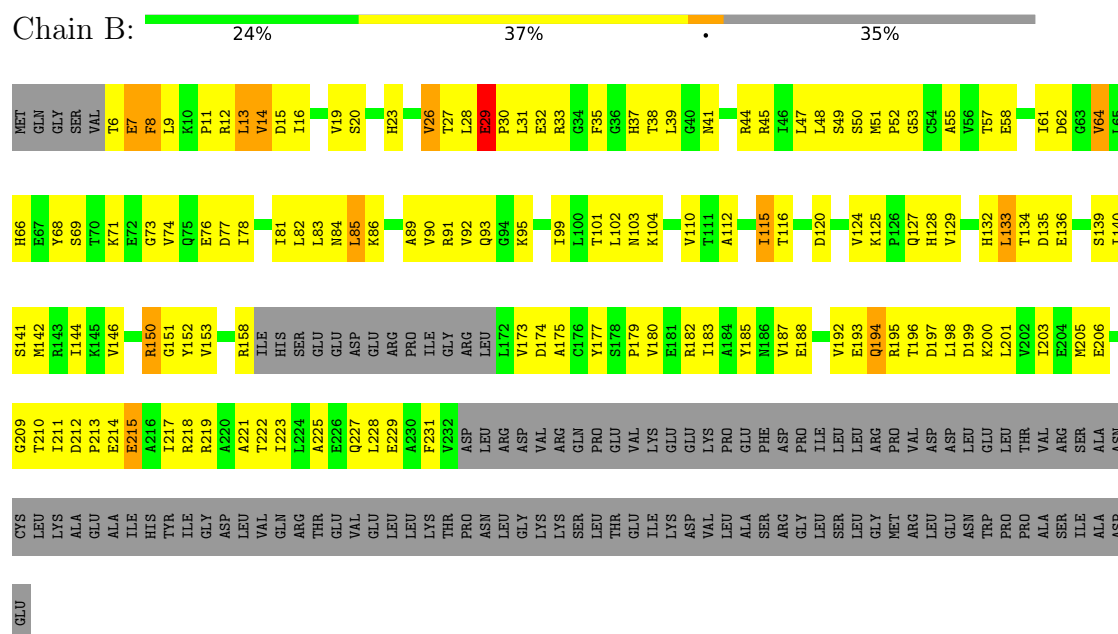
3 Residue-property plots

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

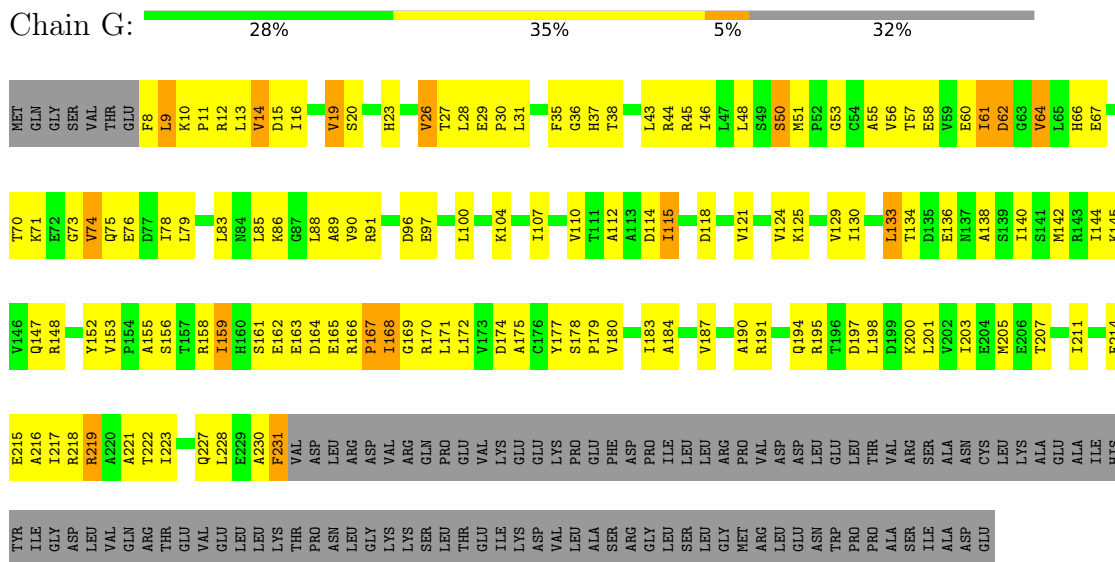
• Molecule 1: DNA-directed RNA polymerase subunit alpha



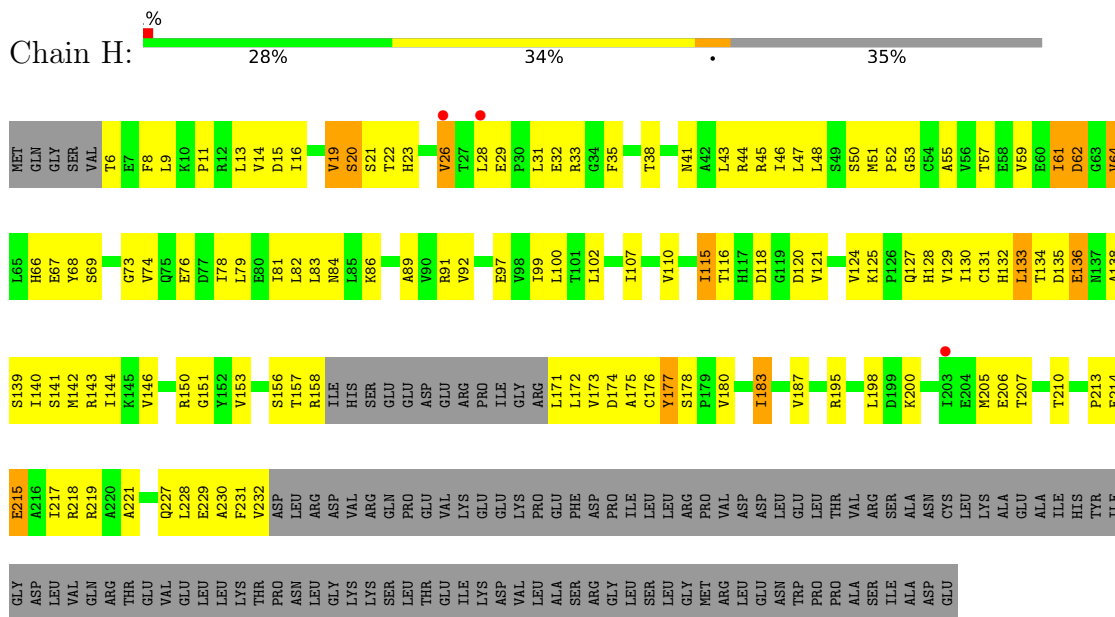
• Molecule 1: DNA-directed RNA polymerase subunit alpha



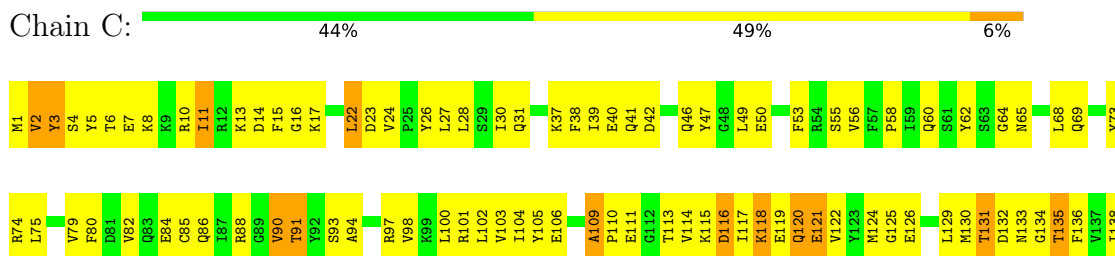
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 2: DNA-directed RNA polymerase subunit beta

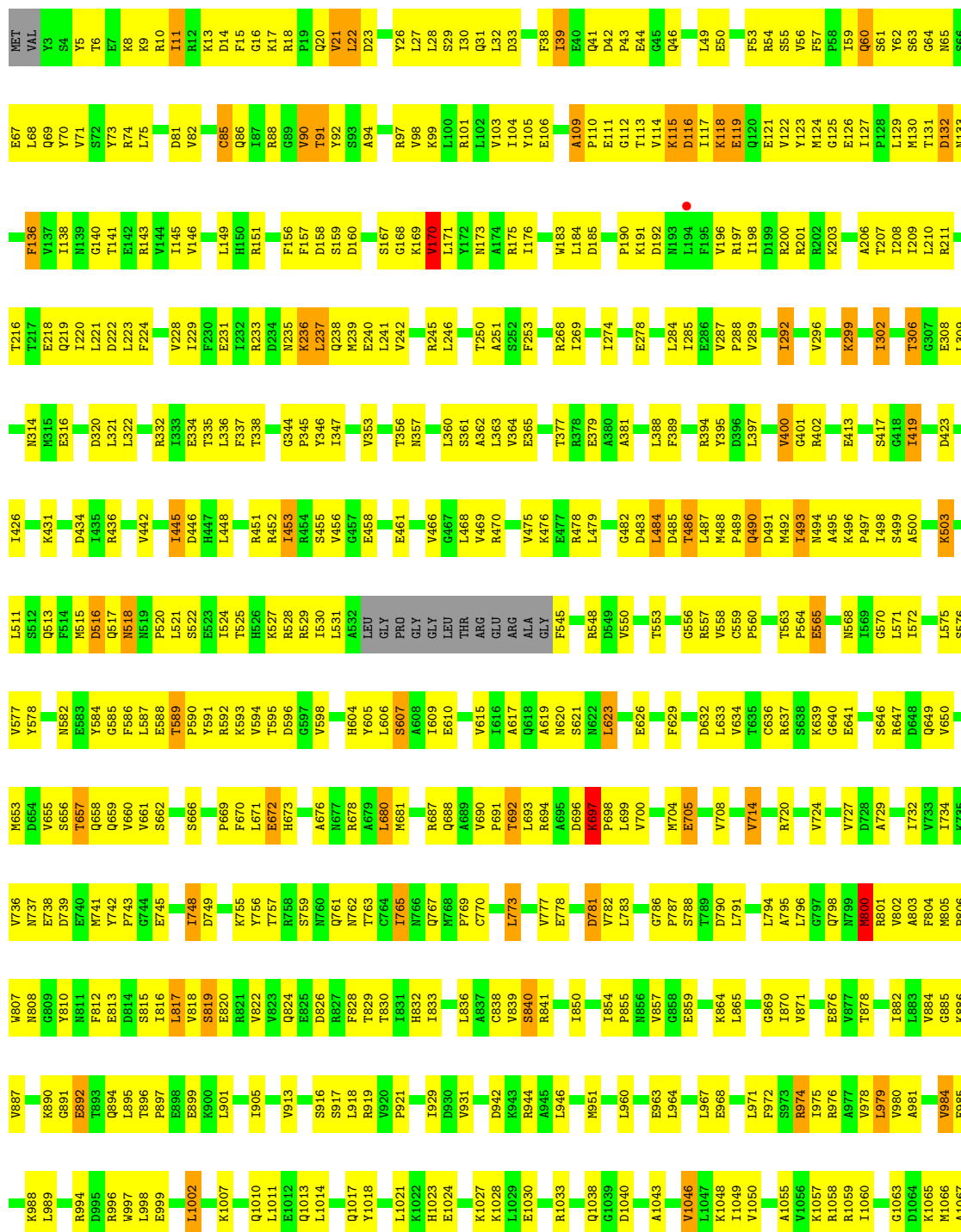


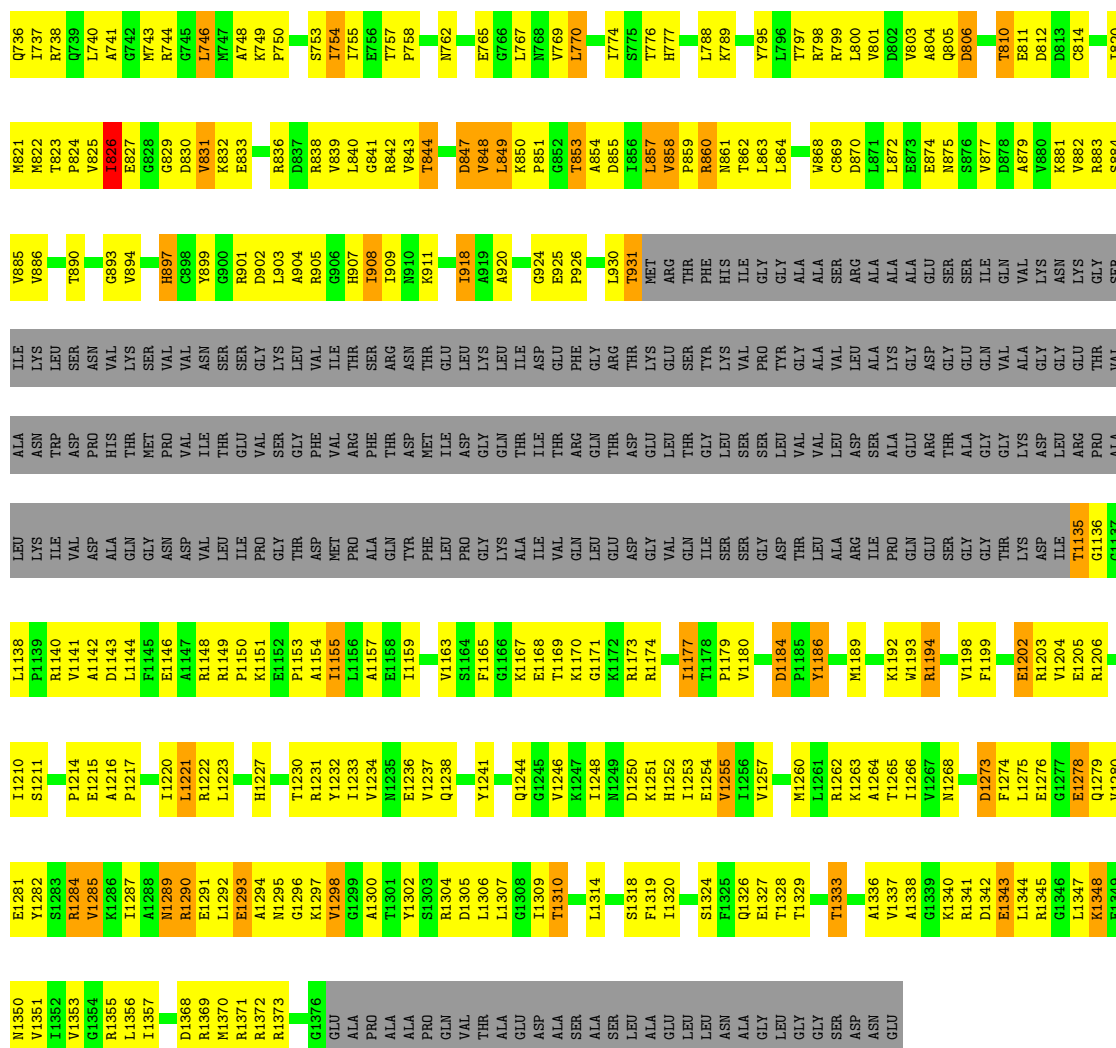
G1218	D1154	I1079	E985	V823	K755	M681	S607	ARG	R485	K369	K299	D222	N139
E1219	V1155	N1080	A986	V826	T756	M684	A608	GLU	V466	M370	D300	L223	G140
E1222	Q1157	P1081	E987	D826	T757	M685	E610	ARG	G467	E374	Y301	F224	I145
R1223	E1082	I1082	K988	R827				A643	L468	E374	I302	F225	V146
P1224	K1158	E1083	K988	E827				G544	V469	P376	D303	E226	S147
V1225	V1159	D1084	K991	H832	Q761	Q688	Y614	F545	R470	R377	T306	K227	Q148
T1226	D1160	M1085	L992	L836	T762	A689	V615		V471	R378	G307	V228	L149
V1227	P1086	P1086	L1002	A837	G764	V690	A617	R548	E472	E379	E308	I229	H150
G1228	D1088	C838	K989	E837	T765	P691	A617	D549	E477	E379	L309	F230	R151
V1229	F1164	E1089	K1007	V839	N766	T692	Q618	V550	E478	E382	I310	E231	
M1230	S1165	Q1008	Q1008	R694	Q767	L693	A619	H551	R477		C311	I232	S152
Y1231		Y1013	Q1008	M768	M768		M620	P552	L479	F365	A312	R233	P153
M1232	V1169	Y913	L1011			A695		T553	S480				
L1233	T843	D696	L1011	L823	L773	D696			L481	F390	A313	K236	F156
K1234	S917	R697	L1014	F629	G774	R697	F629	G556	D482	F390	A313	K236	F157
L1235	R844	P698	L1014	V630	E775	P698	V630	R557	D483	M315	M315	Q238	D158
N1236	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	Q238	S159
N1237	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	D160
H1237	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	K161
L1238	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	G162
V1239	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	K163
D1240	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	S167
D1241	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	K168
K1242	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	K169
													K170
R1246	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	L171
S1247	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	R175
T1248	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	I176
G1249	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	I177
Y1253	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	Y262
V1254	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	V263
T1255	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	D185
Q1256	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	F188
L1259	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	D192
K1262	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	N193
A1263	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	L194
Q1264	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	F195
F1265	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	V196
G1266	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	R197
G1267	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	I198
Q1268	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	
R1269	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	
F1270	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	
G1271	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	
E1272	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	
E1273	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	
M1273	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	
E1274	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	
V1275	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	
W1276	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	
E1279	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	
A1280	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	
Y1281	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	
G1282	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	
Y1285	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	
T1286	R844	P698	L1014	E631	E775	P698	E631	V558	L484	D393	E316	E240	



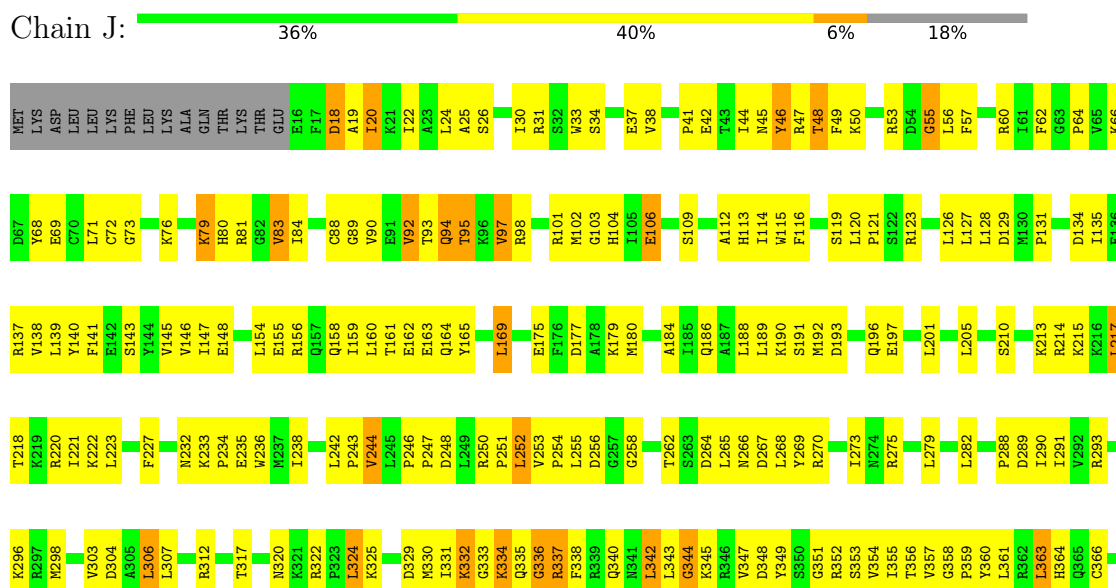
● Molecule 2: DNA-directed RNA polymerase subunit beta

Chain I: 47% 46% 6% .





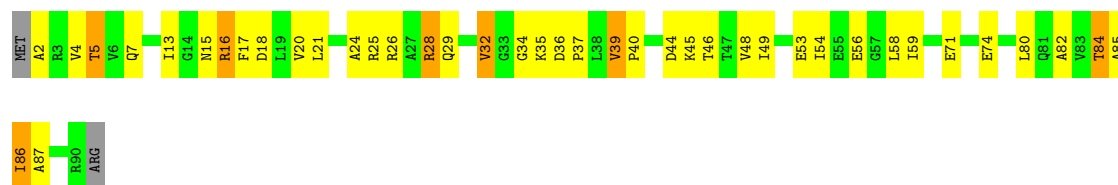
• Molecule 3: DNA-directed RNA polymerase subunit beta'



P369	C454	V526	R610	A688	T757	K832	G906	SER	ILE	P153	H1227	E1293	M1370
M372	D460	L527	I611	D691	P758	E833	H907	GLY	PRO	A1153	H1228	A1294	R1371
A373	F461	T528	G612	S693	N762	V839	T909	LEU	THR	I1155	V1229	M1296	R1372
L374	D462	K531	L614	S694	E765	V843	E913	VAL	ASP	A1156	Y1232	K1297	R1373
E375	G463	E532	K615	G695	G766	T844	A914	THR	ILE	A1157	I1233	V1298	A1374
P379	D464	R535	P616	K696	L767	A845	A915	ARG	ALA	E1158	V1234	R1304	A1375
P379	Q465	L536	F620	A697	S768	E846	G916	THR	THR	V1163	N1235	D1305	GLY
Y382	Q466	L536	F620	M697	P769	D847	G917	ASP	THR	S1164	E1236	L1306	ALA
K384	V468	G540	Q623	D698	L770	V848	P917	MET	THR	F1165	V1237	L1307	PRO
R388	P471	L541	T627	N700	Q771	L849	A919	ILE	LEU	G1166	Q1238	G1308	ALA
I394	L472	A542	G628	L701	F773	K850	A920	ASP	PRO	K1167	D1239	T1309	ALA
K395	L473	S543	P629	Q702	I774	T853	Q921	GLY	GLY	E1168	V1240	T1310	PRO
K399	L474	L544	A630	T703		A854	S922	LEU	LYS	T1169	Y1241	K1311	GLN
M400	L475	H545	A630	E704			G924	THR	ILE	K1170	R1242	A1312	VAL
V401	E475	A546	A633	T705	H777	L857	E925	ASP	ILE	G1171	V1246	S1313	THR
E405	A481	R547	T641	Q712		V858	E925	PHE	VAL	R1174	K1247	A1315	ALA
V408	L482	V548	R634	T707	R730	P859	P926	GLY	GLN	L1175	I1248		ASP
E414	M485	T567	M644	K715	N792	E866	L930	THR	ARG	V1176		S1318	ALA
V415	A486	S568	V645	Q716		E867	NE1	ASP	THR	I1177	K1251	S1324	SER
I416	T487	L569	I646	T717	T797	K868	T931	GLY	VAL	D1181	I1252	F1325	ALA
R417	N488	K570	P647	S718	R798	E888	NE1	THR	THR	G1182	I1253	L1326	SER
E418	N489	T571	K650	T719	R799	K869	ARG	GLY	THR	S1183	E1254	Q1326	LEU
H419	I490	T572		N720	L800	D870	THR	THR	THR	D1184	V1255	E1327	ALA
P420	L491	T573	I653	S721	R801	L871	ALA	ALA	ALA	P1191	I1261	T1328	GLU
L422	S492	V574	I654	T722	R802	E873	ALA	VAL	VAL	K1192	R1262	T1329	LEU
L423	A494	G575	P654	M724	V803	E874	ALA	ARG	ARG	W1193	K1263	L1330	LEU
M424	A494	R576	A657	M725	A804	N875	ALA	ALA	PRO	R1194	A1264	V1331	LEU
R425	P498	L579	E658	S728	Q805	S876	ALA	GLY	GLN	M1197	T1265	L1332	ALA
A426	I499		E659		D806	V877	GLU	ASP	GLU	V1198	I1266	T1333	ALA
P427	V500		E660		L807	D878	GLU	THR	THR	F1199	V1267		GLY
T428	V501		V661		V808	A879	SER	GLY	SER	E1200	N1268	A1336	GLY
L429	P502		A662		V809	V880	ILE	GLN	GLY	G1201	E1269	E1343	GLY
H430			E663		T810	K881	GLN	VAL	THR	R1203	D1273		SER
R431	D505	L587	I664		E811	V882	VAL	ALA	LYS	V1204	L1275	G1339	ASN
E438	V506	P588		R738		K883	LYS	ASP	ASP	E1205	E1276	K1340	ASN
P439	V507	Y589	G671	Q739	C814	S894	ASN	GLY	ILE	R1206	E1277	R1341	ASN
V440	L510	S590	L672	L740	T816	V885	LYS	GLU	THR	G1207	Q1279	D1342	ASN
L441	Y511	V592	T674	G742	M743	T890	ALA	VAL	THR	D1208	V1280	L1344	GLU
I442	Y512	N593	T674	R744	M821	T890	ILE	ALA	GLY	V1209	E1281	G1346	GLY
E443	M513	A596	E677	G745	M822	G893	LYS	ASN	ASP	S1211	Y1282	L1347	ASP
G444	T514	L596	R678	L746	T823	V894	LEU	TRP	ILE	E1215		K1355	ASP
A446	G517	K598	Y679	M747	P824	H897	SER	THR	VAL	A1142	S1283	L1356	ASN
I447	V518		N680	A748	V825		VAL	HIS	ASP	D1143	V1284	P1358	ASN
H450	A520	I601	K681	K749	V825		VAL	THR	GLY	L1144	K1286	G1360	ASN
P451	K521		V682	P750	E827	R901	SER	MET	GLY	P1217		T1361	ASN
L452			I683		G828	D902	VAL	VAL	ASN	D1219	N1289	G1362	ASN
V453	M525		D684	I754	G829	L903	VAL	VAL	ASP	A1147	R1290	Y1363	ASN
			I685	E756	V831	A904	ASN	ILE	THR	L1221	E1291		ASN
						R905	SER	THR	THR	R1222	L1292	H1366	ASN

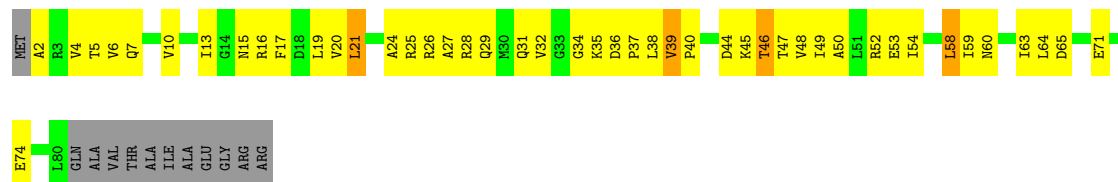
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:  53% 37% 8%



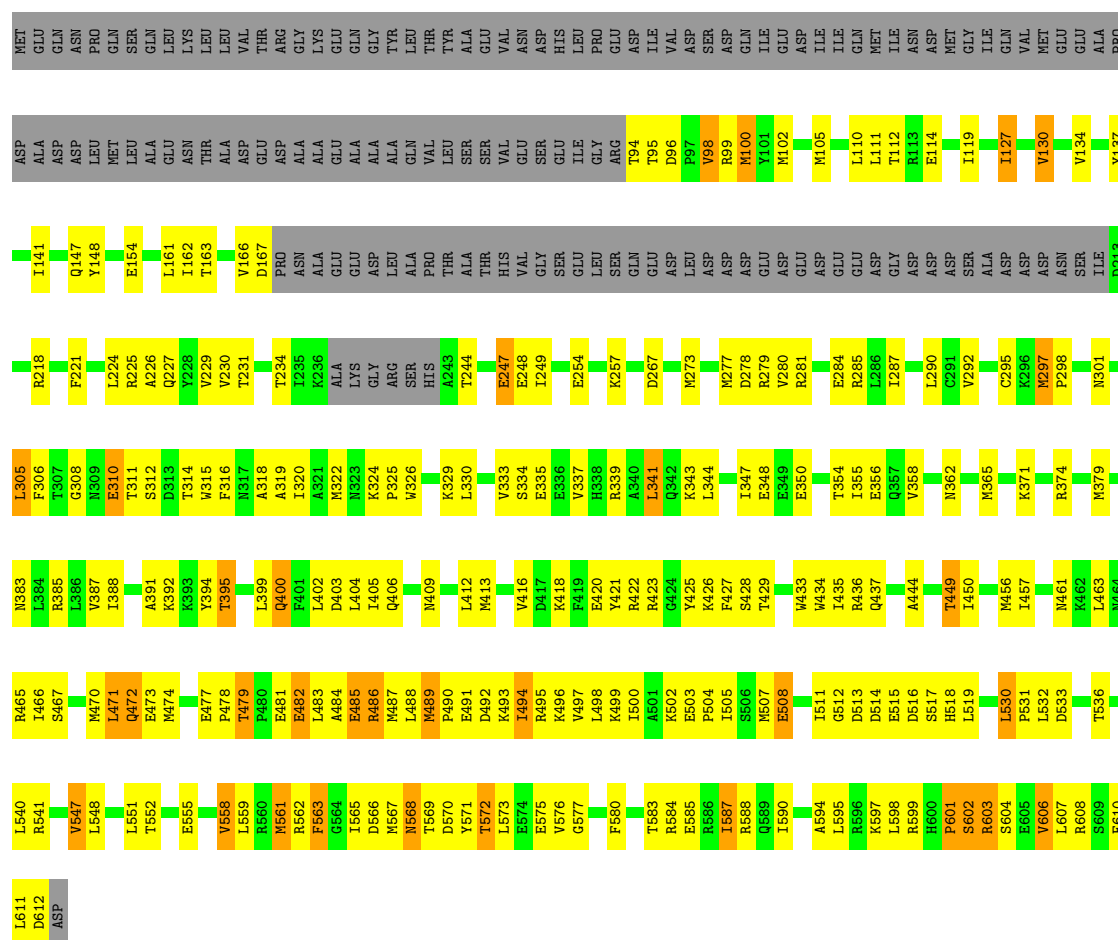
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K: 36% 46% 13%

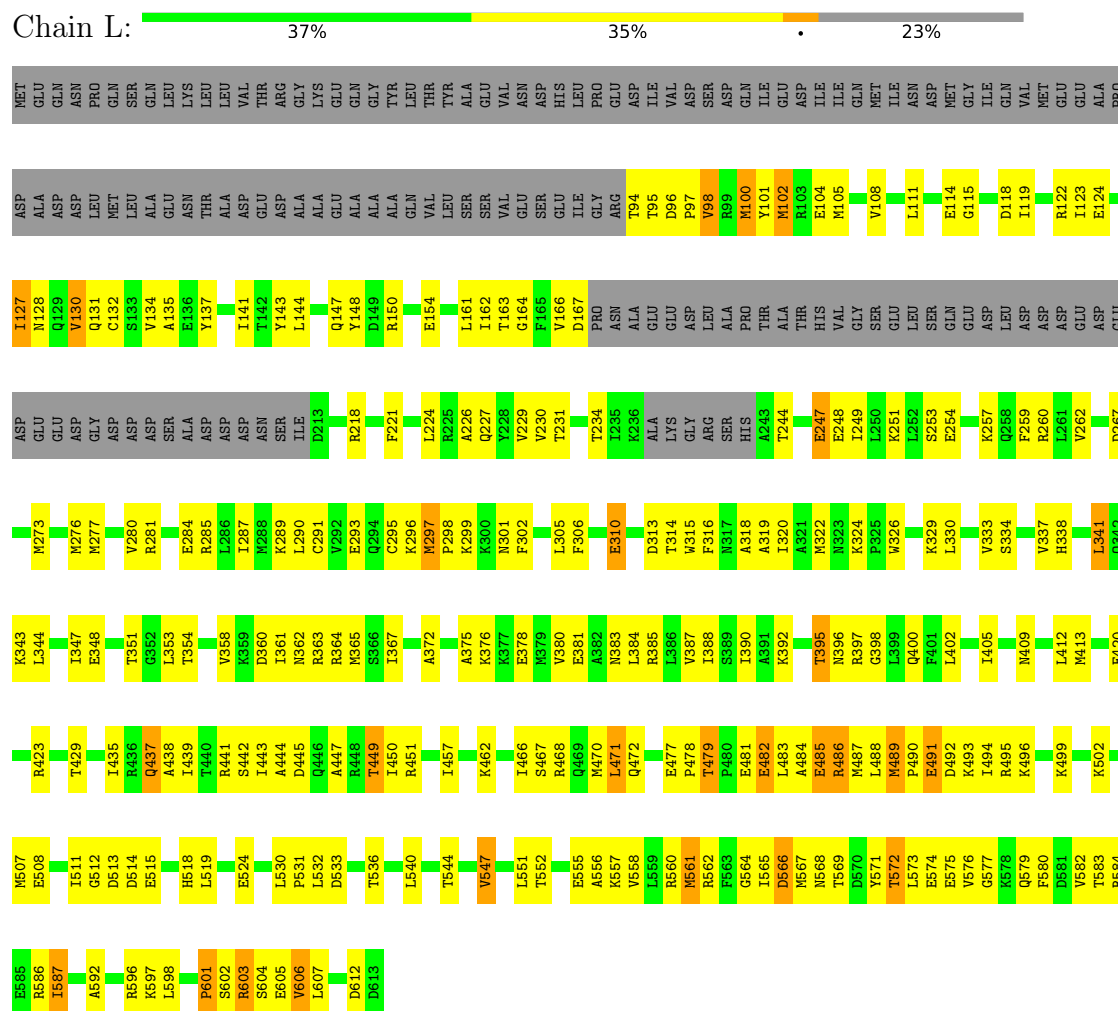


- Molecule 5: RNA polymerase sigma factor RpoD

Chain F: 38% 33% 5% 24%



- Molecule 5: RNA polymerase sigma factor RpoD



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	188.17Å 204.69Å 311.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.03 – 4.10 45.03 – 4.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (45.03-4.10) 98.9 (45.03-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 4.13Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.210 , 0.255 0.212 , 0.255	Depositor DCC
R_{free} test set	2002 reflections (2.12%)	wwPDB-VP
Wilson B-factor (Å ²)	190.5	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 206.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	55005	wwPDB-VP
Average B, all atoms (Å ²)	241.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.64	0/1774	1.11	3/2405 (0.1%)
1	B	0.63	0/1668	1.18	2/2260 (0.1%)
1	G	0.44	0/1751	0.85	0/2373
1	H	0.45	0/1678	0.90	0/2274
2	C	0.65	0/10716	1.07	15/14458 (0.1%)
2	I	0.53	0/10653	0.93	6/14373 (0.0%)
3	D	0.70	1/9229 (0.0%)	1.17	11/12459 (0.1%)
3	J	0.58	0/9140	1.03	10/12341 (0.1%)
4	E	0.63	0/693	0.94	0/935
4	K	0.26	0/629	0.54	0/847
5	F	0.49	0/3864	0.89	5/5194 (0.1%)
5	L	0.45	0/3872	0.83	1/5205 (0.0%)
All	All	0.59	1/55667 (0.0%)	1.02	53/75124 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	C	0	2
2	I	0	2
3	D	0	2
3	J	0	2
4	E	0	1
5	F	0	1
5	L	0	1
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	426	ALA	C-N	-5.45	1.21	1.33

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	42	GLU	CA-CB-CG	7.93	129.96	114.10
5	F	563	PHE	CA-C-N	-7.82	106.09	121.41
5	F	563	PHE	C-N-CA	-7.82	106.09	121.41
1	A	177	TYR	CA-CB-CG	7.31	127.06	113.90
3	D	344	GLY	CA-C-N	6.46	133.88	121.54
3	D	344	GLY	C-N-CA	6.46	133.88	121.54
1	A	177	TYR	CB-CA-C	-6.31	101.29	110.06
2	C	1151	LEU	CA-CB-CG	-6.27	94.34	116.30
5	L	602	SER	N-CA-C	-6.06	97.89	110.80
3	D	503	SER	N-CA-C	5.99	123.56	110.80
2	C	1233	LEU	CA-CB-CG	5.91	137.00	116.30
2	I	697	LYS	N-CA-C	-5.88	96.81	109.81
2	I	516	ASP	N-CA-C	-5.82	97.75	107.99
2	C	1291	LEU	CA-CB-CG	5.81	136.63	116.30
3	D	1348	LYS	CA-CB-CG	5.76	125.63	114.10
3	J	42	GLU	N-CA-CB	5.71	118.44	109.83
2	I	1235	LEU	CA-C-N	-5.64	114.42	122.77
2	I	1235	LEU	C-N-CA	-5.64	114.42	122.77
2	C	1241	ASP	N-CA-C	-5.63	98.82	110.80
3	D	460	ASP	CB-CA-C	-5.62	98.76	110.40
5	F	565	ILE	CA-C-N	5.59	132.23	121.54
5	F	565	ILE	C-N-CA	5.59	132.23	121.54
3	D	331	ILE	CA-C-N	5.58	132.21	121.54
3	D	331	ILE	C-N-CA	5.58	132.21	121.54
2	C	1058	ARG	CA-C-N	-5.55	110.94	121.54
2	C	1058	ARG	C-N-CA	-5.55	110.94	121.54
2	C	1106	ARG	CA-C-N	-5.53	113.49	122.34
2	C	1106	ARG	C-N-CA	-5.53	113.49	122.34
2	C	1179	GLY	N-CA-C	-5.51	100.11	113.18
3	J	55	GLY	N-CA-C	-5.51	100.39	110.97
3	D	426	ALA	N-CA-C	5.48	119.62	112.17
5	F	602	SER	N-CA-C	-5.48	99.14	110.80
1	B	150	ARG	CB-CG-CD	5.43	123.78	111.30
2	C	529	ARG	CG-CD-NE	-5.41	100.11	112.00
2	C	1259	LEU	CA-CB-CG	-5.37	97.50	116.30
3	D	727	ASP	N-CA-C	-5.34	105.13	111.69
2	C	1159	VAL	CA-C-N	5.33	131.72	121.54
2	C	1159	VAL	C-N-CA	5.33	131.72	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	CYS	CB-CA-C	5.33	119.73	110.94
2	I	136	PHE	N-CA-C	-5.32	101.22	109.72
3	D	1168	GLU	CA-CB-CG	5.29	124.68	114.10
3	J	811	GLU	CA-C-N	-5.29	114.36	121.71
3	J	811	GLU	C-N-CA	-5.29	114.36	121.71
2	C	1076	ILE	CB-CA-C	5.28	119.92	111.69
1	B	85	LEU	CA-CB-CG	-5.25	97.93	116.30
2	I	800	MET	CB-CG-SD	-5.20	97.10	112.70
2	C	135	THR	N-CA-C	-5.14	101.73	109.85
3	D	1290	ARG	CB-CG-CD	-5.13	99.49	111.30
3	J	472	LEU	CA-CB-CG	5.11	134.17	116.30
3	J	48	THR	CA-C-N	-5.09	112.12	122.31
3	J	48	THR	C-N-CA	-5.09	112.12	122.31
3	J	789	LYS	CB-CG-CD	5.04	122.89	111.30
3	J	789	LYS	CA-CB-CG	-5.02	104.06	114.10

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	29	GLU	Peptide
2	C	109	ALA	Peptide
2	C	236	LYS	Peptide
3	D	1184	ASP	Peptide
3	D	1296	GLY	Peptide
4	E	32	VAL	Peptide
5	F	601	PRO	Peptide
2	I	109	ALA	Peptide
2	I	236	LYS	Peptide
3	J	1184	ASP	Peptide
3	J	1296	GLY	Peptide
5	L	601	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1780	158	0
1	B	1649	0	1674	187	0
1	G	1730	0	1756	196	0
1	H	1659	0	1692	176	0
2	C	10548	0	10553	876	0
2	I	10486	0	10496	764	0
3	D	9089	0	9265	796	0
3	J	9001	0	9169	779	0
4	E	691	0	695	40	0
4	K	627	0	634	62	0
5	F	3813	0	3880	275	0
5	L	3821	0	3884	263	0
6	C	70	62	0	10	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	0	0
8	J	2	0	0	2	0
All	All	54943	62	55478	4146	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 38.

All (4146) 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:C:65:ASN:HB3	2:C:105:TYR:HB2	1.21	1.21
2:C:1271:GLY:HA2	3:D:343:LEU:HD11	1.22	1.16
2:I:942:ASP:OD2	2:I:1048:LYS:NZ	1.78	1.16
1:B:183:ILE:HD11	1:B:205:MET:HG3	1.21	1.15
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.30	1.14
1:H:83:LEU:HD11	3:J:526:VAL:HG23	1.28	1.14
1:H:79:LEU:HD11	3:J:526:VAL:HG21	1.24	1.13
5:F:490:PRO:HG2	5:F:493:LYS:HE3	1.31	1.13
1:G:45:ARG:HG2	1:H:38:THR:HB	1.17	1.12
3:D:1280:VAL:HG11	3:D:1304:ARG:HH21	1.16	1.11
3:D:342:LEU:HA	3:D:343:LEU:HD13	1.20	1.11
5:F:484:ALA:HB1	5:F:491:GLU:HB2	1.32	1.10
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.10	1.10
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.14	1.10
2:C:1271:GLY:CA	3:D:343:LEU:HD11	1.80	1.09
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.11	1.09
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.31	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:342:LEU:HA	3:D:343:LEU:CD1	1.84	1.08
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.36	1.07
1:B:23:HIS:HB2	1:B:205:MET:O	1.51	1.07
3:D:1289:ASN:OD1	3:D:1290:ARG:NH1	1.86	1.07
2:C:1080:ASN:HB3	2:C:1085:MET:HE3	1.35	1.06
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.15	1.06
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.33	1.06
1:G:118:ASP:HB3	1:G:121:VAL:HG23	1.36	1.06
2:C:1131:MET:HE2	2:C:1141:LEU:CD1	1.86	1.05
2:C:1289:GLU:OE2	3:D:473:THR:HG22	1.57	1.05
2:C:1291:LEU:HD21	3:D:1351:VAL:HG13	1.33	1.05
2:C:1131:MET:CE	2:C:1141:LEU:HD12	1.85	1.05
5:L:105:MET:HE1	5:L:385:ARG:HG2	1.34	1.05
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.37	1.05
1:B:35:PHE:HA	1:B:38:THR:HG22	1.39	1.04
2:C:109:ALA:HB1	2:C:110:PRO:C	1.82	1.04
3:D:848:VAL:HG23	3:D:858:VAL:HG13	1.39	1.04
2:I:98:VAL:HG21	2:I:124:MET:HE3	1.36	1.04
2:I:125:GLY:HA2	2:I:499:SER:HB2	1.34	1.04
1:G:70:THR:HG21	2:I:755:LYS:HE2	1.36	1.03
5:L:561:MET:HA	5:L:567:MET:HE1	1.39	1.03
2:I:1234:LYS:HE2	2:I:1238:LEU:HD23	1.40	1.02
5:L:470:MET:CE	5:L:478:PRO:HB3	1.89	1.02
1:H:57:THR:HG21	1:H:158:ARG:HE	1.22	1.02
2:I:1289:GLU:OE2	3:J:473:THR:HG22	1.58	1.02
1:B:29:GLU:HB3	1:B:30:PRO:HD3	1.37	1.02
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.41	1.02
3:J:384:LYS:NZ	3:J:414:GLU:OE1	1.93	1.02
3:J:863:LEU:HD11	3:J:901:ARG:HB3	1.39	1.02
3:D:1227:HIS:HB2	3:J:1293:GLU:HG2	1.41	1.02
3:D:697:MET:HE1	3:D:737:ILE:HG22	1.42	1.01
5:F:280:VAL:HG22	5:F:347:ILE:HD13	1.38	1.01
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.43	1.01
2:C:1304:MET:HE3	3:D:472:LEU:HD12	1.42	1.01
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.43	1.01
2:I:1291:LEU:HD21	3:J:1351:VAL:HG13	1.42	1.01
2:I:109:ALA:HB1	2:I:110:PRO:C	1.85	1.00
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.40	1.00
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.43	1.00
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	1.77	1.00
1:G:48:LEU:HA	1:G:180:VAL:HG21	1.43	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.41	0.99
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.38	0.99
5:F:492:ASP:HB2	5:F:495:ARG:HH12	1.24	0.99
1:G:45:ARG:HG2	1:H:38:THR:CB	1.92	0.99
2:C:1269:ARG:HD3	3:D:343:LEU:HB3	1.43	0.99
1:G:66:HIS:HA	1:G:171:LEU:HD11	1.40	0.99
2:I:1240:ASP:HB3	3:J:445:LYS:HD2	1.42	0.99
5:L:231:THR:HG23	5:L:249:ILE:HG12	1.43	0.98
3:J:363:LEU:HD23	3:J:487:THR:HG22	1.42	0.98
1:H:83:LEU:HD11	3:J:526:VAL:CG2	1.94	0.98
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.46	0.98
2:I:972:PHE:CE2	2:I:998:LEU:HD11	1.99	0.97
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.44	0.97
2:I:1293:VAL:HG11	2:I:1304:MET:HE2	1.46	0.97
2:C:490:GLN:HG3	5:F:472:GLN:HE21	1.29	0.97
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	1.80	0.97
3:J:186:GLN:HG3	3:J:238:ILE:HB	1.46	0.97
3:J:1266:ILE:HB	3:J:1274:PHE:O	1.65	0.97
2:I:593:LYS:HE3	2:I:595:THR:HG22	1.44	0.96
1:A:13:LEU:H	1:A:13:LEU:HD23	1.31	0.96
5:F:105:MET:HE1	5:F:385:ARG:HG2	1.46	0.96
1:H:91:ARG:NH1	1:H:210:THR:O	1.97	0.96
2:I:1131:MET:HE2	2:I:1141:LEU:HD12	1.45	0.96
3:D:1290:ARG:HG2	3:D:1298:VAL:HG12	1.47	0.96
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.45	0.96
2:C:17:LYS:HE3	2:C:1154:ASP:HB3	1.47	0.95
1:H:23:HIS:HB2	1:H:205:MET:O	1.66	0.95
1:B:29:GLU:OE1	1:B:200:LYS:HE2	1.64	0.95
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.48	0.95
2:C:529:ARG:HH12	6:C:2001:KNG:C18	1.80	0.95
1:A:45:ARG:HG2	1:B:38:THR:HB	1.47	0.95
5:L:492:ASP:HB2	5:L:495:ARG:HH12	1.28	0.95
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.48	0.95
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.48	0.95
2:I:929:ILE:HD13	2:I:1055:ALA:HB2	1.46	0.95
2:I:1080:ASN:HB3	2:I:1085:MET:HE3	1.45	0.95
3:J:526:VAL:HG12	3:J:549:LYS:HB2	1.46	0.94
2:C:593:LYS:HE3	2:C:595:THR:HG22	1.48	0.94
2:C:519:ASN:HB3	2:C:522:SER:HB2	1.46	0.94
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.49	0.94
5:L:280:VAL:HG22	5:L:347:ILE:HD13	1.47	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:23:HIS:HB2	1:G:205:MET:O	1.66	0.94
1:A:211:ILE:HG21	1:A:216:ALA:HB2	1.48	0.94
2:C:1297:ASP:OD1	2:C:1300:GLY:N	2.01	0.94
1:H:62:ASP:HB2	1:H:141:SER:O	1.67	0.94
2:C:510:GLN:HA	6:C:2001:KNG:C49	1.98	0.93
3:D:576:ARG:NH1	3:D:593:ASN:O	2.02	0.93
5:F:484:ALA:HB1	5:F:491:GLU:CB	1.98	0.93
2:I:176:ILE:HD12	2:I:184:LEU:HD23	1.50	0.93
3:D:18:ASP:HB2	3:D:1373:ARG:NH2	1.83	0.93
3:D:1149:ARG:CZ	3:D:1153:PRO:HG2	1.97	0.93
1:H:55:ALA:O	1:H:146:VAL:HG13	1.68	0.93
2:C:145:ILE:CG2	2:C:456:VAL:HG22	1.99	0.93
2:C:1248:THR:HG21	5:F:531:PRO:CG	1.98	0.93
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.51	0.93
2:I:125:GLY:CA	2:I:499:SER:HB2	1.99	0.93
2:C:745:GLU:CG	2:C:1017:GLN:HB3	1.99	0.93
2:C:818:VAL:CG2	2:C:1076:ILE:HD13	1.98	0.93
2:C:1271:GLY:HA2	3:D:343:LEU:CD1	1.98	0.93
2:C:151:ARG:NE	2:C:445:ILE:HD11	1.84	0.92
2:I:732:ILE:HD11	2:I:769:PRO:HB3	1.50	0.92
3:J:517:CYS:HA	3:J:716:GLN:HE22	1.33	0.92
3:J:693:VAL:HG21	3:J:743:MET:HE3	1.49	0.92
3:D:1280:VAL:HG21	3:D:1304:ARG:NE	1.83	0.92
2:I:8:LYS:HE3	2:I:1171:ARG:NH2	1.85	0.92
5:L:281:ARG:HG2	5:L:285:ARG:HD2	1.49	0.92
2:I:98:VAL:CG2	2:I:124:MET:HE3	1.99	0.92
3:D:1273:ASP:HB3	3:D:1276:GLU:HG3	1.52	0.91
3:D:460:ASP:HB2	3:D:464:ASP:OD2	1.71	0.91
3:J:45:ASN:HB3	3:J:48:THR:O	1.71	0.91
2:I:1158:LYS:O	2:I:1159:VAL:HG13	1.70	0.91
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.52	0.91
1:A:23:HIS:HB2	1:A:205:MET:O	1.71	0.91
1:B:183:ILE:CD1	1:B:205:MET:HG3	2.01	0.91
5:F:297:MET:HE3	5:F:330:LEU:HD21	1.52	0.91
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.52	0.91
3:J:507:VAL:HG11	3:J:598:LYS:HG3	1.52	0.91
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.00	0.90
3:D:536:LEU:HD13	3:D:541:LEU:HB2	1.52	0.90
3:J:186:GLN:HB2	3:J:238:ILE:HG21	1.53	0.90
3:J:418:GLU:HG3	4:K:44:ASP:HA	1.53	0.90
1:B:104:LYS:HG2	1:B:110:VAL:HG22	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:126:LEU:HD13	3:J:223:LEU:CD2	2.01	0.90
3:D:930:LEU:HD12	3:D:1138:LEU:HD13	1.53	0.90
3:D:74:LYS:NZ	3:D:86:GLU:OE1	2.05	0.90
5:F:287:ILE:HG12	5:F:337:VAL:HG13	1.50	0.90
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.52	0.89
2:C:5:TYR:HD1	2:C:8:LYS:HD3	1.38	0.89
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.54	0.89
2:I:175:ARG:HD3	2:I:183:TRP:CZ3	2.08	0.89
5:L:316:PHE:CZ	5:L:334:SER:HA	2.08	0.89
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.08	0.89
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.07	0.89
3:J:98:ARG:HB3	3:J:248:ASP:OD2	1.73	0.89
1:A:211:ILE:CG2	1:A:216:ALA:HB2	2.03	0.89
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.55	0.89
3:J:510:LEU:HD22	3:J:601:ILE:HD11	1.54	0.89
5:F:316:PHE:HZ	5:F:334:SER:HA	1.38	0.89
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.54	0.89
2:C:483:ASP:HB2	2:C:486:THR:HG21	1.51	0.89
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.38	0.89
3:J:1344:LEU:HB3	3:J:1350:ASN:HD21	1.36	0.89
2:C:818:VAL:HG23	2:C:1076:ILE:HD13	1.55	0.89
1:H:51:MET:HG3	1:H:52:PRO:HD2	1.55	0.89
2:C:657:THR:HG21	2:C:1188:ASP:HB2	1.54	0.88
3:D:115:TRP:CE2	3:D:1329:THR:HG23	2.07	0.88
5:F:561:MET:HG2	5:F:576:VAL:HG22	1.55	0.88
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.54	0.88
2:C:1248:THR:HG21	5:F:531:PRO:HG2	1.54	0.88
1:G:70:THR:CG2	2:I:755:LYS:HE2	2.02	0.88
5:L:231:THR:CG2	5:L:249:ILE:HG12	2.03	0.88
5:L:470:MET:HE3	5:L:478:PRO:HB3	1.53	0.88
1:B:53:GLY:HA3	1:B:177:TYR:O	1.73	0.88
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.03	0.88
3:D:363:LEU:HG	3:D:363:LEU:O	1.72	0.88
3:D:746:LEU:HD22	3:D:754:ILE:HD11	1.56	0.88
3:D:859:PRO:HG2	3:D:862:THR:HG21	1.55	0.88
2:I:593:LYS:HE3	2:I:595:THR:CG2	2.04	0.88
2:C:697:LYS:HA	2:C:795:ALA:HB2	1.55	0.87
3:D:336:GLY:HA3	3:D:1324:SER:O	1.74	0.87
3:D:56:LEU:H	3:D:56:LEU:HD12	1.38	0.87
1:A:61:ILE:HB	1:A:64:VAL:CG2	2.03	0.87
2:I:1077:SER:HA	3:J:356:THR:OG1	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:94:GLN:O	3:J:97:VAL:HG23	1.75	0.87
2:C:302:ILE:HG22	2:C:309:LEU:CA	2.04	0.87
2:C:296:VAL:HB	2:C:336:LEU:HD12	1.54	0.87
2:C:887:VAL:HB	2:C:913:VAL:HG21	1.55	0.87
2:C:1066:MET:CE	2:C:1076:ILE:HB	2.03	0.87
5:L:551:LEU:HD11	5:L:598:LEU:HD21	1.57	0.87
2:C:157:PHE:CZ	2:C:431:LYS:HG2	2.10	0.87
2:C:1080:ASN:CB	2:C:1085:MET:HE3	2.03	0.87
3:D:857:LEU:HD23	3:D:875:ASN:ND2	1.90	0.86
1:G:12:ARG:H	1:G:30:PRO:HD2	1.39	0.86
2:I:891:GLY:O	2:I:892:GLU:HG3	1.74	0.86
3:J:510:LEU:HD22	3:J:601:ILE:CD1	2.05	0.86
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.08	0.86
2:I:819:SER:HB2	2:I:1085:MET:SD	2.14	0.86
1:A:61:ILE:HB	1:A:64:VAL:HG21	1.58	0.86
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.57	0.86
3:D:905:ARG:HH21	3:D:907:HIS:CB	1.87	0.86
3:D:799:ARG:NH1	3:D:1146:GLU:OE1	2.09	0.86
1:B:86:LYS:NZ	1:B:174:ASP:OD2	2.08	0.86
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.57	0.86
3:J:1280:VAL:CG2	3:J:1304:ARG:HE	1.89	0.86
1:H:110:VAL:HG21	1:H:140:ILE:HD11	1.58	0.86
2:C:145:ILE:CB	2:C:456:VAL:HG22	2.05	0.86
2:C:483:ASP:HB2	2:C:486:THR:CG2	2.05	0.86
3:J:1157:ALA:HB2	3:J:1210:ILE:HD11	1.56	0.86
2:C:490:GLN:HG3	5:F:472:GLN:NE2	1.91	0.86
3:J:722:ILE:HD11	3:J:740:LEU:HD23	1.58	0.85
5:F:343:LYS:H	5:F:343:LYS:HD2	1.40	0.85
1:A:233:ASP:C	1:A:234:LEU:HD22	2.00	0.85
3:D:1135:THR:OG1	3:D:1136:GLY:N	2.04	0.85
2:I:30:ILE:HD12	2:I:30:ILE:H	1.39	0.85
3:D:97:VAL:HG11	3:D:101:ARG:CZ	2.06	0.85
3:D:1203:ARG:HH22	3:D:1205:GLU:HG2	1.41	0.85
2:I:887:VAL:HB	2:I:913:VAL:HG21	1.58	0.85
2:I:963:GLU:O	2:I:967:LEU:HB2	1.77	0.85
5:L:470:MET:SD	5:L:486:ARG:NH1	2.49	0.85
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.58	0.85
1:H:53:GLY:HA3	1:H:177:TYR:O	1.76	0.85
3:D:140:TYR:HE2	5:F:95:THR:HG22	1.41	0.85
1:G:51:MET:HE1	1:G:216:ALA:HA	1.57	0.85
2:I:887:VAL:HB	2:I:913:VAL:CG2	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:LYS:HE2	1:B:128:HIS:CD2	2.11	0.85
2:C:698:PRO:HG3	2:C:1231:TYR:CE2	2.11	0.85
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.57	0.85
3:J:653:ILE:HD13	3:J:692:ARG:HB3	1.57	0.85
5:L:470:MET:HE2	5:L:478:PRO:HB3	1.58	0.85
2:C:593:LYS:HB3	2:C:602:GLU:HG3	1.58	0.85
5:F:540:LEU:HD12	5:F:610:PHE:CD1	2.11	0.85
2:I:223:LEU:HD13	2:I:426:ILE:HD13	1.59	0.84
1:G:83:LEU:HD23	2:I:694:ARG:NH2	1.92	0.84
5:L:119:ILE:HG23	5:L:375:ALA:HB1	1.58	0.84
5:L:148:TYR:OH	5:L:218:ARG:HA	1.77	0.84
3:D:700:ASN:O	3:D:704:GLU:HB2	1.77	0.84
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.24	0.84
2:C:1129:ASN:OD1	2:C:1177:ARG:NH2	2.11	0.84
3:J:1290:ARG:HG2	3:J:1298:VAL:HG12	1.58	0.84
5:L:316:PHE:HZ	5:L:334:SER:HA	1.40	0.84
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.57	0.84
3:J:425:ARG:NH1	3:J:464:ASP:OD1	2.11	0.84
2:C:890:LYS:HE2	2:C:891:GLY:H	1.41	0.84
3:J:1167:LYS:HD3	3:J:1174:ARG:HD2	1.60	0.84
2:C:1304:MET:HE3	3:D:472:LEU:CD1	2.07	0.84
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.13	0.84
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.13	0.84
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.13	0.84
3:D:905:ARG:HH21	3:D:907:HIS:HB2	1.41	0.84
1:G:231:PHE:HB3	1:H:218:ARG:HH11	1.42	0.84
2:C:120:GLN:HG3	2:C:121:GLU:HG3	1.59	0.83
1:H:29:GLU:OE2	1:H:200:LYS:HE3	1.77	0.83
2:C:2:VAL:O	2:C:3:TYR:HB2	1.79	0.83
2:C:561:ILE:HD11	2:C:665:ALA:HB1	1.58	0.83
3:J:363:LEU:HG	3:J:363:LEU:O	1.77	0.83
1:B:62:ASP:HB2	1:B:141:SER:O	1.77	0.83
1:B:6:THR:HG23	1:B:6:THR:O	1.79	0.83
2:I:839:VAL:HG12	2:I:1049:ILE:HG12	1.60	0.83
2:I:1024:GLU:HG2	2:I:1028:LYS:HD3	1.60	0.83
3:J:843:VAL:HG13	3:J:883:ARG:HD3	1.59	0.83
2:I:972:PHE:HD1	2:I:994:ARG:HH21	1.21	0.83
2:C:745:GLU:HG3	2:C:1017:GLN:CB	2.06	0.83
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.61	0.83
5:L:277:MET:HE3	5:L:281:ARG:NH2	1.93	0.83
5:L:281:ARG:O	5:L:285:ARG:HG3	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:2001:KNG:O07	6:C:2001:KNG:O19	1.90	0.83
5:F:573:LEU:HD23	5:F:573:LEU:H	1.44	0.82
3:J:479:GLU:HG3	4:K:20:VAL:HG11	1.59	0.82
3:J:700:ASN:O	3:J:704:GLU:HB2	1.80	0.82
1:A:166:ARG:O	1:A:168:ILE:N	2.11	0.82
1:H:57:THR:O	1:H:173:VAL:HG22	1.79	0.82
2:I:1248:THR:HG21	5:L:531:PRO:HG3	1.61	0.82
3:D:35:PHE:HD1	3:D:101:ARG:HB3	1.45	0.82
1:G:14:VAL:HG22	1:G:15:ASP:H	1.45	0.82
3:J:1198:VAL:HB	3:J:1210:ILE:HA	1.61	0.82
1:A:228:LEU:HD22	1:B:221:ALA:HB1	1.61	0.82
1:B:11:PRO:HB2	1:B:28:LEU:HD11	1.62	0.82
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.60	0.82
3:J:1263:LYS:HE2	3:J:1279:GLN:HE21	1.43	0.82
1:A:14:VAL:HG22	1:A:15:ASP:H	1.43	0.82
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.60	0.81
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.61	0.81
2:C:453:ILE:HD12	2:C:587:LEU:HD21	1.60	0.81
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.62	0.81
3:D:140:TYR:CE2	5:F:95:THR:HG22	2.15	0.81
1:G:191:ARG:NH1	1:G:197:ASP:HA	1.95	0.81
2:I:1142:ARG:HD3	2:I:1161:LEU:CD1	2.10	0.81
2:C:133:ASN:ND2	2:C:713:GLY:HA3	1.94	0.81
3:D:1290:ARG:HD3	3:D:1294:ALA:HB1	1.63	0.81
2:C:890:LYS:HE2	2:C:891:GLY:N	1.96	0.81
3:J:1140:ARG:NH2	3:J:1236:GLU:HG2	1.92	0.81
2:I:145:ILE:HB	2:I:456:VAL:HG22	1.61	0.81
3:J:138:VAL:HG21	3:J:145:VAL:HB	1.63	0.81
1:G:118:ASP:HB3	1:G:121:VAL:CG2	2.09	0.81
1:H:32:GLU:HA	1:H:198:LEU:HD22	1.61	0.81
3:J:210:SER:O	3:J:214:ARG:HG2	1.79	0.81
3:J:901:ARG:HD2	3:J:906:GLY:O	1.80	0.81
2:C:56:VAL:HG11	2:C:468:LEU:HB3	1.63	0.81
3:D:491:LEU:HD23	3:D:498:PRO:HA	1.62	0.81
5:F:354:THR:O	5:F:358:VAL:HG23	1.80	0.81
2:I:1247:SER:HB3	3:J:375:GLU:O	1.80	0.81
5:L:470:MET:HE1	5:L:482:GLU:HG2	1.63	0.81
2:C:145:ILE:HB	2:C:456:VAL:CG2	2.11	0.80
2:I:69:GLN:HE21	2:I:101:ARG:HD2	1.46	0.80
3:J:363:LEU:CD2	3:J:487:THR:HG22	2.10	0.80
3:J:97:VAL:HG11	3:J:101:ARG:NH2	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:284:GLU:HG2	5:F:310:GLU:OE1	1.81	0.80
2:C:883:LEU:HD11	2:C:920:VAL:HG22	1.63	0.80
2:C:1158:LYS:O	2:C:1159:VAL:HG13	1.81	0.80
5:F:399:LEU:HB3	5:F:404:LEU:HD21	1.61	0.80
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.45	0.80
1:H:35:PHE:HA	1:H:38:THR:HG22	1.63	0.80
3:D:342:LEU:CA	3:D:343:LEU:HD13	2.08	0.80
5:F:466:ILE:HD11	5:F:487:MET:HE3	1.63	0.80
1:H:64:VAL:HG11	1:H:69:SER:OG	1.81	0.80
2:I:237:LEU:HD23	2:I:289:VAL:HG23	1.64	0.80
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.64	0.80
3:D:343:LEU:HD12	3:D:344:GLY:HA3	1.61	0.80
2:I:133:ASN:O	2:I:527:LYS:NZ	2.14	0.80
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.64	0.80
2:C:40:GLU:O	2:C:73:TYR:OH	1.99	0.80
1:H:99:ILE:HD11	1:H:143:ARG:HB3	1.63	0.80
2:I:452:ARG:NH1	2:I:585:GLY:HA3	1.97	0.80
2:I:901:LEU:HD11	2:I:905:ILE:HD11	1.64	0.80
5:F:597:LYS:O	5:F:603:ARG:HG3	1.82	0.79
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.64	0.79
3:J:517:CYS:HA	3:J:716:GLN:NE2	1.98	0.79
5:L:289:LYS:HA	5:L:293:GLU:OE1	1.82	0.79
5:L:489:MET:CE	5:L:493:LYS:HD2	2.12	0.79
3:J:290:ILE:H	3:J:290:ILE:HD12	1.48	0.79
5:L:277:MET:HE3	5:L:281:ARG:HH21	1.47	0.79
2:C:1142:ARG:HD3	2:C:1161:LEU:HD11	1.62	0.79
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	1.63	0.79
3:D:694:SER:OG	3:D:738:ARG:NE	2.13	0.79
2:I:56:VAL:HG11	2:I:468:LEU:HD13	1.64	0.79
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.44	0.79
5:L:128:ASN:HA	5:L:131:GLN:HE21	1.46	0.79
3:D:418:GLU:O	3:D:481:ARG:NH2	2.16	0.79
3:D:709:ARG:C	3:D:711:GLY:H	1.88	0.79
3:D:848:VAL:CG2	3:D:858:VAL:HG13	2.12	0.79
1:B:29:GLU:HB3	1:B:30:PRO:CD	2.12	0.79
2:C:890:LYS:NZ	2:C:891:GLY:O	2.14	0.79
2:C:1157:GLN:O	2:C:1158:LYS:HG2	1.83	0.79
2:I:985:GLU:HG2	2:I:988:LYS:HD2	1.63	0.79
1:A:27:THR:C	1:A:28:LEU:HD12	2.07	0.79
1:B:212:ASP:OD1	1:B:214:GLU:HB3	1.83	0.79
2:C:269:ILE:HG22	2:C:274:ILE:HG13	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.65	0.79
1:B:125:LYS:HE2	1:B:128:HIS:HD2	1.47	0.79
2:C:156:PHE:CE1	2:C:443:ASP:HB2	2.17	0.79
2:C:302:ILE:CG2	2:C:309:LEU:HA	2.12	0.79
5:L:132:CYS:SG	5:L:257:LYS:NZ	2.54	0.79
2:I:192:ASP:OD2	2:I:436:ARG:NH2	2.16	0.79
1:B:89:ALA:HB3	1:B:124:VAL:CG1	2.12	0.78
2:C:151:ARG:CZ	2:C:445:ILE:HD11	2.12	0.78
3:J:416:ILE:HG12	3:J:441:LEU:HD21	1.65	0.78
3:D:1280:VAL:O	3:D:1284:ARG:HB3	1.82	0.78
5:F:148:TYR:OH	5:F:218:ARG:HA	1.84	0.78
2:C:1242:LYS:HD2	3:D:465:GLN:OE1	1.83	0.78
2:C:1276:TRP:CE2	3:D:801:VAL:HG21	2.19	0.78
2:C:1196:LYS:CD	2:C:1206:THR:HG23	2.13	0.78
2:I:724:VAL:HG11	2:I:727:VAL:HG22	1.66	0.78
2:C:748:ILE:HD11	2:C:967:LEU:HD12	1.64	0.78
2:C:817:LEU:CD1	2:C:1085:MET:HE1	2.13	0.78
2:C:3:TYR:CE1	2:C:11:ILE:HD11	2.18	0.78
2:C:93:SER:OG	2:C:126:GLU:OE1	2.00	0.78
1:G:227:GLN:HE21	1:H:35:PHE:HD2	1.32	0.78
2:I:1131:MET:HE2	2:I:1141:LEU:CD1	2.14	0.78
3:J:425:ARG:HG2	3:J:426:ALA:H	1.49	0.78
3:J:814:CYS:HB3	3:J:890:THR:OG1	1.84	0.78
3:D:1280:VAL:HG11	3:D:1304:ARG:NH2	1.98	0.78
1:H:13:LEU:HD12	1:H:16:ILE:HD11	1.65	0.78
3:J:1280:VAL:CG1	3:J:1304:ARG:HH21	1.97	0.78
2:I:985:GLU:CG	2:I:988:LYS:HD2	2.14	0.78
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.64	0.78
1:B:64:VAL:HG11	1:B:69:SER:CB	2.14	0.78
3:J:647:PRO:CG	3:J:697:MET:HB3	2.13	0.78
1:A:38:THR:OG1	1:B:45:ARG:HG2	1.83	0.77
2:C:568:ASN:HB2	2:C:571:LEU:HB2	1.65	0.77
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.17	0.77
5:L:557:LYS:HZ2	5:L:561:MET:HE1	1.47	0.77
3:D:333:GLY:HA3	3:D:338:PHE:CE1	2.19	0.77
3:J:827:GLU:O	3:J:829:GLY:N	2.14	0.77
3:J:872:LEU:CD2	3:J:877:VAL:HG11	2.14	0.77
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.16	0.77
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.65	0.77
2:I:720:ARG:HE	2:I:736:VAL:HG11	1.49	0.77
3:J:97:VAL:HG11	3:J:101:ARG:CZ	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:314:THR:O	5:F:318:ALA:HB3	1.84	0.77
5:F:371:LYS:HA	5:F:374:ARG:NH1	1.99	0.77
3:J:870:ASP:O	3:J:874:GLU:HG2	1.84	0.77
3:J:1269:ALA:HB2	3:J:1274:PHE:CE1	2.19	0.77
2:C:726:TYR:CE2	2:C:728:ASP:HB2	2.19	0.77
3:D:518:VAL:CG1	3:D:707:ILE:HD13	2.14	0.77
2:I:122:VAL:HG11	2:I:493:ILE:HD13	1.64	0.77
1:A:10:LYS:HE2	1:B:229:GLU:OE1	1.85	0.77
1:B:47:LEU:HD13	1:B:183:ILE:HG12	1.65	0.77
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.25	0.77
1:H:51:MET:O	1:H:150:ARG:HA	1.85	0.77
2:I:175:ARG:HD3	2:I:183:TRP:CE3	2.19	0.77
2:I:1234:LYS:CE	2:I:1238:LEU:HD23	2.13	0.77
2:C:243:PRO:HB2	2:C:278:GLU:HG3	1.67	0.76
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.67	0.76
1:G:13:LEU:HD23	1:G:13:LEU:H	1.49	0.76
3:D:45:ASN:HB3	3:D:48:THR:O	1.85	0.76
3:D:1341:ARG:NH1	3:D:1343:GLU:OE2	2.18	0.76
5:F:426:LYS:HE2	5:F:428:SER:OG	1.85	0.76
3:J:698:MET:O	3:J:702:GLN:HB3	1.85	0.76
3:D:1343:GLU:HB3	3:D:1345:ARG:HD3	1.66	0.76
2:I:738:GLU:HG2	2:I:741:MET:CE	2.15	0.76
2:I:494:ASN:HB3	2:I:497:PRO:HD2	1.66	0.76
1:B:41:ASN:OD1	1:B:44:ARG:NH1	2.18	0.76
2:I:136:PHE:CE2	2:I:456:VAL:HG11	2.19	0.76
2:I:698:PRO:HG3	2:I:1231:TYR:CE2	2.20	0.76
3:J:1140:ARG:HH21	3:J:1236:GLU:CG	1.97	0.76
3:D:259:ARG:NH1	5:F:505:ILE:HD11	2.01	0.76
2:I:62:TYR:CZ	2:I:476:LYS:HB3	2.21	0.76
2:I:1038:GLN:HG3	2:I:1038:GLN:O	1.84	0.76
3:J:141:PHE:HA	3:J:180:MET:HE2	1.66	0.76
3:J:258:GLY:HA3	5:L:499:LYS:HD3	1.67	0.76
2:C:453:ILE:HD11	2:C:587:LEU:HD11	1.68	0.76
2:C:703:GLY:N	2:C:705:GLU:OE2	2.18	0.76
2:C:1142:ARG:NH2	2:C:1165:SER:HB2	1.99	0.76
2:I:666:SER:OG	2:I:704:MET:HG3	1.85	0.76
3:J:488:ASN:HD21	4:K:6:VAL:HG22	1.51	0.76
3:D:79:LYS:HG3	3:D:80:HIS:N	1.98	0.76
3:J:1289:ASN:OD1	3:J:1290:ARG:NH1	2.19	0.76
2:C:726:TYR:OH	2:C:728:ASP:OD2	2.03	0.76
2:C:817:LEU:HD11	2:C:1080:ASN:HD22	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:724:VAL:HG23	2:C:775:GLU:O	1.86	0.76
5:F:277:MET:HE3	5:F:281:ARG:NH2	2.01	0.76
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.67	0.75
2:C:1217:THR:OG1	2:C:1219:GLU:HG2	1.85	0.75
3:D:141:PHE:HA	3:D:180:MET:HE2	1.67	0.75
3:D:800:LEU:HB3	3:D:920:ALA:HB1	1.68	0.75
3:D:810:THR:CG2	3:D:893:GLY:HA3	2.16	0.75
3:D:843:VAL:HG11	3:D:897:HIS:O	1.85	0.75
5:F:470:MET:CE	5:F:478:PRO:HB3	2.16	0.75
3:J:1156:LEU:HD23	3:J:1219:ASP:HB3	1.68	0.75
2:C:561:ILE:HD11	2:C:665:ALA:CB	2.15	0.75
3:D:836:ARG:HG3	3:D:869:CYS:HB3	1.67	0.75
1:G:43:LEU:HD13	1:G:217:ILE:HD11	1.67	0.75
5:L:572:THR:HG23	5:L:575:GLU:HB2	1.68	0.75
1:B:183:ILE:HD11	1:B:205:MET:CG	2.12	0.75
2:C:1299:ASN:HD22	2:C:1303:LYS:HE2	1.49	0.75
3:D:1371:ARG:HH21	3:J:854:ALA:HA	1.51	0.75
5:F:444:ALA:HB1	5:F:457:ILE:CD1	2.17	0.75
2:I:896:THR:HB	2:I:897:PRO:HD2	1.68	0.75
3:J:1221:LEU:O	3:J:1221:LEU:HD22	1.86	0.75
2:C:323:ALA:O	2:C:327:GLN:HG3	1.87	0.75
2:C:1280:ALA:HB1	3:D:918:ILE:HG22	1.69	0.75
2:I:250:THR:HA	2:I:268:ARG:HA	1.68	0.75
3:J:903:LEU:HD23	3:J:905:ARG:CG	2.16	0.75
2:C:591:TYR:HD2	2:C:606:LEU:HD13	1.51	0.75
3:D:491:LEU:CD2	3:D:498:PRO:HA	2.17	0.75
2:I:1211:ARG:HD3	2:I:1213:TYR:OH	1.86	0.75
3:J:1205:GLU:O	3:J:1208:ASP:HB2	1.87	0.75
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.51	0.75
1:A:218:ARG:HG3	1:B:231:PHE:O	1.86	0.75
2:C:720:ARG:NH2	2:C:736:VAL:HG21	2.02	0.75
3:D:1174:ARG:HG2	3:D:1189:MET:SD	2.27	0.75
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.68	0.75
3:J:514:THR:CG2	3:J:596:LEU:HB2	2.17	0.75
3:J:517:CYS:CA	3:J:716:GLN:HE22	1.98	0.75
3:J:805:GLN:OE1	3:J:1348:LYS:HD3	1.87	0.75
2:C:1131:MET:HE2	2:C:1141:LEU:HD12	0.91	0.75
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.52	0.75
1:A:179:PRO:HA	1:A:208:ASN:OD1	1.87	0.75
2:I:607:SER:HB3	2:I:610:GLU:OE1	1.87	0.75
2:I:1024:GLU:HG2	2:I:1028:LYS:CD	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:341:LEU:HD23	5:L:344:LEU:HD23	1.66	0.75
1:A:104:LYS:NZ	1:A:114:ASP:OD2	2.14	0.75
3:D:222:LYS:NZ	3:D:1276:GLU:OE1	2.17	0.75
1:H:51:MET:HG3	1:H:52:PRO:CD	2.17	0.75
2:C:98:VAL:CG2	2:C:124:MET:HE3	2.17	0.74
2:C:718:ALA:HB2	2:C:783:LEU:CD2	2.17	0.74
2:C:808:ASN:OD1	2:C:1216:ARG:NH2	2.20	0.74
3:D:872:LEU:HD22	3:D:877:VAL:HG11	1.67	0.74
4:E:35:LYS:NZ	4:E:71:GLU:OE2	2.15	0.74
2:I:13:LYS:NZ	2:I:1148:ALA:O	2.20	0.74
2:I:1304:MET:HE3	3:J:472:LEU:HD12	1.69	0.74
5:L:576:VAL:HG12	5:L:587:ILE:HD11	1.69	0.74
2:C:1219:GLU:OE2	3:D:538:ARG:NH1	2.16	0.74
5:F:379:MET:HG2	5:F:416:VAL:CG2	2.17	0.74
1:H:41:ASN:OD1	1:H:44:ARG:NH1	2.19	0.74
2:I:122:VAL:CG1	2:I:493:ILE:HD13	2.17	0.74
5:L:280:VAL:HG22	5:L:347:ILE:CD1	2.17	0.74
1:B:152:TYR:CE2	3:D:536:LEU:HD21	2.22	0.74
3:D:16:GLU:HG3	3:D:1369:ARG:NH2	2.01	0.74
2:I:829:THR:HG23	2:I:1059:ARG:HA	1.68	0.74
3:J:844:THR:HG23	3:J:864:LEU:HD11	1.68	0.74
5:L:322:MET:HE2	5:L:324:LYS:CG	2.17	0.74
2:C:519:ASN:HB3	2:C:522:SER:CB	2.16	0.74
2:C:634:VAL:HG13	2:C:636:CYS:SG	2.26	0.74
3:D:210:SER:O	3:D:214:ARG:HG2	1.88	0.74
3:D:418:GLU:H	4:E:45:LYS:NZ	1.85	0.74
2:I:886:LYS:HE3	2:I:916:SER:HB3	1.70	0.74
2:I:1086:PRO:O	2:I:1094:VAL:HG12	1.87	0.74
3:J:154:LEU:HD22	3:J:160:LEU:HD11	1.70	0.74
1:B:103:ASN:OD1	1:B:141:SER:OG	2.03	0.74
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.67	0.74
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.70	0.74
5:F:461:ASN:O	5:F:465:ARG:HG2	1.88	0.74
1:G:161:SER:O	1:G:163:GLU:HG3	1.86	0.74
2:I:1114:GLU:OE1	2:I:1230:MET:HA	1.87	0.74
3:J:536:LEU:HD12	3:J:542:ALA:HB2	1.69	0.74
1:B:35:PHE:HA	1:B:38:THR:CG2	2.16	0.74
2:I:175:ARG:NH2	2:I:200:ARG:HH12	1.86	0.74
5:F:316:PHE:CZ	5:F:334:SER:HA	2.20	0.74
2:I:86:GLN:HA	2:I:140:GLY:HA2	1.69	0.74
2:I:594:VAL:HG11	2:I:650:VAL:HG23	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:24:VAL:HG21	2:C:704:MET:SD	2.28	0.74
2:C:74:ARG:NH2	2:C:97:ARG:HG3	2.02	0.74
3:D:252:LEU:HD23	3:D:262:THR:HB	1.68	0.74
3:D:378:LYS:NZ	3:D:382:TYR:OH	2.20	0.74
3:D:810:THR:HG21	3:D:893:GLY:HA3	1.68	0.74
2:I:494:ASN:HD22	2:I:497:PRO:HD3	1.50	0.74
3:J:647:PRO:HG3	3:J:697:MET:CB	2.16	0.74
2:C:86:GLN:HA	2:C:140:GLY:HA2	1.69	0.74
2:C:778:GLU:O	2:C:781:ASP:HB2	1.88	0.74
3:D:97:VAL:HG11	3:D:101:ARG:NH2	2.03	0.74
3:D:709:ARG:O	3:D:711:GLY:N	2.21	0.74
1:G:58:GLU:OE2	1:G:170:ARG:NH1	2.21	0.74
2:I:886:LYS:H	2:I:917:SER:HB3	1.51	0.74
5:L:598:LEU:O	5:L:604:SER:OG	2.06	0.74
3:D:215:LYS:O	3:D:218:THR:HG22	1.88	0.73
3:J:1344:LEU:HB3	3:J:1350:ASN:ND2	2.03	0.73
1:A:36:GLY:HA3	1:A:187:VAL:HG11	1.70	0.73
2:C:593:LYS:HE3	2:C:595:THR:CG2	2.18	0.73
2:C:730:SER:O	2:C:753:LEU:HB2	1.88	0.73
2:C:1142:ARG:CD	2:C:1161:LEU:HD11	2.17	0.73
5:L:561:MET:HA	5:L:567:MET:CE	2.16	0.73
2:C:1196:LYS:HD2	2:C:1206:THR:CG2	2.16	0.73
3:D:331:ILE:HG22	3:D:1328:THR:HG21	1.70	0.73
1:G:145:LYS:NZ	1:G:147:GLN:OE1	2.20	0.73
1:H:102:LEU:O	1:H:141:SER:HA	1.87	0.73
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.52	0.73
5:F:362:ASN:HB2	5:F:365:MET:HE2	1.70	0.73
2:I:738:GLU:HA	2:I:741:MET:HE2	1.70	0.73
3:J:1241:TYR:HD2	3:J:1246:VAL:HG11	1.53	0.73
2:C:980:VAL:O	2:C:984:VAL:HB	1.89	0.73
3:D:647:PRO:CG	3:D:697:MET:HB3	2.19	0.73
2:I:1151:LEU:HD11	2:I:1198:LEU:HD23	1.70	0.73
2:I:1288:GLN:HE21	3:J:1355:ARG:HA	1.54	0.73
3:D:1290:ARG:HD3	3:D:1294:ALA:CB	2.18	0.73
5:L:561:MET:HG2	5:L:576:VAL:HG22	1.70	0.73
1:A:47:LEU:O	1:A:180:VAL:HG21	1.89	0.73
2:C:930:ASP:OD2	2:C:931:VAL:N	2.20	0.73
3:D:797:THR:CG2	3:D:924:GLY:HA3	2.15	0.73
3:D:930:LEU:HD12	3:D:1138:LEU:CD1	2.18	0.73
2:I:745:GLU:HG3	2:I:1017:GLN:HB3	1.70	0.73
3:J:825:VAL:C	3:J:826:ILE:HG13	2.14	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:162:ILE:HD13	5:L:221:PHE:HE2	1.54	0.73
1:B:57:THR:O	1:B:173:VAL:HG22	1.89	0.73
2:C:169:LYS:O	2:C:170:VAL:HG22	1.89	0.73
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.22	0.73
3:D:622:ASP:HB3	3:D:626:TYR:HE2	1.54	0.73
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.70	0.73
2:I:1287:LEU:HD22	3:J:1357:ILE:HD11	1.70	0.73
2:C:1293:VAL:HG11	2:C:1304:MET:HE2	1.69	0.73
3:D:884:SER:OG	3:D:1254:GLU:OE1	2.07	0.73
2:I:974:ARG:HB3	2:I:1014:LEU:HD21	1.71	0.73
1:G:13:LEU:HD22	1:H:231:PHE:CZ	2.23	0.72
2:I:71:VAL:HB	2:I:99:LYS:HB2	1.71	0.72
2:I:136:PHE:CZ	2:I:456:VAL:HG11	2.24	0.72
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.69	0.72
5:F:379:MET:HG2	5:F:416:VAL:HG22	1.69	0.72
3:J:131:PRO:HG2	3:J:134:ASP:HB2	1.71	0.72
1:A:57:THR:HG22	1:A:158:ARG:NH2	2.04	0.72
1:A:62:ASP:OD1	1:A:141:SER:OG	2.06	0.72
2:C:478:ARG:NH1	2:C:482:GLY:HA2	2.03	0.72
3:D:1198:VAL:HB	3:D:1210:ILE:HA	1.70	0.72
1:G:191:ARG:HH12	1:G:197:ASP:HA	1.55	0.72
1:H:79:LEU:CD1	3:J:526:VAL:HG21	2.12	0.72
3:J:232:ASN:HA	3:J:236:TRP:HZ3	1.53	0.72
5:L:420:GLU:OE1	5:L:423:ARG:NH2	2.22	0.72
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.71	0.72
3:D:1257:VAL:HG22	3:D:1260:MET:HE2	1.70	0.72
2:I:1304:MET:HE3	3:J:472:LEU:CD1	2.19	0.72
1:A:14:VAL:CG1	1:A:27:THR:HB	2.19	0.72
2:C:1291:LEU:HD21	3:D:1351:VAL:CG1	2.17	0.72
1:H:16:ILE:HD13	1:H:214:GLU:OE2	1.90	0.72
5:L:289:LYS:HE3	5:L:293:GLU:HG2	1.72	0.72
2:C:14:ASP:HA	2:C:1183:ALA:HB3	1.72	0.72
2:I:149:LEU:HD12	2:I:452:ARG:O	1.88	0.72
3:J:848:VAL:HG23	3:J:858:VAL:HG13	1.72	0.72
1:B:102:LEU:HD11	1:B:110:VAL:HG11	1.70	0.72
2:C:136:PHE:CZ	2:C:456:VAL:HG11	2.25	0.72
1:H:6:THR:O	1:H:6:THR:HG22	1.89	0.72
1:B:51:MET:HG3	1:B:52:PRO:HD2	1.72	0.72
2:C:514:PHE:O	6:C:2001:KNG:C32	2.38	0.72
3:D:267:ASP:HA	3:D:270:ARG:HH21	1.55	0.72
2:I:119:GLU:CG	2:I:489:PRO:HD2	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1023:HIS:O	2:I:1027:LYS:HG2	1.90	0.72
2:I:1065:LYS:CD	2:I:1235:LEU:HD12	2.20	0.72
3:J:479:GLU:CG	4:K:20:VAL:HG11	2.19	0.72
2:C:1212:LEU:HD22	2:C:1225:VAL:HG21	1.71	0.72
2:C:1305:TYR:OH	5:F:532:LEU:HG	1.90	0.72
1:G:38:THR:OG1	1:H:45:ARG:HD3	1.89	0.72
1:H:142:MET:HG3	1:H:144:ILE:HG13	1.72	0.72
2:I:1234:LYS:HE2	2:I:1238:LEU:CD2	2.18	0.72
3:J:1137:GLY:O	3:J:1140:ARG:HB3	1.90	0.72
2:C:98:VAL:HG21	2:C:124:MET:HE3	1.72	0.72
2:C:722:GLY:HA2	2:C:737:ASN:OD1	1.90	0.72
5:L:314:THR:O	5:L:318:ALA:HB3	1.90	0.72
3:D:520:ALA:HB3	3:D:546:ALA:HB2	1.72	0.71
5:F:234:THR:HG21	5:F:248:GLU:OE2	1.89	0.71
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.53	0.71
5:L:341:LEU:CD2	5:L:344:LEU:HD23	2.19	0.71
2:C:582:ASN:HB3	2:C:586:PHE:H	1.54	0.71
3:D:137:ARG:HD3	3:D:143:SER:HB2	1.72	0.71
1:G:46:ILE:HD12	1:H:35:PHE:CZ	2.25	0.71
2:I:338:THR:HG22	2:I:345:PRO:HB3	1.71	0.71
5:L:557:LYS:NZ	5:L:561:MET:HE1	2.05	0.71
2:C:1142:ARG:HH22	2:C:1165:SER:HB2	1.54	0.71
3:J:71:LEU:O	3:J:71:LEU:HD22	1.90	0.71
3:J:1280:VAL:O	3:J:1284:ARG:HB3	1.90	0.71
2:C:496:LYS:HB3	2:C:497:PRO:HD3	1.72	0.71
2:C:1271:GLY:HA3	3:D:343:LEU:HD21	1.70	0.71
2:I:817:LEU:HD11	2:I:1080:ASN:HD22	1.56	0.71
2:I:1131:MET:CE	2:I:1141:LEU:HD12	2.21	0.71
3:D:270:ARG:NH2	5:F:449:THR:HG23	2.05	0.71
3:J:810:THR:HG21	3:J:893:GLY:HA3	1.72	0.71
3:J:903:LEU:HD23	3:J:905:ARG:HG3	1.73	0.71
5:F:466:ILE:HG22	5:F:470:MET:HG3	1.71	0.71
2:I:237:LEU:CD1	2:I:292:ILE:HD11	2.21	0.71
2:I:557:ARG:NH2	2:I:607:SER:O	2.23	0.71
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.26	0.71
2:I:1314:GLN:HG2	4:K:28:ARG:CZ	2.20	0.71
3:D:479:GLU:HG3	4:E:20:VAL:HG11	1.72	0.71
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.71	0.71
5:F:277:MET:HG3	5:F:362:ASN:HD21	1.53	0.71
1:G:155:ALA:HA	1:G:158:ARG:HG3	1.73	0.71
2:I:696:ASP:HB2	2:I:798:GLN:CG	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:518:VAL:CG1	3:J:707:ILE:HD13	2.21	0.71
3:J:799:ARG:NH1	3:J:1146:GLU:OE1	2.24	0.71
5:L:492:ASP:CB	5:L:495:ARG:HH12	2.02	0.71
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.70	0.71
2:I:466:VAL:O	2:I:469:VAL:HG22	1.90	0.71
2:I:1285:TYR:CZ	3:J:1356:LEU:HD11	2.26	0.71
3:J:279:LEU:O	3:J:279:LEU:HD23	1.89	0.71
3:J:647:PRO:HG3	3:J:697:MET:CA	2.20	0.71
2:C:589:THR:OG1	2:C:659:GLN:NE2	2.23	0.71
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.71	0.71
3:D:1241:TYR:HD2	3:D:1246:VAL:HG11	1.54	0.71
2:C:1238:LEU:H	2:C:1238:LEU:HD12	1.56	0.70
5:F:278:ASP:OD1	5:F:281:ARG:NH1	2.23	0.70
3:J:614:LEU:HD23	4:K:7:GLN:HB2	1.73	0.70
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.25	0.70
2:C:1308:ILE:HD12	3:D:380:PHE:CZ	2.26	0.70
3:D:1171:GLY:HA2	3:D:1193:TRP:HZ3	1.55	0.70
2:I:1247:SER:OG	3:J:375:GLU:OE2	2.09	0.70
5:L:384:LEU:HD22	5:L:409:ASN:HD21	1.56	0.70
1:B:83:LEU:HD11	3:D:526:VAL:HG23	1.74	0.70
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.54	0.70
2:C:109:ALA:HB1	2:C:111:GLU:N	2.04	0.70
2:C:887:VAL:HB	2:C:913:VAL:HG22	1.73	0.70
2:C:1101:LEU:O	3:D:731:ARG:HD3	1.91	0.70
3:J:30:ILE:HD13	3:J:243:PRO:HD3	1.71	0.70
2:C:41:GLN:NE2	2:C:73:TYR:O	2.24	0.70
3:D:116:PHE:CE1	3:D:1333:THR:HG22	2.27	0.70
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.27	0.70
3:J:430:HIS:HA	3:J:921:GLN:HB3	1.72	0.70
2:C:980:VAL:HA	2:C:984:VAL:HA	1.74	0.70
2:C:1285:TYR:CE2	3:D:1356:LEU:HD11	2.26	0.70
3:J:72:CYS:HG	8:J:1502:ZN:ZN	1.06	0.70
3:J:126:LEU:HD13	3:J:223:LEU:HD22	1.74	0.70
3:J:658:GLU:O	3:J:661:VAL:HG13	1.92	0.70
2:C:26:TYR:CZ	2:C:28:LEU:HB2	2.27	0.70
2:C:593:LYS:HB3	2:C:602:GLU:CG	2.22	0.70
1:G:57:THR:HG22	1:G:158:ARG:NH2	2.06	0.70
3:J:275:ARG:HD3	3:J:298:MET:HB3	1.74	0.70
3:J:1252:HIS:O	3:J:1255:VAL:HG13	1.91	0.70
1:A:218:ARG:NH1	1:B:231:PHE:HA	2.06	0.70
2:C:197:ARG:NH1	2:C:201:ARG:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1144:PHE:O	2:C:1147:ARG:HB2	1.92	0.70
2:I:1285:TYR:CE2	3:J:1356:LEU:HD11	2.27	0.70
3:J:513:MET:O	3:J:575:GLY:HA3	1.91	0.70
3:D:658:GLU:O	3:D:661:VAL:HG13	1.91	0.70
2:C:818:VAL:HB	2:C:1076:ILE:HD11	1.73	0.70
3:D:121:PRO:HG2	3:D:123:ARG:NH2	2.07	0.70
3:J:460:ASP:HB2	3:J:464:ASP:OD2	1.92	0.70
1:B:89:ALA:HB3	1:B:124:VAL:HG12	1.74	0.70
2:C:1131:MET:HE1	2:C:1141:LEU:HA	1.74	0.70
2:C:1248:THR:HB	5:F:532:LEU:HD11	1.74	0.70
3:D:115:TRP:CZ2	3:D:1329:THR:HG23	2.26	0.70
3:D:507:VAL:HG11	3:D:598:LYS:HG3	1.74	0.70
1:G:228:LEU:HD22	1:H:221:ALA:HB1	1.73	0.70
2:I:1272:GLU:H	3:J:343:LEU:HD12	1.56	0.70
2:C:1246:ARG:NH1	2:C:1266:GLY:HA2	2.06	0.69
3:D:141:PHE:CA	3:D:180:MET:HE2	2.21	0.69
5:F:281:ARG:O	5:F:285:ARG:HG3	1.92	0.69
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.74	0.69
5:F:362:ASN:HB2	5:F:365:MET:CE	2.23	0.69
1:H:57:THR:HG21	1:H:158:ARG:NE	2.04	0.69
1:A:164:ASP:OD1	1:A:166:ARG:HB2	1.92	0.69
1:B:23:HIS:HB3	1:B:206:GLU:HG2	1.74	0.69
2:C:30:ILE:H	2:C:30:ILE:HD12	1.58	0.69
3:D:11:GLN:HG3	3:D:12:THR:H	1.57	0.69
3:D:18:ASP:HB2	3:D:1373:ARG:HH22	1.57	0.69
5:F:281:ARG:HG2	5:F:285:ARG:HD2	1.74	0.69
2:I:1105:SER:HB2	3:J:731:ARG:CG	2.21	0.69
1:B:205:MET:CE	1:B:213:PRO:HB3	2.23	0.69
2:C:618:GLN:OE1	3:D:770:LEU:HD13	1.93	0.69
2:C:619:ALA:CA	2:C:654:ASP:HB2	2.22	0.69
2:C:819:SER:HB2	2:C:1085:MET:HG3	1.74	0.69
3:D:56:LEU:HD12	3:D:56:LEU:N	2.07	0.69
3:D:1290:ARG:HD2	3:D:1295:ASN:HD22	1.58	0.69
5:F:548:LEU:HD23	5:F:551:LEU:HD12	1.75	0.69
1:H:176:CYS:O	1:H:178:SER:N	2.25	0.69
2:I:564:PRO:HG3	2:I:572:ILE:HG13	1.73	0.69
2:I:680:LEU:HD22	3:J:783:LEU:CD1	2.22	0.69
2:C:1281:TYR:HD1	3:D:484:MET:HG2	1.55	0.69
3:D:19:ALA:HA	3:D:1344:LEU:CD1	2.22	0.69
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.74	0.69
1:H:79:LEU:HD11	3:J:526:VAL:CG2	2.14	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:146:VAL:HG13	2:C:529:ARG:HB3	1.74	0.69
3:D:872:LEU:O	3:D:877:VAL:HG12	1.93	0.69
5:F:297:MET:HG3	5:F:326:TRP:HB2	1.75	0.69
2:C:227:LYS:NZ	2:C:298:ALA:HB1	2.08	0.69
1:B:74:VAL:HG13	1:B:132:HIS:O	1.93	0.69
2:C:101:ARG:HH21	2:C:118:LYS:HE3	1.57	0.69
3:D:131:PRO:HG2	3:D:134:ASP:HB2	1.74	0.69
2:I:94:ALA:HB2	2:I:129:LEU:HD11	1.74	0.69
2:I:1246:ARG:NE	3:J:348:ASP:OD1	2.26	0.69
3:J:526:VAL:CG1	3:J:549:LYS:HB2	2.22	0.69
3:J:722:ILE:HA	3:J:725:MET:HE3	1.74	0.69
3:J:1236:GLU:HA	3:J:1236:GLU:OE2	1.91	0.69
1:A:41:ASN:CG	2:C:1218:GLY:HA3	2.17	0.69
2:C:545:PHE:HD1	2:C:548:ARG:HD3	1.57	0.69
6:C:2001:KNG:C33	6:C:2001:KNG:C34	2.71	0.69
3:D:98:ARG:HB3	3:D:248:ASP:OD2	1.93	0.69
3:D:528:THR:O	3:D:551:ARG:HB3	1.93	0.69
1:G:231:PHE:HB3	1:H:218:ARG:HG2	1.74	0.69
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.75	0.69
1:B:83:LEU:HD11	3:D:526:VAL:CG2	2.23	0.69
2:C:812:PHE:CE2	3:D:451:PRO:HB3	2.27	0.69
3:D:623:GLN:O	3:D:627:THR:HG22	1.93	0.69
5:F:479:THR:HG22	5:F:482:GLU:HB2	1.75	0.69
2:I:528:ARG:NH2	2:I:576:SER:O	2.26	0.69
2:I:617:ALA:HB3	2:I:653:MET:HG3	1.73	0.69
2:I:1065:LYS:HD3	2:I:1235:LEU:HD12	1.75	0.69
2:I:1116:HIS:CE1	3:J:641:ILE:H	2.10	0.69
3:J:179:LYS:HB2	3:J:184:ALA:HB2	1.74	0.69
5:L:576:VAL:HG12	5:L:587:ILE:CD1	2.23	0.69
3:D:427:PRO:O	3:D:429:LEU:HD22	1.93	0.68
3:D:1280:VAL:CG1	3:D:1304:ARG:HH21	2.02	0.68
3:J:526:VAL:HA	3:J:549:LYS:O	1.94	0.68
1:A:70:THR:CG2	2:C:755:LYS:HE2	2.23	0.68
2:C:156:PHE:CD1	2:C:443:ASP:HB2	2.26	0.68
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.74	0.68
2:C:582:ASN:HB3	2:C:586:PHE:N	2.07	0.68
1:B:35:PHE:CA	1:B:38:THR:HG22	2.20	0.68
1:B:182:ARG:C	1:B:183:ILE:HD12	2.17	0.68
2:C:299:LYS:HG2	2:C:334:GLU:OE1	1.93	0.68
2:C:1101:LEU:HD23	3:D:725:MET:SD	2.33	0.68
3:D:161:THR:HG23	3:D:164:GLN:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:137:TYR:CE2	5:F:273:MET:HG2	2.27	0.68
1:G:9:LEU:HD21	1:G:195:ARG:HH21	1.58	0.68
3:J:30:ILE:CG2	3:J:243:PRO:HG3	2.24	0.68
2:C:478:ARG:HH12	2:C:482:GLY:HA2	1.57	0.68
3:D:142:GLU:OE2	5:F:100:MET:HE2	1.94	0.68
1:G:43:LEU:HD12	1:G:203:ILE:HD11	1.76	0.68
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.29	0.68
5:L:362:ASN:HB2	5:L:365:MET:HE2	1.74	0.68
3:D:1290:ARG:CG	3:D:1298:VAL:HG12	2.23	0.68
5:F:470:MET:HE3	5:F:478:PRO:HB3	1.75	0.68
3:J:1280:VAL:HG11	3:J:1304:ARG:NH2	2.08	0.68
2:C:564:PRO:HA	2:C:684:ASN:HD21	1.59	0.68
3:D:514:THR:CG2	3:D:596:LEU:HB2	2.23	0.68
3:D:1167:LYS:HD3	3:D:1174:ARG:HD2	1.75	0.68
3:J:514:THR:HG21	3:J:596:LEU:HB2	1.75	0.68
3:J:748:ALA:O	3:J:777:HIS:HD2	1.76	0.68
3:J:1290:ARG:CG	3:J:1298:VAL:HG12	2.23	0.68
1:B:182:ARG:O	1:B:183:ILE:HD12	1.93	0.68
2:C:109:ALA:HB1	2:C:111:GLU:HA	1.75	0.68
2:C:748:ILE:CD1	2:C:967:LEU:HD12	2.22	0.68
2:C:866:ASP:HA	2:C:872:TYR:OH	1.94	0.68
2:C:1066:MET:HE2	2:C:1076:ILE:CG2	2.24	0.68
2:C:1146:GLN:HG2	2:C:1160:ASP:OD1	1.93	0.68
3:D:518:VAL:HG11	3:D:707:ILE:HD13	1.74	0.68
3:D:647:PRO:HG3	3:D:697:MET:CB	2.23	0.68
1:H:84:ASN:ND2	1:H:129:VAL:O	2.27	0.68
2:I:813:GLU:HB2	3:J:461:PHE:HB2	1.75	0.68
3:J:30:ILE:HG23	3:J:243:PRO:HG3	1.76	0.68
3:J:843:VAL:CG1	3:J:883:ARG:HD3	2.22	0.68
3:J:1263:LYS:HE2	3:J:1279:GLN:NE2	2.09	0.68
4:K:10:VAL:HG13	4:K:16:ARG:HB2	1.76	0.68
2:C:817:LEU:HD13	2:C:1085:MET:HE1	1.76	0.68
2:I:1242:LYS:HD2	3:J:465:GLN:OE1	1.93	0.68
3:J:332:LYS:HE2	3:J:1329:THR:OG1	1.94	0.68
3:J:820:ILE:HD11	3:J:822:MET:HE2	1.76	0.68
5:L:94:THR:OG1	5:L:95:THR:N	2.24	0.68
3:D:681:LYS:O	3:D:685:ILE:HG23	1.94	0.68
2:C:1148:ALA:HB1	2:C:1180:MET:HE2	1.75	0.68
3:D:259:ARG:HG2	5:F:502:LYS:HE3	1.76	0.68
3:D:1263:LYS:HE2	3:D:1279:GLN:HE21	1.58	0.68
1:G:166:ARG:O	1:G:168:ILE:N	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:821:MET:HE3	3:J:879:ALA:HB1	1.75	0.68
3:D:259:ARG:CZ	5:F:505:ILE:HD11	2.24	0.67
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.76	0.67
5:F:387:VAL:HG22	5:F:435:ILE:HD13	1.76	0.67
2:I:960:LEU:CD1	2:I:1028:LYS:HE2	2.24	0.67
2:I:971:LEU:HD21	2:I:1014:LEU:O	1.94	0.67
5:L:137:TYR:CE2	5:L:273:MET:HG2	2.28	0.67
1:B:153:VAL:HB	1:B:175:ALA:HB3	1.76	0.67
5:F:493:LYS:HA	5:F:496:LYS:HE2	1.76	0.67
2:I:8:LYS:HE3	2:I:1171:ARG:HH21	1.57	0.67
2:I:452:ARG:NH1	2:I:584:TYR:O	2.26	0.67
2:I:557:ARG:HH21	2:I:607:SER:C	2.02	0.67
3:J:156:ARG:NH2	3:J:191:SER:OG	2.25	0.67
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.76	0.67
5:L:280:VAL:CG2	5:L:347:ILE:HD13	2.24	0.67
2:I:794:LEU:HG	2:I:796:LEU:HD11	1.77	0.67
3:J:1252:HIS:HA	3:J:1255:VAL:CG1	2.23	0.67
4:K:31:GLN:HB2	4:K:46:THR:HG21	1.76	0.67
5:L:601:PRO:HA	5:L:604:SER:HB2	1.77	0.67
1:A:224:LEU:O	1:A:224:LEU:HD23	1.94	0.67
2:C:100:LEU:HD12	2:C:122:VAL:HG11	1.76	0.67
2:C:477:GLU:O	2:C:480:SER:HB3	1.94	0.67
3:D:649:LYS:HD2	3:D:652:GLU:OE1	1.95	0.67
1:H:205:MET:HG2	1:H:206:GLU:H	1.59	0.67
2:I:1284:ALA:HB1	3:J:1356:LEU:HD22	1.74	0.67
3:J:1149:ARG:CZ	3:J:1153:PRO:HG2	2.25	0.67
1:A:50:SER:HB2	1:B:8:PHE:HZ	1.58	0.67
2:C:1202:GLY:O	2:C:1203:ASP:HB2	1.94	0.67
3:D:693:VAL:HG21	3:D:743:MET:HE3	1.75	0.67
1:G:90:VAL:HG22	1:G:91:ARG:H	1.60	0.67
5:L:489:MET:HE3	5:L:493:LYS:HD2	1.76	0.67
2:C:136:PHE:CE2	2:C:456:VAL:HG11	2.29	0.67
2:C:549:ASP:OD1	3:D:750:PRO:HB3	1.94	0.67
3:D:126:LEU:HD11	3:D:223:LEU:HD22	1.77	0.67
2:I:980:VAL:O	2:I:984:VAL:HB	1.94	0.67
2:I:1314:GLN:HG2	4:K:28:ARG:NE	2.10	0.67
3:J:1177:ILE:HD12	3:J:1186:TYR:HB3	1.77	0.67
5:L:484:ALA:HB1	5:L:491:GLU:CG	2.25	0.67
3:D:789:LYS:NZ	3:D:931:THR:O	2.17	0.67
2:I:9:LYS:HA	2:I:1171:ARG:HD2	1.77	0.67
2:I:218:GLU:O	2:I:222:ASP:HB2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:872:LEU:HD22	3:J:877:VAL:CG1	2.22	0.67
5:L:562:ARG:NH2	5:L:573:LEU:HD22	2.09	0.67
3:D:1198:VAL:HG23	3:D:1204:VAL:HG11	1.77	0.67
3:J:1165:PHE:HE1	3:J:1200:GLU:HB3	1.59	0.67
1:B:90:VAL:HG22	1:B:91:ARG:H	1.58	0.67
1:G:50:SER:CB	1:H:8:PHE:HE1	2.07	0.67
2:I:123:TYR:OH	2:I:126:GLU:HG3	1.95	0.67
2:I:770:CYS:HB2	2:I:791:LEU:HD23	1.77	0.67
2:C:1291:LEU:CD2	3:D:1351:VAL:HG13	2.20	0.67
2:I:979:LEU:CD1	2:I:1011:LEU:HD11	2.25	0.67
3:J:71:LEU:HD13	3:J:71:LEU:C	2.20	0.67
3:J:336:GLY:O	3:J:337:ARG:HB2	1.94	0.67
2:I:146:VAL:HG21	2:I:513:GLN:NE2	2.09	0.66
2:I:170:VAL:HG23	2:I:171:LEU:N	2.08	0.66
2:I:338:THR:CG2	2:I:345:PRO:HB3	2.25	0.66
5:L:127:ILE:O	5:L:130:VAL:HG22	1.93	0.66
5:L:483:LEU:HD12	5:L:483:LEU:H	1.59	0.66
1:A:61:ILE:HB	1:A:64:VAL:HG23	1.77	0.66
3:D:161:THR:CG2	3:D:164:GLN:H	2.07	0.66
3:D:1206:ARG:NH2	3:D:1223:LEU:O	2.28	0.66
2:I:1272:GLU:H	3:J:343:LEU:CD1	2.08	0.66
2:I:1287:LEU:HD13	3:J:1357:ILE:HD11	1.77	0.66
3:J:833:GLU:OE1	3:J:1242:ARG:HD3	1.95	0.66
1:B:196:THR:HG23	3:D:443:GLU:HG3	1.76	0.66
5:F:110:LEU:HD21	5:F:385:ARG:HD3	1.76	0.66
5:F:127:ILE:O	5:F:130:VAL:HG22	1.96	0.66
1:H:82:LEU:HD22	1:H:173:VAL:CG1	2.24	0.66
2:I:115:LYS:HG3	2:I:485:ASP:OD2	1.95	0.66
3:J:1169:THR:CG2	3:J:1192:LYS:HD3	2.24	0.66
3:J:1197:ASN:HB2	3:J:1211:SER:HA	1.78	0.66
2:I:138:ILE:HB	2:I:143:ARG:HD3	1.78	0.66
2:I:975:ILE:HG23	2:I:1011:LEU:HD22	1.77	0.66
3:J:1252:HIS:HA	3:J:1255:VAL:HG13	1.77	0.66
5:L:322:MET:HE2	5:L:324:LYS:HG3	1.76	0.66
1:B:73:GLY:C	1:B:134:THR:HG22	2.20	0.66
3:D:75:TYR:CE2	3:D:83:VAL:HG21	2.31	0.66
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.76	0.66
5:F:572:THR:HG23	5:F:575:GLU:HB2	1.78	0.66
2:C:1234:LYS:HE2	2:C:1238:LEU:HD23	1.76	0.66
3:D:1309:ILE:HG13	3:D:1310:THR:N	2.10	0.66
2:I:56:VAL:CG1	2:I:468:LEU:HD13	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1080:ASN:CB	2:I:1085:MET:HE3	2.22	0.66
3:J:1269:ALA:HB2	3:J:1274:PHE:CD1	2.30	0.66
3:J:709:ARG:C	3:J:711:GLY:H	2.02	0.66
1:A:154:PRO:HB2	2:C:1059:ARG:HH21	1.60	0.66
2:C:145:ILE:HA	2:C:511:LEU:O	1.95	0.66
2:C:471:VAL:HG21	2:C:498:ILE:HD11	1.78	0.66
2:C:1248:THR:HG21	5:F:531:PRO:HG3	1.76	0.66
2:I:528:ARG:NH2	2:I:575:LEU:HD23	2.09	0.66
2:I:1202:GLY:O	2:I:1203:ASP:HB2	1.96	0.66
2:C:2:VAL:O	2:C:2:VAL:HG12	1.96	0.66
3:D:11:GLN:O	3:D:12:THR:HG23	1.96	0.66
2:I:1157:GLN:O	2:I:1158:LYS:HG2	1.96	0.66
3:J:767:LEU:HD23	3:J:771:GLN:HB3	1.78	0.66
5:L:166:VAL:O	5:L:167:ASP:HB2	1.96	0.66
5:L:573:LEU:HD23	5:L:573:LEU:H	1.61	0.66
2:C:1132:LEU:HD22	2:C:1177:ARG:NH1	2.11	0.66
2:C:1298:VAL:HG11	3:D:96:LYS:HE3	1.77	0.66
1:H:74:VAL:HG22	1:H:133:LEU:HD12	1.77	0.66
1:H:153:VAL:HB	1:H:175:ALA:HB3	1.76	0.66
3:J:126:LEU:HD13	3:J:223:LEU:HD21	1.78	0.66
5:L:96:ASP:O	5:L:98:VAL:N	2.28	0.66
5:L:544:THR:HG22	5:L:607:LEU:HD21	1.78	0.66
5:F:391:ALA:HB3	5:F:405:ILE:HG22	1.78	0.65
5:F:519:LEU:HD23	5:F:519:LEU:C	2.20	0.65
3:J:494:ALA:CB	3:J:922:SER:HB3	2.25	0.65
2:C:17:LYS:HE3	2:C:1154:ASP:CB	2.23	0.65
2:C:819:SER:HB2	2:C:1085:MET:SD	2.36	0.65
2:C:1131:MET:HB3	2:C:1141:LEU:CD1	2.26	0.65
2:C:1158:LYS:O	2:C:1159:VAL:HG22	1.96	0.65
5:F:280:VAL:CG2	5:F:347:ILE:HD13	2.19	0.65
1:H:13:LEU:CD1	1:H:16:ILE:HD11	2.26	0.65
2:I:145:ILE:CG2	2:I:456:VAL:HG22	2.26	0.65
1:A:45:ARG:HG2	1:B:38:THR:CB	2.22	0.65
1:A:159:ILE:O	1:A:159:ILE:HG12	1.96	0.65
3:D:825:VAL:C	3:D:826:ILE:HG13	2.20	0.65
1:G:167:PRO:HB2	1:G:170:ARG:HB2	1.76	0.65
2:I:237:LEU:CD2	2:I:289:VAL:HG23	2.27	0.65
5:L:277:MET:HG3	5:L:362:ASN:HD21	1.61	0.65
5:L:466:ILE:CD1	5:L:487:MET:HG2	2.26	0.65
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.78	0.65
3:D:129:ASP:HB2	3:D:220:ARG:CZ	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:646:ILE:HG23	3:D:741:ALA:O	1.97	0.65
3:D:854:ALA:HB2	3:J:1372:ARG:HB2	1.77	0.65
2:I:802:VAL:CG2	2:I:1098:LEU:HD13	2.26	0.65
3:D:290:ILE:H	3:D:290:ILE:HD12	1.61	0.65
1:G:86:LYS:HZ3	1:G:174:ASP:HB2	1.61	0.65
2:I:69:GLN:NE2	2:I:101:ARG:HD2	2.10	0.65
2:I:274:ILE:HG22	2:I:278:GLU:OE1	1.97	0.65
5:L:287:ILE:HG21	5:L:315:TRP:CH2	2.31	0.65
1:A:175:ALA:HB1	1:A:177:TYR:CE1	2.32	0.65
2:C:1149:TYR:HD1	2:C:1159:VAL:HG11	1.59	0.65
2:I:197:ARG:NH1	2:I:201:ARG:O	2.29	0.65
3:J:505:ASP:HB2	3:J:629:PHE:HE1	1.60	0.65
4:K:27:ALA:HB2	4:K:50:ALA:HB2	1.78	0.65
3:D:9:LYS:HE2	3:D:11:GLN:C	2.22	0.65
3:D:548:VAL:HG12	3:D:550:VAL:HG13	1.79	0.65
3:D:1262:ARG:HD2	3:D:1279:GLN:OE1	1.96	0.65
5:F:230:VAL:O	5:F:234:THR:HG23	1.96	0.65
2:I:1078:LYS:HG2	2:I:1079:ILE:N	2.10	0.65
3:J:248:ASP:O	3:J:251:PRO:HG3	1.97	0.65
1:A:177:TYR:O	1:A:178:SER:HB2	1.95	0.65
2:C:1331:ARG:HG2	3:D:33:TRP:CH2	2.31	0.65
3:D:97:VAL:HG12	3:D:101:ARG:HG3	1.78	0.65
3:D:536:LEU:HD12	3:D:542:ALA:HB2	1.77	0.65
2:C:545:PHE:CD1	2:C:548:ARG:HD3	2.31	0.65
2:C:873:ILE:HG13	2:C:944:ARG:HH22	1.62	0.65
3:D:797:THR:HG22	3:D:924:GLY:CA	2.17	0.65
3:D:839:VAL:HG12	3:D:839:VAL:O	1.97	0.65
2:I:169:LYS:O	2:I:170:VAL:HG22	1.97	0.65
3:J:518:VAL:HG11	3:J:707:ILE:HD13	1.79	0.65
3:D:744:ARG:HG3	3:D:744:ARG:O	1.96	0.65
3:D:1265:THR:HG23	3:D:1305:ASP:OD2	1.97	0.65
5:F:110:LEU:HD21	5:F:385:ARG:CD	2.27	0.65
5:F:277:MET:HE3	5:F:281:ARG:HH21	1.59	0.65
2:I:6:THR:HG21	2:I:782:VAL:HG23	1.78	0.65
1:B:86:LYS:HD3	1:B:174:ASP:HB2	1.78	0.64
2:I:865:LEU:HD22	2:I:869:GLY:O	1.98	0.64
2:C:338:THR:HB	2:C:345:PRO:HB3	1.79	0.64
3:D:1327:GLU:OE2	3:D:1329:THR:HB	1.97	0.64
2:I:979:LEU:HD13	2:I:1011:LEU:HD21	1.78	0.64
3:J:746:LEU:HD23	3:J:758:PRO:HG3	1.78	0.64
1:B:112:ALA:O	1:B:115:ILE:HG13	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:128:LEU:HA	3:D:192:MET:HE1	1.79	0.64
5:F:418:LYS:HD2	5:F:434:TRP:CZ2	2.32	0.64
1:H:74:VAL:HG13	1:H:132:HIS:O	1.97	0.64
2:I:145:ILE:CB	2:I:456:VAL:HG22	2.26	0.64
1:A:165:GLU:OE2	1:A:172:LEU:HD11	1.97	0.64
2:C:1136:GLN:O	2:C:1137:GLU:HB3	1.96	0.64
3:D:140:TYR:HE2	5:F:95:THR:CG2	2.09	0.64
3:D:248:ASP:O	3:D:251:PRO:HG3	1.97	0.64
3:D:697:MET:HE1	3:D:737:ILE:CG2	2.22	0.64
3:D:1149:ARG:NH2	3:D:1153:PRO:HG2	2.12	0.64
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.78	0.64
5:L:560:ARG:O	5:L:567:MET:HE2	1.97	0.64
1:A:78:ILE:HD13	1:A:81:ILE:HD12	1.79	0.64
2:C:1164:PHE:O	2:C:1169:VAL:HG23	1.98	0.64
2:I:836:LEU:HD21	2:I:921:PRO:HD3	1.78	0.64
3:J:421:VAL:HG22	3:J:439:PRO:HG3	1.80	0.64
1:A:224:LEU:HB3	1:B:228:LEU:HD11	1.79	0.64
2:C:53:PHE:CD1	2:C:468:LEU:HD11	2.32	0.64
2:C:815:SER:HB3	2:C:1077:SER:HB3	1.79	0.64
3:D:94:GLN:O	3:D:97:VAL:HG23	1.97	0.64
1:H:76:GLU:HB3	1:H:81:ILE:CG1	2.27	0.64
1:H:82:LEU:HD22	1:H:173:VAL:HG12	1.77	0.64
1:H:110:VAL:HG21	1:H:140:ILE:CD1	2.27	0.64
2:I:10:ARG:CZ	2:I:697:LYS:HD3	2.28	0.64
3:J:227:PHE:HE1	3:J:234:PRO:HD3	1.61	0.64
5:F:484:ALA:CB	5:F:491:GLU:HB2	2.20	0.64
1:H:118:ASP:HB2	1:H:121:VAL:HG23	1.79	0.64
2:I:231:GLU:HG2	2:I:332:ARG:HD3	1.80	0.64
2:I:671:LEU:HD23	2:I:1186:VAL:CG1	2.27	0.64
2:I:1248:THR:HG21	5:L:531:PRO:CG	2.26	0.64
2:I:1299:ASN:HD22	2:I:1303:LYS:HE2	1.62	0.64
2:C:268:ARG:NH2	2:C:270:THR:HG21	2.13	0.64
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.62	0.64
3:D:205:LEU:C	3:D:205:LEU:HD13	2.22	0.64
2:I:1280:ALA:HB1	3:J:918:ILE:HG22	1.79	0.64
3:J:210:SER:OG	3:J:213:LYS:HD2	1.98	0.64
3:J:405:GLU:O	3:J:408:VAL:HG22	1.98	0.64
3:J:653:ILE:HD13	3:J:692:ARG:CB	2.26	0.64
2:C:296:VAL:HB	2:C:336:LEU:CD1	2.25	0.64
2:I:1272:GLU:HB2	3:J:342:LEU:CB	2.28	0.64
3:J:857:LEU:HD12	3:J:858:VAL:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:137:TYR:HD2	5:L:273:MET:HE2	1.62	0.64
1:A:60:GLU:HB2	1:A:170:ARG:HG2	1.80	0.64
5:F:601:PRO:HA	5:F:604:SER:HB2	1.80	0.64
1:H:86:LYS:HD3	1:H:174:ASP:HB2	1.80	0.64
2:I:819:SER:HB2	2:I:1085:MET:CG	2.27	0.64
3:J:56:LEU:HD21	3:J:269:TYR:HB3	1.80	0.64
2:C:301:TYR:O	2:C:309:LEU:HD12	1.98	0.63
2:C:832:HIS:ND1	2:C:1058:ARG:HD2	2.13	0.63
2:C:1131:MET:HB3	2:C:1141:LEU:HD11	1.80	0.63
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.61	0.63
3:D:1238:GLN:HG2	3:D:1253:ILE:CD1	2.29	0.63
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.79	0.63
2:I:494:ASN:HD22	2:I:497:PRO:CD	2.11	0.63
2:I:1276:TRP:CE2	3:J:801:VAL:HG21	2.33	0.63
3:J:320:ASN:OD1	3:J:322:ARG:HB3	1.97	0.63
3:J:502:PRO:HB3	3:J:506:VAL:HG21	1.79	0.63
3:J:1266:ILE:HD12	3:J:1273:ASP:O	1.99	0.63
2:C:133:ASN:HD21	2:C:713:GLY:HA3	1.60	0.63
1:G:11:PRO:HB3	1:G:31:LEU:CD2	2.27	0.63
2:I:119:GLU:HB2	2:I:489:PRO:CG	2.29	0.63
5:L:316:PHE:O	5:L:320:ILE:HG13	1.97	0.63
2:C:27:LEU:O	2:C:528:ARG:NH1	2.31	0.63
2:C:296:VAL:CB	2:C:336:LEU:HD12	2.27	0.63
2:C:980:VAL:HG13	2:C:984:VAL:HG23	1.81	0.63
2:C:1112:ILE:HD11	3:D:639:VAL:HG13	1.81	0.63
3:D:1198:VAL:HG11	3:D:1210:ILE:HG23	1.80	0.63
5:F:555:GLU:HG2	5:F:590:ILE:CG2	2.27	0.63
3:J:658:GLU:HA	3:J:661:VAL:CG1	2.27	0.63
5:L:315:TRP:CZ2	5:L:341:LEU:HD11	2.32	0.63
2:C:223:LEU:HD13	2:C:426:ILE:HD13	1.81	0.63
2:C:268:ARG:HH21	2:C:270:THR:CG2	2.12	0.63
2:C:741:MET:HE3	2:C:974:ARG:CZ	2.28	0.63
2:C:878:THR:OG1	2:C:879:GLY:N	2.26	0.63
2:C:1158:LYS:C	2:C:1159:VAL:HG22	2.23	0.63
5:F:399:LEU:HB3	5:F:404:LEU:CD2	2.29	0.63
1:H:22:THR:OG1	1:H:207:THR:O	2.16	0.63
2:I:170:VAL:O	2:I:171:LEU:HG	1.98	0.63
2:I:697:LYS:HA	2:I:795:ALA:HB2	1.79	0.63
3:J:270:ARG:NH2	5:L:449:THR:HG23	2.12	0.63
5:L:114:GLU:HG3	5:L:115:GLY:N	2.14	0.63
1:B:33:ARG:HD2	2:C:1081:PRO:HG3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:138:ILE:HG22	2:C:139:ASN:N	2.13	0.63
2:C:290:GLU:HG2	2:C:319:LEU:CD1	2.29	0.63
2:C:896:THR:OG1	2:C:899:GLU:HG3	1.99	0.63
3:D:812:ASP:HB2	3:D:911:LYS:NZ	2.14	0.63
3:D:849:LEU:HB3	3:D:853:THR:HG23	1.79	0.63
5:F:279:ARG:HH12	5:F:350:GLU:CD	2.06	0.63
1:G:16:ILE:HG23	1:G:26:VAL:HG12	1.80	0.63
2:I:17:LYS:NZ	2:I:1154:ASP:HB3	2.13	0.63
3:D:708:ASN:OD1	3:D:708:ASN:N	2.30	0.63
2:I:1291:LEU:HD21	3:J:1351:VAL:CG1	2.25	0.63
3:J:141:PHE:CA	3:J:180:MET:HE2	2.29	0.63
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.81	0.63
1:A:185:TYR:HE1	2:C:1087:TYR:OH	1.82	0.63
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.47	0.63
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.13	0.63
3:D:1287:ILE:HG21	3:D:1300:ALA:O	1.98	0.63
5:F:490:PRO:CG	5:F:493:LYS:HE3	2.21	0.63
3:J:905:ARG:HH21	3:J:907:HIS:CB	2.11	0.63
3:J:1361:THR:HG23	4:K:21:LEU:HD13	1.79	0.63
5:L:97:PRO:HA	5:L:100:MET:HG3	1.80	0.63
5:L:571:TYR:HD1	5:L:575:GLU:HG2	1.64	0.63
2:C:1184:THR:HG23	2:C:1189:GLY:HA3	1.81	0.63
3:D:73:GLY:O	3:D:76:LYS:HG3	1.99	0.63
2:I:42:ASP:OD2	2:I:46:GLN:HB3	1.97	0.63
2:I:119:GLU:HB2	2:I:489:PRO:HG2	1.80	0.63
2:I:819:SER:HB2	2:I:1085:MET:HG3	1.79	0.63
2:I:972:PHE:HE2	2:I:998:LEU:HD11	1.58	0.63
3:J:488:ASN:ND2	4:K:6:VAL:HG22	2.13	0.63
3:J:490:ILE:O	3:J:490:ILE:HG13	1.99	0.63
2:C:818:VAL:HB	2:C:1076:ILE:CD1	2.28	0.63
3:D:285:LEU:HB3	5:F:413:MET:HE1	1.81	0.63
3:D:514:THR:HG21	3:D:596:LEU:HB2	1.80	0.63
3:D:1290:ARG:CD	3:D:1294:ALA:HB1	2.29	0.63
3:D:1345:ARG:HD2	3:D:1370:MET:HE1	1.81	0.63
2:I:146:VAL:HG13	2:I:529:ARG:HB3	1.79	0.63
4:K:26:ARG:NH2	4:K:38:LEU:HD13	2.14	0.63
1:B:73:GLY:O	1:B:134:THR:HG22	1.99	0.62
3:D:146:VAL:HG23	3:D:158:GLN:O	1.99	0.62
3:D:205:LEU:HD13	3:D:205:LEU:O	1.99	0.62
5:F:337:VAL:HG12	5:F:341:LEU:HD12	1.79	0.62
1:G:169:GLY:O	1:G:171:LEU:HD22	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:515:MET:HE3	2:I:517:GLN:HB2	1.81	0.62
3:J:349:TYR:CD1	3:J:472:LEU:HD21	2.34	0.62
3:J:722:ILE:CD1	3:J:740:LEU:HD23	2.29	0.62
2:C:153:PRO:HB3	2:C:177:ILE:O	1.98	0.62
2:C:285:ILE:HD11	2:C:287:VAL:HG12	1.81	0.62
2:C:741:MET:HE3	2:C:974:ARG:NH2	2.13	0.62
2:C:1292:THR:HG21	2:C:1317:PRO:CB	2.29	0.62
3:D:8:LEU:HD23	3:D:9:LYS:H	1.64	0.62
3:D:161:THR:HG22	3:D:164:GLN:CG	2.29	0.62
3:D:232:ASN:ND2	3:D:1337:VAL:O	2.32	0.62
2:I:65:ASN:HB3	2:I:105:TYR:HD2	1.63	0.62
3:J:576:ARG:NH1	3:J:593:ASN:O	2.32	0.62
2:C:886:LYS:H	2:C:917:SER:HB3	1.63	0.62
3:D:19:ALA:HA	3:D:1344:LEU:HD12	1.81	0.62
2:I:175:ARG:HD3	2:I:183:TRP:HZ3	1.61	0.62
2:I:734:ILE:HD12	2:I:777:VAL:HG21	1.81	0.62
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.47	0.62
3:J:56:LEU:HD12	3:J:56:LEU:H	1.62	0.62
5:L:571:TYR:CD1	5:L:575:GLU:HG2	2.34	0.62
1:A:45:ARG:NH2	2:C:1215:GLY:O	2.31	0.62
2:C:338:THR:CG2	2:C:345:PRO:HB3	2.29	0.62
3:D:825:VAL:HG13	3:D:833:GLU:HB3	1.81	0.62
3:D:872:LEU:CD2	3:D:877:VAL:HG11	2.30	0.62
3:J:56:LEU:HD11	3:J:273:ILE:HD12	1.80	0.62
3:J:262:THR:C	5:L:507:MET:HB2	2.23	0.62
3:J:1263:LYS:NZ	3:J:1315:ALA:HB1	2.15	0.62
5:L:395:THR:OG1	5:L:396:ASN:N	2.30	0.62
1:A:31:LEU:CD1	1:A:201:LEU:HB2	2.30	0.62
2:C:309:LEU:HD11	2:C:311:CYS:O	1.99	0.62
3:D:526:VAL:HG12	3:D:549:LYS:HB2	1.80	0.62
5:F:134:VAL:HA	5:F:273:MET:HE1	1.81	0.62
1:H:59:VAL:HG22	1:H:144:ILE:HG23	1.81	0.62
2:I:21:VAL:HG11	2:I:592:ARG:HD2	1.82	0.62
2:I:211:ARG:HD3	2:I:357:ASN:O	2.00	0.62
2:I:832:HIS:ND1	2:I:1058:ARG:HD2	2.14	0.62
2:I:1136:GLN:O	2:I:1137:GLU:HB3	1.97	0.62
3:J:808:VAL:HG13	3:J:913:GLU:O	1.99	0.62
3:D:1203:ARG:NH2	3:D:1205:GLU:HG2	2.13	0.62
5:F:166:VAL:O	5:F:167:ASP:HB2	1.98	0.62
1:H:47:LEU:HD22	1:H:180:VAL:HG11	1.81	0.62
2:I:296:VAL:HB	2:I:336:LEU:HD12	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:770:CYS:HB2	2:I:791:LEU:CD2	2.30	0.62
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.80	0.62
5:L:363:ARG:CZ	5:L:367:ILE:HD11	2.30	0.62
2:C:13:LYS:NZ	2:C:1148:ALA:O	2.32	0.62
3:D:18:ASP:HB2	3:D:1373:ARG:CZ	2.29	0.62
5:F:423:ARG:HD2	5:F:425:TYR:CE2	2.34	0.62
5:F:492:ASP:HB2	5:F:495:ARG:NH1	2.07	0.62
1:G:66:HIS:CA	1:G:171:LEU:HD11	2.22	0.62
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.34	0.62
2:I:494:ASN:HB3	2:I:497:PRO:CD	2.30	0.62
2:I:839:VAL:HG12	2:I:1049:ILE:CG1	2.29	0.62
2:I:1101:LEU:HD23	3:J:725:MET:SD	2.39	0.62
3:J:53:ARG:HH22	3:J:60:ARG:HD2	1.65	0.62
3:J:807:LEU:HD23	3:J:915:ILE:HG13	1.82	0.62
2:C:109:ALA:HB1	2:C:111:GLU:CA	2.29	0.62
2:C:478:ARG:HG2	2:C:492:MET:HG2	1.80	0.62
3:D:849:LEU:H	3:D:849:LEU:HD22	1.65	0.62
3:D:1344:LEU:HD12	3:D:1344:LEU:N	2.15	0.62
1:G:230:ALA:HB3	1:G:231:PHE:CE2	2.35	0.62
1:H:59:VAL:HG13	1:H:144:ILE:HG12	1.82	0.62
2:I:658:GLN:O	2:I:661:VAL:HG22	1.98	0.62
3:J:222:LYS:HE2	3:J:1276:GLU:OE1	2.00	0.62
3:J:611:ILE:HG22	3:J:612:LEU:HD12	1.80	0.62
3:J:1265:THR:HG23	3:J:1305:ASP:OD2	1.99	0.62
5:L:111:LEU:HD11	5:L:119:ILE:HD12	1.82	0.62
2:C:696:ASP:O	2:C:697:LYS:HB3	2.00	0.62
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.35	0.62
2:C:817:LEU:HD11	2:C:1085:MET:HE1	1.81	0.62
1:G:195:ARG:HG2	1:G:198:LEU:HG	1.82	0.62
2:I:389:PHE:O	2:I:419:ILE:HG22	2.00	0.62
2:I:729:ALA:O	2:I:755:LYS:NZ	2.19	0.62
3:J:902:ASP:HB2	3:J:1251:LYS:HE3	1.82	0.62
5:L:354:THR:O	5:L:358:VAL:HG23	2.00	0.62
5:L:384:LEU:HD22	5:L:409:ASN:ND2	2.13	0.62
1:A:74:VAL:HG22	1:A:76:GLU:H	1.64	0.62
1:B:214:GLU:O	1:B:218:ARG:HG3	2.00	0.62
2:C:101:ARG:NH2	2:C:118:LYS:HE3	2.13	0.62
2:C:218:GLU:HG3	2:C:299:LYS:HA	1.81	0.62
2:C:688:GLN:OE1	2:C:1237:HIS:HE1	1.82	0.62
3:D:224:LEU:O	3:D:228:VAL:HG23	2.00	0.62
3:D:242:LEU:HD23	3:D:242:LEU:C	2.25	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:466:ILE:HD11	5:L:487:MET:HE3	1.80	0.62
2:C:42:ASP:OD2	2:C:46:GLN:HB3	2.00	0.61
3:D:800:LEU:HB3	3:D:920:ALA:CB	2.31	0.61
3:D:859:PRO:HG2	3:D:862:THR:CG2	2.30	0.61
2:I:820:GLU:HG2	2:I:824:GLN:HG3	1.80	0.61
3:J:824:PRO:HB2	3:J:826:ILE:HG23	1.81	0.61
3:J:905:ARG:HH21	3:J:907:HIS:HB2	1.65	0.61
4:K:26:ARG:HG2	4:K:59:ILE:HG21	1.81	0.61
5:L:486:ARG:CZ	5:L:486:ARG:HB2	2.29	0.61
1:B:101:THR:HG22	1:B:103:ASN:ND2	2.15	0.61
2:C:157:PHE:CE2	2:C:431:LYS:HG2	2.35	0.61
2:C:563:THR:OG1	2:C:564:PRO:HD2	1.99	0.61
3:D:16:GLU:HG3	3:D:1369:ARG:HH22	1.63	0.61
3:D:697:MET:SD	3:D:741:ALA:HB3	2.39	0.61
5:F:315:TRP:HZ2	5:F:341:LEU:HD21	1.65	0.61
2:I:109:ALA:HB1	2:I:111:GLU:N	2.15	0.61
2:I:344:GLY:HA3	2:I:346:TYR:CE2	2.35	0.61
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.82	0.61
5:F:341:LEU:HD23	5:F:344:LEU:HD23	1.82	0.61
5:F:484:ALA:HB1	5:F:491:GLU:CG	2.30	0.61
2:I:50:GLU:OE1	2:I:54:ARG:NE	2.34	0.61
2:I:452:ARG:HH12	2:I:585:GLY:HA3	1.63	0.61
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.83	0.61
3:J:488:ASN:HD21	4:K:6:VAL:CG2	2.13	0.61
3:J:709:ARG:O	3:J:711:GLY:N	2.32	0.61
2:C:720:ARG:NE	2:C:736:VAL:HG11	2.14	0.61
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.24	0.61
2:C:1289:GLU:OE2	3:D:473:THR:CG2	2.43	0.61
2:C:1308:ILE:HG23	3:D:380:PHE:CE2	2.35	0.61
3:D:156:ARG:NH2	3:D:191:SER:OG	2.33	0.61
4:E:26:ARG:NH1	4:E:29:GLN:OE1	2.32	0.61
5:F:348:GLU:HG2	5:F:354:THR:HA	1.81	0.61
2:I:49:LEU:HD12	2:I:73:TYR:CE2	2.36	0.61
2:I:103:VAL:HG12	2:I:116:ASP:CB	2.25	0.61
2:I:1087:TYR:CE1	2:I:1215:GLY:HA2	2.36	0.61
2:I:1101:LEU:O	3:J:731:ARG:HD3	2.00	0.61
3:J:72:CYS:SG	8:J:1502:ZN:ZN	1.87	0.61
3:J:702:GLN:HA	3:J:723:TYR:CE2	2.34	0.61
3:J:800:LEU:HD11	3:J:1309:ILE:HD13	1.81	0.61
3:J:1215:GLU:HG3	3:J:1220:ILE:HD11	1.82	0.61
2:C:289:VAL:HG13	2:C:319:LEU:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:553:THR:O	2:C:557:ARG:HD2	2.01	0.61
5:F:297:MET:HE3	5:F:330:LEU:HD11	1.83	0.61
5:F:585:GLU:HA	5:F:588:ARG:HD3	1.82	0.61
1:G:71:LYS:HB2	1:G:78:ILE:HD11	1.82	0.61
3:J:664:ILE:HD12	3:J:681:LYS:HG2	1.83	0.61
3:J:1253:ILE:O	3:J:1257:VAL:HG23	2.00	0.61
2:C:726:TYR:CZ	2:C:728:ASP:HB2	2.34	0.61
1:H:73:GLY:C	1:H:134:THR:HG22	2.26	0.61
5:L:492:ASP:O	5:L:495:ARG:NH1	2.33	0.61
2:C:30:ILE:HD11	2:C:575:LEU:HD22	1.82	0.61
2:C:484:LEU:CD1	2:C:485:ASP:H	2.14	0.61
3:J:128:LEU:HD23	3:J:192:MET:CE	2.31	0.61
3:J:325:LYS:HE2	3:J:330:MET:HG2	1.82	0.61
5:L:98:VAL:HA	5:L:402:LEU:HD21	1.83	0.61
1:A:10:LYS:HA	1:B:227:GLN:HE22	1.66	0.61
2:C:15:PHE:CE1	2:C:1194:GLU:HB3	2.36	0.61
2:C:1002:LEU:N	2:C:1008:GLN:OE1	2.33	0.61
2:C:1308:ILE:CG2	3:D:379:PRO:HB2	2.30	0.61
3:D:355:ILE:HG12	3:D:464:ASP:O	2.01	0.61
3:D:425:ARG:HG2	3:D:426:ALA:H	1.63	0.61
3:D:582:ILE:CD1	3:D:627:THR:HG21	2.30	0.61
3:D:647:PRO:HG3	3:D:697:MET:CA	2.31	0.61
2:I:157:PHE:CZ	2:I:431:LYS:HG2	2.35	0.61
3:J:1146:GLU:OE2	3:J:1310:THR:HG22	1.99	0.61
5:L:383:ASN:HB2	5:L:412:LEU:HD21	1.82	0.61
5:L:582:VAL:CG1	5:L:586:ARG:HG2	2.31	0.61
2:C:225:PHE:HZ	2:C:348:SER:H	1.49	0.61
2:C:1120:ALA:HB2	2:C:1199:LEU:HG	1.81	0.61
2:C:1142:ARG:HD3	2:C:1161:LEU:CD1	2.29	0.61
1:G:118:ASP:H	1:G:121:VAL:HB	1.65	0.61
2:I:1220:GLN:HG2	2:I:1221:PHE:H	1.65	0.61
3:J:1241:TYR:CD2	3:J:1246:VAL:HG11	2.35	0.61
2:C:46:GLN:OE1	2:C:47:TYR:N	2.33	0.61
2:C:453:ILE:CD1	2:C:587:LEU:HD11	2.30	0.61
5:F:280:VAL:HG11	5:F:355:ILE:HG23	1.83	0.61
3:J:64:PRO:HG3	3:J:90:VAL:HG12	1.83	0.61
3:J:902:ASP:CB	3:J:1251:LYS:HE3	2.30	0.61
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.82	0.60
2:C:91:THR:HG21	2:C:503:LYS:HZ2	1.65	0.60
2:C:1152:GLY:O	2:C:1153:ALA:HB2	2.01	0.60
3:D:93:THR:HG22	3:D:94:GLN:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:206:ALA:O	2:I:209:ILE:HG22	2.01	0.60
3:J:131:PRO:O	3:J:135:ILE:HG13	2.00	0.60
1:A:43:LEU:HD12	1:A:203:ILE:HD11	1.82	0.60
1:A:228:LEU:O	1:A:232:VAL:HG23	2.01	0.60
2:C:91:THR:HG21	2:C:503:LYS:NZ	2.15	0.60
5:F:137:TYR:CD2	5:F:273:MET:HE2	2.36	0.60
1:H:171:LEU:HB2	1:H:172:LEU:HD12	1.84	0.60
2:I:146:VAL:CG2	2:I:513:GLN:NE2	2.64	0.60
3:J:364:HIS:HB3	4:K:4:VAL:HG23	1.82	0.60
3:J:591:ILE:HG23	3:J:604:MET:HE2	1.83	0.60
2:C:169:LYS:O	2:C:169:LYS:HG2	2.02	0.60
3:D:495:ASN:ND2	3:D:497:GLU:HB2	2.16	0.60
3:D:843:VAL:HG13	3:D:883:ARG:HD3	1.82	0.60
1:G:44:ARG:HG3	1:G:183:ILE:CG2	2.31	0.60
1:H:48:LEU:HD22	3:J:535:ARG:HG3	1.83	0.60
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.83	0.60
4:K:27:ALA:HB1	4:K:46:THR:OG1	2.01	0.60
1:B:19:VAL:HB	1:B:23:HIS:NE2	2.17	0.60
2:C:58:PRO:HB3	2:C:69:GLN:HB3	1.83	0.60
2:C:303:ASP:OD2	2:C:328:SER:HB3	2.02	0.60
2:C:1122:LYS:HG2	2:C:1229:TYR:CE1	2.36	0.60
3:D:615:LYS:HB2	3:D:616:PRO:HD3	1.82	0.60
1:G:50:SER:HB2	1:H:8:PHE:CE1	2.35	0.60
2:I:119:GLU:HG3	2:I:489:PRO:N	2.16	0.60
3:J:883:ARG:NH1	3:J:897:HIS:HD2	2.00	0.60
2:C:832:HIS:CE1	2:C:1058:ARG:HD2	2.37	0.60
3:D:259:ARG:CZ	5:F:505:ILE:CD1	2.79	0.60
3:D:1140:ARG:HH21	3:D:1236:GLU:CG	2.14	0.60
5:F:555:GLU:HG2	5:F:590:ILE:HG22	1.82	0.60
2:I:237:LEU:HD11	2:I:292:ILE:HD11	1.83	0.60
2:I:1279:GLU:HG2	3:J:1357:ILE:HD13	1.83	0.60
3:J:22:ILE:HG23	3:J:1336:ALA:HA	1.82	0.60
2:C:688:GLN:OE1	2:C:1237:HIS:CE1	2.54	0.60
2:C:1247:SER:HB3	3:D:375:GLU:O	2.01	0.60
3:D:279:LEU:HD23	3:D:279:LEU:C	2.27	0.60
5:F:287:ILE:HD11	5:F:341:LEU:HG	1.84	0.60
1:G:57:THR:OG1	1:G:147:GLN:HG2	2.02	0.60
1:G:83:LEU:HD23	2:I:694:ARG:HH21	1.62	0.60
2:I:65:ASN:HB3	2:I:105:TYR:CD2	2.36	0.60
2:I:897:PRO:HB3	5:L:564:GLY:C	2.26	0.60
2:I:1150:ASP:O	2:I:1155:VAL:HG21	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:232:ASN:HA	3:J:236:TRP:CZ3	2.34	0.60
3:J:494:ALA:HB2	3:J:922:SER:HB3	1.83	0.60
2:C:646:SER:HB3	2:C:649:GLN:CG	2.24	0.60
3:D:337:ARG:HH12	3:D:1320:ILE:HG23	1.66	0.60
1:H:118:ASP:H	1:H:121:VAL:HB	1.66	0.60
1:H:206:GLU:OE1	3:J:531:LYS:NZ	2.22	0.60
2:I:619:ALA:CB	2:I:657:THR:HA	2.31	0.60
3:J:154:LEU:HD23	3:J:160:LEU:HD21	1.83	0.60
3:J:215:LYS:O	3:J:218:THR:HG22	2.02	0.60
3:J:1280:VAL:HG21	3:J:1304:ARG:CD	2.31	0.60
5:L:484:ALA:CB	5:L:491:GLU:HB2	2.23	0.60
1:B:49:SER:O	1:B:151:GLY:HA2	2.00	0.60
2:C:130:MET:SD	2:C:134:GLY:HA2	2.42	0.60
2:C:161:LYS:HA	2:C:170:VAL:HA	1.83	0.60
2:C:221:LEU:HD21	2:C:351:LEU:HD12	1.84	0.60
2:C:596:ASP:OD2	2:C:598:VAL:HG23	2.01	0.60
3:D:93:THR:HG22	3:D:94:GLN:H	1.66	0.60
1:G:231:PHE:CB	1:H:218:ARG:HH11	2.14	0.60
3:J:1158:GLU:O	3:J:1206:ARG:NH1	2.35	0.60
3:J:1233:ILE:HG21	3:J:1257:VAL:HG22	1.82	0.60
5:L:147:GLN:HE22	5:L:150:ARG:HH11	1.48	0.60
1:A:50:SER:CB	1:B:8:PHE:HZ	2.15	0.60
1:B:182:ARG:NH1	3:D:534:GLU:OE1	2.34	0.60
1:B:90:VAL:HG22	1:B:91:ARG:N	2.17	0.60
2:C:705:GLU:HB2	2:C:794:LEU:H	1.67	0.60
2:C:1248:THR:HB	5:F:532:LEU:CD1	2.31	0.60
3:D:77:ARG:HG3	3:D:79:LYS:H	1.66	0.60
3:D:363:LEU:HA	3:D:450:HIS:CD2	2.37	0.60
3:D:1347:LEU:HG	3:D:1357:ILE:CG2	2.32	0.60
5:F:137:TYR:CD2	5:F:273:MET:HG2	2.37	0.60
1:G:48:LEU:CA	1:G:180:VAL:HG21	2.25	0.60
3:J:126:LEU:HD12	3:J:127:LEU:N	2.17	0.60
2:C:30:ILE:HD11	2:C:575:LEU:CD2	2.32	0.59
3:D:154:LEU:CD2	3:D:160:LEU:HD11	2.32	0.59
3:D:515:ARG:O	3:D:545:HIS:HB3	2.02	0.59
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.66	0.59
1:H:158:ARG:CG	1:H:172:LEU:HD23	2.31	0.59
2:I:55:SER:OG	2:I:56:VAL:N	2.35	0.59
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.83	0.59
2:I:1280:ALA:CB	3:J:918:ILE:HG22	2.32	0.59
3:J:62:PHE:CD1	3:J:247:PRO:HD3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:121:PRO:HG2	3:J:123:ARG:NH2	2.17	0.59
3:J:416:ILE:HG12	3:J:441:LEU:CD2	2.31	0.59
3:J:426:ALA:CB	3:J:427:PRO:HD3	2.29	0.59
2:C:170:VAL:HG23	2:C:171:LEU:N	2.15	0.59
2:C:698:PRO:HD3	2:C:795:ALA:HA	1.84	0.59
2:C:1116:HIS:CE1	3:D:641:ILE:H	2.20	0.59
3:D:11:GLN:HG2	3:D:15:GLU:CG	2.31	0.59
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.35	0.59
3:J:115:TRP:CE2	3:J:1329:THR:HG23	2.37	0.59
5:L:313:ASP:OD1	5:L:338:HIS:NE2	2.36	0.59
5:L:492:ASP:HB2	5:L:495:ARG:NH1	2.08	0.59
1:A:182:ARG:O	1:A:183:ILE:HD12	2.03	0.59
2:C:30:ILE:CD1	2:C:575:LEU:HD22	2.32	0.59
2:C:243:PRO:HB2	2:C:278:GLU:CG	2.32	0.59
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.35	0.59
3:D:140:TYR:HB3	5:F:100:MET:SD	2.42	0.59
3:D:552:ILE:HG21	3:D:589:TYR:CE1	2.38	0.59
5:F:298:PRO:HD2	5:F:326:TRP:HB3	1.83	0.59
5:F:463:LEU:HD22	5:F:483:LEU:CD2	2.32	0.59
1:G:56:VAL:CG1	1:G:86:LYS:HA	2.32	0.59
2:I:119:GLU:HG3	2:I:489:PRO:CD	2.31	0.59
2:I:802:VAL:HG23	2:I:1098:LEU:HD13	1.84	0.59
2:I:886:LYS:CE	2:I:916:SER:HB3	2.31	0.59
2:I:891:GLY:C	2:I:892:GLU:HG3	2.28	0.59
2:I:1063:GLY:O	3:J:354:VAL:HG11	2.02	0.59
2:I:1288:GLN:NE2	3:J:1355:ARG:HA	2.16	0.59
3:J:1347:LEU:HG	3:J:1357:ILE:CG2	2.32	0.59
1:A:10:LYS:HA	1:B:227:GLN:NE2	2.17	0.59
2:C:149:LEU:HD12	2:C:452:ARG:O	2.02	0.59
2:C:269:ILE:HG23	2:C:273:HIS:CB	2.31	0.59
2:C:901:LEU:HD13	5:F:563:PHE:CE2	2.38	0.59
3:D:418:GLU:H	4:E:45:LYS:HZ3	1.48	0.59
1:H:43:LEU:N	1:H:43:LEU:HD12	2.17	0.59
2:I:302:ILE:HG22	2:I:309:LEU:HA	1.83	0.59
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.84	0.59
5:L:322:MET:HE3	5:L:324:LYS:HZ3	1.66	0.59
1:A:57:THR:O	1:A:173:VAL:HG22	2.02	0.59
2:C:519:ASN:O	2:C:522:SER:HB3	2.01	0.59
2:C:1292:THR:HG21	2:C:1317:PRO:HB2	1.84	0.59
3:D:36:GLY:HA3	3:D:61:ILE:HG23	1.83	0.59
3:D:518:VAL:HG11	3:D:707:ILE:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1273:ASP:HB2	3:D:1276:GLU:CD	2.27	0.59
1:H:83:LEU:HD21	3:J:526:VAL:HB	1.85	0.59
2:I:1287:LEU:HD22	3:J:1357:ILE:CD1	2.33	0.59
3:J:128:LEU:HA	3:J:192:MET:HE1	1.83	0.59
1:A:169:GLY:O	1:A:171:LEU:HD22	2.03	0.59
1:B:77:ASP:O	1:B:81:ILE:HG13	2.02	0.59
2:C:109:ALA:CB	2:C:111:GLU:HA	2.33	0.59
2:C:241:LEU:HD11	2:C:246:LEU:CD1	2.30	0.59
2:C:1285:TYR:CD2	3:D:1356:LEU:HD21	2.37	0.59
3:D:510:LEU:HG	3:D:513:MET:CE	2.31	0.59
3:D:536:LEU:HD13	3:D:541:LEU:CB	2.30	0.59
3:D:722:ILE:HA	3:D:725:MET:HE3	1.84	0.59
3:D:1171:GLY:HA2	3:D:1193:TRP:CZ3	2.35	0.59
3:D:1280:VAL:CG2	3:D:1304:ARG:HE	2.01	0.59
5:F:561:MET:HE2	5:F:567:MET:HE1	1.85	0.59
1:G:159:ILE:O	1:G:159:ILE:HG12	2.02	0.59
2:I:1284:ALA:CB	3:J:1356:LEU:HD22	2.31	0.59
5:L:348:GLU:HA	5:L:353:LEU:O	2.02	0.59
2:C:1281:TYR:CE2	3:D:431:ARG:HG3	2.37	0.59
2:C:1299:ASN:ND2	2:C:1303:LYS:HE2	2.15	0.59
4:K:27:ALA:HB2	4:K:50:ALA:CB	2.32	0.59
1:A:59:VAL:HG21	1:A:85:LEU:CD1	2.33	0.59
2:C:125:GLY:HA2	2:C:499:SER:HB2	1.85	0.59
3:D:812:ASP:HB2	3:D:911:LYS:HZ1	1.68	0.59
5:F:561:MET:HG3	5:F:571:TYR:CD2	2.38	0.59
1:H:64:VAL:HG11	1:H:69:SER:HG	1.66	0.59
2:I:483:ASP:HB2	2:I:486:THR:CG2	2.33	0.59
2:I:806:PRO:HB3	3:J:505:ASP:OD1	2.03	0.59
2:I:1184:THR:HG23	2:I:1189:GLY:HA3	1.85	0.59
3:J:797:THR:CG2	3:J:924:GLY:HA3	2.30	0.59
5:L:362:ASN:HB2	5:L:365:MET:CE	2.32	0.59
1:A:28:LEU:HD12	1:A:28:LEU:N	2.18	0.59
1:B:37:HIS:NE2	2:C:1216:ARG:HD2	2.17	0.59
2:C:1131:MET:CE	2:C:1141:LEU:HA	2.33	0.59
3:D:706:VAL:HG12	3:D:715:LYS:HB3	1.84	0.59
4:E:44:ASP:HB3	4:E:48:VAL:HB	1.85	0.59
2:I:607:SER:N	2:I:610:GLU:OE1	2.33	0.59
3:J:400:MET:HE3	3:J:405:GLU:OE1	2.03	0.59
1:A:9:LEU:HD11	1:A:198:LEU:HD11	1.84	0.59
1:A:187:VAL:HG12	1:A:201:LEU:HD13	1.85	0.59
2:C:397:LEU:HB3	2:C:401:GLY:HA3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1158:LYS:C	2:I:1159:VAL:HG22	2.28	0.59
2:I:1331:ARG:HG2	3:J:33:TRP:CH2	2.37	0.59
2:C:640:GLY:O	2:C:641:GLU:HG3	2.03	0.58
2:C:678:ARG:CZ	2:C:1106:ARG:HG2	2.33	0.58
2:C:819:SER:HB2	2:C:1085:MET:CG	2.33	0.58
2:C:1307:ASN:HB3	2:C:1312:ASN:O	2.03	0.58
3:D:161:THR:HG22	3:D:164:GLN:CB	2.33	0.58
3:D:426:ALA:CB	3:D:427:PRO:HD3	2.31	0.58
3:D:831:VAL:O	3:D:831:VAL:HG13	2.03	0.58
5:F:503:GLU:CD	5:F:504:PRO:HD2	2.27	0.58
2:I:90:VAL:HG12	2:I:91:THR:H	1.67	0.58
2:I:400:VAL:HG22	2:I:584:TYR:HD1	1.68	0.58
1:A:36:GLY:HA3	1:A:187:VAL:CG1	2.33	0.58
3:D:233:LYS:HB3	3:D:235:GLU:OE2	2.02	0.58
3:D:418:GLU:HG3	4:E:45:LYS:H	1.68	0.58
3:D:840:LEU:HG	3:D:841:GLY:N	2.15	0.58
2:I:724:VAL:CG1	2:I:727:VAL:HG22	2.33	0.58
3:J:514:THR:HG21	3:J:596:LEU:CB	2.31	0.58
3:J:850:LYS:HD3	3:J:875:ASN:HD21	1.68	0.58
5:L:470:MET:CE	5:L:482:GLU:HG2	2.31	0.58
1:A:150:ARG:HD2	1:B:8:PHE:CZ	2.38	0.58
1:B:19:VAL:O	1:B:20:SER:HB3	2.01	0.58
3:D:416:ILE:HG12	3:D:441:LEU:HD21	1.85	0.58
3:D:518:VAL:N	3:D:716:GLN:HE22	2.01	0.58
3:D:842:ARG:HB3	3:D:882:VAL:CG1	2.33	0.58
5:F:470:MET:HE2	5:F:478:PRO:HB3	1.85	0.58
2:I:223:LEU:CD1	2:I:426:ILE:HD13	2.31	0.58
3:J:1251:LYS:O	3:J:1254:GLU:HB2	2.02	0.58
5:L:123:ILE:HD13	5:L:376:LYS:HG2	1.85	0.58
5:F:343:LYS:O	5:F:347:ILE:HG13	2.04	0.58
1:G:164:ASP:OD1	1:G:166:ARG:HB2	2.02	0.58
1:H:158:ARG:HB3	1:H:172:LEU:CD2	2.33	0.58
3:J:864:LEU:N	3:J:864:LEU:HD23	2.18	0.58
3:J:1263:LYS:HZ1	3:J:1315:ALA:HB1	1.69	0.58
4:K:60:ASN:ND2	4:K:63:ILE:HD13	2.19	0.58
5:L:281:ARG:HG3	5:L:285:ARG:HH11	1.66	0.58
5:L:284:GLU:HG2	5:L:310:GLU:OE1	2.03	0.58
5:L:372:ALA:O	5:L:376:LYS:HG3	2.03	0.58
5:L:390:ILE:HD12	5:L:435:ILE:HG21	1.84	0.58
2:C:231:GLU:O	2:C:238:GLN:N	2.36	0.58
2:C:324:LYS:HA	2:C:327:GLN:HE21	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1165:SER:HA	2:C:1169:VAL:HG21	1.85	0.58
2:C:1209:GLN:HB3	2:C:1224:PRO:HB2	1.86	0.58
5:F:298:PRO:CD	5:F:326:TRP:HB3	2.34	0.58
1:G:218:ARG:NH1	1:H:232:VAL:H	2.01	0.58
3:J:288:PRO:HG2	3:J:291:ILE:HG13	1.86	0.58
5:L:135:ALA:HB1	5:L:253:SER:HA	1.86	0.58
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.85	0.58
3:D:331:ILE:CG2	3:D:1328:THR:HG21	2.33	0.58
3:D:1150:PRO:HG3	3:D:1214:PRO:HB2	1.85	0.58
1:G:10:LYS:HE2	1:H:229:GLU:OE1	2.03	0.58
1:G:11:PRO:HD3	1:H:227:GLN:CD	2.27	0.58
2:I:91:THR:HA	2:I:138:ILE:O	2.03	0.58
2:C:1256:GLN:HB3	2:C:1301:ARG:HH22	1.69	0.58
3:D:698:MET:O	3:D:702:GLN:HB3	2.04	0.58
3:D:1165:PHE:HD2	3:D:1173:ARG:CD	2.17	0.58
3:D:1314:LEU:HD12	3:D:1326:GLN:CD	2.28	0.58
2:I:854:ILE:HD11	2:I:885:GLY:CA	2.34	0.58
3:J:179:LYS:HB2	3:J:184:ALA:CB	2.33	0.58
3:J:653:ILE:HG21	3:J:692:ARG:HB2	1.86	0.58
3:J:1198:VAL:HG11	3:J:1210:ILE:HG23	1.85	0.58
3:J:1203:ARG:HH12	3:J:1205:GLU:HG2	1.68	0.58
1:B:205:MET:CE	1:B:213:PRO:HA	2.34	0.58
2:C:557:ARG:HH21	2:C:607:SER:C	2.12	0.58
2:C:594:VAL:HG11	2:C:650:VAL:HG23	1.86	0.58
2:C:1336:ASN:CG	3:D:29:MET:HE3	2.29	0.58
3:D:147:ILE:CG2	3:D:188:LEU:HG	2.32	0.58
3:D:697:MET:O	3:D:701:LEU:HB2	2.03	0.58
1:G:161:SER:O	1:G:163:GLU:N	2.36	0.58
2:I:17:LYS:HZ2	2:I:1154:ASP:HB3	1.68	0.58
2:I:556:GLY:HA2	2:I:659:GLN:O	2.04	0.58
3:J:863:LEU:CD1	3:J:901:ARG:HB3	2.26	0.58
2:C:156:PHE:HE1	2:C:443:ASP:HB2	1.65	0.58
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.86	0.58
1:H:20:SER:OG	1:H:21:SER:N	2.36	0.58
2:I:1304:MET:O	2:I:1307:ASN:N	2.37	0.58
3:J:502:PRO:HB3	3:J:506:VAL:CG2	2.33	0.58
3:J:744:ARG:HG3	3:J:744:ARG:O	2.03	0.58
2:C:75:LEU:HD22	2:C:75:LEU:N	2.19	0.58
2:C:84:GLU:OE2	2:C:1032:LYS:HE3	2.04	0.58
2:C:619:ALA:HB2	2:C:654:ASP:CB	2.34	0.58
2:C:798:GLN:OE1	2:C:827:ARG:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:980:VAL:HG13	2:C:984:VAL:CG2	2.34	0.58
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.39	0.58
3:D:11:GLN:HB2	3:D:15:GLU:OE2	2.03	0.58
3:D:342:LEU:HA	3:D:343:LEU:HD12	1.81	0.58
3:D:674:THR:OG1	3:D:677:GLU:HB2	2.04	0.58
3:D:1293:GLU:OE1	3:D:1294:ALA:N	2.34	0.58
5:F:335:GLU:OE2	5:F:339:ARG:HG3	2.04	0.58
1:H:132:HIS:O	1:H:133:LEU:HD12	2.04	0.58
1:H:183:ILE:CD1	1:H:205:MET:HG3	2.34	0.58
1:H:213:PRO:O	1:H:217:ILE:HG13	2.03	0.58
2:I:996:ARG:HD2	2:I:999:GLU:OE1	2.04	0.58
2:I:1256:GLN:HB3	2:I:1301:ARG:HH22	1.67	0.58
3:J:30:ILE:HD13	3:J:243:PRO:CD	2.34	0.58
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.86	0.58
3:J:598:LYS:O	3:J:601:ILE:HG22	2.04	0.58
1:A:110:VAL:HG21	1:A:140:ILE:HD11	1.87	0.57
1:A:166:ARG:N	1:A:167:PRO:HD2	2.18	0.57
2:C:53:PHE:CE1	2:C:468:LEU:HD11	2.39	0.57
2:C:1105:SER:HB2	3:D:731:ARG:CG	2.34	0.57
3:D:514:THR:HG21	3:D:596:LEU:CB	2.34	0.57
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.85	0.57
3:D:1309:ILE:HG13	3:D:1310:THR:H	1.69	0.57
5:F:324:LYS:HG3	5:F:326:TRP:CZ2	2.39	0.57
2:I:688:GLN:O	2:I:1235:LEU:HA	2.03	0.57
2:I:1106:ARG:HD2	2:I:1106:ARG:H	1.69	0.57
2:I:1295:SER:HB2	3:J:347:VAL:HG22	1.86	0.57
2:C:1134:GLN:C	2:C:1135:GLN:HG2	2.28	0.57
3:D:436:ALA:HB3	3:D:485:MET:HA	1.85	0.57
5:F:297:MET:HE2	5:F:326:TRP:CE3	2.39	0.57
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.86	0.57
3:J:422:LEU:HD13	3:J:471:PRO:HG3	1.86	0.57
3:J:423:LEU:CD1	3:J:468:VAL:HG12	2.34	0.57
3:J:583:VAL:HG13	3:J:587:LEU:HD22	1.86	0.57
3:J:1291:GLU:C	3:J:1292:LEU:HD12	2.29	0.57
5:L:137:TYR:CD2	5:L:273:MET:HE2	2.39	0.57
2:C:145:ILE:HG22	2:C:456:VAL:HG22	1.86	0.57
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.86	0.57
2:C:906:PHE:CE2	5:F:608:ARG:HG3	2.38	0.57
2:C:1305:TYR:CZ	5:F:532:LEU:HG	2.39	0.57
2:C:1336:ASN:OD1	3:D:29:MET:HE3	2.04	0.57
3:D:45:ASN:O	3:D:46:TYR:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:166:ARG:N	1:G:167:PRO:HD2	2.19	0.57
1:H:11:PRO:HB2	1:H:28:LEU:HD11	1.86	0.57
2:I:109:ALA:HB1	2:I:110:PRO:O	2.03	0.57
2:I:233:ARG:HH12	2:I:332:ARG:NH1	2.02	0.57
3:J:53:ARG:NH2	3:J:60:ARG:HD2	2.19	0.57
3:J:1144:LEU:HD11	3:J:1236:GLU:HB3	1.86	0.57
1:B:197:ASP:C	1:B:198:LEU:HD22	2.29	0.57
2:C:494:ASN:O	2:C:498:ILE:HD13	2.04	0.57
2:C:673:HIS:HB3	2:C:1109:ILE:CG2	2.33	0.57
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.87	0.57
3:J:275:ARG:HD3	3:J:298:MET:HE2	1.86	0.57
3:J:363:LEU:HD23	3:J:487:THR:CG2	2.27	0.57
3:J:1278:GLU:OE2	3:J:1282:TYR:HD2	1.87	0.57
5:L:108:VAL:HG11	5:L:381:GLU:C	2.29	0.57
2:C:239:MET:O	2:C:284:LEU:HD12	2.04	0.57
2:C:529:ARG:HH12	6:C:2001:KNG:C17	2.18	0.57
2:C:560:PRO:HB3	3:D:776:THR:HG21	1.87	0.57
3:D:870:ASP:O	3:D:874:GLU:HG2	2.04	0.57
1:G:133:LEU:HD11	1:G:138:ALA:O	2.04	0.57
1:G:231:PHE:HB3	1:H:218:ARG:HD3	1.86	0.57
2:I:1246:ARG:CZ	2:I:1258:PRO:HB3	2.35	0.57
5:L:147:GLN:HB3	5:L:161:LEU:CD1	2.35	0.57
3:D:364:HIS:HB3	3:D:487:THR:CG2	2.34	0.57
3:D:514:THR:HG21	3:D:596:LEU:HG	1.86	0.57
2:I:5:TYR:HB2	2:I:781:ASP:OD1	2.05	0.57
2:I:810:TYR:CE1	2:I:1078:LYS:HB2	2.39	0.57
3:J:482:ALA:HB3	4:K:20:VAL:HG22	1.85	0.57
2:C:302:ILE:HG22	2:C:309:LEU:N	2.19	0.57
2:C:599:VAL:HG21	2:C:629:PHE:HE1	1.69	0.57
2:C:1066:MET:HE1	2:C:1076:ILE:HB	1.87	0.57
3:D:218:THR:HA	3:D:221:ILE:HG22	1.86	0.57
3:D:1165:PHE:HD2	3:D:1173:ARG:HD2	1.68	0.57
3:D:1234:VAL:O	3:D:1238:GLN:HB2	2.04	0.57
2:I:696:ASP:CB	2:I:798:GLN:HG2	2.31	0.57
5:L:322:MET:HE2	5:L:324:LYS:HG2	1.86	0.57
2:C:55:SER:OG	2:C:56:VAL:N	2.36	0.57
2:C:1017:GLN:O	2:C:1021:LEU:HG	2.05	0.57
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.87	0.57
3:D:11:GLN:HG2	3:D:15:GLU:HG2	1.85	0.57
3:D:612:LEU:HB3	3:D:616:PRO:HG2	1.87	0.57
3:D:689:ALA:O	3:D:693:VAL:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:547:VAL:HG23	5:F:603:ARG:HH11	1.70	0.57
2:I:62:TYR:CE1	2:I:476:LYS:HB3	2.39	0.57
2:I:487:LEU:CD1	2:I:492:MET:HE2	2.35	0.57
3:J:623:GLN:O	3:J:627:THR:HG22	2.04	0.57
3:J:657:ALA:O	3:J:661:VAL:HG12	2.04	0.57
2:C:231:GLU:HG2	2:C:332:ARG:NH2	2.19	0.57
2:C:488:MET:O	2:C:490:GLN:N	2.35	0.57
2:C:599:VAL:CG2	2:C:629:PHE:HE1	2.18	0.57
2:C:617:ALA:HA	2:C:636:CYS:SG	2.44	0.57
3:D:825:VAL:CG1	3:D:833:GLU:HB3	2.34	0.57
3:D:1372:ARG:HH21	3:J:854:ALA:HB3	1.69	0.57
5:F:483:LEU:H	5:F:483:LEU:HD12	1.70	0.57
2:I:169:LYS:O	2:I:169:LYS:HG2	2.05	0.57
3:J:127:LEU:HD21	3:J:234:PRO:HG3	1.87	0.57
3:J:147:ILE:O	3:J:177:ASP:HB3	2.05	0.57
1:A:166:ARG:O	1:A:167:PRO:C	2.48	0.57
2:C:535:PRO:HG2	2:C:536:GLY:H	1.69	0.57
3:D:901:ARG:HA	3:D:908:ILE:HA	1.87	0.57
5:F:230:VAL:HG13	5:F:231:THR:H	1.70	0.57
5:F:402:LEU:HA	5:F:405:ILE:HG12	1.86	0.57
5:F:569:THR:OG1	5:F:570:ASP:N	2.32	0.57
2:I:17:LYS:HE3	2:I:1154:ASP:HB3	1.86	0.57
2:I:870:ILE:HG21	2:I:931:VAL:HG11	1.86	0.57
2:I:1299:ASN:HD22	2:I:1303:LYS:CE	2.17	0.57
3:J:251:PRO:HD2	5:L:507:MET:HE1	1.86	0.57
3:J:1144:LEU:CD1	3:J:1236:GLU:HB3	2.35	0.57
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.05	0.57
2:C:98:VAL:HB	2:C:124:MET:HE3	1.87	0.56
2:C:657:THR:OG1	2:C:1187:PHE:HB2	2.05	0.56
2:C:1086:PRO:O	2:C:1094:VAL:HG12	2.05	0.56
3:D:294:ASN:HD22	5:F:406:GLN:NE2	2.01	0.56
3:D:392:THR:HG21	5:F:606:VAL:HA	1.87	0.56
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.70	0.56
5:F:315:TRP:O	5:F:319:ALA:HB3	2.05	0.56
1:H:61:ILE:HG23	1:H:142:MET:HE2	1.87	0.56
2:I:30:ILE:HD11	2:I:575:LEU:HD22	1.86	0.56
2:I:101:ARG:HE	2:I:118:LYS:HD2	1.70	0.56
2:I:208:ILE:HD11	2:I:365:GLU:HB3	1.86	0.56
2:I:696:ASP:O	2:I:697:LYS:HB3	2.05	0.56
2:I:832:HIS:CE1	2:I:1058:ARG:HD2	2.40	0.56
2:I:971:LEU:HD22	2:I:1018:TYR:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:165:TYR:O	3:J:169:LEU:HB2	2.05	0.56
3:J:583:VAL:HG21	3:J:592:VAL:HG11	1.87	0.56
3:J:1142:ALA:O	3:J:1146:GLU:HB2	2.05	0.56
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.40	0.56
2:C:1132:LEU:HD22	2:C:1177:ARG:CZ	2.35	0.56
3:D:849:LEU:CB	3:D:853:THR:HG23	2.35	0.56
5:F:311:THR:HG21	5:F:348:GLU:CD	2.30	0.56
1:G:231:PHE:HB3	1:H:218:ARG:CG	2.34	0.56
2:I:62:TYR:C	2:I:64:GLY:H	2.12	0.56
2:I:808:ASN:H	3:J:633:ALA:HB2	1.70	0.56
2:I:1122:LYS:HE2	2:I:1178:LYS:O	2.06	0.56
2:I:1238:LEU:H	2:I:1238:LEU:CD1	2.10	0.56
3:J:233:LYS:HB3	3:J:235:GLU:OE2	2.06	0.56
3:J:521:LYS:HE3	3:J:541:LEU:O	2.04	0.56
3:J:809:VAL:HA	3:J:894:VAL:O	2.05	0.56
4:K:53:GLU:OE1	4:K:59:ILE:HG13	2.05	0.56
1:A:218:ARG:HH12	1:B:231:PHE:HA	1.69	0.56
2:C:2:VAL:O	2:C:3:TYR:CB	2.53	0.56
2:C:211:ARG:HD3	2:C:357:ASN:O	2.05	0.56
2:C:309:LEU:HD21	2:C:312:ALA:CA	2.35	0.56
2:C:469:VAL:O	2:C:472:GLU:HB3	2.04	0.56
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.87	0.56
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.40	0.56
2:C:738:GLU:HA	2:C:741:MET:HE2	1.87	0.56
3:D:19:ALA:O	3:D:20:ILE:HG13	2.05	0.56
3:D:267:ASP:HA	3:D:270:ARG:NH2	2.18	0.56
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.40	0.56
3:D:1142:ALA:O	3:D:1146:GLU:HB2	2.06	0.56
5:F:511:ILE:O	5:F:511:ILE:HG23	2.06	0.56
1:G:50:SER:HB2	1:H:8:PHE:HE1	1.70	0.56
1:H:76:GLU:HB3	1:H:81:ILE:HG12	1.86	0.56
1:H:215:GLU:OE1	1:H:219:ARG:NH1	2.38	0.56
2:I:563:THR:HG22	2:I:680:LEU:HD11	1.88	0.56
2:I:1065:LYS:HE2	3:J:462:ASP:O	2.05	0.56
2:I:1308:ILE:CG2	3:J:379:PRO:HB2	2.35	0.56
3:J:69:GLU:HG3	3:J:76:LYS:HA	1.88	0.56
3:J:615:LYS:HB2	3:J:616:PRO:HD3	1.86	0.56
3:J:832:LYS:HD3	3:J:1242:ARG:HH12	1.69	0.56
2:C:367:TYR:HD2	2:C:376:PRO:HB3	1.70	0.56
2:C:1238:LEU:HD12	2:C:1238:LEU:N	2.20	0.56
2:C:1308:ILE:HG21	3:D:379:PRO:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:357:VAL:HG22	3:D:461:PHE:CD1	2.40	0.56
3:D:905:ARG:HH21	3:D:907:HIS:CG	2.23	0.56
5:F:513:ASP:C	5:F:515:GLU:H	2.13	0.56
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.39	0.56
3:J:1318:SER:OG	3:J:1342:ASP:OD2	2.19	0.56
3:J:1358:PRO:HB3	3:J:1366:HIS:CD2	2.41	0.56
5:F:280:VAL:HG22	5:F:347:ILE:CD1	2.25	0.56
2:I:109:ALA:HB1	2:I:111:GLU:HA	1.87	0.56
2:I:397:LEU:HB3	2:I:401:GLY:HA3	1.87	0.56
3:J:355:ILE:HD13	3:J:466:MET:HG3	1.87	0.56
3:J:650:LYS:NZ	3:J:765:GLU:OE2	2.37	0.56
3:J:1264:ALA:HB2	3:J:1304:ARG:HA	1.88	0.56
5:L:119:ILE:CG2	5:L:375:ALA:HB1	2.32	0.56
1:B:11:PRO:CB	1:B:28:LEU:HD11	2.32	0.56
2:C:1065:LYS:CD	2:C:1235:LEU:HD12	2.35	0.56
5:F:463:LEU:HD22	5:F:483:LEU:HD22	1.86	0.56
1:G:11:PRO:HB3	1:G:31:LEU:HD23	1.86	0.56
1:H:142:MET:SD	1:H:144:ILE:HD11	2.46	0.56
2:I:39:ILE:HD11	2:I:75:LEU:HG	1.87	0.56
3:J:289:ASP:HB3	3:J:293:ARG:NH2	2.20	0.56
3:J:825:VAL:HG13	3:J:833:GLU:HB3	1.87	0.56
5:L:470:MET:HE1	5:L:482:GLU:CG	2.33	0.56
1:B:210:THR:O	1:B:211:ILE:HD13	2.05	0.56
2:C:619:ALA:N	2:C:654:ASP:HB2	2.21	0.56
3:D:1237:VAL:HG13	3:D:1253:ILE:HD13	1.88	0.56
5:F:584:ARG:HA	5:F:584:ARG:HH11	1.71	0.56
2:I:16:GLY:O	2:I:1156:ARG:HG2	2.06	0.56
2:I:109:ALA:HB1	2:I:111:GLU:CA	2.36	0.56
2:I:169:LYS:HE2	2:I:190:PRO:O	2.05	0.56
3:J:863:LEU:C	3:J:864:LEU:HD23	2.30	0.56
5:L:540:LEU:O	5:L:540:LEU:HD23	2.06	0.56
2:C:878:THR:HG23	2:C:881:ASP:OD2	2.05	0.56
2:C:1276:TRP:CZ2	3:D:801:VAL:HG21	2.40	0.56
2:I:495:ALA:HB3	5:L:471:LEU:HD22	1.87	0.56
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.88	0.56
3:J:861:ASN:HD22	3:J:883:ARG:NH1	2.03	0.56
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.87	0.56
1:G:112:ALA:O	1:G:115:ILE:HG13	2.05	0.56
2:I:1327:LEU:HD23	2:I:1331:ARG:HH21	1.69	0.56
5:L:412:LEU:HB2	5:L:435:ILE:HD11	1.88	0.56
2:C:722:GLY:HA3	2:C:735:LYS:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1043:ALA:O	2:C:1046:VAL:HG12	2.06	0.56
2:C:1142:ARG:HH22	2:C:1165:SER:CB	2.17	0.56
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.21	0.56
1:G:51:MET:HE1	1:G:216:ALA:CA	2.31	0.56
1:H:97:GLU:HB2	1:H:146:VAL:O	2.06	0.56
3:J:1241:TYR:HD2	3:J:1246:VAL:CG1	2.19	0.56
1:A:12:ARG:H	1:A:30:PRO:HD2	1.71	0.55
1:A:231:PHE:HE2	1:B:39:LEU:HD13	1.72	0.55
2:C:1124:ILE:HB	2:C:1180:MET:HB2	1.88	0.55
1:G:11:PRO:HD3	1:H:227:GLN:OE1	2.06	0.55
1:G:104:LYS:CG	1:G:110:VAL:HG22	2.30	0.55
1:G:165:GLU:C	1:G:167:PRO:HD2	2.31	0.55
1:H:89:ALA:HB3	1:H:124:VAL:CG1	2.36	0.55
1:H:130:ILE:HG22	1:H:131:CYS:SG	2.47	0.55
2:I:590:PRO:HB2	2:I:655:VAL:HG21	1.89	0.55
2:I:670:PHE:HZ	2:I:1117:LEU:HD13	1.71	0.55
3:J:1197:ASN:CB	3:J:1211:SER:HA	2.36	0.55
3:J:1293:GLU:O	3:J:1294:ALA:C	2.49	0.55
5:L:479:THR:HG23	5:L:481:GLU:H	1.71	0.55
1:A:73:GLY:C	1:A:134:THR:HG22	2.31	0.55
1:A:214:GLU:O	1:A:217:ILE:HG22	2.06	0.55
1:B:23:HIS:CB	1:B:206:GLU:HG2	2.36	0.55
2:C:215:TYR:HE2	2:C:422:LYS:HD2	1.71	0.55
3:D:363:LEU:O	3:D:363:LEU:CG	2.47	0.55
3:D:450:HIS:HE1	3:D:452:LEU:HD12	1.70	0.55
3:D:1273:ASP:HB3	3:D:1276:GLU:CG	2.32	0.55
5:F:551:LEU:HD21	5:F:598:LEU:HD21	1.87	0.55
5:F:552:THR:OG1	5:F:555:GLU:HG3	2.07	0.55
2:I:417:SER:OG	2:I:419:ILE:HG13	2.07	0.55
2:I:1291:LEU:CD2	3:J:1351:VAL:HG13	2.26	0.55
3:J:262:THR:O	5:L:507:MET:HB2	2.05	0.55
1:A:207:THR:HG22	1:A:208:ASN:N	2.21	0.55
2:C:90:VAL:HG12	2:C:91:THR:H	1.71	0.55
3:D:683:ILE:HD11	3:D:754:ILE:HG23	1.87	0.55
3:D:854:ALA:HB2	3:J:1372:ARG:CB	2.37	0.55
4:E:32:VAL:O	4:E:34:GLY:N	2.39	0.55
5:F:392:LYS:O	5:F:395:THR:HG22	2.06	0.55
1:H:158:ARG:HB3	1:H:172:LEU:HD22	1.88	0.55
2:I:59:ILE:HG23	2:I:476:LYS:HE3	1.88	0.55
2:I:1276:TRP:CZ2	3:J:801:VAL:HG21	2.42	0.55
2:I:1297:ASP:O	2:I:1301:ARG:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:513:MET:HE1	3:J:579:LEU:HD13	1.87	0.55
1:B:29:GLU:CB	1:B:30:PRO:CD	2.82	0.55
2:C:11:ILE:HG21	2:C:1149:TYR:CE1	2.42	0.55
2:C:489:PRO:HA	2:C:492:MET:HE3	1.86	0.55
2:C:1238:LEU:H	2:C:1238:LEU:CD1	2.15	0.55
3:D:412:LEU:HA	3:D:415:VAL:HG22	1.86	0.55
3:D:1151:LYS:O	3:D:1153:PRO:HD3	2.07	0.55
5:F:292:VAL:HG13	5:F:297:MET:O	2.07	0.55
2:I:1134:GLN:C	2:I:1135:GLN:HG2	2.31	0.55
3:J:244:VAL:HA	3:J:269:TYR:OH	2.07	0.55
3:J:848:VAL:CG2	3:J:858:VAL:HG13	2.36	0.55
1:B:93:GLN:HB2	1:B:120:ASP:OD1	2.06	0.55
1:B:104:LYS:CG	1:B:110:VAL:HG22	2.29	0.55
2:C:1137:GLU:HG2	2:C:1140:LYS:HG2	1.87	0.55
2:C:1246:ARG:HH11	2:C:1266:GLY:HA2	1.71	0.55
3:D:525:MET:O	3:D:548:VAL:HG13	2.07	0.55
3:D:1159:ILE:HG22	3:D:1177:ILE:HD12	1.89	0.55
4:E:80:LEU:O	4:E:84:THR:OG1	2.25	0.55
5:F:297:MET:HE3	5:F:330:LEU:CD2	2.33	0.55
5:F:606:VAL:HG13	5:F:607:LEU:HD12	1.87	0.55
2:I:1152:GLY:O	2:I:1153:ALA:HB2	2.07	0.55
2:I:1287:LEU:HD22	3:J:1357:ILE:CG1	2.37	0.55
3:J:1221:LEU:HD22	3:J:1221:LEU:C	2.31	0.55
5:L:316:PHE:CZ	5:L:337:VAL:HB	2.42	0.55
2:C:147:SER:OG	2:C:455:SER:HB3	2.07	0.55
3:D:585:LYS:HB2	3:D:612:LEU:HD21	1.87	0.55
5:F:456:MET:SD	5:F:497:VAL:HG13	2.46	0.55
1:G:219:ARG:O	1:G:223:ILE:HG13	2.07	0.55
2:I:17:LYS:CE	2:I:1154:ASP:HB3	2.37	0.55
2:I:767:GLN:HG2	2:I:786:GLY:HA2	1.89	0.55
2:I:800:MET:O	2:I:1229:TYR:HA	2.07	0.55
2:I:960:LEU:HD12	2:I:1028:LYS:HE2	1.89	0.55
2:I:968:GLU:HG3	2:I:1018:TYR:HE1	1.72	0.55
3:J:30:ILE:HD13	3:J:243:PRO:CG	2.36	0.55
3:J:489:ASN:HA	3:J:904:ALA:CB	2.34	0.55
2:C:227:LYS:HZ3	2:C:298:ALA:HB1	1.70	0.55
3:D:161:THR:N	3:D:164:GLN:OE1	2.39	0.55
3:D:317:THR:HB	3:D:324:LEU:HB3	1.88	0.55
3:D:398:LYS:O	3:D:402:GLU:HB2	2.06	0.55
1:H:127:GLN:O	1:H:127:GLN:HG2	2.05	0.55
2:I:887:VAL:HB	2:I:913:VAL:HG22	1.84	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1129:ASN:OD1	2:I:1177:ARG:NH2	2.39	0.55
2:I:1243:MET:CE	3:J:445:LYS:HD3	2.37	0.55
5:L:582:VAL:HG12	5:L:586:ARG:HG2	1.89	0.55
1:B:205:MET:HG2	1:B:206:GLU:N	2.22	0.55
2:C:565:GLU:HB2	2:C:680:LEU:HD21	1.88	0.55
2:C:646:SER:CB	2:C:649:GLN:HG3	2.26	0.55
2:C:1065:LYS:HD3	2:C:1235:LEU:HD12	1.88	0.55
2:C:1119:MET:HB2	2:C:1228:GLY:CA	2.34	0.55
1:G:44:ARG:HG3	1:G:183:ILE:HG22	1.88	0.55
3:J:431:ARG:HH21	3:J:489:ASN:CG	2.14	0.55
2:C:397:LEU:N	2:C:397:LEU:HD12	2.22	0.55
2:C:688:GLN:O	2:C:1235:LEU:HA	2.07	0.55
3:D:316:ILE:HA	3:D:323:PRO:HA	1.87	0.55
3:D:516:ASP:HA	3:D:545:HIS:HB2	1.88	0.55
1:G:218:ARG:NH1	1:H:232:VAL:N	2.55	0.55
2:I:678:ARG:CZ	2:I:1106:ARG:HG2	2.36	0.55
2:I:1116:HIS:CE1	3:J:641:ILE:HB	2.41	0.55
3:J:193:ASP:CG	3:J:196:GLN:HG2	2.31	0.55
4:K:15:ASN:O	4:K:16:ARG:HB3	2.07	0.55
1:A:224:LEU:HD23	1:A:224:LEU:C	2.32	0.55
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.89	0.55
3:D:137:ARG:HD3	3:D:143:SER:CB	2.37	0.55
3:D:291:ILE:HD13	5:F:409:ASN:HB3	1.89	0.55
5:F:513:ASP:OD2	5:F:515:GLU:HB2	2.07	0.55
2:I:672:GLU:HG2	2:I:1187:PHE:HA	1.89	0.55
3:J:186:GLN:CB	3:J:238:ILE:HG21	2.32	0.55
3:J:491:LEU:HD23	3:J:498:PRO:HA	1.89	0.55
3:J:1217:PRO:HG3	3:J:1232:TYR:HE2	1.71	0.55
5:L:441:ARG:HH12	5:L:445:ASP:CG	2.15	0.55
5:L:445:ASP:OD2	5:L:451:ARG:HD2	2.06	0.55
1:A:14:VAL:HG13	1:A:27:THR:HB	1.88	0.54
3:D:132:LEU:HD13	3:D:132:LEU:C	2.32	0.54
5:F:577:GLY:CA	5:F:583:THR:HG23	2.29	0.54
1:G:19:VAL:HG13	1:G:20:SER:H	1.72	0.54
2:I:864:LYS:NZ	2:I:876:GLU:O	2.40	0.54
2:I:884:VAL:O	2:I:917:SER:HB2	2.07	0.54
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.39	0.54
5:L:343:LYS:H	5:L:343:LYS:HD2	1.72	0.54
2:C:548:ARG:CZ	2:C:571:LEU:HD11	2.37	0.54
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.42	0.54
2:C:1142:ARG:NH2	2:C:1165:SER:CB	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1144:PHE:CE1	2:C:1201:LEU:HD11	2.42	0.54
3:D:109:SER:HB2	3:D:296:LYS:HE2	1.88	0.54
3:D:451:PRO:O	3:D:454:CYS:HB2	2.07	0.54
3:D:1193:TRP:HB2	3:D:1194:ARG:CZ	2.36	0.54
5:F:316:PHE:O	5:F:320:ILE:HG13	2.07	0.54
5:F:383:ASN:HB2	5:F:412:LEU:HD21	1.88	0.54
2:I:1115:THR:HG22	2:I:1228:GLY:HA3	1.89	0.54
2:I:1238:LEU:HD12	2:I:1238:LEU:N	2.20	0.54
1:A:154:PRO:CB	2:C:1059:ARG:HH21	2.19	0.54
1:A:231:PHE:CE2	1:B:39:LEU:HD13	2.42	0.54
1:B:196:THR:HG23	3:D:443:GLU:CG	2.38	0.54
2:C:98:VAL:CB	2:C:124:MET:HE3	2.36	0.54
2:C:1089:GLU:OE2	2:C:1211:ARG:HD2	2.07	0.54
3:D:1227:HIS:O	3:D:1230:THR:HG22	2.07	0.54
3:D:1282:TYR:O	3:D:1285:VAL:HG12	2.07	0.54
2:I:840:SER:CB	2:I:850:ILE:HD11	2.37	0.54
3:J:1293:GLU:OE1	3:J:1294:ALA:N	2.38	0.54
2:C:3:TYR:CE1	2:C:11:ILE:CD1	2.90	0.54
2:C:484:LEU:HD12	2:C:485:ASP:H	1.72	0.54
2:C:599:VAL:CG2	2:C:629:PHE:CE1	2.90	0.54
2:C:1210:ILE:HG22	2:C:1211:ARG:H	1.73	0.54
5:F:111:LEU:HD11	5:F:119:ILE:HD12	1.90	0.54
5:F:486:ARG:HB2	5:F:486:ARG:CZ	2.37	0.54
1:H:32:GLU:OE2	1:H:195:ARG:NH2	2.41	0.54
2:I:1191:LYS:O	2:I:1195:ILE:HG13	2.08	0.54
3:J:41:PRO:HB3	3:J:270:ARG:HG3	1.90	0.54
3:J:483:LEU:HD21	4:K:17:PHE:CD1	2.43	0.54
3:J:868:TRP:CZ3	3:J:871:LEU:HD13	2.42	0.54
3:J:1167:LYS:CD	3:J:1174:ARG:HD2	2.36	0.54
5:L:315:TRP:CH2	5:L:341:LEU:HD11	2.43	0.54
1:B:101:THR:HG22	1:B:103:ASN:HD21	1.72	0.54
1:B:127:GLN:HG2	1:B:127:GLN:O	2.08	0.54
2:C:198:ILE:O	2:C:201:ARG:HB2	2.06	0.54
2:C:1113:LEU:CD1	3:D:641:ILE:HG13	2.37	0.54
3:D:126:LEU:CD1	3:D:223:LEU:CD2	2.85	0.54
3:D:129:ASP:HB2	3:D:220:ARG:NH2	2.22	0.54
4:E:36:ASP:HB2	4:E:37:PRO:HD2	1.89	0.54
5:F:505:ILE:HD12	5:F:505:ILE:N	2.23	0.54
3:J:192:MET:HE2	3:J:197:GLU:OE2	2.07	0.54
1:B:140:ILE:HG23	1:B:140:ILE:O	2.07	0.54
2:C:16:GLY:O	2:C:1156:ARG:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:233:ARG:HH12	2:C:332:ARG:HH12	1.56	0.54
4:E:15:ASN:O	4:E:16:ARG:HB3	2.07	0.54
2:I:757:THR:C	2:I:833:ILE:HD12	2.32	0.54
2:I:818:VAL:HG13	2:I:822:VAL:HG21	1.90	0.54
5:L:114:GLU:HG3	5:L:115:GLY:H	1.72	0.54
2:C:106:GLU:OE1	2:C:114:VAL:HG22	2.07	0.54
2:C:518:ASN:O	2:C:691:PRO:HD3	2.08	0.54
3:D:9:LYS:NZ	3:D:11:GLN:HA	2.22	0.54
3:D:384:LYS:NZ	3:D:414:GLU:OE1	2.36	0.54
5:F:277:MET:HG3	5:F:362:ASN:ND2	2.22	0.54
1:H:231:PHE:CD2	1:H:231:PHE:N	2.76	0.54
2:I:478:ARG:NH1	2:I:482:GLY:HA2	2.23	0.54
3:J:205:LEU:C	3:J:205:LEU:HD13	2.32	0.54
3:J:418:GLU:HB3	4:K:48:VAL:HG23	1.89	0.54
3:J:843:VAL:HG11	3:J:897:HIS:O	2.08	0.54
5:L:571:TYR:HB3	5:L:575:GLU:HG2	1.88	0.54
2:C:38:PHE:CZ	2:C:49:LEU:HD21	2.43	0.54
2:C:221:LEU:HD21	2:C:351:LEU:CD1	2.38	0.54
2:C:325:LEU:CD1	2:C:333:ILE:HG12	2.38	0.54
2:C:1151:LEU:CD1	2:C:1198:LEU:HD23	2.38	0.54
5:F:320:ILE:HG12	5:F:330:LEU:HD12	1.89	0.54
2:I:219:GLN:HA	2:I:222:ASP:HB3	1.89	0.54
2:I:738:GLU:HG2	2:I:741:MET:HE2	1.90	0.54
1:A:158:ARG:NH2	1:A:172:LEU:HD23	2.23	0.54
2:C:724:VAL:HG11	2:C:727:VAL:HG22	1.89	0.54
2:C:864:LYS:NZ	2:C:877:VAL:HA	2.23	0.54
3:D:56:LEU:H	3:D:56:LEU:CD1	2.17	0.54
3:D:872:LEU:O	3:D:877:VAL:CG1	2.56	0.54
2:I:60:GLN:O	2:I:476:LYS:HE2	2.07	0.54
3:J:210:SER:HB2	3:J:213:LYS:CG	2.38	0.54
3:J:610:ARG:HG2	3:J:866:GLU:CD	2.33	0.54
5:L:277:MET:CE	5:L:281:ARG:HH21	2.19	0.54
5:L:353:LEU:HD13	5:L:361:ILE:HD12	1.90	0.54
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.22	0.54
1:B:201:LEU:HD21	1:B:203:ILE:HD11	1.89	0.54
2:C:62:TYR:C	2:C:64:GLY:H	2.16	0.54
2:C:231:GLU:HG2	2:C:332:ARG:CZ	2.38	0.54
2:C:813:GLU:HB2	3:D:461:PHE:HB2	1.90	0.54
3:D:1344:LEU:O	3:D:1345:ARG:HB2	2.08	0.54
5:F:598:LEU:HA	5:F:603:ARG:HB2	1.90	0.54
1:G:61:ILE:HG23	1:G:142:MET:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:187:VAL:HG23	1:H:187:VAL:O	2.07	0.54
2:I:192:ASP:CG	2:I:436:ARG:HH21	2.12	0.54
2:I:1129:ASN:OD1	2:I:1177:ARG:NE	2.39	0.54
1:A:73:GLY:O	1:A:134:THR:HG22	2.08	0.53
2:C:103:VAL:HG12	2:C:116:ASP:HB3	1.90	0.53
2:C:228:VAL:HB	2:C:335:THR:OG1	2.08	0.53
2:C:1174:GLU:OE2	2:C:1177:ARG:NH1	2.40	0.53
2:C:1271:GLY:CA	3:D:343:LEU:CD1	2.68	0.53
5:F:96:ASP:CG	5:F:96:ASP:O	2.52	0.53
1:G:70:THR:HG21	2:I:755:LYS:CE	2.26	0.53
3:J:30:ILE:HD13	3:J:243:PRO:HG3	1.90	0.53
3:J:491:LEU:HB2	3:J:904:ALA:HA	1.90	0.53
1:A:48:LEU:HA	1:A:180:VAL:HG21	1.90	0.53
1:A:61:ILE:HG23	1:A:142:MET:HB3	1.89	0.53
1:A:159:ILE:HG12	1:A:162:GLU:OE2	2.08	0.53
2:C:782:VAL:HG11	2:C:792:GLY:HA3	1.90	0.53
2:C:1223:ARG:NH2	3:D:719:PHE:O	2.41	0.53
2:C:1269:ARG:HD3	3:D:343:LEU:CB	2.28	0.53
3:D:670:SER:HB2	3:D:672:LEU:HD13	1.90	0.53
5:F:512:GLY:C	5:F:514:ASP:H	2.16	0.53
2:I:91:THR:HG21	2:I:503:LYS:NZ	2.24	0.53
2:I:796:LEU:H	2:I:796:LEU:HD12	1.71	0.53
3:J:129:ASP:HB2	3:J:220:ARG:CZ	2.38	0.53
3:J:526:VAL:HG12	3:J:549:LYS:CB	2.31	0.53
3:J:592:VAL:HA	3:J:596:LEU:HD21	1.89	0.53
1:A:165:GLU:C	1:A:167:PRO:HD2	2.33	0.53
2:C:782:VAL:HG11	2:C:792:GLY:CA	2.39	0.53
2:C:1212:LEU:HD22	2:C:1225:VAL:CG2	2.39	0.53
3:D:372:MET:O	3:D:376:LEU:HD12	2.08	0.53
3:D:1350:ASN:OD1	3:D:1355:ARG:HD2	2.08	0.53
5:F:137:TYR:HD2	5:F:273:MET:HE2	1.73	0.53
1:H:205:MET:HG2	1:H:206:GLU:N	2.23	0.53
2:I:185:ASP:O	2:I:196:VAL:HG23	2.09	0.53
2:I:563:THR:OG1	2:I:564:PRO:HD2	2.08	0.53
3:J:57:PHE:HB3	3:J:98:ARG:HH22	1.74	0.53
3:J:103:GLY:CA	3:J:244:VAL:HG22	2.39	0.53
3:J:325:LYS:HG3	3:J:329:ASP:HB2	1.90	0.53
3:J:357:VAL:HG22	3:J:461:PHE:CD1	2.44	0.53
3:J:615:LYS:HZ3	4:K:7:GLN:HG2	1.73	0.53
1:A:36:GLY:CA	1:A:187:VAL:HG11	2.36	0.53
2:C:696:ASP:HB2	2:C:798:GLN:CG	2.28	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:161:THR:HG22	3:D:164:GLN:HB2	1.89	0.53
1:G:71:LYS:HZ2	1:G:140:ILE:HG22	1.73	0.53
1:H:67:GLU:OE1	1:H:67:GLU:N	2.42	0.53
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.42	0.53
2:I:21:VAL:HG11	2:I:592:ARG:CD	2.38	0.53
2:I:798:GLN:HB2	2:I:828:PHE:HE1	1.72	0.53
2:I:854:ILE:HD11	2:I:885:GLY:HA3	1.90	0.53
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.08	0.53
3:J:514:THR:OG1	3:J:594:GLN:O	2.27	0.53
4:K:71:GLU:HA	4:K:74:GLU:HG3	1.90	0.53
5:L:315:TRP:HZ2	5:L:341:LEU:HD21	1.72	0.53
1:B:187:VAL:HG13	1:B:199:ASP:HB3	1.90	0.53
2:C:219:GLN:HA	2:C:222:ASP:HB3	1.90	0.53
2:C:1307:ASN:HA	2:C:1310:ASP:HB2	1.89	0.53
3:D:17:PHE:CE2	3:D:1355:ARG:NH2	2.76	0.53
1:G:231:PHE:HB3	1:H:218:ARG:CD	2.38	0.53
3:J:369:PRO:HB3	3:J:444:GLY:O	2.08	0.53
3:J:418:GLU:HB3	4:K:48:VAL:CG2	2.39	0.53
3:J:646:ILE:HG23	3:J:741:ALA:O	2.07	0.53
5:L:134:VAL:HA	5:L:273:MET:HE1	1.91	0.53
2:C:1:MET:O	2:C:2:VAL:HG23	2.07	0.53
2:C:102:LEU:O	2:C:116:ASP:HA	2.08	0.53
2:C:185:ASP:O	2:C:196:VAL:HG23	2.08	0.53
2:C:338:THR:CB	2:C:345:PRO:HB3	2.38	0.53
2:C:516:ASP:O	2:C:522:SER:OG	2.17	0.53
2:C:942:ASP:O	2:C:946:LEU:HB2	2.08	0.53
2:C:1075:VAL:HG23	3:D:461:PHE:O	2.09	0.53
1:G:11:PRO:HG3	1:G:31:LEU:HD21	1.90	0.53
1:H:89:ALA:HB3	1:H:124:VAL:HG12	1.89	0.53
2:I:896:THR:H	2:I:899:GLU:HB2	1.73	0.53
2:I:1073:LYS:HE3	3:J:462:ASP:HB2	1.90	0.53
3:J:44:ILE:HB	3:J:49:PHE:O	2.08	0.53
3:J:525:MET:O	3:J:548:VAL:HG13	2.08	0.53
3:J:1358:PRO:HB3	3:J:1366:HIS:CG	2.43	0.53
2:C:50:GLU:HG2	2:C:73:TYR:HE1	1.74	0.53
3:D:573:THR:OG1	3:D:576:ARG:HG3	2.08	0.53
2:I:224:PHE:CD2	2:I:347:ILE:HG13	2.44	0.53
2:I:985:GLU:HB3	2:I:988:LYS:HD2	1.89	0.53
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.73	0.53
3:J:693:VAL:CG2	3:J:743:MET:HE3	2.32	0.53
5:L:387:VAL:HG22	5:L:435:ILE:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:864:LYS:HZ1	2:C:877:VAL:HA	1.74	0.53
3:D:333:GLY:HA3	3:D:338:PHE:CZ	2.43	0.53
1:G:37:HIS:NE2	1:G:187:VAL:HG21	2.23	0.53
2:I:151:ARG:NH2	2:I:156:PHE:CD2	2.75	0.53
3:J:56:LEU:HD12	3:J:56:LEU:N	2.24	0.53
3:J:210:SER:HB2	3:J:213:LYS:HG3	1.91	0.53
5:L:606:VAL:HG13	5:L:607:LEU:HD12	1.90	0.53
1:A:59:VAL:HG21	1:A:85:LEU:HD13	1.91	0.53
2:C:74:ARG:C	2:C:75:LEU:HD22	2.33	0.53
2:C:810:TYR:CD1	2:C:1078:LYS:HB2	2.44	0.53
2:C:992:LEU:HD23	2:C:992:LEU:H	1.73	0.53
3:D:152:THR:OG1	3:D:153:ASN:N	2.42	0.53
3:D:619:ILE:O	3:D:623:GLN:HG2	2.09	0.53
1:G:35:PHE:CE1	1:H:46:ILE:HG23	2.44	0.53
1:H:74:VAL:HG12	1:H:76:GLU:H	1.74	0.53
2:I:640:GLY:O	2:I:641:GLU:HG3	2.09	0.53
2:I:700:VAL:HG13	2:I:1117:LEU:HD22	1.90	0.53
2:I:817:LEU:HD11	2:I:1080:ASN:ND2	2.24	0.53
2:I:1119:MET:HE2	2:I:1227:VAL:HG23	1.91	0.53
2:I:1196:LYS:HA	2:I:1199:LEU:HD12	1.91	0.53
5:L:513:ASP:C	5:L:515:GLU:H	2.16	0.53
5:L:552:THR:OG1	5:L:555:GLU:HG3	2.08	0.53
2:C:448:LEU:HA	2:C:451:ARG:HB2	1.90	0.53
2:C:629:PHE:CE2	2:C:634:VAL:HG11	2.43	0.53
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.39	0.53
3:D:126:LEU:CD1	3:D:223:LEU:HD22	2.39	0.53
3:D:679:TYR:CE2	3:D:683:ILE:HD12	2.44	0.53
3:D:1273:ASP:CB	3:D:1276:GLU:HG3	2.35	0.53
1:H:116:THR:O	1:H:116:THR:HG23	2.09	0.53
2:I:560:PRO:HG3	3:J:773:PHE:CE2	2.44	0.53
2:I:929:ILE:CD1	2:I:1055:ALA:HB2	2.31	0.53
3:J:41:PRO:CB	3:J:270:ARG:HG3	2.39	0.53
3:J:674:THR:OG1	3:J:677:GLU:HB2	2.09	0.53
2:C:1124:ILE:CG2	2:C:1180:MET:HG3	2.39	0.52
3:D:325:LYS:HB3	5:F:508:GLU:HG2	1.91	0.52
5:F:559:LEU:HD22	5:F:594:ALA:HB1	1.91	0.52
1:G:10:LYS:HA	1:H:227:GLN:NE2	2.24	0.52
1:G:89:ALA:HB3	1:G:125:LYS:CD	2.39	0.52
3:J:19:ALA:O	3:J:20:ILE:HG13	2.09	0.52
3:J:45:ASN:O	3:J:46:TYR:HD2	1.91	0.52
3:J:66:LYS:HE2	3:J:69:GLU:OE1	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:444:ALA:HB1	5:L:457:ILE:HD12	1.91	0.52
1:B:47:LEU:HD22	1:B:180:VAL:HG11	1.90	0.52
1:B:194:GLN:OE1	1:B:194:GLN:HA	2.09	0.52
2:C:31:GLN:O	2:C:130:MET:HE1	2.10	0.52
2:C:486:THR:HG23	2:C:487:LEU:H	1.74	0.52
2:C:1285:TYR:CE1	3:D:475:GLU:HG2	2.44	0.52
5:F:383:ASN:ND2	5:F:427:PHE:HE2	2.06	0.52
5:F:598:LEU:HA	5:F:603:ARG:CB	2.39	0.52
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.91	0.52
3:J:79:LYS:HG3	3:J:80:HIS:N	2.22	0.52
3:J:128:LEU:HD23	3:J:192:MET:HE1	1.90	0.52
3:J:342:LEU:N	3:J:344:GLY:HA2	2.24	0.52
3:J:431:ARG:NH2	3:J:489:ASN:OD1	2.42	0.52
3:J:1343:GLU:C	3:J:1344:LEU:HD12	2.34	0.52
2:C:102:LEU:HB2	2:C:489:PRO:HG3	1.92	0.52
2:C:325:LEU:HD13	2:C:333:ILE:HG12	1.91	0.52
3:D:92:VAL:HG22	3:D:92:VAL:O	2.07	0.52
4:E:82:ALA:O	4:E:85:ALA:HB3	2.09	0.52
5:F:479:THR:HG22	5:F:482:GLU:CB	2.39	0.52
2:I:38:PHE:CZ	2:I:49:LEU:HD21	2.45	0.52
3:J:37:GLU:HB2	3:J:104:HIS:CE1	2.44	0.52
3:J:502:PRO:HB3	3:J:506:VAL:HG11	1.91	0.52
2:C:94:ALA:HB2	2:C:129:LEU:CD1	2.37	0.52
3:D:106:GLU:OE2	3:D:241:VAL:HG22	2.10	0.52
3:D:748:ALA:O	3:D:777:HIS:HD2	1.91	0.52
2:I:871:VAL:O	2:I:944:ARG:NH1	2.40	0.52
2:I:1271:GLY:HA3	3:J:343:LEU:HD12	1.91	0.52
3:J:24:LEU:HD11	3:J:116:PHE:CZ	2.44	0.52
2:C:192:ASP:OD2	2:C:436:ARG:NH2	2.43	0.52
2:C:929:ILE:HD13	2:C:1055:ALA:HB2	1.92	0.52
3:D:227:PHE:O	3:D:230:SER:HB3	2.09	0.52
3:D:514:THR:HG21	3:D:596:LEU:CG	2.40	0.52
3:D:842:ARG:CB	3:D:882:VAL:HG11	2.39	0.52
5:F:551:LEU:HD21	5:F:598:LEU:CD2	2.39	0.52
1:G:9:LEU:HD21	1:G:195:ARG:NH2	2.22	0.52
1:H:125:LYS:HB3	1:H:128:HIS:HB2	1.92	0.52
2:I:65:ASN:CB	2:I:105:TYR:HD2	2.23	0.52
2:I:389:PHE:HA	2:I:395:TYR:CD1	2.44	0.52
3:J:800:LEU:HB3	3:J:920:ALA:HB1	1.92	0.52
3:J:1309:ILE:HG13	3:J:1310:THR:N	2.25	0.52
2:C:619:ALA:HB2	2:C:654:ASP:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:817:LEU:HD11	2:C:1080:ASN:ND2	2.21	0.52
3:D:97:VAL:HG12	3:D:101:ARG:CG	2.40	0.52
3:D:847:ASP:HA	3:D:860:ARG:H	1.75	0.52
3:D:1179:PRO:HD2	3:D:1184:ASP:HA	1.92	0.52
1:H:158:ARG:HG3	1:H:172:LEU:HD23	1.92	0.52
2:I:516:ASP:CG	2:I:522:SER:HG	2.18	0.52
2:I:568:ASN:HB2	2:I:571:LEU:HB2	1.92	0.52
2:I:816:ILE:O	2:I:1076:ILE:HD12	2.10	0.52
2:I:895:LEU:HB2	2:I:899:GLU:HB2	1.91	0.52
3:J:114:ILE:O	3:J:114:ILE:HG13	2.08	0.52
3:J:510:LEU:HG	3:J:513:MET:CE	2.40	0.52
3:J:1269:ALA:HB2	3:J:1274:PHE:HE1	1.73	0.52
5:L:409:ASN:O	5:L:413:MET:HG3	2.10	0.52
1:A:115:ILE:HG22	1:A:116:THR:H	1.74	0.52
1:B:47:LEU:CD1	1:B:183:ILE:HG12	2.35	0.52
1:B:66:HIS:CD2	1:B:68:TYR:OH	2.63	0.52
2:C:202:ARG:HH22	2:C:368:ARG:HH22	1.57	0.52
2:C:324:LYS:O	2:C:327:GLN:NE2	2.43	0.52
2:C:593:LYS:HG3	2:C:595:THR:HG23	1.91	0.52
3:D:79:LYS:HE3	3:D:80:HIS:HA	1.91	0.52
3:D:490:ILE:HB	3:D:500:ILE:HG13	1.91	0.52
3:D:1149:ARG:HG3	3:D:1216:ALA:HB2	1.91	0.52
5:F:379:MET:HG2	5:F:416:VAL:HG21	1.90	0.52
5:F:547:VAL:HG22	5:F:598:LEU:HD22	1.91	0.52
2:I:619:ALA:HB1	2:I:657:THR:HA	1.90	0.52
3:J:517:CYS:C	3:J:716:GLN:HE22	2.16	0.52
3:J:1145:PHE:HB3	3:J:1309:ILE:CG2	2.40	0.52
5:L:147:GLN:HE22	5:L:150:ARG:NH1	2.07	0.52
1:B:64:VAL:HG11	1:B:69:SER:HB2	1.91	0.52
2:C:768:MET:O	2:C:784:ALA:HB1	2.10	0.52
2:C:796:LEU:H	2:C:796:LEU:HD12	1.75	0.52
3:D:161:THR:H	3:D:164:GLN:HB2	1.74	0.52
1:G:89:ALA:HB3	1:G:125:LYS:HD2	1.91	0.52
1:G:90:VAL:HG22	1:G:91:ARG:N	2.22	0.52
1:G:133:LEU:CD1	1:G:138:ALA:HB3	2.39	0.52
1:G:219:ARG:HG2	1:G:223:ILE:HD11	1.90	0.52
2:I:839:VAL:HG12	2:I:1049:ILE:CD1	2.40	0.52
2:I:1272:GLU:N	3:J:343:LEU:HD12	2.25	0.52
3:J:363:LEU:O	3:J:363:LEU:CG	2.56	0.52
3:J:827:GLU:HG2	3:J:832:LYS:HD2	1.91	0.52
4:K:29:GLN:CD	4:K:35:LYS:HE2	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:ALA:O	1:B:146:VAL:HG13	2.10	0.52
2:C:1113:LEU:HD11	3:D:641:ILE:HG13	1.90	0.52
3:D:97:VAL:CG1	3:D:101:ARG:CZ	2.85	0.52
1:G:64:VAL:HG11	1:G:78:ILE:HG13	1.92	0.52
1:G:231:PHE:N	1:G:231:PHE:CD2	2.76	0.52
2:I:680:LEU:HD22	3:J:783:LEU:HD11	1.92	0.52
2:I:1142:ARG:HH12	2:I:1169:VAL:HG21	1.75	0.52
3:J:1233:ILE:HG21	3:J:1257:VAL:CG2	2.40	0.52
5:L:290:LEU:HD12	5:L:337:VAL:HG22	1.92	0.52
1:A:16:ILE:HG23	1:A:26:VAL:HG12	1.92	0.52
2:C:958:LYS:O	2:C:962:GLU:HG2	2.10	0.52
3:D:287:ALA:HB1	3:D:288:PRO:HD2	1.92	0.52
3:D:357:VAL:HG22	3:D:461:PHE:CE1	2.45	0.52
3:D:1154:ALA:N	3:D:1214:PRO:O	2.33	0.52
3:D:1241:TYR:CD2	3:D:1246:VAL:HG11	2.41	0.52
3:D:1250:ASP:O	3:D:1251:LYS:C	2.51	0.52
2:I:197:ARG:NH2	2:I:203:LYS:HB2	2.25	0.52
2:I:778:GLU:O	2:I:781:ASP:HB2	2.10	0.52
2:I:836:LEU:CD2	2:I:921:PRO:HD3	2.40	0.52
2:I:968:GLU:HG3	2:I:1018:TYR:CE1	2.45	0.52
2:I:971:LEU:HG	2:I:1014:LEU:HD23	1.92	0.52
3:J:825:VAL:O	3:J:826:ILE:HG13	2.10	0.52
2:C:490:GLN:CG	5:F:472:GLN:NE2	2.71	0.51
3:D:392:THR:CG2	5:F:606:VAL:HA	2.40	0.51
3:D:658:GLU:HA	3:D:661:VAL:CG1	2.40	0.51
3:D:810:THR:HG22	3:D:893:GLY:HA3	1.92	0.51
5:F:337:VAL:HG12	5:F:341:LEU:CD1	2.40	0.51
5:F:547:VAL:HG23	5:F:603:ARG:NH1	2.25	0.51
1:G:61:ILE:HG23	1:G:142:MET:HE2	1.92	0.51
2:I:568:ASN:CB	2:I:571:LEU:HD12	2.40	0.51
2:I:836:LEU:N	2:I:836:LEU:HD12	2.24	0.51
3:J:92:VAL:HG22	3:J:92:VAL:O	2.11	0.51
3:J:331:ILE:HG22	3:J:1328:THR:HG21	1.92	0.51
1:B:66:HIS:HB3	1:B:68:TYR:CE2	2.45	0.51
2:C:302:ILE:HG22	2:C:308:GLU:C	2.35	0.51
2:C:1080:ASN:CB	2:C:1085:MET:CE	2.84	0.51
6:C:2001:KNG:C34	6:C:2001:KNG:C29	2.88	0.51
3:D:115:TRP:NE1	3:D:1329:THR:HG23	2.24	0.51
3:D:487:THR:OG1	4:E:4:VAL:O	2.27	0.51
3:D:821:MET:HE3	3:D:879:ALA:HB1	1.90	0.51
3:D:823:THR:HB	3:D:824:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:842:ARG:HB3	3:D:882:VAL:HG11	1.92	0.51
3:D:843:VAL:CG1	3:D:883:ARG:HD3	2.39	0.51
5:L:513:ASP:OD2	5:L:515:GLU:OE1	2.29	0.51
1:A:49:SER:OG	1:A:50:SER:N	2.43	0.51
2:C:17:LYS:CE	2:C:1154:ASP:HB3	2.32	0.51
2:C:255:ILE:HG23	2:C:285:ILE:HD13	1.92	0.51
2:C:309:LEU:HD21	2:C:312:ALA:HA	1.92	0.51
2:C:678:ARG:NE	2:C:1106:ARG:HG2	2.26	0.51
2:C:696:ASP:O	2:C:697:LYS:CB	2.59	0.51
3:D:317:THR:HG22	3:D:322:ARG:O	2.10	0.51
3:D:500:ILE:HG22	3:D:500:ILE:O	2.09	0.51
3:D:1314:LEU:CD1	3:D:1326:GLN:OE1	2.58	0.51
5:F:230:VAL:HG13	5:F:231:THR:N	2.25	0.51
1:G:48:LEU:HA	1:G:180:VAL:CG2	2.27	0.51
2:I:124:MET:HB2	2:I:498:ILE:HD13	1.92	0.51
2:I:810:TYR:CD1	2:I:1078:LYS:HB2	2.45	0.51
2:I:1132:LEU:HD11	2:I:1174:GLU:HG2	1.92	0.51
2:I:1273:MET:HA	2:I:1276:TRP:CE3	2.45	0.51
3:J:361:LEU:CD1	3:J:366:CYS:HA	2.41	0.51
3:J:521:LYS:NZ	3:J:540:GLY:O	2.33	0.51
1:B:74:VAL:HG22	1:B:133:LEU:HD12	1.92	0.51
2:C:241:LEU:CD1	2:C:246:LEU:HD11	2.38	0.51
2:C:1299:ASN:HD22	2:C:1303:LYS:CE	2.22	0.51
3:D:48:THR:HB	3:D:50:LYS:HG3	1.92	0.51
3:D:56:LEU:HD21	3:D:269:TYR:HB3	1.91	0.51
3:D:103:GLY:CA	3:D:244:VAL:HG22	2.40	0.51
3:D:108:ALA:HB1	3:D:279:LEU:HD22	1.92	0.51
3:D:129:ASP:HB2	3:D:220:ARG:NE	2.25	0.51
5:F:540:LEU:HA	5:F:610:PHE:CZ	2.46	0.51
2:I:62:TYR:O	2:I:64:GLY:N	2.43	0.51
2:I:598:VAL:HG13	2:I:626:GLU:O	2.10	0.51
2:I:975:ILE:HG13	2:I:1014:LEU:HD22	1.92	0.51
3:J:493:PRO:HB2	3:J:918:ILE:HD12	1.92	0.51
5:L:105:MET:HE1	5:L:385:ARG:CG	2.24	0.51
5:L:132:CYS:SG	5:L:257:LYS:CE	2.99	0.51
1:A:14:VAL:HG12	1:A:27:THR:HB	1.91	0.51
1:A:154:PRO:HB2	2:C:1059:ARG:NH2	2.25	0.51
1:B:205:MET:HE3	1:B:213:PRO:HA	1.92	0.51
2:C:1281:TYR:HE2	3:D:431:ARG:HG3	1.75	0.51
3:D:165:TYR:O	3:D:169:LEU:HB2	2.09	0.51
3:D:190:LYS:HD3	3:D:235:GLU:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:573:LEU:H	5:F:573:LEU:CD2	2.19	0.51
1:H:9:LEU:HB3	1:H:32:GLU:HG3	1.93	0.51
3:J:382:TYR:HE2	5:L:532:LEU:HD23	1.75	0.51
3:J:821:MET:CE	3:J:879:ALA:HB1	2.40	0.51
3:J:1263:LYS:CE	3:J:1279:GLN:HE21	2.20	0.51
1:A:231:PHE:HZ	1:B:201:LEU:HD23	1.76	0.51
1:B:58:GLU:OE1	1:B:158:ARG:NH2	2.43	0.51
2:C:268:ARG:HH21	2:C:270:THR:HG21	1.73	0.51
5:F:105:MET:CE	5:F:385:ARG:HG2	2.31	0.51
5:F:310:GLU:O	5:F:344:LEU:HD21	2.11	0.51
2:I:487:LEU:HD12	2:I:492:MET:HE2	1.92	0.51
2:I:518:ASN:O	2:I:691:PRO:HD3	2.11	0.51
2:I:815:SER:CB	3:J:357:VAL:CG2	2.88	0.51
2:I:978:VAL:CG1	2:I:1007:LYS:HB3	2.40	0.51
3:J:474:LEU:HD23	4:K:28:ARG:HG2	1.93	0.51
3:J:697:MET:SD	3:J:741:ALA:HB3	2.50	0.51
3:J:843:VAL:HG13	3:J:883:ARG:CD	2.37	0.51
1:B:197:ASP:OD1	1:B:197:ASP:N	2.42	0.51
2:C:316:GLU:H	2:C:316:GLU:CD	2.19	0.51
2:C:557:ARG:NH2	2:C:608:ALA:HA	2.26	0.51
2:C:1043:ALA:O	2:C:1046:VAL:CG1	2.58	0.51
2:C:1149:TYR:HB3	2:C:1159:VAL:HG11	1.93	0.51
3:D:160:LEU:HA	3:D:164:GLN:OE1	2.10	0.51
3:D:859:PRO:CG	3:D:862:THR:HG21	2.35	0.51
1:H:41:ASN:ND2	2:I:1217:THR:HA	2.26	0.51
1:H:57:THR:CG2	1:H:158:ARG:HE	2.10	0.51
2:I:132:ASP:OD1	2:I:132:ASP:N	2.28	0.51
2:I:159:SER:HB2	2:I:442:VAL:HG21	1.92	0.51
2:I:1109:ILE:HG12	3:J:644:MET:SD	2.51	0.51
2:I:1158:LYS:O	2:I:1159:VAL:CG1	2.52	0.51
3:J:129:ASP:HB2	3:J:220:ARG:NH2	2.25	0.51
3:J:614:LEU:HB3	4:K:7:GLN:HG2	1.93	0.51
3:J:660:GLU:O	3:J:664:ILE:HG12	2.11	0.51
3:J:843:VAL:HG23	3:J:862:THR:C	2.35	0.51
4:K:60:ASN:H	4:K:63:ILE:HB	1.76	0.51
2:C:356:THR:HG21	2:C:362:ALA:HA	1.93	0.51
3:D:83:VAL:HG13	3:D:92:VAL:HG13	1.93	0.51
3:D:127:LEU:HD22	3:D:237:MET:HE3	1.91	0.51
3:D:1221:LEU:O	3:D:1221:LEU:HD22	2.10	0.51
1:H:133:LEU:HD11	1:H:140:ILE:HD13	1.93	0.51
2:I:146:VAL:HG11	2:I:531:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:455:SER:O	2:I:456:VAL:C	2.54	0.51
2:I:646:SER:HB3	2:I:649:GLN:CG	2.34	0.51
3:J:19:ALA:HA	3:J:1344:LEU:CD1	2.40	0.51
3:J:1328:THR:HG22	3:J:1332:LEU:HD23	1.93	0.51
2:C:1331:ARG:HA	2:C:1335:ILE:O	2.11	0.51
3:D:108:ALA:CB	3:D:279:LEU:HD22	2.40	0.51
3:D:858:VAL:HA	3:D:868:TRP:CZ3	2.46	0.51
3:D:1298:VAL:O	3:D:1298:VAL:HG22	2.11	0.51
4:E:15:ASN:HB3	4:E:18:ASP:HB2	1.92	0.51
1:G:27:THR:C	1:G:28:LEU:HD12	2.36	0.51
1:G:166:ARG:O	1:G:167:PRO:C	2.54	0.51
2:I:119:GLU:CB	2:I:489:PRO:HB2	2.40	0.51
3:J:709:ARG:C	3:J:711:GLY:N	2.69	0.51
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.92	0.51
2:C:26:TYR:OH	2:C:28:LEU:HD12	2.10	0.51
2:C:192:ASP:CG	2:C:436:ARG:HH21	2.19	0.51
2:C:802:VAL:HG12	2:C:1228:GLY:O	2.10	0.51
2:C:1062:PRO:HA	2:C:1076:ILE:O	2.10	0.51
3:D:418:GLU:H	4:E:45:LYS:HZ2	1.58	0.51
3:D:805:GLN:OE1	3:D:1348:LYS:HD3	2.11	0.51
1:G:9:LEU:HD11	1:G:198:LEU:HD21	1.93	0.51
1:G:50:SER:CB	1:H:8:PHE:CE1	2.91	0.51
1:G:73:GLY:O	1:G:134:THR:HG22	2.10	0.51
2:I:68:LEU:HD23	2:I:475:VAL:HG11	1.93	0.51
2:I:1174:GLU:OE2	2:I:1177:ARG:HD2	2.11	0.51
3:J:140:TYR:HB3	5:L:100:MET:SD	2.51	0.51
3:J:750:PRO:HA	3:J:777:HIS:CE1	2.46	0.51
3:J:850:LYS:HG2	3:J:857:LEU:HD23	1.93	0.51
3:J:1345:ARG:HD2	3:J:1370:MET:HE1	1.93	0.51
5:L:123:ILE:CD1	5:L:376:LYS:HG2	2.40	0.51
5:L:492:ASP:HA	5:L:495:ARG:NH2	2.26	0.51
2:C:529:ARG:NH1	6:C:2001:KNG:C17	2.74	0.50
2:C:1007:LYS:O	2:C:1011:LEU:HG	2.10	0.50
3:D:40:LYS:HB2	3:D:54:ASP:O	2.11	0.50
3:D:495:ASN:HD21	3:D:497:GLU:HB2	1.75	0.50
3:D:1266:ILE:HA	3:D:1302:TYR:HA	1.92	0.50
1:G:211:ILE:HG21	1:G:216:ALA:HB2	1.93	0.50
1:H:13:LEU:HD23	1:H:13:LEU:H	1.76	0.50
2:I:26:TYR:OH	2:I:28:LEU:HD12	2.10	0.50
2:I:151:ARG:HH21	2:I:156:PHE:HD2	1.54	0.50
2:I:216:THR:HG23	2:I:219:GLN:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:974:ARG:HB3	2:I:1014:LEU:CD2	2.40	0.50
2:I:985:GLU:CB	2:I:988:LYS:HD2	2.41	0.50
2:I:994:ARG:HD2	2:I:997:TRP:CH2	2.46	0.50
3:J:233:LYS:N	3:J:236:TRP:CZ3	2.76	0.50
3:J:288:PRO:HG2	3:J:291:ILE:CG1	2.41	0.50
3:J:514:THR:HG23	3:J:596:LEU:HB2	1.90	0.50
3:J:797:THR:O	3:J:801:VAL:HG13	2.12	0.50
3:J:810:THR:HG23	3:J:811:GLU:H	1.76	0.50
3:J:902:ASP:HB2	3:J:1251:LYS:CE	2.40	0.50
3:J:1177:ILE:HG13	3:J:1186:TYR:O	2.10	0.50
1:B:86:LYS:HD3	1:B:174:ASP:CB	2.41	0.50
2:C:11:ILE:HG22	2:C:1149:TYR:OH	2.11	0.50
2:C:689:ALA:HB2	2:C:1233:LEU:HG	1.93	0.50
2:C:1077:SER:HA	3:D:356:THR:OG1	2.11	0.50
2:I:796:LEU:HD12	2:I:796:LEU:N	2.25	0.50
2:I:841:ARG:CZ	3:J:256:ASP:HB3	2.41	0.50
2:I:1280:ALA:CB	3:J:431:ARG:HB3	2.42	0.50
3:J:115:TRP:CZ2	3:J:1329:THR:HG23	2.46	0.50
3:J:227:PHE:HE1	3:J:234:PRO:CD	2.23	0.50
3:J:527:LEU:HD23	3:J:532:GLU:HG3	1.92	0.50
3:J:1261:LEU:HD12	3:J:1261:LEU:C	2.36	0.50
5:L:299:LYS:HA	5:L:302:PHE:HB3	1.93	0.50
2:C:310:ILE:HD13	2:C:325:LEU:HA	1.93	0.50
2:C:678:ARG:HG3	2:C:1108:ASN:HD22	1.77	0.50
2:C:1109:ILE:HD11	3:D:644:MET:SD	2.50	0.50
2:C:1333:LEU:HD21	3:D:327:LEU:HB3	1.93	0.50
3:D:364:HIS:HB3	3:D:487:THR:HG23	1.92	0.50
3:D:686:TRP:HA	3:D:686:TRP:CE3	2.45	0.50
3:D:770:LEU:O	3:D:774:ILE:HG13	2.11	0.50
3:D:820:ILE:HG22	3:D:1227:HIS:ND1	2.26	0.50
3:D:1155:ILE:HD11	3:D:1211:SER:HB3	1.94	0.50
1:G:221:ALA:HB1	1:H:228:LEU:HD22	1.92	0.50
2:I:229:ILE:HG21	2:I:240:GLU:OE2	2.11	0.50
2:I:478:ARG:HG2	2:I:492:MET:HG2	1.92	0.50
2:I:815:SER:OG	3:J:357:VAL:CG2	2.59	0.50
3:J:908:ILE:HD13	3:J:909:ILE:O	2.11	0.50
4:K:4:VAL:HG13	4:K:5:THR:HG23	1.93	0.50
4:K:19:LEU:HD13	4:K:54:ILE:HG21	1.93	0.50
1:A:83:LEU:HD23	2:C:694:ARG:HH21	1.77	0.50
1:A:187:VAL:HG23	1:A:187:VAL:O	2.11	0.50
2:C:402:ARG:HD2	2:C:406:ASN:ND2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:45:ASN:O	3:D:46:TYR:HB3	2.10	0.50
3:D:349:TYR:CD1	3:D:472:LEU:HD21	2.46	0.50
3:D:491:LEU:CD2	3:D:498:PRO:CA	2.88	0.50
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.92	0.50
1:G:214:GLU:HA	1:G:217:ILE:HG22	1.94	0.50
1:G:219:ARG:HA	1:G:222:THR:HB	1.92	0.50
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	1.92	0.50
3:J:146:VAL:HG23	3:J:158:GLN:O	2.11	0.50
5:L:147:GLN:CB	5:L:161:LEU:HD11	2.41	0.50
1:A:39:LEU:O	1:A:43:LEU:N	2.39	0.50
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.45	0.50
2:C:619:ALA:HA	2:C:654:ASP:HB2	1.90	0.50
2:C:1191:LYS:O	2:C:1195:ILE:HG13	2.12	0.50
2:C:1280:ALA:HB3	3:D:431:ARG:HB3	1.94	0.50
1:G:55:ALA:HB3	1:G:177:TYR:CD1	2.47	0.50
2:I:20:GLN:O	2:I:20:GLN:HG3	2.11	0.50
3:J:483:LEU:HD21	4:K:17:PHE:HD1	1.76	0.50
5:L:462:LYS:O	5:L:466:ILE:HG13	2.12	0.50
5:L:467:SER:HB2	5:L:483:LEU:HD21	1.93	0.50
2:C:215:TYR:CE2	2:C:422:LYS:HD2	2.47	0.50
2:C:306:THR:OG1	2:C:308:GLU:HB2	2.12	0.50
2:C:670:PHE:CE2	2:C:1113:LEU:HB3	2.46	0.50
2:C:750:ILE:HD13	2:C:963:GLU:CD	2.37	0.50
2:C:1323:PHE:CZ	2:C:1327:LEU:CD1	2.95	0.50
2:C:1323:PHE:CE1	2:C:1327:LEU:HD13	2.47	0.50
3:J:418:GLU:CG	4:K:44:ASP:HA	2.32	0.50
3:J:903:LEU:HD23	3:J:905:ARG:CD	2.40	0.50
5:L:364:ARG:HA	5:L:367:ILE:HD12	1.94	0.50
1:A:65:LEU:HD22	1:A:65:LEU:N	2.25	0.50
2:C:1075:VAL:O	2:C:1076:ILE:C	2.54	0.50
2:C:1315:MET:CE	2:C:1317:PRO:HB3	2.42	0.50
3:D:45:ASN:O	3:D:46:TYR:CD2	2.65	0.50
3:D:141:PHE:C	3:D:180:MET:HE2	2.37	0.50
3:D:438:GLU:OE1	4:E:2:ALA:HB2	2.10	0.50
3:D:801:VAL:HG12	3:D:920:ALA:HB3	1.94	0.50
1:G:187:VAL:HG23	1:G:187:VAL:O	2.12	0.50
2:I:149:LEU:HB2	2:I:530:ILE:CG2	2.42	0.50
2:I:836:LEU:HD21	2:I:921:PRO:CD	2.41	0.50
2:I:1245:ALA:HB2	3:J:372:MET:HE3	1.94	0.50
3:J:388:ARG:CZ	3:J:414:GLU:OE2	2.59	0.50
3:J:735:ALA:O	3:J:738:ARG:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1171:GLY:HA2	3:J:1193:TRP:HZ3	1.75	0.50
2:C:231:GLU:HG2	2:C:332:ARG:HD3	1.94	0.50
2:C:1210:ILE:HG13	2:C:1227:VAL:HG22	1.93	0.50
3:D:141:PHE:CD1	3:D:293:ARG:HD3	2.47	0.50
3:D:165:TYR:CE2	3:D:178:ALA:HB3	2.47	0.50
3:D:275:ARG:HD3	3:D:298:MET:HB3	1.93	0.50
3:D:398:LYS:HG2	3:D:402:GLU:OE2	2.11	0.50
5:F:392:LYS:O	5:F:395:THR:CG2	2.60	0.50
1:G:38:THR:HA	1:H:45:ARG:HD3	1.94	0.50
2:I:26:TYR:CE2	2:I:32:LEU:HD12	2.41	0.50
2:I:998:LEU:HD12	2:I:998:LEU:N	2.27	0.50
3:J:45:ASN:O	3:J:46:TYR:HB3	2.11	0.50
3:J:425:ARG:HG2	3:J:426:ALA:N	2.20	0.50
3:J:708:ASN:OD1	3:J:708:ASN:N	2.45	0.50
3:J:848:VAL:HG23	3:J:857:LEU:CD1	2.41	0.50
5:L:287:ILE:HD11	5:L:341:LEU:HG	1.94	0.50
5:L:392:LYS:O	5:L:395:THR:HG22	2.11	0.50
1:A:86:LYS:HD3	1:A:176:CYS:HB2	1.94	0.50
2:C:5:TYR:HD1	2:C:8:LYS:CD	2.19	0.50
3:D:810:THR:HG23	3:D:811:GLU:H	1.77	0.50
5:F:226:ALA:O	5:F:229:VAL:HG22	2.12	0.50
2:I:996:ARG:HD2	2:I:999:GLU:CD	2.37	0.50
2:I:1220:GLN:HG2	2:I:1221:PHE:N	2.26	0.50
3:J:19:ALA:HA	3:J:1344:LEU:HD12	1.92	0.50
3:J:64:PRO:HG3	3:J:90:VAL:CG1	2.41	0.50
3:J:500:ILE:HG22	3:J:500:ILE:O	2.12	0.50
3:J:511:TYR:CD2	3:J:728:SER:HB3	2.47	0.50
3:J:903:LEU:HD13	3:J:909:ILE:CD1	2.42	0.50
1:A:38:THR:OG1	1:B:45:ARG:CG	2.58	0.49
2:C:981:ALA:HB1	2:C:1007:LYS:NZ	2.26	0.49
3:D:827:GLU:O	3:D:829:GLY:N	2.34	0.49
3:D:1278:GLU:OE1	3:D:1278:GLU:HA	2.11	0.49
1:G:14:VAL:HG13	1:G:27:THR:HB	1.93	0.49
3:J:250:ARG:HB3	3:J:265:LEU:HD12	1.93	0.49
3:J:360:TYR:OH	3:J:442:ILE:HD11	2.12	0.49
3:J:361:LEU:HD13	3:J:366:CYS:HA	1.93	0.49
3:J:1273:ASP:HB3	3:J:1276:GLU:HG3	1.92	0.49
1:A:53:GLY:O	1:A:177:TYR:HB3	2.12	0.49
2:C:471:VAL:CG2	2:C:498:ILE:HD11	2.41	0.49
2:I:31:GLN:OE1	2:I:456:VAL:HG23	2.12	0.49
2:I:62:TYR:C	2:I:64:GLY:N	2.70	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:700:VAL:HG13	2:I:1117:LEU:CD2	2.42	0.49
2:I:1280:ALA:HB3	3:J:431:ARG:HB3	1.94	0.49
3:J:451:PRO:O	3:J:454:CYS:HB2	2.12	0.49
3:J:827:GLU:CG	3:J:832:LYS:HD2	2.41	0.49
5:L:597:LYS:O	5:L:603:ARG:HG3	2.12	0.49
2:C:661:VAL:HB	2:C:665:ALA:HB3	1.94	0.49
2:C:848:GLU:CD	2:C:888:THR:HG22	2.37	0.49
2:C:921:PRO:O	2:C:924:VAL:HG22	2.12	0.49
3:D:450:HIS:CE1	3:D:452:LEU:HD12	2.47	0.49
3:D:709:ARG:C	3:D:711:GLY:N	2.58	0.49
3:D:741:ALA:O	3:D:762:ASN:ND2	2.45	0.49
3:D:814:CYS:HB3	3:D:890:THR:OG1	2.12	0.49
1:H:43:LEU:HD21	1:H:221:ALA:HB2	1.92	0.49
1:H:59:VAL:N	1:H:171:LEU:O	2.35	0.49
2:I:796:LEU:O	2:I:1233:LEU:HD12	2.12	0.49
2:I:824:GLN:HE22	2:I:1082:ILE:HD11	1.77	0.49
3:J:290:ILE:H	3:J:290:ILE:CD1	2.23	0.49
3:J:609:TYR:HD1	3:J:610:ARG:HH11	1.60	0.49
3:J:820:ILE:HG22	3:J:1227:HIS:ND1	2.27	0.49
3:J:1191:PRO:HB2	3:J:1194:ARG:HH11	1.77	0.49
5:L:224:LEU:HB2	5:L:259:PHE:CE1	2.48	0.49
5:L:281:ARG:CG	5:L:285:ARG:HH11	2.24	0.49
2:C:593:LYS:CB	2:C:602:GLU:HG3	2.38	0.49
2:C:705:GLU:H	2:C:705:GLU:CD	2.20	0.49
2:C:891:GLY:O	2:C:892:GLU:HG3	2.12	0.49
2:C:1146:GLN:NE2	2:C:1150:ASP:OD2	2.45	0.49
2:C:1272:GLU:N	3:D:343:LEU:HD11	2.27	0.49
3:D:279:LEU:HD23	3:D:279:LEU:O	2.12	0.49
3:D:536:LEU:CD1	3:D:541:LEU:HB2	2.33	0.49
3:D:755:ILE:HG22	3:D:757:THR:H	1.76	0.49
3:D:885:VAL:HG12	3:D:894:VAL:CG1	2.43	0.49
5:F:494:ILE:O	5:F:498:LEU:CB	2.60	0.49
1:G:27:THR:HG21	1:G:200:LYS:HD3	1.94	0.49
1:G:230:ALA:HB3	1:G:231:PHE:CD2	2.46	0.49
2:I:1164:PHE:O	2:I:1169:VAL:HG23	2.12	0.49
2:I:1250:SER:OG	5:L:524:GLU:OE1	2.30	0.49
3:J:545:HIS:NE2	3:J:719:PHE:HE1	2.10	0.49
2:C:188:PHE:CE1	2:C:194:LEU:HD13	2.48	0.49
2:C:227:LYS:HZ2	2:C:298:ALA:HB1	1.74	0.49
2:C:1292:THR:HG22	2:C:1293:VAL:N	2.28	0.49
3:D:16:GLU:CG	3:D:1369:ARG:NH2	2.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.94	0.49
3:D:536:LEU:HD12	3:D:542:ALA:CB	2.42	0.49
3:D:583:VAL:HG13	3:D:587:LEU:HD22	1.95	0.49
1:G:134:THR:O	2:I:773:LEU:HD11	2.13	0.49
2:I:39:ILE:CD1	2:I:75:LEU:HG	2.42	0.49
2:I:208:ILE:HD11	2:I:365:GLU:CB	2.42	0.49
2:I:245:ARG:HG2	2:I:337:PHE:CZ	2.48	0.49
2:I:761:GLN:O	2:I:762:ASN:HB2	2.12	0.49
2:I:1080:ASN:HB3	2:I:1085:MET:CE	2.32	0.49
3:J:418:GLU:HG3	4:K:45:LYS:H	1.77	0.49
3:J:658:GLU:C	3:J:661:VAL:HG13	2.37	0.49
4:K:26:ARG:NE	4:K:53:GLU:OE1	2.46	0.49
1:A:57:THR:CG2	1:A:158:ARG:CZ	2.90	0.49
1:B:41:ASN:ND2	2:C:1217:THR:HA	2.27	0.49
2:C:1180:MET:O	2:C:1182:ILE:HG13	2.11	0.49
3:D:510:LEU:O	3:D:514:THR:HG23	2.13	0.49
1:G:89:ALA:H	1:G:125:LYS:HD3	1.77	0.49
1:H:183:ILE:HD11	1:H:205:MET:HG3	1.94	0.49
2:I:979:LEU:HD13	2:I:1011:LEU:CD2	2.42	0.49
2:I:981:ALA:HB1	2:I:1007:LYS:HZ2	1.77	0.49
3:J:917:VAL:O	3:J:921:GLN:HG3	2.12	0.49
5:L:144:LEU:HG	5:L:221:PHE:HE1	1.77	0.49
5:L:287:ILE:CD1	5:L:344:LEU:HD22	2.42	0.49
5:L:519:LEU:C	5:L:519:LEU:HD23	2.37	0.49
2:C:520:PRO:HB3	2:C:714:VAL:HG21	1.95	0.49
2:C:691:PRO:HB3	2:C:788:SER:OG	2.13	0.49
2:C:733:VAL:HG11	2:C:966:ILE:HG21	1.93	0.49
2:C:854:ILE:HD11	2:C:885:GLY:HA3	1.94	0.49
3:D:518:VAL:HG13	3:D:519:ASN:N	2.26	0.49
3:D:824:PRO:HB2	3:D:826:ILE:HG23	1.94	0.49
3:D:1371:ARG:CZ	3:D:1371:ARG:HB3	2.43	0.49
5:F:297:MET:CE	5:F:330:LEU:HD11	2.42	0.49
5:F:583:THR:HG22	5:F:584:ARG:H	1.76	0.49
3:J:113:HIS:HD1	3:J:115:TRP:H	1.60	0.49
3:J:420:PRO:O	3:J:471:PRO:HD2	2.12	0.49
3:J:1344:LEU:HD12	3:J:1344:LEU:N	2.27	0.49
5:L:348:GLU:HG2	5:L:354:THR:HA	1.95	0.49
5:L:493:LYS:HA	5:L:496:LYS:HE2	1.95	0.49
1:A:61:ILE:HD12	1:A:64:VAL:HG21	1.95	0.49
1:B:51:MET:HG3	1:B:52:PRO:CD	2.41	0.49
2:C:215:TYR:CE1	2:C:223:LEU:HD11	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:634:VAL:HG13	2:C:636:CYS:HG	1.77	0.49
2:C:886:LYS:HE3	2:C:916:SER:HB3	1.95	0.49
3:D:799:ARG:HB3	3:D:1309:ILE:HD12	1.93	0.49
5:F:420:GLU:OE1	5:F:423:ARG:NH2	2.45	0.49
2:I:629:PHE:CE2	2:I:650:VAL:HG21	2.47	0.49
2:I:1043:ALA:HB3	2:I:1046:VAL:HG11	1.94	0.49
3:J:1298:VAL:O	3:J:1298:VAL:HG13	2.13	0.49
1:A:185:TYR:CE1	2:C:1087:TYR:OH	2.64	0.49
1:B:19:VAL:HB	1:B:23:HIS:CD2	2.48	0.49
2:C:836:LEU:HD12	2:C:836:LEU:N	2.27	0.49
2:C:985:GLU:HG2	2:C:988:LYS:HD2	1.95	0.49
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.94	0.49
3:D:842:ARG:HD3	3:D:882:VAL:HG11	1.95	0.49
1:G:172:LEU:HD12	1:G:172:LEU:H	1.77	0.49
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.95	0.49
2:I:490:GLN:HG2	2:I:491:ASP:N	2.27	0.49
2:I:1246:ARG:HG2	2:I:1247:SER:N	2.26	0.49
3:J:755:ILE:HD12	3:J:774:ILE:HG21	1.93	0.49
3:J:1371:ARG:HB3	3:J:1371:ARG:CZ	2.43	0.49
1:B:51:MET:O	1:B:150:ARG:HA	2.13	0.49
2:C:1158:LYS:O	2:C:1159:VAL:CG1	2.55	0.49
3:D:11:GLN:HG3	3:D:12:THR:N	2.28	0.49
3:D:72:CYS:HB3	3:D:88:CYS:SG	2.52	0.49
3:D:91:GLU:HG3	3:D:91:GLU:O	2.13	0.49
3:D:559:ALA:HB3	3:D:562:GLU:HB3	1.93	0.49
3:D:795:TYR:CE2	3:D:799:ARG:NE	2.81	0.49
5:F:147:GLN:HB3	5:F:161:LEU:CD2	2.43	0.49
1:G:16:ILE:CG2	1:G:26:VAL:HG12	2.42	0.49
1:G:38:THR:HA	1:H:45:ARG:CD	2.43	0.49
1:H:35:PHE:HA	1:H:38:THR:CG2	2.36	0.49
2:I:91:THR:CA	2:I:138:ILE:O	2.61	0.49
2:I:105:TYR:HA	2:I:113:THR:HA	1.94	0.49
2:I:488:MET:O	2:I:490:GLN:N	2.43	0.49
2:I:1294:LYS:HB3	3:J:347:VAL:HG13	1.94	0.49
3:J:190:LYS:HD3	3:J:235:GLU:HG2	1.94	0.49
1:A:90:VAL:HG23	1:A:123:ILE:HD13	1.94	0.48
2:C:510:GLN:CA	6:C:2001:KNG:C49	2.83	0.48
2:C:1264:GLN:O	2:C:1264:GLN:HG2	2.12	0.48
3:D:1143:ASP:OD1	3:D:1148:ARG:NH1	2.45	0.48
5:F:568:ASN:O	5:F:569:THR:HG22	2.12	0.48
1:H:125:LYS:HE2	1:H:128:HIS:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.52	0.48
3:J:885:VAL:HG12	3:J:894:VAL:CG1	2.43	0.48
3:J:1263:LYS:NZ	3:J:1315:ALA:CB	2.76	0.48
4:K:36:ASP:HB2	4:K:37:PRO:HD2	1.95	0.48
5:L:341:LEU:O	5:L:344:LEU:HB3	2.12	0.48
2:C:452:ARG:HH21	2:C:458:GLU:CD	2.20	0.48
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.95	0.48
2:C:737:ASN:HB3	2:C:739:ASP:OD1	2.13	0.48
3:D:622:ASP:HB3	3:D:626:TYR:CE2	2.41	0.48
3:D:899:TYR:CE2	3:D:1251:LYS:HD2	2.48	0.48
5:F:494:ILE:O	5:F:498:LEU:HB3	2.13	0.48
2:I:91:THR:HG21	2:I:503:LYS:HZ2	1.77	0.48
2:I:975:ILE:HG23	2:I:1011:LEU:CD2	2.43	0.48
3:J:288:PRO:HD2	3:J:291:ILE:HD12	1.94	0.48
3:J:831:VAL:HG13	3:J:831:VAL:O	2.13	0.48
5:L:533:ASP:O	5:L:536:THR:N	2.46	0.48
1:A:14:VAL:HG22	1:A:15:ASP:N	2.21	0.48
2:C:4:SER:HB2	2:C:7:GLU:HG3	1.95	0.48
2:C:62:TYR:C	2:C:64:GLY:N	2.70	0.48
2:C:548:ARG:HB3	2:C:569:ILE:O	2.12	0.48
2:C:650:VAL:HG23	2:C:650:VAL:O	2.13	0.48
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.41	0.48
3:D:291:ILE:CD1	5:F:409:ASN:HB3	2.43	0.48
3:D:518:VAL:H	3:D:716:GLN:HE22	1.60	0.48
3:D:587:LEU:HD11	3:D:608:CYS:HA	1.95	0.48
5:F:362:ASN:O	5:F:365:MET:HB3	2.13	0.48
2:I:886:LYS:NZ	2:I:916:SER:HB3	2.28	0.48
3:J:71:LEU:HD22	3:J:71:LEU:C	2.36	0.48
3:J:97:VAL:HG12	3:J:101:ARG:HG3	1.94	0.48
3:J:141:PHE:C	3:J:180:MET:HE2	2.38	0.48
3:J:352:ARG:O	3:J:353:SER:HB3	2.14	0.48
5:L:147:GLN:HB3	5:L:161:LEU:HD13	1.95	0.48
1:A:172:LEU:H	1:A:172:LEU:HD12	1.78	0.48
1:B:144:ILE:HG23	1:B:144:ILE:O	2.12	0.48
2:C:1066:MET:CE	2:C:1076:ILE:CB	2.86	0.48
2:C:1148:ALA:HB1	2:C:1180:MET:CE	2.42	0.48
1:G:71:LYS:NZ	1:G:140:ILE:HG22	2.28	0.48
2:I:119:GLU:HG2	2:I:489:PRO:HD2	1.96	0.48
2:I:141:THR:O	2:I:143:ARG:HG3	2.13	0.48
2:I:737:ASN:HB3	2:I:739:ASP:OD1	2.13	0.48
2:I:1172:LEU:O	2:I:1172:LEU:HD22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:507:VAL:HG21	3:J:598:LYS:HB2	1.94	0.48
3:J:1237:VAL:CG1	3:J:1253:ILE:HD13	2.43	0.48
5:L:468:ARG:O	5:L:471:LEU:HB2	2.13	0.48
5:L:544:THR:HG22	5:L:607:LEU:CD2	2.44	0.48
1:A:36:GLY:C	1:A:187:VAL:HG11	2.38	0.48
1:B:205:MET:CG	1:B:206:GLU:N	2.76	0.48
2:C:180:ARG:NH1	2:C:465:ARG:HH12	2.12	0.48
2:C:805:MET:O	2:C:805:MET:HG3	2.13	0.48
2:C:980:VAL:HG13	2:C:984:VAL:HB	1.96	0.48
2:C:1327:LEU:HD23	2:C:1331:ARG:HH21	1.78	0.48
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.96	0.48
5:F:162:ILE:HD13	5:F:221:PHE:HE2	1.78	0.48
5:F:231:THR:HG23	5:F:249:ILE:HG12	1.95	0.48
5:F:312:SER:O	5:F:315:TRP:NE1	2.47	0.48
1:G:197:ASP:O	1:G:198:LEU:HD23	2.13	0.48
1:H:124:VAL:HG11	1:H:210:THR:HG23	1.96	0.48
2:I:31:GLN:O	2:I:130:MET:HE1	2.13	0.48
2:I:106:GLU:HA	2:I:114:VAL:CG2	2.43	0.48
2:I:478:ARG:CZ	2:I:487:LEU:HD13	2.43	0.48
2:I:998:LEU:HD12	2:I:998:LEU:H	1.79	0.48
2:I:1142:ARG:HD3	2:I:1161:LEU:HD11	1.90	0.48
3:J:355:ILE:HG22	3:J:447:ILE:HB	1.96	0.48
1:A:57:THR:CG2	1:A:158:ARG:NH2	2.76	0.48
1:B:210:THR:C	1:B:211:ILE:HG12	2.39	0.48
2:C:241:LEU:CD2	2:C:246:LEU:HD11	2.36	0.48
2:C:911:SER:OG	2:C:913:VAL:HG12	2.13	0.48
2:C:1271:GLY:HA3	3:D:343:LEU:HD11	1.87	0.48
3:D:854:ALA:CB	3:J:1372:ARG:HE	2.26	0.48
3:D:1141:VAL:HG13	3:D:1237:VAL:HG23	1.96	0.48
5:F:163:THR:O	5:F:163:THR:HG22	2.13	0.48
5:F:400:GLN:HB2	5:F:403:ASP:OD2	2.13	0.48
2:I:101:ARG:NE	2:I:118:LYS:HD2	2.28	0.48
2:I:470:ARG:CZ	2:I:497:PRO:HA	2.44	0.48
2:I:478:ARG:HH12	2:I:482:GLY:HA2	1.77	0.48
2:I:720:ARG:NH2	2:I:736:VAL:HG21	2.28	0.48
3:J:510:LEU:O	3:J:514:THR:HG23	2.14	0.48
3:J:805:GLN:CD	3:J:1348:LYS:HD3	2.37	0.48
3:J:820:ILE:CD1	3:J:822:MET:HE2	2.41	0.48
3:J:1171:GLY:HA2	3:J:1193:TRP:CZ3	2.47	0.48
4:K:25:ARG:NH1	4:K:65:ASP:OD1	2.39	0.48
2:C:194:LEU:HA	2:C:194:LEU:HD12	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:566:GLY:O	2:C:569:ILE:HG13	2.13	0.48
2:C:594:VAL:HG22	2:C:599:VAL:HA	1.95	0.48
2:C:614:TYR:CE1	2:C:652:TYR:CE1	3.01	0.48
2:C:672:GLU:HB3	3:D:767:LEU:O	2.13	0.48
2:C:1149:TYR:HD1	2:C:1159:VAL:CG1	2.25	0.48
3:D:77:ARG:NH1	3:D:78:LEU:HG	2.29	0.48
3:D:214:ARG:HA	3:D:217:LEU:HB2	1.96	0.48
3:D:412:LEU:O	3:D:415:VAL:HG22	2.13	0.48
3:D:514:THR:HG23	3:D:596:LEU:HB2	1.95	0.48
3:D:750:PRO:HA	3:D:777:HIS:NE2	2.28	0.48
3:D:1169:THR:CG2	3:D:1192:LYS:HD3	2.43	0.48
5:F:298:PRO:HD2	5:F:326:TRP:CB	2.43	0.48
1:G:71:LYS:HB3	1:G:74:VAL:CG1	2.44	0.48
1:G:75:GLN:HA	2:I:729:ALA:N	2.28	0.48
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	1.96	0.48
3:J:336:GLY:HA3	3:J:1324:SER:O	2.14	0.48
3:J:481:ARG:O	3:J:485:MET:HB2	2.13	0.48
3:J:528:THR:HG22	3:J:532:GLU:CD	2.39	0.48
3:J:930:LEU:HD12	3:J:1138:LEU:HD13	1.94	0.48
3:J:1175:LEU:O	3:J:1187:GLU:HA	2.13	0.48
3:J:1184:ASP:OD2	3:J:1185:PRO:N	2.47	0.48
3:J:1309:ILE:HG13	3:J:1310:THR:H	1.79	0.48
1:A:207:THR:HG22	1:A:209:GLY:H	1.78	0.48
2:C:757:THR:HG22	2:C:765:ILE:O	2.13	0.48
2:C:1165:SER:HA	2:C:1169:VAL:CG2	2.44	0.48
2:C:1262:LYS:HD3	2:C:1262:LYS:HA	1.62	0.48
3:D:858:VAL:HG22	3:D:858:VAL:O	2.13	0.48
3:D:1203:ARG:HH12	3:D:1205:GLU:HG2	1.77	0.48
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.47	0.48
4:E:71:GLU:HA	4:E:74:GLU:HG3	1.96	0.48
1:H:76:GLU:HB3	1:H:81:ILE:HG13	1.95	0.48
1:H:142:MET:HG3	1:H:144:ILE:CG1	2.41	0.48
2:I:582:ASN:HB3	2:I:586:PHE:N	2.29	0.48
2:I:697:LYS:HD2	2:I:1181:PRO:HG3	1.96	0.48
2:I:896:THR:OG1	2:I:899:GLU:HG3	2.14	0.48
2:I:1112:ILE:HD11	3:J:639:VAL:HG13	1.96	0.48
3:J:186:GLN:HG3	3:J:238:ILE:CB	2.30	0.48
3:J:839:VAL:O	3:J:839:VAL:HG12	2.12	0.48
3:J:1167:LYS:HB2	3:J:1174:ARG:HD3	1.95	0.48
1:A:82:LEU:HD11	1:A:171:LEU:HG	1.96	0.48
2:C:1149:TYR:CB	2:C:1159:VAL:HG11	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:905:ARG:NH2	3:D:907:HIS:HB2	2.17	0.48
1:G:13:LEU:HD23	1:H:230:ALA:HB1	1.96	0.48
1:G:38:THR:CB	1:H:45:ARG:HD3	2.43	0.48
1:G:163:GLU:O	1:G:164:ASP:HB3	2.14	0.48
2:I:38:PHE:HE1	2:I:461:GLU:HA	1.79	0.48
2:I:43:PRO:O	2:I:44:GLU:HB3	2.13	0.48
2:I:292:ILE:HD12	2:I:322:LEU:HD11	1.96	0.48
2:I:815:SER:OG	3:J:357:VAL:HG22	2.14	0.48
2:I:979:LEU:HD12	2:I:1011:LEU:HD11	1.95	0.48
2:I:981:ALA:O	2:I:1002:LEU:HD11	2.13	0.48
2:I:1134:GLN:O	2:I:1135:GLN:HG2	2.14	0.48
2:I:1151:LEU:CD1	2:I:1198:LEU:HD23	2.41	0.48
3:J:1221:LEU:C	3:J:1221:LEU:HD13	2.38	0.48
5:L:290:LEU:CD1	5:L:337:VAL:HG22	2.43	0.48
5:L:444:ALA:HB1	5:L:457:ILE:CD1	2.44	0.48
5:L:583:THR:HG22	5:L:584:ARG:H	1.78	0.48
1:A:13:LEU:H	1:A:13:LEU:CD2	2.06	0.48
1:A:27:THR:HA	1:A:201:LEU:O	2.13	0.48
1:B:14:VAL:O	1:B:16:ILE:HG13	2.14	0.48
2:C:243:PRO:CB	2:C:278:GLU:HG3	2.41	0.48
2:C:397:LEU:HD12	2:C:397:LEU:H	1.77	0.48
2:C:494:ASN:HB3	2:C:497:PRO:HD2	1.96	0.48
2:C:699:LEU:HD23	2:C:699:LEU:HA	1.60	0.48
2:C:883:LEU:HD23	2:C:883:LEU:HA	1.57	0.48
3:D:113:HIS:HE1	3:D:115:TRP:HB2	1.69	0.48
5:F:513:ASP:OD2	5:F:515:GLU:OE1	2.32	0.48
2:I:168:GLY:C	2:I:170:VAL:H	2.22	0.48
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.96	0.48
3:J:399:LYS:HZ1	5:L:612:ASP:HB3	1.77	0.48
3:J:518:VAL:N	3:J:716:GLN:HE22	2.12	0.48
3:J:615:LYS:NZ	4:K:7:GLN:CG	2.77	0.48
1:A:54:CYS:HB3	1:A:148:ARG:HG3	1.96	0.47
1:B:198:LEU:HD13	1:B:198:LEU:HA	1.56	0.47
2:C:91:THR:CB	2:C:138:ILE:O	2.62	0.47
2:C:159:SER:O	2:C:160:ASP:HB2	2.13	0.47
2:C:393:ASP:OD1	2:C:394:ARG:HD3	2.13	0.47
2:C:852:ALA:HB2	2:C:869:GLY:HA2	1.96	0.47
3:D:147:ILE:HG22	3:D:188:LEU:CG	2.43	0.47
3:D:197:GLU:O	3:D:201:LEU:HG	2.14	0.47
3:D:1273:ASP:CB	3:D:1276:GLU:CD	2.87	0.47
1:G:165:GLU:HG3	1:G:165:GLU:O	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:55:ALA:CB	1:H:176:CYS:H	2.27	0.47
2:I:756:TYR:H	2:I:756:TYR:HD1	1.62	0.47
2:I:1304:MET:HE3	3:J:472:LEU:HD13	1.94	0.47
3:J:1165:PHE:CE1	3:J:1200:GLU:HB3	2.45	0.47
3:J:1314:LEU:HD11	3:J:1330:ARG:HH22	1.79	0.47
3:J:1356:LEU:HD23	3:J:1356:LEU:HA	1.72	0.47
5:L:96:ASP:O	5:L:98:VAL:HG13	2.14	0.47
5:L:101:TYR:CE2	5:L:405:ILE:HD12	2.49	0.47
5:L:297:MET:HA	5:L:326:TRP:HB3	1.95	0.47
5:L:315:TRP:O	5:L:319:ALA:HB3	2.14	0.47
5:L:397:ARG:HB3	5:L:443:ILE:HD13	1.97	0.47
5:L:513:ASP:OD2	5:L:515:GLU:HB2	2.13	0.47
1:B:89:ALA:CB	1:B:124:VAL:CG1	2.90	0.47
2:C:17:LYS:NZ	2:C:1154:ASP:HB2	2.29	0.47
2:C:374:GLU:HG3	2:C:374:GLU:O	2.13	0.47
2:C:818:VAL:HG23	2:C:1076:ILE:CD1	2.38	0.47
2:C:1271:GLY:C	3:D:343:LEU:HD11	2.38	0.47
3:D:394:ILE:HG13	5:F:536:THR:HG22	1.96	0.47
3:D:421:VAL:HG13	3:D:439:PRO:HG3	1.95	0.47
3:D:664:ILE:HG22	3:D:678:ARG:HG2	1.96	0.47
5:F:388:ILE:O	5:F:392:LYS:HG3	2.13	0.47
2:I:14:ASP:OD2	2:I:1156:ARG:NE	2.46	0.47
2:I:60:GLN:HB3	2:I:67:GLU:HG3	1.96	0.47
2:I:1299:ASN:ND2	2:I:1303:LYS:HE2	2.29	0.47
3:J:148:GLU:H	3:J:156:ARG:HG3	1.78	0.47
3:J:1174:ARG:NH2	3:J:1187:GLU:OE2	2.47	0.47
4:K:38:LEU:HD23	4:K:58:LEU:HD13	1.96	0.47
1:A:43:LEU:CD1	1:A:203:ILE:HD11	2.44	0.47
1:B:29:GLU:HG2	1:B:30:PRO:HG3	1.96	0.47
1:B:85:LEU:HA	1:B:85:LEU:HD23	1.33	0.47
1:B:195:ARG:HB2	1:B:198:LEU:CD2	2.45	0.47
2:C:6:THR:HG21	2:C:782:VAL:HG23	1.94	0.47
2:C:564:PRO:HG3	2:C:572:ILE:HG13	1.95	0.47
3:D:126:LEU:C	3:D:126:LEU:HD12	2.38	0.47
3:D:654:ILE:O	3:D:658:GLU:HB2	2.14	0.47
3:D:678:ARG:CD	3:D:678:ARG:C	2.86	0.47
3:D:1372:ARG:HA	3:J:853:THR:HB	1.96	0.47
1:H:16:ILE:HG23	1:H:26:VAL:HG13	1.96	0.47
1:H:22:THR:O	1:H:207:THR:OG1	2.31	0.47
2:I:765:ILE:HG13	2:I:787:PRO:HG3	1.96	0.47
2:I:1066:MET:CE	2:I:1076:ILE:HB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:102:MET:HE2	3:J:102:MET:HB3	1.73	0.47
3:J:290:ILE:HD12	3:J:290:ILE:N	2.22	0.47
3:J:572:THR:HG21	3:J:589:TYR:OH	2.14	0.47
1:A:40:GLY:HA3	1:A:185:TYR:CD2	2.49	0.47
1:B:31:LEU:O	1:B:198:LEU:HD12	2.14	0.47
2:C:23:ASP:OD1	2:C:23:ASP:N	2.44	0.47
2:C:530:ILE:HG23	2:C:530:ILE:HD12	1.59	0.47
2:C:564:PRO:HG2	2:C:568:ASN:O	2.14	0.47
2:C:738:GLU:HG2	2:C:741:MET:CE	2.44	0.47
2:C:882:ILE:HD12	2:C:882:ILE:N	2.29	0.47
3:D:22:ILE:HG23	3:D:1336:ALA:HA	1.95	0.47
3:D:291:ILE:HG12	5:F:409:ASN:HD22	1.79	0.47
3:D:525:MET:HE3	3:D:525:MET:HB2	1.82	0.47
5:F:280:VAL:HG13	5:F:355:ILE:HD12	1.95	0.47
5:F:540:LEU:HB2	5:F:610:PHE:CE1	2.49	0.47
1:G:73:GLY:C	1:G:134:THR:HG22	2.39	0.47
2:I:218:GLU:OE1	2:I:299:LYS:HE2	2.14	0.47
2:I:582:ASN:HB3	2:I:586:PHE:H	1.78	0.47
2:I:671:LEU:HD23	2:I:1186:VAL:HG12	1.97	0.47
2:I:681:MET:HE1	2:I:1073:LYS:NZ	2.29	0.47
2:I:705:GLU:HB2	2:I:794:LEU:H	1.80	0.47
2:I:738:GLU:HG2	2:I:741:MET:HE1	1.92	0.47
2:I:828:PHE:HB3	2:I:1060:ILE:HD12	1.96	0.47
3:J:438:GLU:OE1	4:K:2:ALA:CB	2.62	0.47
3:J:502:PRO:HB3	3:J:506:VAL:CG1	2.44	0.47
3:J:615:LYS:NZ	4:K:7:GLN:HG2	2.29	0.47
3:J:1145:PHE:HB3	3:J:1309:ILE:HG23	1.95	0.47
1:A:59:VAL:HG21	1:A:85:LEU:HD12	1.97	0.47
1:B:89:ALA:O	1:B:124:VAL:HG12	2.14	0.47
1:B:152:TYR:HE2	3:D:536:LEU:HD21	1.75	0.47
1:B:210:THR:O	1:B:211:ILE:CD1	2.63	0.47
2:C:22:LEU:HD22	2:C:22:LEU:HA	1.61	0.47
2:C:894:GLN:O	2:C:894:GLN:HG3	2.14	0.47
3:D:92:VAL:O	3:D:92:VAL:CG2	2.63	0.47
3:D:684:ASP:O	3:D:687:ALA:HB3	2.15	0.47
3:D:705:THR:OG1	3:D:718:SER:HA	2.14	0.47
5:F:394:TYR:OH	5:F:436:ARG:HG3	2.13	0.47
5:F:562:ARG:HE	5:F:573:LEU:HB3	1.80	0.47
1:G:194:GLN:O	1:G:195:ARG:HB2	2.13	0.47
2:I:104:ILE:O	2:I:114:VAL:N	2.45	0.47
2:I:146:VAL:HG11	2:I:531:LEU:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:692:THR:OG1	2:I:693:LEU:N	2.47	0.47
3:J:267:ASP:HA	3:J:270:ARG:HH21	1.80	0.47
3:J:552:ILE:HG12	3:J:570:LYS:HG3	1.96	0.47
5:L:124:GLU:O	5:L:127:ILE:HG13	2.13	0.47
1:A:76:GLU:HB3	1:A:81:ILE:HG12	1.97	0.47
2:C:104:ILE:O	2:C:113:THR:HA	2.14	0.47
2:C:1151:LEU:HD23	2:C:1197:GLU:OE2	2.14	0.47
3:D:35:PHE:HD1	3:D:101:ARG:CB	2.23	0.47
3:D:1184:ASP:O	3:D:1186:TYR:N	2.48	0.47
5:F:490:PRO:HB2	5:F:493:LYS:HG3	1.96	0.47
1:G:56:VAL:HG11	1:G:86:LYS:HA	1.97	0.47
1:G:85:LEU:HD22	1:G:144:ILE:HD13	1.95	0.47
3:J:48:THR:HB	3:J:50:LYS:HG3	1.97	0.47
3:J:201:LEU:HD11	3:J:220:ARG:NH1	2.30	0.47
3:J:218:THR:HA	3:J:221:ILE:HG22	1.97	0.47
3:J:746:LEU:CD2	3:J:758:PRO:HG3	2.45	0.47
3:J:1291:GLU:HB3	3:J:1292:LEU:HD12	1.97	0.47
5:L:390:ILE:HD12	5:L:435:ILE:CG2	2.44	0.47
1:A:150:ARG:CD	1:B:8:PHE:CE2	2.98	0.47
1:B:192:VAL:CG1	1:B:193:GLU:N	2.77	0.47
1:B:205:MET:HE3	1:B:213:PRO:HB3	1.96	0.47
2:C:22:LEU:HD13	2:C:23:ASP:N	2.29	0.47
2:C:185:ASP:O	2:C:196:VAL:HA	2.14	0.47
2:C:230:PHE:O	2:C:332:ARG:HA	2.15	0.47
2:C:697:LYS:CA	2:C:795:ALA:HB2	2.36	0.47
2:C:739:ASP:OD1	2:C:739:ASP:N	2.47	0.47
2:C:741:MET:HG2	2:C:974:ARG:NH2	2.29	0.47
2:C:972:PHE:CD2	2:C:975:ILE:HD12	2.50	0.47
2:C:987:GLU:HG2	2:C:991:LYS:HE3	1.97	0.47
2:C:1024:GLU:HA	2:C:1027:LYS:HG2	1.95	0.47
2:C:1191:LYS:HD3	2:C:1193:ALA:N	2.24	0.47
2:C:1279:GLU:HG2	3:D:1357:ILE:HD13	1.97	0.47
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.48	0.47
3:D:490:ILE:O	3:D:491:LEU:HD23	2.15	0.47
3:D:580:TRP:CZ3	3:D:589:TYR:HA	2.49	0.47
3:D:795:TYR:HE2	3:D:799:ARG:NE	2.12	0.47
3:D:839:VAL:HG13	3:D:882:VAL:HG21	1.96	0.47
3:D:861:ASN:O	3:D:861:ASN:OD1	2.33	0.47
3:D:1233:ILE:HG12	3:D:1260:MET:HE1	1.95	0.47
5:F:481:GLU:O	5:F:485:GLU:OE2	2.32	0.47
1:G:61:ILE:HG22	1:G:62:ASP:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:67:GLU:OE2	1:H:171:LEU:N	2.47	0.47
2:I:27:LEU:HD12	2:I:524:ILE:HD11	1.96	0.47
2:I:176:ILE:HB	2:I:184:LEU:HB3	1.97	0.47
2:I:452:ARG:NH2	2:I:458:GLU:OE1	2.44	0.47
2:I:1272:GLU:CG	3:J:342:LEU:CB	2.92	0.47
2:I:1307:ASN:HB3	2:I:1312:ASN:O	2.15	0.47
3:J:479:GLU:HG3	4:K:20:VAL:CG1	2.37	0.47
3:J:858:VAL:HG22	3:J:858:VAL:O	2.14	0.47
3:J:1350:ASN:OD1	3:J:1355:ARG:HD2	2.14	0.47
5:L:96:ASP:O	5:L:96:ASP:CG	2.57	0.47
5:L:511:ILE:HG23	5:L:511:ILE:O	2.14	0.47
5:L:573:LEU:HG	5:L:574:GLU:OE1	2.14	0.47
1:A:56:VAL:HG21	1:A:144:ILE:HG23	1.97	0.47
1:A:165:GLU:HG3	1:A:165:GLU:O	2.15	0.47
1:B:92:VAL:HA	1:B:120:ASP:O	2.15	0.47
2:C:842:ASP:HB2	2:C:1045:GLY:O	2.14	0.47
2:C:848:GLU:HG2	2:C:888:THR:HB	1.97	0.47
2:C:854:ILE:HD11	2:C:885:GLY:CA	2.45	0.47
2:C:896:THR:HG23	2:C:899:GLU:OE2	2.14	0.47
5:F:277:MET:CE	5:F:281:ARG:HH21	2.26	0.47
1:G:14:VAL:HG22	1:G:15:ASP:N	2.23	0.47
2:I:894:GLN:HG3	2:I:894:GLN:O	2.14	0.47
2:I:1196:LYS:O	2:I:1199:LEU:HB2	2.14	0.47
3:J:418:GLU:OE1	4:K:2:ALA:HA	2.15	0.47
3:J:1146:GLU:HG2	3:J:1148:ARG:NH2	2.30	0.47
3:J:1263:LYS:CE	3:J:1279:GLN:NE2	2.78	0.47
5:L:490:PRO:HG2	5:L:493:LYS:HE3	1.97	0.47
1:A:61:ILE:CD1	1:A:64:VAL:HG21	2.45	0.47
2:C:360:LEU:O	2:C:364:VAL:HG23	2.15	0.47
2:C:518:ASN:ND2	2:C:761:GLN:HG2	2.30	0.47
2:C:796:LEU:HB2	2:C:1233:LEU:CD1	2.45	0.47
2:C:810:TYR:HD1	2:C:1078:LYS:HB2	1.78	0.47
2:C:1268:GLN:HE22	3:D:352:ARG:NH1	2.13	0.47
3:D:139:LEU:HA	3:D:139:LEU:HD23	1.58	0.47
4:E:16:ARG:O	4:E:16:ARG:HG2	2.14	0.47
5:F:568:ASN:C	5:F:569:THR:HG22	2.40	0.47
1:G:67:GLU:OE1	2:I:1057:LYS:NZ	2.48	0.47
1:G:177:TYR:O	1:G:178:SER:HB2	2.15	0.47
1:H:66:HIS:HB3	1:H:68:TYR:CE2	2.49	0.47
2:I:578:TYR:HB3	2:I:590:PRO:HG2	1.95	0.47
2:I:805:MET:HE1	2:I:1221:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1043:ALA:O	2:I:1046:VAL:CG1	2.63	0.47
2:I:1337:ILE:O	2:I:1337:ILE:HG23	2.14	0.47
3:J:303:VAL:O	3:J:307:LEU:HG	2.14	0.47
3:J:800:LEU:CD1	3:J:1309:ILE:CD1	2.93	0.47
5:L:111:LEU:HD23	5:L:111:LEU:HA	1.48	0.47
2:C:103:VAL:HB	2:C:113:THR:HG21	1.97	0.47
2:C:1142:ARG:HH12	2:C:1169:VAL:HG21	1.79	0.47
3:D:45:ASN:O	3:D:46:TYR:CB	2.61	0.47
3:D:192:MET:HE2	3:D:197:GLU:OE2	2.15	0.47
3:D:440:VAL:O	3:D:442:ILE:HG12	2.15	0.47
3:D:598:LYS:O	3:D:601:ILE:HG22	2.15	0.47
3:D:686:TRP:CE3	3:D:758:PRO:HG2	2.49	0.47
3:D:857:LEU:CD2	3:D:875:ASN:ND2	2.71	0.47
5:F:423:ARG:CD	5:F:425:TYR:CE2	2.98	0.47
1:G:110:VAL:O	1:G:130:ILE:HB	2.14	0.47
2:I:238:GLN:HB3	2:I:284:LEU:HD11	1.96	0.47
2:I:724:VAL:HG11	2:I:727:VAL:CG2	2.39	0.47
3:J:755:ILE:HG22	3:J:757:THR:H	1.80	0.47
1:A:59:VAL:CG2	1:A:85:LEU:HD13	2.44	0.46
1:B:33:ARG:HH11	2:C:1081:PRO:HG3	1.80	0.46
2:C:1184:THR:HG23	2:C:1189:GLY:CA	2.45	0.46
2:C:1246:ARG:NH2	2:C:1249:GLY:H	2.13	0.46
3:D:333:GLY:CA	3:D:338:PHE:CZ	2.98	0.46
3:D:614:LEU:O	3:D:615:LYS:C	2.56	0.46
3:D:1290:ARG:HA	3:D:1294:ALA:HB3	1.95	0.46
5:F:244:THR:O	5:F:247:GLU:HG2	2.15	0.46
1:H:6:THR:O	1:H:6:THR:CG2	2.61	0.46
1:H:151:GLY:O	1:H:177:TYR:HB2	2.15	0.46
2:I:53:PHE:O	2:I:57:PHE:HB2	2.16	0.46
3:J:45:ASN:O	3:J:46:TYR:CD2	2.68	0.46
3:J:218:THR:HA	3:J:221:ILE:CG2	2.45	0.46
1:A:112:ALA:O	1:A:115:ILE:HG13	2.16	0.46
1:B:89:ALA:HB3	1:B:124:VAL:HG11	1.94	0.46
3:D:1290:ARG:HA	3:D:1294:ALA:CB	2.45	0.46
1:G:50:SER:HB3	1:H:8:PHE:HE1	1.79	0.46
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.97	0.46
2:I:745:GLU:HG3	2:I:1017:GLN:CB	2.42	0.46
2:I:855:PRO:HG3	2:I:913:VAL:HG13	1.96	0.46
2:I:870:ILE:HG12	2:I:1050:VAL:HG11	1.95	0.46
3:J:128:LEU:HD23	3:J:192:MET:HE3	1.96	0.46
3:J:201:LEU:HD11	3:J:220:ARG:HH11	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:820:ILE:HD11	3:J:822:MET:CE	2.45	0.46
3:J:847:ASP:OD1	3:J:847:ASP:N	2.26	0.46
3:J:1203:ARG:NH1	3:J:1205:GLU:HG2	2.30	0.46
3:J:1280:VAL:CB	3:J:1304:ARG:HE	2.28	0.46
3:J:1307:LEU:HB3	3:J:1312:ALA:HB2	1.96	0.46
5:L:482:GLU:HA	5:L:485:GLU:OE2	2.15	0.46
5:L:601:PRO:HB2	5:L:605:GLU:HG2	1.97	0.46
1:A:50:SER:HB2	1:B:8:PHE:CZ	2.44	0.46
1:A:233:ASP:CA	1:A:234:LEU:HD22	2.45	0.46
1:B:6:THR:N	1:B:7:GLU:OE2	2.48	0.46
2:C:632:ASP:O	2:C:647:ARG:HB2	2.15	0.46
2:C:882:ILE:HG13	2:C:919:ARG:NH1	2.30	0.46
3:D:58:CYS:SG	3:D:60:ARG:HB3	2.55	0.46
3:D:490:ILE:O	3:D:490:ILE:HG13	2.14	0.46
3:D:537:TYR:CZ	3:D:544:LEU:HD22	2.50	0.46
3:D:857:LEU:CD1	3:D:858:VAL:HG13	2.45	0.46
3:D:1319:PHE:HB3	3:D:1340:LYS:HD2	1.97	0.46
4:E:54:ILE:HD13	4:E:59:ILE:O	2.16	0.46
5:F:292:VAL:HA	5:F:297:MET:O	2.16	0.46
1:G:38:THR:CA	1:H:45:ARG:HD3	2.44	0.46
1:H:100:LEU:HB3	1:H:115:ILE:CG2	2.45	0.46
2:I:106:GLU:HA	2:I:114:VAL:HG22	1.97	0.46
2:I:159:SER:O	2:I:160:ASP:HB2	2.15	0.46
2:I:516:ASP:CG	2:I:522:SER:OG	2.58	0.46
3:J:518:VAL:HG12	3:J:707:ILE:HD13	1.97	0.46
3:J:681:LYS:O	3:J:685:ILE:HG23	2.16	0.46
3:J:1264:ALA:CB	3:J:1304:ARG:HA	2.44	0.46
5:L:137:TYR:CD2	5:L:273:MET:HG2	2.50	0.46
1:A:71:LYS:HB3	1:A:74:VAL:CG1	2.45	0.46
1:A:85:LEU:HD22	1:A:144:ILE:HD13	1.97	0.46
2:C:883:LEU:CD1	2:C:920:VAL:HG22	2.41	0.46
2:C:1151:LEU:HD23	2:C:1151:LEU:HA	1.71	0.46
2:C:1327:LEU:O	2:C:1331:ARG:HB2	2.15	0.46
3:D:902:ASP:OD1	3:D:903:LEU:N	2.48	0.46
5:F:584:ARG:HA	5:F:584:ARG:NH1	2.31	0.46
2:I:109:ALA:CB	2:I:111:GLU:HA	2.44	0.46
2:I:238:GLN:OE1	2:I:284:LEU:HD21	2.16	0.46
2:I:251:ALA:CA	2:I:269:ILE:HD11	2.45	0.46
2:I:681:MET:HE2	2:I:681:MET:HB3	1.76	0.46
3:J:210:SER:HB2	3:J:213:LYS:HB2	1.97	0.46
3:J:816:THR:HB	3:J:889:ASP:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1237:VAL:HG11	3:J:1253:ILE:HD13	1.96	0.46
1:A:104:LYS:HG2	1:A:110:VAL:HG22	1.97	0.46
2:C:466:VAL:O	2:C:470:ARG:HG2	2.15	0.46
2:C:591:TYR:CD2	2:C:606:LEU:HD13	2.40	0.46
2:C:719:LYS:O	2:C:779:ARG:HG3	2.15	0.46
2:C:1217:THR:C	2:C:1219:GLU:H	2.22	0.46
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.48	0.46
3:D:416:ILE:O	3:D:417:ARG:C	2.58	0.46
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.98	0.46
3:D:1372:ARG:HH21	3:J:854:ALA:CB	2.27	0.46
1:G:179:PRO:CG	1:G:211:ILE:HG13	2.45	0.46
2:I:56:VAL:HG11	2:I:468:LEU:CD1	2.41	0.46
2:I:253:PHE:CD1	2:I:288:PRO:HD3	2.50	0.46
2:I:905:ILE:CD1	5:L:598:LEU:HD13	2.46	0.46
3:J:34:SER:HB2	3:J:104:HIS:HB3	1.98	0.46
3:J:514:THR:HG21	3:J:596:LEU:CG	2.46	0.46
3:J:664:ILE:HG21	3:J:681:LYS:HB3	1.97	0.46
3:J:930:LEU:HB2	3:J:1138:LEU:HB2	1.97	0.46
3:J:1145:PHE:CE1	3:J:1256:ILE:HG21	2.51	0.46
4:K:50:ALA:O	4:K:54:ILE:HG12	2.16	0.46
5:L:582:VAL:HG11	5:L:586:ARG:HG2	1.95	0.46
2:C:188:PHE:CZ	2:C:194:LEU:HD13	2.51	0.46
2:C:274:ILE:HG22	2:C:278:GLU:OE1	2.15	0.46
2:C:820:GLU:O	2:C:823:VAL:HG12	2.16	0.46
2:C:972:PHE:HD2	2:C:975:ILE:HD12	1.79	0.46
2:C:1341:ASP:HB3	3:D:18:ASP:OD2	2.16	0.46
3:D:1167:LYS:CD	3:D:1174:ARG:HD2	2.42	0.46
4:E:49:ILE:O	4:E:53:GLU:HG3	2.16	0.46
5:F:479:THR:HG23	5:F:481:GLU:H	1.79	0.46
2:I:30:ILE:H	2:I:30:ILE:CD1	2.13	0.46
2:I:237:LEU:HD11	2:I:292:ILE:CD1	2.45	0.46
2:I:1149:TYR:CB	2:I:1159:VAL:HG11	2.46	0.46
3:J:925:GLU:HB3	3:J:926:PRO:HD3	1.98	0.46
3:J:1167:LYS:NZ	3:J:1170:LYS:HB2	2.30	0.46
3:J:1341:ARG:NH1	3:J:1343:GLU:OE2	2.47	0.46
5:L:322:MET:SD	5:L:326:TRP:HH2	2.39	0.46
1:B:86:LYS:HD3	1:B:174:ASP:OD2	2.16	0.46
1:B:116:THR:HG23	1:B:116:THR:O	2.16	0.46
2:C:109:ALA:HB1	2:C:110:PRO:O	2.13	0.46
2:C:562:GLU:OE2	2:C:662:SER:OG	2.28	0.46
3:D:16:GLU:HB3	3:D:1369:ARG:NH2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:56:LEU:CD2	3:D:269:TYR:HB3	2.46	0.46
3:D:100:GLU:O	3:D:246:PRO:HG3	2.15	0.46
1:G:60:GLU:HB2	1:G:170:ARG:HG2	1.96	0.46
1:G:172:LEU:HD12	1:G:172:LEU:N	2.31	0.46
2:I:151:ARG:CZ	2:I:445:ILE:HD11	2.46	0.46
2:I:577:VAL:HG23	2:I:661:VAL:O	2.15	0.46
5:L:101:TYR:O	5:L:102:MET:C	2.56	0.46
1:B:32:GLU:HA	1:B:198:LEU:HD12	1.97	0.46
2:C:494:ASN:HD22	2:C:497:PRO:CD	2.28	0.46
2:C:818:VAL:CB	2:C:1076:ILE:CD1	2.94	0.46
2:C:836:LEU:HD21	2:C:921:PRO:HD3	1.98	0.46
2:C:980:VAL:HG13	2:C:984:VAL:CB	2.46	0.46
3:D:478:LEU:HD12	4:E:24:ALA:HA	1.98	0.46
5:F:568:ASN:O	5:F:569:THR:CG2	2.64	0.46
1:G:156:SER:O	1:G:159:ILE:HG22	2.16	0.46
1:G:179:PRO:O	1:G:207:THR:HG23	2.15	0.46
1:G:223:ILE:HD13	1:H:8:PHE:CZ	2.50	0.46
2:I:470:ARG:HE	2:I:497:PRO:HB3	1.79	0.46
2:I:806:PRO:O	3:J:633:ALA:HA	2.15	0.46
2:I:850:ILE:O	2:I:850:ILE:HG22	2.16	0.46
2:I:1067:ALA:HB1	2:I:1072:ASN:O	2.16	0.46
3:J:1359:ALA:HA	3:J:1363:TYR:HB2	1.96	0.46
1:A:145:LYS:HB2	1:A:170:ARG:HH12	1.80	0.46
2:C:593:LYS:O	2:C:600:THR:HB	2.15	0.46
2:C:697:LYS:HB3	2:C:697:LYS:HE2	1.75	0.46
2:C:794:LEU:HD21	2:C:796:LEU:HD21	1.97	0.46
2:C:1178:LYS:HD3	2:C:1178:LYS:HA	1.75	0.46
3:D:9:LYS:HE2	3:D:11:GLN:O	2.15	0.46
3:D:26:SER:HB2	3:D:236:TRP:CZ2	2.51	0.46
3:D:64:PRO:HG3	3:D:90:VAL:CG1	2.46	0.46
3:D:126:LEU:CD1	3:D:223:LEU:HD23	2.46	0.46
3:D:517:CYS:HA	3:D:716:GLN:NE2	2.31	0.46
5:F:551:LEU:HD11	5:F:598:LEU:HD21	1.98	0.46
2:I:1103:VAL:HG21	3:J:639:VAL:HG11	1.97	0.46
2:I:1119:MET:HG3	2:I:1204:LEU:HD13	1.97	0.46
3:J:242:LEU:C	3:J:242:LEU:HD23	2.41	0.46
3:J:741:ALA:O	3:J:762:ASN:ND2	2.49	0.46
1:B:26:VAL:HG21	1:B:217:ILE:HD12	1.98	0.46
1:B:192:VAL:HG12	1:B:193:GLU:N	2.30	0.46
2:C:407:ARG:HH21	2:C:414:ILE:HG22	1.81	0.46
2:C:448:LEU:HD23	2:C:451:ARG:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1101:LEU:CD2	3:D:725:MET:SD	3.03	0.46
3:D:515:ARG:HH21	3:D:717:VAL:HG23	1.79	0.46
3:D:905:ARG:NH2	3:D:907:HIS:ND1	2.63	0.46
5:F:315:TRP:CH2	5:F:341:LEU:HD11	2.51	0.46
5:F:394:TYR:OH	5:F:436:ARG:CG	2.64	0.46
2:I:6:THR:HG21	2:I:782:VAL:CG2	2.44	0.46
2:I:81:ASP:O	2:I:85:CYS:HB2	2.15	0.46
2:I:88:ARG:NH1	2:I:88:ARG:HB2	2.30	0.46
2:I:521:LEU:O	2:I:524:ILE:HG22	2.16	0.46
3:J:72:CYS:SG	3:J:73:GLY:N	2.89	0.46
3:J:1198:VAL:CG1	3:J:1210:ILE:HG23	2.46	0.46
5:L:439:ILE:O	5:L:442:SER:HB3	2.16	0.46
5:L:470:MET:HE3	5:L:470:MET:HB3	1.91	0.46
1:A:145:LYS:HB3	1:A:145:LYS:HE3	1.65	0.45
1:A:232:VAL:O	1:A:233:ASP:HB3	2.16	0.45
1:B:142:MET:HE2	1:B:142:MET:HB3	1.80	0.45
2:C:197:ARG:NH2	2:C:203:LYS:HB2	2.31	0.45
3:D:357:VAL:HA	3:D:461:PHE:CE1	2.50	0.45
3:D:850:LYS:HB3	3:D:851:PRO:HD2	1.97	0.45
3:D:1343:GLU:C	3:D:1344:LEU:HD12	2.41	0.45
5:F:297:MET:CE	5:F:330:LEU:HD21	2.33	0.45
2:I:127:ILE:HG13	2:I:127:ILE:O	2.14	0.45
2:I:356:THR:HG21	2:I:362:ALA:HA	1.97	0.45
2:I:560:PRO:O	3:J:780:ARG:NH2	2.48	0.45
2:I:660:VAL:HG11	3:J:769:VAL:CG1	2.46	0.45
3:J:38:VAL:HG13	3:J:55:GLY:C	2.41	0.45
3:J:127:LEU:CD2	3:J:234:PRO:HB3	2.46	0.45
3:J:357:VAL:HA	3:J:461:PHE:CE1	2.51	0.45
3:J:358:GLY:N	3:J:359:PRO:HD3	2.31	0.45
3:J:706:VAL:HG12	3:J:715:LYS:HB3	1.97	0.45
3:J:1234:VAL:HG23	3:J:1235:ASN:N	2.29	0.45
5:L:134:VAL:HG22	5:L:273:MET:HE1	1.98	0.45
1:A:19:VAL:HG11	1:A:23:HIS:CE1	2.50	0.45
1:B:51:MET:HG2	1:B:179:PRO:CD	2.47	0.45
2:C:11:ILE:HG22	2:C:1149:TYR:CZ	2.51	0.45
2:C:593:LYS:HG2	2:C:602:GLU:OE2	2.15	0.45
2:C:677:ASN:O	2:C:681:MET:HG3	2.16	0.45
2:C:808:ASN:H	3:D:633:ALA:HB2	1.80	0.45
2:C:818:VAL:CG2	2:C:1076:ILE:CD1	2.85	0.45
3:D:821:MET:CE	3:D:879:ALA:HB1	2.47	0.45
3:D:930:LEU:HA	3:D:1244:GLN:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1291:GLU:CG	3:D:1297:LYS:HZ3	2.29	0.45
5:F:483:LEU:HB2	5:F:494:ILE:CD1	2.46	0.45
5:F:499:LYS:HE3	5:F:499:LYS:HB2	1.70	0.45
1:H:76:GLU:CB	1:H:81:ILE:HG12	2.45	0.45
1:H:99:ILE:HG23	1:H:99:ILE:O	2.15	0.45
2:I:974:ARG:HD3	2:I:1010:GLN:NE2	2.32	0.45
2:I:978:VAL:HG21	2:I:1010:GLN:CD	2.41	0.45
2:I:1043:ALA:HB3	2:I:1046:VAL:CG1	2.47	0.45
2:I:1120:ALA:HB2	2:I:1199:LEU:HG	1.97	0.45
3:J:95:THR:O	3:J:98:ARG:HB2	2.16	0.45
1:A:218:ARG:NH1	1:B:231:PHE:C	2.75	0.45
2:C:101:ARG:HH21	2:C:118:LYS:CE	2.25	0.45
2:C:1298:VAL:HG21	3:D:96:LYS:NZ	2.30	0.45
2:C:1333:LEU:HD21	3:D:327:LEU:CB	2.47	0.45
3:D:688:ALA:O	3:D:692:ARG:HG3	2.16	0.45
5:F:387:VAL:HG22	5:F:435:ILE:CD1	2.46	0.45
1:G:171:LEU:HD22	1:G:171:LEU:N	2.32	0.45
1:G:218:ARG:HH11	1:H:232:VAL:N	2.15	0.45
3:J:843:VAL:O	3:J:883:ARG:HG3	2.16	0.45
3:J:931:THR:O	3:J:931:THR:HG22	2.16	0.45
3:J:1252:HIS:C	3:J:1255:VAL:HG13	2.41	0.45
5:L:227:GLN:O	5:L:230:VAL:CG1	2.64	0.45
5:L:577:GLY:CA	5:L:583:THR:HG23	2.31	0.45
1:B:205:MET:CE	1:B:213:PRO:CB	2.94	0.45
2:C:614:TYR:CE1	2:C:652:TYR:HE1	2.34	0.45
2:C:981:ALA:HB1	2:C:1007:LYS:HZ1	1.81	0.45
2:C:1271:GLY:HA2	3:D:343:LEU:CG	2.46	0.45
2:C:1285:TYR:CD1	3:D:475:GLU:HB3	2.52	0.45
3:D:112:ALA:HB3	3:D:300:GLN:HE22	1.82	0.45
3:D:664:ILE:HG21	3:D:681:LYS:HB3	1.99	0.45
3:D:1140:ARG:NH2	3:D:1236:GLU:HG2	2.30	0.45
3:D:1151:LYS:C	3:D:1153:PRO:HD3	2.41	0.45
5:F:399:LEU:CB	5:F:404:LEU:HD21	2.39	0.45
5:F:515:GLU:C	5:F:517:SER:N	2.74	0.45
1:H:118:ASP:HB2	1:H:121:VAL:CG2	2.46	0.45
2:I:591:TYR:HD2	2:I:606:LEU:HD13	1.81	0.45
2:I:634:VAL:HG13	2:I:636:CYS:SG	2.57	0.45
2:I:736:VAL:HG23	2:I:748:ILE:HA	1.97	0.45
2:I:815:SER:OG	3:J:461:PHE:CD1	2.70	0.45
2:I:1103:VAL:HB	2:I:1104:PRO:HD3	1.97	0.45
2:I:1246:ARG:NH1	2:I:1266:GLY:HA2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1313:HIS:HD2	3:J:477:GLN:NE2	2.14	0.45
3:J:788:LEU:HG	3:J:792:ASN:ND2	2.31	0.45
3:J:804:ALA:HB1	3:J:916:GLY:HA3	1.98	0.45
3:J:850:LYS:HD3	3:J:875:ASN:ND2	2.29	0.45
3:J:908:ILE:HD13	3:J:909:ILE:N	2.32	0.45
3:J:1252:HIS:CA	3:J:1255:VAL:HG13	2.46	0.45
4:K:49:ILE:HA	4:K:52:ARG:HD3	1.98	0.45
2:C:852:ALA:HB2	2:C:869:GLY:CA	2.47	0.45
3:D:646:ILE:H	3:D:646:ILE:HG12	1.60	0.45
3:D:1203:ARG:HH22	3:D:1205:GLU:CG	2.19	0.45
3:D:1280:VAL:HG21	3:D:1304:ARG:CD	2.45	0.45
5:F:290:LEU:HD12	5:F:337:VAL:HG22	1.97	0.45
5:F:587:ILE:HG22	5:F:588:ARG:N	2.31	0.45
1:G:14:VAL:CG1	1:G:27:THR:HB	2.46	0.45
1:H:86:LYS:CD	1:H:174:ASP:HB2	2.45	0.45
1:H:139:SER:O	1:H:140:ILE:HG23	2.16	0.45
2:I:617:ALA:HB3	2:I:653:MET:CG	2.43	0.45
2:I:660:VAL:HG13	2:I:661:VAL:HG13	1.99	0.45
3:J:79:LYS:HB2	5:L:569:THR:H	1.82	0.45
3:J:114:ILE:HB	3:J:304:ASP:OD1	2.16	0.45
3:J:447:ILE:HG21	3:J:447:ILE:HD13	1.64	0.45
3:J:902:ASP:HB3	3:J:1251:LYS:HE3	1.96	0.45
5:L:119:ILE:HA	5:L:122:ARG:HD3	1.97	0.45
1:B:197:ASP:O	1:B:197:ASP:CG	2.59	0.45
2:C:202:ARG:NH2	2:C:368:ARG:HH12	2.14	0.45
2:C:964:LEU:HA	2:C:964:LEU:HD12	1.73	0.45
3:D:1291:GLU:HG2	3:D:1297:LYS:HD3	1.98	0.45
3:D:1368:ASP:HA	3:D:1371:ARG:HH22	1.81	0.45
5:F:607:LEU:HD12	5:F:607:LEU:N	2.31	0.45
1:G:67:GLU:H	1:G:67:GLU:HG2	1.41	0.45
1:G:74:VAL:HG22	1:G:76:GLU:H	1.81	0.45
2:I:593:LYS:HE3	2:I:595:THR:HG23	1.94	0.45
2:I:669:PRO:O	2:I:1070:HIS:HE1	1.99	0.45
2:I:1236:ASN:HB2	2:I:1238:LEU:HD11	1.99	0.45
2:I:1293:VAL:CG1	2:I:1304:MET:HE2	2.33	0.45
2:I:1326:LEU:HA	2:I:1326:LEU:HD12	1.82	0.45
3:J:45:ASN:O	3:J:46:TYR:CB	2.64	0.45
3:J:364:HIS:CB	4:K:4:VAL:HG23	2.45	0.45
3:J:800:LEU:CD1	3:J:1309:ILE:HD13	2.47	0.45
5:L:518:HIS:O	5:L:519:LEU:C	2.59	0.45
1:A:154:PRO:O	1:A:158:ARG:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:VAL:O	1:B:15:ASP:C	2.60	0.45
1:B:29:GLU:CG	1:B:30:PRO:HG3	2.46	0.45
1:B:37:HIS:HA	1:B:185:TYR:HE1	1.82	0.45
1:B:205:MET:HE1	1:B:213:PRO:HA	1.97	0.45
2:C:100:LEU:HD12	2:C:122:VAL:CG1	2.47	0.45
2:C:210:LEU:CD1	2:C:224:PHE:HE2	2.30	0.45
2:C:494:ASN:O	2:C:498:ILE:CD1	2.64	0.45
2:C:678:ARG:HG3	2:C:1106:ARG:HB3	1.98	0.45
2:C:1269:ARG:CD	3:D:343:LEU:HB3	2.30	0.45
3:D:557:LYS:HE3	3:D:557:LYS:HB2	1.67	0.45
3:D:848:VAL:CG2	3:D:858:VAL:CG1	2.88	0.45
3:D:1350:ASN:OD1	3:D:1355:ARG:CD	2.65	0.45
5:F:308:GLY:HA2	5:F:356:GLU:OE1	2.17	0.45
5:F:547:VAL:CG2	5:F:603:ARG:HH11	2.30	0.45
5:F:583:THR:HG22	5:F:584:ARG:N	2.31	0.45
5:F:602:SER:OG	5:F:603:ARG:N	2.49	0.45
1:G:195:ARG:HG2	1:G:198:LEU:CG	2.45	0.45
1:H:79:LEU:C	1:H:79:LEU:HD13	2.41	0.45
2:I:445:ILE:HG22	2:I:446:ASP:OD1	2.16	0.45
2:I:854:ILE:O	2:I:857:VAL:HG22	2.17	0.45
3:J:242:LEU:HD23	3:J:243:PRO:O	2.16	0.45
3:J:827:GLU:HB3	3:J:832:LYS:HD2	1.99	0.45
2:C:796:LEU:HB2	2:C:1233:LEU:HD12	1.99	0.45
2:C:1061:GLN:HB2	2:C:1062:PRO:HD2	1.98	0.45
2:C:1149:TYR:CG	2:C:1159:VAL:HG11	2.50	0.45
3:D:137:ARG:HG2	3:D:142:GLU:HB2	1.99	0.45
3:D:641:ILE:O	3:D:641:ILE:HD13	2.17	0.45
5:F:467:SER:O	5:F:471:LEU:HB2	2.17	0.45
2:I:10:ARG:NH2	2:I:697:LYS:HD3	2.31	0.45
2:I:158:ASP:HB3	2:I:173:ASN:OD1	2.17	0.45
2:I:361:SER:O	2:I:364:VAL:HB	2.17	0.45
3:J:109:SER:HB2	3:J:296:LYS:HE2	1.99	0.45
3:J:750:PRO:HA	3:J:777:HIS:NE2	2.32	0.45
2:C:5:TYR:CD1	2:C:8:LYS:HD3	2.30	0.45
3:D:830:ASP:C	3:D:831:VAL:HG12	2.42	0.45
5:F:322:MET:HE2	5:F:324:LYS:HZ3	1.82	0.45
1:H:22:THR:O	1:H:213:PRO:HG3	2.17	0.45
2:I:57:PHE:CE2	2:I:70:TYR:HB2	2.51	0.45
2:I:565:GLU:HB2	2:I:680:LEU:HD21	1.98	0.45
3:J:205:LEU:HD13	3:J:205:LEU:O	2.16	0.45
3:J:351:GLY:O	3:J:352:ARG:HB3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:908:ILE:HD13	3:J:908:ILE:HG23	1.77	0.45
3:J:1193:TRP:HB2	3:J:1194:ARG:NH1	2.32	0.45
5:L:316:PHE:CE2	5:L:334:SER:HA	2.48	0.45
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.99	0.45
1:A:64:VAL:HG11	1:A:78:ILE:HG21	1.99	0.45
1:A:227:GLN:HB3	1:B:39:LEU:HD11	1.99	0.45
1:B:151:GLY:H	1:B:177:TYR:HB2	1.81	0.45
1:B:205:MET:HE2	1:B:213:PRO:HB3	1.98	0.45
2:C:233:ARG:NH1	2:C:332:ARG:HH12	2.15	0.45
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.52	0.45
2:C:1159:VAL:HB	2:C:1160:ASP:H	1.57	0.45
3:D:115:TRP:NE1	3:D:1329:THR:CG2	2.79	0.45
3:D:174:ASP:O	3:D:175:GLU:HG2	2.16	0.45
3:D:505:ASP:HB2	3:D:629:PHE:HE1	1.81	0.45
3:D:514:THR:CG2	3:D:596:LEU:CB	2.94	0.45
3:D:825:VAL:HG21	3:D:832:LYS:CB	2.47	0.45
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.81	0.45
2:I:801:ARG:HG2	2:I:1094:VAL:HG23	1.98	0.45
3:J:450:HIS:HE1	3:J:452:LEU:HD12	1.80	0.45
5:L:298:PRO:HD2	5:L:326:TRP:CD1	2.52	0.45
1:A:57:THR:HG22	1:A:158:ARG:HH21	1.80	0.44
2:C:80:PHE:CE2	2:C:88:ARG:HD2	2.53	0.44
2:C:262:TYR:CZ	2:C:282:VAL:HG21	2.51	0.44
2:C:1119:MET:HE1	2:C:1210:ILE:HD11	1.99	0.44
2:C:1259:LEU:HD12	2:C:1259:LEU:HA	1.63	0.44
2:C:1294:LYS:HB3	3:D:347:VAL:HG13	1.98	0.44
3:D:209:ASN:HA	3:D:214:ARG:HE	1.82	0.44
3:D:863:LEU:HD12	3:D:863:LEU:HA	1.58	0.44
3:D:1221:LEU:HD13	3:D:1221:LEU:C	2.42	0.44
5:F:227:GLN:O	5:F:230:VAL:HG12	2.17	0.44
1:H:205:MET:SD	1:H:217:ILE:HG12	2.57	0.44
2:I:207:THR:HA	2:I:210:LEU:HD12	1.99	0.44
2:I:1271:GLY:CA	3:J:343:LEU:HD12	2.47	0.44
3:J:141:PHE:CD1	3:J:293:ARG:HD3	2.52	0.44
3:J:518:VAL:O	3:J:547:ARG:NH1	2.50	0.44
3:J:647:PRO:HG3	3:J:697:MET:N	2.32	0.44
3:J:748:ALA:O	3:J:777:HIS:CD2	2.64	0.44
3:J:1280:VAL:O	3:J:1280:VAL:HG12	2.17	0.44
3:J:1344:LEU:HD23	3:J:1350:ASN:CG	2.42	0.44
5:L:562:ARG:HH21	5:L:573:LEU:HB3	1.82	0.44
1:B:205:MET:CE	1:B:213:PRO:CA	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:42:ASP:CG	2:C:46:GLN:HB3	2.42	0.44
2:C:62:TYR:O	2:C:64:GLY:N	2.50	0.44
2:C:163:LYS:HB3	2:C:163:LYS:HE3	1.60	0.44
2:C:481:LEU:HD22	2:C:481:LEU:N	2.32	0.44
2:C:587:LEU:HD23	2:C:587:LEU:HA	1.73	0.44
2:C:1142:ARG:CG	2:C:1161:LEU:HD11	2.47	0.44
2:C:1151:LEU:HD11	2:C:1198:LEU:HD23	1.98	0.44
3:D:74:LYS:HD3	3:D:75:TYR:HE1	1.82	0.44
3:D:114:ILE:HB	3:D:304:ASP:OD1	2.17	0.44
3:D:140:TYR:CE2	5:F:95:THR:CG2	2.92	0.44
3:D:140:TYR:O	3:D:141:PHE:HB2	2.17	0.44
5:F:421:TYR:CE2	5:F:422:ARG:HG3	2.53	0.44
5:F:513:ASP:C	5:F:515:GLU:N	2.75	0.44
1:G:45:ARG:HH22	2:I:1216:ARG:HA	1.80	0.44
2:I:10:ARG:HH12	2:I:697:LYS:NZ	2.15	0.44
2:I:208:ILE:CD1	2:I:365:GLU:HB3	2.47	0.44
2:I:520:PRO:HB3	2:I:714:VAL:HG21	1.99	0.44
2:I:1101:LEU:HD12	3:J:505:ASP:OD2	2.17	0.44
2:I:1301:ARG:HH11	2:I:1301:ARG:HD2	1.66	0.44
2:I:1334:GLY:O	3:J:25:ALA:CB	2.65	0.44
3:J:83:VAL:HG13	3:J:92:VAL:HG13	1.99	0.44
3:J:317:THR:HB	3:J:324:LEU:HB3	1.99	0.44
3:J:520:ALA:HB1	3:J:543:SER:HB3	1.99	0.44
5:L:592:ALA:O	5:L:596:ARG:HB2	2.17	0.44
3:D:825:VAL:HG21	3:D:832:LYS:HB3	1.99	0.44
3:D:1193:TRP:HB2	3:D:1194:ARG:HH12	1.73	0.44
5:F:279:ARG:NH2	5:F:350:GLU:OE2	2.42	0.44
5:F:399:LEU:HA	5:F:399:LEU:HD12	1.53	0.44
3:J:930:LEU:HA	3:J:930:LEU:HD23	1.72	0.44
3:J:1346:GLY:O	3:J:1358:PRO:HG3	2.17	0.44
1:B:152:TYR:HA	1:B:175:ALA:O	2.18	0.44
2:C:13:LYS:NZ	2:C:1151:LEU:HB2	2.32	0.44
2:C:120:GLN:HE21	2:C:120:GLN:HB2	1.59	0.44
2:C:289:VAL:HG13	2:C:319:LEU:CD1	2.47	0.44
2:C:393:ASP:OD1	2:C:394:ARG:HG2	2.17	0.44
2:C:1149:TYR:CD1	2:C:1159:VAL:CG1	2.92	0.44
2:C:1199:LEU:HD23	2:C:1204:LEU:HD12	1.99	0.44
3:D:706:VAL:HG12	3:D:715:LYS:CB	2.47	0.44
1:G:79:LEU:HD13	1:G:83:LEU:HD13	2.00	0.44
1:G:218:ARG:HH12	1:H:232:VAL:H	1.65	0.44
2:I:17:LYS:NZ	2:I:1154:ASP:CB	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:119:GLU:CG	2:I:489:PRO:CD	2.88	0.44
3:J:137:ARG:HD3	3:J:143:SER:OG	2.16	0.44
3:J:244:VAL:O	3:J:244:VAL:CG2	2.64	0.44
3:J:615:LYS:HZ3	4:K:7:GLN:CG	2.30	0.44
3:J:638:SER:OG	3:J:639:VAL:N	2.50	0.44
3:J:670:SER:HB2	3:J:672:LEU:HD13	1.99	0.44
3:J:1156:LEU:CD2	3:J:1219:ASP:HB3	2.44	0.44
1:A:78:ILE:HD12	1:A:78:ILE:HG23	1.64	0.44
2:C:1117:LEU:HD12	2:C:1195:ILE:HG12	1.99	0.44
2:C:1240:ASP:HB3	3:D:445:LYS:CD	2.40	0.44
3:D:121:PRO:HG2	3:D:123:ARG:HH22	1.83	0.44
3:D:450:HIS:HE1	3:D:452:LEU:CD1	2.30	0.44
3:D:857:LEU:HD13	3:D:858:VAL:CG1	2.47	0.44
3:D:1318:SER:OG	3:D:1342:ASP:OD2	2.27	0.44
5:F:611:LEU:HD23	5:F:611:LEU:HA	1.78	0.44
1:H:28:LEU:HD21	1:H:31:LEU:HD21	2.00	0.44
2:I:18:ARG:NH1	2:I:621:SER:O	2.48	0.44
2:I:250:THR:HG23	2:I:268:ARG:N	2.33	0.44
3:J:213:LYS:O	3:J:217:LEU:HB2	2.18	0.44
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.88	0.44
3:J:425:ARG:NH1	3:J:464:ASP:CG	2.73	0.44
3:J:478:LEU:HD12	4:K:24:ALA:HA	1.99	0.44
1:A:38:THR:CG2	1:B:45:ARG:HG2	2.48	0.44
1:A:218:ARG:HH11	1:B:231:PHE:C	2.26	0.44
1:B:219:ARG:O	1:B:223:ILE:HG13	2.17	0.44
2:C:448:LEU:HA	2:C:448:LEU:HD23	1.81	0.44
2:C:818:VAL:CB	2:C:1076:ILE:HD13	2.46	0.44
2:C:848:GLU:CG	2:C:888:THR:HG22	2.47	0.44
2:C:886:LYS:HZ1	2:C:916:SER:HB3	1.82	0.44
3:D:66:LYS:HE2	3:D:69:GLU:OE1	2.17	0.44
3:D:242:LEU:C	3:D:242:LEU:CD2	2.91	0.44
3:D:422:LEU:C	3:D:423:LEU:HD12	2.43	0.44
3:D:733:SER:O	3:D:734:ALA:C	2.59	0.44
3:D:839:VAL:CG1	3:D:864:LEU:HD12	2.44	0.44
5:F:295:CYS:O	5:F:329:LYS:HB3	2.17	0.44
1:H:67:GLU:HG2	1:H:82:LEU:HD11	1.99	0.44
1:H:83:LEU:HD11	3:J:526:VAL:HG21	1.92	0.44
1:H:172:LEU:HD12	1:H:172:LEU:H	1.83	0.44
2:I:228:VAL:HG13	2:I:239:MET:HE3	1.99	0.44
2:I:494:ASN:ND2	2:I:497:PRO:HD3	2.26	0.44
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1272:GLU:CB	3:J:342:LEU:CB	2.95	0.44
2:I:1279:GLU:CG	3:J:1357:ILE:HD13	2.47	0.44
3:J:162:GLU:O	3:J:163:GLU:C	2.58	0.44
3:J:474:LEU:HB2	4:K:28:ARG:NH1	2.33	0.44
3:J:1286:LYS:HD3	3:J:1286:LYS:HA	1.85	0.44
3:J:1314:LEU:HD12	3:J:1326:GLN:OE1	2.18	0.44
5:L:118:ASP:O	5:L:122:ARG:HG3	2.18	0.44
5:L:388:ILE:O	5:L:392:LYS:HG3	2.18	0.44
5:L:556:ALA:O	5:L:560:ARG:HG3	2.18	0.44
1:A:149:GLY:HA3	1:A:177:TYR:CE2	2.52	0.44
2:C:68:LEU:HD11	2:C:489:PRO:HB3	2.00	0.44
2:C:847:PRO:HB3	2:C:1047:LEU:HD11	1.99	0.44
2:C:1066:MET:HE2	2:C:1076:ILE:HG22	1.98	0.44
3:D:352:ARG:O	3:D:353:SER:HB3	2.17	0.44
3:D:385:LEU:HA	3:D:385:LEU:HD23	1.83	0.44
5:F:147:GLN:HB3	5:F:161:LEU:CD1	2.48	0.44
5:F:512:GLY:C	5:F:514:ASP:N	2.76	0.44
1:H:67:GLU:HA	1:H:78:ILE:HG21	1.99	0.44
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.99	0.44
2:I:453:ILE:HD12	2:I:587:LEU:HD21	2.00	0.44
2:I:496:LYS:HB3	2:I:496:LYS:HE3	1.63	0.44
3:J:127:LEU:HD21	3:J:234:PRO:CG	2.47	0.44
5:L:227:GLN:O	5:L:230:VAL:HG12	2.18	0.44
1:A:182:ARG:C	1:A:183:ILE:HD12	2.43	0.44
1:B:92:VAL:HG21	1:B:95:LYS:O	2.17	0.44
1:B:99:ILE:O	1:B:99:ILE:HG23	2.18	0.44
2:C:13:LYS:HA	2:C:1157:GLN:OE1	2.18	0.44
2:C:495:ALA:HB3	5:F:471:LEU:HD22	1.99	0.44
2:C:854:ILE:O	2:C:857:VAL:HG22	2.18	0.44
3:D:74:LYS:HD3	3:D:75:TYR:CE1	2.53	0.44
3:D:294:ASN:HD22	5:F:406:GLN:HE21	1.66	0.44
5:F:96:ASP:O	5:F:98:VAL:N	2.50	0.44
1:G:168:ILE:H	1:G:168:ILE:HG12	1.60	0.44
2:I:149:LEU:HD11	2:I:451:ARG:HB3	1.98	0.44
2:I:191:LYS:HB3	2:I:191:LYS:HE2	1.79	0.44
2:I:253:PHE:CZ	2:I:287:VAL:HG12	2.52	0.44
2:I:838:CYS:HB2	2:I:918:LEU:HB2	2.00	0.44
3:J:56:LEU:HD11	3:J:273:ILE:CD1	2.47	0.44
3:J:279:LEU:HD23	3:J:279:LEU:C	2.41	0.44
3:J:334:LYS:HA	3:J:335:GLN:HA	1.76	0.44
3:J:825:VAL:CG1	3:J:833:GLU:HB3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1241:TYR:CE2	3:J:1248:ILE:HD11	2.52	0.44
3:J:1344:LEU:HA	3:J:1349:GLU:HG3	2.00	0.44
5:L:443:ILE:O	5:L:447:ALA:HB3	2.18	0.44
1:A:9:LEU:CD1	1:A:198:LEU:HD11	2.48	0.44
1:A:27:THR:O	1:A:28:LEU:HD12	2.17	0.44
1:B:6:THR:O	1:B:6:THR:CG2	2.52	0.44
2:C:496:LYS:HE3	2:C:497:PRO:HD3	2.00	0.44
2:C:589:THR:HG1	2:C:659:GLN:HE22	1.62	0.44
2:C:591:TYR:O	2:C:603:ILE:HA	2.18	0.44
2:C:1217:THR:CB	2:C:1219:GLU:HG2	2.48	0.44
3:D:16:GLU:HB3	3:D:1369:ARG:HH21	1.82	0.44
3:D:875:ASN:OD1	3:D:875:ASN:N	2.51	0.44
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.17	0.44
3:D:1264:ALA:HB2	3:D:1304:ARG:HA	2.00	0.44
3:D:1290:ARG:HD3	3:D:1290:ARG:HA	1.77	0.44
5:F:518:HIS:O	5:F:519:LEU:C	2.60	0.44
1:G:169:GLY:O	1:G:171:LEU:CD2	2.66	0.44
1:G:218:ARG:HG3	1:H:231:PHE:HB3	1.99	0.44
2:I:1165:SER:HA	2:I:1169:VAL:HG21	2.00	0.44
3:J:596:LEU:HD11	3:J:604:MET:CE	2.48	0.44
3:J:755:ILE:HD12	3:J:774:ILE:CG2	2.48	0.44
5:L:322:MET:CE	5:L:324:LYS:HZ3	2.31	0.44
1:B:48:LEU:HA	1:B:48:LEU:HD23	1.77	0.43
2:C:338:THR:HG22	2:C:345:PRO:HB3	2.00	0.43
3:D:43:THR:OG1	3:D:44:ILE:N	2.51	0.43
3:D:259:ARG:CG	5:F:502:LYS:HE3	2.44	0.43
3:D:334:LYS:HA	3:D:335:GLN:HA	1.75	0.43
5:F:400:GLN:O	5:F:404:LEU:HG	2.18	0.43
5:F:561:MET:HG3	5:F:571:TYR:HD2	1.82	0.43
1:G:88:LEU:CD1	1:G:112:ALA:HB1	2.47	0.43
1:G:231:PHE:CB	1:H:218:ARG:HG2	2.45	0.43
2:I:156:PHE:CZ	2:I:445:ILE:HG13	2.52	0.43
2:I:198:ILE:HD13	2:I:388:LEU:HD13	2.00	0.43
2:I:241:LEU:HD21	2:I:246:LEU:HD11	2.00	0.43
2:I:895:LEU:H	2:I:895:LEU:HG	1.56	0.43
2:I:1179:GLY:O	2:I:1181:PRO:HD3	2.18	0.43
3:J:349:TYR:CG	3:J:472:LEU:HD21	2.52	0.43
5:L:291:CYS:SG	5:L:330:LEU:HD22	2.58	0.43
1:A:218:ARG:NH1	1:B:231:PHE:CA	2.78	0.43
1:B:225:ALA:O	1:B:228:LEU:HB2	2.18	0.43
2:C:74:ARG:HG2	2:C:75:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:800:MET:HE1	2:C:822:VAL:CG2	2.48	0.43
2:C:961:SER:O	2:C:965:GLN:HG3	2.18	0.43
2:C:1269:ARG:NE	3:D:343:LEU:O	2.48	0.43
3:D:394:ILE:CG1	5:F:536:THR:HG22	2.48	0.43
3:D:419:HIS:CE1	3:D:477:GLN:OE1	2.71	0.43
3:D:695:LYS:HA	3:D:695:LYS:HD3	1.55	0.43
3:D:697:MET:CE	3:D:737:ILE:HG22	2.30	0.43
3:D:1287:ILE:O	3:D:1291:GLU:HG3	2.18	0.43
5:F:225:ARG:O	5:F:229:VAL:HG13	2.18	0.43
5:F:595:LEU:O	5:F:599:ARG:HB2	2.17	0.43
1:G:89:ALA:HB3	1:G:124:VAL:CG1	2.48	0.43
2:I:109:ALA:CB	2:I:110:PRO:C	2.75	0.43
2:I:235:ASN:OD1	2:I:236:LYS:HG2	2.18	0.43
2:I:545:PHE:HA	2:I:548:ARG:CD	2.47	0.43
2:I:1160:ASP:CG	2:I:1161:LEU:N	2.72	0.43
2:I:1327:LEU:HD21	2:I:1339:LEU:HD11	2.00	0.43
3:J:192:MET:HE3	3:J:192:MET:HB2	1.80	0.43
3:J:1259:GLN:NE2	3:J:1262:ARG:HH12	2.17	0.43
5:L:276:MET:O	5:L:280:VAL:HG23	2.18	0.43
5:L:380:VAL:HG13	5:L:412:LEU:HD23	2.01	0.43
1:A:150:ARG:HD2	1:B:8:PHE:CE2	2.53	0.43
2:C:101:ARG:HE	2:C:118:LYS:HD2	1.83	0.43
2:C:844:LYS:HD3	3:D:49:PHE:CD2	2.53	0.43
3:D:140:TYR:OH	3:D:312:ARG:CZ	2.65	0.43
3:D:218:THR:HA	3:D:221:ILE:CG2	2.47	0.43
3:D:250:ARG:HB3	3:D:265:LEU:HD12	2.00	0.43
3:D:1248:ILE:HD13	3:D:1248:ILE:HG21	1.69	0.43
1:G:53:GLY:O	1:G:148:ARG:HG3	2.18	0.43
1:G:100:LEU:HD23	1:G:115:ILE:HG21	2.00	0.43
1:G:158:ARG:NH2	1:G:172:LEU:HD23	2.33	0.43
1:H:68:TYR:O	1:H:69:SER:HB3	2.18	0.43
2:I:737:ASN:O	2:I:741:MET:HB2	2.18	0.43
2:I:1271:GLY:HA2	3:J:344:GLY:HA3	1.99	0.43
3:J:31:ARG:NH2	3:J:106:GLU:OE2	2.49	0.43
5:L:244:THR:O	5:L:244:THR:HG22	2.18	0.43
5:L:360:ASP:O	5:L:361:ILE:C	2.58	0.43
5:L:575:GLU:O	5:L:579:GLN:HG2	2.18	0.43
1:A:49:SER:HB3	2:C:1083:GLU:CD	2.44	0.43
1:A:134:THR:HG23	2:C:726:TYR:HE1	1.83	0.43
2:C:109:ALA:CB	2:C:110:PRO:C	2.72	0.43
2:C:866:ASP:HB3	2:C:872:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:898:GLU:OE1	2:C:898:GLU:N	2.47	0.43
3:D:884:SER:OG	3:D:886:VAL:HG12	2.18	0.43
5:F:254:GLU:HA	5:F:257:LYS:HD3	2.00	0.43
1:G:57:THR:CG2	1:G:158:ARG:CZ	2.96	0.43
2:I:119:GLU:HB2	2:I:489:PRO:HB2	2.00	0.43
2:I:208:ILE:O	2:I:362:ALA:HB1	2.19	0.43
2:I:981:ALA:HB1	2:I:1007:LYS:NZ	2.33	0.43
2:I:1103:VAL:HG11	2:I:1112:ILE:HD11	2.01	0.43
3:J:165:TYR:CE2	3:J:169:LEU:HD12	2.53	0.43
3:J:421:VAL:CG2	3:J:439:PRO:HG3	2.45	0.43
3:J:825:VAL:O	3:J:826:ILE:C	2.60	0.43
5:L:132:CYS:SG	5:L:257:LYS:HE3	2.58	0.43
5:L:489:MET:CB	5:L:490:PRO:HD2	2.48	0.43
1:A:232:VAL:O	1:A:233:ASP:CB	2.66	0.43
2:C:807:TRP:O	2:C:808:ASN:C	2.60	0.43
2:C:967:LEU:HD12	2:C:967:LEU:HA	1.38	0.43
2:C:1112:ILE:CD1	3:D:639:VAL:HG22	2.48	0.43
3:D:75:TYR:CD2	3:D:83:VAL:HG21	2.52	0.43
3:D:156:ARG:NH1	3:D:157:GLN:NE2	2.67	0.43
3:D:205:LEU:C	3:D:205:LEU:CD1	2.91	0.43
3:D:360:TYR:OH	3:D:442:ILE:HD11	2.18	0.43
4:E:39:VAL:HG22	4:E:40:PRO:HD2	2.00	0.43
5:F:141:ILE:HG23	5:F:224:LEU:HD11	2.00	0.43
5:F:280:VAL:HG22	5:F:347:ILE:HG21	1.99	0.43
1:G:231:PHE:CA	1:H:218:ARG:HH11	2.31	0.43
2:I:27:LEU:CD1	2:I:524:ILE:HD11	2.48	0.43
2:I:131:THR:HG22	2:I:132:ASP:N	2.34	0.43
2:I:145:ILE:HB	2:I:456:VAL:CG2	2.39	0.43
2:I:650:VAL:HG23	2:I:650:VAL:O	2.19	0.43
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.84	0.43
3:J:490:ILE:HD13	3:J:490:ILE:HG21	1.80	0.43
3:J:1237:VAL:HG13	3:J:1238:GLN:N	2.33	0.43
2:C:98:VAL:HB	2:C:124:MET:CE	2.47	0.43
2:C:231:GLU:HG2	2:C:332:ARG:CD	2.48	0.43
2:C:556:GLY:HA2	2:C:659:GLN:O	2.18	0.43
2:C:754:THR:O	2:C:755:LYS:HD2	2.19	0.43
2:C:1152:GLY:O	2:C:1153:ALA:CB	2.65	0.43
2:C:1336:ASN:ND2	3:D:29:MET:HE3	2.34	0.43
3:D:291:ILE:CD1	5:F:409:ASN:HD22	2.31	0.43
3:D:647:PRO:CD	3:D:697:MET:HB3	2.49	0.43
3:D:909:ILE:O	3:D:909:ILE:HG23	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:290:LEU:HD13	5:F:333:VAL:HG22	2.01	0.43
5:F:470:MET:HE1	5:F:482:GLU:HG2	2.00	0.43
5:F:558:VAL:HG21	5:F:587:ILE:HG12	2.00	0.43
2:I:49:LEU:HD12	2:I:73:TYR:HE2	1.84	0.43
2:I:74:ARG:NH2	2:I:97:ARG:HG3	2.33	0.43
2:I:720:ARG:HB2	2:I:749:ASP:OD1	2.19	0.43
2:I:759:SER:OG	2:I:763:THR:N	2.48	0.43
2:I:817:LEU:HD13	2:I:1085:MET:HE1	1.99	0.43
2:I:974:ARG:HD2	2:I:1014:LEU:HD11	2.01	0.43
2:I:1013:GLN:O	2:I:1017:GLN:HG2	2.18	0.43
3:J:24:LEU:HD11	3:J:116:PHE:CE2	2.54	0.43
3:J:179:LYS:CB	3:J:184:ALA:HB2	2.47	0.43
5:L:491:GLU:O	5:L:491:GLU:HG3	2.17	0.43
1:A:224:LEU:C	1:A:224:LEU:CD2	2.92	0.43
2:C:325:LEU:HD13	2:C:333:ILE:CG1	2.48	0.43
2:C:407:ARG:HH21	2:C:414:ILE:CG2	2.31	0.43
2:C:848:GLU:OE1	2:C:886:LYS:NZ	2.51	0.43
2:C:934:PHE:N	2:C:934:PHE:CD2	2.85	0.43
2:C:1124:ILE:HG22	2:C:1180:MET:HG3	2.01	0.43
2:C:1131:MET:CB	2:C:1141:LEU:HD11	2.47	0.43
2:C:1160:ASP:HB2	2:C:1163:THR:OG1	2.19	0.43
2:C:1236:ASN:O	2:C:1236:ASN:CG	2.61	0.43
3:D:578:ILE:HG21	3:D:631:TYR:OH	2.18	0.43
3:D:609:TYR:HD1	3:D:610:ARG:HH11	1.65	0.43
3:D:653:ILE:HD13	3:D:692:ARG:HB3	2.01	0.43
3:D:722:ILE:HG21	3:D:722:ILE:HD13	1.62	0.43
3:D:903:LEU:HD22	3:D:909:ILE:HD12	2.01	0.43
5:F:606:VAL:HG13	5:F:607:LEU:CD1	2.49	0.43
1:G:8:PHE:N	1:H:150:ARG:HH12	2.16	0.43
1:G:13:LEU:HD22	1:H:231:PHE:CE1	2.54	0.43
2:I:20:GLN:NE2	2:I:23:ASP:HB3	2.34	0.43
2:I:548:ARG:HH21	2:I:568:ASN:HA	1.83	0.43
2:I:548:ARG:O	2:I:570:GLY:HA3	2.19	0.43
2:I:742:TYR:HD2	2:I:743:PRO:HD2	1.83	0.43
2:I:817:LEU:CD1	2:I:1085:MET:HE1	2.48	0.43
3:J:123:ARG:O	3:J:126:LEU:HD12	2.18	0.43
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.70	0.43
3:J:400:MET:HE2	3:J:400:MET:HB3	1.80	0.43
3:J:474:LEU:HD12	3:J:474:LEU:HA	1.81	0.43
3:J:647:PRO:CD	3:J:697:MET:HB3	2.49	0.43
5:L:244:THR:O	5:L:247:GLU:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:VAL:O	1:B:14:VAL:HG13	2.19	0.43
1:B:51:MET:HB3	1:B:179:PRO:HD3	2.00	0.43
1:B:188:GLU:O	1:B:200:LYS:N	2.49	0.43
1:B:205:MET:HE2	1:B:205:MET:HB3	1.71	0.43
2:C:74:ARG:HH22	2:C:97:ARG:HG3	1.81	0.43
2:C:590:PRO:CB	2:C:655:VAL:HG21	2.48	0.43
2:C:800:MET:HE1	2:C:822:VAL:CG1	2.48	0.43
3:D:81:ARG:C	3:D:83:VAL:H	2.26	0.43
3:D:342:LEU:CB	3:D:343:LEU:HD13	2.47	0.43
3:D:599:LYS:HD3	3:D:599:LYS:HA	1.78	0.43
5:F:305:LEU:HD13	5:F:315:TRP:HA	2.00	0.43
1:G:26:VAL:HG22	1:G:203:ILE:HB	2.01	0.43
1:G:35:PHE:HE1	1:H:46:ILE:HG23	1.83	0.43
1:G:175:ALA:HB1	1:G:177:TYR:CZ	2.54	0.43
2:I:149:LEU:HB2	2:I:530:ILE:HG21	1.99	0.43
2:I:708:VAL:CG1	2:I:794:LEU:HD22	2.48	0.43
2:I:802:VAL:HA	2:I:1096:ILE:O	2.19	0.43
2:I:805:MET:HE1	2:I:1221:PHE:CE1	2.54	0.43
2:I:1222:GLU:O	2:I:1223:ARG:CB	2.64	0.43
3:J:119:SER:O	3:J:120:LEU:C	2.62	0.43
3:J:138:VAL:CG2	3:J:145:VAL:HB	2.43	0.43
3:J:161:THR:HG22	3:J:164:GLN:CD	2.42	0.43
3:J:478:LEU:HD21	4:K:47:THR:O	2.18	0.43
3:J:505:ASP:HB2	3:J:629:PHE:CE1	2.47	0.43
3:J:514:THR:HG21	3:J:596:LEU:HG	2.00	0.43
1:B:221:ALA:O	1:B:222:THR:C	2.60	0.43
2:C:488:MET:HE3	2:C:488:MET:HB2	1.71	0.43
2:C:607:SER:H	2:C:610:GLU:HB2	1.84	0.43
3:D:9:LYS:CE	3:D:11:GLN:HA	2.49	0.43
3:D:510:LEU:O	3:D:514:THR:CG2	2.67	0.43
5:F:391:ALA:CB	5:F:405:ILE:HG22	2.46	0.43
5:F:588:ARG:H	5:F:588:ARG:HG3	1.48	0.43
1:G:38:THR:OG1	1:H:45:ARG:HB3	2.18	0.43
1:H:33:ARG:HD2	2:I:1081:PRO:HG3	2.00	0.43
2:I:483:ASP:HB2	2:I:486:THR:HG21	1.99	0.43
2:I:496:LYS:O	2:I:500:ALA:CB	2.67	0.43
2:I:755:LYS:O	2:I:757:THR:HG22	2.19	0.43
2:I:807:TRP:HE1	2:I:1086:PRO:HD3	1.84	0.43
2:I:815:SER:HB3	2:I:1077:SER:HB3	2.00	0.43
3:J:372:MET:HB3	3:J:372:MET:HE2	1.29	0.43
1:B:84:ASN:ND2	1:B:129:VAL:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:8:LYS:HE3	2:C:1171:ARG:NH2	2.34	0.43
2:C:145:ILE:HG21	2:C:456:VAL:HG22	1.96	0.43
2:C:1066:MET:HE2	2:C:1076:ILE:HB	1.96	0.43
3:D:479:GLU:CG	4:E:20:VAL:HG11	2.46	0.43
3:D:755:ILE:HD12	3:D:774:ILE:HG21	1.99	0.43
3:D:1252:HIS:HA	3:D:1255:VAL:HG13	2.01	0.43
5:F:470:MET:HA	5:F:473:GLU:HB3	2.01	0.43
2:I:125:GLY:HA3	2:I:499:SER:HB2	1.90	0.43
2:I:228:VAL:HB	2:I:335:THR:OG1	2.19	0.43
2:I:316:GLU:H	2:I:316:GLU:CD	2.27	0.43
2:I:870:ILE:HG22	2:I:944:ARG:NH1	2.33	0.43
2:I:1142:ARG:NH2	2:I:1165:SER:HB2	2.33	0.43
3:J:72:CYS:HB3	3:J:88:CYS:SG	2.59	0.43
3:J:810:THR:CG2	3:J:893:GLY:HA3	2.44	0.43
3:J:1229:VAL:HG22	3:J:1233:ILE:HD13	2.01	0.43
5:L:111:LEU:CD1	5:L:119:ILE:HD12	2.49	0.43
5:L:234:THR:HG21	5:L:248:GLU:OE2	2.19	0.43
5:L:490:PRO:O	5:L:491:GLU:HG2	2.18	0.43
5:L:499:LYS:HA	5:L:502:LYS:HE2	2.00	0.43
2:C:37:LYS:HD3	2:C:37:LYS:HA	1.62	0.42
2:C:91:THR:HB	2:C:138:ILE:O	2.19	0.42
2:C:103:VAL:HA	2:C:116:ASP:HB3	2.00	0.42
2:C:230:PHE:HE1	2:C:287:VAL:HG21	1.83	0.42
2:C:412:GLU:HB3	2:C:413:GLU:OE1	2.18	0.42
2:C:515:MET:HE3	2:C:517:GLN:HB2	2.01	0.42
2:C:593:LYS:O	2:C:600:THR:CB	2.67	0.42
3:D:262:THR:C	5:F:507:MET:HB2	2.44	0.42
4:E:4:VAL:HG13	4:E:5:THR:HG23	2.01	0.42
5:F:322:MET:CE	5:F:324:LYS:NZ	2.82	0.42
5:F:362:ASN:HB2	5:F:365:MET:HE1	1.99	0.42
1:G:191:ARG:HH12	1:G:197:ASP:CA	2.28	0.42
2:I:13:LYS:HD3	2:I:1149:TYR:HA	2.01	0.42
2:I:44:GLU:HA	2:I:54:ARG:NH1	2.34	0.42
2:I:676:ALA:HB3	3:J:779:ALA:HB2	2.01	0.42
3:J:1191:PRO:CB	3:J:1194:ARG:HH11	2.31	0.42
5:L:226:ALA:O	5:L:229:VAL:HG22	2.19	0.42
5:L:341:LEU:CG	5:L:344:LEU:HD23	2.49	0.42
1:A:154:PRO:CB	2:C:1059:ARG:NH2	2.82	0.42
1:B:12:ARG:O	1:B:13:LEU:HG	2.19	0.42
1:B:64:VAL:HG11	1:B:69:SER:HB3	1.98	0.42
1:B:102:LEU:HD22	1:B:103:ASN:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:528:ARG:NH2	2:C:576:SER:O	2.51	0.42
3:D:8:LEU:HD22	3:D:9:LYS:O	2.19	0.42
3:D:372:MET:HE2	3:D:372:MET:HB3	1.71	0.42
3:D:382:TYR:HE2	5:F:532:LEU:HD23	1.84	0.42
3:D:536:LEU:CD1	3:D:541:LEU:CB	2.96	0.42
3:D:804:ALA:O	3:D:805:GLN:C	2.62	0.42
3:D:842:ARG:CD	3:D:882:VAL:HG11	2.49	0.42
1:G:13:LEU:H	1:G:13:LEU:CD2	2.24	0.42
1:G:29:GLU:HB3	1:G:30:PRO:HD3	2.01	0.42
1:G:61:ILE:CG2	1:G:142:MET:HE2	2.49	0.42
2:I:29:SER:HB3	2:I:33:ASP:OD2	2.19	0.42
2:I:595:THR:O	2:I:596:ASP:C	2.62	0.42
2:I:979:LEU:HA	2:I:1002:LEU:HD12	2.01	0.42
3:J:62:PHE:CG	3:J:247:PRO:CG	3.02	0.42
3:J:357:VAL:HG22	3:J:461:PHE:CE1	2.54	0.42
3:J:494:ALA:HB2	3:J:922:SER:CB	2.49	0.42
3:J:660:GLU:O	3:J:663:GLU:HB2	2.19	0.42
4:K:32:VAL:O	4:K:34:GLY:N	2.52	0.42
5:L:127:ILE:HG13	5:L:127:ILE:H	1.64	0.42
1:A:47:LEU:HD23	1:A:47:LEU:HA	1.78	0.42
1:B:19:VAL:HG21	1:B:23:HIS:CE1	2.55	0.42
1:B:140:ILE:O	1:B:140:ILE:CG2	2.67	0.42
2:C:218:GLU:O	2:C:222:ASP:HB2	2.19	0.42
2:C:530:ILE:C	2:C:531:LEU:HD23	2.44	0.42
2:C:817:LEU:HD23	2:C:1078:LYS:HB3	2.01	0.42
2:C:1080:ASN:HD22	2:C:1085:MET:CE	2.32	0.42
2:C:1332:SER:HB3	3:D:245:LEU:HD13	2.01	0.42
3:D:364:HIS:CD2	4:E:4:VAL:HG23	2.54	0.42
3:D:369:PRO:HB3	3:D:444:GLY:O	2.19	0.42
3:D:441:LEU:HA	3:D:441:LEU:HD13	1.70	0.42
3:D:664:ILE:HD12	3:D:681:LYS:HG2	2.01	0.42
3:D:1144:LEU:HA	3:D:1144:LEU:HD23	1.77	0.42
3:D:1314:LEU:HD12	3:D:1326:GLN:OE1	2.19	0.42
2:I:250:THR:HG23	2:I:268:ARG:CA	2.49	0.42
2:I:560:PRO:HG3	3:J:773:PHE:HE2	1.85	0.42
2:I:568:ASN:HB3	2:I:571:LEU:HD12	2.01	0.42
2:I:590:PRO:HG3	2:I:605:TYR:CE2	2.53	0.42
2:I:696:ASP:O	2:I:697:LYS:CB	2.67	0.42
2:I:812:PHE:CE2	3:J:451:PRO:HB3	2.55	0.42
2:I:818:VAL:HG12	2:I:819:SER:O	2.18	0.42
3:J:47:ARG:HD2	3:J:47:ARG:HA	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:650:LYS:HE2	3:J:654:ILE:HD11	2.02	0.42
3:J:808:VAL:HG12	3:J:809:VAL:N	2.35	0.42
3:J:827:GLU:C	3:J:829:GLY:H	2.14	0.42
3:J:903:LEU:HD23	3:J:905:ARG:HD3	2.00	0.42
1:B:14:VAL:HA	1:B:27:THR:O	2.19	0.42
2:C:175:ARG:HG2	2:C:177:ILE:CG1	2.50	0.42
2:C:271:ALA:O	2:C:275:ARG:HG3	2.19	0.42
2:C:496:LYS:HB3	2:C:496:LYS:HE3	1.77	0.42
2:C:680:LEU:O	2:C:684:ASN:HB2	2.18	0.42
2:C:1115:THR:HG22	2:C:1228:GLY:HA3	2.01	0.42
3:D:64:PRO:HG3	3:D:90:VAL:HG12	2.01	0.42
3:D:614:LEU:HD23	4:E:7:GLN:HB2	2.01	0.42
3:D:1217:PRO:HG3	3:D:1232:TYR:HE2	1.84	0.42
4:E:59:ILE:HD12	4:E:59:ILE:HG23	1.55	0.42
1:H:158:ARG:HB3	1:H:172:LEU:HD23	2.01	0.42
2:I:62:TYR:OH	2:I:476:LYS:HB3	2.19	0.42
2:I:233:ARG:HH12	2:I:332:ARG:HH12	1.66	0.42
2:I:830:THR:HG22	2:I:1234:LYS:NZ	2.35	0.42
1:A:172:LEU:HD12	1:A:172:LEU:N	2.34	0.42
2:C:2:VAL:O	2:C:2:VAL:CG1	2.66	0.42
2:C:886:LYS:NZ	2:C:916:SER:HB3	2.34	0.42
2:C:1124:ILE:HG21	2:C:1180:MET:HG3	2.02	0.42
3:D:253:VAL:HA	3:D:254:PRO:HD3	1.71	0.42
3:D:412:LEU:HD23	3:D:412:LEU:C	2.45	0.42
3:D:438:GLU:OE1	4:E:2:ALA:CB	2.68	0.42
3:D:520:ALA:HB1	3:D:543:SER:HB3	2.00	0.42
5:F:444:ALA:HB1	5:F:457:ILE:HD13	1.96	0.42
1:G:195:ARG:HG2	1:G:198:LEU:CD1	2.50	0.42
2:I:22:LEU:HD22	2:I:22:LEU:HA	1.69	0.42
2:I:556:GLY:O	2:I:589:THR:HB	2.18	0.42
2:I:804:PHE:O	2:I:805:MET:HB3	2.19	0.42
2:I:1337:ILE:O	2:I:1337:ILE:CG2	2.67	0.42
3:J:800:LEU:HB3	3:J:920:ALA:CB	2.49	0.42
3:J:846:GLU:HA	3:J:860:ARG:HD2	2.00	0.42
3:J:1146:GLU:O	3:J:1147:ALA:HB3	2.19	0.42
4:K:26:ARG:HB2	4:K:64:LEU:HD21	2.01	0.42
5:L:147:GLN:CB	5:L:161:LEU:CD1	2.97	0.42
5:L:470:MET:HB2	5:L:478:PRO:HG3	2.00	0.42
2:C:13:LYS:HZ3	2:C:1151:LEU:HB2	1.84	0.42
3:D:141:PHE:CG	3:D:293:ARG:HD3	2.54	0.42
3:D:342:LEU:HA	3:D:343:LEU:HA	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:848:VAL:HG22	3:D:858:VAL:HG22	2.00	0.42
3:D:1241:TYR:HD2	3:D:1246:VAL:CG1	2.28	0.42
3:D:1295:ASN:CB	3:D:1298:VAL:HB	2.49	0.42
5:F:423:ARG:HD2	5:F:425:TYR:CD2	2.54	0.42
1:G:13:LEU:CD2	1:H:230:ALA:HB1	2.50	0.42
1:G:86:LYS:HB2	1:G:86:LYS:HE3	1.83	0.42
1:G:156:SER:HB2	2:I:1059:ARG:NH2	2.35	0.42
1:H:9:LEU:HB3	1:H:32:GLU:CG	2.49	0.42
2:I:85:CYS:SG	2:I:92:TYR:HA	2.60	0.42
2:I:606:LEU:HD12	2:I:606:LEU:N	2.35	0.42
2:I:807:TRP:NE1	2:I:1086:PRO:HD3	2.34	0.42
2:I:1043:ALA:O	2:I:1046:VAL:HG12	2.19	0.42
2:I:1327:LEU:HG	2:I:1337:ILE:HG23	2.00	0.42
3:J:81:ARG:C	3:J:83:VAL:H	2.27	0.42
3:J:97:VAL:CG1	3:J:101:ARG:CZ	2.91	0.42
3:J:282:LEU:HA	3:J:282:LEU:HD23	1.84	0.42
3:J:702:GLN:HG2	3:J:703:THR:N	2.31	0.42
3:J:1158:GLU:HB3	3:J:1186:TYR:CE1	2.54	0.42
3:J:1280:VAL:HG11	3:J:1304:ARG:HE	1.83	0.42
3:J:1361:THR:CG2	4:K:21:LEU:HD13	2.46	0.42
5:L:324:LYS:HG3	5:L:326:TRP:CZ2	2.54	0.42
2:C:245:ARG:O	2:C:249:GLU:OE1	2.37	0.42
2:C:250:THR:HA	2:C:268:ARG:HA	2.02	0.42
2:C:363:LEU:HD13	2:C:382:GLU:HG2	2.01	0.42
2:C:719:LYS:HD2	2:C:751:TYR:HE1	1.84	0.42
3:D:527:LEU:HD21	3:D:536:LEU:HG	2.02	0.42
3:D:527:LEU:HB3	3:D:532:GLU:CG	2.49	0.42
3:D:625:MET:HE2	3:D:625:MET:HB3	1.96	0.42
3:D:749:LYS:HG2	3:D:753:SER:HB2	2.01	0.42
5:F:405:ILE:HG21	5:F:405:ILE:HD13	1.60	0.42
5:F:561:MET:HA	5:F:567:MET:HE1	2.02	0.42
1:H:47:LEU:HD22	1:H:180:VAL:CG1	2.47	0.42
2:I:170:VAL:CG2	2:I:171:LEU:N	2.76	0.42
2:I:494:ASN:HB3	2:I:497:PRO:HG2	2.01	0.42
2:I:794:LEU:HG	2:I:796:LEU:CD1	2.49	0.42
2:I:1119:MET:CE	2:I:1210:ILE:HD11	2.50	0.42
2:I:1246:ARG:NH2	2:I:1258:PRO:HB3	2.34	0.42
2:I:1250:SER:HB3	2:I:1259:LEU:O	2.20	0.42
3:J:418:GLU:HG3	4:K:44:ASP:CA	2.36	0.42
3:J:1221:LEU:HD13	3:J:1222:ARG:N	2.34	0.42
5:L:143:TYR:CD2	5:L:143:TYR:C	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:405:ILE:HG21	5:L:405:ILE:HD13	1.61	0.42
1:A:44:ARG:CZ	1:A:48:LEU:HD11	2.50	0.42
1:B:152:TYR:HD2	3:D:541:LEU:CD1	2.33	0.42
2:C:840:SER:CB	2:C:850:ILE:HD11	2.50	0.42
2:C:850:ILE:HG22	2:C:850:ILE:O	2.19	0.42
2:C:1158:LYS:C	2:C:1159:VAL:CG2	2.92	0.42
2:C:1222:GLU:H	2:C:1222:GLU:HG3	1.47	0.42
2:C:1225:VAL:HG23	2:C:1227:VAL:HG13	2.01	0.42
3:D:137:ARG:CD	3:D:143:SER:HB2	2.45	0.42
3:D:733:SER:O	3:D:736:GLN:N	2.53	0.42
3:D:826:ILE:HD12	3:D:826:ILE:O	2.20	0.42
5:F:94:THR:O	5:F:95:THR:OG1	2.33	0.42
5:F:105:MET:HE2	5:F:105:MET:HB2	1.85	0.42
5:F:112:THR:OG1	5:F:114:GLU:HG3	2.19	0.42
2:I:587:LEU:HA	2:I:587:LEU:HD23	1.75	0.42
2:I:617:ALA:HA	2:I:636:CYS:SG	2.60	0.42
2:I:996:ARG:NH1	2:I:999:GLU:OE2	2.49	0.42
3:J:528:THR:O	3:J:551:ARG:HB3	2.20	0.42
3:J:610:ARG:HG2	3:J:866:GLU:OE1	2.19	0.42
3:J:1144:LEU:HD23	3:J:1144:LEU:HA	1.83	0.42
5:L:289:LYS:HG2	5:L:293:GLU:OE1	2.19	0.42
5:L:583:THR:HG22	5:L:584:ARG:N	2.34	0.42
1:A:38:THR:CB	1:B:45:ARG:HG2	2.49	0.42
2:C:690:VAL:HG23	2:C:763:THR:HG21	2.01	0.42
2:C:1042:LEU:HD23	2:C:1042:LEU:HA	1.81	0.42
3:D:116:PHE:CD1	3:D:1333:THR:HG22	2.55	0.42
3:D:423:LEU:HD12	3:D:423:LEU:N	2.34	0.42
3:D:544:LEU:O	3:D:574:VAL:HB	2.20	0.42
3:D:609:TYR:HA	3:D:617:THR:OG1	2.19	0.42
3:D:765:GLU:H	3:D:765:GLU:HG3	1.66	0.42
3:D:1287:ILE:HG22	3:D:1300:ALA:H	1.84	0.42
3:D:1289:ASN:O	3:D:1292:LEU:O	2.38	0.42
4:E:86:ILE:HG22	4:E:86:ILE:O	2.20	0.42
1:G:201:LEU:HA	1:G:201:LEU:HD12	1.75	0.42
2:I:678:ARG:NH2	2:I:1106:ARG:HG2	2.33	0.42
2:I:830:THR:HG22	2:I:1234:LYS:HZ3	1.85	0.42
2:I:1285:TYR:CD1	3:J:475:GLU:HB3	2.54	0.42
3:J:93:THR:HG22	3:J:94:GLN:H	1.84	0.42
3:J:252:LEU:HD23	3:J:262:THR:HB	2.00	0.42
3:J:357:VAL:HA	3:J:461:PHE:CZ	2.54	0.42
3:J:1177:ILE:CD1	3:J:1186:TYR:HB3	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1183:SER:OG	3:J:1185:PRO:HD3	2.19	0.42
5:L:111:LEU:HD11	5:L:119:ILE:CD1	2.49	0.42
5:L:141:ILE:HG23	5:L:224:LEU:HD11	2.00	0.42
5:L:512:GLY:C	5:L:514:ASP:H	2.27	0.42
1:B:101:THR:CG2	1:B:103:ASN:HD21	2.32	0.42
2:C:516:ASP:CG	2:C:522:SER:OG	2.63	0.42
2:C:629:PHE:CD2	2:C:634:VAL:HG11	2.55	0.42
2:C:685:MET:HE3	2:C:685:MET:HB2	1.76	0.42
2:C:1176:LEU:HA	2:C:1176:LEU:HD23	1.69	0.42
2:C:1285:TYR:CZ	3:D:1356:LEU:HD11	2.53	0.42
2:C:1333:LEU:HD23	3:D:327:LEU:HD13	2.01	0.42
3:D:395:LYS:O	3:D:398:LYS:HB3	2.20	0.42
3:D:646:ILE:CD1	3:D:741:ALA:HA	2.50	0.42
3:D:702:GLN:O	3:D:718:SER:N	2.35	0.42
3:D:843:VAL:CG2	3:D:861:ASN:HB2	2.50	0.42
3:D:853:THR:C	3:D:855:ASP:H	2.26	0.42
2:I:229:ILE:CD1	2:I:334:GLU:HG2	2.50	0.42
2:I:402:ARG:NH2	2:I:419:ILE:O	2.52	0.42
2:I:478:ARG:NH2	2:I:487:LEU:HB3	2.35	0.42
2:I:967:LEU:HD23	2:I:1021:LEU:HD22	2.01	0.42
2:I:1287:LEU:HD21	3:J:1351:VAL:HG22	2.02	0.42
3:J:645:VAL:HB	3:J:701:LEU:HD23	2.02	0.42
3:J:1286:LYS:HD2	3:J:1290:ARG:HH22	1.85	0.42
3:J:1343:GLU:O	3:J:1344:LEU:HB2	2.20	0.42
5:L:161:LEU:O	5:L:262:VAL:HG23	2.20	0.42
5:L:363:ARG:NH2	5:L:367:ILE:HD11	2.34	0.42
5:L:375:ALA:O	5:L:378:GLU:HB3	2.20	0.42
5:L:489:MET:HE1	5:L:493:LYS:HD2	1.98	0.42
1:A:41:ASN:ND2	2:C:1217:THR:C	2.78	0.41
1:A:51:MET:HE3	1:A:51:MET:HB3	1.88	0.41
1:A:153:VAL:HB	1:A:175:ALA:HB3	2.02	0.41
2:C:24:VAL:CG1	2:C:27:LEU:HD21	2.49	0.41
2:C:80:PHE:CZ	2:C:88:ARG:HD2	2.54	0.41
2:C:100:LEU:HA	2:C:100:LEU:HD23	1.84	0.41
2:C:724:VAL:HA	2:C:734:ILE:HD13	2.02	0.41
2:C:808:ASN:CG	2:C:1216:ARG:HH22	2.27	0.41
2:C:867:GLU:H	2:C:867:GLU:HG3	1.46	0.41
2:C:1337:ILE:HD13	2:C:1337:ILE:HG21	1.88	0.41
3:D:35:PHE:CD1	3:D:101:ARG:CD	2.94	0.41
3:D:49:PHE:HE1	5:F:500:ILE:HD12	1.85	0.41
3:D:1337:VAL:HG23	3:D:1338:ALA:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:548:LEU:CD2	5:F:551:LEU:HD12	2.47	0.41
1:G:44:ARG:CG	1:G:183:ILE:HG22	2.50	0.41
2:I:448:LEU:HG	2:I:553:THR:OG1	2.20	0.41
2:I:964:LEU:CD1	2:I:1021:LEU:HB3	2.49	0.41
3:J:68:TYR:HA	3:J:92:VAL:HG23	2.02	0.41
3:J:416:ILE:O	3:J:417:ARG:C	2.62	0.41
3:J:1198:VAL:HG11	3:J:1210:ILE:CG2	2.48	0.41
3:J:1219:ASP:O	3:J:1220:ILE:C	2.62	0.41
5:L:287:ILE:HG21	5:L:315:TRP:HH2	1.82	0.41
1:B:82:LEU:HD23	1:B:82:LEU:HA	1.74	0.41
1:B:104:LYS:O	1:B:140:ILE:HG22	2.19	0.41
1:B:205:MET:CG	1:B:206:GLU:H	2.32	0.41
2:C:315:MET:HE3	2:C:315:MET:HB2	1.85	0.41
3:D:430:HIS:ND1	3:D:430:HIS:N	2.65	0.41
3:D:553:THR:OG1	3:D:567:THR:OG1	2.36	0.41
4:E:85:ALA:C	4:E:87:ALA:H	2.28	0.41
5:F:298:PRO:HD3	5:F:326:TRP:HB3	2.02	0.41
1:G:97:GLU:OE2	1:G:145:LYS:HD3	2.18	0.41
1:G:221:ALA:HB1	1:H:228:LEU:CD2	2.50	0.41
2:I:511:LEU:CD2	2:I:531:LEU:HD13	2.49	0.41
2:I:978:VAL:HG21	2:I:1010:GLN:OE1	2.21	0.41
2:I:1219:GLU:OE2	3:J:634:ARG:NE	2.52	0.41
3:J:112:ALA:HA	3:J:238:ILE:HD13	2.01	0.41
3:J:596:LEU:HD11	3:J:604:MET:HE1	2.01	0.41
3:J:930:LEU:HD22	3:J:1240:VAL:HG12	2.02	0.41
4:K:32:VAL:C	4:K:34:GLY:H	2.29	0.41
2:C:46:GLN:O	2:C:47:TYR:C	2.64	0.41
2:C:135:THR:HG21	2:C:515:MET:SD	2.60	0.41
2:C:1301:ARG:HG3	2:C:1302:THR:N	2.35	0.41
3:D:9:LYS:HE2	3:D:11:GLN:CA	2.51	0.41
3:D:156:ARG:NH1	3:D:157:GLN:HE21	2.18	0.41
3:D:639:VAL:HG13	3:D:639:VAL:O	2.19	0.41
3:D:1237:VAL:CG1	3:D:1253:ILE:HD13	2.48	0.41
2:I:5:TYR:CD1	2:I:8:LYS:NZ	2.87	0.41
2:I:1290:MET:SD	2:I:1294:LYS:HE3	2.59	0.41
2:I:1305:TYR:OH	5:L:532:LEU:HG	2.20	0.41
3:J:147:ILE:HD11	3:J:177:ASP:OD2	2.20	0.41
3:J:244:VAL:O	3:J:244:VAL:HG23	2.19	0.41
3:J:418:GLU:OE2	4:K:44:ASP:CG	2.64	0.41
4:K:26:ARG:HH22	4:K:38:LEU:HD13	1.85	0.41
5:L:362:ASN:O	5:L:365:MET:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:HA	1:A:31:LEU:HD23	1.81	0.41
1:A:161:SER:O	1:A:163:GLU:N	2.52	0.41
1:B:153:VAL:HB	1:B:175:ALA:CB	2.46	0.41
1:B:212:ASP:OD2	1:B:215:GLU:HB2	2.20	0.41
2:C:122:VAL:O	2:C:122:VAL:HG13	2.20	0.41
2:C:488:MET:C	2:C:490:GLN:H	2.26	0.41
2:C:596:ASP:O	2:C:648:ASP:OD1	2.38	0.41
2:C:1332:SER:HB3	3:D:245:LEU:CD1	2.50	0.41
3:D:478:LEU:CD1	4:E:24:ALA:N	2.83	0.41
3:D:581:MET:HB3	3:D:581:MET:HE2	1.77	0.41
5:F:231:THR:CG2	5:F:249:ILE:HG12	2.50	0.41
5:F:489:MET:H	5:F:489:MET:HG2	1.41	0.41
5:F:533:ASP:O	5:F:536:THR:N	2.54	0.41
1:G:27:THR:HA	1:G:201:LEU:O	2.21	0.41
1:G:89:ALA:O	1:G:124:VAL:HG12	2.20	0.41
1:H:14:VAL:HG13	1:H:15:ASP:N	2.35	0.41
2:I:353:VAL:O	2:I:353:VAL:HG12	2.20	0.41
2:I:588:GLU:HA	2:I:606:LEU:O	2.21	0.41
2:I:1209:GLN:HB3	2:I:1224:PRO:HB2	2.02	0.41
3:J:138:VAL:HG13	3:J:180:MET:HA	2.03	0.41
3:J:210:SER:HB2	3:J:213:LYS:CB	2.50	0.41
3:J:591:ILE:HG23	3:J:592:VAL:HG13	2.03	0.41
3:J:832:LYS:HD3	3:J:1242:ARG:NH1	2.32	0.41
5:L:101:TYR:O	5:L:104:GLU:N	2.49	0.41
5:L:322:MET:SD	5:L:326:TRP:CH2	3.13	0.41
1:A:90:VAL:HG22	1:A:91:ARG:H	1.84	0.41
1:B:57:THR:HA	1:B:173:VAL:HG22	2.02	0.41
2:C:131:THR:OG1	2:C:135:THR:O	2.37	0.41
2:C:498:ILE:H	2:C:498:ILE:HD12	1.85	0.41
2:C:569:ILE:HD13	2:C:569:ILE:HG21	1.79	0.41
2:C:755:LYS:HA	2:C:766:ASN:OD1	2.21	0.41
2:C:848:GLU:CD	2:C:888:THR:CG2	2.93	0.41
2:C:1087:TYR:O	2:C:1213:TYR:N	2.41	0.41
3:D:68:TYR:HA	3:D:92:VAL:HG23	2.03	0.41
3:D:317:THR:CG2	3:D:320:ASN:HB3	2.42	0.41
3:D:667:GLN:HB3	3:D:673:VAL:HG22	2.02	0.41
3:D:748:ALA:HB1	3:D:753:SER:O	2.20	0.41
3:D:844:THR:HB	3:D:860:ARG:O	2.19	0.41
3:D:1150:PRO:O	3:D:1153:PRO:HG3	2.20	0.41
3:D:1350:ASN:HA	3:D:1353:VAL:HG12	2.02	0.41
5:F:515:GLU:HG2	5:F:516:ASP:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:210:LEU:CD1	2:I:220:ILE:HD13	2.50	0.41
2:I:239:MET:HG2	2:I:240:GLU:O	2.20	0.41
2:I:498:ILE:H	2:I:498:ILE:HD12	1.86	0.41
2:I:802:VAL:HG21	2:I:1098:LEU:HD13	2.01	0.41
2:I:803:ALA:HB2	2:I:1094:VAL:HG21	2.02	0.41
2:I:1067:ALA:CB	2:I:1072:ASN:O	2.69	0.41
2:I:1142:ARG:HD3	2:I:1161:LEU:HD13	1.97	0.41
2:I:1153:ALA:O	2:I:1154:ASP:C	2.63	0.41
2:I:1184:THR:O	2:I:1184:THR:HG22	2.20	0.41
3:J:18:ASP:HB2	3:J:1373:ARG:NH1	2.35	0.41
3:J:264:ASP:O	3:J:265:LEU:C	2.62	0.41
3:J:337:ARG:HB3	3:J:340:GLN:CB	2.50	0.41
3:J:707:ILE:H	3:J:707:ILE:HD12	1.86	0.41
3:J:800:LEU:HD12	3:J:1309:ILE:HD12	2.01	0.41
3:J:1328:THR:O	3:J:1332:LEU:HD23	2.20	0.41
2:C:28:LEU:HA	2:C:28:LEU:HD23	1.56	0.41
2:C:75:LEU:HA	2:C:75:LEU:HD13	1.79	0.41
2:C:484:LEU:H	2:C:484:LEU:HG	1.56	0.41
2:C:796:LEU:HD12	2:C:796:LEU:N	2.35	0.41
2:C:888:THR:HG23	2:C:916:SER:OG	2.21	0.41
2:C:1082:ILE:HD12	2:C:1082:ILE:H	1.85	0.41
3:D:60:ARG:HA	3:D:89:GLY:O	2.20	0.41
3:D:1221:LEU:HD13	3:D:1222:ARG:N	2.36	0.41
4:E:34:GLY:C	4:E:35:LYS:HG3	2.45	0.41
1:G:153:VAL:HB	1:G:175:ALA:HB3	2.01	0.41
2:I:196:VAL:HG12	2:I:206:ALA:HA	2.00	0.41
2:I:1211:ARG:HB2	2:I:1220:GLN:HE21	1.85	0.41
3:J:1280:VAL:HG21	3:J:1304:ARG:HD3	2.02	0.41
5:L:163:THR:HG22	5:L:163:THR:O	2.21	0.41
1:B:78:ILE:HA	1:B:81:ILE:HD12	2.02	0.41
2:C:201:ARG:HE	2:C:370:MET:HA	1.86	0.41
2:C:496:LYS:HD2	2:C:496:LYS:C	2.46	0.41
2:C:1101:LEU:HD23	2:C:1101:LEU:HA	1.62	0.41
2:C:1144:PHE:HE1	2:C:1201:LEU:HD11	1.85	0.41
3:D:55:GLY:O	3:D:56:LEU:C	2.63	0.41
3:D:147:ILE:HG22	3:D:188:LEU:CD2	2.51	0.41
3:D:518:VAL:CG1	3:D:519:ASN:N	2.84	0.41
5:F:99:ARG:HD3	5:F:99:ARG:HA	1.89	0.41
5:F:474:MET:HE3	5:F:474:MET:HB3	1.95	0.41
1:G:51:MET:HE1	1:G:216:ALA:CB	2.51	0.41
1:G:152:TYR:CD1	2:I:824:GLN:HG2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:105:TYR:HA	2:I:112:GLY:O	2.21	0.41
2:I:157:PHE:CE2	2:I:431:LYS:NZ	2.89	0.41
2:I:720:ARG:HB3	2:I:736:VAL:HG13	2.01	0.41
2:I:791:LEU:HD23	2:I:791:LEU:HA	1.88	0.41
2:I:1289:GLU:OE2	3:J:473:THR:CG2	2.48	0.41
3:J:60:ARG:HA	3:J:89:GLY:O	2.20	0.41
3:J:695:LYS:HD3	3:J:695:LYS:HA	1.72	0.41
3:J:808:VAL:HG13	3:J:913:GLU:C	2.45	0.41
3:J:913:GLU:CD	4:K:17:PHE:HZ	2.27	0.41
3:J:1311:LYS:O	3:J:1314:LEU:HB3	2.21	0.41
5:L:164:GLY:O	5:L:260:ARG:HB2	2.21	0.41
1:B:195:ARG:HB2	1:B:198:LEU:HD21	2.02	0.41
2:C:958:LYS:O	2:C:962:GLU:CG	2.69	0.41
2:C:1065:LYS:HD2	2:C:1235:LEU:HD12	2.01	0.41
2:C:1142:ARG:CZ	2:C:1142:ARG:HB2	2.50	0.41
3:D:161:THR:HG22	3:D:164:GLN:HG3	2.02	0.41
3:D:255:LEU:HD13	3:D:255:LEU:HA	1.85	0.41
3:D:442:ILE:HA	3:D:442:ILE:HD13	1.85	0.41
3:D:931:THR:HG22	3:D:1244:GLN:HE21	1.84	0.41
3:D:1291:GLU:CG	3:D:1297:LYS:NZ	2.84	0.41
1:G:79:LEU:HD13	1:G:79:LEU:O	2.21	0.41
1:G:86:LYS:HE2	1:G:174:ASP:O	2.21	0.41
1:H:43:LEU:N	1:H:43:LEU:CD1	2.83	0.41
1:H:133:LEU:CD1	1:H:140:ILE:HD13	2.50	0.41
2:I:660:VAL:HG11	3:J:769:VAL:HG13	2.03	0.41
2:I:699:LEU:HD23	2:I:699:LEU:HA	1.44	0.41
2:I:882:ILE:HG13	2:I:919:ARG:NH1	2.36	0.41
2:I:1069:ARG:NH2	2:I:1231:TYR:HB3	2.35	0.41
3:J:57:PHE:CD2	3:J:57:PHE:N	2.87	0.41
3:J:582:ILE:HG22	3:J:620:PHE:CE1	2.55	0.41
3:J:814:CYS:SG	3:J:889:ASP:N	2.93	0.41
3:J:1372:ARG:O	3:J:1375:ALA:HB3	2.20	0.41
5:L:289:LYS:HB3	5:L:289:LYS:HE2	1.77	0.41
5:L:557:LYS:O	5:L:561:MET:HB2	2.20	0.41
1:B:95:LYS:HG3	1:B:120:ASP:OD2	2.21	0.41
2:C:247:ARG:HB2	2:C:274:ILE:CD1	2.51	0.41
2:C:531:LEU:HD11	6:C:2001:KNG:C14	2.50	0.41
2:C:568:ASN:HA	2:C:571:LEU:HD12	2.03	0.41
2:C:637:ARG:HB3	2:C:642:SER:HB3	2.02	0.41
2:C:857:VAL:HB	2:C:861:ALA:HB3	2.01	0.41
2:C:898:GLU:OE2	5:F:541:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:953:LEU:HA	2:C:953:LEU:HD12	1.76	0.41
2:C:1037:THR:HG22	2:C:1037:THR:O	2.20	0.41
2:C:1112:ILE:HD11	3:D:639:VAL:CG1	2.50	0.41
2:C:1240:ASP:HB3	3:D:445:LYS:NZ	2.35	0.41
2:C:1273:MET:HE3	2:C:1273:MET:HB2	1.78	0.41
2:C:1308:ILE:HG23	3:D:380:PHE:CD2	2.56	0.41
3:D:93:THR:CG2	3:D:94:GLN:N	2.84	0.41
3:D:124:ILE:HG12	3:D:237:MET:SD	2.61	0.41
3:D:147:ILE:HG13	3:D:147:ILE:O	2.21	0.41
3:D:239:LEU:HA	3:D:239:LEU:HD23	1.77	0.41
3:D:298:MET:SD	5:F:406:GLN:HG3	2.61	0.41
3:D:310:GLY:HA2	3:D:314:ARG:HD2	2.02	0.41
3:D:337:ARG:O	3:D:341:ASN:CB	2.68	0.41
3:D:363:LEU:HD23	3:D:487:THR:HG22	2.02	0.41
3:D:474:LEU:HD23	4:E:28:ARG:HG2	2.03	0.41
3:D:517:CYS:CA	3:D:716:GLN:HE22	2.34	0.41
3:D:528:THR:HG23	3:D:529:GLY:N	2.36	0.41
3:D:1306:LEU:C	3:D:1307:LEU:HD12	2.45	0.41
5:F:433:TRP:CD2	5:F:433:TRP:C	2.99	0.41
5:F:490:PRO:O	5:F:491:GLU:HG2	2.21	0.41
1:G:86:LYS:HZ3	1:G:174:ASP:CB	2.32	0.41
1:H:28:LEU:HD23	1:H:31:LEU:HD11	2.03	0.41
1:H:107:ILE:HG13	1:H:136:GLU:O	2.21	0.41
1:H:176:CYS:C	1:H:178:SER:N	2.79	0.41
2:I:26:TYR:HE2	2:I:32:LEU:CD1	2.28	0.41
2:I:27:LEU:HD12	2:I:524:ILE:CD1	2.50	0.41
2:I:41:GLN:NE2	2:I:73:TYR:O	2.53	0.41
2:I:169:LYS:HZ1	2:I:192:ASP:CG	2.29	0.41
2:I:239:MET:O	2:I:284:LEU:HD12	2.21	0.41
2:I:496:LYS:O	2:I:500:ALA:HB2	2.21	0.41
2:I:590:PRO:CB	2:I:655:VAL:HG21	2.50	0.41
2:I:623:LEU:HD23	2:I:623:LEU:N	2.36	0.41
2:I:1287:LEU:HD22	3:J:1357:ILE:HG13	2.02	0.41
2:I:1294:LYS:CB	3:J:347:VAL:HG13	2.51	0.41
3:J:22:ILE:O	3:J:1339:GLY:HA2	2.20	0.41
3:J:93:THR:HG22	3:J:94:GLN:N	2.35	0.41
3:J:139:LEU:HA	3:J:139:LEU:HD23	1.84	0.41
3:J:701:LEU:HD13	3:J:723:TYR:HB2	2.01	0.41
3:J:722:ILE:HD11	3:J:740:LEU:CD2	2.40	0.41
3:J:923:ILE:HD13	3:J:923:ILE:HG21	1.81	0.41
3:J:1181:ASP:OD1	3:J:1182:GLY:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1263:LYS:HZ2	3:J:1315:ALA:CB	2.32	0.41
5:L:276:MET:HG2	5:L:351:THR:HG21	2.03	0.41
5:L:296:LYS:HB2	5:L:329:LYS:HD3	2.03	0.41
5:L:396:ASN:C	5:L:398:GLY:H	2.28	0.41
5:L:489:MET:CB	5:L:490:PRO:CD	2.99	0.41
1:A:65:LEU:HA	1:A:65:LEU:HD13	1.63	0.41
1:B:125:LYS:HG3	1:B:128:HIS:HB2	2.03	0.41
2:C:290:GLU:HG2	2:C:319:LEU:HD12	1.99	0.41
2:C:385:PHE:CE2	2:C:390:PHE:HE2	2.39	0.41
2:C:615:VAL:HG21	2:C:645:PHE:CD2	2.55	0.41
2:C:741:MET:HE3	2:C:974:ARG:NH1	2.35	0.41
3:D:657:ALA:O	3:D:661:VAL:HG12	2.21	0.41
3:D:664:ILE:CD1	3:D:681:LYS:HG2	2.51	0.41
3:D:801:VAL:O	3:D:805:GLN:HB2	2.21	0.41
3:D:806:ASP:HA	3:D:1347:LEU:HD13	2.02	0.41
5:F:324:LYS:HB3	5:F:325:PRO:HD2	2.03	0.41
1:H:124:VAL:HB	1:H:210:THR:HG22	2.03	0.41
2:I:619:ALA:HB1	2:I:656:SER:C	2.46	0.41
2:I:972:PHE:CZ	2:I:1018:TYR:CE1	3.09	0.41
2:I:976:ARG:HD2	2:I:989:LEU:HD23	2.02	0.41
3:J:883:ARG:HH12	3:J:897:HIS:HD2	1.66	0.41
5:L:513:ASP:C	5:L:515:GLU:N	2.79	0.41
5:L:565:ILE:HG22	5:L:566:ASP:CG	2.45	0.41
1:B:51:MET:HG2	1:B:179:PRO:HD2	2.03	0.40
1:B:210:THR:O	1:B:211:ILE:HG12	2.20	0.40
2:C:606:LEU:N	2:C:606:LEU:HD12	2.36	0.40
2:C:653:MET:HG2	2:C:654:ASP:N	2.35	0.40
2:C:716:ALA:HB2	2:C:767:GLN:HE22	1.86	0.40
2:C:803:ALA:HB2	2:C:1094:VAL:HG21	2.03	0.40
3:D:174:ASP:O	3:D:175:GLU:CG	2.69	0.40
3:D:349:TYR:CG	3:D:472:LEU:HD21	2.56	0.40
3:D:478:LEU:HD12	4:E:24:ALA:CA	2.51	0.40
3:D:647:PRO:HD3	3:D:697:MET:HB3	2.03	0.40
1:G:31:LEU:HD23	1:G:31:LEU:HA	1.79	0.40
1:G:36:GLY:C	1:G:187:VAL:HG11	2.45	0.40
1:G:46:ILE:HD11	1:H:38:THR:HG21	2.03	0.40
1:G:104:LYS:HG2	1:G:110:VAL:CG2	2.38	0.40
1:G:231:PHE:CB	1:H:218:ARG:HD3	2.51	0.40
2:I:11:ILE:HG22	2:I:1149:TYR:CZ	2.56	0.40
2:I:971:LEU:CD2	2:I:1018:TYR:HB2	2.50	0.40
2:I:1113:LEU:N	2:I:1113:LEU:HD12	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:629:PHE:O	3:J:630:ALA:C	2.64	0.40
3:J:688:ALA:O	3:J:691:ASP:HB2	2.20	0.40
3:J:1264:ALA:HB3	3:J:1280:VAL:HG22	2.02	0.40
5:L:277:MET:HG3	5:L:362:ASN:ND2	2.31	0.40
1:B:11:PRO:HB2	1:B:28:LEU:CD1	2.44	0.40
2:C:13:LYS:O	2:C:1183:ALA:N	2.47	0.40
2:C:513:GLN:HG3	2:C:526:HIS:CE1	2.56	0.40
2:C:548:ARG:NH2	2:C:571:LEU:CD1	2.84	0.40
2:C:571:LEU:C	2:C:572:ILE:HG12	2.47	0.40
2:C:1015:ALA:O	2:C:1018:TYR:HB3	2.21	0.40
2:C:1271:GLY:CA	3:D:343:LEU:HD21	2.45	0.40
2:C:1271:GLY:HA3	3:D:343:LEU:CD2	2.45	0.40
2:C:1315:MET:HE3	2:C:1315:MET:HB2	1.92	0.40
3:D:34:SER:HB2	3:D:104:HIS:HB3	2.02	0.40
3:D:245:LEU:HA	3:D:245:LEU:HD12	1.84	0.40
3:D:278:ARG:HD2	3:D:295:GLU:CD	2.46	0.40
3:D:564:VAL:HG12	3:D:565:ALA:N	2.36	0.40
3:D:678:ARG:C	3:D:678:ARG:HD3	2.46	0.40
3:D:844:THR:HG21	3:D:858:VAL:HG21	2.02	0.40
3:D:902:ASP:O	3:D:903:LEU:HB2	2.20	0.40
4:E:39:VAL:HG21	4:E:56:GLU:HG3	2.03	0.40
1:G:13:LEU:HB3	1:H:231:PHE:HZ	1.85	0.40
1:G:228:LEU:HD23	1:G:228:LEU:HA	1.79	0.40
1:G:231:PHE:CE1	1:H:221:ALA:HB3	2.56	0.40
1:H:228:LEU:HA	1:H:228:LEU:HD23	1.45	0.40
2:I:9:LYS:HG2	2:I:1171:ARG:HD3	2.03	0.40
2:I:306:THR:OG1	2:I:308:GLU:HB2	2.21	0.40
2:I:525:THR:HG21	2:I:687:ARG:HD2	2.02	0.40
2:I:905:ILE:HD11	5:L:598:LEU:HD13	2.03	0.40
2:I:1290:MET:O	3:J:347:VAL:HG21	2.21	0.40
5:L:224:LEU:HB2	5:L:259:PHE:CZ	2.57	0.40
5:L:437:GLN:HG3	5:L:438:ALA:N	2.35	0.40
5:L:481:GLU:O	5:L:484:ALA:HB3	2.22	0.40
5:L:484:ALA:CB	5:L:491:GLU:OE2	2.69	0.40
1:B:74:VAL:HG12	1:B:76:GLU:H	1.86	0.40
1:B:112:ALA:O	1:B:115:ILE:CD1	2.68	0.40
2:C:11:ILE:HG22	2:C:11:ILE:O	2.21	0.40
2:C:79:VAL:HG23	2:C:80:PHE:H	1.86	0.40
2:C:971:LEU:HG	2:C:1014:LEU:HD23	2.03	0.40
2:C:1151:LEU:HD12	2:C:1198:LEU:HD23	2.01	0.40
3:D:79:LYS:CD	3:D:79:LYS:C	2.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:238:ILE:HD13	3:D:238:ILE:HA	1.82	0.40
3:D:242:LEU:HD23	3:D:243:PRO:N	2.36	0.40
3:D:254:PRO:C	3:D:255:LEU:HD22	2.47	0.40
3:D:478:LEU:CD1	4:E:24:ALA:HA	2.52	0.40
3:D:638:SER:O	3:D:721:SER:CB	2.70	0.40
3:D:755:ILE:HD12	3:D:774:ILE:CG2	2.50	0.40
3:D:1231:ARG:HA	3:D:1234:VAL:HG22	2.02	0.40
4:E:26:ARG:NE	4:E:53:GLU:OE1	2.55	0.40
1:H:19:VAL:HB	1:H:23:HIS:NE2	2.37	0.40
1:H:92:VAL:HA	1:H:120:ASP:O	2.21	0.40
1:H:156:SER:C	1:H:158:ARG:H	2.30	0.40
2:I:15:PHE:CE1	2:I:1151:LEU:HD13	2.57	0.40
2:I:208:ILE:HD11	2:I:356:THR:HG21	2.04	0.40
2:I:299:LYS:HG2	2:I:334:GLU:OE1	2.21	0.40
2:I:617:ALA:HB3	2:I:653:MET:CB	2.52	0.40
2:I:646:SER:CB	2:I:649:GLN:HG3	2.36	0.40
3:J:288:PRO:CG	3:J:291:ILE:HD12	2.52	0.40
3:J:427:PRO:O	3:J:429:LEU:HD22	2.21	0.40
5:L:295:CYS:SG	5:L:333:VAL:HB	2.61	0.40
1:A:211:ILE:HG22	1:A:216:ALA:HB2	1.98	0.40
1:B:71:LYS:HE2	1:B:139:SER:O	2.21	0.40
1:B:89:ALA:CB	1:B:124:VAL:HG12	2.49	0.40
1:B:152:TYR:CE2	3:D:536:LEU:CD2	2.99	0.40
2:C:263:VAL:CG2	2:C:273:HIS:HB3	2.52	0.40
2:C:557:ARG:HH21	2:C:608:ALA:HA	1.86	0.40
2:C:592:ARG:O	2:C:652:TYR:HA	2.22	0.40
2:C:623:LEU:HA	2:C:630:VAL:HG23	2.02	0.40
2:C:1112:ILE:CD1	3:D:639:VAL:HG13	2.50	0.40
3:D:161:THR:HG22	3:D:164:GLN:H	1.86	0.40
3:D:221:ILE:HG23	3:D:222:LYS:N	2.37	0.40
3:D:522:GLY:O	3:D:525:MET:HG2	2.21	0.40
5:F:530:LEU:O	5:F:533:ASP:HB2	2.22	0.40
1:G:96:ASP:OD2	1:G:148:ARG:NH2	2.39	0.40
1:G:110:VAL:HG13	1:G:114:ASP:OD2	2.21	0.40
2:I:632:ASP:O	2:I:647:ARG:HB2	2.21	0.40
2:I:870:ILE:CG1	2:I:1050:VAL:HG11	2.51	0.40
2:I:978:VAL:HG13	2:I:1007:LYS:HB3	2.03	0.40
2:I:996:ARG:HA	2:I:996:ARG:HD3	1.73	0.40
2:I:1065:LYS:HD3	2:I:1235:LEU:CD1	2.47	0.40
2:I:1301:ARG:HG3	2:I:1302:THR:N	2.36	0.40
3:J:127:LEU:HD23	3:J:189:LEU:HD22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:395:LYS:HG2	5:L:536:THR:HG21	2.04	0.40
3:J:611:ILE:CG2	3:J:612:LEU:HD12	2.48	0.40
3:J:914:ALA:O	3:J:918:ILE:HG23	2.21	0.40
4:K:10:VAL:CG1	4:K:16:ARG:HB2	2.49	0.40
5:L:253:SER:O	5:L:257:LYS:HG3	2.22	0.40
1:B:124:VAL:HG21	1:B:209:GLY:O	2.21	0.40
2:C:209:ILE:HG21	2:C:209:ILE:HD13	1.81	0.40
2:C:325:LEU:O	2:C:330:HIS:HB2	2.21	0.40
2:C:698:PRO:HD3	2:C:795:ALA:CA	2.51	0.40
2:C:818:VAL:O	2:C:1079:ILE:HD12	2.20	0.40
2:C:1106:ARG:HD2	2:C:1106:ARG:N	2.34	0.40
3:D:8:LEU:CD2	3:D:9:LYS:N	2.85	0.40
3:D:434:ILE:HG21	3:D:434:ILE:HD13	1.73	0.40
3:D:461:PHE:C	3:D:463:GLY:H	2.29	0.40
3:D:822:MET:SD	3:D:838:ARG:HB3	2.61	0.40
4:E:24:ALA:O	4:E:25:ARG:C	2.63	0.40
5:F:311:THR:HG21	5:F:348:GLU:OE2	2.21	0.40
1:G:107:ILE:HG13	1:G:136:GLU:HA	2.02	0.40
2:I:690:VAL:HG22	2:I:691:PRO:HD2	2.04	0.40
2:I:708:VAL:HG11	2:I:794:LEU:HD22	2.03	0.40
2:I:1246:ARG:NH2	2:I:1249:GLY:H	2.19	0.40
2:I:1334:GLY:O	3:J:25:ALA:HB3	2.21	0.40
3:J:126:LEU:HD12	3:J:126:LEU:C	2.46	0.40
3:J:557:LYS:CD	3:J:611:ILE:HG23	2.52	0.40
3:J:814:CYS:SG	3:J:889:ASP:HB3	2.61	0.40
3:J:850:LYS:CD	3:J:875:ASN:ND2	2.85	0.40
5:L:251:LYS:HA	5:L:254:GLU:HG2	2.03	0.40
5:L:296:LYS:HD3	5:L:296:LYS:HA	1.97	0.40
5:L:544:THR:HA	5:L:547:VAL:HG12	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	225/329 (68%)	198 (88%)	20 (9%)	7 (3%)	3	25
1	B	210/329 (64%)	186 (89%)	19 (9%)	5 (2%)	4	30
1	G	222/329 (68%)	194 (87%)	23 (10%)	5 (2%)	5	31
1	H	211/329 (64%)	187 (89%)	17 (8%)	7 (3%)	3	24
2	C	1335/1342 (100%)	1226 (92%)	100 (8%)	9 (1%)	18	55
2	I	1324/1342 (99%)	1220 (92%)	96 (7%)	8 (1%)	21	58
3	D	1162/1407 (83%)	1068 (92%)	86 (7%)	8 (1%)	18	55
3	J	1151/1407 (82%)	1060 (92%)	78 (7%)	13 (1%)	11	44
4	E	87/91 (96%)	82 (94%)	4 (5%)	1 (1%)	11	44
4	K	77/91 (85%)	74 (96%)	3 (4%)	0	100	100
5	F	462/613 (75%)	426 (92%)	35 (8%)	1 (0%)	43	76
5	L	463/613 (76%)	426 (92%)	36 (8%)	1 (0%)	43	76
All	All	6929/8222 (84%)	6347 (92%)	517 (8%)	65 (1%)	14	49

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	PRO
1	B	13	LEU
1	B	29	GLU
2	C	2	VAL
2	C	3	TYR
2	C	535	PRO
2	C	697	LYS
2	C	1159	VAL
3	D	332	LYS
1	G	162	GLU
1	G	167	PRO
1	H	135	ASP
2	I	1159	VAL
3	J	332	LYS
1	A	162	GLU
1	A	233	ASP
1	B	135	ASP
1	B	136	GLU
2	C	170	VAL
1	G	14	VAL
1	H	136	GLU
1	H	177	TYR

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Mol	Chain	Res	Type
2	I	170	VAL
3	J	334	LYS
2	C	1158	LYS
2	I	697	LYS
3	J	337	ARG
2	C	484	LEU
3	D	710	ASP
3	D	806	ASP
1	G	62	ASP
1	H	20	SER
1	H	62	ASP
1	H	138	ALA
1	H	157	THR
2	I	484	LEU
3	J	338	PHE
3	J	342	LEU
3	J	344	GLY
3	J	710	ASP
1	A	14	VAL
1	A	196	THR
1	A	232	VAL
3	D	12	THR
2	I	1136	GLN
2	I	1158	LYS
3	J	333	GLY
3	J	345	LYS
3	J	806	ASP
1	B	14	VAL
3	D	345	LYS
3	D	831	VAL
2	I	63	SER
2	C	1186	VAL
4	E	86	ILE
3	J	831	VAL
5	F	477	GLU
1	G	159	ILE
3	J	826	ILE
3	D	826	ILE
5	L	477	GLU
3	D	1180	VAL
2	I	1186	VAL
3	J	336	GLY

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Mol	Chain	Res	Type
1	A	159	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/286 (68%)	179 (92%)	15 (8%)	12	34
1	B	182/286 (64%)	171 (94%)	11 (6%)	17	42
1	G	191/286 (67%)	177 (93%)	14 (7%)	13	36
1	H	184/286 (64%)	175 (95%)	9 (5%)	22	46
2	C	1151/1157 (100%)	1035 (90%)	116 (10%)	7	25
2	I	1147/1157 (99%)	1034 (90%)	113 (10%)	7	26
3	D	970/1168 (83%)	859 (89%)	111 (11%)	5	21
3	J	960/1168 (82%)	852 (89%)	108 (11%)	5	22
4	E	72/75 (96%)	63 (88%)	9 (12%)	4	19
4	K	67/75 (89%)	62 (92%)	5 (8%)	12	35
5	F	417/540 (77%)	375 (90%)	42 (10%)	7	25
5	L	418/540 (77%)	376 (90%)	42 (10%)	7	26
All	All	5953/7024 (85%)	5358 (90%)	595 (10%)	7	26

All (595) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	19	VAL
1	A	26	VAL
1	A	50	SER
1	A	61	ILE
1	A	64	VAL
1	A	71	LYS
1	A	74	VAL
1	A	115	ILE

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Mol	Chain	Res	Type
1	A	129	VAL
1	A	133	LEU
1	A	168	ILE
1	A	215	GLU
1	A	219	ARG
1	A	231	PHE
1	B	7	GLU
1	B	8	PHE
1	B	9	LEU
1	B	26	VAL
1	B	50	SER
1	B	61	ILE
1	B	64	VAL
1	B	115	ILE
1	B	133	LEU
1	B	194	GLN
1	B	215	GLU
2	C	11	ILE
2	C	22	LEU
2	C	39	ILE
2	C	60	GLN
2	C	82	VAL
2	C	85	CYS
2	C	90	VAL
2	C	91	THR
2	C	115	LYS
2	C	116	ASP
2	C	117	ILE
2	C	118	LYS
2	C	119	GLU
2	C	120	GLN
2	C	121	GLU
2	C	131	THR
2	C	132	ASP
2	C	167	SER
2	C	170	VAL
2	C	237	LEU
2	C	285	ILE
2	C	292	ILE
2	C	299	LYS
2	C	302	ILE
2	C	306	THR

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Mol	Chain	Res	Type
2	C	320	ASP
2	C	321	LEU
2	C	353	VAL
2	C	360	LEU
2	C	377	THR
2	C	379	GLU
2	C	394	ARG
2	C	400	VAL
2	C	413	GLU
2	C	419	ILE
2	C	423	ASP
2	C	434	ASP
2	C	445	ILE
2	C	453	ILE
2	C	484	LEU
2	C	486	THR
2	C	490	GLN
2	C	493	ILE
2	C	503	LYS
2	C	518	ASN
2	C	531	LEU
2	C	550	VAL
2	C	558	VAL
2	C	565	GLU
2	C	589	THR
2	C	604	HIS
2	C	607	SER
2	C	609	ILE
2	C	615	VAL
2	C	620	ASN
2	C	623	LEU
2	C	633	LEU
2	C	639	LYS
2	C	657	THR
2	C	672	GLU
2	C	680	LEU
2	C	692	THR
2	C	697	LYS
2	C	705	GLU
2	C	714	VAL
2	C	748	ILE
2	C	765	ILE

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Mol	Chain	Res	Type
2	C	773	LEU
2	C	781	ASP
2	C	788	SER
2	C	800	MET
2	C	817	LEU
2	C	819	SER
2	C	826	ASP
2	C	840	SER
2	C	859	GLU
2	C	878	THR
2	C	890	LYS
2	C	892	GLU
2	C	946	LEU
2	C	951	MET
2	C	974	ARG
2	C	979	LEU
2	C	984	VAL
2	C	1002	LEU
2	C	1040	ASP
2	C	1046	VAL
2	C	1073	LYS
2	C	1082	ILE
2	C	1083	GLU
2	C	1108	ASN
2	C	1109	ILE
2	C	1114	GLU
2	C	1134	GLN
2	C	1146	GLN
2	C	1151	LEU
2	C	1156	ARG
2	C	1159	VAL
2	C	1161	LEU
2	C	1174	GLU
2	C	1180	MET
2	C	1198	LEU
2	C	1204	LEU
2	C	1210	ILE
2	C	1238	LEU
2	C	1248	THR
2	C	1253	LEU
2	C	1254	VAL
2	C	1264	GLN

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Mol	Chain	Res	Type
2	C	1293	VAL
2	C	1310	ASP
2	C	1327	LEU
2	C	1331	ARG
2	C	1340	GLU
2	C	1341	ASP
2	C	1342	GLU
3	D	8	LEU
3	D	13	LYS
3	D	18	ASP
3	D	20	ILE
3	D	26	SER
3	D	46	TYR
3	D	79	LYS
3	D	83	VAL
3	D	84	ILE
3	D	92	VAL
3	D	94	GLN
3	D	95	THR
3	D	97	VAL
3	D	106	GLU
3	D	159	ILE
3	D	169	LEU
3	D	175	GLU
3	D	217	LEU
3	D	244	VAL
3	D	252	LEU
3	D	255	LEU
3	D	306	LEU
3	D	312	ARG
3	D	324	LEU
3	D	363	LEU
3	D	374	LEU
3	D	394	ILE
3	D	401	VAL
3	D	416	ILE
3	D	425	ARG
3	D	429	LEU
3	D	454	CYS
3	D	490	ILE
3	D	501	VAL
3	D	506	VAL

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Mol	Chain	Res	Type
3	D	507	VAL
3	D	510	LEU
3	D	513	MET
3	D	514	THR
3	D	536	LEU
3	D	545	HIS
3	D	547	ARG
3	D	567	THR
3	D	568	SER
3	D	573	THR
3	D	594	GLN
3	D	641	ILE
3	D	646	ILE
3	D	660	GLU
3	D	661	VAL
3	D	678	ARG
3	D	680	ASN
3	D	683	ILE
3	D	685	ILE
3	D	697	MET
3	D	698	MET
3	D	701	LEU
3	D	702	GLN
3	D	707	ILE
3	D	708	ASN
3	D	710	ASP
3	D	712	GLN
3	D	717	VAL
3	D	720	ASN
3	D	740	LEU
3	D	746	LEU
3	D	754	ILE
3	D	769	VAL
3	D	770	LEU
3	D	788	LEU
3	D	798	ARG
3	D	803	VAL
3	D	810	THR
3	D	826	ILE
3	D	844	THR
3	D	847	ASP
3	D	848	VAL

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Mol	Chain	Res	Type
3	D	849	LEU
3	D	853	THR
3	D	857	LEU
3	D	858	VAL
3	D	860	ARG
3	D	881	LYS
3	D	897	HIS
3	D	908	ILE
3	D	918	ILE
3	D	931	THR
3	D	1135	THR
3	D	1155	ILE
3	D	1163	VAL
3	D	1170	LYS
3	D	1177	ILE
3	D	1186	TYR
3	D	1194	ARG
3	D	1202	GLU
3	D	1221	LEU
3	D	1255	VAL
3	D	1268	ASN
3	D	1273	ASP
3	D	1274	PHE
3	D	1275	LEU
3	D	1278	GLU
3	D	1281	GLU
3	D	1284	ARG
3	D	1285	VAL
3	D	1289	ASN
3	D	1293	GLU
3	D	1298	VAL
3	D	1310	THR
3	D	1333	THR
3	D	1343	GLU
4	E	5	THR
4	E	13	ILE
4	E	16	ARG
4	E	21	LEU
4	E	28	ARG
4	E	39	VAL
4	E	46	THR
4	E	58	LEU

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Mol	Chain	Res	Type
4	E	84	THR
5	F	98	VAL
5	F	100	MET
5	F	102	MET
5	F	127	ILE
5	F	130	VAL
5	F	154	GLU
5	F	247	GLU
5	F	267	ASP
5	F	297	MET
5	F	301	ASN
5	F	305	LEU
5	F	306	PHE
5	F	310	GLU
5	F	341	LEU
5	F	395	THR
5	F	400	GLN
5	F	429	THR
5	F	437	GLN
5	F	449	THR
5	F	450	ILE
5	F	471	LEU
5	F	472	GLN
5	F	479	THR
5	F	482	GLU
5	F	485	GLU
5	F	486	ARG
5	F	488	LEU
5	F	489	MET
5	F	494	ILE
5	F	508	GLU
5	F	530	LEU
5	F	547	VAL
5	F	558	VAL
5	F	561	MET
5	F	566	ASP
5	F	568	ASN
5	F	572	THR
5	F	580	PHE
5	F	587	ILE
5	F	603	ARG
5	F	606	VAL

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Mol	Chain	Res	Type
5	F	612	ASP
1	G	9	LEU
1	G	19	VAL
1	G	26	VAL
1	G	50	SER
1	G	61	ILE
1	G	64	VAL
1	G	74	VAL
1	G	115	ILE
1	G	129	VAL
1	G	133	LEU
1	G	168	ILE
1	G	215	GLU
1	G	219	ARG
1	G	231	PHE
1	H	19	VAL
1	H	26	VAL
1	H	50	SER
1	H	61	ILE
1	H	64	VAL
1	H	115	ILE
1	H	133	LEU
1	H	183	ILE
1	H	215	GLU
2	I	11	ILE
2	I	21	VAL
2	I	22	LEU
2	I	39	ILE
2	I	60	GLN
2	I	82	VAL
2	I	85	CYS
2	I	90	VAL
2	I	91	THR
2	I	115	LYS
2	I	116	ASP
2	I	117	ILE
2	I	118	LYS
2	I	119	GLU
2	I	121	GLU
2	I	132	ASP
2	I	167	SER
2	I	170	VAL

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Mol	Chain	Res	Type
2	I	237	LEU
2	I	285	ILE
2	I	292	ILE
2	I	299	LYS
2	I	302	ILE
2	I	306	THR
2	I	320	ASP
2	I	321	LEU
2	I	360	LEU
2	I	377	THR
2	I	379	GLU
2	I	394	ARG
2	I	400	VAL
2	I	413	GLU
2	I	419	ILE
2	I	423	ASP
2	I	434	ASP
2	I	445	ILE
2	I	453	ILE
2	I	484	LEU
2	I	486	THR
2	I	490	GLN
2	I	493	ILE
2	I	503	LYS
2	I	518	ASN
2	I	550	VAL
2	I	558	VAL
2	I	565	GLU
2	I	589	THR
2	I	604	HIS
2	I	607	SER
2	I	609	ILE
2	I	615	VAL
2	I	620	ASN
2	I	623	LEU
2	I	633	LEU
2	I	639	LYS
2	I	657	THR
2	I	672	GLU
2	I	680	LEU
2	I	692	THR
2	I	697	LYS

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Mol	Chain	Res	Type
2	I	705	GLU
2	I	714	VAL
2	I	748	ILE
2	I	765	ILE
2	I	773	LEU
2	I	781	ASP
2	I	788	SER
2	I	800	MET
2	I	817	LEU
2	I	819	SER
2	I	826	ASP
2	I	840	SER
2	I	859	GLU
2	I	878	THR
2	I	890	LYS
2	I	892	GLU
2	I	946	LEU
2	I	951	MET
2	I	974	ARG
2	I	979	LEU
2	I	984	VAL
2	I	1002	LEU
2	I	1040	ASP
2	I	1046	VAL
2	I	1073	LYS
2	I	1076	ILE
2	I	1082	ILE
2	I	1083	GLU
2	I	1108	ASN
2	I	1109	ILE
2	I	1114	GLU
2	I	1134	GLN
2	I	1146	GLN
2	I	1151	LEU
2	I	1156	ARG
2	I	1159	VAL
2	I	1161	LEU
2	I	1174	GLU
2	I	1180	MET
2	I	1198	LEU
2	I	1204	LEU
2	I	1210	ILE

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Mol	Chain	Res	Type
2	I	1238	LEU
2	I	1253	LEU
2	I	1254	VAL
2	I	1264	GLN
2	I	1293	VAL
2	I	1310	ASP
2	I	1327	LEU
2	I	1331	ARG
2	I	1340	GLU
2	I	1341	ASP
2	I	1342	GLU
3	J	18	ASP
3	J	20	ILE
3	J	26	SER
3	J	46	TYR
3	J	79	LYS
3	J	83	VAL
3	J	84	ILE
3	J	92	VAL
3	J	94	GLN
3	J	95	THR
3	J	97	VAL
3	J	106	GLU
3	J	159	ILE
3	J	169	LEU
3	J	175	GLU
3	J	217	LEU
3	J	244	VAL
3	J	252	LEU
3	J	255	LEU
3	J	306	LEU
3	J	312	ARG
3	J	324	LEU
3	J	363	LEU
3	J	374	LEU
3	J	394	ILE
3	J	401	VAL
3	J	416	ILE
3	J	425	ARG
3	J	429	LEU
3	J	454	CYS
3	J	490	ILE

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Mol	Chain	Res	Type
3	J	501	VAL
3	J	506	VAL
3	J	507	VAL
3	J	510	LEU
3	J	513	MET
3	J	514	THR
3	J	536	LEU
3	J	545	HIS
3	J	547	ARG
3	J	567	THR
3	J	568	SER
3	J	573	THR
3	J	594	GLN
3	J	641	ILE
3	J	646	ILE
3	J	660	GLU
3	J	661	VAL
3	J	678	ARG
3	J	680	ASN
3	J	683	ILE
3	J	685	ILE
3	J	697	MET
3	J	698	MET
3	J	701	LEU
3	J	702	GLN
3	J	707	ILE
3	J	708	ASN
3	J	710	ASP
3	J	712	GLN
3	J	717	VAL
3	J	720	ASN
3	J	740	LEU
3	J	746	LEU
3	J	754	ILE
3	J	769	VAL
3	J	770	LEU
3	J	788	LEU
3	J	798	ARG
3	J	803	VAL
3	J	810	THR
3	J	826	ILE
3	J	844	THR

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Mol	Chain	Res	Type
3	J	847	ASP
3	J	848	VAL
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	858	VAL
3	J	860	ARG
3	J	881	LYS
3	J	897	HIS
3	J	908	ILE
3	J	918	ILE
3	J	931	THR
3	J	1155	ILE
3	J	1163	VAL
3	J	1170	LYS
3	J	1177	ILE
3	J	1186	TYR
3	J	1194	ARG
3	J	1202	GLU
3	J	1221	LEU
3	J	1255	VAL
3	J	1268	ASN
3	J	1273	ASP
3	J	1274	PHE
3	J	1275	LEU
3	J	1278	GLU
3	J	1281	GLU
3	J	1284	ARG
3	J	1285	VAL
3	J	1289	ASN
3	J	1293	GLU
3	J	1298	VAL
3	J	1310	THR
3	J	1333	THR
3	J	1343	GLU
4	K	13	ILE
4	K	21	LEU
4	K	39	VAL
4	K	46	THR
4	K	58	LEU
5	L	98	VAL
5	L	100	MET

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Mol	Chain	Res	Type
5	L	102	MET
5	L	127	ILE
5	L	130	VAL
5	L	154	GLU
5	L	247	GLU
5	L	267	ASP
5	L	297	MET
5	L	301	ASN
5	L	305	LEU
5	L	306	PHE
5	L	310	GLU
5	L	341	LEU
5	L	395	THR
5	L	400	GLN
5	L	429	THR
5	L	437	GLN
5	L	449	THR
5	L	450	ILE
5	L	471	LEU
5	L	472	GLN
5	L	479	THR
5	L	482	GLU
5	L	485	GLU
5	L	486	ARG
5	L	488	LEU
5	L	489	MET
5	L	491	GLU
5	L	494	ILE
5	L	508	GLU
5	L	530	LEU
5	L	547	VAL
5	L	558	VAL
5	L	561	MET
5	L	566	ASP
5	L	568	ASN
5	L	572	THR
5	L	580	PHE
5	L	587	ILE
5	L	603	ARG
5	L	606	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	117	HIS
1	A	132	HIS
1	B	66	HIS
1	B	132	HIS
2	C	69	GLN
2	C	120	GLN
2	C	139	ASN
2	C	148	GLN
2	C	150	HIS
2	C	165	HIS
2	C	276	GLN
2	C	327	GLN
2	C	494	ASN
2	C	513	GLN
2	C	518	ASN
2	C	620	ASN
2	C	628	HIS
2	C	659	GLN
2	C	677	ASN
2	C	684	ASN
2	C	725	GLN
2	C	1017	GLN
2	C	1080	ASN
2	C	1116	HIS
2	C	1136	GLN
2	C	1146	GLN
2	C	1237	HIS
2	C	1299	ASN
2	C	1312	ASN
2	C	1313	HIS
3	D	94	GLN
3	D	157	GLN
3	D	200	GLN
3	D	419	HIS
3	D	435	GLN
3	D	450	HIS
3	D	489	ASN
3	D	560	ASN
3	D	593	ASN
3	D	669	GLN
3	D	702	GLN
3	D	716	GLN

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Mol	Chain	Res	Type
3	D	736	GLN
3	D	777	HIS
3	D	929	GLN
3	D	1197	ASN
3	D	1244	GLN
3	D	1295	ASN
3	D	1367	GLN
4	E	61	ASN
4	E	62	GLN
5	F	131	GLN
5	F	331	HIS
5	F	346	GLN
5	F	362	ASN
5	F	406	GLN
5	F	409	ASN
5	F	446	GLN
5	F	455	HIS
5	F	461	ASN
5	F	464	ASN
5	F	472	GLN
5	F	518	HIS
5	F	545	HIS
5	F	579	GLN
1	H	66	HIS
1	H	132	HIS
2	I	20	GLN
2	I	69	GLN
2	I	139	ASN
2	I	165	HIS
2	I	343	HIS
2	I	494	ASN
2	I	513	GLN
2	I	658	GLN
2	I	761	GLN
2	I	766	ASN
2	I	799	ASN
2	I	824	GLN
2	I	1017	GLN
2	I	1038	GLN
2	I	1061	GLN
2	I	1080	ASN
2	I	1116	HIS

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Mol	Chain	Res	Type
2	I	1134	GLN
2	I	1136	GLN
2	I	1146	GLN
2	I	1288	GLN
2	I	1299	ASN
2	I	1312	ASN
2	I	1313	HIS
3	J	94	GLN
3	J	158	GLN
3	J	200	GLN
3	J	364	HIS
3	J	450	HIS
3	J	594	GLN
3	J	665	GLN
3	J	669	GLN
3	J	702	GLN
3	J	716	GLN
3	J	777	HIS
3	J	792	ASN
3	J	861	ASN
3	J	897	HIS
3	J	907	HIS
3	J	1235	ASN
3	J	1259	GLN
3	J	1279	GLN
3	J	1366	HIS
3	J	1367	GLN
4	K	61	ASN
5	L	128	ASN
5	L	131	GLN
5	L	147	GLN
5	L	227	GLN
5	L	317	ASN
5	L	345	GLN
5	L	362	ASN
5	L	446	GLN
5	L	455	HIS
5	L	464	ASN
5	L	472	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 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$
6	KNG	C	2001	-	75,75,75	3.81	30 (40%)	107,114,114	2.95	42 (39%)

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
6	KNG	C	2001	-	-	36/76/113/113	0/5/6/6

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	2001	KNG	O18-C46	-14.51	1.20	1.44
6	C	2001	KNG	O03-C06	10.20	1.56	1.37
6	C	2001	KNG	O17-C47	-10.11	1.21	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	2001	KNG	C04-C10	9.74	1.59	1.43
6	C	2001	KNG	O16-C37	7.88	1.62	1.42
6	C	2001	KNG	C12-C11	-5.83	1.31	1.54
6	C	2001	KNG	O11-C04	-5.77	1.19	1.36
6	C	2001	KNG	C02-C01	5.63	1.55	1.40
6	C	2001	KNG	C01-C09	5.53	1.59	1.43
6	C	2001	KNG	O17-C50	5.46	1.50	1.41
6	C	2001	KNG	C19-C18	-5.36	1.35	1.53
6	C	2001	KNG	O18-C50	5.27	1.50	1.41
6	C	2001	KNG	C03-C02	5.26	1.47	1.39
6	C	2001	KNG	O12-C39	5.18	1.44	1.34
6	C	2001	KNG	O06-C37	-5.06	1.27	1.41
6	C	2001	KNG	C03-C04	5.03	1.49	1.37
6	C	2001	KNG	O07-C25	-4.92	1.37	1.44
6	C	2001	KNG	O01-C01	-4.78	1.20	1.35
6	C	2001	KNG	C47-C48	4.30	1.60	1.52
6	C	2001	KNG	C47-C46	3.55	1.62	1.52
6	C	2001	KNG	C15-N01	3.39	1.42	1.35
6	C	2001	KNG	C02-N01	3.19	1.48	1.41
6	C	2001	KNG	C32-C22	-2.81	1.47	1.53
6	C	2001	KNG	O10-C15	-2.78	1.18	1.23
6	C	2001	KNG	C27-C28	2.72	1.59	1.50
6	C	2001	KNG	O04-C11	-2.43	1.18	1.21
6	C	2001	KNG	O05-C29	2.35	1.45	1.39
6	C	2001	KNG	C49-C48	-2.27	1.46	1.51
6	C	2001	KNG	O16-C48	2.25	1.49	1.44
6	C	2001	KNG	O06-C27	-2.02	1.39	1.44

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	2001	KNG	C34-C26-C27	-8.81	93.15	110.95
6	C	2001	KNG	C49-C48-C47	8.72	126.36	113.39
6	C	2001	KNG	C25-C26-C27	7.51	132.41	111.99
6	C	2001	KNG	C24-C23-C22	7.51	127.92	115.41
6	C	2001	KNG	O07-C35-C36	7.06	123.69	111.09
6	C	2001	KNG	O03-C06-C07	6.94	132.93	121.16
6	C	2001	KNG	C23-C22-C21	-6.81	98.90	112.55
6	C	2001	KNG	C12-C11-C05	6.26	119.42	107.30
6	C	2001	KNG	C25-O07-C35	-6.12	108.21	117.72
6	C	2001	KNG	O07-C25-C26	-5.76	94.25	107.52
6	C	2001	KNG	C45-C46-C47	-5.50	107.46	114.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	2001	KNG	O04-C11-C05	-4.82	122.75	131.63
6	C	2001	KNG	O12-C39-C40	4.66	122.15	112.03
6	C	2001	KNG	O10-C15-N01	-4.62	112.92	123.89
6	C	2001	KNG	C33-C24-C23	-4.40	102.78	111.43
6	C	2001	KNG	C34-C26-C25	-4.23	103.96	111.40
6	C	2001	KNG	C23-C24-C25	3.80	117.84	110.58
6	C	2001	KNG	C18-C19-C20	3.76	122.11	114.56
6	C	2001	KNG	C02-N01-C15	-3.64	116.70	126.84
6	C	2001	KNG	O07-C35-O08	-3.53	116.17	122.99
6	C	2001	KNG	O13-C39-C40	-3.32	112.56	123.55
6	C	2001	KNG	C19-C20-C21	3.29	118.28	112.43
6	C	2001	KNG	C37-C45-C46	-3.12	105.25	111.20
6	C	2001	KNG	C18-C17-C16	-3.08	121.72	128.94
6	C	2001	KNG	C01-C02-N01	3.00	125.80	117.46
6	C	2001	KNG	C13-C12-C11	-2.94	106.67	113.90
6	C	2001	KNG	C26-C25-C24	2.85	120.44	114.68
6	C	2001	KNG	C16-C15-N01	2.79	125.85	116.19
6	C	2001	KNG	C03-C02-N01	-2.76	114.71	121.95
6	C	2001	KNG	O19-C23-C24	-2.74	103.47	109.56
6	C	2001	KNG	O09-C21-C22	-2.65	103.67	109.56
6	C	2001	KNG	C38-C31-C20	2.56	117.98	113.39
6	C	2001	KNG	O03-C06-C05	-2.47	106.80	113.56
6	C	2001	KNG	O11-C04-C03	-2.41	114.16	121.38
6	C	2001	KNG	O18-C50-O17	-2.30	103.41	107.44
6	C	2001	KNG	C40-C43-C44	-2.27	109.91	114.95
6	C	2001	KNG	O16-C48-C47	-2.23	105.07	109.19
6	C	2001	KNG	C32-C22-C23	2.17	115.69	111.43
6	C	2001	KNG	O16-C48-C49	-2.16	101.95	106.74
6	C	2001	KNG	C05-C06-C07	-2.10	120.23	125.29
6	C	2001	KNG	C30-C16-C15	2.03	120.21	115.22
6	C	2001	KNG	C12-O03-C06	-2.01	104.33	107.69

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	2001	KNG	C21-C22-C23-O19
6	C	2001	KNG	O19-C23-C24-C25
6	C	2001	KNG	O19-C23-C24-C33
6	C	2001	KNG	C23-C24-C25-C26
6	C	2001	KNG	C23-C24-C25-O07
6	C	2001	KNG	C33-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
6	C	2001	KNG	C33-C24-C25-O07
6	C	2001	KNG	C26-C27-C28-C29
6	C	2001	KNG	O06-C27-C28-C29
6	C	2001	KNG	C38-C31-O12-C39
6	C	2001	KNG	C32-C22-C23-C24
6	C	2001	KNG	C32-C22-C23-O19
6	C	2001	KNG	C36-C35-O07-C25
6	C	2001	KNG	C22-C23-C24-C33
6	C	2001	KNG	C21-C22-C23-C24
6	C	2001	KNG	C22-C23-C24-C25
6	C	2001	KNG	O08-C35-O07-C25
6	C	2001	KNG	C31-C20-C21-O09
6	C	2001	KNG	O10-C15-C16-C30
6	C	2001	KNG	C40-C39-O12-C31
6	C	2001	KNG	N01-C15-C16-C17
6	C	2001	KNG	C20-C21-C22-C23
6	C	2001	KNG	C41-C40-C43-C44
6	C	2001	KNG	C20-C21-C22-C32
6	C	2001	KNG	O13-C39-O12-C31
6	C	2001	KNG	N01-C15-C16-C30
6	C	2001	KNG	C11-C12-O05-C29
6	C	2001	KNG	O03-C12-O05-C29
6	C	2001	KNG	C01-C02-N01-C15
6	C	2001	KNG	O09-C21-C22-C32
6	C	2001	KNG	O10-C15-C16-C17
6	C	2001	KNG	C42-C40-C43-C44
6	C	2001	KNG	C28-C29-O05-C12
6	C	2001	KNG	O12-C39-C40-C43
6	C	2001	KNG	C03-C02-N01-C15
6	C	2001	KNG	C39-C40-C43-C44

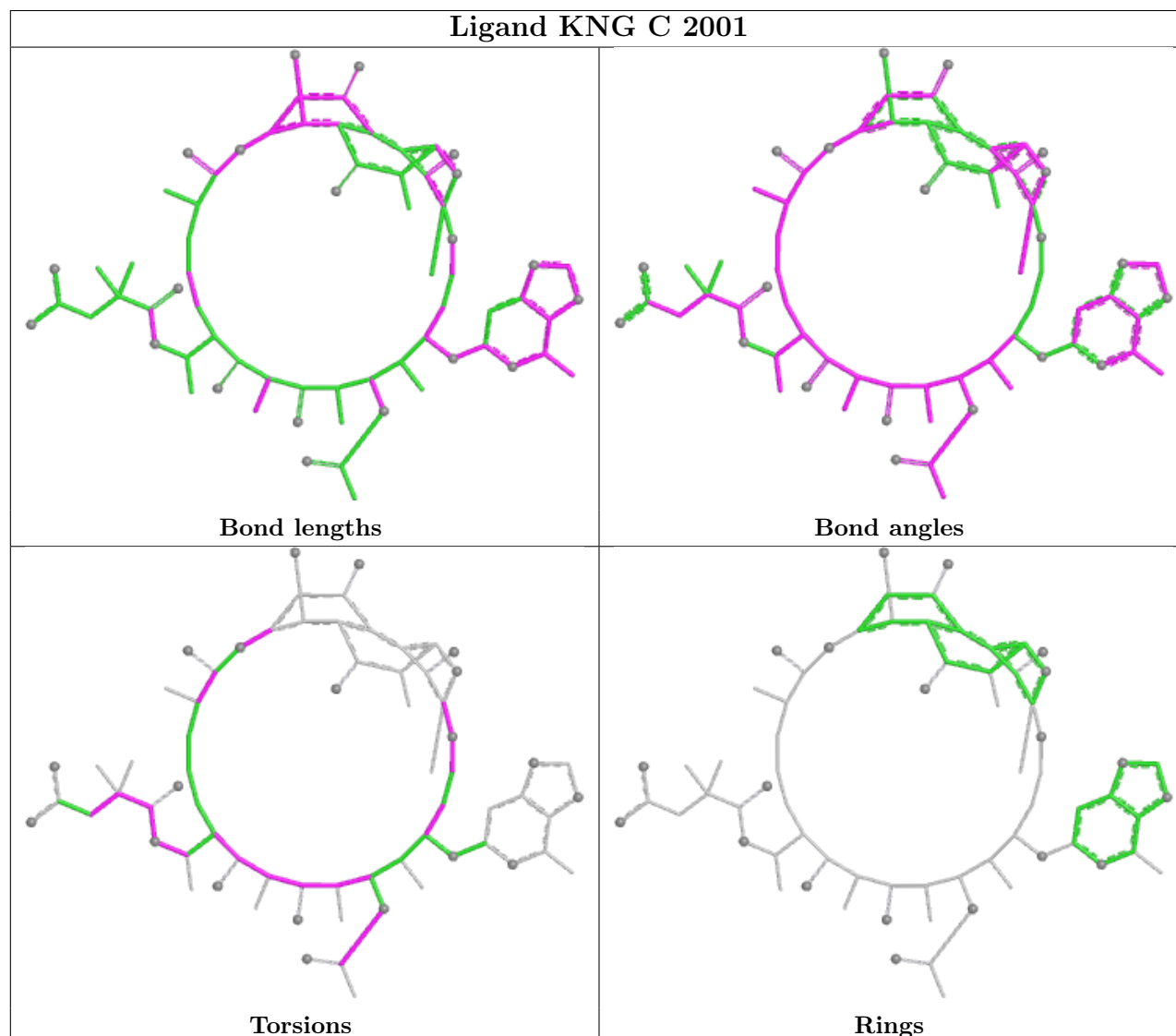
There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	2001	KNG	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	227/329 (68%)	-0.66	0 100 100	160, 212, 279, 349	0
1	B	214/329 (65%)	-0.61	0 100 100	155, 250, 349, 390	0
1	G	224/329 (68%)	-0.73	0 100 100	194, 274, 328, 348	0
1	H	215/329 (65%)	-0.56	3 (1%) 73 56	247, 309, 348, 370	0
2	C	1339/1342 (99%)	-0.66	0 100 100	124, 208, 314, 382	0
2	I	1328/1342 (98%)	-0.70	1 (0%) 92 87	186, 241, 336, 473	0
3	D	1166/1407 (82%)	-0.69	0 100 100	129, 188, 298, 360	0
3	J	1155/1407 (82%)	-0.71	0 100 100	164, 229, 312, 374	0
4	E	89/91 (97%)	-0.72	0 100 100	198, 267, 290, 306	0
4	K	79/91 (86%)	-0.78	0 100 100	329, 403, 484, 493	0
5	F	468/613 (76%)	-0.75	0 100 100	156, 283, 413, 445	0
5	L	469/613 (76%)	-0.75	0 100 100	193, 275, 393, 414	0
All	All	6973/8222 (84%)	-0.69	4 (0%) 92 87	124, 232, 349, 493	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	203	ILE	3.5
1	H	28	LEU	2.7
1	H	26	VAL	2.4
2	I	194	LEU	2.0

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

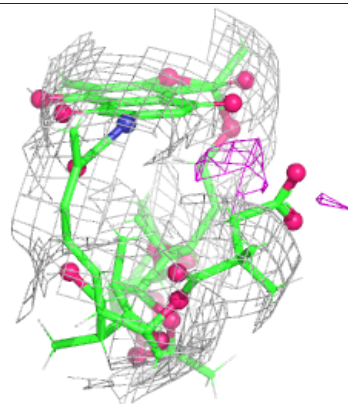
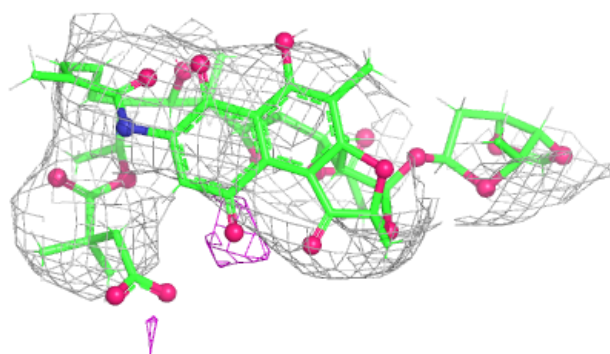
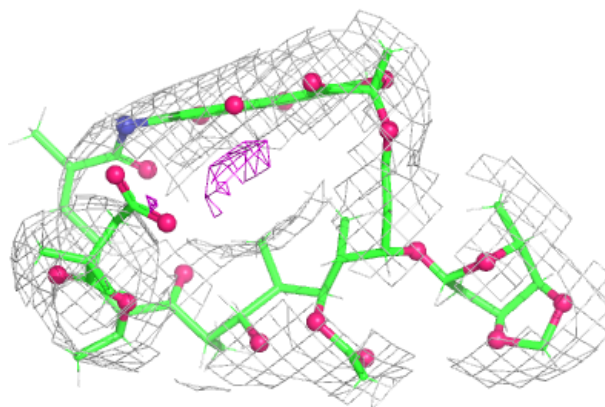
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MG	J	1501	1/1	0.87	0.10	154,154,154,154	0
6	KNG	C	2001	70/70	0.88	0.07	155,226,287,292	0
7	MG	D	1501	1/1	0.94	0.08	196,196,196,196	0
8	ZN	J	1502	1/1	0.99	0.02	215,215,215,215	0
8	ZN	D	1503	1/1	1.00	0.04	258,258,258,258	0
8	ZN	D	1502	1/1	1.00	0.03	192,192,192,192	0
8	ZN	J	1503	1/1	1.00	0.03	197,197,197,197	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around KNG C 2001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.