



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 06:15 AM EDT

PDB ID : 6CUX
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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

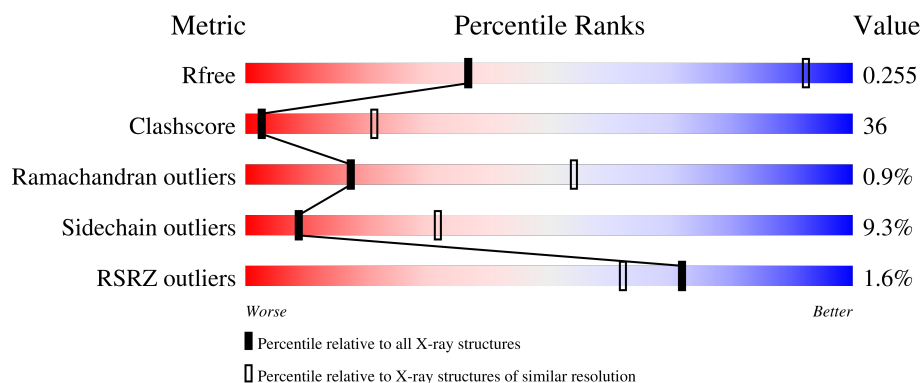
1 Overall quality at a glance

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}	130704	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)

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	<div> <div></div> <div>33%</div> <div>29%</div> <div>7%</div> <div>31%</div> </div>
1	B	329	<div> <div>23%</div> <div>39%</div> <div>•</div> <div>35%</div> </div>
1	G	329	<div> <div>29%</div> <div>34%</div> <div>6%</div> <div>32%</div> </div>
1	H	329	<div> <div>28%</div> <div>34%</div> <div>•</div> <div>35%</div> </div>
2	C	1342	<div> <div>44%</div> <div>49%</div> <div>6%</div> </div>

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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			

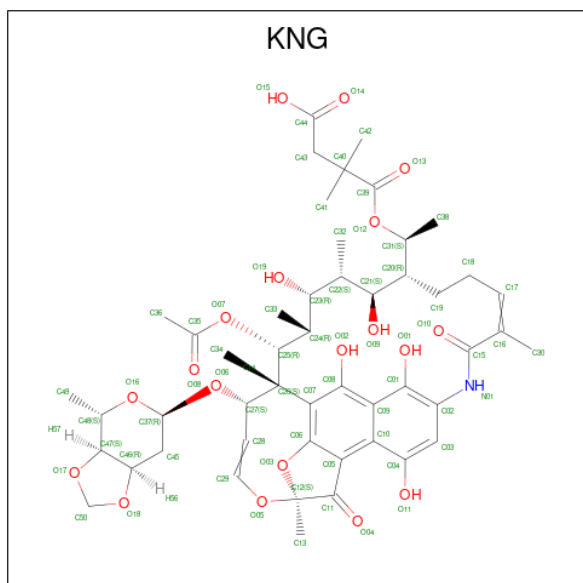
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

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 (three-letter code: 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 (three-letter code: 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		

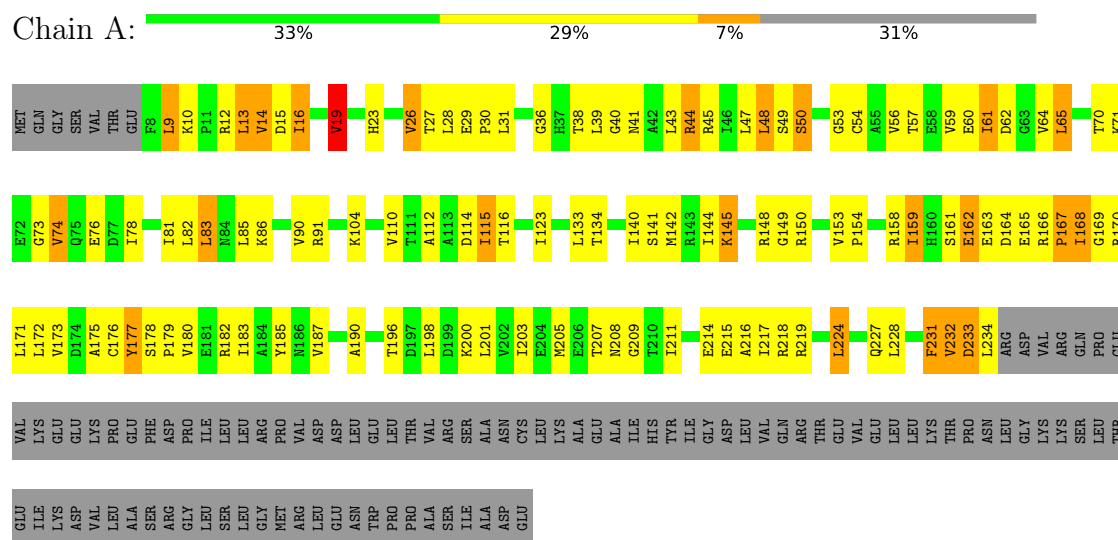
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

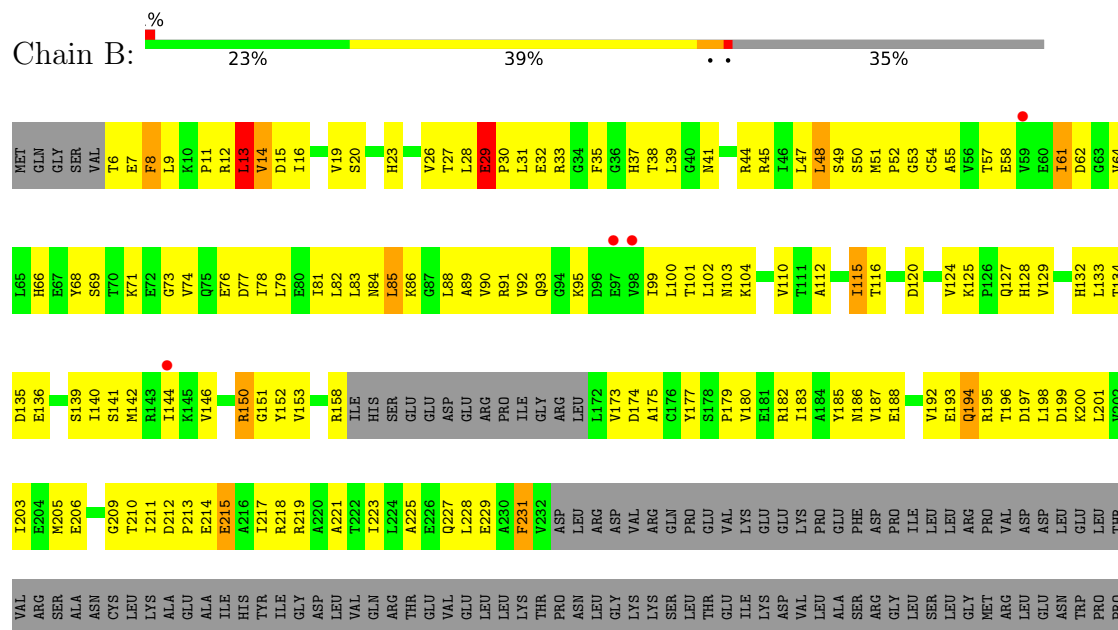
3 Residue-property plots

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.

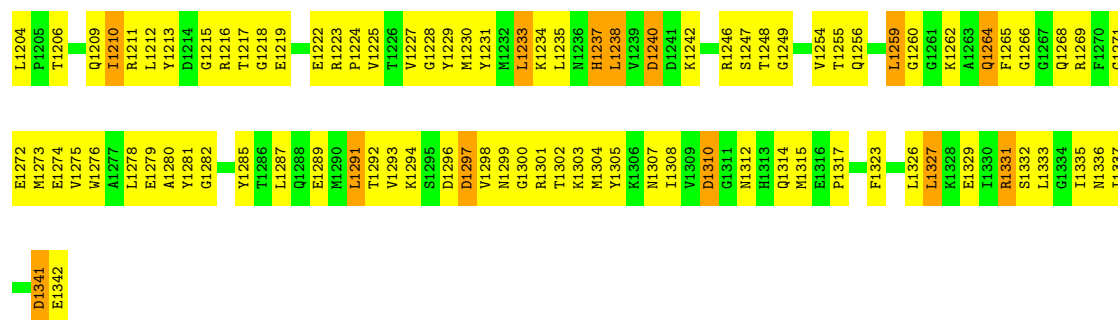
• Molecule 1: DNA-directed RNA polymerase subunit alpha



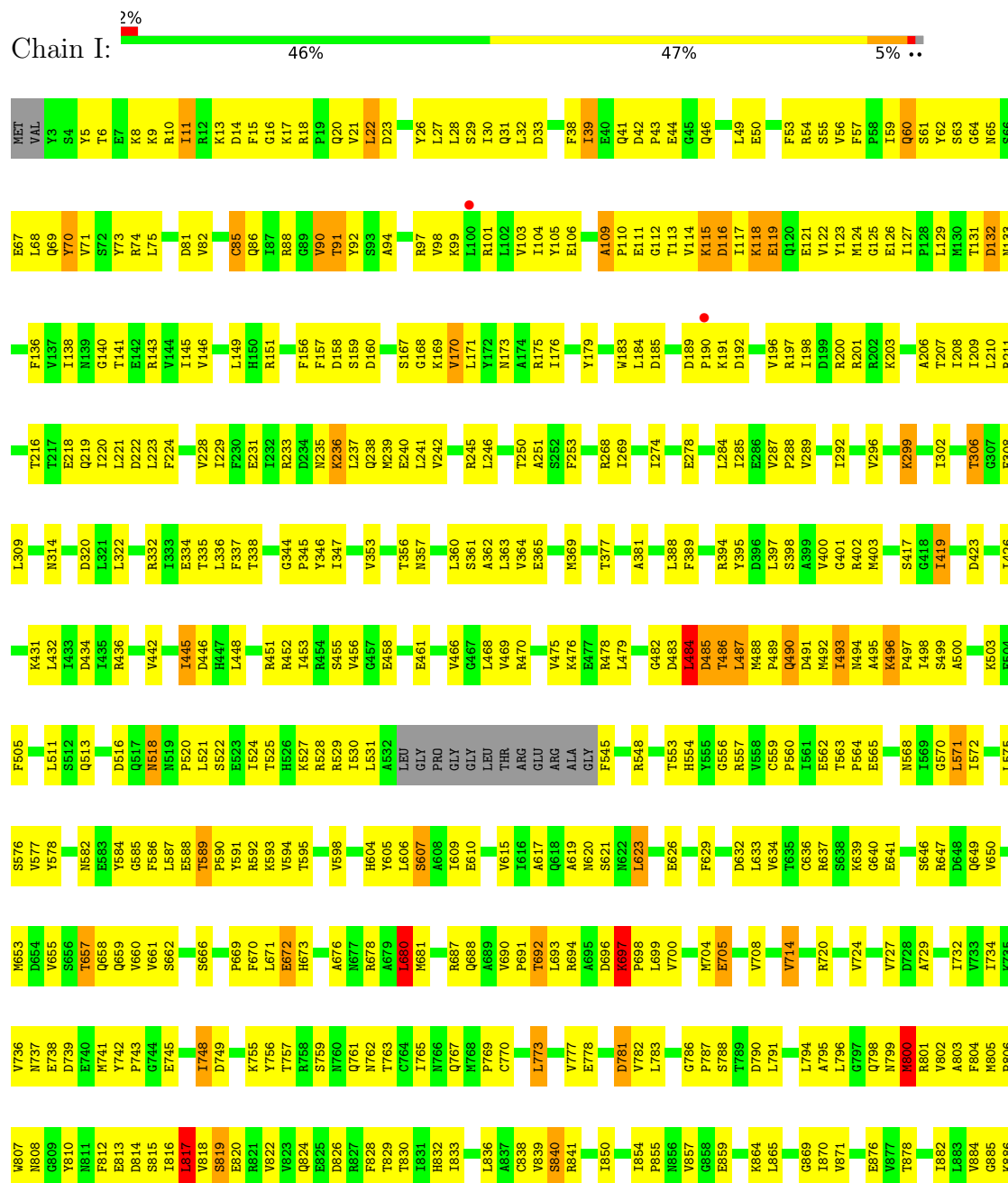
• Molecule 1: DNA-directed RNA polymerase subunit alpha

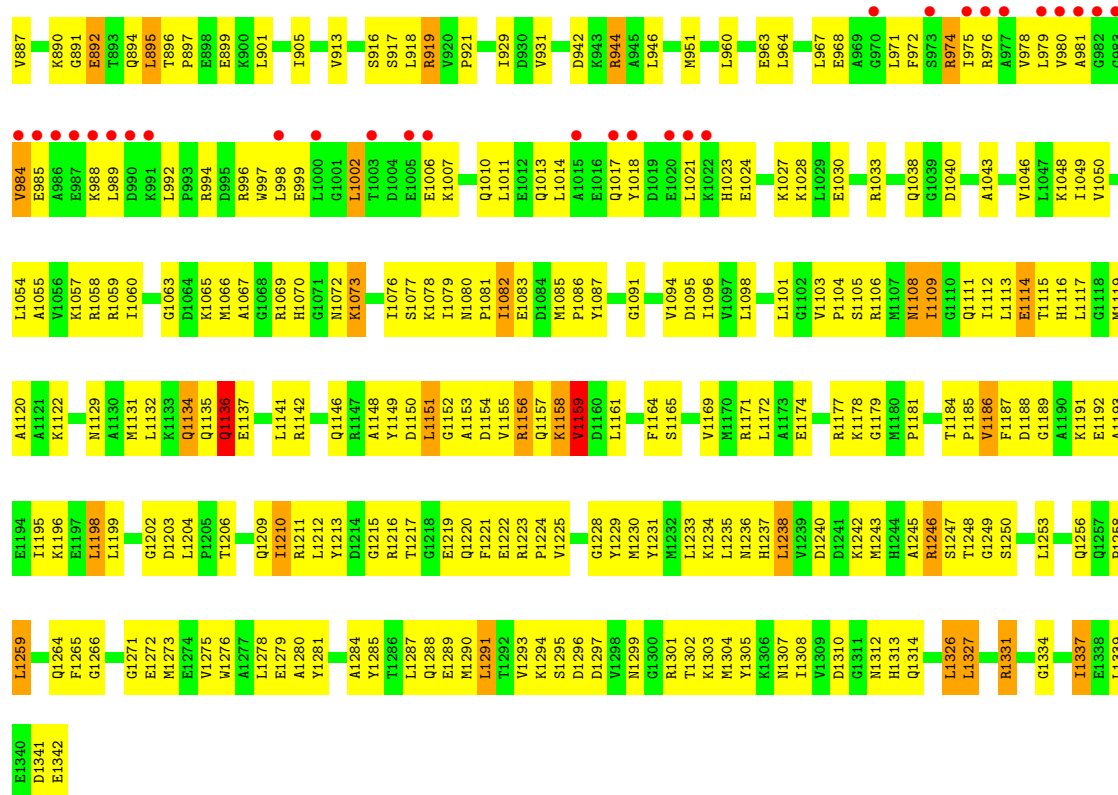




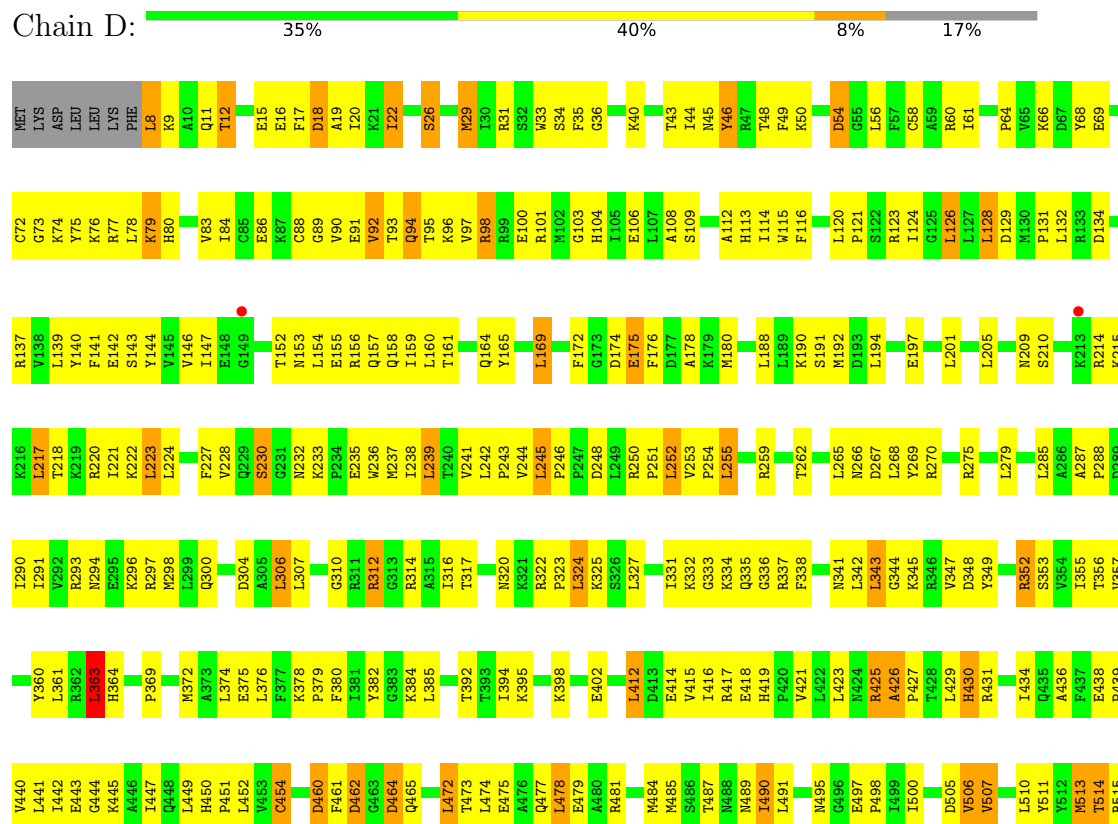


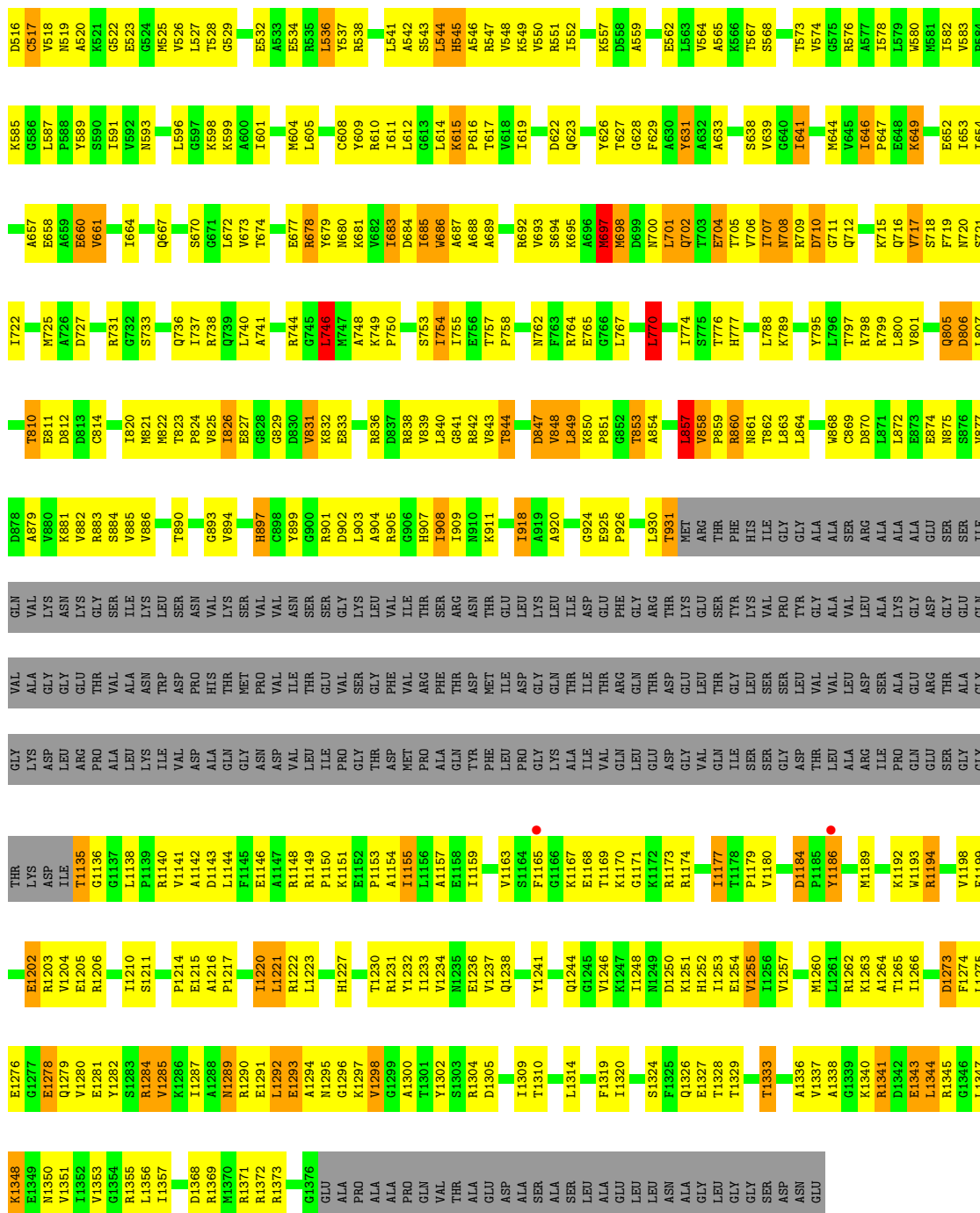
- Molecule 2: DNA-directed RNA polymerase subunit beta



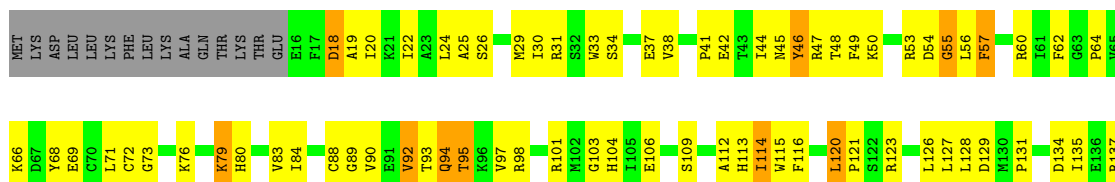


• Molecule 3: DNA-directed RNA polymerase subunit beta'

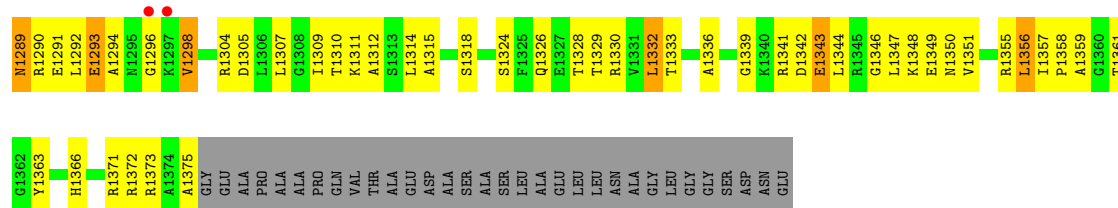




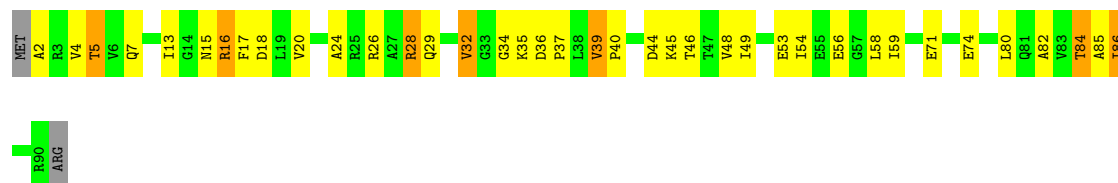
- Molecule 3: DNA-directed RNA polymerase subunit beta'



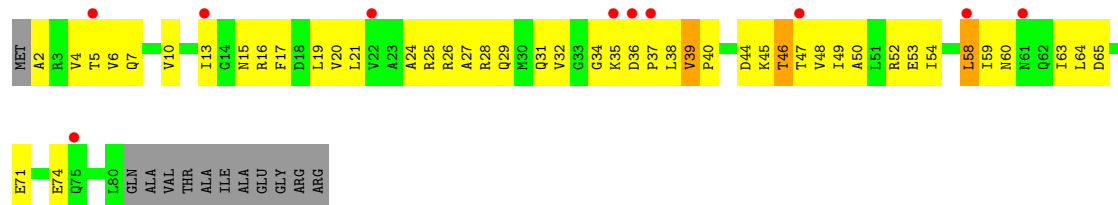
H1218	R1148	VAL	ILE	ASN	A904	D830	I755	A688	V609	V526	D460	P369	E297	T218	V138
D1219	R1149	LEU	THR	SER	R905	V831	E756		R610	L527	F461	P372	M296	K219	L139
I1220	P1150	ILE	GLU	SER	G906	R332	I757	D691	I611	T528	D462	A373	V303	R220	I140
L1221	K1151	PRO	VAL	GLY	H907	E933	P758	R692	L612		G463	L374	D304	I221	F141
R1222	E1152	GLY	SER	LYS	I908	V839		V693	G613	K531	D464	E375	A305	K222	E142
H1227	P1153	THR	GLY	LEU	I909	V839	N762	S694	L614	E532	D465		L306	L223	S143
A1228	A1154	ASP	PHE	VAL			E763	K695	K615	R535	M466	P379	L307	F227	Y144
I1155	I1155	MET	VAL	ILE	E913	V843	R764	A696	P620	L536	A467		R312		V145
L1156	A1157	PRO	ARG	THR	A914	T844	R765	M697	F620	G540	P471	Y382	R312	N232	V146
E1158	E1158	ALA	PHE	ARG	I915	A845	G766	M698		L541	L472	K384	T317	K233	I147
		GLN	THR	ARG	G916	E846	L767	D699	T627	A542	T473	R388		E234	E148
V1163	V1163	TYR	ASP	ASN	V917	D847	N768	N700	G623	S543	L474		M320	P235	L154
S1164	S1164	LEU	ILE	THR	I918	V848	V769	L701		A546	A475	R321	R321	E236	E155
F1165	F1165	LEU	ILE	GLU	A819	L849	L770	Q702	T627	A547	Q477	R322	R322	W237	R156
E1236	E1236	PRO	ASP	LEU	A920	K850	Y771	T703	G628	L544	A476	K395	K395	I238	Q157
V1237	K1167	GLY	GLY	LYS	S922		Y772	E704	F629	A546	Q477		R323	Q158	Q158
Q1238	E1168	THR	GLN	LEU	I923	T853	I774	V705		A547	L478		R324	I159	L160
D1239	V1169	ALA	THR	ILE	S924	A854	I774	T707	G633	V548	E479	H400	K325	L242	L242
V1240	T1170	ASP	ILE	ASP	G924			N708	R634	K549	A480		K325	P243	P243
Y1241	K1171	GLU	ILE	GLU	E925		H777	R709	S638	V550	R481	E405	D329	V244	V244
R1242	G1171	THR	ARG	PHE	P926		G778	R709	V639	R551	A482		M330	L245	L245
		GLN	THR	GLY			R779	D710		L552	L483	V408	I331	P246	P246
V1246	R1174	GLU	THR	ARG	L930	N861	R780	G711	I641		M484		K332	P247	P247
K1247	L1175	THR	ASP	THR	T931	T862		Q712		K557	M485	E414	G333	D248	D248
I1248	V1176	GLY	LYS	LYS	MET	L863	L783		R644		S486	V415	K334	L249	L249
I1177	I1177	VAL	GLU	GLU	ARG	L864		K715		T567	L487	I416	K334	R250	R250
		GLN	THR	THR	THR	L865	L788	Q716	V645	T567	L487	I416	K335	P251	P251
K1251	D1181	THR	GLY	TYR	PHE	H865		R717	P646	S568	N488	R417	G336	L252	L252
H1252	I1182	SER	LEU	LYS	THR	E866	N792	S718	P647	L569	N489	E418	R337	P253	P253
I1253	S1183	SER	SER	VAL	ILE	Q867		F719		K570	L490	H419	F338	P254	P254
V1255	D1184	GLY	SER	PRO	GLY	V868	T797	N720	K650	R571	L491	P420	R339	L255	L255
I1256	P1185	ASP	LEU	TYR	GLY	C869	R798	S721		T572	S492	V421	Q340	D256	D256
V1257	T1186	VAL	VAL	GLY	ALA	D870	R799	I722	L653	T573	P493	L422	R341	A178	A178
R1258	Y1186	LEU	VAL	ALA	SER	L871	L800	Y724	L654	V574	A494	N423	L342	K179	K179
E1187	E1187	ALA	LEU	VAL	ALA	L872	R801	M724		G575	A494	N423	L343	G258	G258
		ARG	ASP	LEU	ALA	E873	D802	M725	A657	R576	P498	R425	G344	T262	T262
P1191	K1191	SER	ASP	ALA	ALA	E874	V803	A726	E658	L579	L499	A426	K345	A184	A184
L1261	K1192	ILE	SER	ALA	ALA	N875	A804	A727			I500	P427	R346	I185	I185
R1262	V1193	PRO	ALA	LYS	ALA	S876	Q805	S728	E659		V501	T428	V347	L265	L265
K1263	R1194	GLN	GLU	ASP	GLU	S877	D806	S728	E660	T582	P502	L429	D348	N266	N266
A1264	Q1195	GLU	ARG	GLY	GLY	D878	L807	R731	V661	V583		H430	Y349	D267	D267
T1265	L1196	SER	THR	GLY	SER	R879	V808	G732	E663		D505	R431	S350	L268	L268
I1266	N1197	GLY	ALA	GLU	SER	A879	V808		E663	L587	V506		S350	Y269	Y269
	V1198	GLY	GLN	GLN	ILE	V880	V609		I664		V507		G351	R270	R270
A1269	F1199	THR	VAL	VAL	GLN	K881	T810	A735		P588	V507	E438	R352		
	E1200	LYS	ALA	ALA	VAL	V882	E911		S670	Y589		P439	R352	I273	I273
D1273	G1201	ASP	LYS	LYS	LYS	R883		Q738	G671		L510	V440	S353	N274	N274
F1274	E1202	ILE	LEU	ASN	ASN	S884	C914	R738		T591	V511	L441	I355	R275	R275
L1275	R1203	THR	ARG	GLY	LYS	V885	G815	L740	V673	V592	V512	I442	T356	Q196	Q196
E1276	V1204	GLY	PRO	GLY	GLY		T816	A741	T674	N593	M513	G443	V357	L279	L279
G1277	E1205	VAL	ALA	SER	SER	D889	G742			O594	T514	G444	G358		
A1278	R1206	LEU	ALA	ILE	ILE	T890	T620	N743	E677	A595	C517	K445	P359	L282	L282
Q1279	G1207	LYS	ASN	LYS	LYS		M821	R744	R678	L596	V518	A446	Y360	L282	L282
V1280	D1208	ILE	TRP	LEU	LEU	G893	M822	G745	V679	G597	N519	I447	L361	P288	P288
E1281	V1209	VAL	ASP	SER	SER	V894	T823	L746	N680	K598	N519		L362	D289	D289
I1210	V1210	ASP	PRO	ASN	ASN	K681	P824	M747	K681		A520	H450	R363	I290	I290
S1211	S1211	VAL	VAL	VAL	VAL	V825	V825	M748	V682	I601	K521	P451	H364	I291	I291
		GLN	THR	THR	LYS		T826	K749			G522	L452	Q385	V292	V292
R1284	S1283	ALA	GLN	THR	LYS		T826	K749			G522	L452	Q385	V292	V292
V1285	F1144	GLY	GLY	MET	SER	R901	E827	P750		M604	G523	V453	C386	R293	R293
K1286	E1215	VAL	ASN	PRO	VAL	D902	G828				E524	C454	G387	K216	K216
	A1216	VAL	VAL	VAL	VAL			I754		C608	M525		L368	K216	K216
	P1217	ASP	ASP	VAL	VAL		G829							L217	L217



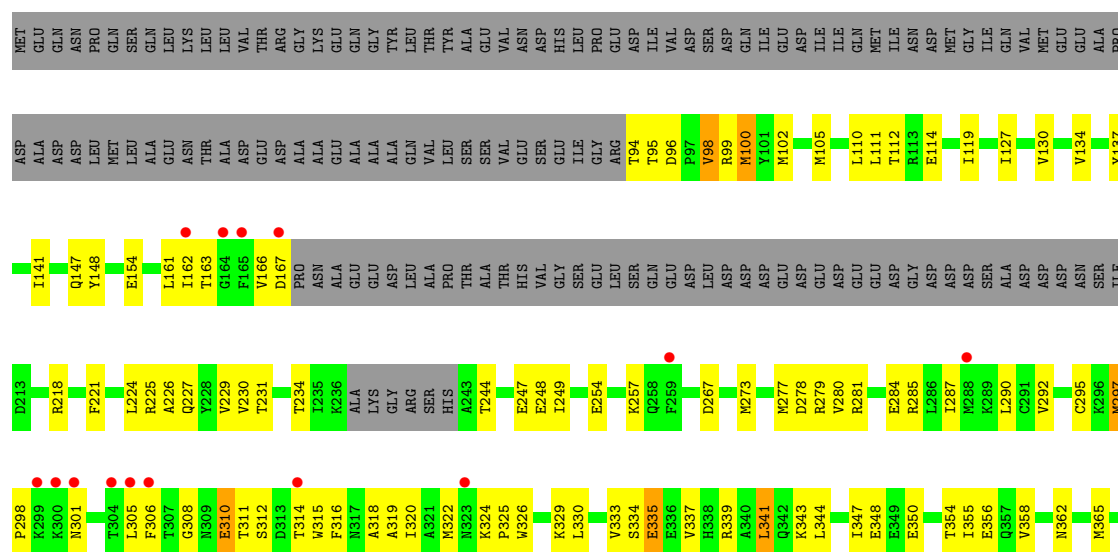
- Molecule 4: DNA-directed RNA polymerase subunit omega

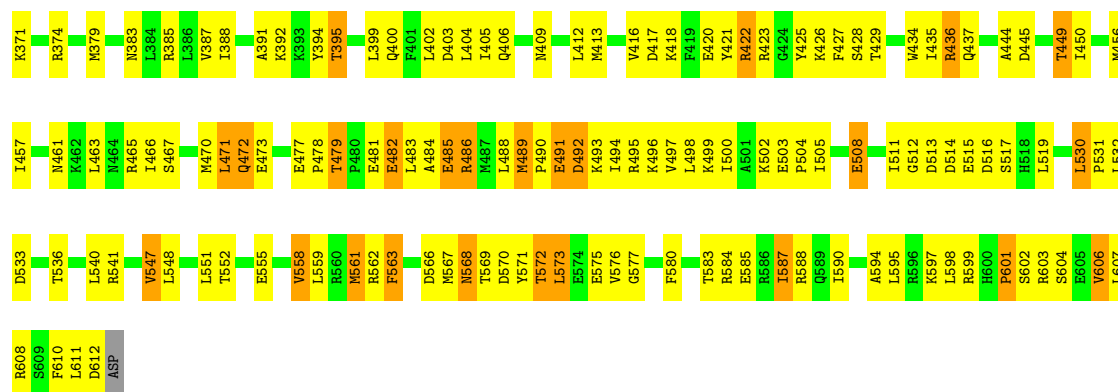


- Molecule 4: DNA-directed RNA polymerase subunit omega

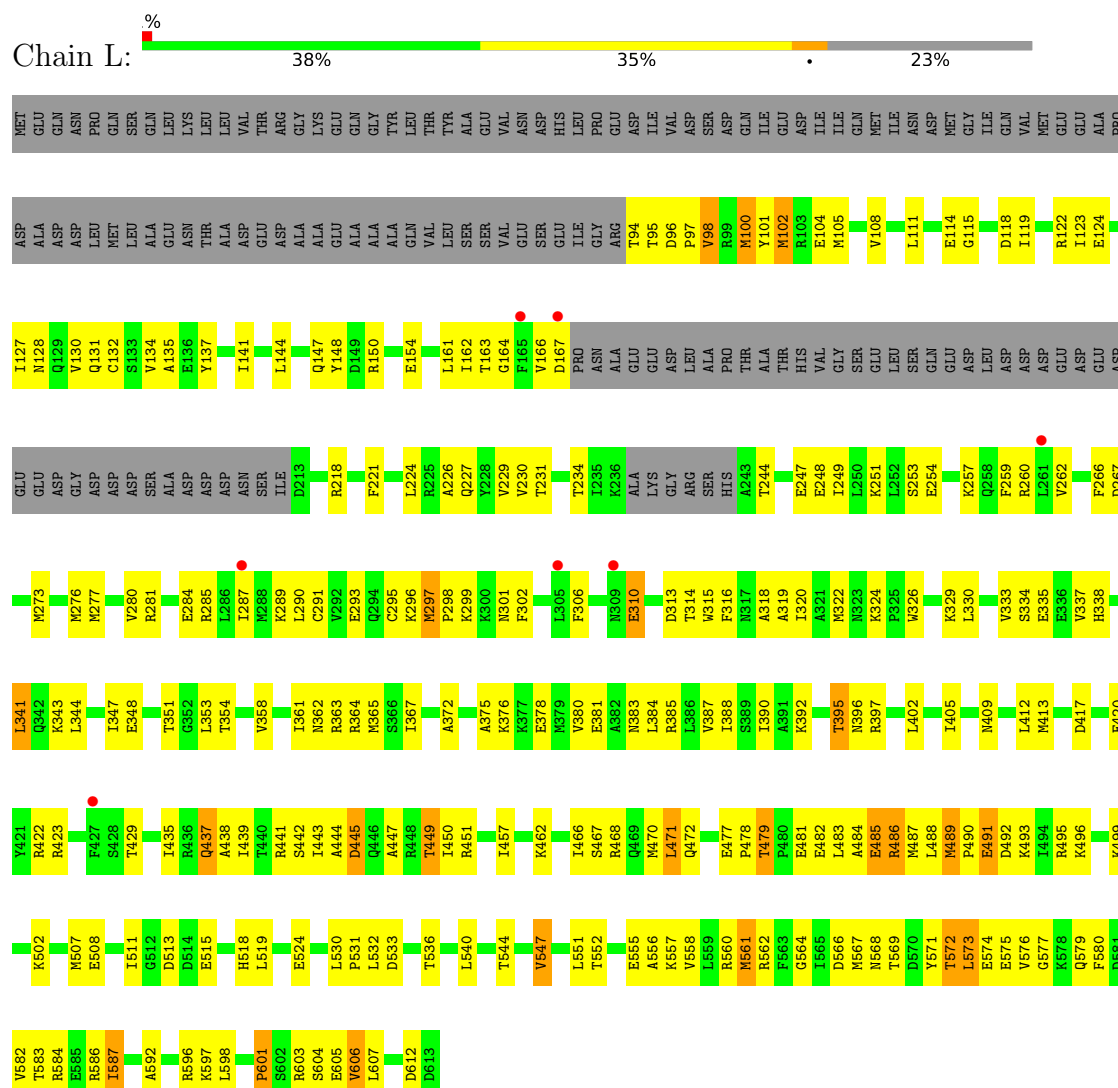


- Molecule 5: RNA polymerase sigma factor RpoD





- 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) 99.0 (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 0.210 , 0.255	Depositor DCC
R_{free} test set	2001 reflections (2.14%)	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)	0.27 , 182.8	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: KNG, MG, ZN

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	0.67	1/1774 (0.1%)	1.07	9/2405 (0.4%)
1	B	0.63	0/1668	1.07	7/2260 (0.3%)
1	G	0.50	0/1751	0.82	2/2373 (0.1%)
1	H	0.47	0/1678	0.79	0/2274
2	C	0.67	6/10716 (0.1%)	0.98	24/14458 (0.2%)
2	I	0.56	2/10653 (0.0%)	0.85	14/14373 (0.1%)
3	D	0.71	8/9229 (0.1%)	1.08	42/12459 (0.3%)
3	J	0.60	1/9140 (0.0%)	0.92	16/12341 (0.1%)
4	E	0.62	0/693	0.85	0/935
4	K	0.30	0/629	0.50	0/847
5	F	0.51	0/3864	0.79	2/5194 (0.0%)
5	L	0.48	0/3872	0.76	0/5205
All	All	0.61	18/55667 (0.0%)	0.93	116/75124 (0.2%)

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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	517	CYS	CB-SG	-9.59	1.66	1.82
2	C	1274	GLU	CG-CD	7.89	1.63	1.51
3	D	426	ALA	C-N	-6.92	1.21	1.34
3	D	727	ASP	CB-CG	5.86	1.64	1.51
2	C	838	CYS	CB-SG	-5.63	1.72	1.81
2	C	1329	GLU	CB-CG	-5.61	1.41	1.52
2	C	807	TRP	CB-CG	-5.60	1.40	1.50
3	D	511	TYR	CB-CG	-5.44	1.43	1.51
2	I	562	GLU	CB-CG	5.42	1.62	1.52
3	D	686	TRP	CB-CG	-5.36	1.40	1.50
2	C	1064	ASP	CB-CG	5.26	1.62	1.51
3	D	464	ASP	CB-CG	5.21	1.62	1.51
3	J	57	PHE	CB-CG	-5.17	1.42	1.51
1	A	19	VAL	CB-CG1	-5.13	1.42	1.52
3	D	511	TYR	CD1-CE1	-5.13	1.31	1.39
2	C	1329	GLU	CG-CD	-5.06	1.44	1.51
2	I	505	PHE	CB-CG	-5.05	1.42	1.51
3	D	144	TYR	CD2-CE2	-5.04	1.31	1.39

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1296	ASP	CB-CG-OD2	-10.40	108.94	118.30
2	C	1233	LEU	CA-CB-CG	9.43	137.00	115.30
2	C	1291	LEU	CA-CB-CG	9.27	136.63	115.30
2	C	1151	LEU	CA-CB-CG	-9.11	94.34	115.30
3	D	605	LEU	CB-CG-CD2	-8.72	96.18	111.00
3	D	727	ASP	CB-CG-OD1	8.36	125.83	118.30
3	J	472	LEU	CA-CB-CG	8.21	134.17	115.30
3	D	770	LEU	CB-CG-CD2	-8.00	97.41	111.00
3	D	807	LEU	CB-CG-CD2	-7.90	97.58	111.00
2	C	1259	LEU	CA-CB-CG	-7.74	97.50	115.30
5	F	563	PHE	C-N-CA	-7.72	106.09	122.30
1	B	85	LEU	CA-CB-CG	-7.55	97.93	115.30
3	J	42	GLU	CA-CB-CG	7.53	129.96	113.40
3	D	1344	LEU	CB-CG-CD2	7.52	123.78	111.00
1	A	177	TYR	CA-CB-CG	7.19	127.06	113.40
3	J	343	LEU	CA-CB-CG	7.13	131.69	115.30
3	D	297	ARG	NE-CZ-NH1	-7.11	116.75	120.30
2	I	1259	LEU	CA-CB-CG	-7.01	99.17	115.30
3	J	114	ILE	CG1-CB-CG2	-6.99	96.01	111.40
2	C	529	ARG	NE-CZ-NH1	-6.85	116.88	120.30
1	A	177	TYR	CB-CG-CD1	6.85	125.11	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	126	LEU	CB-CG-CD1	-6.79	99.46	111.00
2	C	1278	LEU	CB-CG-CD1	-6.76	99.51	111.00
3	D	128	LEU	CA-CB-CG	6.66	130.62	115.30
3	D	857	LEU	CA-CB-CG	6.57	130.41	115.30
2	I	1253	LEU	CA-CB-CG	6.56	130.40	115.30
1	B	150	ARG	NE-CZ-NH1	6.55	123.58	120.30
3	D	412	LEU	CB-CG-CD2	-6.55	99.87	111.00
3	D	307	LEU	CB-CG-CD2	-6.52	99.91	111.00
3	J	483	LEU	CB-CG-CD2	-6.52	99.92	111.00
3	J	1156	LEU	CA-CB-CG	6.47	130.19	115.30
3	D	478	LEU	CB-CG-CD2	-6.44	100.05	111.00
3	D	1344	LEU	CA-CB-CG	-6.42	100.54	115.30
3	D	361	LEU	CB-CG-CD1	-6.41	100.11	111.00
3	D	306	LEU	CA-CB-CG	6.39	130.00	115.30
5	F	436	ARG	NE-CZ-NH1	-6.27	117.17	120.30
2	I	1326	LEU	CB-CG-CD1	-6.23	100.41	111.00
3	D	631	TYR	CB-CG-CD2	-6.17	117.30	121.00
1	B	100	LEU	CA-CB-CG	6.10	129.34	115.30
3	D	746	LEU	CA-CB-CG	6.10	129.34	115.30
2	I	432	LEU	CB-CG-CD1	-6.09	100.65	111.00
3	J	727	ASP	CB-CG-OD1	6.08	123.77	118.30
3	D	245	LEU	CB-CG-CD1	-6.08	100.67	111.00
2	I	1291	LEU	CA-CB-CG	6.01	129.13	115.30
2	C	883	LEU	CA-CB-CG	-5.98	101.54	115.30
1	B	79	LEU	CA-CB-CG	5.96	129.00	115.30
2	C	17	LYS	CD-CE-NZ	5.94	125.36	111.70
1	A	48	LEU	CA-CB-CG	5.92	128.92	115.30
2	C	790	ASP	CB-CG-OD1	5.89	123.60	118.30
3	D	460	ASP	CB-CA-C	-5.82	98.76	110.40
3	J	120	LEU	CA-CB-CG	5.76	128.55	115.30
1	B	88	LEU	CB-CG-CD2	-5.73	101.26	111.00
1	G	88	LEU	CA-CB-CG	5.73	128.48	115.30
3	J	1332	LEU	CA-CB-CG	5.73	128.47	115.30
3	D	363	LEU	CA-CB-CG	-5.72	102.15	115.30
2	I	1054	LEU	CB-CG-CD2	-5.69	101.33	111.00
3	D	343	LEU	CB-CG-CD1	-5.66	101.37	111.00
3	D	239	LEU	CB-CG-CD2	-5.66	101.38	111.00
1	G	228	LEU	CA-CB-CG	-5.65	102.30	115.30
2	I	571	LEU	CB-CG-CD2	-5.62	101.45	111.00
3	J	268	LEU	CB-CG-CD1	-5.60	101.48	111.00
2	C	1297	ASP	CB-CG-OD1	-5.58	113.28	118.30
2	C	529	ARG	CG-CD-NE	-5.57	100.11	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1348	LYS	CA-CB-CG	5.56	125.63	113.40
3	D	1341	ARG	NE-CZ-NH2	-5.55	117.52	120.30
2	C	1326	LEU	CB-CG-CD2	5.55	120.43	111.00
1	A	224	LEU	CA-CB-CG	-5.51	102.63	115.30
3	D	223	LEU	CB-CG-CD2	5.50	120.35	111.00
2	C	1240	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	177	TYR	CB-CG-CD2	-5.48	117.71	121.00
3	D	447	ILE	CG1-CB-CG2	-5.48	99.35	111.40
1	A	16	ILE	CG1-CB-CG2	5.43	123.34	111.40
3	D	194	LEU	CB-CG-CD2	-5.40	101.83	111.00
1	B	48	LEU	CB-CG-CD2	-5.39	101.83	111.00
2	C	1066	MET	CG-SD-CE	5.38	108.81	100.20
3	J	536	LEU	CA-CB-CG	5.35	127.61	115.30
3	D	615	LYS	CD-CE-NZ	5.33	123.95	111.70
3	D	22	ILE	CG1-CB-CG2	-5.30	99.73	111.40
2	C	680	LEU	CB-CG-CD1	-5.30	102.00	111.00
2	I	680	LEU	CB-CG-CD1	-5.29	102.00	111.00
2	I	1337	ILE	CG1-CB-CG2	-5.28	99.79	111.40
3	J	863	LEU	CA-CB-CG	5.26	127.41	115.30
2	I	697	LYS	N-CA-C	-5.26	96.81	111.00
2	C	1274	GLU	OE1-CD-OE2	-5.25	117.00	123.30
3	J	368	LEU	CB-CG-CD2	-5.24	102.08	111.00
2	I	1296	ASP	CB-CG-OD2	-5.24	113.58	118.30
2	C	1132	LEU	CA-CB-CG	5.24	127.34	115.30
3	D	649	LYS	CD-CE-NZ	5.24	123.74	111.70
3	D	472	LEU	CA-CB-CG	5.21	127.27	115.30
2	C	1179	GLY	N-CA-C	-5.19	100.11	113.10
3	D	544	LEU	CB-CG-CD2	-5.18	102.19	111.00
2	C	1069	ARG	NE-CZ-NH1	-5.17	117.71	120.30
2	C	836	LEU	CB-CG-CD2	-5.17	102.22	111.00
3	D	126	LEU	CA-CB-CG	5.16	127.16	115.30
3	J	830	ASP	CB-CG-OD1	5.16	122.94	118.30
1	B	54	CYS	CA-CB-SG	5.15	123.27	114.00
3	D	449	LEU	CB-CG-CD2	-5.14	102.27	111.00
2	I	817	LEU	CA-CB-CG	5.13	127.09	115.30
1	A	44	ARG	NE-CZ-NH2	-5.12	117.74	120.30
3	D	255	LEU	CB-CG-CD2	-5.12	102.29	111.00
3	D	1168	GLU	CA-CB-CG	5.12	124.68	113.40
2	C	1273	MET	CG-SD-CE	-5.12	92.01	100.20
3	D	631	TYR	CB-CG-CD1	5.11	124.07	121.00
3	D	1220	ILE	CG1-CB-CG2	-5.11	100.16	111.40
2	I	800	MET	CB-CG-SD	-5.10	97.10	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	462	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	83	LEU	CB-CG-CD2	5.09	119.65	111.00
2	C	1326	LEU	CB-CG-CD1	-5.09	102.35	111.00
3	J	55	GLY	N-CA-C	-5.08	100.39	113.10
2	I	484	LEU	CA-CB-CG	5.08	126.98	115.30
3	D	1292	LEU	CA-CB-CG	5.07	126.97	115.30
3	D	697	MET	CB-CG-SD	5.05	127.56	112.40
3	D	464	ASP	CB-CG-OD2	5.04	122.83	118.30
3	J	1356	LEU	CB-CG-CD2	-5.01	102.48	111.00
2	C	1291	LEU	CB-CG-CD2	-5.00	102.49	111.00
1	A	65	LEU	CB-CG-CD1	-5.00	102.50	111.00

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	152	0
1	B	1649	0	1674	184	0
1	G	1730	0	1756	191	0
1	H	1659	0	1692	173	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	10548	0	10553	852	0
2	I	10486	0	10496	746	0
3	D	9089	0	9265	765	0
3	J	9001	0	9169	751	0
4	E	691	0	695	36	0
4	K	627	0	634	59	0
5	F	3813	0	3880	264	0
5	L	3821	0	3884	246	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	4003	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 36.

All (4003) 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
5:L:561:MET:HA	5:L:567:MET:HE1	1.27	1.17
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
2:C:1131:MET:HE2	2:C:1141:LEU:HD12	1.35	1.08
3:D:342:LEU:HA	3:D:343:LEU:CD1	1.84	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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
3:J:128:LEU:HD23	3:J:192:MET:HE3	1.34	1.04
3:D:848:VAL:HG23	3:D:858:VAL:HG13	1.39	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
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
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: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: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
2:C:109:ALA:HB1	2:C:110:PRO:C	1.82	1.00
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:L:470:MET:HE2	5:L:478:PRO:HB3	1.42	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: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
1:H:91:ARG:NH1	1:H:210:THR:O	1.97	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:I:109:ALA:HB1	2:I:110:PRO:C	1.85	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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:I:1131:MET:HE1	2:I:1141:LEU:HD12	1.53	0.90
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
5:L:105:MET:HE1	5:L:385:ARG:HG2	1.56	0.85
3:D:140:TYR:HE2	5:F:95:THR:HG22	1.41	0.85
2:I:887:VAL:HB	2:I:913:VAL:CG2	2.07	0.85
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:281:ARG:O	5:L:285:ARG:HG3	1.78	0.83
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:233:ASP:C	1:A:234:LEU:HD22	2.00	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
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
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
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
2:C:1131:MET:HE2	2:C:1141:LEU:HA	1.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
5:F:362:ASN:HB2	5:F:365:MET:HE2	1.65	0.79
2:I:985:GLU:HG2	2:I:988:LYS:HD2	1.63	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
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
1:B:205:MET:HE1	1:B:213:PRO:HA	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
5:L:470:MET:HE1	5:L:482:GLU:HG2	1.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:C:724:VAL:HG23	2:C:775:GLU:O	1.86	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:1080:ASN:HB3	2:C:1085:MET:HE2	1.68	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
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: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
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
3:D:709:ARG:C	3:D:711:GLY:H	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:27:THR:C	1:A:28:LEU:HD12	2.07	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
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: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
5:L:470:MET:HE3	5:L:478:PRO:HB3	1.69	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.52	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
2:C:1131:MET:HE3	2:C:1141:LEU:HD12	1.70	0.73
3:D:1290:ARG:HD3	3:D:1294:ALA:CB	2.18	0.73
5:F:470:MET:HE2	5:F:478:PRO:HB3	1.68	0.73
1:G:51:MET:HE1	1:G:216:ALA:HA	1.71	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
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
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:378:LYS:NZ	3:D:382:TYR:OH	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
5:L:489:MET:HE3	5:L:493:LYS:HD2	1.70	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
3:D:418:GLU:H	4:E:45:LYS:HZ3	1.38	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:94:THR:OG1	5:L:95:THR:N	2.24	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:1304:MET:HE2	3:D:472:LEU:HD12	1.73	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:98:VAL:HG21	2:I:124:MET:HE3	1.75	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:1236:GLU:HA	3:J:1236:GLU:OE2	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
3:D:1290:ARG:CG	3:D:1298:VAL:HG12	2.23	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: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: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:D:681:LYS:O	3:D:685:ILE:HG23	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:J:825:VAL:C	3:J:826:ILE:HG13	2.14	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
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
1:G:90:VAL:HG22	1:G:91:ARG:H	1.60	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
2:C:1148:ALA:HB1	2:C:1180:MET:HE2	1.75	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: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
2:I:738:GLU:HG2	2:I:741:MET:HE2	1.77	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
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)
3:J:1269:ALA:HB2	3:J:1274:PHE:CD1	2.30	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:1078:LYS:HG2	2:I:1079:ILE:N	2.10	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
2:C:832:HIS:HD1	2:C:1058:ARG:HD2	1.61	0.65
5:F:391:ALA:HB3	5:F:405:ILE:HG22	1.78	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:HE2	2:C:1141:LEU:CD1	2.21	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
1:G:86:LYS:HZ3	1:G:174:ASP:HB2	1.59	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
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: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
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
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
5:L:105:MET:CE	5:L:385:ARG:HG2	2.26	0.64
1:B:112:ALA:O	1:B:115:ILE:HG13	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:41:ASN:CG	2:C:1218:GLY:HA3	2.17	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
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
1:B:182:ARG:C	1:B:183:ILE:HD12	2.17	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1136:GLN:O	2:I:1137:GLU:HB3	1.97	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
5:L:470:MET:HE1	5:L:482:GLU:CG	2.28	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:878:THR:OG1	2:C:879:GLY:N	2.26	0.63
5:F:134:VAL:HG13	5:F:273:MET:HE3	1.79	0.63
5:F:166:VAL:O	5:F:167:ASP:HB2	1.98	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:849:LEU:HB3	3:D:853:THR:HG23	1.79	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: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: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
2:I:146:VAL:HG13	2:I:529:ARG:HB3	1.79	0.63
2:I:557:ARG:HH21	2:I:607:SER:C	2.02	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:O	3:D:205:LEU:HD13	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:C:1080:ASN:HB3	2:C:1085:MET:CE	2.28	0.62
3:D:526:VAL:HG12	3:D:549:LYS:HB2	1.80	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:53:ARG:HH22	3:J:60:ARG:HD2	1.65	0.62
3:J:71:LEU:HD13	3:J:71:LEU:C	2.20	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
3:D:825:VAL:C	3:D:826:ILE:HG13	2.20	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:73:GLY:C	1:B:134:THR:HG22	2.20	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
2:C:553:THR:O	2:C:557:ARG:HD2	2.01	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
2:I:98:VAL:HG21	2:I:124:MET:CE	2.29	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
3:J:709:ARG:C	3:J:711:GLY:H	2.02	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
5:F:105:MET:CE	5:F:385:ARG:HG2	2.31	0.61
3:J:325:LYS:HE2	3:J:330:MET:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:697:MET:CE	3:D:737:ILE:HG22	2.30	0.61
5:F:519:LEU:HD23	5:F:519:LEU:C	2.20	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
5:L:362:ASN:HB2	5:L:365:MET:HE2	1.81	0.61
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.82	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
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
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
5:L:134:VAL:HG22	5:L:273:MET:HE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:9:LYS:HE2	3:D:11:GLN:C	2.22	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
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:1150:ASP:O	2:I:1155:VAL:HG21	2.02	0.60
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
5:L:561:MET:HA	5:L:567:MET:CE	2.16	0.60
1:B:49:SER:O	1:B:151:GLY:HA2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:L:277:MET:HE3	5:L:281:ARG:HH21	1.66	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
2:I:1080:ASN:HB3	2:I:1085:MET:HE2	1.82	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
1:H:83:LEU:HD21	3:J:526:VAL:HB	1.85	0.59
2:I:1080:ASN:HB3	2:I:1085:MET:CE	2.32	0.59
2:I:1287:LEU:HD22	3:J:1357:ILE:CD1	2.33	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:205:LEU:HD13	3:D:205:LEU:C	2.22	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
1:B:19:VAL:O	1:B:20:SER:HB3	2.01	0.59
2:C:397:LEU:HB3	2:C:401:GLY:HA3	1.84	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
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
2:C:1158:LYS:C	2:C:1159:VAL:HG22	2.23	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
5:F:279:ARG:HH12	5:F:350:GLU:CD	2.06	0.58
2:I:724:VAL:CG1	2:I:727:VAL:HG22	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:150:ARG:HD2	1:B:8:PHE:CZ	2.38	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
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
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:72:CYS:HG	8:J:1502:ZN:ZN	1.16	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
2:I:91:THR:HA	2:I:138:ILE:O	2.03	0.58
1:B:205:MET:HE3	1:B:213:PRO:HB3	1.85	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1203:ARG:HH12	3:J:1205:GLU:HG2	1.68	0.58
5:L:470:MET:CE	5:L:482:GLU:HG2	2.31	0.58
1:B:205:MET:CE	1:B:213:PRO:HA	2.34	0.58
2:C:594:VAL:HG11	2:C:650:VAL:HG23	1.86	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: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
5:F:105:MET:HE1	5:F:385:ARG:HG2	1.85	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:J:262:THR:C	5:L:507:MET:HB2	2.23	0.57
3:D:436:ALA:HB3	3:D:485:MET:HA	1.85	0.57
5:F:297:MET:CE	5:F:330:LEU:HD21	2.33	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
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
3:D:45:ASN:O	3:D:46:TYR:HD2	1.87	0.57
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
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: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
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
3:J:141:PHE:HA	3:J:180:MET:HE2	1.85	0.57
5:L:147:GLN:HB3	5:L:161:LEU:CD1	2.35	0.57
3:D:142:GLU:CG	5:F:100:MET:HE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:218:THR:HA	3:D:221:ILE:HG22	1.86	0.57
3:D:242:LEU:HD23	3:D:242:LEU:C	2.25	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
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
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
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: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:657:THR:OG1	2:C:1187:PHE:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:G:231:PHE:HB3	1:H:218:ARG:CG	2.34	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
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:73:GLY:C	1:H:134:THR:HG22	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:G:140:ILE:HD12	1:G:142:MET:HE3	1.87	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:709:ARG:C	3:D:711:GLY:N	2.58	0.56
1:G:112:ALA:O	1:G:115:ILE:HG13	2.05	0.56
1:H:127:GLN:O	1:H:127:GLN:HG2	2.05	0.56
2:I:17:LYS:HZ2	2:I:1154:ASP:HB3	1.70	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
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: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: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
5:L:479:THR:HG23	5:L:481:GLU:H	1.71	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
2:C:1131:MET:CE	2:C:1141:LEU:HA	2.33	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:897:PRO:HB3	5:L:564:GLY:C	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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:HD21	1.87	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
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:141:PHE:O	3:D:180:MET:HE1	2.07	0.55
3:D:585:LYS:HB2	3:D:612:LEU:HD21	1.87	0.55
4:E:15:ASN:O	4:E:16:ARG:HB3	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:I:887:VAL:HB	2:I:913:VAL:HG22	1.84	0.55
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:277:MET:CE	5:L:281:ARG:HH21	2.19	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
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:279:LEU:HD23	3:D:279:LEU:C	2.27	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:891:GLY:C	2:I:892:GLU:HG3	2.28	0.55
2:I:1116:HIS:CE1	3:J:641:ILE:HB	2.41	0.55
4:K:15:ASN:O	4:K:16:ARG:HB3	2.07	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: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
2:C:1080:ASN:CB	2:C:1085:MET:CE	2.84	0.54
2:C:1304:MET:CE	3:D:472:LEU:HD12	2.37	0.54
3:D:1273:ASP:HB2	3:D:1276:GLU:CD	2.27	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:884:VAL:O	2:I:917:SER:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:697:MET:HE2	3:D:737:ILE:HG22	1.89	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
3:J:591:ILE:HG23	3:J:604:MET:HE2	1.88	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:1089:GLU:OE2	2:C:1211:ARG:HD2	2.07	0.54
3:D:92:VAL:HG22	3:D:92:VAL:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:233:ARG:HH12	2:C:332:ARG:HH12	1.56	0.54
2:I:818:VAL:HG13	2:I:822:VAL:HG21	1.90	0.54
2:I:1158:LYS:C	2:I:1159:VAL:HG22	2.28	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: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
5:F:503:GLU:CD	5:F:504:PRO:HD2	2.27	0.54
2:I:219:GLN:HA	2:I:222:ASP:HB3	1.89	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
2:I:864:LYS:NZ	2:I:876:GLU:O	2.40	0.54
3:J:210:SER:HB2	3:J:213:LYS:CG	2.38	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:H:187:VAL:HG23	1:H:187:VAL:O	2.07	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
3:D:1314:LEU:HD12	3:D:1326:GLN:CD	2.28	0.53
1:G:11:PRO:HD3	1:H:227:GLN:CD	2.27	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
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
3:J:1291:GLU:C	3:J:1292:LEU:HD12	2.29	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
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:729:ALA:O	2:I:755:LYS:NZ	2.19	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:1134:GLN:C	2:C:1135:GLN:HG2	2.28	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
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:557:ARG:HH21	2:C:607:SER:C	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:387:VAL:HG22	5:L:435:ILE:HD13	1.90	0.53
3:D:141:PHE:HA	3:D:180:MET:HE2	1.90	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: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:1196:LYS:HA	2:I:1199:LEU:HD12	1.91	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:132:ASP:OD1	2:I:132:ASP:N	2.28	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
5:L:108:VAL:HG11	5:L:381:GLU:C	2.29	0.53
1:B:197:ASP:C	1:B:198:LEU:HD22	2.29	0.52
2:C:1080:ASN:CB	2:C:1085:MET:HE3	2.38	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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
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
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
1:B:205:MET:HE1	1:B:213:PRO:CA	2.35	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
2:C:817:LEU:HD11	2:C:1080:ASN:ND2	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:166:ARG:O	1:A:167:PRO:C	2.48	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: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
5:F:311:THR:HG21	5:F:348:GLU:CD	2.30	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:62:TYR:C	2:I:64:GLY:H	2.12	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
1:B:55:ALA:O	1:B:146:VAL:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:513:MET:HE1	3:J:579:LEU:HD13	1.91	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
5:F:513:ASP:C	5:F:515:GLU:H	2.13	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
2:C:864:LYS:HZ1	2:C:877:VAL:HA	1.75	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
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
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:823:THR:HB	3:D:824:PRO:HD2	1.92	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:F:470:MET:HE3	5:F:478:PRO:HB3	1.92	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: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
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
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:863:LEU:C	3:J:864:LEU:HD23	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:310:GLU:O	5:F:344:LEU:HD21	2.11	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:557:ARG:NH2	2:C:608:ALA:HA	2.26	0.51
2:C:634:VAL:HG13	2:C:636:CYS:HG	1.75	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: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
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: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
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:1293:GLU:O	3:J:1294:ALA:C	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:165:GLU:C	1:G:167:PRO:HD2	2.31	0.51
2:I:119:GLU:CB	2:I:489:PRO:HB2	2.40	0.51
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.92	0.51
1:A:73:GLY:C	1:A:134:THR:HG22	2.31	0.51
2:C:26:TYR:OH	2:C:28:LEU:HD12	2.10	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:128:LEU:HD23	3:D:192:MET:HE3	1.91	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
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
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
2:I:1134:GLN:C	2:I:1135:GLN:HG2	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1221:LEU:HD22	3:J:1221:LEU:C	2.31	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
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
3:J:205:LEU:C	3:J:205:LEU:HD13	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:193:ASP:CG	3:J:196:GLN:HG2	2.31	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: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:D:812:ASP:HB2	3:D:911:LYS:HZ2	1.77	0.50
5:F:297:MET:CE	5:F:330:LEU:HD11	2.42	0.50
3:J:418:GLU:CG	4:K:44:ASP:HA	2.32	0.50
3:J:431:ARG:HH21	3:J:489:ASN:CG	2.14	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
1:A:224:LEU:HD23	1:A:224:LEU:C	2.32	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: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
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
3:J:1171:GLY:HA2	3:J:1193:TRP:HZ3	1.75	0.50
5:L:441:ARG:HH12	5:L:445:ASP:CG	2.15	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:132:LEU:HD13	3:D:132:LEU:C	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1278:GLU:OE1	3:D:1278:GLU:HA	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: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
2:C:1080:ASN:HB2	2:C:1085:MET:HE3	1.94	0.49
3:D:827:GLU:O	3:D:829:GLY:N	2.34	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:757:THR:C	2:I:833:ILE:HD12	2.32	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
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
3:J:418:GLU:HG3	4:K:45:LYS:H	1.77	0.49
4:K:26:ARG:NE	4:K:53:GLU:OE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1066:MET:HE1	2:C:1076:ILE:HB	1.88	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
2:C:98:VAL:HB	2:C:124:MET:HE2	1.95	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: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:610:ARG:HG2	3:J:866:GLU:CD	2.33	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
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:192:ASP:CG	2:I:436:ARG:HH21	2.12	0.49
2:I:516:ASP:CG	2:I:522:SER:HG	2.16	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
2:I:1293:VAL:HG11	2:I:1304:MET:CE	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:F:96:ASP:CG	5:F:96:ASP:O	2.52	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:91:THR:HG21	2:C:503:LYS:HZ1	1.77	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
5:F:512:GLY:C	5:F:514:ASP:H	2.16	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
1:A:165:GLU:C	1:A:167:PRO:HD2	2.33	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:560:ARG:O	5:L:567:MET:HE2	2.13	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
2:C:1131:MET:HE2	2:C:1141:LEU:CA	2.37	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: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: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:97:VAL:HG12	3:J:101:ARG:HG3	1.94	0.48
3:J:352:ARG:O	3:J:353:SER:HB3	2.14	0.48
3:J:839:VAL:O	3:J:839:VAL:HG12	2.12	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:62:TYR:C	2:C:64:GLY:H	2.16	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
5:F:277:MET:CE	5:F:281:ARG:HH21	2.26	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
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:B:205:MET:CG	1:B:206:GLU:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1080:ASN:CB	2:I:1085:MET:HE3	2.44	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
3:J:400:MET:HE2	3:J:405:GLU:OE1	2.14	0.48
5:L:513:ASP:C	5:L:515:GLU:H	2.16	0.48
1:A:57:THR:CG2	1:A:158:ARG:NH2	2.76	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: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:74:ARG:C	2:C:75:LEU:HD22	2.33	0.48
2:C:194:LEU:HA	2:C:194:LEU:HD12	1.62	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:1304:MET:HE2	3:D:472:LEU:CD1	2.44	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:673:HIS:HB3	2:I:1109:ILE:HG22	1.96	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
1:G:165:GLU:HG3	1:G:165:GLU:O	2.12	0.47
1:H:55:ALA:CB	1:H:176:CYS:H	2.27	0.47
2:I:179:TYR:OH	2:I:458:GLU:OE2	2.20	0.47
2:I:756:TYR:H	2:I:756:TYR:HD1	1.62	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:1343:GLU:C	3:J:1344:LEU:HD12	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:654:ILE:O	3:D:658:GLU:HB2	2.14	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
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
3:J:693:VAL:HG21	3:J:743:MET:CE	2.45	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:490:ILE:O	3:D:490:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:705:GLU:HB2	2:I:794:LEU:H	1.80	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:608:CYS:HG	3:J:620:PHE:HD2	1.62	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
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:510:LEU:HA	3:J:513:MET:HE2	1.96	0.47
3:J:517:CYS:C	3:J:716:GLN:HE22	2.16	0.47
3:J:552:ILE:HG12	3:J:570:LYS:HG3	1.96	0.47
4:K:29:GLN:CD	4:K:35:LYS:HE2	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:9:LYS:HE2	3:D:11:GLN:O	2.15	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:1250:ASP:O	3:D:1251:LYS:C	2.51	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:302:ILE:HG22	2:C:308:GLU:C	2.35	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:C:316:GLU:H	2:C:316:GLU:CD	2.19	0.46
3:D:1290:ARG:HA	3:D:1294:ALA:CB	2.45	0.46
5:F:470:MET:HE1	5:F:482:GLU:HG2	1.97	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
2:I:1293:VAL:HG11	2:I:1304:MET:HE2	1.97	0.46
3:J:201:LEU:HD11	3:J:220:ARG:HH11	1.79	0.46
3:J:709:ARG:C	3:J:711:GLY:N	2.69	0.46
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:537:TYR:CZ	3:D:544:LEU:HD22	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:F:297:MET:HE3	5:F:330:LEU:HD11	1.96	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
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
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
3:J:843:VAL:HG23	3:J:862:THR:C	2.35	0.46
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:800:MET:HE1	2:C:822:VAL:HG21	1.96	0.46
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.48	0.46
3:D:142:GLU:HG3	5:F:100:MET:HE1	1.98	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
5:F:567:MET:HB2	5:F:567:MET:HE3	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:27:THR:C	1:G:28:LEU:HD12	2.36	0.46
1:G:166:ARG:O	1:G:167:PRO:C	2.54	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:455:SER:O	2:I:456:VAL:C	2.54	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:192:ASP:CG	2:C:436:ARG:HH21	2.19	0.46
3:D:16:GLU:HB3	3:D:1369:ARG:NH2	2.30	0.46
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
1:H:99:ILE:HG23	1:H:99:ILE:O	2.15	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:62:TYR:C	2:I:64:GLY:N	2.70	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: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:741:ALA:O	3:J:762:ASN:ND2	2.49	0.46
3:J:1261:LEU:HD12	3:J:1261:LEU:C	2.36	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:439:ILE:O	5:L:442:SER:HB3	2.16	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
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
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: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
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:91:THR:HG21	2:C:503:LYS:HZ2	1.80	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
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
2:I:974:ARG:HD3	2:I:1010:GLN:NE2	2.32	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
2:C:101:ARG:HH21	2:C:118:LYS:CE	2.25	0.45
2:C:750:ILE:HD13	2:C:963:GLU:CD	2.37	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:322:MET:HE3	5:F:324:LYS:NZ	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1075:VAL:O	2:C:1076:ILE:C	2.54	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
5:F:399:LEU:CB	5:F:404:LEU:HD21	2.39	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
2:I:1313:HIS:HD2	3:J:477:GLN:NE2	2.14	0.45
3:J:644:MET:HE3	3:J:764:ARG:HG2	1.98	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:322:MET:HE3	5:F:324:LYS:HZ1	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:996:ARG:HD2	2:I:999:GLU:CD	2.37	0.45
2:I:1236:ASN:HB2	2:I:1238:LEU:HD11	1.99	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
1:A:154:PRO:O	1:A:158:ARG:HG3	2.17	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
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:1257:VAL:HG22	3:D:1260:MET:HE1	1.97	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:489:PRO:HA	2:C:492:MET:HE3	1.99	0.45
2:C:848:GLU:CD	2:C:888:THR:HG22	2.37	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
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
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:705:GLU:H	2:C:705:GLU:CD	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:262:TYR:CZ	2:C:282:VAL:HG21	2.51	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:591:ILE:HG13	3:D:604:MET:HE2	1.98	0.44
3:D:863:LEU:HD12	3:D:863:LEU:HA	1.58	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:658:GLU:C	3:J:661:VAL:HG13	2.37	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
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
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:562:GLU:OE2	2:C:662:SER:OG	2.28	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:277:MET:HE3	5:F:281:ARG:HH21	1.81	0.44
5:F:421:TYR:CE2	5:F:422:ARG:HG3	2.53	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:1077:SER:HA	3:J:356:THR:HG1	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:520:ALA:HB1	3:J:543:SER:HB3	1.99	0.44
5:L:519:LEU:C	5:L:519:LEU:HD23	2.37	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
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:654:ILE:HG12	3:J:743:MET:HE1	1.99	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
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:478:LEU:HD12	4:K:24:ALA:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:THR:CG2	1:B:45:ARG:HG2	2.48	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: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: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
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: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
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
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: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:452:ARG:HH21	2:C:458:GLU:CD	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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
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:71:LEU:HD22	3:J:71:LEU:C	2.36	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
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:9:LYS:HZ3	3:D:11:GLN:HA	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:36:GLY:C	1:A:187:VAL:HG11	2.38	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
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: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: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:1327:LEU:HD21	2:I:1339:LEU:HD11	2.00	0.43
3:J:1221:LEU:C	3:J:1221:LEU:HD13	2.38	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
1:B:210:THR:C	1:B:211:ILE:HG12	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:596:LEU:HD11	3:J:604:MET:HE3	2.00	0.43
5:L:244:THR:O	5:L:244:THR:HG22	2.18	0.43
5:L:575:GLU:O	5:L:579:GLN:HG2	2.18	0.43
1:A:134:THR:HG23	2:C:726:TYR:HE1	1.83	0.43
2:C:866:ASP:HB3	2:C:872:TYR:CE1	2.53	0.43
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:137:TYR:HD2	5:F:273:MET:HE2	1.82	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:528:THR:HG22	3:J:532:GLU:CD	2.39	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:62:TYR:C	2:C:64:GLY:N	2.70	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:244:VAL:O	3:D:244:VAL:HG23	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
5:F:290:LEU:HD13	5:F:333:VAL:HG22	2.01	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: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
2:C:157:PHE:HE2	2:C:431:LYS:HZ3	1.66	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:589:THR:HG1	2:C:659:GLN:NE2	2.14	0.43
2:C:800:MET:HE1	2:C:822:VAL:CG2	2.49	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
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:168:GLY:C	2:I:170:VAL:H	2.22	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:J:820:ILE:HD11	3:J:822:MET:HE3	2.01	0.43
5:L:244:THR:O	5:L:247:GLU:HG2	2.19	0.43
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
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:1336:ASN:ND2	3:D:29:MET:HE2	2.34	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
3:D:1273:ASP:CB	3:D:1276:GLU:CD	2.87	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:1222:GLU:O	2:I:1223:ARG:CB	2.64	0.43
3:J:138:VAL:CG2	3:J:145:VAL:HB	2.43	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
2:C:607:SER:H	2:C:610:GLU:HB2	1.84	0.43
2:C:1271:GLY:C	3:D:343:LEU:HD11	2.38	0.43
3:D:9:LYS:CE	3:D:11:GLN:HA	2.49	0.43
3:D:126:LEU:C	3:D:126:LEU:HD12	2.38	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:98:VAL:CG2	2:I:124:MET:CE	2.96	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
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
3:D:479:GLU:CG	4:E:20:VAL:HG11	2.46	0.43
3:D:678:ARG:CD	3:D:678:ARG:C	2.86	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: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
2:I:1245:ALA:HB2	3:J:372:MET:HE3	2.00	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:821:MET:HE3	3:J:879:ALA:HB1	2.01	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:593:LYS:O	2:C:600:THR:CB	2.67	0.42
3:D:639:VAL:HG13	3:D:639:VAL:O	2.19	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
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:805:GLN:CD	3:J:1348:LYS:HD3	2.37	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: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:842:ARG:CD	3:D:882:VAL:HG11	2.49	0.42
3:D:1314:LEU:HD12	3:D:1326:GLN:OE1	2.19	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
2:I:29:SER:HB3	2:I:33:ASP:OD2	2.19	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
1:B:183:ILE:HD12	1:B:183:ILE:N	2.34	0.42
2:C:218:GLU:O	2:C:222:ASP:HB2	2.19	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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:800:MET:HE2	2:C:1095:ASP:HB3	2.01	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
5:L:96:ASP:O	5:L:96:ASP:CG	2.57	0.42
5:L:101:TYR:O	5:L:102:MET:C	2.56	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: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:73:GLY:C	1:G:134:THR:HG22	2.39	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:681:MET:HE1	2:I:1073:LYS:NZ	2.35	0.42
2:I:804:PHE:O	2:I:805:MET:HB3	2.19	0.42
2:I:1080:ASN:CB	2:I:1085:MET:CE	2.97	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:277:MET:CE	5:L:281:ARG:NH2	2.81	0.42
5:L:470:MET:HB2	5:L:478:PRO:HG3	2.00	0.42
1:B:61:ILE:HG23	1:B:142:MET:HE2	2.02	0.42
2:C:1111:GLN:HB2	2:C:1230:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:397:LEU:O	2:I:398:SER:OG	2.34	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:97:VAL:CG1	3:J:101:ARG:CZ	2.91	0.42
3:J:141:PHE:O	3:J:180:MET:HE1	2.20	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: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:568:ASN:C	5:F:569:THR:HG22	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1221:LEU:HD13	3:J:1222:ARG:N	2.34	0.42
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:1217:THR:C	2:C:1219:GLU:H	2.22	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: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:242:LEU:HD23	3:J:242:LEU:C	2.41	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:285:LEU:HD23	5:F:413:MET:HE2	2.02	0.42
3:D:423:LEU:N	3:D:423:LEU:HD12	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:HZ2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:B:101:THR:CG2	1:B:103:ASN:HD21	2.32	0.42
2:C:122:VAL:HG13	2:C:122:VAL:O	2.20	0.42
2:C:629:PHE:CD2	2:C:634:VAL:HG11	2.55	0.42
2:C:653:MET:HG2	2:C:654:ASP:N	2.35	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:614:LEU:O	3:D:615:LYS:C	2.56	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
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:800:MET:HE2	2:I:1095:ASP:HB3	2.00	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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:403:MET:HE3	2:I:403:MET:HB3	1.98	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:1198:VAL:HG11	3:J:1210:ILE:CG2	2.48	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
3:D:430:HIS:ND1	3:D:430:HIS:N	2.65	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:91:THR:HG21	2:I:503:LYS:HZ1	1.85	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:693:VAL:HG21	3:J:743:MET:HE2	2.02	0.41
3:J:930:LEU:HD22	3:J:1240:VAL:HG12	2.02	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:416:ILE:O	3:D:417:ARG:C	2.58	0.41
3:D:1237:VAL:CG1	3:D:1253:ILE:HD13	2.48	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
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
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:131:THR:OG1	2:C:135:THR:O	2.37	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
5:F:231:THR:CG2	5:F:249:ILE:HG12	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1066:MET:HE3	2:C:1076:ILE:HB	1.92	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:C	5:F:517:SER:N	2.74	0.41
5:F:515:GLU:HG2	5:F:516:ASP:N	2.35	0.41
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:418:GLU:N	4:E:45:LYS:HZ3	2.11	0.41
3:D:1221:LEU:HD13	3:D:1222:ARG:N	2.36	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: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: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
1:G:152:TYR:CD1	2:I:824:GLN:HG2	2.55	0.41
2:I:105:TYR:HA	2:I:112:GLY:O	2.21	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:821:MET:HE2	3:J:879:ALA:HB1	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:I:1278:LEU:HD21	3:J:484:MET:HE1	2.03	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
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:1259:LEU:HG	2:C:1260:GLY:N	2.31	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:825:VAL:O	3:D:826:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1343:GLU:C	3:D:1344:LEU:HD12	2.41	0.41
5:F:490:PRO:O	5:F:491:GLU:HG2	2.21	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
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: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:516:ASP:CG	2:I:522:SER:OG	2.58	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:978:VAL:HG21	2:I:1010:GLN:CD	2.41	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:38:VAL:HG13	3:J:55:GLY:C	2.41	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
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: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:A:218:ARG:NH1	1:B:231:PHE:C	2.75	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:883:ARG:HH12	3:J:897:HIS:HD2	1.66	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: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
2:C:1293:VAL:HG11	2:C:1304:MET:HE2	2.02	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: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
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
5:L:470:MET:HE2	5:L:478:PRO:CB	2.32	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:738:GLU:HG2	2:C:741:MET:HE1	2.02	0.40
2:C:1015:ALA:O	2:C:1018:TYR:HB3	2.21	0.40
2:C:1158:LYS:O	2:C:1159:VAL:CB	2.69	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
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:564:VAL:HG12	3:D:565:ALA:N	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:J:162:GLU:O	3:J:163:GLU:C	2.58	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
1:B:197:ASP:O	1:B:197:ASP:CG	2.59	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: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: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
5:F:105:MET:HE2	5:F:385:ARG:HG2	2.00	0.40
1:H:19:VAL:HB	1:H:23:HIS:NE2	2.37	0.40
1:H:79:LEU:C	1:H:79:LEU:HD13	2.41	0.40
1:H:92:VAL:HA	1:H:120:ASP:O	2.21	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
5:L:518:HIS:O	5:L:519:LEU:C	2.59	0.40
1:A:211:ILE:HG22	1:A:216:ALA:HB2	1.98	0.40
1:B:14:VAL:O	1:B:15:ASP:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:517:GLN:HG2	2:C:517:GLN:O	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:822:MET:SD	3:D:838:ARG:HB3	2.61	0.40
3:D:1291:GLU:CG	3:D:1297:LYS:HZ3	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	225/329 (68%)	198 (88%)	20 (9%)	7 (3%)	4	31
1	B	210/329 (64%)	186 (89%)	19 (9%)	5 (2%)	6	35
1	G	222/329 (68%)	194 (87%)	23 (10%)	5 (2%)	6	36
1	H	211/329 (64%)	187 (89%)	17 (8%)	7 (3%)	4	29
2	C	1335/1342 (100%)	1226 (92%)	100 (8%)	9 (1%)	22	60
2	I	1324/1342 (99%)	1220 (92%)	96 (7%)	8 (1%)	25	63
3	D	1162/1407 (83%)	1068 (92%)	86 (7%)	8 (1%)	22	60
3	J	1151/1407 (82%)	1060 (92%)	78 (7%)	13 (1%)	14	50
4	E	87/91 (96%)	82 (94%)	4 (5%)	1 (1%)	14	50
4	K	77/91 (85%)	74 (96%)	3 (4%)	0	100	100
5	F	462/613 (75%)	426 (92%)	35 (8%)	1 (0%)	47	80
5	L	463/613 (76%)	426 (92%)	36 (8%)	1 (0%)	47	80
All	All	6929/8222 (84%)	6347 (92%)	517 (8%)	65 (1%)	17	54

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
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

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Mol	Chain	Res	Type
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
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%)	180 (93%)	14 (7%)	14	42
1	B	182/286 (64%)	172 (94%)	10 (6%)	21	50
1	G	191/286 (67%)	177 (93%)	14 (7%)	14	41
1	H	184/286 (64%)	176 (96%)	8 (4%)	29	56
2	C	1151/1157 (100%)	1045 (91%)	106 (9%)	9	32
2	I	1147/1157 (99%)	1042 (91%)	105 (9%)	9	32
3	D	970/1168 (83%)	868 (90%)	102 (10%)	7	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	J	960/1168 (82%)	863 (90%)	97 (10%)	7	28
4	E	72/75 (96%)	64 (89%)	8 (11%)	6	25
4	K	67/75 (89%)	63 (94%)	4 (6%)	19	47
5	F	417/540 (77%)	375 (90%)	42 (10%)	7	28
5	L	418/540 (77%)	377 (90%)	41 (10%)	8	29
All	All	5953/7024 (85%)	5402 (91%)	551 (9%)	9	32

All (551) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	13	LEU
1	A	19	VAL
1	A	26	VAL
1	A	50	SER
1	A	61	ILE
1	A	74	VAL
1	A	115	ILE
1	A	133	LEU
1	A	145	LYS
1	A	168	ILE
1	A	215	GLU
1	A	219	ARG
1	A	231	PHE
1	B	8	PHE
1	B	9	LEU
1	B	13	LEU
1	B	50	SER
1	B	61	ILE
1	B	115	ILE
1	B	186	ASN
1	B	194	GLN
1	B	215	GLU
1	B	231	PHE
2	C	11	ILE
2	C	22	LEU
2	C	39	ILE
2	C	46	GLN
2	C	60	GLN
2	C	70	TYR

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Mol	Chain	Res	Type
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	132	ASP
2	C	167	SER
2	C	189	ASP
2	C	285	ILE
2	C	299	LYS
2	C	306	THR
2	C	320	ASP
2	C	360	LEU
2	C	369	MET
2	C	377	THR
2	C	394	ARG
2	C	419	ILE
2	C	423	ASP
2	C	434	ASP
2	C	445	ILE
2	C	484	LEU
2	C	485	ASP
2	C	486	THR
2	C	490	GLN
2	C	493	ILE
2	C	496	LYS
2	C	518	ASN
2	C	531	LEU
2	C	554	HIS
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

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Mol	Chain	Res	Type
2	C	633	LEU
2	C	639	LYS
2	C	657	THR
2	C	672	GLU
2	C	680	LEU
2	C	684	ASN
2	C	692	THR
2	C	697	LYS
2	C	705	GLU
2	C	714	VAL
2	C	748	ILE
2	C	773	LEU
2	C	781	ASP
2	C	788	SER
2	C	799	ASN
2	C	800	MET
2	C	814	ASP
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	895	LEU
2	C	919	ARG
2	C	944	ARG
2	C	946	LEU
2	C	951	MET
2	C	974	ARG
2	C	992	LEU
2	C	1002	LEU
2	C	1006	GLU
2	C	1040	ASP
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

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Mol	Chain	Res	Type
2	C	1136	GLN
2	C	1146	GLN
2	C	1151	LEU
2	C	1156	ARG
2	C	1159	VAL
2	C	1198	LEU
2	C	1210	ILE
2	C	1237	HIS
2	C	1238	LEU
2	C	1264	GLN
2	C	1265	PHE
2	C	1310	ASP
2	C	1327	LEU
2	C	1331	ARG
2	C	1341	ASP
2	C	1342	GLU
3	D	8	LEU
3	D	18	ASP
3	D	26	SER
3	D	29	MET
3	D	46	TYR
3	D	54	ASP
3	D	79	LYS
3	D	84	ILE
3	D	92	VAL
3	D	94	GLN
3	D	95	THR
3	D	98	ARG
3	D	159	ILE
3	D	169	LEU
3	D	172	PHE
3	D	175	GLU
3	D	176	PHE
3	D	217	LEU
3	D	230	SER
3	D	252	LEU
3	D	312	ARG
3	D	324	LEU
3	D	352	ARG
3	D	363	LEU
3	D	374	LEU
3	D	425	ARG

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Mol	Chain	Res	Type
3	D	430	HIS
3	D	454	CYS
3	D	490	ILE
3	D	506	VAL
3	D	507	VAL
3	D	513	MET
3	D	514	THR
3	D	523	GLU
3	D	536	LEU
3	D	545	HIS
3	D	547	ARG
3	D	567	THR
3	D	568	SER
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	704	GLU
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	764	ARG
3	D	770	LEU
3	D	788	LEU
3	D	798	ARG
3	D	805	GLN
3	D	810	THR
3	D	844	THR

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Mol	Chain	Res	Type
3	D	847	ASP
3	D	848	VAL
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	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	1333	THR
3	D	1343	GLU
4	E	5	THR
4	E	13	ILE
4	E	16	ARG
4	E	28	ARG
4	E	39	VAL
4	E	46	THR
4	E	58	LEU
4	E	84	THR

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Mol	Chain	Res	Type
5	F	98	VAL
5	F	100	MET
5	F	102	MET
5	F	154	GLU
5	F	267	ASP
5	F	297	MET
5	F	301	ASN
5	F	306	PHE
5	F	310	GLU
5	F	335	GLU
5	F	341	LEU
5	F	395	THR
5	F	417	ASP
5	F	422	ARG
5	F	429	THR
5	F	437	GLN
5	F	445	ASP
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	491	GLU
5	F	492	ASP
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	573	LEU
5	F	580	PHE
5	F	587	ILE
5	F	606	VAL
5	F	612	ASP

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Mol	Chain	Res	Type
1	G	9	LEU
1	G	13	LEU
1	G	19	VAL
1	G	26	VAL
1	G	50	SER
1	G	61	ILE
1	G	74	VAL
1	G	115	ILE
1	G	133	LEU
1	G	145	LYS
1	G	168	ILE
1	G	215	GLU
1	G	219	ARG
1	G	231	PHE
1	H	13	LEU
1	H	19	VAL
1	H	26	VAL
1	H	45	ARG
1	H	50	SER
1	H	61	ILE
1	H	115	ILE
1	H	215	GLU
2	I	11	ILE
2	I	22	LEU
2	I	39	ILE
2	I	60	GLN
2	I	70	TYR
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	189	ASP
2	I	285	ILE
2	I	299	LYS

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Mol	Chain	Res	Type
2	I	306	THR
2	I	320	ASP
2	I	360	LEU
2	I	369	MET
2	I	377	THR
2	I	394	ARG
2	I	419	ILE
2	I	423	ASP
2	I	434	ASP
2	I	445	ILE
2	I	484	LEU
2	I	485	ASP
2	I	486	THR
2	I	487	LEU
2	I	490	GLN
2	I	493	ILE
2	I	496	LYS
2	I	518	ASN
2	I	554	HIS
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
2	I	705	GLU
2	I	714	VAL
2	I	748	ILE
2	I	773	LEU
2	I	781	ASP
2	I	788	SER
2	I	799	ASN
2	I	800	MET
2	I	814	ASP

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Mol	Chain	Res	Type
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	895	LEU
2	I	919	ARG
2	I	944	ARG
2	I	946	LEU
2	I	951	MET
2	I	974	ARG
2	I	984	VAL
2	I	992	LEU
2	I	1002	LEU
2	I	1006	GLU
2	I	1040	ASP
2	I	1073	LYS
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	1136	GLN
2	I	1146	GLN
2	I	1151	LEU
2	I	1156	ARG
2	I	1159	VAL
2	I	1198	LEU
2	I	1210	ILE
2	I	1237	HIS
2	I	1238	LEU
2	I	1246	ARG
2	I	1264	GLN
2	I	1265	PHE
2	I	1310	ASP
2	I	1327	LEU
2	I	1331	ARG
2	I	1341	ASP

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Mol	Chain	Res	Type
2	I	1342	GLU
3	J	18	ASP
3	J	26	SER
3	J	29	MET
3	J	46	TYR
3	J	54	ASP
3	J	79	LYS
3	J	84	ILE
3	J	92	VAL
3	J	94	GLN
3	J	95	THR
3	J	159	ILE
3	J	169	LEU
3	J	172	PHE
3	J	175	GLU
3	J	217	LEU
3	J	251	PRO
3	J	252	LEU
3	J	312	ARG
3	J	324	LEU
3	J	352	ARG
3	J	363	LEU
3	J	374	LEU
3	J	394	ILE
3	J	425	ARG
3	J	454	CYS
3	J	490	ILE
3	J	507	VAL
3	J	513	MET
3	J	514	THR
3	J	523	GLU
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	641	ILE
3	J	646	ILE
3	J	660	GLU
3	J	661	VAL
3	J	678	ARG

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Mol	Chain	Res	Type
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	704	GLU
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	770	LEU
3	J	788	LEU
3	J	798	ARG
3	J	803	VAL
3	J	805	GLN
3	J	810	THR
3	J	844	THR
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

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Mol	Chain	Res	Type
3	J	1221	LEU
3	J	1255	VAL
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	1333	THR
3	J	1343	GLU
4	K	13	ILE
4	K	39	VAL
4	K	46	THR
4	K	58	LEU
5	L	98	VAL
5	L	100	MET
5	L	102	MET
5	L	154	GLU
5	L	266	PHE
5	L	267	ASP
5	L	297	MET
5	L	301	ASN
5	L	306	PHE
5	L	310	GLU
5	L	335	GLU
5	L	341	LEU
5	L	395	THR
5	L	417	ASP
5	L	422	ARG
5	L	429	THR
5	L	437	GLN
5	L	445	ASP
5	L	449	THR
5	L	450	ILE
5	L	471	LEU
5	L	472	GLN
5	L	479	THR
5	L	485	GLU

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Mol	Chain	Res	Type
5	L	486	ARG
5	L	488	LEU
5	L	489	MET
5	L	491	GLU
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	573	LEU
5	L	580	PHE
5	L	587	ILE
5	L	606	VAL
5	L	612	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	132	HIS
1	B	66	HIS
1	B	227	GLN
2	C	69	GLN
2	C	120	GLN
2	C	133	ASN
2	C	139	ASN
2	C	150	HIS
2	C	327	GLN
2	C	494	ASN
2	C	513	GLN
2	C	620	ASN
2	C	628	HIS
2	C	659	GLN
2	C	684	ASN
2	C	725	GLN
2	C	1080	ASN
2	C	1116	HIS
2	C	1134	GLN
2	C	1136	GLN

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Mol	Chain	Res	Type
2	C	1146	GLN
2	C	1237	HIS
2	C	1299	ASN
2	C	1313	HIS
3	D	94	GLN
3	D	200	GLN
3	D	419	HIS
3	D	424	ASN
3	D	435	GLN
3	D	560	ASN
3	D	669	GLN
3	D	702	GLN
3	D	716	GLN
3	D	777	HIS
3	D	929	GLN
3	D	1244	GLN
3	D	1295	ASN
5	F	131	GLN
5	F	362	ASN
5	F	383	ASN
5	F	406	GLN
5	F	409	ASN
5	F	446	GLN
5	F	455	HIS
5	F	472	GLN
5	F	518	HIS
1	H	66	HIS
1	H	132	HIS
2	I	20	GLN
2	I	69	GLN
2	I	139	ASN
2	I	343	HIS
2	I	494	ASN
2	I	513	GLN
2	I	824	GLN
2	I	1038	GLN
2	I	1116	HIS
2	I	1134	GLN
2	I	1136	GLN
2	I	1146	GLN
2	I	1220	GLN
2	I	1288	GLN

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Mol	Chain	Res	Type
2	I	1299	ASN
2	I	1313	HIS
2	I	1314	GLN
3	J	94	GLN
3	J	200	GLN
3	J	419	HIS
3	J	450	HIS
3	J	469	HIS
3	J	488	ASN
3	J	594	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	1259	GLN
3	J	1279	GLN
3	J	1366	HIS
4	K	61	ASN
5	L	131	GLN
5	L	147	GLN
5	L	227	GLN
5	L	362	ASN
5	L	446	GLN
5	L	455	HIS
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 monosaccharides 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	3.77	29 (38%)	104,114,114	2.96	39 (37%)

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 (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	2001	KNG	O18-C46	-14.63	1.20	1.44
6	C	2001	KNG	O17-C47	-9.86	1.21	1.43
6	C	2001	KNG	O03-C06	9.82	1.56	1.37
6	C	2001	KNG	C04-C10	8.96	1.59	1.43
6	C	2001	KNG	O16-C37	8.26	1.62	1.42
6	C	2001	KNG	O11-C04	-6.12	1.19	1.36
6	C	2001	KNG	C12-C11	-5.77	1.31	1.54
6	C	2001	KNG	C02-C01	5.38	1.55	1.40
6	C	2001	KNG	O17-C50	5.38	1.50	1.41
6	C	2001	KNG	O06-C37	-5.36	1.27	1.41
6	C	2001	KNG	O12-C39	5.36	1.44	1.34
6	C	2001	KNG	C03-C02	5.32	1.47	1.39
6	C	2001	KNG	C03-C04	5.31	1.49	1.37
6	C	2001	KNG	O18-C50	5.18	1.50	1.41
6	C	2001	KNG	C19-C18	-5.18	1.35	1.53
6	C	2001	KNG	C01-C09	5.14	1.59	1.43
6	C	2001	KNG	O07-C25	-4.83	1.37	1.44
6	C	2001	KNG	O01-C01	-4.65	1.20	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	2001	KNG	C47-C48	4.24	1.60	1.52
6	C	2001	KNG	C47-C46	3.44	1.62	1.52
6	C	2001	KNG	C02-N01	3.28	1.48	1.41
6	C	2001	KNG	C15-N01	3.25	1.42	1.35
6	C	2001	KNG	O10-C15	-2.78	1.18	1.23
6	C	2001	KNG	C32-C22	-2.75	1.47	1.53
6	C	2001	KNG	C27-C28	2.61	1.59	1.50
6	C	2001	KNG	O05-C29	2.34	1.45	1.39
6	C	2001	KNG	C49-C48	-2.28	1.46	1.51
6	C	2001	KNG	O04-C11	-2.25	1.18	1.21
6	C	2001	KNG	O16-C48	2.25	1.49	1.44

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	2001	KNG	C34-C26-C27	-8.72	93.15	110.93
6	C	2001	KNG	C49-C48-C47	8.51	126.36	113.41
6	C	2001	KNG	C25-C26-C27	7.48	132.41	112.02
6	C	2001	KNG	C24-C23-C22	7.46	127.92	115.43
6	C	2001	KNG	O03-C06-C07	6.85	132.93	121.14
6	C	2001	KNG	O07-C35-C36	6.85	123.69	111.09
6	C	2001	KNG	C23-C22-C21	-6.79	98.90	112.54
6	C	2001	KNG	C45-C46-C47	-6.21	107.46	114.78
6	C	2001	KNG	C12-C11-C05	6.19	119.42	107.30
6	C	2001	KNG	C25-O07-C35	-6.14	108.21	117.72
6	C	2001	KNG	O07-C25-C26	-5.70	94.25	107.50
6	C	2001	KNG	O10-C15-N01	-5.16	112.92	123.92
6	C	2001	KNG	O04-C11-C05	-4.75	122.75	131.81
6	C	2001	KNG	C33-C24-C23	-4.26	102.78	111.39
6	C	2001	KNG	C34-C26-C25	-4.15	103.96	111.40
6	C	2001	KNG	O13-C39-C40	-4.03	112.56	123.82
6	C	2001	KNG	C18-C19-C20	3.95	122.11	114.59
6	C	2001	KNG	C23-C24-C25	3.70	117.84	110.61
6	C	2001	KNG	C02-N01-C15	-3.62	116.70	126.80
6	C	2001	KNG	C18-C17-C16	-3.46	121.72	129.08
6	C	2001	KNG	O07-C35-O08	-3.42	116.17	122.96
6	C	2001	KNG	C19-C20-C21	3.29	118.28	112.43
6	C	2001	KNG	C37-C45-C46	-3.04	105.25	111.11
6	C	2001	KNG	C13-C12-C11	-2.92	106.67	113.90
6	C	2001	KNG	C26-C25-C24	2.82	120.44	114.68
6	C	2001	KNG	C01-C02-N01	2.80	125.80	117.45
6	C	2001	KNG	C16-C15-N01	2.75	125.85	116.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	2001	KNG	C03-C02-N01	-2.72	114.71	121.90
6	C	2001	KNG	O19-C23-C24	-2.70	103.47	109.49
6	C	2001	KNG	O09-C21-C22	-2.61	103.67	109.49
6	C	2001	KNG	C38-C31-C20	2.56	117.98	113.39
6	C	2001	KNG	O03-C06-C05	-2.44	106.80	113.57
6	C	2001	KNG	O11-C04-C03	-2.39	114.16	121.17
6	C	2001	KNG	O18-C50-O17	-2.30	103.41	107.44
6	C	2001	KNG	C40-C43-C44	-2.23	109.91	114.86
6	C	2001	KNG	O16-C48-C49	-2.20	101.95	106.70
6	C	2001	KNG	O16-C48-C47	-2.18	105.07	109.13
6	C	2001	KNG	C32-C22-C23	2.13	115.69	111.39
6	C	2001	KNG	C05-C06-C07	-2.07	120.23	125.29

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
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	C36-C35-O07-C25
6	C	2001	KNG	C32-C22-C23-O19
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	C40-C39-O12-C31
6	C	2001	KNG	C31-C20-C21-O09
6	C	2001	KNG	C20-C21-C22-C23
6	C	2001	KNG	O10-C15-C16-C30
6	C	2001	KNG	O13-C39-O12-C31
6	C	2001	KNG	N01-C15-C16-C17
6	C	2001	KNG	C41-C40-C43-C44
6	C	2001	KNG	C20-C21-C22-C32

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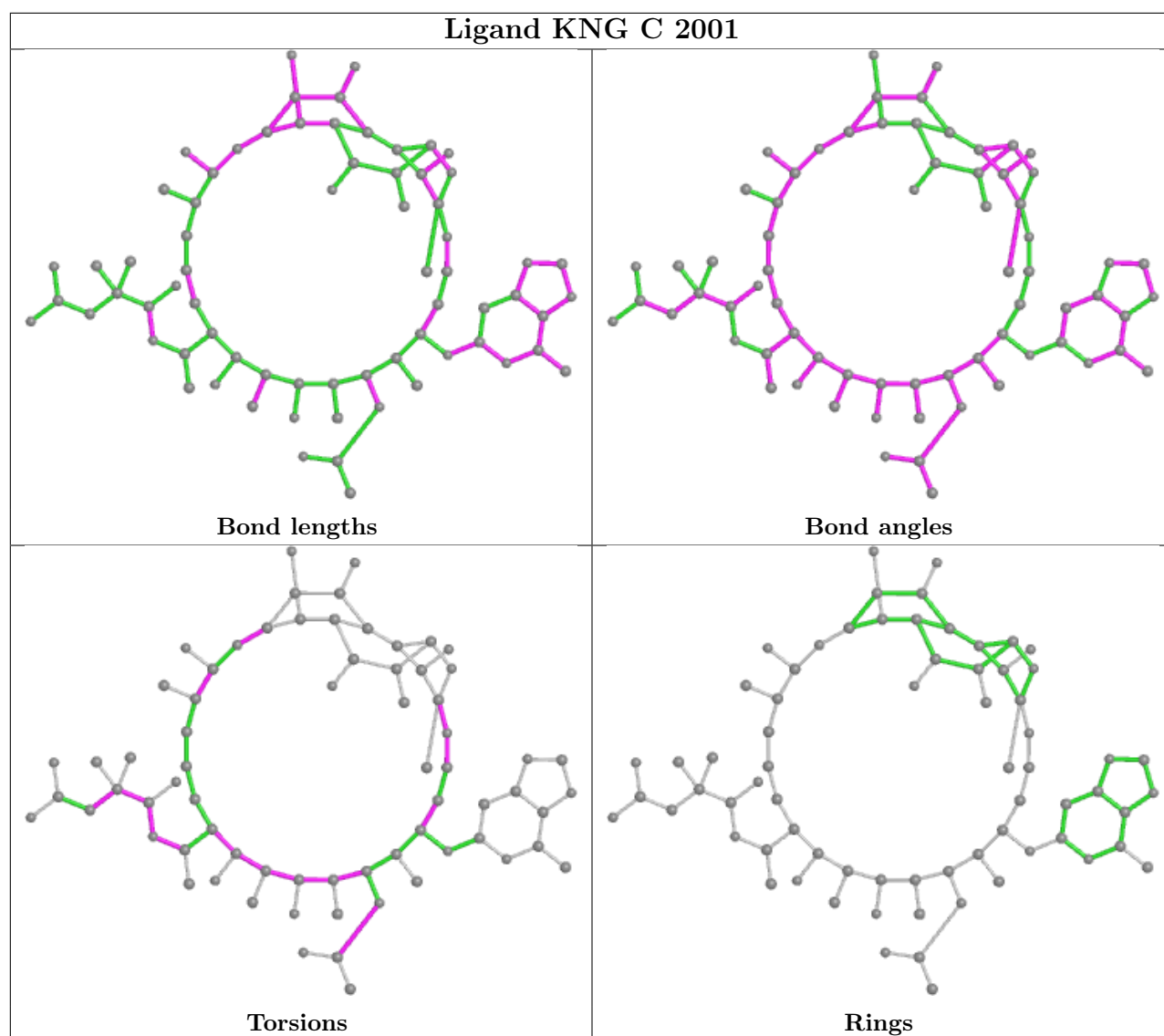
Mol	Chain	Res	Type	Atoms
6	C	2001	KNG	N01-C15-C16-C30
6	C	2001	KNG	C28-C29-O05-C12
6	C	2001	KNG	C11-C12-O05-C29
6	C	2001	KNG	O03-C12-O05-C29
6	C	2001	KNG	O09-C21-C22-C32
6	C	2001	KNG	C01-C02-N01-C15
6	C	2001	KNG	O10-C15-C16-C17
6	C	2001	KNG	C42-C40-C43-C44
6	C	2001	KNG	O12-C39-C40-C43
6	C	2001	KNG	C03-C02-N01-C15
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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	227/329 (68%)	-0.31	0 100 100	160, 212, 279, 349	0
1	B	214/329 (65%)	-0.19	4 (1%) 66 58	155, 250, 349, 390	0
1	G	224/329 (68%)	-0.28	2 (0%) 84 77	194, 274, 328, 348	0
1	H	215/329 (65%)	0.09	8 (3%) 41 33	247, 309, 348, 370	0
2	C	1339/1342 (99%)	-0.21	17 (1%) 77 68	124, 208, 314, 382	0
2	I	1328/1342 (98%)	-0.13	31 (2%) 60 51	186, 241, 336, 473	0
3	D	1166/1407 (82%)	-0.29	4 (0%) 94 90	129, 188, 298, 360	0
3	J	1155/1407 (82%)	-0.20	15 (1%) 77 68	164, 229, 312, 374	0
4	E	89/91 (97%)	-0.10	0 100 100	198, 267, 290, 306	0
4	K	79/91 (86%)	0.73	10 (12%) 3 5	329, 403, 484, 493	0
5	F	468/613 (76%)	-0.18	14 (2%) 50 39	156, 283, 413, 445	0
5	L	469/613 (76%)	-0.23	7 (1%) 73 63	193, 275, 393, 414	0
All	All	6973/8222 (84%)	-0.19	112 (1%) 72 62	124, 232, 349, 493	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	982	GLY	9.5
2	I	983	GLY	6.9
2	I	987	GLU	6.3
2	I	980	VAL	5.6
2	I	976	ARG	5.3
5	F	167	ASP	5.2
5	F	165	PHE	5.0
2	I	986	ALA	4.7
3	J	1175	LEU	4.5
2	I	981	ALA	4.5
2	I	979	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
5	F	301	ASN	3.8
2	C	1	MET	3.7
5	F	162	ILE	3.6
1	H	96	ASP	3.5
1	H	112	ALA	3.5
2	C	317	LEU	3.4
2	I	1003	THR	3.3
5	F	300	LYS	3.3
1	H	205	MET	3.2
4	K	5	THR	3.2
2	C	248	GLY	3.2
1	H	28	LEU	3.2
3	J	1296	GLY	3.1
5	F	305	LEU	3.1
2	C	1000	LEU	3.1
2	C	116	ASP	3.0
2	I	991	LYS	3.0
2	I	985	GLU	3.0
2	I	1006	GLU	3.0
2	I	984	VAL	2.8
2	I	1018	TYR	2.8
2	I	998	LEU	2.8
5	F	164	GLY	2.8
4	K	37	PRO	2.8
1	H	12	ARG	2.8
2	I	990	ASP	2.7
2	I	988	LYS	2.7
2	I	1020	GLU	2.7
1	H	98	VAL	2.7
2	I	973	SER	2.6
2	I	1021	LEU	2.6
3	J	849	LEU	2.6
4	K	36	ASP	2.6
5	F	259	PHE	2.6
2	C	282	VAL	2.5
4	K	61	ASN	2.5
1	H	24	ALA	2.5
2	C	272	ARG	2.5
5	F	288	MET	2.5
3	J	1151	LYS	2.4
5	L	165	PHE	2.4
2	C	292	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	I	100	LEU	2.4
4	K	22	VAL	2.4
2	C	206	ALA	2.4
2	I	977	ALA	2.4
2	I	975	ILE	2.3
3	J	1196	LEU	2.3
4	K	75	GLN	2.3
1	G	95	LYS	2.3
1	B	59	VAL	2.3
5	L	167	ASP	2.3
2	I	970	GLY	2.3
4	K	35	LYS	2.3
3	D	1165	PHE	2.3
2	C	266	GLY	2.3
2	C	265	LYS	2.3
3	D	213	LYS	2.3
5	F	314	THR	2.3
2	I	190	PRO	2.2
3	J	312	ARG	2.2
3	J	880	VAL	2.2
3	J	732	GLY	2.2
3	J	1297	LYS	2.2
2	C	322	LEU	2.2
2	I	989	LEU	2.2
5	L	287	ILE	2.2
5	L	427	PHE	2.2
3	D	149	GLY	2.2
4	K	47	THR	2.2
2	C	376	PRO	2.2
2	C	115	LYS	2.1
5	F	299	LYS	2.1
5	F	323	ASN	2.1
1	B	98	VAL	2.1
3	J	857	LEU	2.1
5	L	305	LEU	2.1
3	J	1165	PHE	2.1
3	J	1152	GLU	2.1
2	I	1022	LYS	2.1
2	C	253	PHE	2.1
4	K	13	ILE	2.1
2	I	1005	GLU	2.1
2	I	1017	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
3	J	747	MET	2.1
5	F	304	THR	2.1
3	J	1198	VAL	2.1
5	L	261	LEU	2.1
1	G	211	ILE	2.1
3	J	1201	GLY	2.0
5	L	309	ASN	2.0
1	B	97	GLU	2.0
2	I	1000	LEU	2.0
4	K	58	LEU	2.0
1	B	144	ILE	2.0
2	C	276	GLN	2.0
3	D	1186	TYR	2.0
1	H	26	VAL	2.0
2	I	1015	ALA	2.0
2	C	261	VAL	2.0
5	F	306	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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.

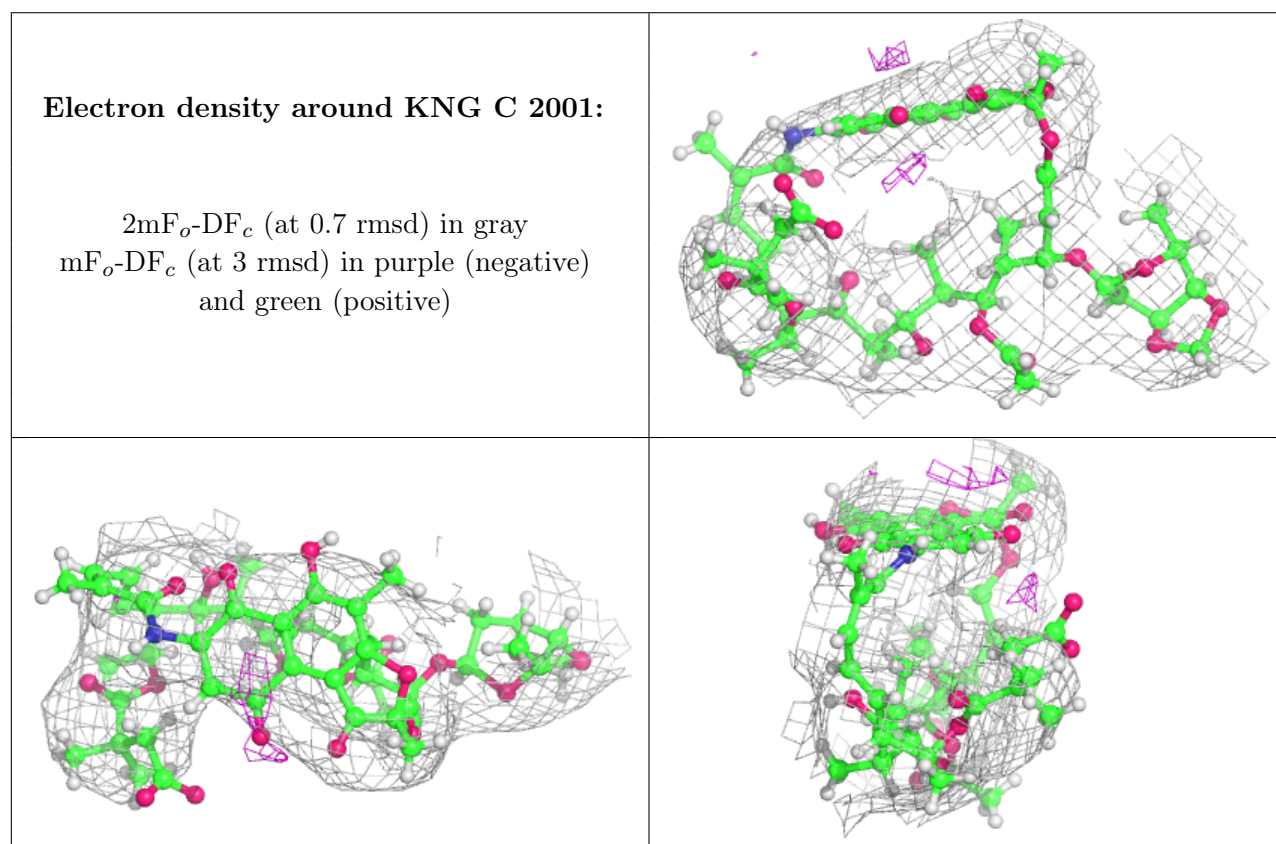
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	KNG	C	2001	70/70	0.93	0.28	155,226,287,292	0
8	ZN	D	1502	1/1	0.95	0.11	192,192,192,192	0
7	MG	J	1501	1/1	0.96	0.34	154,154,154,154	0
8	ZN	J	1502	1/1	0.96	0.06	215,215,215,215	0
7	MG	D	1501	1/1	0.98	0.46	196,196,196,196	0
8	ZN	D	1503	1/1	0.99	0.29	258,258,258,258	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	ZN	J	1503	1/1	0.99	0.28	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.