



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 06:57 PM GMT

PDB ID : 3N6R
Title : CRYSTAL STRUCTURE OF the holoenzyme of PROPIONYL-COA CARBOXYLASE (PCC)
Authors : Huang, C.S.; Sadre-Bazzaz, K.; Tong, L.
Deposited on : 2010-05-26
Resolution : 3.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

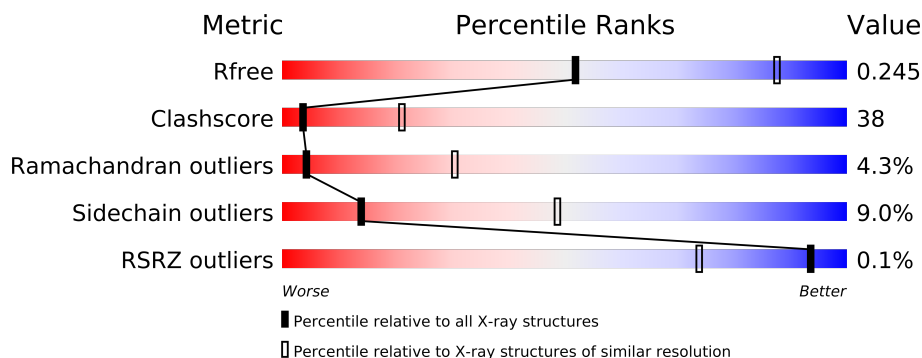
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.20 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}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	681	
1	C	681	
1	E	681	
1	G	681	
1	I	681	
1	K	681	
2	B	531	
2	D	531	
2	F	531	
2	H	531	
2	J	531	
2	L	531	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 51921 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Propionyl-CoA carboxylase, alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	591	Total	C	N	O	S	0	0	0
			4507	2828	794	857	28			
1	C	591	Total	C	N	O	S	0	0	0
			4507	2828	794	857	28			
1	E	591	Total	C	N	O	S	0	0	0
			4507	2828	794	857	28			
1	G	646	Total	C	N	O	S	0	0	0
			4950	3108	869	942	31			
1	I	646	Total	C	N	O	S	0	0	0
			4950	3108	869	942	31			
1	K	646	Total	C	N	O	S	0	0	0
			4950	3108	869	942	31			

- Molecule 2 is a protein called Propionyl-CoA carboxylase, beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	506	Total	C	N	O	S	0	0	0
			3910	2462	683	744	21			
2	D	506	Total	C	N	O	S	0	0	0
			3910	2462	683	744	21			
2	F	506	Total	C	N	O	S	0	0	0
			3910	2462	683	744	21			
2	H	506	Total	C	N	O	S	0	0	0
			3910	2462	683	744	21			
2	J	506	Total	C	N	O	S	0	0	0
			3910	2462	683	744	21			
2	L	506	Total	C	N	O	S	0	0	0
			3910	2462	683	744	21			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	11	MET	-	EXPRESSION TAG	UNP Q168G2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	12	GLY	-	EXPRESSION TAG	UNP Q168G2
B	13	SER	-	EXPRESSION TAG	UNP Q168G2
B	14	SER	-	EXPRESSION TAG	UNP Q168G2
B	15	HIS	-	EXPRESSION TAG	UNP Q168G2
B	16	HIS	-	EXPRESSION TAG	UNP Q168G2
B	17	HIS	-	EXPRESSION TAG	UNP Q168G2
B	18	HIS	-	EXPRESSION TAG	UNP Q168G2
B	19	HIS	-	EXPRESSION TAG	UNP Q168G2
B	20	HIS	-	EXPRESSION TAG	UNP Q168G2
B	21	SER	-	EXPRESSION TAG	UNP Q168G2
B	22	SER	-	EXPRESSION TAG	UNP Q168G2
B	23	GLY	-	EXPRESSION TAG	UNP Q168G2
B	24	LEU	-	EXPRESSION TAG	UNP Q168G2
B	25	VAL	-	EXPRESSION TAG	UNP Q168G2
B	26	PRO	-	EXPRESSION TAG	UNP Q168G2
B	27	ARG	-	EXPRESSION TAG	UNP Q168G2
B	28	GLY	-	EXPRESSION TAG	UNP Q168G2
B	29	SER	-	EXPRESSION TAG	UNP Q168G2
B	30	HIS	-	EXPRESSION TAG	UNP Q168G2
B	31	MET	-	EXPRESSION TAG	UNP Q168G2
D	11	MET	-	EXPRESSION TAG	UNP Q168G2
D	12	GLY	-	EXPRESSION TAG	UNP Q168G2
D	13	SER	-	EXPRESSION TAG	UNP Q168G2
D	14	SER	-	EXPRESSION TAG	UNP Q168G2
D	15	HIS	-	EXPRESSION TAG	UNP Q168G2
D	16	HIS	-	EXPRESSION TAG	UNP Q168G2
D	17	HIS	-	EXPRESSION TAG	UNP Q168G2
D	18	HIS	-	EXPRESSION TAG	UNP Q168G2
D	19	HIS	-	EXPRESSION TAG	UNP Q168G2
D	20	HIS	-	EXPRESSION TAG	UNP Q168G2
D	21	SER	-	EXPRESSION TAG	UNP Q168G2
D	22	SER	-	EXPRESSION TAG	UNP Q168G2
D	23	GLY	-	EXPRESSION TAG	UNP Q168G2
D	24	LEU	-	EXPRESSION TAG	UNP Q168G2
D	25	VAL	-	EXPRESSION TAG	UNP Q168G2
D	26	PRO	-	EXPRESSION TAG	UNP Q168G2
D	27	ARG	-	EXPRESSION TAG	UNP Q168G2
D	28	GLY	-	EXPRESSION TAG	UNP Q168G2
D	29	SER	-	EXPRESSION TAG	UNP Q168G2
D	30	HIS	-	EXPRESSION TAG	UNP Q168G2
D	31	MET	-	EXPRESSION TAG	UNP Q168G2
F	11	MET	-	EXPRESSION TAG	UNP Q168G2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	12	GLY	-	EXPRESSION TAG	UNP Q168G2
F	13	SER	-	EXPRESSION TAG	UNP Q168G2
F	14	SER	-	EXPRESSION TAG	UNP Q168G2
F	15	HIS	-	EXPRESSION TAG	UNP Q168G2
F	16	HIS	-	EXPRESSION TAG	UNP Q168G2
F	17	HIS	-	EXPRESSION TAG	UNP Q168G2
F	18	HIS	-	EXPRESSION TAG	UNP Q168G2
F	19	HIS	-	EXPRESSION TAG	UNP Q168G2
F	20	HIS	-	EXPRESSION TAG	UNP Q168G2
F	21	SER	-	EXPRESSION TAG	UNP Q168G2
F	22	SER	-	EXPRESSION TAG	UNP Q168G2
F	23	GLY	-	EXPRESSION TAG	UNP Q168G2
F	24	LEU	-	EXPRESSION TAG	UNP Q168G2
F	25	VAL	-	EXPRESSION TAG	UNP Q168G2
F	26	PRO	-	EXPRESSION TAG	UNP Q168G2
F	27	ARG	-	EXPRESSION TAG	UNP Q168G2
F	28	GLY	-	EXPRESSION TAG	UNP Q168G2
F	29	SER	-	EXPRESSION TAG	UNP Q168G2
F	30	HIS	-	EXPRESSION TAG	UNP Q168G2
F	31	MET	-	EXPRESSION TAG	UNP Q168G2
H	11	MET	-	EXPRESSION TAG	UNP Q168G2
H	12	GLY	-	EXPRESSION TAG	UNP Q168G2
H	13	SER	-	EXPRESSION TAG	UNP Q168G2
H	14	SER	-	EXPRESSION TAG	UNP Q168G2
H	15	HIS	-	EXPRESSION TAG	UNP Q168G2
H	16	HIS	-	EXPRESSION TAG	UNP Q168G2
H	17	HIS	-	EXPRESSION TAG	UNP Q168G2
H	18	HIS	-	EXPRESSION TAG	UNP Q168G2
H	19	HIS	-	EXPRESSION TAG	UNP Q168G2
H	20	HIS	-	EXPRESSION TAG	UNP Q168G2
H	21	SER	-	EXPRESSION TAG	UNP Q168G2
H	22	SER	-	EXPRESSION TAG	UNP Q168G2
H	23	GLY	-	EXPRESSION TAG	UNP Q168G2
H	24	LEU	-	EXPRESSION TAG	UNP Q168G2
H	25	VAL	-	EXPRESSION TAG	UNP Q168G2
H	26	PRO	-	EXPRESSION TAG	UNP Q168G2
H	27	ARG	-	EXPRESSION TAG	UNP Q168G2
H	28	GLY	-	EXPRESSION TAG	UNP Q168G2
H	29	SER	-	EXPRESSION TAG	UNP Q168G2
H	30	HIS	-	EXPRESSION TAG	UNP Q168G2
H	31	MET	-	EXPRESSION TAG	UNP Q168G2
J	11	MET	-	EXPRESSION TAG	UNP Q168G2

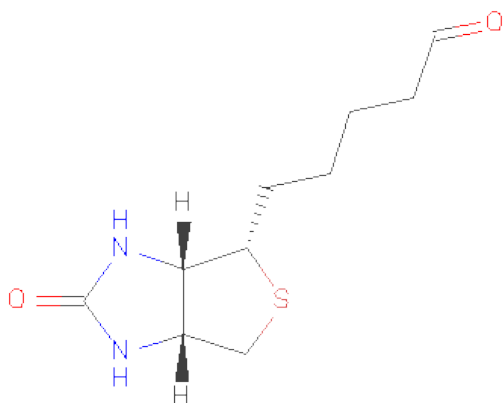
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Chain	Residue	Modelled	Actual	Comment	Reference
J	12	GLY	-	EXPRESSION TAG	UNP Q168G2
J	13	SER	-	EXPRESSION TAG	UNP Q168G2
J	14	SER	-	EXPRESSION TAG	UNP Q168G2
J	15	HIS	-	EXPRESSION TAG	UNP Q168G2
J	16	HIS	-	EXPRESSION TAG	UNP Q168G2
J	17	HIS	-	EXPRESSION TAG	UNP Q168G2
J	18	HIS	-	EXPRESSION TAG	UNP Q168G2
J	19	HIS	-	EXPRESSION TAG	UNP Q168G2
J	20	HIS	-	EXPRESSION TAG	UNP Q168G2
J	21	SER	-	EXPRESSION TAG	UNP Q168G2
J	22	SER	-	EXPRESSION TAG	UNP Q168G2
J	23	GLY	-	EXPRESSION TAG	UNP Q168G2
J	24	LEU	-	EXPRESSION TAG	UNP Q168G2
J	25	VAL	-	EXPRESSION TAG	UNP Q168G2
J	26	PRO	-	EXPRESSION TAG	UNP Q168G2
J	27	ARG	-	EXPRESSION TAG	UNP Q168G2
J	28	GLY	-	EXPRESSION TAG	UNP Q168G2
J	29	SER	-	EXPRESSION TAG	UNP Q168G2
J	30	HIS	-	EXPRESSION TAG	UNP Q168G2
J	31	MET	-	EXPRESSION TAG	UNP Q168G2
L	11	MET	-	EXPRESSION TAG	UNP Q168G2
L	12	GLY	-	EXPRESSION TAG	UNP Q168G2
L	13	SER	-	EXPRESSION TAG	UNP Q168G2
L	14	SER	-	EXPRESSION TAG	UNP Q168G2
L	15	HIS	-	EXPRESSION TAG	UNP Q168G2
L	16	HIS	-	EXPRESSION TAG	UNP Q168G2
L	17	HIS	-	EXPRESSION TAG	UNP Q168G2
L	18	HIS	-	EXPRESSION TAG	UNP Q168G2
L	19	HIS	-	EXPRESSION TAG	UNP Q168G2
L	20	HIS	-	EXPRESSION TAG	UNP Q168G2
L	21	SER	-	EXPRESSION TAG	UNP Q168G2
L	22	SER	-	EXPRESSION TAG	UNP Q168G2
L	23	GLY	-	EXPRESSION TAG	UNP Q168G2
L	24	LEU	-	EXPRESSION TAG	UNP Q168G2
L	25	VAL	-	EXPRESSION TAG	UNP Q168G2
L	26	PRO	-	EXPRESSION TAG	UNP Q168G2
L	27	ARG	-	EXPRESSION TAG	UNP Q168G2
L	28	GLY	-	EXPRESSION TAG	UNP Q168G2
L	29	SER	-	EXPRESSION TAG	UNP Q168G2
L	30	HIS	-	EXPRESSION TAG	UNP Q168G2
L	31	MET	-	EXPRESSION TAG	UNP Q168G2

- Molecule 3 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL

(three-letter code: BTI) (formula: C₁₀H₁₆N₂O₂S).



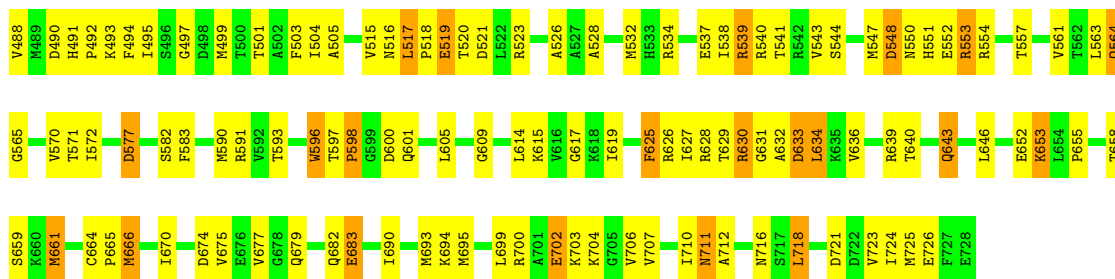
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	C	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	E	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	G	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	I	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	K	1	Total	C	N	O	S	0	0
			15	10	2	2	1		

T571	K493	ALA	R375	A315	K126
A573	F494	PRO	V376	G316	V127
L572	L495	SER	A377	M317	M128
D577	M499	GLY	A378	E318	P192
		GLU	Q379	Q319	P193
V581	T500	A428K	E380	A320	A130
F582	F501	A428L	P381	V321	I131
P583	A502	T433	L382	A322	R132
M590	F503		G434	L323	GLY
R591	L504	V435	Q386	A324	A133
V592	V615	Y436	V389	K325	A136
		G439	K390	A326	ASP
T593	N516	E440	L391	V327	Q137
W596	L517	E441	T392	G328	A138
T597	P518	I441	G393	V329	V139
P598	E519	S442	W394	A330	GLU
G599	T520	M443	A395	S331	A141
D600	D521	Y444	I396	A332	VAL
L602	L522	Y445	E397	A332	G142
L605	R523	D446	R398	G335	Y143
	R524	P447	R399	T334	G144
L605	V525	M448	L400	F337	F145
	A526	I449	Y401	I338	L146
G609	A527	L452	A402	V339	S150
	E403		G340	K151	
L614	A528	C453	D404	G341	K151
	A530	Q450	P405	Q342	F152
K615	K451	W455	Y406	K343	A155
V616	M532	A456	R407	N344	L156
G617	H533	P457	L411	F345	E157
F618	R534	T458	L414	G346	A158
L619	V535	A461		L347	GLY
F625	A536	A462	G415	L285	E159
	E537	I463	R416	G286	A160
R626	T538	E463	L417	E287	V161
I627	R539	E464	T418	R288	F163
R628	R540	A465	G148	G352	A164
T629	T541	M466	R419	T352	G165
R630	R542	R467	Y420	R353	P166
G631	V543	I468	R421	I292	P167
A632	S544	D471	P422	Q355	K168
D633	M547	S472	P423A	R293	G169
L634		F473	E422C	R294	ARG
R642	N550	F474	A422A	R295	A170
Q643	H551	W475	R420	R296	I171
E552	E552	E476	R421	Q297	E172
	R553	G477	I478	K298	ASN
L646	R554	I478	PRO	V299	ASP
	M650	T557	LEU	T361	GLN
P651	E558	H480	LEU	L362	GLU
K653	L654	M481	VAL	T364	ALA
L654	P655	L482	ASN	G366	ARG
P655	T652	P483	GLY	V367	GLY
	L563	F484	LYS	D368	PHE
T658	Q564	L485	TRP	V370	GLN
	G565	H491	GLN	E371	SER
S659	N570	P492	ASP	Q372	LYS
K660	L666	L493	V376	K372	ASN
		P493	A377	M373	GLY
L666	L668	L494	E379	L374	ALA
		P494	A379	L375	ALA

● Molecule 1: Propionyl-CoA carboxylase, alpha subunit

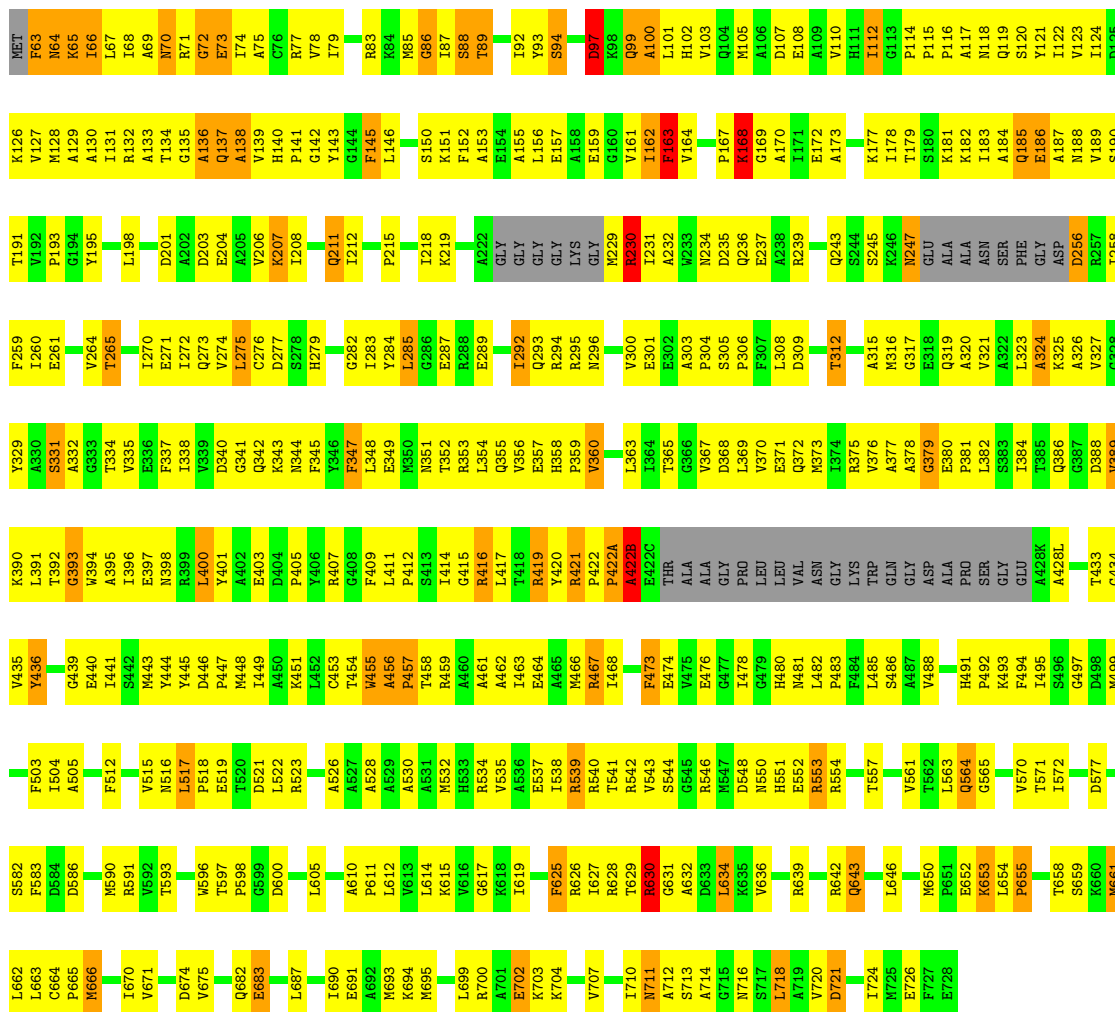
Chain E:

GLY	ASP	ALA	PRO	SER	GLY	GLU	A428K	A428L	T433	G434	V435	Y436	G439	E440	I441	S442	M443	Y444	Y445	D446	P447	M448	I449	A450	K451	L452	C453	T454	W455	A456	P457	T458	R459	A460	A461	A462	I463	E464	R467	I468	D471	S472	F473	E474	V475	E476	G477	I478	H479	H480	N481	L482	P483	F484	L485	S486	A487																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
I374	R375	V376	A377	A378	Q379	E380	V381	P381	L382	Q386	V387	D388	V389	K390	L391	T392	G393	W394	A395	I396	E397	N398	R399	L400	Y401	A402	E403	D404	P405	L411	I414	G415	R416	R417	T418	R419	Y420	P421	P422	P423A	E422B	E422C	THR	ALA	ALA	GLY	PRO	LEU	LEU	VAL	ASN	GLY	LYS	TRP	GLN	GLY	ASP	ASP	ASP	GLY	PHE	V264	T265	Q266	P267	R268	H269	E270	E271	I272	Q273	V274	L275	C276	D277	S278	H279	G280	N281	G282	L283	Y284	L285	G286	E287	R288	E289	I292	Q293	R294	R295	H296	T297	V298	N299	V300	E301	A302	A303	G304	P305	P306	F307	L308	LYS	D309	T310	R311	R312	R313	R314	R315	R316	R317	R318	R319	R320	R321	R322	R323	R324	R325	R326	R327	R328	R329	R330	R331	R332	R333	R334	R335	R336	R337	R338	R339	R340	R341	R342	R343	R344	R345	R346	R347	R348	R349	R350	R351	R352	R353	R354	R355	R356	R357	R358	R359	R360	R361	R362	R363	R364	R365	R366	R367	R368	R369	R370	R371	R372	R373	R374	R375	R376	R377	R378	R379	R380	R381	R382	R383	R384	R385	R386	R387	R388	R389	R390	R391	R392	R393	R394	R395	R396	R397	R398	R399	R400	R401	R402	R403	R404	R405	R406	R407	R408	R409	R410	R411	R412	R413	R414	R415	R416	R417	R418	R419	R420	R421	R422	R423	R424	R425	R426	R427	R428	R429	R430	R431	R432	R433	R434	R435	R436	R437	R438	R439	R440	R441	R442	R443	R444	R445	R446	R447	R448	R449	R450	R451	R452	R453	R454	R455	R456	R457	R458	R459	R460	R461	R462	R463	R464	R465	R466	R467	R468	R469	R470	R471	R472	R473	R474	R475	R476	R477	R478	R479	R480	R481	R482	R483	R484	R485	R486	R487	R488	R489	R490	R491	R492	R493	R494	R495	R496	R497	R498	R499	R500	R501	R502	R503	R504	R505	R506	R507	R508	R509	R510	R511	R512	R513	R514	R515	R516	R517	R518	R519	R520	R521	R522	R523	R524	R525	R526	R527	R528	R529	R530	R531	R532	R533	R534	R535	R536	R537	R538	R539	R540	R541	R542	R543	R544	R545	R546	R547	R548	R549	R550	R551	R552	R553	R554	R555	R556	R557	R558	R559	R560	R561	R562	R563	R564	R565	R566	R567	R568	R569	R570	R571	R572	R573	R574	R575	R576	R577	R578	R579	R580	R581	R582	R583	R584	R585	R586	R587	R588	R589	R590	R591	R592	R593	R594	R595	R596	R597	R598	R599	R600	R601	R602	R603	R604	R605	R606	R607	R608	R609	R610	R611	R612	R613	R614	R615	R616	R617	R618	R619	R620	R621	R622	R623	R624	R625	R626	R627	R628	R629	R630	R631	R632	R633	R634	R635	R636	R637	R638	R639	R640	R641	R642	R643	R644	R645	R646	R647	R648	R649	R650	R651	R652	R653	R654	R655	R656	R657	R658	R659	R660	R661	R662	R663	R664	R665	R666	R667	R668	R669	R670	R671	R672	R673	R674	R675	R676	R677	R678	R679	R680	R681	R682	R683	R684	R685	R686	R687	R688	R689	R690	R691	R692	R693	R694	R695	R696	R697	R698	R699	R700	R701	R702	R703	R704	R705	R706	R707	R708	R709	R710	R711	R712	R713	R714	R715	R716	R717	R718	R719	R720	R721	R722	R723	R724	R725	R726	R727	R728	R729	R730	R731	R732	R733	R734	R735	R736	R737	R738	R739	R740	R741	R742	R743	R744	R745	R746	R747	R748	R749	R750	R751	R752	R753	R754	R755	R756	R757	R758	R759	R760	R761	R762	R763	R764	R765	R766	R767	R768	R769	R770	R771	R772	R773	R774	R775	R776	R777	R778	R779	R780	R781	R782	R783	R784	R785	R786	R787	R788	R789	R790	R791	R792	R793	R794	R795	R796	R797	R798	R799	R800	R801	R802	R803	R804	R805	R806	R807	R808	R809	R810	R811	R812	R813	R814	R815	R816	R817	R818	R819	R820	R821	R822	R823	R824	R825	R826	R827	R828	R829	R830	R831	R832	R833	R834	R835	R836	R837	R838	R839	R840	R841	R842	R843	R844	R845	R846	R847	R848	R849	R850	R851	R852	R853	R854	R855	R856	R857	R858	R859	R860	R861	R862	R863	R864	R865	R866	R867	R868	R869	R870	R871	R872	R873	R874	R875	R876	R877	R878	R879	R880	R881	R882	R883	R884	R885	R886	R887	R888	R889	R890	R891	R892	R893	R894	R895	R896	R897	R898	R899	R900	R901	R902	R903	R904	R905	R906	R907	R908	R909	R910	R911	R912	R913	R914	R915	R916	R917	R918	R919	R920	R921	R922	R923	R924	R925	R926	R927	R928	R929	R930	R931	R932	R933	R934	R935	R936	R937	R938	R939	R940	R941	R942	R943	R944	R945	R946	R947	R948	R949	R950	R951	R952	R953	R954	R955	R956	R957	R958	R959	R960	R961	R962	R963	R964	R965	R966	R967	R968	R969	R970	R971	R972	R973	R974	R975	R976	R977	R978	R979	R980	R981	R982	R983	R984	R985	R986	R987	R988	R989	R990	R991	R992	R993	R994	R995	R996	R997	R998	R999	R1000
ALA	ALA	ASN	SER	PHE	GLY	ASP	MET	GLY	LEU	ILE	PHE	ILE	GLU	ASP	ALA	ASP	ASP	ASN	SER	GLN	GLN	GLY	TYR	PRO	VAL	MET	ILE	LYS	LYS	ALA	ALA	SER	ALA	G282	L283	Y284	L285	G286	E287	R288	E289	I292	Q293	R294	R295	H296	T297	V298	N299	V300	E301	A302	A303	G304	P305	P306	F307	L308	LYS	D309	T310	R311	R312	R313	R314	R315	R316	R317	R318	R319	R320	R321	R322	R323	R324	R325	R326	R327	R328	R329	R330	R331	R332	R333	R334	R335	R336	R337	R338	R339	R340	R341	R342	R343	R344	R345	R346	R347	R348	R349	R350	R351	R352	R353	R354	R355	R356	R357	R358	R359	R360	R361	R362	R363	R364	R365	R366	R367	R368	R369	R370	R371	R372	R373	R374	R375	R376	R377	R378	R379	R380	R381	R382	R383	R384	R385	R386	R387	R388	R389	R390	R391	R392	R393	R394	R395	R396	R397	R398	R399	R400	R401	R402	R403	R404	R405	R406	R407	R408	R409	R410	R411	R412	R413	R414	R415	R416	R417	R418	R419	R420	R421	R422	R423	R424	R425	R426	R427	R428	R429	R430	R431	R432	R433	R434	R435	R436	R437	R438	R439	R440	R441	R442	R443	R444	R445	R446	R447	R448	R449	R450	R451	R452	R453	R454	R455	R456	R457	R458	R459	R460	R461	R462	R463	R464	R465	R466	R467	R468	R469	R470	R471	R472	R473	R474	R475	R476	R477	R478	R479	R480	R481	R482	R483	R484	R485	R486	R487	R488	R489	R490	R491	R492	R493	R494	R495	R496	R497	R498	R499	R500	R501	R502	R503	R504	R505	R506	R507	R508	R509	R510	R511	R512	R513	R514	R515	R516	R517	R518	R519	R520	R521	R522	R523	R524	R525	R526	R527	R528	R529	R530	R531	R532	R533	R534	R535	R536	R537	R538	R539	R540	R541	R542	R543	R544	R545	R546	R547	R548	R549	R550	R551	R552	R553	R554	R555	R556	R557	R558	R559	R560	R561	R562	R563	R564	R565	R566	R567	R568	R569	R570	R571	R572	R573	R574	R575	R576	R577	R578	R579	R580	R581	R582	R583	R584	R585	R586	R587	R588	R589	R590	R591	R592	R593	R594	R595	R596	R597	R598	R599	R600	R601	R602	R603	R604	R605	R606	R607	R608	R609	R610	R611	R612	R613	R614	R615	R616	R617	R618	R619	R620	R621	R622	R623	R624	R625	R626	R627	R628	R629	R630	R631	R632	R633	R634	R635	R636	R637	R638	R639	R640	R641	R642	R643	R644	R645	R646	R647	R648	R649	R650	R651	R652	R653	R654	R655	R656	R657	R658	R659	R660	R661	R662	R663	R664	R665	R666	R667	R668	R669	R670	R671	R672	R673	R674	R675	R676	R677	R678	R679	R680	R681	R682	R683	R684	R685	R686	R687	R688	R689	R690	R691	R692	R693	R694	R695	R696	R697	R698	R699	R700	R701	R702	R703	R704	R705	R706	R707	R708	R709	R710	R711	R712	R713	R714	R715	R716	R717	R718	R719	R720	R721	R722	R723	R724	R725	R726	R727	R728	R729	R730	R731	R732	R733	R734	R735	R736	R737	R738	R739	R740	R741	R742	R743	R744	R745	R746	R747	R748	R749	R750	R751	R752	R753	R754	R755	R756	R757	R758	R759	R760	R761	R762	R763	R764	R765	R766	R767	R768	R769	R770	R771	R772	R773	R774	R775	R776	R777	R778	R779	R780	R781	R782	R783	R784	R785	R786	R787	R788	R789	R790	R791	R792	R793	R794	R795	R796	R797	R798	R799	R800	R801	R802	R803	R804	R805	R806	R807	R808	R809	R810	R811	R812	R813	R814	R815	R816	R817	R818	R819	R820	R821	R822	R823	R824	R825	R826	R827	R828	R829	R830	R831	R832	R833	R834	R835	R836	R837	R838	R839	R840	R841	R842	R843	R844	R845	R846	R847	R848	R849	R850	R851	R852	R853	R854	R855	R856	R857	R858	R859	R860	R861	R862	R863	R864	R865	R866	R867	R868	R869	R870	R871	R872	R873	R874	R875	R876	R877	R878	R879	R880	R881	R882	R883	R884	R885	R886	R887	R888	R889	R890	R891	R892	R893	R894	R895	R896	R897	R898	R899	R900	R901	R902	R903	R904	R905	R906	R907	R908	R909	R910	R911	R912	R913	R914	R915	R916	R917	R918	R919	R920	R921	R922	R923	R924	R925	R926	R927	R928	R929	R930	R931	R932	R933	R934	R935	R936	R937	R938	R939	R940	R941	R942	R943	R944	R945	R946	R947	R948	R9																																																																																																	



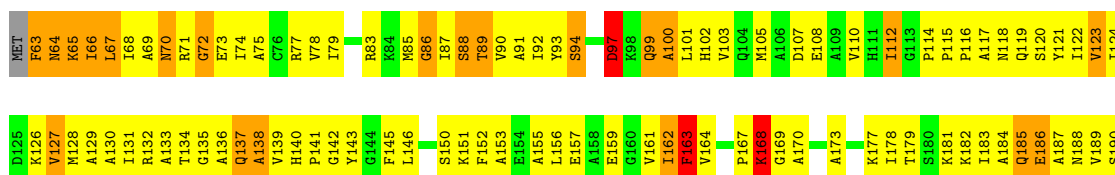
• Molecule 1: Propionyl-CoA carboxylase, alpha subunit

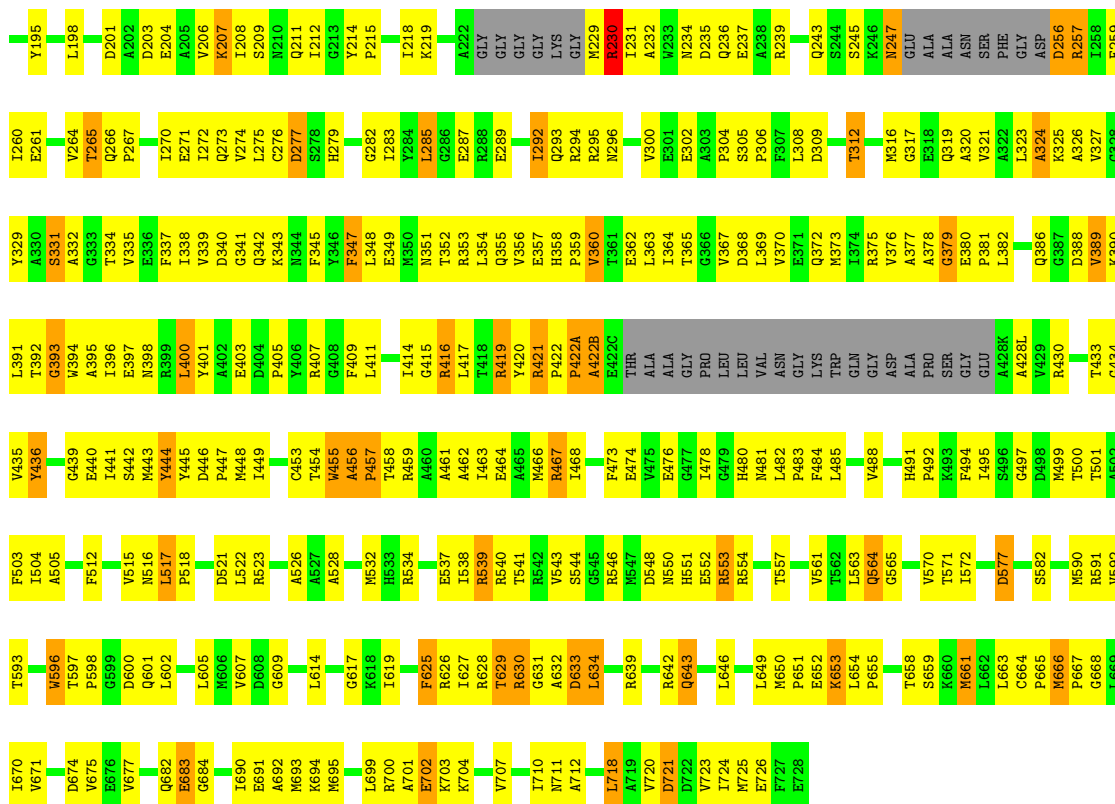
Chain G:



• Molecule 1: Propionyl-CoA carboxylase, alpha subunit

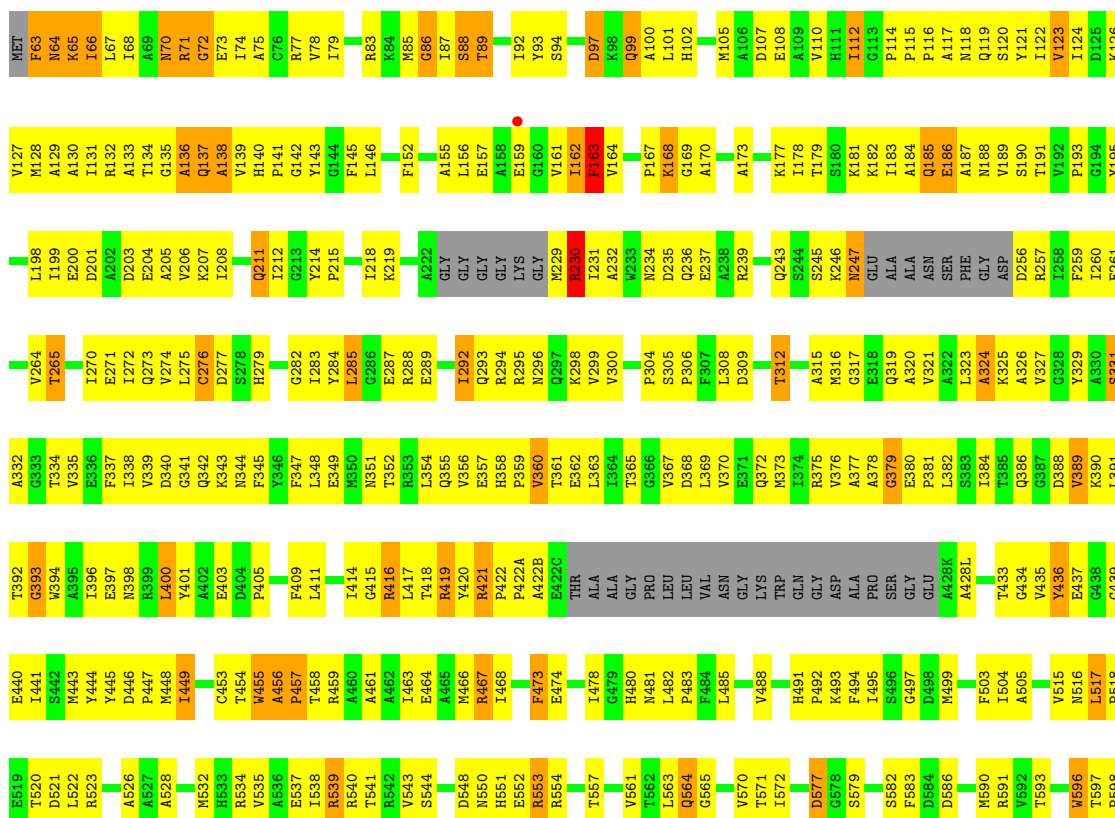
Chain I:

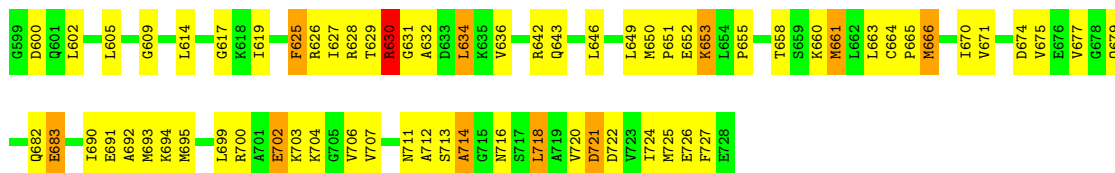




• Molecule 1: Propionyl-CoA carboxylase, alpha subunit

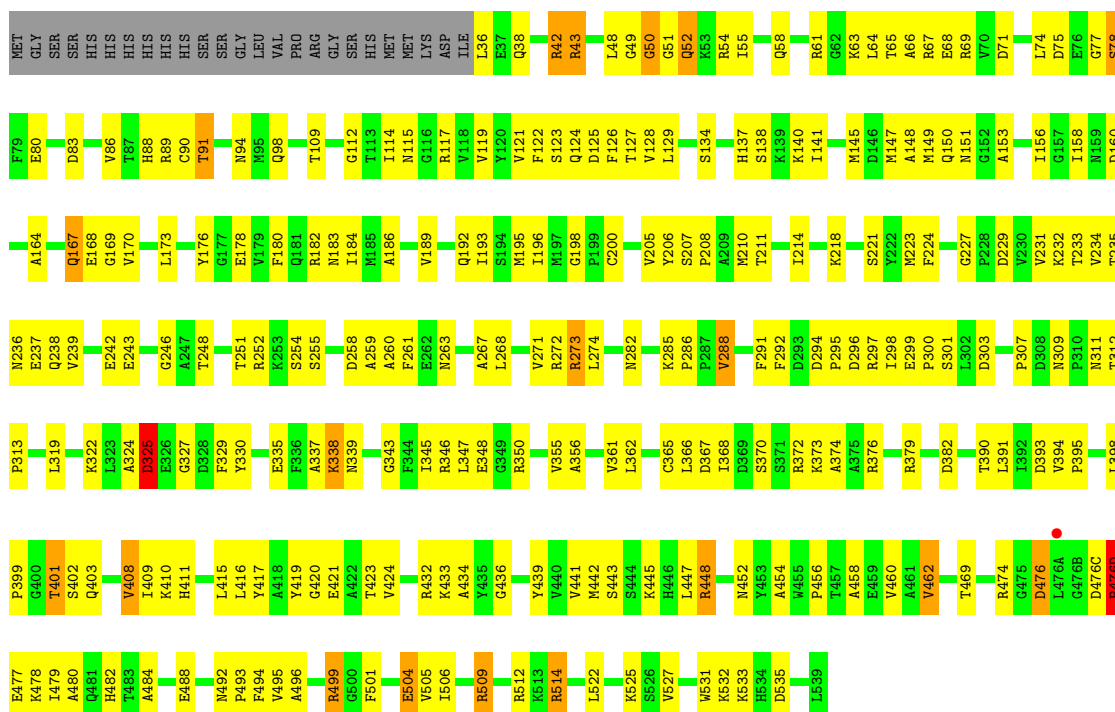
Chain K:





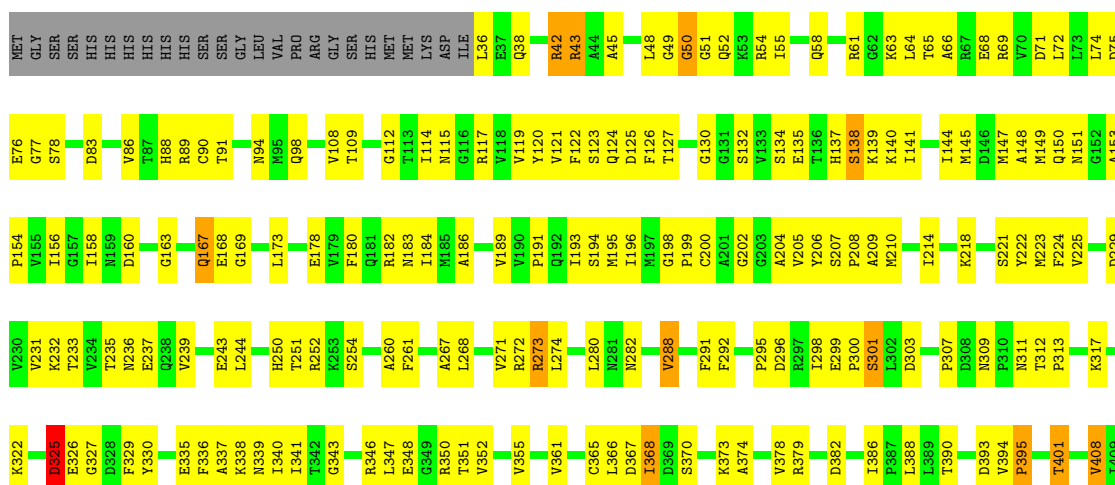
• Molecule 2: Propionyl-CoA carboxylase, beta subunit

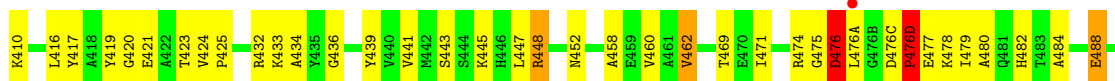
Chain B:



• Molecule 2: Propionyl-CoA carboxylase, beta subunit

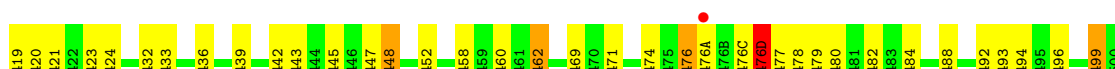
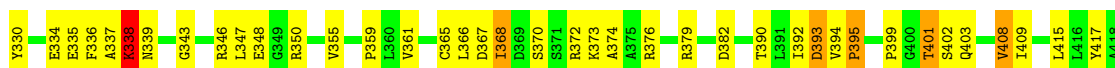
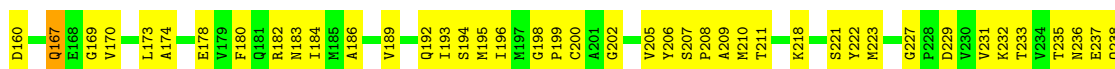
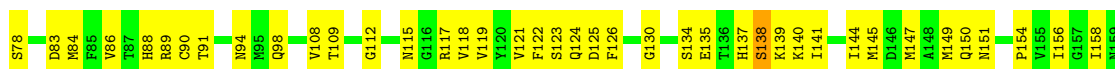
Chain D:





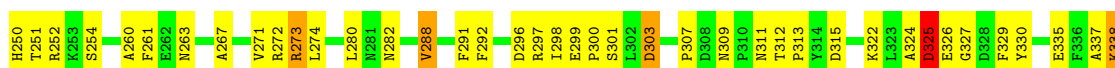
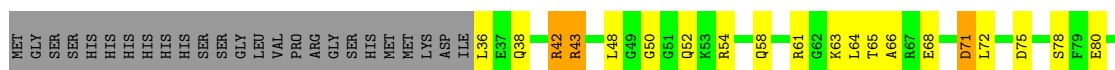
• Molecule 2: Propionyl-CoA carboxylase, beta subunit

Chain F:



• Molecule 2: Propionyl-CoA carboxylase, beta subunit

Chain H:



Y505	R509	R512	R513	R514	R517	L522	R523	M524	K525	S526	V527	K532	D535	N536	I537	P538	L539
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	133.89Å 159.17Å 153.74Å 113.87° 101.03° 108.99°	Depositor
Resolution (Å)	29.36 – 3.20 29.36 – 3.14	Depositor EDS
% Data completeness (in resolution range)	92.4 (29.36-3.20) 90.7 (29.36-3.14)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.11Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.212 , 0.245 0.213 , 0.245	Depositor DCC
R_{free} test set	12030 reflections (8.07%)	DCC
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 23.3	EDS
Estimated twinning fraction	0.017 for -h,h+k+l,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 169648 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	51921	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: BTI

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	0.51	0/4586	0.73	1/6209 (0.0%)
1	C	0.51	0/4586	0.74	1/6209 (0.0%)
1	E	0.52	0/4586	0.74	1/6209 (0.0%)
1	G	0.52	0/5036	0.74	1/6811 (0.0%)
1	I	0.51	0/5036	0.74	1/6811 (0.0%)
1	K	0.51	0/5036	0.73	1/6811 (0.0%)
2	B	0.62	1/3990 (0.0%)	0.81	0/5399
2	D	0.61	1/3990 (0.0%)	0.82	0/5399
2	F	0.61	1/3990 (0.0%)	0.82	0/5399
2	H	0.61	0/3990	0.80	0/5399
2	J	0.61	0/3990	0.82	0/5399
2	L	0.61	0/3990	0.81	0/5399
All	All	0.56	3/52806 (0.0%)	0.77	6/71454 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	E	0	1
1	G	0	1
1	I	0	1
1	K	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	365	CYS	CB-SG	-6.58	1.71	1.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	365	CYS	CB-SG	-5.84	1.72	1.81
2	F	365	CYS	CB-SG	-5.36	1.73	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	422(B)	ALA	N-CA-C	5.95	127.07	111.00
1	K	422(B)	ALA	N-CA-C	5.46	125.75	111.00
1	G	422(B)	ALA	N-CA-C	5.44	125.69	111.00
1	I	422(B)	ALA	N-CA-C	5.36	125.48	111.00
1	E	422(B)	ALA	N-CA-C	5.19	125.01	111.00
1	C	422(B)	ALA	N-CA-C	5.12	124.83	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	420	TYR	Sidechain
1	E	420	TYR	Sidechain
1	G	420	TYR	Sidechain
1	I	420	TYR	Sidechain
1	K	420	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4507	0	4511	424	0
1	C	4507	0	4512	449	0
1	E	4507	0	4512	449	0
1	G	4950	0	4944	491	0
1	I	4950	0	4943	486	0
1	K	4950	0	4943	474	0
2	B	3910	0	3851	260	0
2	D	3910	0	3851	251	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	3910	0	3851	229	0
2	H	3910	0	3851	239	0
2	J	3910	0	3851	233	0
2	L	3910	0	3851	230	0
3	A	15	0	15	1	0
3	C	15	0	15	0	0
3	E	15	0	15	1	0
3	G	15	0	15	0	0
3	I	15	0	15	2	0
3	K	15	0	15	0	0
All	All	51921	0	51561	3984	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 38.

All (3984) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:338:ILE:HD11	1:E:348:LEU:HB2	1.25	1.17
1:A:338:ILE:HD11	1:A:348:LEU:HB2	1.26	1.16
1:C:115:PRO:HG2	1:C:116:PRO:HD3	1.29	1.14
1:A:433:THR:HG22	1:A:435:VAL:H	1.06	1.11
1:G:400:LEU:HD13	1:G:449:ILE:HD11	1.33	1.11
1:K:338:ILE:HD11	1:K:348:LEU:HB2	1.22	1.10
1:I:400:LEU:HD13	1:I:449:ILE:HD11	1.32	1.10
1:I:338:ILE:HD11	1:I:348:LEU:HB2	1.23	1.09
1:C:338:ILE:HD11	1:C:348:LEU:HB2	1.25	1.09
2:L:167:GLN:N	2:L:167:GLN:HE21	1.51	1.09
1:I:433:THR:HG22	1:I:435:VAL:H	1.10	1.09
2:L:167:GLN:NE2	2:L:167:GLN:H	1.51	1.08
1:E:400:LEU:HD13	1:E:449:ILE:HD11	1.35	1.08
1:A:79:ILE:HG23	1:A:89:THR:HG21	1.36	1.07
1:E:433:THR:HG22	1:E:435:VAL:H	1.12	1.07
2:H:167:GLN:N	2:H:167:GLN:HE21	1.53	1.06
1:A:400:LEU:HD13	1:A:449:ILE:HD11	1.34	1.06
1:G:338:ILE:HD11	1:G:348:LEU:HB2	1.35	1.06
1:C:400:LEU:HD13	1:C:449:ILE:HD11	1.34	1.06
1:E:115:PRO:HG2	1:E:116:PRO:HD3	1.34	1.04
1:G:433:THR:HG22	1:G:435:VAL:H	1.23	1.04
1:A:115:PRO:HG2	1:A:116:PRO:HD3	1.37	1.04
1:K:433:THR:HG22	1:K:435:VAL:H	1.19	1.04
1:E:79:ILE:HG23	1:E:89:THR:HG21	1.38	1.03
1:C:433:THR:HG22	1:C:435:VAL:H	1.16	1.03

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:115:PRO:HG2	1:K:116:PRO:HD3	1.39	1.03
1:I:115:PRO:HG2	1:I:116:PRO:HD3	1.36	1.02
1:I:653:LYS:HD3	1:I:653:LYS:H	1.20	1.01
1:C:653:LYS:HD3	1:C:653:LYS:H	1.23	1.01
1:C:292:ILE:H	1:C:292:ILE:HD12	1.25	1.01
2:B:167:GLN:H	2:B:167:GLN:NE2	1.58	1.01
2:H:167:GLN:NE2	2:H:167:GLN:H	1.58	1.01
1:E:653:LYS:HD3	1:E:653:LYS:H	1.25	1.01
2:B:167:GLN:N	2:B:167:GLN:HE21	1.60	0.99
2:J:167:GLN:HE21	2:J:167:GLN:N	1.60	0.99
1:E:162:ILE:HG21	1:E:377:ALA:O	1.62	0.99
1:G:292:ILE:HD12	1:G:292:ILE:H	1.27	0.99
1:G:653:LYS:H	1:G:653:LYS:HD3	1.26	0.99
1:G:309:ASP:OD1	1:G:312:THR:HG22	1.63	0.98
1:E:308:LEU:HD22	1:E:316:MET:SD	2.03	0.98
1:I:309:ASP:OD1	1:I:312:THR:HG22	1.64	0.98
2:F:167:GLN:HE21	2:F:167:GLN:N	1.59	0.98
1:G:79:ILE:HG23	1:G:89:THR:HG21	1.44	0.98
1:A:653:LYS:H	1:A:653:LYS:HD3	1.23	0.98
2:D:167:GLN:H	2:D:167:GLN:HE21	0.98	0.98
1:C:79:ILE:HG23	1:C:89:THR:HG21	1.46	0.98
1:G:115:PRO:HG2	1:G:116:PRO:HD3	1.42	0.98
2:F:167:GLN:NE2	2:F:167:GLN:H	1.61	0.98
1:E:670:ILE:HG13	1:E:718:LEU:HD21	1.45	0.97
1:E:419:ARG:HD2	1:E:601:GLN:OE1	1.63	0.97
1:C:66:ILE:HD12	1:C:87:ILE:HG22	1.46	0.97
1:K:162:ILE:HG21	1:K:377:ALA:O	1.63	0.97
1:I:473:PHE:HB3	1:I:482:LEU:HD21	1.46	0.97
1:K:653:LYS:H	1:K:653:LYS:HD3	1.28	0.97
1:G:178:ILE:H	1:G:178:ILE:HD12	1.30	0.96
1:C:178:ILE:H	1:C:178:ILE:HD12	1.30	0.96
1:K:540:ARG:O	1:K:543:VAL:HG23	1.65	0.96
2:J:167:GLN:H	2:J:167:GLN:NE2	1.62	0.96
1:I:670:ILE:HG13	1:I:718:LEU:HD21	1.48	0.95
1:E:665:PRO:HG2	1:E:666:MET:HE1	1.45	0.95
1:G:162:ILE:HG21	1:G:377:ALA:O	1.67	0.95
1:K:292:ILE:HD12	1:K:292:ILE:H	1.30	0.95
1:K:400:LEU:HD13	1:K:449:ILE:HD11	1.45	0.95
1:I:528:ALA:O	1:I:532:MET:HG3	1.67	0.95
1:E:617:GLY:O	1:E:625:PHE:HB3	1.67	0.94
1:I:540:ARG:O	1:I:543:VAL:HG23	1.66	0.94
1:E:456:ALA:HB1	1:E:457:PRO:HD2	1.47	0.94

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:178:ILE:HD12	1:A:178:ILE:H	1.32	0.94
1:K:456:ALA:HB1	1:K:457:PRO:HD2	1.48	0.94
1:C:456:ALA:HB1	1:C:457:PRO:HD2	1.50	0.94
1:I:162:ILE:HG21	1:I:377:ALA:O	1.66	0.94
1:K:617:GLY:O	1:K:625:PHE:HB3	1.68	0.94
1:K:178:ILE:H	1:K:178:ILE:HD12	1.31	0.94
1:E:178:ILE:HD12	1:E:178:ILE:H	1.29	0.93
1:A:162:ILE:HG21	1:A:377:ALA:O	1.66	0.93
1:I:131:ILE:HG22	1:I:136:ALA:HB2	1.50	0.93
1:I:136:ALA:HB1	1:I:161:VAL:HG13	1.51	0.93
1:G:66:ILE:HD12	1:G:87:ILE:HG22	1.50	0.93
1:G:131:ILE:HG22	1:G:136:ALA:HB2	1.50	0.93
1:I:178:ILE:HD12	1:I:178:ILE:H	1.31	0.93
1:I:292:ILE:H	1:I:292:ILE:HD12	1.33	0.93
1:C:540:ARG:O	1:C:543:VAL:HG23	1.69	0.93
2:F:325:ASP:HA	2:F:512:ARG:HH12	1.32	0.93
1:K:309:ASP:OD1	1:K:312:THR:HG22	1.68	0.93
1:A:670:ILE:HG13	1:A:718:LEU:HD21	1.51	0.93
1:I:456:ALA:HB1	1:I:457:PRO:HD2	1.51	0.92
1:E:540:ARG:O	1:E:543:VAL:HG23	1.68	0.92
1:K:308:LEU:HD22	1:K:316:MET:SD	2.08	0.92
1:A:136:ALA:HB1	1:A:161:VAL:HG13	1.51	0.92
1:K:264:VAL:HG13	1:K:340:ASP:HB3	1.52	0.92
1:G:540:ARG:O	1:G:543:VAL:HG23	1.68	0.92
1:C:162:ILE:HG21	1:C:377:ALA:O	1.70	0.92
1:K:131:ILE:HG22	1:K:136:ALA:HB2	1.52	0.92
1:K:528:ALA:O	1:K:532:MET:HG3	1.67	0.92
1:C:308:LEU:HD22	1:C:316:MET:SD	2.10	0.91
2:F:207:SER:HB3	2:F:208:PRO:HD3	1.50	0.91
1:K:136:ALA:HB1	1:K:161:VAL:HG13	1.51	0.91
2:L:479:ILE:HD12	2:L:480:ALA:N	1.84	0.91
1:I:79:ILE:HG23	1:I:89:THR:HG21	1.52	0.91
1:K:66:ILE:HD12	1:K:87:ILE:HG22	1.53	0.91
1:E:528:ALA:O	1:E:532:MET:HG3	1.71	0.91
2:F:499:ARG:HG2	2:F:499:ARG:HH11	1.34	0.91
1:I:523:ARG:HB3	1:I:590:MET:HE1	1.53	0.91
1:E:66:ILE:HD12	1:E:87:ILE:HG22	1.53	0.91
1:A:665:PRO:HG2	1:A:666:MET:HE1	1.53	0.91
1:E:136:ALA:HB1	1:E:161:VAL:HG13	1.51	0.91
2:F:420:GLY:HA3	2:H:184:ILE:HD12	1.53	0.90
2:D:167:GLN:HE21	2:D:167:GLN:N	1.69	0.90
2:B:36:LEU:HD22	2:B:38:GLN:HG3	1.53	0.90

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:66:ILE:HD12	1:A:87:ILE:HG22	1.54	0.90
2:J:479:ILE:HD12	2:J:480:ALA:N	1.85	0.90
1:A:265:THR:O	1:A:267:PRO:HD3	1.72	0.90
1:C:457:PRO:HG2	1:C:458:THR:H	1.37	0.90
1:G:456:ALA:HB1	1:G:457:PRO:HD2	1.51	0.90
2:D:325:ASP:HA	2:D:512:ARG:HH12	1.37	0.90
2:B:88:HIS:HD2	2:B:90:CYS:H	1.17	0.89
1:A:617:GLY:O	1:A:625:PHE:HB3	1.72	0.89
2:F:83:ASP:HB2	2:F:140:LYS:HE3	1.52	0.89
2:B:325:ASP:HA	2:B:512:ARG:HH12	1.38	0.89
1:A:292:ILE:HD12	1:A:292:ILE:H	1.36	0.89
2:F:167:GLN:H	2:F:167:GLN:HE21	0.92	0.89
1:G:264:VAL:HG13	1:G:340:ASP:HB3	1.52	0.88
1:G:457:PRO:HG2	1:G:458:THR:H	1.38	0.88
1:G:390:LYS:HD3	1:G:391:LEU:N	1.87	0.88
1:G:136:ALA:HB1	1:G:161:VAL:HG13	1.55	0.88
2:L:207:SER:HB3	2:L:208:PRO:HD3	1.55	0.88
1:C:136:ALA:HB1	1:C:161:VAL:HG13	1.55	0.88
2:H:499:ARG:HH21	2:J:89:ARG:HH11	1.21	0.88
2:H:325:ASP:HA	2:H:512:ARG:HH12	1.36	0.88
1:A:456:ALA:HB1	1:A:457:PRO:HD2	1.55	0.88
2:H:499:ARG:HG2	2:H:499:ARG:HH11	1.39	0.88
2:J:499:ARG:HH11	2:J:499:ARG:HG2	1.39	0.88
1:G:528:ALA:O	1:G:532:MET:HG3	1.74	0.88
2:D:167:GLN:H	2:D:167:GLN:NE2	1.70	0.88
1:C:617:GLY:O	1:C:625:PHE:HB3	1.73	0.88
1:G:127:VAL:HG12	1:G:131:ILE:HD11	1.55	0.88
2:B:207:SER:HB3	2:B:208:PRO:HD3	1.56	0.88
1:E:457:PRO:HG2	1:E:458:THR:H	1.40	0.87
1:I:390:LYS:HD3	1:I:391:LEU:N	1.89	0.87
1:K:665:PRO:HG2	1:K:666:MET:HE1	1.57	0.87
1:G:557:THR:HG23	1:G:572:ILE:O	1.74	0.87
1:A:127:VAL:HG12	1:A:131:ILE:HD11	1.56	0.87
2:B:189:VAL:HA	2:B:282:ASN:ND2	1.89	0.87
1:I:66:ILE:HD12	1:I:87:ILE:HG22	1.55	0.86
2:H:207:SER:HB3	2:H:208:PRO:HD3	1.55	0.86
2:F:184:ILE:HD12	2:H:420:GLY:HA3	1.57	0.86
2:B:151:ASN:HD21	2:D:522:LEU:HD23	1.37	0.86
1:C:390:LYS:HD3	1:C:391:LEU:N	1.90	0.86
2:H:479:ILE:HD12	2:H:480:ALA:N	1.90	0.86
1:I:127:VAL:HG12	1:I:131:ILE:HD11	1.58	0.86
1:K:390:LYS:HD3	1:K:391:LEU:N	1.90	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:665:PRO:HG2	1:A:666:MET:CE	2.06	0.86
2:B:499:ARG:HH21	2:F:89:ARG:HH11	1.23	0.86
2:B:479:ILE:HD12	2:B:480:ALA:N	1.90	0.86
1:A:433:THR:HG22	1:A:435:VAL:N	1.91	0.85
1:I:400:LEU:HB3	1:I:449:ILE:HG12	1.58	0.85
2:J:499:ARG:HH21	2:L:89:ARG:HH11	1.23	0.85
1:A:517:LEU:HD22	1:A:517:LEU:H	1.38	0.85
1:A:131:ILE:HG22	1:A:136:ALA:HB2	1.58	0.85
1:A:308:LEU:HD22	1:A:316:MET:SD	2.16	0.85
1:E:665:PRO:HG2	1:E:666:MET:CE	2.06	0.85
1:C:517:LEU:HD22	1:C:517:LEU:H	1.40	0.85
2:L:504:GLU:HG3	2:L:505:VAL:N	1.89	0.85
1:E:131:ILE:HG22	1:E:136:ALA:HB2	1.56	0.85
1:E:156:LEU:HD12	1:E:163:PHE:HB2	1.59	0.85
1:G:396:ILE:HG12	1:G:463:ILE:HD13	1.58	0.84
1:E:557:THR:HG23	1:E:572:ILE:O	1.77	0.84
1:C:309:ASP:OD1	1:C:312:THR:HG22	1.76	0.84
1:K:517:LEU:HD22	1:K:517:LEU:H	1.40	0.84
2:H:417:TYR:OH	2:H:535:ASP:HB2	1.76	0.84
2:B:499:ARG:HH11	2:B:499:ARG:HG2	1.41	0.84
1:A:309:ASP:OD1	1:A:312:THR:HG22	1.78	0.84
1:E:421:ARG:HB3	1:E:474:GLU:HB2	1.59	0.84
1:C:131:ILE:HG22	1:C:136:ALA:HB2	1.56	0.84
1:K:112:ILE:HG13	1:K:120:SER:HB2	1.59	0.84
2:D:420:GLY:HA3	2:L:184:ILE:HD12	1.59	0.84
1:A:528:ALA:O	1:A:532:MET:HG3	1.78	0.84
2:J:207:SER:HB3	2:J:208:PRO:HD3	1.59	0.84
2:B:420:GLY:HA3	2:J:184:ILE:HD12	1.59	0.83
1:K:457:PRO:HG2	1:K:458:THR:H	1.43	0.83
2:J:417:TYR:OH	2:J:535:ASP:HB2	1.76	0.83
2:J:91:THR:HA	2:J:98:GLN:HG3	1.60	0.83
1:G:665:PRO:HG2	1:G:666:MET:HE1	1.61	0.83
1:G:665:PRO:HG2	1:G:666:MET:CE	2.09	0.83
1:E:596:TRP:CZ3	1:E:600:ASP:O	2.32	0.83
1:G:400:LEU:HB3	1:G:449:ILE:HG12	1.59	0.83
2:J:36:LEU:HD22	2:J:38:GLN:HG3	1.60	0.83
1:K:665:PRO:HG2	1:K:666:MET:CE	2.07	0.83
2:J:42:ARG:HG2	2:J:42:ARG:HH11	1.42	0.83
2:B:167:GLN:H	2:B:167:GLN:HE21	0.85	0.83
1:C:357:GLU:O	1:C:360:VAL:HG23	1.78	0.83
2:L:499:ARG:HH11	2:L:499:ARG:HG2	1.42	0.83
1:E:292:ILE:H	1:E:292:ILE:HD12	1.44	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:79:ILE:HG23	1:K:89:THR:HG21	1.60	0.83
1:G:670:ILE:HG13	1:G:718:LEU:HD21	1.61	0.82
2:J:325:ASP:HA	2:J:512:ARG:HH12	1.44	0.82
1:K:321:VAL:O	1:K:324:ALA:HB3	1.79	0.82
2:F:479:ILE:HD12	2:F:480:ALA:N	1.94	0.82
1:G:473:PHE:HB3	1:G:482:LEU:HD21	1.61	0.82
1:I:112:ILE:HG13	1:I:120:SER:HB2	1.62	0.82
1:A:419:ARG:HH11	1:A:421:ARG:HB2	1.45	0.82
1:G:112:ILE:HG13	1:G:120:SER:HB2	1.62	0.82
1:C:127:VAL:HG12	1:C:131:ILE:HD11	1.61	0.82
1:C:528:ALA:O	1:C:532:MET:HG3	1.79	0.82
1:K:198:LEU:HD13	1:K:256:ASP:O	1.79	0.82
1:K:473:PHE:HB3	1:K:482:LEU:HD21	1.61	0.81
1:G:321:VAL:O	1:G:324:ALA:HB3	1.81	0.81
1:C:665:PRO:HG2	1:C:666:MET:CE	2.10	0.81
1:C:718:LEU:HD23	1:C:718:LEU:N	1.95	0.81
1:I:517:LEU:HD22	1:I:517:LEU:H	1.45	0.81
1:I:357:GLU:O	1:I:360:VAL:HG23	1.81	0.81
1:C:321:VAL:O	1:C:324:ALA:HB3	1.80	0.81
1:C:294:ARG:HB2	1:C:504:ILE:HG12	1.63	0.81
1:E:127:VAL:HG12	1:E:131:ILE:HD11	1.61	0.81
1:C:156:LEU:HD12	1:C:163:PHE:HB2	1.62	0.81
1:A:338:ILE:CD1	1:A:348:LEU:HB2	2.09	0.81
1:G:123:VAL:O	1:G:127:VAL:HG23	1.80	0.81
2:F:184:ILE:HD13	2:H:417:TYR:HA	1.61	0.81
1:A:321:VAL:O	1:A:324:ALA:HB3	1.81	0.81
1:K:596:TRP:CZ3	1:K:600:ASP:O	2.34	0.81
2:D:88:HIS:HD2	2:D:90:CYS:H	1.27	0.81
2:D:151:ASN:HD21	2:F:522:LEU:HD23	1.45	0.80
1:C:523:ARG:HB3	1:C:590:MET:HE1	1.63	0.80
1:E:516:ASN:HB2	1:E:564:GLN:NE2	1.97	0.80
1:E:321:VAL:O	1:E:324:ALA:HB3	1.79	0.80
1:K:338:ILE:CD1	1:K:348:LEU:HB2	2.08	0.80
1:G:614:LEU:HD22	1:G:627:ILE:CG2	2.10	0.80
1:E:294:ARG:HB2	1:E:504:ILE:HG12	1.64	0.80
1:E:718:LEU:N	1:E:718:LEU:HD23	1.97	0.80
1:C:557:THR:HG23	1:C:572:ILE:O	1.80	0.80
1:I:293:GLN:O	1:I:504:ILE:HG21	1.80	0.80
1:C:156:LEU:CD1	1:C:163:PHE:HB2	2.12	0.80
1:I:156:LEU:HD12	1:I:163:PHE:HB2	1.62	0.80
1:E:517:LEU:HD22	1:E:517:LEU:H	1.47	0.80
1:I:321:VAL:O	1:I:324:ALA:HB3	1.81	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:156:LEU:CD1	1:E:163:PHE:HB2	2.12	0.80
1:E:596:TRP:HZ3	1:E:600:ASP:O	1.63	0.79
1:K:480:HIS:CD2	1:K:482:LEU:HB2	2.18	0.79
1:K:419:ARG:HH11	1:K:421:ARG:HB2	1.47	0.79
2:D:499:ARG:HH11	2:D:499:ARG:HG2	1.48	0.79
1:A:357:GLU:O	1:A:360:VAL:HG23	1.80	0.79
1:I:308:LEU:HD22	1:I:316:MET:SD	2.22	0.79
1:I:665:PRO:HG2	1:I:666:MET:CE	2.12	0.79
1:I:94:SER:HB2	1:I:114:PRO:O	1.82	0.79
1:E:130:ALA:HA	1:E:133:ALA:HB3	1.63	0.79
1:A:540:ARG:O	1:A:543:VAL:HG23	1.82	0.79
1:K:294:ARG:HB2	1:K:504:ILE:HG12	1.65	0.79
1:K:421:ARG:HB3	1:K:474:GLU:HB2	1.64	0.79
2:D:207:SER:HB3	2:D:208:PRO:HD3	1.65	0.79
1:I:123:VAL:O	1:I:127:VAL:HG23	1.81	0.79
1:K:557:THR:HG23	1:K:572:ILE:O	1.83	0.79
1:I:198:LEU:HD13	1:I:256:ASP:O	1.82	0.79
1:E:596:TRP:CZ3	1:E:600:ASP:HB2	2.17	0.79
1:K:614:LEU:HD22	1:K:627:ILE:CG2	2.13	0.78
1:I:419:ARG:HH11	1:I:421:ARG:HB2	1.47	0.78
1:I:421:ARG:HB3	1:I:474:GLU:HB2	1.63	0.78
1:C:115:PRO:CG	1:C:116:PRO:HD3	2.11	0.78
2:L:251:THR:HG21	2:L:260:ALA:HB2	1.64	0.78
2:D:479:ILE:HD12	2:D:480:ALA:N	1.97	0.78
2:B:409:ILE:HD13	2:J:205:VAL:HB	1.64	0.78
1:A:396:ILE:HG12	1:A:463:ILE:HD13	1.66	0.78
2:H:88:HIS:HD2	2:H:90:CYS:H	1.32	0.78
2:J:504:GLU:HG3	2:J:505:VAL:N	1.97	0.78
1:E:400:LEU:HB3	1:E:449:ILE:HG12	1.65	0.78
1:G:163:PHE:O	1:G:163:PHE:HD1	1.67	0.78
1:C:665:PRO:HG2	1:C:666:MET:HE1	1.65	0.78
2:L:36:LEU:HD22	2:L:38:GLN:HG3	1.64	0.78
1:I:433:THR:HG22	1:I:435:VAL:N	1.95	0.78
1:A:419:ARG:NH1	1:A:421:ARG:HB2	1.96	0.78
2:F:460:VAL:HG21	2:F:496:ALA:HB2	1.65	0.78
1:G:517:LEU:H	1:G:517:LEU:HD22	1.46	0.78
1:K:123:VAL:O	1:K:127:VAL:HG23	1.84	0.78
2:F:337:ALA:HB3	2:F:373:LYS:HD2	1.65	0.78
1:A:433:THR:CG2	1:A:435:VAL:HG12	2.13	0.78
1:C:400:LEU:HB3	1:C:449:ILE:HG12	1.66	0.78
1:A:614:LEU:HD22	1:A:627:ILE:CG2	2.13	0.78
1:A:557:THR:HG23	1:A:572:ILE:O	1.82	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:433:THR:CG2	1:E:435:VAL:HG12	2.13	0.78
1:E:419:ARG:NH1	1:E:421:ARG:HB2	1.98	0.78
1:C:516:ASN:HB2	1:C:564:GLN:NE2	1.99	0.78
1:K:433:THR:HG23	1:K:449:ILE:O	1.83	0.78
1:E:653:LYS:N	1:E:653:LYS:HD3	1.98	0.78
2:B:88:HIS:CD2	2:B:90:CYS:H	2.00	0.78
1:K:357:GLU:O	1:K:360:VAL:HG23	1.84	0.78
2:L:417:TYR:OH	2:L:535:ASP:HB2	1.83	0.78
1:G:419:ARG:HH11	1:G:421:ARG:HB2	1.48	0.78
1:I:457:PRO:HG2	1:I:458:THR:H	1.49	0.77
2:D:89:ARG:HH11	2:F:499:ARG:HH21	1.31	0.77
1:A:400:LEU:HB3	1:A:449:ILE:HG12	1.65	0.77
2:F:210:MET:HE2	2:H:417:TYR:HB2	1.66	0.77
2:B:460:VAL:HG21	2:B:496:ALA:HB2	1.66	0.77
2:B:83:ASP:HB2	2:B:140:LYS:HE3	1.65	0.77
1:E:309:ASP:OD1	1:E:312:THR:HG22	1.83	0.77
1:E:77:ARG:NH1	1:E:370:VAL:HG21	2.00	0.77
2:D:36:LEU:HD22	2:D:38:GLN:HG3	1.65	0.77
1:I:557:THR:HG23	1:I:572:ILE:O	1.83	0.77
1:I:596:TRP:CZ3	1:I:600:ASP:O	2.37	0.77
1:A:390:LYS:HD3	1:A:391:LEU:N	1.98	0.77
1:E:390:LYS:HD3	1:E:391:LEU:N	2.00	0.77
2:D:83:ASP:HB2	2:D:140:LYS:HE3	1.66	0.77
2:J:339:ASN:HD21	2:J:370:SER:HB3	1.49	0.77
2:D:88:HIS:CD2	2:D:90:CYS:H	2.02	0.77
1:G:293:GLN:O	1:G:504:ILE:HG21	1.85	0.77
1:C:130:ALA:HA	1:C:133:ALA:HB3	1.67	0.77
1:G:523:ARG:HB3	1:G:590:MET:HE1	1.64	0.77
1:K:523:ARG:HB3	1:K:590:MET:HE1	1.67	0.77
2:J:88:HIS:HD2	2:J:90:CYS:H	1.32	0.77
1:I:653:LYS:HD3	1:I:653:LYS:N	2.00	0.77
1:G:94:SER:HB2	1:G:114:PRO:O	1.85	0.77
2:F:189:VAL:HG23	2:H:532:LYS:HE2	1.67	0.77
1:C:264:VAL:HG13	1:C:340:ASP:HB3	1.67	0.77
1:E:115:PRO:CG	1:E:116:PRO:HD3	2.14	0.77
1:C:433:THR:CG2	1:C:435:VAL:HG12	2.15	0.76
1:K:334:THR:HG21	1:K:355:GLN:NE2	2.01	0.76
2:D:184:ILE:HD13	2:L:417:TYR:HA	1.67	0.76
1:I:617:GLY:O	1:I:625:PHE:HB3	1.84	0.76
1:A:163:PHE:O	1:A:163:PHE:HD1	1.67	0.76
1:I:156:LEU:CD1	1:I:163:PHE:HB2	2.15	0.76
1:G:433:THR:CG2	1:G:435:VAL:HG12	2.16	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:334:THR:HG21	1:G:355:GLN:NE2	1.99	0.76
1:K:397:GLU:HG3	1:K:453:CYS:SG	2.25	0.76
1:I:264:VAL:HG13	1:I:340:ASP:HB3	1.65	0.76
1:G:308:LEU:HD22	1:G:316:MET:SD	2.25	0.76
1:E:163:PHE:HD1	1:E:163:PHE:O	1.69	0.76
1:K:433:THR:HG22	1:K:435:VAL:N	1.98	0.76
1:K:419:ARG:NH1	1:K:421:ARG:HB2	2.01	0.76
2:D:492:ASN:HD22	2:D:494:PHE:H	1.34	0.76
1:A:467:ARG:HB3	1:A:467:ARG:HH11	1.51	0.76
1:A:130:ALA:HA	1:A:133:ALA:HB3	1.68	0.76
1:I:130:ALA:HA	1:I:133:ALA:HB3	1.66	0.76
2:J:189:VAL:HA	2:J:282:ASN:ND2	2.00	0.76
1:E:523:ARG:HB3	1:E:590:MET:HE1	1.66	0.76
1:E:94:SER:HB2	1:E:114:PRO:O	1.86	0.75
1:G:198:LEU:HD13	1:G:256:ASP:O	1.85	0.75
1:I:491:HIS:O	1:I:495:ILE:HG13	1.85	0.75
1:E:123:VAL:O	1:E:127:VAL:HG23	1.87	0.75
1:E:357:GLU:O	1:E:360:VAL:HG23	1.87	0.75
1:G:130:ALA:HA	1:G:133:ALA:HB3	1.68	0.75
1:C:101:LEU:O	1:C:105:MET:HG3	1.87	0.75
1:I:163:PHE:HD1	1:I:163:PHE:O	1.69	0.75
1:K:658:THR:HB	1:K:703:LYS:HD3	1.69	0.75
2:D:504:GLU:HG3	2:D:505:VAL:N	2.02	0.75
1:C:614:LEU:HD22	1:C:627:ILE:CG2	2.16	0.75
1:K:456:ALA:HB1	1:K:457:PRO:CD	2.16	0.75
1:C:670:ILE:HG13	1:C:718:LEU:HD21	1.68	0.75
1:G:653:LYS:N	1:G:653:LYS:HD3	2.02	0.75
1:A:294:ARG:HB2	1:A:504:ILE:HG12	1.69	0.75
1:C:596:TRP:CZ3	1:C:600:ASP:O	2.40	0.75
1:I:316:MET:HE3	1:I:337:PHE:HD1	1.52	0.75
2:B:184:ILE:HD12	2:J:420:GLY:HA3	1.69	0.75
1:G:614:LEU:HD22	1:G:627:ILE:HG23	1.67	0.75
2:J:492:ASN:HD22	2:J:494:PHE:H	1.33	0.75
1:G:101:LEU:O	1:G:105:MET:HG3	1.87	0.75
2:H:288:VAL:HG13	2:H:350:ARG:HG3	1.67	0.75
1:G:398:ASN:HB3	1:G:485:LEU:HD13	1.68	0.75
1:A:128:MET:HA	1:A:131:ILE:HD12	1.69	0.74
1:I:66:ILE:HB	1:I:138:ALA:O	1.86	0.74
2:B:522:LEU:HD23	2:F:151:ASN:HD21	1.52	0.74
2:J:348:GLU:OE1	1:K:550:ASN:HB2	1.86	0.74
1:G:334:THR:HG21	1:G:355:GLN:HE21	1.49	0.74
1:A:115:PRO:CG	1:A:116:PRO:HD3	2.17	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:123:VAL:O	1:C:127:VAL:HG23	1.86	0.74
1:C:127:VAL:O	1:C:131:ILE:HG13	1.87	0.74
1:I:596:TRP:HZ3	1:I:600:ASP:O	1.71	0.74
1:E:334:THR:HG21	1:E:355:GLN:NE2	2.02	0.74
1:C:661:MET:HE2	1:C:726:GLU:HA	1.68	0.74
2:D:417:TYR:HA	2:L:184:ILE:HD13	1.70	0.74
2:H:251:THR:HG21	2:H:260:ALA:HB2	1.69	0.74
1:G:516:ASN:HB2	1:G:564:GLN:NE2	2.03	0.74
1:K:401:TYR:HE2	1:K:448:MET:HB2	1.51	0.74
1:K:234:ASN:ND2	1:K:236:GLN:HB2	2.03	0.74
2:J:251:THR:HG21	2:J:260:ALA:HB2	1.70	0.74
1:C:94:SER:HB2	1:C:114:PRO:O	1.88	0.74
1:I:528:ALA:HB1	1:I:605:LEU:HD22	1.69	0.74
2:D:173:LEU:HD21	2:L:436:GLY:HA2	1.68	0.74
2:B:288:VAL:HG13	2:B:350:ARG:HG3	1.70	0.74
1:C:66:ILE:HD12	1:C:87:ILE:CG2	2.18	0.74
1:G:294:ARG:HB2	1:G:504:ILE:HG12	1.69	0.74
1:A:661:MET:HE2	1:A:726:GLU:HA	1.70	0.74
1:I:338:ILE:CD1	1:I:348:LEU:HB2	2.12	0.74
2:J:445:LYS:HE2	2:J:452:ASN:OD1	1.88	0.74
1:G:421:ARG:HB3	1:G:474:GLU:HB2	1.70	0.73
1:E:115:PRO:HB2	1:E:444:TYR:CD2	2.24	0.73
1:K:94:SER:HB2	1:K:114:PRO:O	1.87	0.73
1:K:334:THR:HG21	1:K:355:GLN:HE21	1.54	0.73
1:A:428(L):ALA:HB3	1:A:455:TRP:HD1	1.53	0.73
1:I:516:ASN:HB2	1:I:564:GLN:NE2	2.03	0.73
1:I:419:ARG:NH1	1:I:421:ARG:HB2	2.04	0.73
2:F:504:GLU:HG3	2:F:505:VAL:N	2.03	0.73
2:F:296:ASP:O	2:F:298:ILE:HD12	1.88	0.73
1:I:661:MET:HE2	1:I:726:GLU:HA	1.71	0.73
2:L:88:HIS:HD2	2:L:90:CYS:H	1.34	0.73
1:C:115:PRO:HB2	1:C:444:TYR:CD2	2.23	0.73
1:A:653:LYS:N	1:A:653:LYS:HD3	2.01	0.73
1:C:433:THR:HG22	1:C:435:VAL:N	1.99	0.73
1:C:163:PHE:HD1	1:C:163:PHE:O	1.71	0.73
2:F:83:ASP:HB3	2:F:86:VAL:CG2	2.18	0.73
1:C:658:THR:HB	1:C:703:LYS:HD3	1.71	0.73
1:E:189:VAL:HG21	1:E:323:LEU:HB2	1.69	0.73
1:E:433:THR:HG22	1:E:435:VAL:N	1.97	0.73
1:A:115:PRO:HB2	1:A:444:TYR:CD2	2.23	0.73
1:A:264:VAL:HG13	1:A:340:ASP:HB3	1.71	0.73
2:D:75:ASP:OD1	2:D:272:ARG:NH2	2.20	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:473:PHE:HB3	1:A:482:LEU:HD21	1.68	0.73
1:I:614:LEU:HD22	1:I:627:ILE:HG23	1.70	0.73
2:L:460:VAL:HG21	2:L:496:ALA:HB2	1.71	0.73
1:C:419:ARG:HH11	1:C:421:ARG:HB2	1.54	0.73
2:L:58:GLN:OE1	2:L:63:LYS:HE3	1.89	0.73
2:F:65:THR:HG23	2:F:68:GLU:OE1	1.89	0.73
1:C:159:GLU:HB2	1:C:161:VAL:HG23	1.71	0.73
1:A:614:LEU:HD22	1:A:627:ILE:HG23	1.71	0.73
1:G:74:ILE:HD13	1:G:143:TYR:CE2	2.23	0.72
1:E:419:ARG:HH11	1:E:421:ARG:HB2	1.52	0.72
1:I:159:GLU:HB2	1:I:161:VAL:HG23	1.71	0.72
2:F:379:ARG:NH2	2:H:535:ASP:OD2	2.22	0.72
1:C:110:VAL:HG21	1:C:130:ALA:HB1	1.71	0.72
2:F:36:LEU:HD22	2:F:38:GLN:HG3	1.71	0.72
1:K:122:ILE:HA	1:K:146:LEU:HD11	1.70	0.72
1:K:127:VAL:HG12	1:K:131:ILE:HD11	1.69	0.72
1:K:163:PHE:O	1:K:163:PHE:HD1	1.71	0.72
1:K:415:GLY:O	1:K:440:GLU:HG3	1.88	0.72
1:K:417:LEU:HD21	1:K:478:ILE:HD13	1.70	0.72
2:H:36:LEU:HD22	2:H:38:GLN:HG3	1.70	0.72
2:H:504:GLU:HG3	2:H:505:VAL:N	2.03	0.72
1:G:550:ASN:HB2	2:L:348:GLU:OE1	1.88	0.72
1:G:283:ILE:HD12	1:G:389:VAL:HG21	1.69	0.72
2:H:65:THR:HG23	2:H:68:GLU:OE1	1.89	0.72
1:I:276:CYS:HA	1:I:282:GLY:HA2	1.72	0.72
1:G:494:PHE:HA	1:G:499:MET:HE2	1.69	0.72
1:I:665:PRO:HG2	1:I:666:MET:HE1	1.72	0.72
1:I:494:PHE:HA	1:I:499:MET:HE1	1.71	0.72
2:F:288:VAL:HG13	2:F:350:ARG:HG3	1.72	0.72
1:G:480:HIS:CD2	1:G:482:LEU:HB2	2.25	0.72
1:C:653:LYS:HD3	1:C:653:LYS:N	2.03	0.72
1:A:718:LEU:HD23	1:A:718:LEU:N	2.04	0.72
1:K:596:TRP:HZ3	1:K:600:ASP:O	1.71	0.72
1:E:473:PHE:HB3	1:E:482:LEU:HD21	1.70	0.72
1:I:115:PRO:CG	1:I:116:PRO:HD3	2.16	0.72
1:K:66:ILE:H	1:K:66:ILE:HD13	1.52	0.72
1:G:456:ALA:HB1	1:G:457:PRO:CD	2.19	0.72
1:E:419:ARG:CD	1:E:601:GLN:OE1	2.38	0.72
2:F:417:TYR:HA	2:H:184:ILE:HD13	1.70	0.72
2:J:83:ASP:HB2	2:J:140:LYS:HE3	1.70	0.72
1:G:338:ILE:CD1	1:G:348:LEU:HB2	2.17	0.72
2:D:417:TYR:OH	2:D:535:ASP:HB2	1.89	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:532:LYS:HE2	2:H:189:VAL:HG23	1.72	0.72
1:A:596:TRP:CZ3	1:A:600:ASP:HB2	2.24	0.72
1:G:66:ILE:HD12	1:G:87:ILE:CG2	2.20	0.72
1:C:522:LEU:HD22	1:C:563:LEU:HD13	1.71	0.72
1:C:419:ARG:NH1	1:C:421:ARG:HB2	2.04	0.72
1:I:658:THR:HB	1:I:703:LYS:HD3	1.71	0.72
1:E:112:ILE:HG13	1:E:120:SER:HB2	1.71	0.71
1:I:718:LEU:HD23	1:I:718:LEU:N	2.05	0.71
1:E:66:ILE:HD13	1:E:66:ILE:H	1.55	0.71
1:A:457:PRO:HG2	1:A:458:THR:H	1.54	0.71
1:G:419:ARG:NH1	1:G:421:ARG:HB2	2.05	0.71
1:I:101:LEU:O	1:I:105:MET:HG3	1.89	0.71
2:B:504:GLU:HG3	2:B:505:VAL:N	2.03	0.71
2:B:462:VAL:CG2	2:J:169:GLY:HA2	2.19	0.71
1:A:112:ILE:HG13	1:A:120:SER:HB2	1.72	0.71
1:K:400:LEU:HB3	1:K:449:ILE:HG12	1.71	0.71
1:G:156:LEU:CD1	1:G:163:PHE:HB2	2.20	0.71
1:G:156:LEU:HD12	1:G:163:PHE:HB2	1.72	0.71
1:C:596:TRP:HZ3	1:C:600:ASP:O	1.73	0.71
2:F:492:ASN:HD22	2:F:494:PHE:H	1.36	0.71
1:E:338:ILE:CD1	1:E:348:LEU:HB2	2.15	0.71
2:J:123:SER:HA	2:J:158:ILE:HB	1.73	0.71
1:I:334:THR:HG21	1:I:355:GLN:NE2	2.05	0.71
1:K:293:GLN:O	1:K:504:ILE:HG21	1.90	0.71
1:I:219:LYS:HE2	1:I:229:MET:N	2.06	0.71
1:K:115:PRO:HB2	1:K:444:TYR:CD2	2.25	0.71
1:C:550:ASN:HB2	2:F:348:GLU:OE1	1.90	0.71
1:K:292:ILE:H	1:K:292:ILE:CD1	2.00	0.71
1:K:66:ILE:HB	1:K:138:ALA:O	1.90	0.71
1:C:646:LEU:HD12	2:D:72:LEU:HD21	1.73	0.71
1:A:179:THR:HG22	1:A:183:ILE:HD11	1.73	0.71
1:I:329:TYR:HE2	1:I:352:THR:HG22	1.56	0.71
1:K:433:THR:CG2	1:K:435:VAL:HG12	2.20	0.71
1:E:456:ALA:HB1	1:E:457:PRO:CD	2.20	0.71
1:A:127:VAL:O	1:A:131:ILE:HG13	1.91	0.71
1:E:85:MET:O	1:E:87:ILE:HG13	1.91	0.71
1:E:596:TRP:CE3	1:E:600:ASP:HB2	2.25	0.71
1:E:658:THR:HB	1:E:703:LYS:HD3	1.71	0.71
1:C:480:HIS:CD2	1:C:482:LEU:HB2	2.26	0.70
1:I:294:ARG:HB2	1:I:504:ILE:HG12	1.72	0.70
2:F:462:VAL:CG2	2:H:169:GLY:HA2	2.21	0.70
1:C:112:ILE:HG13	1:C:120:SER:HB2	1.72	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:467:ARG:HB3	1:C:467:ARG:HH11	1.56	0.70
1:C:293:GLN:O	1:C:504:ILE:HG21	1.90	0.70
2:J:88:HIS:CD2	2:J:90:CYS:H	2.08	0.70
2:F:156:ILE:HD12	2:F:156:ILE:N	2.06	0.70
1:C:396:ILE:HG12	1:C:463:ILE:HD13	1.71	0.70
1:I:695:MET:SD	2:J:313:PRO:HG3	2.31	0.70
2:F:83:ASP:HB3	2:F:86:VAL:HG21	1.71	0.70
1:I:83:ARG:HG2	1:I:83:ARG:HH11	1.55	0.70
1:K:661:MET:HE2	1:K:726:GLU:HA	1.73	0.70
2:D:288:VAL:HG13	2:D:350:ARG:HG3	1.72	0.70
2:F:499:ARG:HG2	2:F:499:ARG:NH1	2.02	0.70
2:J:42:ARG:NH1	2:J:42:ARG:HG2	2.05	0.70
2:D:189:VAL:HG23	2:L:532:LYS:HE2	1.73	0.70
1:K:614:LEU:HD22	1:K:627:ILE:HG23	1.73	0.70
1:G:718:LEU:HD23	1:G:718:LEU:N	2.06	0.70
1:G:329:TYR:HE2	1:G:352:THR:HG22	1.56	0.70
2:H:348:GLU:OE1	1:I:550:ASN:HB2	1.91	0.70
1:C:456:ALA:HB1	1:C:457:PRO:CD	2.20	0.70
1:C:596:TRP:CZ3	1:C:600:ASP:HB2	2.27	0.70
1:A:596:TRP:CZ3	1:A:600:ASP:O	2.45	0.70
2:D:460:VAL:HG21	2:D:496:ALA:HB2	1.72	0.70
1:K:130:ALA:HA	1:K:133:ALA:HB3	1.73	0.70
1:K:219:LYS:HE2	1:K:229:MET:N	2.05	0.70
2:F:417:TYR:OH	2:F:535:ASP:HB2	1.91	0.70
1:G:464:GLU:O	1:G:468:ILE:HG13	1.92	0.70
1:I:396:ILE:HG12	1:I:463:ILE:HD13	1.73	0.70
2:D:532:LYS:HE2	2:L:189:VAL:CG2	2.22	0.70
1:C:85:MET:O	1:C:87:ILE:HG13	1.92	0.70
1:K:543:VAL:HG11	2:L:117:ARG:HD2	1.74	0.70
1:E:110:VAL:HG21	1:E:130:ALA:HB1	1.72	0.70
1:I:329:TYR:CE2	1:I:352:THR:HG22	2.26	0.70
1:G:234:ASN:ND2	1:G:236:GLN:HB2	2.07	0.70
1:K:204:GLU:O	1:K:208:ILE:HG13	1.92	0.70
1:K:670:ILE:HG13	1:K:718:LEU:HD21	1.73	0.69
2:B:348:GLU:OE1	1:E:550:ASN:HB2	1.91	0.69
1:A:123:VAL:O	1:A:127:VAL:HG23	1.92	0.69
1:K:218:ILE:HD12	1:K:260:ILE:HG12	1.73	0.69
2:B:210:MET:HE2	2:J:417:TYR:HB2	1.74	0.69
1:G:617:GLY:O	1:G:625:PHE:HB3	1.93	0.69
2:D:379:ARG:NH2	2:L:535:ASP:OD2	2.25	0.69
1:C:494:PHE:HA	1:C:499:MET:HE2	1.73	0.69
1:E:639:ARG:HB3	1:E:643:GLN:HB3	1.74	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:66:ILE:H	1:G:66:ILE:HD13	1.58	0.69
1:E:66:ILE:HB	1:E:138:ALA:O	1.92	0.69
1:A:658:THR:HB	1:A:703:LYS:HD3	1.74	0.69
2:H:499:ARG:HG2	2:H:499:ARG:NH1	2.06	0.69
1:I:534:ARG:HG3	1:I:534:ARG:HH11	1.56	0.69
2:L:65:THR:HG23	2:L:68:GLU:OE1	1.91	0.69
1:A:523:ARG:HB3	1:A:590:MET:HE1	1.74	0.69
1:E:467:ARG:HB3	1:E:467:ARG:HH11	1.58	0.69
2:B:89:ARG:HH11	2:D:499:ARG:HH21	1.40	0.69
1:I:614:LEU:HD22	1:I:627:ILE:CG2	2.21	0.69
1:G:433:THR:HG22	1:G:435:VAL:N	2.03	0.69
1:E:159:GLU:HB2	1:E:161:VAL:HG23	1.73	0.69
1:G:159:GLU:HB2	1:G:161:VAL:HG23	1.75	0.69
1:A:550:ASN:HB2	2:D:348:GLU:OE1	1.93	0.69
1:G:219:LYS:HE2	1:G:229:MET:N	2.06	0.69
1:A:334:THR:HG21	1:A:355:GLN:NE2	2.08	0.69
1:E:614:LEU:HD22	1:E:627:ILE:CG2	2.21	0.69
1:K:695:MET:SD	2:L:313:PRO:HG3	2.33	0.69
1:E:337:PHE:C	1:E:338:ILE:HD12	2.13	0.69
1:E:128:MET:HA	1:E:131:ILE:HD12	1.74	0.69
1:G:74:ILE:HD13	1:G:143:TYR:HE2	1.57	0.69
1:A:66:ILE:HD13	1:A:66:ILE:H	1.57	0.69
1:C:122:ILE:HA	1:C:146:LEU:HD11	1.74	0.69
1:A:516:ASN:HB2	1:A:564:GLN:NE2	2.07	0.69
2:B:417:TYR:OH	2:B:535:ASP:HB2	1.93	0.69
1:G:596:TRP:CZ3	1:G:600:ASP:O	2.46	0.69
2:F:445:LYS:HE2	2:F:452:ASN:OD1	1.92	0.69
2:L:42:ARG:HH11	2:L:42:ARG:HG2	1.57	0.69
1:E:117:ALA:HB1	1:E:121:TYR:HB2	1.75	0.69
2:B:499:ARG:HH21	2:F:89:ARG:NH1	1.90	0.69
1:G:658:THR:HB	1:G:703:LYS:HD3	1.75	0.69
1:C:179:THR:HG22	1:C:183:ILE:HD11	1.73	0.69
1:C:338:ILE:CD1	1:C:348:LEU:HB2	2.13	0.69
1:A:74:ILE:HD13	1:A:143:TYR:CE2	2.27	0.69
2:B:184:ILE:HD13	2:J:417:TYR:HA	1.74	0.69
2:L:189:VAL:HA	2:L:282:ASN:ND2	2.08	0.69
2:L:445:LYS:HE2	2:L:452:ASN:OD1	1.93	0.69
2:L:83:ASP:HB2	2:L:140:LYS:HE3	1.74	0.69
1:K:201:ASP:OD1	1:K:203:ASP:HB2	1.92	0.69
1:C:538:ILE:O	1:C:541:THR:HB	1.93	0.69
1:A:670:ILE:CG1	1:A:718:LEU:HD21	2.23	0.68
2:L:149:MET:SD	2:L:186:ALA:HB2	2.32	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:334:THR:HG21	1:A:355:GLN:HE21	1.58	0.68
1:E:101:LEU:O	1:E:105:MET:HG3	1.93	0.68
1:K:115:PRO:CG	1:K:116:PRO:HD3	2.21	0.68
1:I:74:ILE:O	1:I:77:ARG:HB3	1.93	0.68
1:A:156:LEU:CD1	1:A:163:PHE:HB2	2.22	0.68
1:A:110:VAL:HG21	1:A:130:ALA:HB1	1.73	0.68
2:B:50:GLY:O	2:B:54:ARG:HD2	1.94	0.68
1:G:661:MET:HE2	1:G:726:GLU:HA	1.74	0.68
1:E:396:ILE:HG12	1:E:463:ILE:HD13	1.73	0.68
1:G:357:GLU:O	1:G:360:VAL:HG23	1.94	0.68
1:A:417:LEU:HD21	1:A:478:ILE:HD13	1.74	0.68
1:I:117:ALA:HB1	1:I:121:TYR:HB2	1.75	0.68
1:C:66:ILE:HD13	1:C:66:ILE:H	1.58	0.68
1:A:159:GLU:HB2	1:A:161:VAL:HG23	1.75	0.68
1:K:235:ASP:O	1:K:239:ARG:HG2	1.93	0.68
2:B:445:LYS:HE2	2:B:452:ASN:OD1	1.93	0.68
1:I:456:ALA:HB1	1:I:457:PRO:CD	2.23	0.68
1:I:129:ALA:O	1:I:133:ALA:HB2	1.93	0.68
2:H:329:PHE:CE1	2:H:343:GLY:HA3	2.28	0.68
1:A:122:ILE:HA	1:A:146:LEU:HD11	1.74	0.68
1:K:159:GLU:HB2	1:K:161:VAL:HG23	1.76	0.68
2:J:339:ASN:ND2	2:J:370:SER:HB3	2.08	0.68
1:A:140:HIS:CE1	1:A:142:GLY:H	2.12	0.68
2:H:445:LYS:HE2	2:H:452:ASN:OD1	1.94	0.68
2:B:65:THR:HG23	2:B:68:GLU:OE1	1.93	0.68
1:I:433:THR:CG2	1:I:435:VAL:HG12	2.24	0.68
1:K:179:THR:HG22	1:K:183:ILE:HD11	1.76	0.68
2:D:65:THR:HG23	2:D:68:GLU:OE1	1.94	0.68
1:I:538:ILE:O	1:I:541:THR:HB	1.93	0.68
1:E:312:THR:O	1:E:316:MET:HG3	1.93	0.68
1:I:596:TRP:CZ3	1:I:600:ASP:HB2	2.29	0.68
2:F:189:VAL:HA	2:F:282:ASN:ND2	2.08	0.68
2:B:368:ILE:HG13	2:B:408:VAL:HG13	1.76	0.68
1:G:112:ILE:HD12	1:G:120:SER:O	1.93	0.67
2:D:476(C):ASP:O	2:D:477:GLU:N	2.27	0.67
1:I:464:GLU:O	1:I:468:ILE:HG13	1.95	0.67
2:D:42:ARG:HH11	2:D:42:ARG:HG2	1.58	0.67
1:A:77:ARG:NH1	1:A:370:VAL:HG21	2.09	0.67
2:J:499:ARG:NH1	2:J:499:ARG:HG2	2.06	0.67
1:G:329:TYR:CE2	1:G:352:THR:HG22	2.30	0.67
1:K:718:LEU:HD23	1:K:718:LEU:N	2.08	0.67
2:L:65:THR:OG1	2:L:68:GLU:HG3	1.93	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:276:CYS:HA	1:K:282:GLY:HA2	1.76	0.67
1:E:397:GLU:HG3	1:E:453:CYS:SG	2.34	0.67
1:K:140:HIS:CE1	1:K:142:GLY:H	2.12	0.67
1:A:480:HIS:CD2	1:A:482:LEU:HB2	2.30	0.67
1:G:115:PRO:CG	1:G:116:PRO:HD3	2.21	0.67
1:K:156:LEU:CD1	1:K:163:PHE:HB2	2.25	0.67
1:I:670:ILE:CG1	1:I:718:LEU:HD21	2.22	0.67
1:I:66:ILE:HD13	1:I:66:ILE:H	1.59	0.67
2:B:416:LEU:HG	2:J:210:MET:HE1	1.76	0.67
2:B:83:ASP:HB3	2:B:86:VAL:CG2	2.24	0.67
2:F:532:LYS:HE2	2:H:189:VAL:CG2	2.25	0.67
2:J:167:GLN:H	2:J:167:GLN:HE21	0.79	0.67
1:G:264:VAL:HG13	1:G:340:ASP:CB	2.23	0.67
1:G:528:ALA:HB1	1:G:605:LEU:HD22	1.75	0.67
1:E:661:MET:HE2	1:E:726:GLU:HA	1.75	0.67
2:B:91:THR:HG21	2:L:91:THR:HG21	1.76	0.67
1:I:122:ILE:HA	1:I:146:LEU:HD11	1.76	0.67
2:J:58:GLN:OE1	2:J:63:LYS:HE3	1.94	0.67
2:F:476(C):ASP:O	2:F:477:GLU:N	2.26	0.67
1:A:642:ARG:HH11	2:B:71:ASP:HB3	1.60	0.67
1:I:334:THR:HG21	1:I:355:GLN:HE21	1.57	0.67
1:A:66:ILE:HB	1:A:138:ALA:O	1.95	0.67
1:E:464:GLU:O	1:E:468:ILE:HG13	1.94	0.67
2:B:83:ASP:HB3	2:B:86:VAL:HG21	1.76	0.67
1:I:204:GLU:O	1:I:208:ILE:HG13	1.95	0.67
2:L:423:THR:O	2:L:525:LYS:HE2	1.95	0.67
1:A:329:TYR:HE2	1:A:352:THR:HG22	1.59	0.67
1:C:276:CYS:HA	1:C:282:GLY:HA2	1.75	0.67
2:D:329:PHE:CE1	2:D:343:GLY:HA3	2.30	0.67
2:D:169:GLY:HA2	2:L:462:VAL:CG2	2.24	0.67
1:G:117:ALA:HB1	1:G:121:TYR:HB2	1.76	0.67
1:G:64:ASN:O	1:G:66:ILE:HG23	1.93	0.67
2:J:121:VAL:HG22	2:J:122:PHE:N	2.09	0.67
1:A:83:ARG:HH11	1:A:83:ARG:HG2	1.59	0.67
1:K:396:ILE:HG12	1:K:463:ILE:HD13	1.76	0.67
1:K:401:TYR:CE2	1:K:448:MET:HB2	2.30	0.67
2:J:43:ARG:HH11	2:J:43:ARG:HG2	1.60	0.67
1:I:235:ASP:O	1:I:239:ARG:HG2	1.95	0.67
1:K:101:LEU:O	1:K:105:MET:HG3	1.95	0.67
1:I:92:ILE:HB	1:I:112:ILE:HG21	1.77	0.66
2:H:492:ASN:HD22	2:H:494:PHE:H	1.41	0.66
1:K:189:VAL:HG21	1:K:323:LEU:HB2	1.76	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:101:LEU:O	1:A:105:MET:HG3	1.94	0.66
1:C:443:MET:HG3	1:C:444:TYR:CD1	2.30	0.66
1:A:117:ALA:C	1:A:119:GLN:H	1.96	0.66
1:A:64:ASN:O	1:A:66:ILE:HG23	1.95	0.66
2:D:462:VAL:CG2	2:L:169:GLY:HA2	2.26	0.66
2:L:141:ILE:O	2:L:145:MET:HG3	1.96	0.66
1:A:397:GLU:HG3	1:A:453:CYS:SG	2.35	0.66
2:H:368:ILE:HG13	2:H:408:VAL:HG13	1.77	0.66
1:K:516:ASN:HB2	1:K:564:GLN:NE2	2.10	0.66
1:E:64:ASN:O	1:E:66:ILE:HG23	1.95	0.66
2:L:499:ARG:HG2	2:L:499:ARG:NH1	2.11	0.66
2:H:150:GLN:HG2	2:L:527:VAL:HG22	1.77	0.66
2:H:151:ASN:HD21	2:L:522:LEU:HD23	1.61	0.66
1:C:329:TYR:HE2	1:C:352:THR:HG22	1.59	0.66
1:I:397:GLU:HG3	1:I:453:CYS:SG	2.35	0.66
1:E:122:ILE:HA	1:E:146:LEU:HD11	1.78	0.66
1:C:358:HIS:ND1	1:C:359:PRO:HD3	2.11	0.66
1:G:110:VAL:HG21	1:G:130:ALA:HB1	1.77	0.66
2:D:291:PHE:CE1	2:D:348:GLU:HA	2.30	0.66
2:J:368:ILE:HG13	2:J:408:VAL:HG13	1.77	0.66
1:A:156:LEU:HD12	1:A:163:PHE:HB2	1.76	0.66
1:G:232:ALA:HA	1:G:237:GLU:HG2	1.76	0.66
2:H:324:ALA:HA	2:H:345:ILE:HD12	1.78	0.66
1:C:614:LEU:HD22	1:C:627:ILE:HG23	1.77	0.66
1:K:264:VAL:HG13	1:K:340:ASP:CB	2.23	0.66
1:G:129:ALA:O	1:G:133:ALA:HB2	1.95	0.66
2:D:339:ASN:HB3	2:D:361:VAL:HG12	1.77	0.66
1:C:140:HIS:CE1	1:C:142:GLY:H	2.13	0.66
1:G:276:CYS:HA	1:G:282:GLY:HA2	1.78	0.66
1:K:400:LEU:HD11	1:K:482:LEU:HD13	1.78	0.66
1:K:117:ALA:HB1	1:K:121:TYR:HB2	1.77	0.66
1:A:456:ALA:HB1	1:A:457:PRO:CD	2.26	0.66
1:E:398:ASN:HB3	1:E:485:LEU:HD13	1.78	0.66
1:A:312:THR:O	1:A:316:MET:HG3	1.96	0.66
1:K:265:THR:HB	1:K:341:GLY:H	1.61	0.66
2:D:210:MET:HE2	2:L:417:TYR:HB2	1.78	0.66
2:H:231:VAL:O	2:H:235:THR:HB	1.96	0.66
1:E:270:ILE:HG12	1:E:289:GLU:HG3	1.76	0.65
1:C:117:ALA:C	1:C:119:GLN:H	1.98	0.65
1:E:433:THR:HG21	1:E:435:VAL:HG12	1.77	0.65
1:G:235:ASP:O	1:G:239:ARG:HG2	1.96	0.65
1:E:276:CYS:HA	1:E:282:GLY:HA2	1.78	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:339:ASN:HD21	2:L:370:SER:HB3	1.60	0.65
2:B:231:VAL:O	2:B:235:THR:HB	1.96	0.65
1:I:480:HIS:CD2	1:I:482:LEU:HB2	2.31	0.65
1:C:337:PHE:C	1:C:338:ILE:HD12	2.16	0.65
1:E:92:ILE:HB	1:E:112:ILE:HG21	1.79	0.65
1:I:115:PRO:HB2	1:I:444:TYR:CD2	2.31	0.65
1:K:596:TRP:CZ3	1:K:600:ASP:HB2	2.31	0.65
2:D:58:GLN:HE21	2:D:61:ARG:HH21	1.43	0.65
2:D:445:LYS:HE2	2:D:452:ASN:OD1	1.95	0.65
1:A:464:GLU:O	1:A:468:ILE:HG13	1.96	0.65
1:C:117:ALA:HB1	1:C:121:TYR:HB2	1.76	0.65
1:G:443:MET:HG3	1:G:444:TYR:CD1	2.32	0.65
1:K:522:LEU:HD22	1:K:563:LEU:HD13	1.79	0.65
2:D:416:LEU:HB2	2:D:441:VAL:HG22	1.79	0.65
1:E:504:ILE:HG23	1:E:505:ALA:N	2.11	0.65
1:A:276:CYS:HA	1:A:282:GLY:HA2	1.77	0.65
2:D:123:SER:HA	2:D:158:ILE:HB	1.77	0.65
1:K:232:ALA:HA	1:K:237:GLU:HG2	1.79	0.65
1:A:143:TYR:CZ	1:A:356:VAL:HG22	2.31	0.65
1:I:77:ARG:NH1	1:I:370:VAL:HG21	2.10	0.65
1:E:670:ILE:CG1	1:E:718:LEU:HD21	2.24	0.65
1:K:110:VAL:HG21	1:K:130:ALA:HB1	1.77	0.65
1:I:634:LEU:N	1:I:634:LEU:HD23	2.11	0.65
1:E:177:LYS:HB3	1:E:181:LYS:NZ	2.12	0.65
1:I:411:LEU:HD22	1:I:682:GLN:HB2	1.78	0.65
1:I:401:TYR:HE2	1:I:448:MET:HB2	1.61	0.65
2:F:189:VAL:CG2	2:H:532:LYS:HE2	2.26	0.65
2:F:199:PRO:HB3	2:F:222:TYR:CZ	2.31	0.65
1:C:428(L):ALA:HB3	1:C:455:TRP:HD1	1.61	0.65
1:G:265:THR:HB	1:G:341:GLY:H	1.61	0.65
1:E:107:ASP:O	1:E:108:GLU:HG3	1.97	0.65
1:K:312:THR:HG21	1:K:343:LYS:HD3	1.79	0.65
1:E:117:ALA:C	1:E:119:GLN:H	2.00	0.65
2:H:189:VAL:HA	2:H:282:ASN:ND2	2.12	0.65
2:D:532:LYS:HE2	2:L:189:VAL:HG23	1.78	0.65
2:F:123:SER:HA	2:F:158:ILE:HB	1.79	0.65
2:B:156:ILE:HD12	2:B:156:ILE:N	2.12	0.65
1:E:480:HIS:CD2	1:E:482:LEU:HB2	2.32	0.65
1:C:66:ILE:HB	1:C:138:ALA:O	1.96	0.65
2:H:65:THR:OG1	2:H:68:GLU:HG3	1.97	0.65
2:L:288:VAL:HG13	2:L:350:ARG:HG3	1.79	0.65
1:G:179:THR:HG22	1:G:183:ILE:HD11	1.78	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:400:LEU:HD11	1:I:482:LEU:HD13	1.78	0.65
2:F:231:VAL:O	2:F:235:THR:HB	1.97	0.65
2:J:229:ASP:O	2:J:233:THR:HG23	1.97	0.65
1:K:308:LEU:CD2	1:K:316:MET:SD	2.84	0.64
1:A:94:SER:HB2	1:A:114:PRO:O	1.97	0.64
2:F:325:ASP:HA	2:F:512:ARG:NH1	2.10	0.64
2:H:88:HIS:CD2	2:H:90:CYS:H	2.14	0.64
1:K:283:ILE:HD12	1:K:389:VAL:HG21	1.77	0.64
1:I:234:ASN:ND2	1:I:236:GLN:HB2	2.11	0.64
2:L:121:VAL:O	2:L:144:ILE:HD13	1.96	0.64
1:I:308:LEU:HD12	1:I:308:LEU:O	1.97	0.64
1:C:433:THR:HG23	1:C:449:ILE:O	1.97	0.64
2:B:416:LEU:HB2	2:B:441:VAL:HG22	1.79	0.64
1:A:421:ARG:HB3	1:A:474:GLU:HB2	1.78	0.64
1:E:293:GLN:O	1:E:504:ILE:HG21	1.96	0.64
2:L:325:ASP:HA	2:L:512:ARG:HH12	1.62	0.64
1:E:634:LEU:HD23	1:E:634:LEU:N	2.12	0.64
1:C:304:PRO:O	1:C:394:TRP:CH2	2.50	0.64
2:H:83:ASP:HB2	2:H:140:LYS:HE3	1.78	0.64
2:D:296:ASP:O	2:D:298:ILE:HD12	1.97	0.64
2:D:401:THR:HB	2:L:237:GLU:OE1	1.98	0.64
1:C:338:ILE:N	1:C:338:ILE:HD12	2.13	0.64
1:K:117:ALA:C	1:K:119:GLN:H	1.99	0.64
1:E:127:VAL:O	1:E:131:ILE:HG13	1.97	0.64
2:F:291:PHE:CE1	2:F:348:GLU:HA	2.32	0.64
1:E:83:ARG:HH11	1:E:83:ARG:HG2	1.61	0.64
1:C:397:GLU:HG3	1:C:453:CYS:SG	2.37	0.64
1:K:443:MET:HG3	1:K:444:TYR:CD1	2.32	0.64
1:A:163:PHE:O	1:A:163:PHE:CD1	2.49	0.64
2:F:227:GLY:O	2:F:231:VAL:HG23	1.98	0.64
2:D:251:THR:HG21	2:D:260:ALA:HB2	1.79	0.64
2:H:460:VAL:HG21	2:H:496:ALA:HB2	1.78	0.64
1:E:443:MET:HG3	1:E:444:TYR:CD1	2.32	0.64
1:G:66:ILE:HB	1:G:138:ALA:O	1.96	0.64
1:A:528:ALA:HB1	1:A:605:LEU:HD22	1.77	0.64
2:F:88:HIS:CD2	2:F:90:CYS:H	2.15	0.64
2:F:169:GLY:HA2	2:H:462:VAL:CG2	2.27	0.64
1:G:181:LYS:O	1:G:185:GLN:HG3	1.98	0.64
1:E:308:LEU:CD2	1:E:316:MET:SD	2.83	0.64
1:A:630:ARG:C	1:A:632:ALA:H	2.01	0.64
1:C:421:ARG:HB3	1:C:474:GLU:HB2	1.79	0.64
1:K:526:ALA:HA	1:K:561:VAL:HG11	1.79	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:382:ASP:OD1	2:B:424:VAL:HG13	1.98	0.64
1:E:358:HIS:ND1	1:E:359:PRO:HD3	2.12	0.64
1:G:178:ILE:CD1	1:G:178:ILE:H	2.07	0.64
1:K:234:ASN:HD22	1:K:236:GLN:HB2	1.62	0.64
1:G:164:VAL:HG23	1:G:377:ALA:HB2	1.80	0.64
1:I:128:MET:HA	1:I:131:ILE:HD12	1.78	0.64
1:A:66:ILE:HD12	1:A:87:ILE:CG2	2.26	0.64
2:F:346:ARG:HA	2:F:350:ARG:O	1.98	0.64
1:A:596:TRP:CE3	1:A:600:ASP:HB2	2.32	0.64
2:L:329:PHE:CE1	2:L:343:GLY:HA3	2.32	0.64
1:E:338:ILE:N	1:E:338:ILE:HD12	2.13	0.64
1:I:143:TYR:CZ	1:I:356:VAL:HG22	2.33	0.64
1:G:163:PHE:CD1	1:G:163:PHE:O	2.49	0.64
2:F:346:ARG:HH11	2:F:346:ARG:HG3	1.61	0.64
1:C:83:ARG:HG2	1:C:83:ARG:HH11	1.63	0.64
2:B:124:GLN:HE21	2:B:137:HIS:CE1	2.16	0.64
2:B:261:PHE:CD1	2:B:267:ALA:HA	2.33	0.64
2:F:419:TYR:CE1	2:F:443:SER:HB2	2.33	0.64
1:I:337:PHE:C	1:I:338:ILE:HD12	2.19	0.64
1:I:443:MET:HG3	1:I:444:TYR:CD1	2.33	0.64
1:A:265:THR:O	1:A:267:PRO:CD	2.46	0.64
2:F:339:ASN:HD21	2:F:370:SER:HB3	1.61	0.64
1:K:275:LEU:HD23	1:K:331:SER:O	1.98	0.64
2:B:123:SER:HA	2:B:158:ILE:HB	1.78	0.64
1:I:97:ASP:OD1	1:I:102:HIS:HE1	1.81	0.64
1:C:189:VAL:HG21	1:C:323:LEU:HB2	1.79	0.64
2:B:476(C):ASP:O	2:B:477:GLU:N	2.31	0.63
2:L:379:ARG:HD2	2:L:421:GLU:OE2	1.98	0.63
1:I:630:ARG:C	1:I:632:ALA:H	2.00	0.63
2:L:88:HIS:CD2	2:L:90:CYS:H	2.16	0.63
1:C:329:TYR:CE2	1:C:352:THR:HG22	2.33	0.63
1:K:329:TYR:HE2	1:K:352:THR:HG22	1.62	0.63
2:J:65:THR:HG23	2:J:68:GLU:OE1	1.98	0.63
2:F:307:PRO:O	2:F:432:ARG:NH2	2.30	0.63
1:G:128:MET:HA	1:G:131:ILE:HD12	1.80	0.63
2:F:382:ASP:OD1	2:F:424:VAL:HG13	1.98	0.63
2:D:49:GLY:C	2:D:51:GLY:H	2.00	0.63
2:D:200:CYS:HB3	2:D:223:MET:HB3	1.79	0.63
2:B:169:GLY:HA2	2:J:462:VAL:CG2	2.28	0.63
2:H:273:ARG:HD2	2:H:330:TYR:HD1	1.64	0.63
1:I:110:VAL:HG21	1:I:130:ALA:HB1	1.81	0.63
1:C:473:PHE:HB3	1:C:482:LEU:HD21	1.81	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:124:ILE:HG23	1:E:152:PHE:HD2	1.64	0.63
1:A:85:MET:O	1:A:87:ILE:HG13	1.98	0.63
1:E:66:ILE:HD12	1:E:87:ILE:CG2	2.28	0.63
1:K:275:LEU:HG	1:K:332:ALA:HB2	1.81	0.63
1:K:329:TYR:CE2	1:K:352:THR:HG22	2.32	0.63
2:L:193:ILE:HD13	2:L:274:LEU:HD23	1.80	0.63
2:L:476(C):ASP:O	2:L:477:GLU:N	2.32	0.63
2:D:91:THR:HG21	2:H:91:THR:HG21	1.80	0.63
1:E:163:PHE:CD1	1:E:163:PHE:O	2.49	0.63
1:C:143:TYR:CZ	1:C:356:VAL:HG22	2.33	0.63
1:G:414:ILE:HD11	1:G:443:MET:N	2.14	0.63
1:C:64:ASN:O	1:C:66:ILE:HG23	1.98	0.63
2:H:476(C):ASP:O	2:H:477:GLU:N	2.30	0.63
2:B:532:LYS:HE2	2:J:189:VAL:CG2	2.28	0.63
2:J:58:GLN:HE21	2:J:61:ARG:HH21	1.46	0.63
1:A:329:TYR:CE2	1:A:352:THR:HG22	2.33	0.63
1:G:177:LYS:HB3	1:G:181:LYS:NZ	2.14	0.63
2:L:242:GLU:OE2	2:L:246:GLY:HA3	1.99	0.63
1:E:411:LEU:HD22	1:E:682:GLN:HB2	1.81	0.63
1:I:316:MET:CE	1:I:337:PHE:HD1	2.11	0.63
1:K:517:LEU:N	1:K:564:GLN:HE22	1.96	0.63
1:I:231:ILE:HD12	1:I:231:ILE:H	1.64	0.63
1:E:308:LEU:HD12	1:E:308:LEU:O	1.99	0.63
1:K:156:LEU:HD12	1:K:163:PHE:HB2	1.81	0.63
1:C:695:MET:SD	2:D:313:PRO:HG3	2.39	0.63
2:H:167:GLN:HE21	2:H:167:GLN:H	0.75	0.63
1:C:517:LEU:N	1:C:564:GLN:HE22	1.95	0.63
2:H:89:ARG:HH11	2:L:499:ARG:HH21	1.46	0.63
1:G:467:ARG:HH11	1:G:467:ARG:HB3	1.64	0.63
1:E:334:THR:HG21	1:E:355:GLN:HE21	1.63	0.63
2:B:65:THR:OG1	2:B:68:GLU:HG3	1.98	0.63
1:E:526:ALA:HA	1:E:561:VAL:HG11	1.80	0.63
1:G:433:THR:HG23	1:G:449:ILE:O	1.98	0.62
1:K:653:LYS:HD3	1:K:653:LYS:N	2.08	0.62
1:K:467:ARG:HB3	1:K:467:ARG:HH11	1.63	0.62
1:I:64:ASN:O	1:I:66:ILE:HG23	1.99	0.62
2:B:151:ASN:ND2	2:D:522:LEU:HD23	2.12	0.62
2:F:91:THR:HG21	2:J:91:THR:HG21	1.80	0.62
1:E:630:ARG:C	1:E:632:ALA:H	2.00	0.62
1:G:522:LEU:HD22	1:G:563:LEU:HD13	1.81	0.62
1:I:398:ASN:HB3	1:I:485:LEU:HD13	1.81	0.62
2:J:419:TYR:CE1	2:J:443:SER:HB2	2.34	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:66:ILE:HD12	1:I:87:ILE:CG2	2.28	0.62
1:I:259:PHE:CE2	1:I:261:GLU:HB2	2.34	0.62
2:D:300:PRO:HA	2:D:509:ARG:NH1	2.14	0.62
2:H:527:VAL:HG22	2:J:150:GLN:HG2	1.81	0.62
2:F:58:GLN:CD	2:F:63:LYS:HE3	2.20	0.62
1:E:78:VAL:HG13	1:E:79:ILE:N	2.14	0.62
1:E:304:PRO:O	1:E:394:TRP:CH2	2.51	0.62
1:E:304:PRO:HG2	1:E:394:TRP:CZ2	2.33	0.62
2:J:43:ARG:NH1	2:J:43:ARG:HG2	2.13	0.62
1:E:329:TYR:HE2	1:E:352:THR:HG22	1.65	0.62
1:I:177:LYS:HB3	1:I:181:LYS:NZ	2.14	0.62
1:A:433:THR:HG23	1:A:449:ILE:O	1.99	0.62
1:E:143:TYR:CZ	1:E:356:VAL:HG22	2.34	0.62
2:D:189:VAL:CG2	2:L:532:LYS:HE2	2.28	0.62
1:I:232:ALA:HA	1:I:237:GLU:HG2	1.80	0.62
2:D:193:ILE:HD13	2:D:274:LEU:HD23	1.81	0.62
1:G:292:ILE:HD13	1:G:300:VAL:O	1.99	0.62
1:K:517:LEU:HD21	1:K:632:ALA:CB	2.28	0.62
1:I:146:LEU:HD23	1:I:152:PHE:CG	2.35	0.62
2:B:499:ARG:NH1	2:B:499:ARG:HG2	2.07	0.62
1:E:517:LEU:HD21	1:E:632:ALA:CB	2.30	0.62
1:I:264:VAL:HG13	1:I:340:ASP:CB	2.29	0.62
1:E:179:THR:HG22	1:E:183:ILE:HD11	1.80	0.62
1:K:181:LYS:O	1:K:185:GLN:HG3	2.00	0.62
1:A:337:PHE:C	1:A:338:ILE:HD12	2.19	0.62
1:G:400:LEU:HD11	1:G:482:LEU:HD13	1.82	0.62
1:K:66:ILE:HD12	1:K:87:ILE:CG2	2.26	0.62
1:K:64:ASN:O	1:K:66:ILE:HG23	2.00	0.62
1:G:596:TRP:CZ3	1:G:600:ASP:HB2	2.35	0.62
1:K:83:ARG:HG2	1:K:83:ARG:HH11	1.64	0.62
1:G:259:PHE:CE2	1:G:261:GLU:HB2	2.35	0.62
2:J:231:VAL:O	2:J:235:THR:HB	2.00	0.62
2:J:288:VAL:HG13	2:J:350:ARG:HG3	1.81	0.62
1:E:433:THR:HG23	1:E:449:ILE:O	2.00	0.62
1:A:74:ILE:HD13	1:A:143:TYR:HE2	1.64	0.62
1:E:186:GLU:C	1:E:188:ASN:H	2.02	0.62
1:G:170:ALA:O	1:G:173:ALA:HB3	1.99	0.62
1:K:480:HIS:HD2	1:K:482:LEU:HB2	1.65	0.62
2:H:379:ARG:HD2	2:H:421:GLU:OE2	1.99	0.62
1:I:112:ILE:HD12	1:I:120:SER:O	2.00	0.62
2:D:492:ASN:HB2	2:D:493:PRO:HD2	1.82	0.62
1:I:275:LEU:HD23	1:I:276:CYS:N	2.14	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:368:ILE:HG13	2:F:408:VAL:HG13	1.79	0.62
1:I:414:ILE:HD11	1:I:443:MET:N	2.14	0.62
1:A:124:ILE:HG23	1:A:152:PHE:HD2	1.65	0.62
2:D:499:ARG:NH1	2:D:499:ARG:HG2	2.12	0.62
1:I:665:PRO:HG2	1:I:666:MET:HE2	1.81	0.62
1:I:140:HIS:CE1	1:I:142:GLY:H	2.18	0.62
1:A:181:LYS:O	1:A:185:GLN:HG3	1.99	0.62
1:C:334:THR:HG21	1:C:355:GLN:NE2	2.14	0.62
1:G:397:GLU:HG3	1:G:453:CYS:SG	2.39	0.62
1:C:186:GLU:C	1:C:188:ASN:H	2.02	0.62
1:E:323:LEU:O	1:E:326:ALA:HB3	1.99	0.62
1:C:128:MET:HA	1:C:131:ILE:HD12	1.82	0.62
1:C:417:LEU:HD21	1:C:478:ILE:HD13	1.82	0.62
1:C:401:TYR:HE2	1:C:448:MET:HB2	1.65	0.62
2:J:527:VAL:HG22	2:L:150:GLN:HG2	1.81	0.62
1:G:403:GLU:O	1:G:405:PRO:HD3	1.99	0.61
1:C:75:ALA:O	1:C:78:VAL:HG12	1.99	0.61
2:D:89:ARG:NH1	2:F:499:ARG:HH21	1.98	0.61
2:H:325:ASP:HA	2:H:512:ARG:NH1	2.12	0.61
1:C:661:MET:HE1	1:C:726:GLU:HB3	1.81	0.61
1:G:275:LEU:HG	1:G:332:ALA:HB2	1.80	0.61
2:F:88:HIS:HD2	2:F:90:CYS:H	1.47	0.61
1:G:292:ILE:CD1	1:G:292:ILE:H	1.97	0.61
1:C:163:PHE:CD1	1:C:163:PHE:O	2.53	0.61
1:A:293:GLN:O	1:A:504:ILE:HG21	2.00	0.61
2:F:42:ARG:HG2	2:F:42:ARG:HH11	1.65	0.61
1:C:320:ALA:HB1	1:C:335:VAL:HG21	1.82	0.61
1:G:74:ILE:O	1:G:77:ARG:HB3	1.99	0.61
1:A:358:HIS:ND1	1:A:359:PRO:HD3	2.16	0.61
2:B:88:HIS:HD2	2:B:90:CYS:N	1.95	0.61
1:A:292:ILE:CD1	1:A:292:ILE:H	2.05	0.61
2:J:499:ARG:HH21	2:L:89:ARG:NH1	1.95	0.61
1:K:596:TRP:CE3	1:K:600:ASP:HB2	2.35	0.61
2:B:532:LYS:HE2	2:J:189:VAL:HG23	1.82	0.61
2:B:346:ARG:HA	2:B:350:ARG:O	2.00	0.61
2:J:83:ASP:HB3	2:J:86:VAL:CG2	2.30	0.61
2:H:229:ASP:O	2:H:233:THR:HG23	2.00	0.61
1:G:642:ARG:HH11	2:H:71:ASP:HB3	1.66	0.61
1:A:117:ALA:HB1	1:A:121:TYR:HB2	1.81	0.61
2:D:58:GLN:OE1	2:D:63:LYS:HE3	2.00	0.61
2:J:83:ASP:HB3	2:J:86:VAL:HG21	1.81	0.61
1:C:275:LEU:HG	1:C:332:ALA:HB2	1.83	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:189:VAL:HA	1:G:319:GLN:OE1	2.01	0.61
1:C:283:ILE:HD12	1:C:389:VAL:HG21	1.82	0.61
1:C:78:VAL:HG13	1:C:79:ILE:N	2.15	0.61
2:H:499:ARG:HH21	2:J:89:ARG:NH1	1.95	0.61
1:K:74:ILE:O	1:K:77:ARG:HB3	2.00	0.61
2:D:184:ILE:HD12	2:L:420:GLY:HA3	1.83	0.61
2:F:65:THR:OG1	2:F:68:GLU:HG3	2.00	0.61
1:A:596:TRP:HZ3	1:A:600:ASP:O	1.82	0.61
2:L:339:ASN:ND2	2:L:370:SER:HB3	2.15	0.61
1:K:97:ASP:OD1	1:K:102:HIS:HE1	1.84	0.61
1:G:122:ILE:HA	1:G:146:LEU:HD11	1.81	0.61
2:F:184:ILE:CD1	2:H:417:TYR:HA	2.30	0.61
1:G:229:MET:HG3	1:G:229:MET:O	2.01	0.61
1:A:275:LEU:HD11	1:A:372:GLN:HB2	1.82	0.61
2:H:156:ILE:HD12	2:H:156:ILE:N	2.14	0.61
1:K:538:ILE:O	1:K:541:THR:HB	2.00	0.61
1:I:400:LEU:HD23	1:I:481:ASN:OD1	2.00	0.61
1:K:497:GLY:HA2	1:K:499:MET:HE3	1.83	0.61
1:I:163:PHE:CD1	1:I:163:PHE:O	2.52	0.61
2:L:346:ARG:HH11	2:L:346:ARG:HG3	1.64	0.61
1:E:164:VAL:HG23	1:E:377:ALA:HB2	1.82	0.61
1:G:77:ARG:NH1	1:G:370:VAL:HG21	2.16	0.61
2:F:535:ASP:OD2	2:H:379:ARG:NH2	2.33	0.61
1:C:129:ALA:O	1:C:133:ALA:HB2	2.01	0.61
1:C:596:TRP:CE3	1:C:600:ASP:HB2	2.35	0.61
1:C:275:LEU:HD11	1:C:372:GLN:HB2	1.83	0.61
1:A:184:ALA:HB1	1:A:189:VAL:HB	1.83	0.61
1:C:433:THR:HG21	1:C:435:VAL:HG12	1.83	0.61
1:I:67:LEU:HG	1:I:68:ILE:H	1.64	0.61
1:G:115:PRO:HB2	1:G:444:TYR:CD2	2.36	0.61
1:K:376:VAL:C	1:K:378:ALA:H	2.04	0.61
1:E:66:ILE:O	1:E:66:ILE:HG12	2.00	0.61
1:A:661:MET:HE1	1:A:726:GLU:HB3	1.83	0.61
2:D:50:GLY:O	2:D:54:ARG:HD2	2.01	0.61
2:F:329:PHE:CE1	2:F:343:GLY:HA3	2.35	0.61
2:L:123:SER:HA	2:L:158:ILE:HB	1.82	0.61
1:E:75:ALA:O	1:E:78:VAL:HG12	2.00	0.60
1:G:365:THR:HG22	1:G:391:LEU:CD2	2.31	0.60
1:C:630:ARG:C	1:C:632:ALA:H	2.02	0.60
2:B:42:ARG:HH11	2:B:42:ARG:HG2	1.66	0.60
2:J:460:VAL:HG21	2:J:496:ALA:HB2	1.82	0.60
2:L:324:ALA:HA	2:L:345:ILE:HD12	1.82	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:201:ASP:OD1	1:I:203:ASP:HB2	2.01	0.60
1:I:74:ILE:HD13	1:I:143:TYR:CE2	2.36	0.60
1:A:164:VAL:HG23	1:A:377:ALA:HB2	1.83	0.60
1:G:458:THR:O	1:G:461:ALA:HB3	2.02	0.60
1:K:658:THR:OG1	1:K:702:GLU:HG2	2.00	0.60
1:A:464:GLU:OE2	1:A:464:GLU:HA	2.01	0.60
1:A:411:LEU:HD22	1:A:682:GLN:HB2	1.83	0.60
2:F:409:ILE:HD13	2:H:205:VAL:HB	1.82	0.60
1:E:74:ILE:O	1:E:77:ARG:HB3	2.01	0.60
1:K:127:VAL:O	1:K:131:ILE:HG13	2.01	0.60
1:K:619:ILE:HD12	1:K:625:PHE:C	2.21	0.60
2:D:417:TYR:HB2	2:L:210:MET:HE2	1.83	0.60
2:D:535:ASP:OD2	2:L:379:ARG:NH2	2.34	0.60
1:K:77:ARG:NH1	1:K:370:VAL:HG21	2.16	0.60
1:K:596:TRP:CG	1:K:597:THR:N	2.69	0.60
2:D:307:PRO:O	2:D:432:ARG:NH2	2.34	0.60
1:G:401:TYR:HE2	1:G:448:MET:HB2	1.66	0.60
2:H:423:THR:O	2:H:525:LYS:HE2	2.01	0.60
2:H:337:ALA:HB1	2:H:370:SER:HA	1.83	0.60
2:D:436:GLY:HA2	2:L:173:LEU:HD21	1.82	0.60
1:I:189:VAL:HG21	1:I:323:LEU:HB2	1.83	0.60
1:K:414:ILE:HD11	1:K:443:MET:N	2.15	0.60
1:K:517:LEU:H	1:K:564:GLN:HE22	1.46	0.60
1:C:467:ARG:HE	1:C:630:ARG:HG3	1.66	0.60
1:I:492:PRO:HA	1:I:495:ILE:HD12	1.83	0.60
1:E:181:LYS:O	1:E:185:GLN:HG3	2.00	0.60
2:L:231:VAL:O	2:L:235:THR:HB	2.01	0.60
1:I:215:PRO:HB2	1:I:231:ILE:CG2	2.32	0.60
1:E:329:TYR:CE2	1:E:352:THR:HG22	2.37	0.60
2:B:173:LEU:HD21	2:J:436:GLY:HA2	1.83	0.60
1:I:526:ALA:HA	1:I:561:VAL:HG11	1.83	0.60
1:C:653:LYS:H	1:C:653:LYS:CD	2.08	0.60
1:C:504:ILE:HG23	1:C:505:ALA:N	2.15	0.60
1:E:517:LEU:N	1:E:564:GLN:HE22	2.00	0.60
2:D:156:ILE:HD12	2:D:156:ILE:N	2.16	0.60
1:C:400:LEU:HD21	1:C:482:LEU:HD13	1.83	0.60
1:I:543:VAL:HG12	1:I:544:SER:O	2.02	0.60
2:F:417:TYR:HB2	2:H:210:MET:HE2	1.82	0.60
1:G:670:ILE:CG1	1:G:718:LEU:HD21	2.29	0.60
1:G:275:LEU:HD23	1:G:331:SER:O	2.01	0.60
1:I:186:GLU:C	1:I:188:ASN:H	2.04	0.60
2:L:156:ILE:HD12	2:L:156:ILE:N	2.15	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:417:LEU:HD21	1:G:478:ILE:HD13	1.83	0.60
1:G:538:ILE:O	1:G:541:THR:HB	2.02	0.60
1:A:283:ILE:HD12	1:A:389:VAL:HG21	1.83	0.60
2:B:237:GLU:OE1	2:J:401:THR:HB	2.01	0.60
1:E:494:PHE:HA	1:E:499:MET:HE2	1.84	0.60
1:A:304:PRO:O	1:A:394:TRP:CH2	2.54	0.60
1:C:92:ILE:HB	1:C:112:ILE:HG21	1.83	0.60
2:F:169:GLY:HA2	2:H:462:VAL:HG22	1.82	0.60
1:E:97:ASP:OD1	1:E:102:HIS:HE1	1.85	0.60
1:E:265:THR:HG22	1:E:266:GLN:HG2	1.83	0.60
1:A:480:HIS:HD2	1:A:482:LEU:HB2	1.67	0.60
1:E:403:GLU:O	1:E:405:PRO:HD3	2.02	0.60
1:A:74:ILE:O	1:A:77:ARG:HB3	2.02	0.60
2:F:339:ASN:ND2	2:F:370:SER:HB3	2.17	0.60
2:D:58:GLN:CD	2:D:63:LYS:HE3	2.22	0.60
2:B:169:GLY:HA2	2:J:462:VAL:HG22	1.83	0.60
1:C:414:ILE:HD11	1:C:443:MET:N	2.16	0.60
1:K:128:MET:HA	1:K:131:ILE:HD12	1.83	0.60
1:K:163:PHE:O	1:K:163:PHE:CD1	2.54	0.60
1:C:464:GLU:O	1:C:468:ILE:HG13	2.02	0.60
2:B:460:VAL:CG2	2:B:496:ALA:HB2	2.32	0.60
2:D:337:ALA:HB3	2:D:373:LYS:HD2	1.84	0.60
1:A:276:CYS:O	1:A:382:LEU:HD21	2.01	0.60
1:G:97:ASP:OD1	1:G:102:HIS:HE1	1.85	0.60
1:E:118:ASN:HD21	1:E:119:GLN:HE21	1.50	0.59
1:C:392:THR:O	1:C:455:TRP:HZ3	1.84	0.59
2:L:42:ARG:NH1	2:L:42:ARG:HG2	2.17	0.59
1:C:276:CYS:O	1:C:382:LEU:HD21	2.01	0.59
2:L:337:ALA:HB3	2:L:373:LYS:HD2	1.84	0.59
2:L:124:GLN:HE21	2:L:137:HIS:CE1	2.19	0.59
1:A:267:PRO:O	1:A:501:THR:HG23	2.02	0.59
2:D:151:ASN:ND2	2:F:522:LEU:HD23	2.15	0.59
1:E:129:ALA:O	1:E:133:ALA:HB2	2.01	0.59
2:B:348:GLU:OE2	1:E:551:HIS:HE1	1.85	0.59
2:H:83:ASP:HB3	2:H:86:VAL:CG2	2.32	0.59
2:H:273:ARG:HD2	2:H:330:TYR:CD1	2.37	0.59
2:L:193:ILE:CD1	2:L:274:LEU:HD23	2.33	0.59
2:D:261:PHE:CD1	2:D:267:ALA:HA	2.37	0.59
2:J:476(C):ASP:O	2:J:477:GLU:N	2.35	0.59
2:F:50:GLY:O	2:F:54:ARG:HD2	2.01	0.59
1:E:414:ILE:HD11	1:E:443:MET:N	2.18	0.59
2:B:121:VAL:HG22	2:B:122:PHE:N	2.17	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:417:TYR:HA	2:J:184:ILE:HD13	1.83	0.59
1:E:459:ARG:O	1:E:463:ILE:HG12	2.03	0.59
1:A:695:MET:SD	2:B:313:PRO:HG3	2.43	0.59
2:D:237:GLU:OE1	2:L:401:THR:HB	2.03	0.59
1:C:265:THR:HB	1:C:341:GLY:H	1.67	0.59
1:E:619:ILE:HD12	1:E:625:PHE:C	2.23	0.59
1:I:164:VAL:HG23	1:I:377:ALA:HB2	1.84	0.59
1:K:178:ILE:CD1	1:K:178:ILE:H	2.07	0.59
2:H:149:MET:SD	2:H:186:ALA:HB2	2.43	0.59
1:E:275:LEU:HG	1:E:332:ALA:HB2	1.84	0.59
2:H:42:ARG:HH11	2:H:42:ARG:HG2	1.67	0.59
2:F:239:VAL:HG22	2:F:243:GLU:HB2	1.84	0.59
1:K:577:ASP:HB2	1:K:591:ARG:NH2	2.16	0.59
1:C:679:GLN:O	1:C:706:VAL:HG13	2.02	0.59
2:J:160:ASP:OD1	2:J:198:GLY:HA3	2.03	0.59
1:K:467:ARG:HE	1:K:630:ARG:HG3	1.67	0.59
1:K:528:ALA:HB1	1:K:605:LEU:HD22	1.84	0.59
2:H:291:PHE:CE1	2:H:348:GLU:HA	2.36	0.59
2:L:325:ASP:C	2:L:327:GLY:H	2.06	0.59
2:J:65:THR:OG1	2:J:68:GLU:HG3	2.03	0.59
1:E:179:THR:O	1:E:183:ILE:HG13	2.02	0.59
2:D:160:ASP:OD1	2:D:198:GLY:HA3	2.02	0.59
2:F:173:LEU:HD21	2:H:436:GLY:HA2	1.84	0.59
1:G:83:ARG:HH11	1:G:83:ARG:HG2	1.66	0.59
2:D:83:ASP:HB3	2:D:86:VAL:CG2	2.32	0.59
2:J:492:ASN:HB2	2:J:493:PRO:HD2	1.83	0.59
2:B:462:VAL:HG22	2:J:169:GLY:HA2	1.85	0.59
2:B:54:ARG:HH11	2:B:54:ARG:HG2	1.67	0.59
1:G:275:LEU:HD23	1:G:276:CYS:N	2.18	0.59
1:G:189:VAL:HG21	1:G:323:LEU:HB2	1.83	0.59
1:G:167:PRO:O	1:G:169:GLY:N	2.36	0.59
2:B:527:VAL:HG22	2:F:150:GLN:HG2	1.84	0.59
1:K:598:PRO:HD2	2:L:292:PHE:CE1	2.38	0.59
1:I:543:VAL:HG11	2:J:117:ARG:HD2	1.85	0.59
1:K:428(L):ALA:HB3	1:K:455:TRP:HD1	1.67	0.59
1:G:131:ILE:CG2	1:G:136:ALA:HB2	2.27	0.59
2:F:460:VAL:CG2	2:F:496:ALA:HB2	2.33	0.59
2:F:334:GLU:O	2:F:338:LYS:HD2	2.02	0.59
2:H:346:ARG:HA	2:H:350:ARG:O	2.03	0.59
1:E:334:THR:HG22	1:E:351:ASN:HB2	1.84	0.59
2:F:462:VAL:HG22	2:H:169:GLY:HA2	1.84	0.59
1:E:614:LEU:HD22	1:E:627:ILE:HG23	1.84	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:634:LEU:H	1:I:634:LEU:HD23	1.67	0.59
1:G:634:LEU:HD23	1:G:634:LEU:N	2.17	0.59
2:B:61:ARG:HB2	2:B:63:LYS:HG3	1.85	0.59
1:I:117:ALA:C	1:I:119:GLN:H	2.03	0.59
1:K:358:HIS:ND1	1:K:359:PRO:HD3	2.18	0.59
1:G:543:VAL:HG12	1:G:544:SER:O	2.03	0.59
1:A:619:ILE:HD12	1:A:625:PHE:C	2.23	0.59
1:A:433:THR:HG22	1:A:434:GLY:N	2.18	0.59
1:K:400:LEU:HD23	1:K:481:ASN:OD1	2.02	0.59
1:G:234:ASN:HD22	1:G:236:GLN:HB2	1.66	0.59
1:E:275:LEU:HD11	1:E:372:GLN:HB2	1.85	0.59
2:D:368:ILE:HG13	2:D:408:VAL:HG13	1.85	0.59
2:F:261:PHE:CD1	2:F:267:ALA:HA	2.38	0.59
2:D:121:VAL:HG22	2:D:122:PHE:N	2.18	0.59
1:G:132:ARG:HD3	1:G:159:GLU:OE1	2.03	0.58
1:G:392:THR:O	1:G:455:TRP:HZ3	1.86	0.58
1:K:259:PHE:CE2	1:K:261:GLU:HB2	2.38	0.58
1:K:275:LEU:HD11	1:K:372:GLN:HB2	1.84	0.58
1:G:117:ALA:C	1:G:119:GLN:H	2.06	0.58
1:C:181:LYS:O	1:C:185:GLN:HG3	2.03	0.58
2:F:436:GLY:HA2	2:H:173:LEU:HD21	1.85	0.58
1:K:642:ARG:HH11	2:L:71:ASP:HB3	1.68	0.58
1:I:338:ILE:HD12	1:I:338:ILE:N	2.19	0.58
1:I:78:VAL:HG23	1:I:370:VAL:CG1	2.33	0.58
1:I:653:LYS:H	1:I:653:LYS:CD	2.06	0.58
1:C:178:ILE:H	1:C:178:ILE:CD1	2.08	0.58
2:B:325:ASP:HA	2:B:512:ARG:NH1	2.15	0.58
1:K:365:THR:HG22	1:K:391:LEU:CD2	2.33	0.58
1:G:596:TRP:HZ3	1:G:600:ASP:O	1.86	0.58
2:D:436:GLY:O	2:D:439:TYR:HB3	2.03	0.58
2:L:298:ILE:HG23	2:L:509:ARG:HB2	1.83	0.58
1:A:320:ALA:HB1	1:A:335:VAL:HG21	1.85	0.58
1:E:492:PRO:HA	1:E:495:ILE:HD12	1.84	0.58
2:J:324:ALA:HA	2:J:345:ILE:HD12	1.85	0.58
1:A:433:THR:HG21	1:A:435:VAL:HG12	1.83	0.58
1:G:124:ILE:HG23	1:G:152:PHE:HD2	1.68	0.58
1:A:517:LEU:N	1:A:564:GLN:HE22	2.01	0.58
1:A:112:ILE:HD12	1:A:120:SER:O	2.03	0.58
2:F:58:GLN:OE1	2:F:63:LYS:HE3	2.03	0.58
1:I:181:LYS:O	1:I:185:GLN:HG3	2.02	0.58
1:A:189:VAL:HG21	1:A:323:LEU:HB2	1.85	0.58
2:H:43:ARG:HH11	2:H:43:ARG:HG2	1.69	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:398:ASN:HB3	1:C:485:LEU:HD13	1.84	0.58
1:K:411:LEU:HD22	1:K:682:GLN:HB2	1.85	0.58
1:I:170:ALA:O	1:I:173:ALA:HB3	2.03	0.58
1:C:308:LEU:CD2	1:C:316:MET:SD	2.90	0.58
1:K:128:MET:SD	1:K:131:ILE:HD12	2.44	0.58
1:I:467:ARG:HE	1:I:630:ARG:HG3	1.68	0.58
1:K:186:GLU:C	1:K:188:ASN:H	2.07	0.58
2:J:199:PRO:HB3	2:J:222:TYR:CZ	2.38	0.58
1:E:400:LEU:HD21	1:E:482:LEU:HD13	1.84	0.58
1:C:66:ILE:CD1	1:C:87:ILE:HG22	2.29	0.58
1:C:365:THR:HG22	1:C:391:LEU:HD22	1.85	0.58
1:I:467:ARG:HH11	1:I:467:ARG:HB3	1.68	0.58
2:H:348:GLU:OE2	1:I:551:HIS:HE1	1.86	0.58
1:I:553:ARG:NH1	2:J:115:ASN:OD1	2.37	0.58
1:A:724:ILE:HG22	1:A:725:MET:HG3	1.85	0.58
1:A:78:VAL:HG13	1:A:79:ILE:N	2.18	0.58
1:I:157:GLU:C	1:I:159:GLU:H	2.06	0.58
1:C:264:VAL:CG1	1:C:340:ASP:HB3	2.34	0.58
2:L:149:MET:CE	2:L:189:VAL:HG11	2.33	0.58
1:K:552:GLU:H	1:K:552:GLU:CD	2.07	0.58
1:C:526:ALA:HA	1:C:561:VAL:HG11	1.85	0.58
1:G:140:HIS:CE1	1:G:142:GLY:H	2.21	0.58
2:F:182:ARG:HG3	2:F:182:ARG:HH11	1.69	0.58
1:K:543:VAL:HG12	1:K:544:SER:O	2.04	0.58
1:K:304:PRO:O	1:K:394:TRP:CH2	2.57	0.58
1:A:363:LEU:HD13	1:A:455:TRP:HB3	1.85	0.58
1:G:528:ALA:HB1	1:G:605:LEU:CD2	2.32	0.58
2:D:416:LEU:HG	2:L:210:MET:HE1	1.85	0.58
2:F:346:ARG:NH1	2:F:346:ARG:HG3	2.18	0.58
2:D:337:ALA:HB1	2:D:370:SER:HA	1.85	0.58
2:B:329:PHE:CE1	2:B:343:GLY:HA3	2.38	0.58
1:C:598:PRO:HD2	2:D:292:PHE:CE1	2.38	0.58
1:I:335:VAL:O	1:I:335:VAL:HG23	2.04	0.58
1:I:179:THR:O	1:I:183:ILE:HG13	2.04	0.58
1:C:312:THR:O	1:C:316:MET:HG3	2.03	0.58
1:A:128:MET:SD	1:A:131:ILE:HD12	2.44	0.58
1:G:396:ILE:HG12	1:G:463:ILE:CD1	2.31	0.58
1:K:212:ILE:HD12	1:K:260:ILE:HG22	1.86	0.58
2:L:346:ARG:HG3	2:L:346:ARG:NH1	2.16	0.58
1:C:634:LEU:HD23	1:C:634:LEU:N	2.18	0.58
1:C:577:ASP:HB2	1:C:591:ARG:NH2	2.19	0.58
2:D:150:GLN:HG2	2:F:527:VAL:HG22	1.86	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:218:ILE:HD12	1:G:260:ILE:HG12	1.86	0.58
1:E:140:HIS:CE1	1:E:142:GLY:H	2.20	0.58
1:G:143:TYR:CZ	1:G:356:VAL:HG22	2.39	0.58
1:C:74:ILE:HD13	1:C:143:TYR:CE2	2.39	0.58
1:I:128:MET:SD	1:I:131:ILE:HD12	2.44	0.58
1:G:146:LEU:HD23	1:G:152:PHE:CG	2.38	0.58
1:K:78:VAL:HG23	1:K:370:VAL:CG1	2.33	0.58
2:D:42:ARG:NH1	2:D:42:ARG:HG2	2.18	0.58
2:H:43:ARG:NH1	2:H:43:ARG:HG2	2.18	0.58
2:D:195:MET:SD	2:D:271:VAL:HG21	2.43	0.58
1:E:170:ALA:O	1:E:173:ALA:HB3	2.04	0.58
2:D:199:PRO:HB3	2:D:222:TYR:CZ	2.39	0.58
1:I:365:THR:HG22	1:I:391:LEU:CD2	2.34	0.58
1:C:365:THR:HG22	1:C:391:LEU:CD2	2.34	0.58
1:I:275:LEU:HG	1:I:332:ALA:HB2	1.86	0.58
1:G:204:GLU:O	1:G:208:ILE:HG13	2.04	0.58
1:C:272:ILE:HB	1:C:335:VAL:HG23	1.85	0.58
2:B:170:VAL:HG11	2:J:460:VAL:HG23	1.86	0.58
1:I:179:THR:HG22	1:I:183:ILE:HD11	1.85	0.58
2:H:148:ALA:HB1	2:H:153:ALA:O	2.04	0.58
2:H:87:THR:HG23	2:L:498:GLU:HG2	1.86	0.58
1:A:380:GLU:CG	1:A:381:PRO:HD2	2.33	0.58
1:E:543:VAL:HG12	1:E:544:SER:O	2.04	0.57
1:K:92:ILE:HB	1:K:112:ILE:HG21	1.86	0.57
1:A:504:ILE:HG23	1:A:505:ALA:N	2.19	0.57
1:G:596:TRP:CE3	1:G:600:ASP:HB2	2.39	0.57
1:G:658:THR:OG1	1:G:702:GLU:HG2	2.04	0.57
1:K:184:ALA:HB1	1:K:189:VAL:HB	1.85	0.57
2:L:300:PRO:HA	2:L:509:ARG:NH1	2.18	0.57
1:G:231:ILE:H	1:G:231:ILE:HD12	1.69	0.57
1:K:67:LEU:HG	1:K:68:ILE:H	1.69	0.57
1:K:74:ILE:HD13	1:K:143:TYR:CE2	2.39	0.57
1:K:415:GLY:C	1:K:440:GLU:HG3	2.24	0.57
1:C:304:PRO:HG2	1:C:394:TRP:CZ2	2.39	0.57
1:G:358:HIS:HB2	1:G:369:LEU:HD12	1.85	0.57
1:G:128:MET:SD	1:G:131:ILE:HD12	2.44	0.57
1:C:124:ILE:HG23	1:C:152:PHE:HD2	1.69	0.57
2:L:58:GLN:HE21	2:L:61:ARG:HH21	1.52	0.57
2:F:178:GLU:O	2:F:182:ARG:HG3	2.04	0.57
1:C:74:ILE:O	1:C:77:ARG:HB3	2.03	0.57
1:C:157:GLU:C	1:C:159:GLU:H	2.06	0.57
1:I:630:ARG:C	1:I:632:ALA:N	2.55	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:630:ARG:C	1:E:632:ALA:N	2.57	0.57
1:I:596:TRP:CE3	1:I:600:ASP:HB2	2.39	0.57
1:A:551:HIS:HE1	2:D:348:GLU:OE2	1.86	0.57
1:G:275:LEU:HD11	1:G:372:GLN:HB2	1.85	0.57
2:B:401:THR:HB	2:J:237:GLU:OE1	2.04	0.57
1:I:670:ILE:HD11	1:I:718:LEU:HD11	1.85	0.57
1:I:137:GLN:O	1:I:138:ALA:HB2	2.03	0.57
1:K:504:ILE:HG23	1:K:505:ALA:N	2.19	0.57
2:J:307:PRO:O	2:J:432:ARG:NH2	2.37	0.57
1:K:230:ARG:HG2	1:K:230:ARG:HH11	1.69	0.57
2:F:401:THR:HB	2:H:237:GLU:OE1	2.04	0.57
1:A:275:LEU:HD23	1:A:331:SER:O	2.04	0.57
1:G:304:PRO:HG2	1:G:394:TRP:CZ2	2.40	0.57
1:E:279:HIS:NE2	1:E:380:GLU:N	2.52	0.57
1:K:464:GLU:O	1:K:468:ILE:HG13	2.05	0.57
1:K:398:ASN:HB3	1:K:485:LEU:HD13	1.86	0.57
1:A:400:LEU:HD21	1:A:482:LEU:HD13	1.85	0.57
1:E:131:ILE:CG2	1:E:136:ALA:HB2	2.32	0.57
1:A:517:LEU:HD22	1:A:517:LEU:N	2.15	0.57
2:D:193:ILE:CD1	2:D:274:LEU:HD23	2.35	0.57
1:C:279:HIS:NE2	1:C:380:GLU:N	2.53	0.57
2:L:419:TYR:CE1	2:L:443:SER:HB2	2.39	0.57
2:B:251:THR:HG21	2:B:260:ALA:HB2	1.86	0.57
1:A:526:ALA:HA	1:A:561:VAL:HG11	1.85	0.57
1:A:491:HIS:O	1:A:495:ILE:HG13	2.04	0.57
2:B:501:PHE:CE1	2:J:174:ALA:HB2	2.40	0.57
1:G:400:LEU:HD21	1:G:482:LEU:HD13	1.85	0.57
1:C:619:ILE:HD12	1:C:625:PHE:C	2.25	0.57
1:I:121:TYR:HE2	1:I:445:TYR:HH	1.53	0.57
1:I:78:VAL:HG13	1:I:79:ILE:N	2.19	0.57
1:E:365:THR:HG22	1:E:391:LEU:HD22	1.86	0.57
1:A:157:GLU:C	1:A:159:GLU:H	2.05	0.57
1:K:137:GLN:O	1:K:138:ALA:HB2	2.04	0.57
1:K:177:LYS:O	1:K:181:LYS:HG2	2.04	0.57
1:I:189:VAL:HA	1:I:319:GLN:OE1	2.04	0.57
1:A:634:LEU:N	1:A:634:LEU:HD23	2.19	0.57
2:H:75:ASP:OD1	2:H:272:ARG:NH2	2.38	0.57
1:K:337:PHE:C	1:K:338:ILE:HD12	2.24	0.57
1:G:85:MET:O	1:G:87:ILE:HG13	2.05	0.57
1:C:164:VAL:HG23	1:C:377:ALA:HB2	1.86	0.57
2:F:207:SER:HB3	2:F:208:PRO:CD	2.26	0.57
1:G:276:CYS:O	1:G:382:LEU:HD21	2.05	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:400:LEU:HD23	1:G:481:ASN:OD1	2.05	0.57
1:K:348:LEU:O	1:K:348:LEU:HD23	2.05	0.57
1:E:117:ALA:CB	1:E:121:TYR:HB2	2.35	0.57
1:E:417:LEU:HD21	1:E:478:ILE:HD13	1.87	0.57
1:I:283:ILE:HA	1:I:386:GLN:NE2	2.19	0.57
1:E:264:VAL:CG1	1:E:340:ASP:HB3	2.35	0.57
1:G:683:GLU:HB2	1:G:704:LYS:HG3	1.86	0.57
2:B:160:ASP:OD1	2:B:198:GLY:HA3	2.04	0.57
1:K:400:LEU:HD21	1:K:482:LEU:HD13	1.86	0.57
1:A:123:VAL:HG12	1:A:126:LYS:H	1.70	0.57
1:E:137:GLN:O	1:E:138:ALA:HB2	2.05	0.57
1:I:85:MET:O	1:I:87:ILE:HG13	2.05	0.57
1:G:395:ALA:C	1:G:396:ILE:HD12	2.25	0.57
1:K:112:ILE:HD12	1:K:120:SER:O	2.05	0.57
1:A:365:THR:HG22	1:A:391:LEU:CD2	2.35	0.57
1:K:218:ILE:CD1	1:K:260:ILE:HG12	2.35	0.57
1:K:492:PRO:HA	1:K:495:ILE:HD12	1.85	0.57
2:F:200:CYS:HB3	2:F:223:MET:HB3	1.86	0.57
1:G:201:ASP:OD1	1:G:203:ASP:HB2	2.05	0.57
1:E:190:SER:N	1:E:319:GLN:OE1	2.34	0.56
1:C:270:ILE:HG12	1:C:289:GLU:HG3	1.87	0.56
1:K:457:PRO:CG	1:K:458:THR:H	2.17	0.56
1:I:146:LEU:HD23	1:I:152:PHE:CD2	2.40	0.56
2:J:458:ALA:HB3	2:J:493:PRO:HB3	1.86	0.56
1:K:215:PRO:HB2	1:K:231:ILE:CG2	2.35	0.56
1:K:642:ARG:NH1	2:L:71:ASP:OD2	2.38	0.56
1:I:279:HIS:NE2	1:I:380:GLU:N	2.53	0.56
1:E:400:LEU:HD11	1:E:482:LEU:HD13	1.86	0.56
1:G:308:LEU:HD12	1:G:308:LEU:O	2.05	0.56
1:I:74:ILE:HD13	1:I:143:TYR:HE2	1.70	0.56
1:C:137:GLN:O	1:C:138:ALA:HB2	2.05	0.56
2:D:83:ASP:HB3	2:D:86:VAL:HG21	1.87	0.56
2:F:58:GLN:HE21	2:F:61:ARG:HH21	1.52	0.56
2:B:492:ASN:HB2	2:B:493:PRO:HD2	1.86	0.56
1:G:207:LYS:O	1:G:211:GLN:HB2	2.04	0.56
1:I:66:ILE:O	1:I:66:ILE:HG12	2.05	0.56
1:G:712:ALA:HA	1:G:716:ASN:ND2	2.20	0.56
1:G:92:ILE:HB	1:G:112:ILE:HG21	1.88	0.56
2:L:83:ASP:HB3	2:L:86:VAL:HG21	1.87	0.56
1:I:401:TYR:CE2	1:I:448:MET:HB2	2.40	0.56
1:E:634:LEU:HD23	1:E:634:LEU:H	1.69	0.56
2:H:337:ALA:HB3	2:H:373:LYS:HD2	1.86	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:74:LEU:HD13	2:B:112:GLY:HA3	1.87	0.56
2:F:237:GLU:OE1	2:H:401:THR:HB	2.06	0.56
1:K:675:VAL:CG1	1:K:707:VAL:HG21	2.35	0.56
2:H:141:ILE:O	2:H:145:MET:HG3	2.06	0.56
1:C:292:ILE:HD13	1:C:300:VAL:O	2.04	0.56
1:G:517:LEU:HB3	1:G:521:ASP:HB3	1.87	0.56
2:D:458:ALA:HB3	2:D:493:PRO:HB3	1.87	0.56
1:I:275:LEU:HD23	1:I:331:SER:O	2.05	0.56
2:D:484:ALA:O	2:D:488:GLU:OE1	2.24	0.56
1:K:167:PRO:O	1:K:169:GLY:N	2.38	0.56
1:A:598:PRO:HD2	2:B:292:PHE:CE1	2.40	0.56
1:C:457:PRO:CG	1:C:458:THR:H	2.13	0.56
1:I:354:LEU:HD11	1:I:358:HIS:CE1	2.41	0.56
1:I:127:VAL:O	1:I:131:ILE:HG13	2.05	0.56
2:L:291:PHE:CE1	2:L:348:GLU:HA	2.40	0.56
1:A:275:LEU:HG	1:A:332:ALA:HB2	1.88	0.56
1:E:380:GLU:CG	1:E:381:PRO:HD2	2.36	0.56
2:B:492:ASN:HD22	2:B:494:PHE:H	1.53	0.56
1:K:553:ARG:NH1	2:L:115:ASN:OD1	2.39	0.56
1:I:675:VAL:CG1	1:I:707:VAL:HG21	2.36	0.56
2:B:447:LEU:C	2:B:448:ARG:HG2	2.25	0.56
1:E:157:GLU:C	1:E:159:GLU:H	2.08	0.56
1:E:358:HIS:HB2	1:E:369:LEU:HD12	1.87	0.56
1:A:522:LEU:HD22	1:A:563:LEU:HD13	1.87	0.56
1:K:74:ILE:HD13	1:K:143:TYR:HE2	1.69	0.56
1:G:441:ILE:HD12	1:G:478:ILE:HD13	1.88	0.56
1:E:287:GLU:OE2	1:E:305:SER:N	2.38	0.56
1:G:335:VAL:HG23	1:G:335:VAL:O	2.06	0.56
2:J:75:ASP:OD1	2:J:272:ARG:NH2	2.37	0.56
1:E:400:LEU:HD23	1:E:481:ASN:OD1	2.05	0.56
1:E:428(L):ALA:HB3	1:E:455:TRP:HD1	1.71	0.56
2:B:479:ILE:C	2:B:479:ILE:HD12	2.26	0.56
1:I:92:ILE:HB	1:I:112:ILE:CG2	2.34	0.56
2:J:149:MET:SD	2:J:186:ALA:HB2	2.45	0.56
1:C:272:ILE:HB	1:C:335:VAL:CG2	2.36	0.56
2:B:501:PHE:N	2:B:501:PHE:CD2	2.69	0.56
2:L:250:HIS:HA	2:L:254:SER:OG	2.06	0.56
1:G:337:PHE:C	1:G:338:ILE:HD12	2.26	0.56
1:A:152:PHE:CE1	1:A:156:LEU:HD11	2.41	0.56
2:D:339:ASN:HD21	2:D:370:SER:HB3	1.71	0.56
1:A:67:LEU:HG	1:A:68:ILE:H	1.71	0.56
2:H:154:PRO:HG3	2:H:191:PRO:HD2	1.88	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:296:ASP:O	2:H:298:ILE:HD12	2.06	0.56
1:K:157:GLU:C	1:K:159:GLU:H	2.07	0.56
1:K:517:LEU:HD21	1:K:632:ALA:HB1	1.87	0.56
2:B:189:VAL:CG2	2:J:532:LYS:HE2	2.36	0.56
1:E:324:ALA:O	1:E:327:VAL:HG12	2.05	0.56
2:L:460:VAL:CG2	2:L:496:ALA:HB2	2.36	0.56
1:E:552:GLU:CD	1:E:552:GLU:H	2.09	0.56
2:H:121:VAL:HG22	2:H:122:PHE:N	2.20	0.56
1:A:639:ARG:HB3	1:A:643:GLN:HB3	1.88	0.56
1:I:117:ALA:CB	1:I:121:TYR:HB2	2.36	0.56
1:K:354:LEU:HD13	1:K:354:LEU:C	2.26	0.56
1:E:363:LEU:HD13	1:E:455:TRP:HB3	1.88	0.56
1:K:497:GLY:O	1:K:499:MET:HG2	2.05	0.56
1:G:157:GLU:C	1:G:159:GLU:H	2.09	0.56
1:A:92:ILE:HB	1:A:112:ILE:HG21	1.86	0.56
2:H:492:ASN:ND2	2:H:494:PHE:H	2.03	0.56
1:G:186:GLU:C	1:G:188:ASN:H	2.07	0.56
2:F:436:GLY:O	2:F:439:TYR:HB3	2.05	0.56
1:G:683:GLU:H	1:G:704:LYS:HG2	1.71	0.56
1:K:537:GLU:HG3	1:K:553:ARG:NH2	2.21	0.56
1:C:70:ASN:ND2	1:C:145:PHE:CD1	2.74	0.56
2:B:148:ALA:HB1	2:B:153:ALA:O	2.05	0.56
1:E:335:VAL:O	1:E:335:VAL:HG23	2.07	0.55
1:G:433:THR:HG22	1:G:434:GLY:N	2.21	0.55
1:E:123:VAL:HG12	1:E:126:LYS:H	1.71	0.55
1:C:630:ARG:C	1:C:632:ALA:N	2.58	0.55
1:G:670:ILE:CD1	1:G:718:LEU:HD21	2.36	0.55
2:D:432:ARG:HG2	2:D:433:LYS:N	2.21	0.55
1:I:283:ILE:HD12	1:I:389:VAL:HG21	1.88	0.55
1:E:283:ILE:HG22	1:E:386:GLN:HG2	1.87	0.55
1:E:646:LEU:HD12	2:F:72:LEU:HD21	1.88	0.55
1:A:443:MET:HG3	1:A:444:TYR:CD1	2.41	0.55
1:G:70:ASN:ND2	1:G:145:PHE:CD1	2.74	0.55
1:C:66:ILE:O	1:C:66:ILE:HG12	2.05	0.55
1:G:137:GLN:O	1:G:138:ALA:HB2	2.06	0.55
1:G:528:ALA:CB	1:G:605:LEU:HD22	2.36	0.55
2:B:189:VAL:HA	2:B:282:ASN:HD22	1.67	0.55
1:K:177:LYS:HB3	1:K:181:LYS:NZ	2.21	0.55
1:A:70:ASN:ND2	1:A:145:PHE:CD1	2.75	0.55
2:L:307:PRO:HG3	2:L:312:THR:O	2.06	0.55
1:A:75:ALA:O	1:A:78:VAL:HG12	2.06	0.55
1:E:421:ARG:HD2	1:E:474:GLU:HG3	1.87	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:394:TRP:CE3	1:K:459:ARG:HG3	2.41	0.55
1:A:630:ARG:C	1:A:632:ALA:N	2.58	0.55
1:K:75:ALA:O	1:K:78:VAL:HG12	2.06	0.55
1:I:517:LEU:HD21	1:I:632:ALA:CB	2.36	0.55
1:A:129:ALA:O	1:A:133:ALA:HB2	2.06	0.55
1:I:185:GLN:O	1:I:188:ASN:N	2.38	0.55
1:A:177:LYS:HB3	1:A:181:LYS:NZ	2.21	0.55
1:A:272:ILE:HB	1:A:335:VAL:CG2	2.35	0.55
1:E:484:PHE:O	1:E:487:ALA:HB3	2.06	0.55
1:A:538:ILE:O	1:A:541:THR:HB	2.06	0.55
2:H:78:SER:O	2:H:112:GLY:HA2	2.07	0.55
1:A:338:ILE:N	1:A:338:ILE:HD12	2.21	0.55
1:G:380:GLU:CG	1:G:381:PRO:HD2	2.36	0.55
1:G:283:ILE:HD12	1:G:389:VAL:CG2	2.37	0.55
2:F:492:ASN:HB2	2:F:493:PRO:HD2	1.88	0.55
1:K:491:HIS:O	1:K:495:ILE:HG13	2.07	0.55
1:A:683:GLU:H	1:A:704:LYS:HG2	1.70	0.55
1:A:78:VAL:HA	1:A:370:VAL:HG11	1.88	0.55
1:G:443:MET:HG3	1:G:444:TYR:CE1	2.41	0.55
1:A:517:LEU:HD21	1:A:632:ALA:CB	2.37	0.55
1:G:92:ILE:HD12	1:G:112:ILE:HD13	1.87	0.55
2:D:346:ARG:HA	2:D:350:ARG:O	2.06	0.55
1:E:275:LEU:HD23	1:E:331:SER:O	2.06	0.55
2:D:307:PRO:HG3	2:D:312:THR:O	2.07	0.55
1:G:534:ARG:HG3	1:G:534:ARG:HH11	1.70	0.55
1:I:598:PRO:HD2	2:J:292:PHE:CE1	2.42	0.55
2:B:419:TYR:CE1	2:B:443:SER:HB2	2.42	0.55
1:G:78:VAL:HG23	1:G:370:VAL:CG1	2.36	0.55
1:I:124:ILE:O	1:I:128:MET:HB2	2.05	0.55
1:G:127:VAL:O	1:G:131:ILE:HG13	2.06	0.55
2:F:379:ARG:HD2	2:F:421:GLU:OE2	2.07	0.55
1:G:324:ALA:O	1:G:327:VAL:HG12	2.06	0.55
1:A:324:ALA:O	1:A:327:VAL:HG12	2.06	0.55
1:K:229:MET:O	1:K:229:MET:HG3	2.06	0.55
1:G:661:MET:HE1	1:G:726:GLU:HB3	1.88	0.55
2:D:65:THR:OG1	2:D:68:GLU:HG3	2.07	0.55
1:G:401:TYR:CD2	1:G:448:MET:HA	2.42	0.55
1:G:215:PRO:HB2	1:G:231:ILE:CG2	2.36	0.55
1:I:528:ALA:HB1	1:I:605:LEU:CD2	2.35	0.55
1:K:392:THR:O	1:K:455:TRP:HZ3	1.89	0.55
1:C:123:VAL:HG12	1:C:126:LYS:H	1.70	0.55
1:G:504:ILE:HG23	1:G:505:ALA:N	2.20	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:186:GLU:C	1:A:188:ASN:H	2.09	0.55
2:D:154:PRO:HG3	2:D:191:PRO:HD2	1.89	0.55
2:F:160:ASP:OD1	2:F:198:GLY:HA3	2.06	0.55
2:F:196:ILE:HG22	2:F:221:SER:HB2	1.89	0.55
1:E:156:LEU:HD22	1:E:161:VAL:HB	1.89	0.55
1:G:517:LEU:HD21	1:G:632:ALA:CB	2.37	0.55
2:B:398:LEU:O	2:B:403:GLN:HG3	2.07	0.55
2:J:250:HIS:HA	2:J:254:SER:OG	2.07	0.55
1:C:443:MET:HG3	1:C:444:TYR:CE1	2.42	0.55
1:K:517:LEU:N	1:K:517:LEU:HD22	2.17	0.55
1:A:358:HIS:HB2	1:A:369:LEU:HD12	1.88	0.55
1:G:464:GLU:HA	1:G:464:GLU:OE2	2.05	0.55
1:E:275:LEU:HD23	1:E:276:CYS:N	2.21	0.55
1:G:179:THR:O	1:G:183:ILE:HG13	2.07	0.55
1:C:334:THR:HG22	1:C:351:ASN:HB2	1.87	0.55
1:G:401:TYR:HD2	1:G:448:MET:HA	1.71	0.55
1:E:401:TYR:HE2	1:E:448:MET:HB2	1.72	0.55
1:K:433:THR:HG21	1:K:435:VAL:HG12	1.88	0.55
1:I:417:LEU:HD21	1:I:478:ILE:HD13	1.88	0.55
2:J:94:ASN:HA	2:J:98:GLN:OE1	2.06	0.55
1:I:602:LEU:HD12	1:I:614:LEU:O	2.06	0.55
2:B:235:THR:HG22	2:B:237:GLU:HB2	1.88	0.55
2:L:121:VAL:HG22	2:L:122:PHE:N	2.22	0.55
2:D:43:ARG:HH11	2:D:43:ARG:HG2	1.72	0.55
2:L:382:ASP:OD1	2:L:424:VAL:HG13	2.06	0.55
2:B:307:PRO:O	2:B:432:ARG:NH2	2.39	0.55
2:H:498:GLU:HG2	2:J:87:THR:HG23	1.89	0.55
1:C:539:ARG:NH2	2:D:326:GLU:OE2	2.40	0.55
2:L:229:ASP:O	2:L:233:THR:HG23	2.06	0.55
1:G:480:HIS:HD2	1:G:482:LEU:HB2	1.72	0.54
1:C:316:MET:CE	1:C:337:PHE:HD1	2.19	0.54
1:E:405:PRO:HG2	1:E:481:ASN:HA	1.89	0.54
2:L:117:ARG:HH21	2:L:280:LEU:HG	1.72	0.54
1:G:358:HIS:ND1	1:G:359:PRO:HD3	2.22	0.54
1:G:376:VAL:C	1:G:378:ALA:H	2.09	0.54
1:I:276:CYS:O	1:I:382:LEU:HD21	2.07	0.54
1:C:275:LEU:HD23	1:C:331:SER:O	2.06	0.54
2:B:324:ALA:HA	2:B:345:ILE:HD12	1.89	0.54
1:C:598:PRO:HD2	2:D:292:PHE:CD1	2.42	0.54
2:D:309:ASN:HD21	2:D:311:ASN:HB2	1.72	0.54
1:K:563:LEU:O	1:K:565:GLY:N	2.40	0.54
1:A:376:VAL:C	1:A:378:ALA:N	2.59	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:264:VAL:HG13	1:A:340:ASP:CB	2.37	0.54
2:J:522:LEU:HD23	2:L:151:ASN:HD21	1.71	0.54
1:A:97:ASP:OD1	1:A:102:HIS:HE1	1.90	0.54
1:E:73:GLU:OE1	1:E:451:LYS:NZ	2.37	0.54
3:I:801:BTI:H63	2:J:399:PRO:HD3	1.89	0.54
2:B:182:ARG:HG3	2:B:182:ARG:HH11	1.72	0.54
1:E:365:THR:HG22	1:E:391:LEU:CD2	2.38	0.54
1:I:458:THR:O	1:I:461:ALA:HB3	2.07	0.54
1:K:532:MET:O	1:K:535:VAL:HB	2.07	0.54
2:L:207:SER:HB3	2:L:208:PRO:CD	2.32	0.54
1:A:543:VAL:HG12	1:A:544:SER:O	2.08	0.54
1:G:517:LEU:N	1:G:564:GLN:HE22	2.05	0.54
2:B:434:ALA:HB3	2:B:460:VAL:HG12	1.87	0.54
1:K:231:ILE:H	1:K:231:ILE:HD12	1.72	0.54
1:C:266:GLN:HG2	1:C:341:GLY:CA	2.38	0.54
2:D:43:ARG:HG2	2:D:43:ARG:NH1	2.22	0.54
1:G:646:LEU:HD12	2:H:72:LEU:HD11	1.89	0.54
2:L:75:ASP:OD1	2:L:272:ARG:NH2	2.39	0.54
1:G:526:ALA:HA	1:G:561:VAL:HG11	1.90	0.54
2:L:492:ASN:ND2	2:L:494:PHE:HB2	2.22	0.54
1:K:335:VAL:HG23	1:K:335:VAL:O	2.08	0.54
1:G:78:VAL:HG13	1:G:79:ILE:N	2.21	0.54
1:K:304:PRO:HG2	1:K:394:TRP:CZ2	2.43	0.54
1:G:66:ILE:HD13	1:G:88:SER:O	2.06	0.54
2:F:293:ASP:OD1	2:F:325:ASP:O	2.25	0.54
1:A:92:ILE:HD12	1:A:112:ILE:HD13	1.89	0.54
2:D:169:GLY:HA2	2:L:462:VAL:HG22	1.90	0.54
2:J:156:ILE:HD12	2:J:156:ILE:N	2.21	0.54
1:E:577:ASP:HB2	1:E:591:ARG:NH2	2.23	0.54
1:G:491:HIS:O	1:G:495:ILE:HG13	2.06	0.54
1:A:287:GLU:OE2	1:A:305:SER:N	2.36	0.54
1:G:75:ALA:O	1:G:78:VAL:HG12	2.07	0.54
1:K:376:VAL:C	1:K:378:ALA:N	2.60	0.54
1:K:378:ALA:O	1:K:379:GLY:C	2.46	0.54
2:F:83:ASP:HB3	2:F:86:VAL:HG23	1.90	0.54
2:D:492:ASN:ND2	2:D:494:PHE:H	2.01	0.54
1:C:411:LEU:HD22	1:C:682:GLN:HB2	1.90	0.54
1:G:312:THR:O	1:G:316:MET:HG3	2.08	0.54
1:I:670:ILE:HD12	1:I:712:ALA:HB1	1.88	0.54
2:B:141:ILE:O	2:B:145:MET:HG3	2.06	0.54
2:B:291:PHE:CE1	2:B:348:GLU:HA	2.43	0.54
2:B:200:CYS:HB3	2:B:223:MET:HB3	1.88	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:436:GLY:O	2:B:439:TYR:HB3	2.07	0.54
1:G:316:MET:CE	1:G:337:PHE:HD1	2.21	0.54
1:K:444:TYR:O	1:K:445:TYR:CG	2.61	0.54
1:G:378:ALA:O	1:G:379:GLY:C	2.46	0.54
1:E:178:ILE:H	1:E:178:ILE:CD1	2.06	0.54
2:L:325:ASP:O	2:L:327:GLY:N	2.40	0.54
1:C:380:GLU:CG	1:C:381:PRO:HD2	2.38	0.54
2:J:296:ASP:O	2:J:298:ILE:HD12	2.08	0.54
1:I:683:GLU:HB2	1:I:704:LYS:HG3	1.88	0.54
2:F:193:ILE:CD1	2:F:274:LEU:HD23	2.37	0.54
1:E:74:ILE:HD13	1:E:143:TYR:CE2	2.42	0.54
1:K:123:VAL:HG12	1:K:126:LYS:H	1.73	0.54
1:A:376:VAL:C	1:A:378:ALA:H	2.10	0.54
1:C:543:VAL:HG12	1:C:544:SER:O	2.08	0.54
1:I:518:PRO:HD2	1:I:521:ASP:HB2	1.89	0.54
2:H:307:PRO:O	2:H:432:ARG:NH2	2.41	0.54
1:C:184:ALA:HB1	1:C:189:VAL:HB	1.90	0.54
2:D:49:GLY:O	2:D:51:GLY:N	2.41	0.54
1:C:401:TYR:CE2	1:C:448:MET:HB2	2.43	0.54
1:G:347:PHE:CD1	1:G:347:PHE:O	2.61	0.54
2:L:239:VAL:HG22	2:L:243:GLU:HB2	1.89	0.54
2:F:374:ALA:HB3	2:F:415:LEU:HD13	1.90	0.54
1:E:189:VAL:CG2	1:E:323:LEU:HB2	2.36	0.54
1:C:444:TYR:CD1	1:C:444:TYR:N	2.76	0.54
1:I:358:HIS:ND1	1:I:359:PRO:HD3	2.21	0.54
1:A:392:THR:O	1:A:455:TRP:HZ3	1.90	0.54
1:I:324:ALA:O	1:I:327:VAL:HG12	2.08	0.54
2:J:149:MET:CE	2:J:189:VAL:HG11	2.38	0.54
1:G:695:MET:SD	2:H:313:PRO:HG3	2.48	0.54
1:K:190:SER:N	1:K:319:GLN:OE1	2.34	0.54
2:D:298:ILE:HG23	2:D:509:ARG:HB2	1.90	0.54
1:E:491:HIS:CE1	1:E:493:LYS:HB2	2.43	0.54
1:A:534:ARG:HG3	1:A:534:ARG:HH11	1.72	0.54
2:L:285:LYS:HB3	2:L:286:PRO:HD2	1.89	0.54
1:E:92:ILE:HB	1:E:112:ILE:CG2	2.37	0.54
1:C:464:GLU:OE2	1:C:464:GLU:HA	2.08	0.54
1:I:155:ALA:O	1:I:159:GLU:HG2	2.08	0.54
1:G:66:ILE:HG12	1:G:66:ILE:O	2.06	0.54
2:F:337:ALA:HB1	2:F:370:SER:HA	1.90	0.54
1:K:441:ILE:HD12	1:K:478:ILE:HD13	1.89	0.54
1:E:283:ILE:CG2	1:E:386:GLN:HG2	2.38	0.54
1:I:367:VAL:HG12	1:I:368:ASP:N	2.22	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:245:SER:C	1:K:247:ASN:H	2.11	0.54
1:A:444:TYR:CD1	1:A:444:TYR:N	2.76	0.53
1:I:670:ILE:CD1	1:I:718:LEU:HD21	2.38	0.53
1:I:354:LEU:HD11	1:I:358:HIS:ND1	2.23	0.53
1:C:517:LEU:H	1:C:564:GLN:HE22	1.55	0.53
1:K:143:TYR:CZ	1:K:356:VAL:HG22	2.43	0.53
1:E:517:LEU:HD21	1:E:632:ALA:HB1	1.90	0.53
1:G:619:ILE:HD12	1:G:625:PHE:C	2.29	0.53
2:L:436:GLY:O	2:L:439:TYR:HB3	2.07	0.53
1:K:670:ILE:CD1	1:K:718:LEU:HD21	2.38	0.53
2:D:42:ARG:O	2:D:45:ALA:HB3	2.08	0.53
2:H:83:ASP:HB3	2:H:86:VAL:HG21	1.88	0.53
1:G:304:PRO:O	1:G:394:TRP:CH2	2.61	0.53
1:E:63:PHE:N	1:E:63:PHE:CD1	2.76	0.53
2:B:298:ILE:N	2:B:298:ILE:HD12	2.23	0.53
2:J:200:CYS:HB3	2:J:223:MET:HB3	1.90	0.53
1:C:267:PRO:O	1:C:501:THR:HG23	2.07	0.53
1:A:99:GLN:HB2	1:A:436:TYR:OH	2.08	0.53
1:C:400:LEU:HD11	1:C:482:LEU:HD13	1.90	0.53
1:E:457:PRO:CG	1:E:458:THR:H	2.14	0.53
1:C:358:HIS:HB2	1:C:369:LEU:HD12	1.90	0.53
2:B:109:THR:HG22	2:B:122:PHE:CB	2.38	0.53
1:G:518:PRO:O	1:G:521:ASP:N	2.36	0.53
1:K:129:ALA:O	1:K:133:ALA:HB2	2.07	0.53
1:G:218:ILE:CD1	1:G:260:ILE:HG12	2.38	0.53
1:K:537:GLU:HG3	1:K:553:ARG:HH21	1.72	0.53
1:E:283:ILE:HD12	1:E:389:VAL:HG21	1.89	0.53
1:E:534:ARG:HH11	1:E:534:ARG:HG3	1.73	0.53
2:H:193:ILE:CD1	2:H:274:LEU:HD23	2.38	0.53
1:E:272:ILE:HB	1:E:335:VAL:CG2	2.38	0.53
1:G:312:THR:HG21	1:G:343:LYS:HD3	1.90	0.53
1:I:378:ALA:O	1:I:379:GLY:C	2.46	0.53
1:K:66:ILE:O	1:K:66:ILE:HG12	2.08	0.53
1:G:457:PRO:HG2	1:G:458:THR:N	2.17	0.53
1:A:463:ILE:HD12	1:A:494:PHE:CE1	2.44	0.53
2:H:346:ARG:HH11	2:H:346:ARG:HG3	1.72	0.53
1:K:670:ILE:HD12	1:K:712:ALA:HB1	1.90	0.53
1:E:276:CYS:O	1:E:382:LEU:HD21	2.08	0.53
2:L:43:ARG:HG2	2:L:43:ARG:HH11	1.74	0.53
1:E:136:ALA:HB1	1:E:161:VAL:CG1	2.33	0.53
1:E:625:PHE:CD1	1:E:625:PHE:N	2.76	0.53
1:E:543:VAL:HG11	2:F:117:ARG:HD2	1.89	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:285:LEU:N	1:I:285:LEU:HD12	2.23	0.53
1:K:71:ARG:HG3	1:K:72:GLY:N	2.24	0.53
1:E:334:THR:CG2	1:E:351:ASN:HB2	2.39	0.53
2:H:149:MET:CE	2:H:189:VAL:HG11	2.39	0.53
2:D:339:ASN:ND2	2:D:370:SER:HB3	2.24	0.53
1:G:177:LYS:O	1:G:181:LYS:HG2	2.08	0.53
1:I:304:PRO:O	1:I:394:TRP:CH2	2.61	0.53
1:I:304:PRO:HG2	1:I:394:TRP:CZ2	2.44	0.53
2:B:94:ASN:HA	2:B:98:GLN:OE1	2.08	0.53
2:B:299:GLU:HG3	2:B:322:LYS:HB3	1.89	0.53
1:E:312:THR:O	1:E:315:ALA:HB3	2.09	0.53
1:K:338:ILE:N	1:K:338:ILE:HD12	2.23	0.53
1:I:78:VAL:HG23	1:I:370:VAL:HG11	1.90	0.53
1:K:132:ARG:HD3	1:K:159:GLU:OE1	2.08	0.53
1:I:392:THR:O	1:I:455:TRP:HZ3	1.91	0.53
2:B:460:VAL:HG21	2:B:496:ALA:CB	2.35	0.53
1:I:661:MET:HE1	1:I:726:GLU:HB3	1.91	0.53
2:D:337:ALA:HB3	2:D:373:LYS:CD	2.39	0.53
1:C:334:THR:HG21	1:C:355:GLN:HE21	1.72	0.53
1:I:184:ALA:HB1	1:I:189:VAL:HB	1.91	0.53
2:D:145:MET:HE3	2:D:183:ASN:HD21	1.73	0.53
1:A:272:ILE:HB	1:A:335:VAL:HG23	1.90	0.53
1:A:683:GLU:HB2	1:A:704:LYS:HG3	1.90	0.53
1:A:295:ARG:O	1:A:296:ASN:HB2	2.09	0.53
1:A:400:LEU:HD11	1:A:482:LEU:HD13	1.90	0.53
1:E:443:MET:HG3	1:E:444:TYR:CE1	2.44	0.53
1:E:67:LEU:HG	1:E:68:ILE:H	1.72	0.53
1:K:292:ILE:HD13	1:K:300:VAL:O	2.09	0.53
1:A:670:ILE:HD12	1:A:712:ALA:HB1	1.90	0.53
1:E:292:ILE:HG23	1:E:503:PHE:CD2	2.43	0.53
1:A:494:PHE:HA	1:A:499:MET:HE1	1.90	0.53
1:G:598:PRO:HD2	2:H:292:PHE:CE1	2.44	0.53
1:G:642:ARG:NH1	2:H:71:ASP:OD2	2.41	0.53
2:F:54:ARG:O	2:F:57:ALA:HB3	2.07	0.53
1:A:380:GLU:HG2	1:A:381:PRO:HD2	1.90	0.53
1:E:283:ILE:HA	1:E:386:GLN:NE2	2.24	0.53
1:G:552:GLU:H	1:G:552:GLU:CD	2.12	0.53
2:F:251:THR:HG21	2:F:260:ALA:HB2	1.90	0.53
1:C:444:TYR:O	1:C:445:TYR:CG	2.62	0.53
1:I:376:VAL:C	1:I:378:ALA:H	2.12	0.53
1:A:66:ILE:HG12	1:A:66:ILE:O	2.08	0.53
2:B:149:MET:CE	2:B:189:VAL:HG11	2.39	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:184:ILE:CD1	2:L:417:TYR:HA	2.39	0.53
2:B:346:ARG:HH11	2:B:346:ARG:HG3	1.74	0.53
2:J:346:ARG:HA	2:J:350:ARG:O	2.08	0.53
1:E:279:HIS:HD2	1:E:380:GLU:O	1.92	0.53
1:K:279:HIS:NE2	1:K:380:GLU:N	2.57	0.53
2:F:469:THR:HG23	2:F:482:HIS:HB3	1.91	0.53
2:F:484:ALA:O	2:F:488:GLU:OE1	2.27	0.53
1:E:155:ALA:O	1:E:159:GLU:HG2	2.09	0.53
1:I:131:ILE:CG2	1:I:136:ALA:HB2	2.29	0.53
1:A:137:GLN:O	1:A:138:ALA:HB2	2.08	0.53
1:C:128:MET:SD	1:C:131:ILE:HD12	2.48	0.53
1:A:458:THR:O	1:A:461:ALA:HB3	2.09	0.53
2:J:379:ARG:HD2	2:J:421:GLU:OE2	2.09	0.53
2:H:346:ARG:HG3	2:H:346:ARG:NH1	2.23	0.53
1:A:140:HIS:ND1	1:A:141:PRO:HD2	2.24	0.53
1:A:308:LEU:HD12	1:A:308:LEU:O	2.09	0.53
1:C:289:GLU:OE1	1:C:306:PRO:HD2	2.08	0.53
1:G:338:ILE:N	1:G:338:ILE:HD12	2.23	0.53
1:E:70:ASN:OD1	1:E:74:ILE:HG21	2.09	0.53
1:G:444:TYR:O	1:G:445:TYR:CG	2.62	0.53
1:I:528:ALA:CB	1:I:605:LEU:HD22	2.36	0.53
1:K:85:MET:O	1:K:87:ILE:HG13	2.09	0.53
1:I:504:ILE:HG23	1:I:505:ALA:N	2.24	0.53
2:L:83:ASP:HB3	2:L:86:VAL:CG2	2.38	0.53
2:J:109:THR:HG22	2:J:122:PHE:HB2	1.91	0.53
1:I:411:LEU:HD22	1:I:682:GLN:CB	2.38	0.53
1:C:534:ARG:HG3	1:C:534:ARG:HH11	1.74	0.53
1:G:675:VAL:CG1	1:G:707:VAL:HG21	2.38	0.53
2:L:501:PHE:CD2	2:L:501:PHE:N	2.75	0.53
1:C:114:PRO:HB2	1:C:115:PRO:HD2	1.91	0.53
1:I:444:TYR:O	1:I:445:TYR:CG	2.62	0.53
1:K:124:ILE:O	1:K:128:MET:HB2	2.09	0.53
1:C:393:GLY:HA2	1:C:457:PRO:O	2.09	0.53
1:G:66:ILE:CD1	1:G:87:ILE:HG22	2.33	0.53
1:G:146:LEU:HD23	1:G:152:PHE:CD2	2.43	0.53
1:C:156:LEU:HD22	1:C:161:VAL:HB	1.91	0.53
2:H:325:ASP:C	2:H:327:GLY:H	2.12	0.53
1:K:78:VAL:HG13	1:K:79:ILE:N	2.24	0.53
2:H:390:THR:HG23	2:H:419:TYR:OH	2.09	0.53
2:H:160:ASP:OD1	2:H:198:GLY:HA3	2.09	0.53
1:E:272:ILE:HB	1:E:335:VAL:HG23	1.90	0.52
1:E:78:VAL:CG1	1:E:79:ILE:N	2.72	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:71:ARG:HG3	1:G:72:GLY:N	2.24	0.52
1:K:393:GLY:HA2	1:K:457:PRO:O	2.09	0.52
1:I:66:ILE:HD13	1:I:88:SER:O	2.09	0.52
2:J:207:SER:HB3	2:J:208:PRO:CD	2.34	0.52
1:I:112:ILE:O	1:I:120:SER:HA	2.09	0.52
1:I:517:LEU:HD21	1:I:632:ALA:HB1	1.92	0.52
2:D:114:ILE:O	2:D:115:ASN:HB2	2.08	0.52
2:F:458:ALA:HB3	2:F:493:PRO:HB3	1.90	0.52
1:C:335:VAL:O	1:C:335:VAL:HG23	2.09	0.52
2:B:58:GLN:HE21	2:B:61:ARG:HH21	1.58	0.52
2:J:501:PHE:N	2:J:501:PHE:CD2	2.75	0.52
1:I:65:LYS:HE2	1:I:134:THR:O	2.10	0.52
1:K:271:GLU:O	1:K:287:GLU:HB2	2.10	0.52
2:B:469:THR:HG23	2:B:482:HIS:HB3	1.91	0.52
2:H:58:GLN:HE21	2:H:61:ARG:HH21	1.57	0.52
1:E:289:GLU:OE1	1:E:306:PRO:HD2	2.09	0.52
1:K:312:THR:O	1:K:316:MET:HG3	2.09	0.52
1:K:122:ILE:HA	1:K:146:LEU:CD1	2.39	0.52
1:K:543:VAL:CG1	2:L:117:ARG:HD2	2.37	0.52
1:I:132:ARG:HD3	1:I:159:GLU:OE1	2.09	0.52
1:K:528:ALA:HB1	1:K:605:LEU:CD2	2.39	0.52
1:I:390:LYS:HD3	1:I:391:LEU:H	1.71	0.52
1:C:517:LEU:HD22	1:C:517:LEU:N	2.17	0.52
2:B:535:ASP:OD2	2:J:379:ARG:NH2	2.41	0.52
2:L:416:LEU:HB2	2:L:441:VAL:HG22	1.91	0.52
2:F:300:PRO:HA	2:F:509:ARG:NH1	2.24	0.52
1:I:275:LEU:HD11	1:I:372:GLN:HB2	1.90	0.52
1:K:670:ILE:CG1	1:K:718:LEU:HD21	2.39	0.52
2:B:297:ARG:HG2	2:B:297:ARG:HH11	1.74	0.52
2:H:484:ALA:O	2:H:488:GLU:OE1	2.28	0.52
2:F:394:VAL:HG23	2:F:395:PRO:HD2	1.92	0.52
2:J:178:GLU:HB3	2:J:182:ARG:NH1	2.24	0.52
1:E:393:GLY:HA3	1:E:455:TRP:CZ3	2.45	0.52
1:A:132:ARG:HD3	1:A:159:GLU:OE1	2.09	0.52
1:C:317:GLY:O	1:C:321:VAL:HG12	2.10	0.52
1:G:283:ILE:HA	1:G:386:GLN:NE2	2.24	0.52
2:L:149:MET:CE	2:L:189:VAL:CG1	2.87	0.52
1:A:658:THR:OG1	1:A:702:GLU:HG2	2.10	0.52
1:E:186:GLU:C	1:E:188:ASN:N	2.63	0.52
1:C:189:VAL:HA	1:C:319:GLN:OE1	2.09	0.52
1:K:464:GLU:HA	1:K:464:GLU:OE2	2.10	0.52
2:H:239:VAL:HG22	2:H:243:GLU:HB2	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:646:LEU:HD12	2:J:72:LEU:HD21	1.92	0.52
2:D:239:VAL:HG22	2:D:243:GLU:HB2	1.91	0.52
1:K:70:ASN:ND2	1:K:145:PHE:CD1	2.78	0.52
1:A:78:VAL:HG23	1:A:370:VAL:CG1	2.40	0.52
1:G:316:MET:HE3	1:G:337:PHE:HD1	1.74	0.52
1:E:444:TYR:CD1	1:E:444:TYR:N	2.78	0.52
1:K:458:THR:O	1:K:461:ALA:HB3	2.09	0.52
1:I:358:HIS:N	1:I:359:PRO:CD	2.72	0.52
2:J:492:ASN:ND2	2:J:494:PHE:H	2.06	0.52
2:D:367:ASP:O	2:D:368:ILE:C	2.46	0.52
2:F:193:ILE:HD13	2:F:274:LEU:HD23	1.90	0.52
2:H:123:SER:HA	2:H:158:ILE:HB	1.91	0.52
2:F:141:ILE:O	2:F:145:MET:HG3	2.08	0.52
1:C:614:LEU:HD22	1:C:627:ILE:HG21	1.91	0.52
1:A:543:VAL:HG11	2:B:117:ARG:HD2	1.91	0.52
1:C:646:LEU:HD13	2:D:64:LEU:HD13	1.92	0.52
1:I:401:TYR:CD2	1:I:448:MET:HA	2.44	0.52
1:C:177:LYS:O	1:C:181:LYS:HG2	2.10	0.52
1:C:68:ILE:HG22	1:C:70:ASN:H	1.74	0.52
2:B:296:ASP:O	2:B:298:ILE:HD12	2.09	0.52
1:A:401:TYR:HE2	1:A:448:MET:HB2	1.74	0.52
2:B:192:GLN:O	2:B:211:THR:HB	2.10	0.52
2:F:309:ASN:HD21	2:F:311:ASN:HB2	1.74	0.52
1:A:316:MET:CE	1:A:337:PHE:HD1	2.23	0.52
1:G:405:PRO:HG2	1:G:481:ASN:HA	1.90	0.52
1:I:480:HIS:HD2	1:I:482:LEU:HB2	1.73	0.52
1:E:70:ASN:ND2	1:E:145:PHE:CD1	2.77	0.52
1:E:78:VAL:HG23	1:E:370:VAL:CG1	2.39	0.52
1:C:292:ILE:H	1:C:292:ILE:CD1	1.96	0.52
1:I:428(L):ALA:HB3	1:I:455:TRP:HD1	1.75	0.52
1:C:92:ILE:HB	1:C:112:ILE:CG2	2.38	0.52
1:I:140:HIS:ND1	1:I:141:PRO:HD2	2.25	0.52
1:A:335:VAL:O	1:A:335:VAL:HG23	2.10	0.52
1:I:295:ARG:O	1:I:296:ASN:HB2	2.10	0.52
1:E:628:ARG:HG3	1:E:633:ASP:HA	1.90	0.52
2:F:254:SER:OG	2:F:256:VAL:HG23	2.10	0.52
1:E:189:VAL:HA	1:E:319:GLN:OE1	2.09	0.52
1:I:75:ALA:O	1:I:78:VAL:HG12	2.10	0.52
1:K:494:PHE:CD2	1:K:499:MET:HE1	2.45	0.52
1:C:543:VAL:HG11	2:D:117:ARG:HD2	1.92	0.52
1:C:376:VAL:C	1:C:378:ALA:H	2.13	0.52
1:A:517:LEU:H	1:A:564:GLN:HE22	1.58	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:712:ALA:HA	1:C:716:ASN:ND2	2.25	0.52
2:H:492:ASN:HB2	2:H:493:PRO:HD2	1.91	0.52
2:F:42:ARG:NH1	2:F:42:ARG:HG2	2.24	0.52
2:B:42:ARG:NH1	2:B:42:ARG:HG2	2.24	0.52
1:A:283:ILE:HA	1:A:386:GLN:NE2	2.24	0.52
1:E:362:GLU:HG2	1:E:367:VAL:O	2.09	0.52
1:K:99:GLN:HB2	1:K:436:TYR:OH	2.09	0.52
1:C:117:ALA:CB	1:C:121:TYR:HB2	2.40	0.52
1:G:444:TYR:CD1	1:G:444:TYR:N	2.77	0.52
1:K:463:ILE:HD12	1:K:494:PHE:CE1	2.44	0.52
1:A:66:ILE:HD13	1:A:88:SER:O	2.09	0.52
1:C:131:ILE:CG2	1:C:136:ALA:HB2	2.34	0.52
1:C:156:LEU:HD13	1:C:163:PHE:HB2	1.91	0.52
1:C:164:VAL:HG23	1:C:373:MET:O	2.09	0.52
2:D:417:TYR:HA	2:L:184:ILE:CD1	2.39	0.52
1:E:504:ILE:CG2	1:E:505:ALA:N	2.73	0.52
2:D:180:PHE:O	2:D:184:ILE:HG13	2.09	0.52
1:I:596:TRP:CG	1:I:597:THR:N	2.77	0.52
2:D:189:VAL:HA	2:D:282:ASN:ND2	2.24	0.52
2:D:51:GLY:O	2:D:55:ILE:HG13	2.10	0.52
2:D:109:THR:HG22	2:D:122:PHE:HB2	1.90	0.52
1:K:634:LEU:HD23	1:K:634:LEU:N	2.24	0.52
2:H:200:CYS:HB3	2:H:223:MET:HB3	1.92	0.52
1:E:320:ALA:HB1	1:E:335:VAL:HG21	1.91	0.52
2:F:117:ARG:HH21	2:F:280:LEU:HG	1.74	0.52
1:I:395:ALA:C	1:I:396:ILE:HD12	2.30	0.52
1:K:140:HIS:ND1	1:K:141:PRO:HD2	2.24	0.52
1:C:177:LYS:HB3	1:C:181:LYS:NZ	2.25	0.52
1:C:185:GLN:O	1:C:188:ASN:N	2.41	0.52
2:D:231:VAL:O	2:D:235:THR:HB	2.10	0.52
1:K:534:ARG:HH11	1:K:534:ARG:HG3	1.74	0.52
2:L:261:PHE:CD1	2:L:267:ALA:HA	2.44	0.52
2:D:124:GLN:HE21	2:D:137:HIS:CE1	2.27	0.52
2:H:261:PHE:CD1	2:H:267:ALA:HA	2.45	0.52
1:C:93:TYR:HA	1:C:121:TYR:OH	2.10	0.52
1:E:71:ARG:HG3	1:E:72:GLY:N	2.24	0.52
1:G:457:PRO:CG	1:G:458:THR:H	2.14	0.52
1:G:630:ARG:C	1:G:632:ALA:H	2.11	0.52
1:A:83:ARG:HB3	1:A:83:ARG:CZ	2.40	0.52
1:K:289:GLU:OE1	1:K:306:PRO:HD2	2.10	0.52
2:H:335:GLU:HA	2:H:338:LYS:HE2	1.91	0.52
1:G:577:ASP:HB2	1:G:591:ARG:NH2	2.24	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:501:PHE:CD2	2:F:501:PHE:N	2.74	0.52
1:I:403:GLU:O	1:I:405:PRO:HD3	2.09	0.51
1:I:316:MET:HB3	1:I:337:PHE:CE1	2.44	0.51
1:E:354:LEU:HD11	1:E:358:HIS:ND1	2.25	0.51
1:K:189:VAL:HA	1:K:319:GLN:OE1	2.09	0.51
2:L:368:ILE:HG13	2:L:408:VAL:HG13	1.92	0.51
2:B:78:SER:O	2:B:112:GLY:HA2	2.10	0.51
2:J:340:ILE:HD13	2:J:374:ALA:HB2	1.92	0.51
2:D:182:ARG:HH11	2:D:182:ARG:HG3	1.73	0.51
2:B:51:GLY:O	2:B:55:ILE:HG13	2.09	0.51
1:E:146:LEU:HD23	1:E:152:PHE:CD2	2.44	0.51
1:A:653:LYS:H	1:A:653:LYS:CD	2.09	0.51
1:G:376:VAL:C	1:G:378:ALA:N	2.62	0.51
1:A:378:ALA:O	1:A:379:GLY:C	2.49	0.51
1:G:363:LEU:HD13	1:G:455:TRP:HB3	1.92	0.51
1:A:393:GLY:HA3	1:A:455:TRP:CZ3	2.45	0.51
1:G:117:ALA:CB	1:G:121:TYR:HB2	2.39	0.51
1:I:177:LYS:O	1:I:181:LYS:HG2	2.09	0.51
1:A:190:SER:N	1:A:319:GLN:OE1	2.33	0.51
2:D:145:MET:CE	2:D:183:ASN:ND2	2.74	0.51
2:J:222:TYR:HB2	2:J:245:GLY:O	2.10	0.51
2:B:458:ALA:HB3	2:B:493:PRO:HB3	1.93	0.51
2:B:232:LYS:O	2:B:236:ASN:N	2.37	0.51
1:I:71:ARG:HG3	1:I:72:GLY:N	2.25	0.51
1:K:124:ILE:HG23	1:K:152:PHE:HD2	1.74	0.51
1:C:665:PRO:HG2	1:C:666:MET:HE2	1.91	0.51
1:A:497:GLY:O	1:A:499:MET:HG2	2.11	0.51
2:J:445:LYS:HE3	2:J:503:ASP:OD1	2.10	0.51
1:K:189:VAL:CG2	1:K:323:LEU:HB2	2.40	0.51
1:A:275:LEU:HD23	1:A:276:CYS:N	2.25	0.51
1:C:186:GLU:C	1:C:188:ASN:N	2.63	0.51
2:H:42:ARG:HG2	2:H:42:ARG:NH1	2.24	0.51
2:B:300:PRO:HA	2:B:509:ARG:NH1	2.26	0.51
1:K:63:PHE:N	1:K:63:PHE:CD1	2.78	0.51
1:E:538:ILE:O	1:E:541:THR:HB	2.11	0.51
2:J:382:ASP:OD1	2:J:424:VAL:HG13	2.10	0.51
2:F:94:ASN:HA	2:F:98:GLN:OE1	2.11	0.51
1:I:415:GLY:C	1:I:440:GLU:HG3	2.30	0.51
1:I:639:ARG:HB3	1:I:643:GLN:HB3	1.90	0.51
1:I:400:LEU:HD21	1:I:482:LEU:HD13	1.92	0.51
1:C:347:PHE:CD1	1:C:347:PHE:O	2.63	0.51
1:K:563:LEU:HD23	1:K:636:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:467:ARG:HD2	1:A:467:ARG:O	2.11	0.51
1:E:517:LEU:N	1:E:517:LEU:HD22	2.22	0.51
1:E:517:LEU:H	1:E:564:GLN:HE22	1.58	0.51
2:B:522:LEU:HD23	2:F:151:ASN:ND2	2.24	0.51
1:E:661:MET:HE1	1:E:726:GLU:HB3	1.91	0.51
1:E:464:GLU:HA	1:E:464:GLU:OE2	2.10	0.51
2:L:367:ASP:O	2:L:368:ILE:C	2.49	0.51
1:K:380:GLU:CG	1:K:381:PRO:HD2	2.40	0.51
2:B:376:ARG:HH11	2:J:410:LYS:HZ2	1.58	0.51
2:J:273:ARG:HD2	2:J:330:TYR:HD1	1.75	0.51
1:G:400:LEU:HD11	1:G:482:LEU:CD1	2.39	0.51
1:C:528:ALA:HB1	1:C:605:LEU:HD22	1.92	0.51
1:I:441:ILE:HD12	1:I:478:ILE:HD13	1.91	0.51
1:K:358:HIS:N	1:K:359:PRO:CD	2.74	0.51
1:G:123:VAL:HG12	1:G:126:LYS:H	1.76	0.51
1:G:163:PHE:CD1	1:G:163:PHE:C	2.84	0.51
2:B:207:SER:HB3	2:B:208:PRO:CD	2.35	0.51
2:B:89:ARG:NH1	2:D:499:ARG:HH21	2.08	0.51
1:I:658:THR:OG1	1:I:702:GLU:HG2	2.11	0.51
1:K:319:GLN:NE2	1:K:345:PHE:CE1	2.78	0.51
1:I:186:GLU:C	1:I:188:ASN:N	2.64	0.51
1:E:401:TYR:CE2	1:E:448:MET:HB2	2.46	0.51
1:A:71:ARG:HG3	1:A:72:GLY:N	2.25	0.51
1:C:403:GLU:O	1:C:405:PRO:HD3	2.11	0.51
1:G:303:ALA:HB3	1:G:360:VAL:HG12	1.93	0.51
1:C:275:LEU:HD23	1:C:276:CYS:N	2.26	0.51
2:J:108:VAL:O	2:J:122:PHE:HA	2.09	0.51
1:A:189:VAL:HA	1:A:319:GLN:OE1	2.10	0.51
2:B:178:GLU:HB3	2:B:182:ARG:NH1	2.25	0.51
2:L:43:ARG:HG2	2:L:43:ARG:NH1	2.25	0.51
1:K:679:GLN:O	1:K:706:VAL:HG13	2.11	0.51
2:B:150:GLN:HG2	2:D:527:VAL:HG22	1.93	0.51
1:K:207:LYS:O	1:K:207:LYS:HD2	2.11	0.51
1:C:433:THR:HG22	1:C:434:GLY:N	2.24	0.51
1:C:551:HIS:HE1	2:F:348:GLU:OE2	1.94	0.51
1:C:304:PRO:HD2	1:C:394:TRP:CE2	2.46	0.51
2:H:196:ILE:HD13	2:H:214:ILE:HG23	1.93	0.51
1:K:418:THR:O	1:K:437:GLU:HG3	2.11	0.51
1:C:400:LEU:HD21	1:C:482:LEU:CD1	2.41	0.51
1:I:444:TYR:N	1:I:444:TYR:CD1	2.78	0.51
1:E:124:ILE:O	1:E:128:MET:HB2	2.11	0.51
1:E:392:THR:O	1:E:455:TRP:HZ3	1.94	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:363:LEU:HD13	1:K:455:TRP:HB3	1.93	0.51
2:B:379:ARG:HD2	2:B:421:GLU:OE2	2.11	0.51
1:G:665:PRO:HG2	1:G:666:MET:HE2	1.91	0.51
1:K:206:VAL:HG13	1:K:235:ASP:HB3	1.93	0.51
1:G:177:LYS:HB3	1:G:181:LYS:HZ1	1.76	0.51
1:E:140:HIS:ND1	1:E:141:PRO:HD2	2.26	0.51
1:E:264:VAL:O	1:E:267:PRO:HD3	2.11	0.51
1:I:415:GLY:O	1:I:440:GLU:HG3	2.10	0.51
2:H:356:ALA:CB	2:H:391:LEU:HB2	2.41	0.51
2:D:501:PHE:CD2	2:D:501:PHE:N	2.77	0.51
1:C:362:GLU:HG2	1:C:367:VAL:O	2.11	0.51
1:K:316:MET:O	1:K:320:ALA:HB2	2.11	0.51
1:K:403:GLU:O	1:K:405:PRO:HD3	2.10	0.51
1:E:458:THR:O	1:E:461:ALA:HB3	2.10	0.51
1:A:614:LEU:HD22	1:A:627:ILE:HG21	1.92	0.51
2:H:416:LEU:HB2	2:H:441:VAL:HG22	1.92	0.51
1:K:365:THR:HG22	1:K:391:LEU:HD22	1.92	0.51
1:A:517:LEU:CD2	1:A:517:LEU:H	2.15	0.51
1:C:324:ALA:O	1:C:327:VAL:HG12	2.11	0.51
1:E:517:LEU:CD2	1:E:517:LEU:H	2.21	0.51
2:J:307:PRO:HG3	2:J:312:THR:O	2.10	0.51
1:K:179:THR:O	1:K:183:ILE:HG13	2.11	0.51
1:C:279:HIS:HD2	1:C:380:GLU:O	1.93	0.51
2:F:43:ARG:NH1	2:F:43:ARG:HG2	2.26	0.51
2:B:75:ASP:OD1	2:B:272:ARG:NH2	2.43	0.51
1:E:164:VAL:HG23	1:E:373:MET:O	2.10	0.51
1:A:139:VAL:O	1:A:164:VAL:HG12	2.11	0.51
2:L:346:ARG:HA	2:L:350:ARG:O	2.10	0.51
1:K:283:ILE:HA	1:K:386:GLN:NE2	2.24	0.51
1:I:283:ILE:HG22	1:I:386:GLN:HG2	1.93	0.51
1:G:320:ALA:HB1	1:G:335:VAL:HG21	1.94	0.51
1:I:362:GLU:HG2	1:I:367:VAL:O	2.11	0.51
1:C:97:ASP:OD1	1:C:102:HIS:HE1	1.94	0.51
2:H:50:GLY:O	2:H:54:ARG:HD2	2.11	0.51
2:F:539:LEU:OXT	2:H:372:ARG:NH2	2.44	0.51
1:E:378:ALA:O	1:E:379:GLY:C	2.50	0.51
1:I:693:MET:O	1:I:694:LYS:HB2	2.11	0.51
1:A:515:VAL:HG21	1:A:631:GLY:HA3	1.93	0.51
1:G:100:ALA:HB3	1:G:103:VAL:HG23	1.93	0.50
1:G:400:LEU:HD21	1:G:482:LEU:CD1	2.40	0.50
1:I:405:PRO:HG2	1:I:481:ASN:HA	1.92	0.50
1:K:400:LEU:HD11	1:K:482:LEU:CD1	2.41	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:71:ARG:HG3	1:C:72:GLY:N	2.26	0.50
1:A:393:GLY:HA2	1:A:457:PRO:O	2.11	0.50
2:F:210:MET:HE1	2:H:416:LEU:HG	1.94	0.50
2:L:149:MET:HE1	2:L:189:VAL:HG11	1.91	0.50
1:K:206:VAL:HG13	1:K:235:ASP:CB	2.41	0.50
2:D:462:VAL:HG22	2:L:169:GLY:HA2	1.93	0.50
1:G:275:LEU:HD23	1:G:276:CYS:H	1.75	0.50
1:I:272:ILE:HB	1:I:335:VAL:CG2	2.41	0.50
2:D:178:GLU:O	2:D:182:ARG:HG3	2.10	0.50
3:E:801:BTI:H63	2:F:399:PRO:HD3	1.92	0.50
1:A:537:GLU:HG3	1:A:553:ARG:NH2	2.26	0.50
1:K:316:MET:CE	1:K:337:PHE:HD1	2.24	0.50
1:I:348:LEU:O	1:I:349:GLU:HB3	2.11	0.50
1:C:348:LEU:O	1:C:348:LEU:HD23	2.11	0.50
1:G:139:VAL:O	1:G:164:VAL:HG12	2.12	0.50
1:C:376:VAL:C	1:C:378:ALA:N	2.63	0.50
1:E:292:ILE:HD13	1:E:300:VAL:O	2.11	0.50
1:I:625:PHE:CD1	1:I:625:PHE:N	2.79	0.50
1:E:185:GLN:O	1:E:188:ASN:N	2.42	0.50
1:C:334:THR:CG2	1:C:351:ASN:HB2	2.41	0.50
2:B:58:GLN:CD	2:B:63:LYS:HE3	2.31	0.50
2:L:148:ALA:HB1	2:L:153:ALA:O	2.11	0.50
1:C:295:ARG:O	1:C:296:ASN:HB2	2.11	0.50
2:H:232:LYS:O	2:H:236:ASN:N	2.36	0.50
1:K:405:PRO:HG2	1:K:481:ASN:HA	1.93	0.50
1:C:74:ILE:HD13	1:C:143:TYR:HE2	1.77	0.50
1:G:380:GLU:HG2	1:G:381:PRO:HD2	1.93	0.50
1:C:363:LEU:HD13	1:C:455:TRP:HB3	1.93	0.50
1:G:92:ILE:CD1	1:G:112:ILE:HD13	2.42	0.50
1:A:334:THR:HG22	1:A:351:ASN:HB2	1.93	0.50
1:K:276:CYS:O	1:K:382:LEU:HD21	2.10	0.50
2:L:94:ASN:HA	2:L:98:GLN:OE1	2.11	0.50
1:E:177:LYS:HB3	1:E:181:LYS:HZ3	1.74	0.50
1:A:634:LEU:HD23	1:A:634:LEU:H	1.76	0.50
2:D:273:ARG:HD2	2:D:330:TYR:CD1	2.47	0.50
1:I:577:ASP:HB2	1:I:591:ARG:NH2	2.26	0.50
1:K:683:GLU:HB2	1:K:704:LYS:HG3	1.92	0.50
1:I:671:VAL:CG2	1:I:691:GLU:HB2	2.41	0.50
2:L:66:ALA:HB2	2:L:125:ASP:HA	1.93	0.50
1:E:693:MET:O	1:E:694:LYS:HB2	2.11	0.50
1:I:348:LEU:O	1:I:348:LEU:HD23	2.11	0.50
1:E:433:THR:HG22	1:E:434:GLY:N	2.23	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:287:GLU:HG3	1:G:308:LEU:HD21	1.93	0.50
1:K:400:LEU:HD13	1:K:449:ILE:CD1	2.32	0.50
1:G:74:ILE:HG23	1:G:75:ALA:N	2.27	0.50
1:C:155:ALA:O	1:C:159:GLU:HG2	2.11	0.50
1:K:78:VAL:HG23	1:K:370:VAL:HG11	1.93	0.50
1:K:317:GLY:O	1:K:321:VAL:HG12	2.11	0.50
1:G:112:ILE:O	1:G:120:SER:HA	2.12	0.50
2:F:156:ILE:CD1	2:F:156:ILE:N	2.73	0.50
1:K:283:ILE:HG22	1:K:386:GLN:HG2	1.93	0.50
1:E:675:VAL:CG1	1:E:707:VAL:HG21	2.41	0.50
1:K:664:CYS:SG	1:K:690:ILE:HD13	2.51	0.50
1:E:515:VAL:CG2	1:E:631:GLY:HA3	2.41	0.50
1:G:99:GLN:HB2	1:G:436:TYR:OH	2.10	0.50
1:E:74:ILE:HD13	1:E:143:TYR:HE2	1.76	0.50
1:G:67:LEU:HG	1:G:68:ILE:H	1.77	0.50
1:G:354:LEU:HD11	1:G:358:HIS:ND1	2.27	0.50
1:K:393:GLY:HA3	1:K:455:TRP:CZ3	2.47	0.50
1:A:665:PRO:HG2	1:A:666:MET:HE2	1.89	0.50
1:A:304:PRO:HG2	1:A:394:TRP:CZ2	2.46	0.50
1:K:92:ILE:HB	1:K:112:ILE:CG2	2.42	0.50
1:G:467:ARG:HE	1:G:630:ARG:HG3	1.76	0.50
2:J:121:VAL:O	2:J:144:ILE:HD13	2.11	0.50
1:K:380:GLU:HG2	1:K:381:PRO:HD2	1.93	0.50
2:J:196:ILE:HG22	2:J:221:SER:HB2	1.93	0.50
2:D:469:THR:HG23	2:D:482:HIS:HB3	1.92	0.50
1:I:167:PRO:O	1:I:169:GLY:N	2.45	0.50
2:J:423:THR:O	2:J:525:LYS:HE2	2.11	0.50
1:K:312:THR:O	1:K:315:ALA:HB3	2.10	0.50
1:A:117:ALA:C	1:A:119:GLN:N	2.65	0.50
1:I:292:ILE:HG23	1:I:503:PHE:CD2	2.46	0.50
1:C:163:PHE:C	1:C:163:PHE:CD1	2.85	0.50
1:K:65:LYS:HE2	1:K:134:THR:O	2.11	0.50
1:A:83:ARG:CG	1:A:83:ARG:HH11	2.23	0.50
2:F:367:ASP:O	2:F:368:ILE:C	2.48	0.50
1:I:380:GLU:CG	1:I:381:PRO:HD2	2.41	0.50
2:B:356:ALA:CB	2:B:391:LEU:HB2	2.42	0.50
2:F:229:ASP:O	2:F:233:THR:HG23	2.12	0.50
1:I:433:THR:HG22	1:I:434:GLY:N	2.26	0.50
1:C:312:THR:O	1:C:315:ALA:HB3	2.12	0.50
1:E:414:ILE:HD12	1:E:441:ILE:O	2.12	0.50
1:A:95:ASP:OD2	1:A:114:PRO:HA	2.12	0.50
1:K:358:HIS:HB2	1:K:369:LEU:HD12	1.92	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:456:ALA:CB	1:K:457:PRO:CD	2.90	0.50
1:A:625:PHE:N	1:A:625:PHE:CD1	2.77	0.50
2:H:207:SER:HB3	2:H:208:PRO:CD	2.33	0.50
2:J:91:THR:HA	2:J:98:GLN:CG	2.39	0.50
2:D:379:ARG:HD2	2:D:421:GLU:OE2	2.12	0.50
1:A:365:THR:HG22	1:A:391:LEU:HD22	1.93	0.50
1:G:334:THR:HG22	1:G:351:ASN:HB2	1.93	0.50
2:B:346:ARG:NH1	2:B:346:ARG:HG3	2.27	0.50
1:I:83:ARG:CG	1:I:83:ARG:HH11	2.22	0.50
1:K:661:MET:HE1	1:K:726:GLU:HB3	1.93	0.50
2:B:54:ARG:HG2	2:B:54:ARG:NH1	2.27	0.50
2:D:49:GLY:C	2:D:51:GLY:N	2.65	0.50
1:K:579:SER:O	1:K:591:ARG:HD2	2.12	0.50
1:G:306:PRO:HG3	1:G:394:TRP:CH2	2.46	0.50
2:L:335:GLU:HA	2:L:338:LYS:HE2	1.94	0.50
1:C:671:VAL:CG2	1:C:691:GLU:HB2	2.42	0.50
2:B:335:GLU:HA	2:B:338:LYS:HE2	1.94	0.50
1:E:415:GLY:C	1:E:440:GLU:HG3	2.32	0.50
1:E:369:LEU:O	1:E:373:MET:HB2	2.12	0.50
1:C:124:ILE:O	1:C:128:MET:HB2	2.12	0.50
1:G:517:LEU:CD2	1:G:517:LEU:H	2.22	0.50
1:A:293:GLN:HB3	1:A:298:LYS:HA	1.94	0.50
1:A:63:PHE:N	1:A:63:PHE:CD1	2.79	0.50
2:D:474:ARG:O	2:D:476:ASP:N	2.45	0.50
1:I:265:THR:HB	1:I:341:GLY:H	1.76	0.50
1:E:167:PRO:O	1:E:169:GLY:N	2.44	0.50
1:E:184:ALA:HB1	1:E:189:VAL:HB	1.93	0.50
1:K:348:LEU:O	1:K:349:GLU:HB3	2.12	0.50
1:I:312:THR:O	1:I:316:MET:HG3	2.12	0.50
1:I:114:PRO:HB2	1:I:115:PRO:HD2	1.94	0.50
1:K:334:THR:HG22	1:K:351:ASN:HB2	1.94	0.50
1:I:376:VAL:C	1:I:378:ALA:N	2.64	0.50
1:A:376:VAL:HG23	1:A:377:ALA:N	2.26	0.50
1:A:92:ILE:HB	1:A:112:ILE:CG2	2.42	0.50
1:A:185:GLN:O	1:A:188:ASN:N	2.44	0.50
1:I:320:ALA:HB1	1:I:335:VAL:HG21	1.94	0.50
1:C:380:GLU:HG2	1:C:381:PRO:HD2	1.93	0.50
2:B:69:ARG:HA	2:B:268:LEU:HD11	1.94	0.50
1:A:405:PRO:HG2	1:A:481:ASN:HA	1.94	0.50
1:K:170:ALA:O	1:K:173:ALA:HB3	2.11	0.50
1:C:642:ARG:HH11	2:D:71:ASP:HB3	1.77	0.50
2:J:49:GLY:C	2:J:51:GLY:H	2.16	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:239:VAL:HG22	2:B:243:GLU:HB2	1.93	0.50
1:A:646:LEU:HD13	2:B:64:LEU:HD13	1.94	0.50
1:G:162:ILE:O	1:G:164:VAL:N	2.45	0.49
1:G:369:LEU:O	1:G:373:MET:HB2	2.12	0.49
1:K:517:LEU:CD2	1:K:517:LEU:H	2.18	0.49
1:I:467:ARG:HE	1:I:630:ARG:CG	2.25	0.49
1:C:658:THR:HG22	1:C:659:SER:O	2.12	0.49
1:I:234:ASN:HD22	1:I:236:GLN:HB2	1.74	0.49
1:K:185:GLN:O	1:K:188:ASN:N	2.45	0.49
1:G:190:SER:N	1:G:319:GLN:OE1	2.36	0.49
1:E:380:GLU:HG2	1:E:381:PRO:HD2	1.94	0.49
1:E:283:ILE:HB	1:E:386:GLN:CD	2.32	0.49
2:B:178:GLU:O	2:B:182:ARG:HG3	2.12	0.49
2:H:390:THR:CG2	2:H:419:TYR:OH	2.60	0.49
2:F:43:ARG:HH11	2:F:43:ARG:HG2	1.76	0.49
2:L:252:ARG:NH2	2:L:335:GLU:HG3	2.27	0.49
1:I:207:LYS:O	1:I:211:GLN:HB2	2.12	0.49
2:H:250:HIS:HA	2:H:254:SER:OG	2.11	0.49
1:G:537:GLU:HG3	1:G:553:ARG:HH21	1.77	0.49
1:G:342:GLN:O	1:G:343:LYS:HB2	2.11	0.49
1:E:118:ASN:O	1:E:119:GLN:HG3	2.11	0.49
1:K:146:LEU:HD23	1:K:152:PHE:CG	2.47	0.49
1:K:155:ALA:O	1:K:159:GLU:HG2	2.12	0.49
2:F:417:TYR:HA	2:H:184:ILE:CD1	2.40	0.49
2:F:479:ILE:C	2:F:479:ILE:HD12	2.32	0.49
1:C:583:PHE:CZ	1:C:590:MET:HE3	2.47	0.49
1:A:396:ILE:HD13	1:A:462:ALA:CB	2.42	0.49
2:H:189:VAL:HA	2:H:282:ASN:HD22	1.76	0.49
1:G:596:TRP:CG	1:G:597:THR:N	2.80	0.49
1:E:177:LYS:O	1:E:181:LYS:HG2	2.12	0.49
2:D:109:THR:HG22	2:D:122:PHE:CB	2.42	0.49
2:L:432:ARG:HG2	2:L:433:LYS:N	2.27	0.49
2:L:492:ASN:HD22	2:L:494:PHE:HB2	1.77	0.49
1:I:407:ARG:HG2	1:I:407:ARG:HH11	1.77	0.49
1:A:65:LYS:HE2	1:A:134:THR:O	2.12	0.49
1:E:288:ARG:HD3	1:E:361:THR:OG1	2.12	0.49
1:G:415:GLY:C	1:G:440:GLU:HG3	2.32	0.49
1:G:454:THR:HG21	1:G:466:MET:HA	1.94	0.49
2:J:232:LYS:O	2:J:236:ASN:N	2.36	0.49
1:G:78:VAL:HA	1:G:370:VAL:HG11	1.94	0.49
1:G:279:HIS:NE2	1:G:380:GLU:N	2.60	0.49
1:G:358:HIS:N	1:G:359:PRO:CD	2.75	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:71:ARG:O	1:K:75:ALA:CB	2.60	0.49
1:G:92:ILE:HB	1:G:112:ILE:CG2	2.42	0.49
1:K:670:ILE:HD11	1:K:718:LEU:HD11	1.94	0.49
1:K:712:ALA:HA	1:K:716:ASN:ND2	2.28	0.49
1:I:634:LEU:N	1:I:634:LEU:CD2	2.75	0.49
1:A:177:LYS:O	1:A:181:LYS:HG2	2.12	0.49
1:G:83:ARG:CZ	1:G:83:ARG:HB3	2.42	0.49
1:E:69:ALA:HB3	1:E:141:PRO:HA	1.94	0.49
1:C:491:HIS:O	1:C:495:ILE:HG13	2.12	0.49
2:H:351:THR:HG22	2:H:386:ILE:HG23	1.94	0.49
2:D:382:ASP:OD1	2:D:424:VAL:HG13	2.13	0.49
1:C:347:PHE:CD1	1:C:347:PHE:C	2.85	0.49
1:A:444:TYR:O	1:A:445:TYR:CG	2.66	0.49
1:G:455:TRP:CG	1:G:456:ALA:N	2.79	0.49
1:I:463:ILE:HD12	1:I:494:PHE:CE1	2.47	0.49
1:A:179:THR:O	1:A:183:ILE:HG13	2.13	0.49
1:I:534:ARG:HG3	1:I:534:ARG:NH1	2.25	0.49
1:I:283:ILE:CG2	1:I:386:GLN:HG2	2.42	0.49
1:G:415:GLY:O	1:G:440:GLU:HG3	2.13	0.49
1:A:552:GLU:CD	1:A:552:GLU:H	2.16	0.49
2:J:66:ALA:HB2	2:J:125:ASP:HA	1.95	0.49
2:B:337:ALA:HB1	2:B:370:SER:HA	1.92	0.49
2:B:337:ALA:HB3	2:B:373:LYS:HD2	1.94	0.49
1:I:664:CYS:HB2	1:I:724:ILE:HD11	1.93	0.49
1:K:117:ALA:CB	1:K:121:TYR:HB2	2.40	0.49
2:B:417:TYR:HA	2:J:184:ILE:CD1	2.42	0.49
1:K:324:ALA:O	1:K:327:VAL:HG12	2.12	0.49
2:D:88:HIS:CD2	2:D:88:HIS:C	2.85	0.49
2:L:189:VAL:HA	2:L:282:ASN:HD22	1.77	0.49
1:G:537:GLU:HG3	1:G:553:ARG:NH2	2.28	0.49
2:J:356:ALA:HB2	2:J:391:LEU:HB2	1.94	0.49
1:G:416:ARG:HG3	1:G:439:GLY:O	2.12	0.49
1:A:71:ARG:O	1:A:75:ALA:CB	2.61	0.49
1:C:78:VAL:CG1	1:C:79:ILE:N	2.76	0.49
1:E:317:GLY:O	1:E:321:VAL:HG12	2.12	0.49
2:F:492:ASN:ND2	2:F:494:PHE:H	2.05	0.49
2:L:403:GLN:O	2:L:408:VAL:HG22	2.12	0.49
2:L:227:GLY:O	2:L:231:VAL:HG23	2.13	0.49
2:B:300:PRO:HB3	2:B:509:ARG:HH12	1.77	0.49
2:D:273:ARG:HD2	2:D:330:TYR:HD1	1.78	0.49
1:G:693:MET:O	1:G:694:LYS:HB2	2.13	0.49
2:H:507:GLN:OE1	2:J:39:LEU:HD23	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:515:VAL:CG2	1:I:631:GLY:HA3	2.42	0.49
1:G:639:ARG:HB3	1:G:643:GLN:HB3	1.93	0.49
2:J:329:PHE:CE1	2:J:343:GLY:HA3	2.47	0.49
1:A:650:MET:SD	2:B:263:ASN:HB2	2.53	0.49
2:J:447:LEU:C	2:J:448:ARG:HG2	2.32	0.49
1:I:358:HIS:HB2	1:I:369:LEU:HD12	1.94	0.49
2:F:338:LYS:HB3	2:F:361:VAL:HG21	1.93	0.49
1:E:658:THR:OG1	1:E:702:GLU:HG2	2.13	0.49
1:E:394:TRP:CE3	1:E:459:ARG:HG3	2.48	0.49
2:F:476(C):ASP:C	2:F:477:GLU:H	2.15	0.49
1:I:411:LEU:HB2	1:I:682:GLN:HG3	1.95	0.49
1:E:265:THR:HB	1:E:341:GLY:H	1.76	0.49
1:I:283:ILE:HB	1:I:386:GLN:CD	2.33	0.49
2:H:109:THR:HG22	2:H:122:PHE:HB2	1.93	0.49
2:L:307:PRO:O	2:L:432:ARG:NH2	2.45	0.49
2:B:307:PRO:HG3	2:B:312:THR:O	2.13	0.49
1:C:411:LEU:HB2	1:C:682:GLN:HG3	1.94	0.49
2:L:273:ARG:HD2	2:L:330:TYR:HD1	1.77	0.49
1:C:107:ASP:O	1:C:108:GLU:HG3	2.11	0.49
2:J:78:SER:O	2:J:112:GLY:HA2	2.12	0.49
1:E:354:LEU:C	1:E:354:LEU:HD13	2.33	0.49
1:I:163:PHE:C	1:I:163:PHE:CD1	2.86	0.49
1:E:518:PRO:O	1:E:521:ASP:HB2	2.13	0.49
1:E:517:LEU:HD21	1:E:632:ALA:HB2	1.93	0.49
1:G:563:LEU:O	1:G:565:GLY:N	2.46	0.49
1:K:658:THR:CB	1:K:703:LYS:HD3	2.42	0.49
1:C:179:THR:O	1:C:183:ILE:HG13	2.13	0.49
1:K:275:LEU:HD23	1:K:276:CYS:N	2.28	0.49
2:J:235:THR:HG22	2:J:237:GLU:HB2	1.93	0.49
1:C:283:ILE:HA	1:C:386:GLN:NE2	2.28	0.49
2:D:108:VAL:O	2:D:122:PHE:HA	2.12	0.49
2:J:273:ARG:HD2	2:J:330:TYR:CD1	2.46	0.49
1:K:207:LYS:O	1:K:211:GLN:HB2	2.12	0.49
1:C:720:VAL:HG22	1:C:721:ASP:H	1.78	0.49
1:A:312:THR:O	1:A:315:ALA:HB3	2.13	0.49
1:C:615:LYS:HB2	1:C:628:ARG:HB2	1.95	0.49
1:E:421:ARG:O	1:E:421:ARG:CD	2.61	0.49
2:B:180:PHE:O	2:B:184:ILE:HG13	2.13	0.49
2:B:499:ARG:NH2	2:F:89:ARG:HH11	2.01	0.49
1:A:467:ARG:CB	1:A:467:ARG:HH11	2.22	0.49
1:I:517:LEU:N	1:I:564:GLN:HE22	2.09	0.49
2:L:434:ALA:HB3	2:L:460:VAL:HG12	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:206:VAL:HG13	1:I:235:ASP:HB3	1.95	0.49
2:L:339:ASN:ND2	2:L:367:ASP:OD1	2.45	0.49
2:H:460:VAL:O	2:H:460:VAL:HG23	2.13	0.49
1:E:271:GLU:O	1:E:287:GLU:HB2	2.12	0.49
1:C:63:PHE:N	1:C:63:PHE:CD1	2.81	0.49
1:G:411:LEU:HD22	1:G:682:GLN:HB2	1.95	0.49
1:C:675:VAL:CG1	1:C:707:VAL:HG21	2.42	0.49
1:A:342:GLN:O	1:A:343:LYS:HB2	2.12	0.49
2:B:193:ILE:HD13	2:B:274:LEU:HD23	1.94	0.49
1:C:117:ALA:C	1:C:119:GLN:N	2.66	0.49
1:G:482:LEU:N	1:G:483:PRO:HD2	2.27	0.49
1:K:117:ALA:C	1:K:119:GLN:N	2.66	0.49
1:K:626:ARG:NE	1:K:628:ARG:HD2	2.27	0.49
1:A:155:ALA:O	1:A:159:GLU:HG2	2.12	0.49
1:G:543:VAL:HG11	2:H:117:ARG:HD2	1.94	0.49
1:G:428(L):ALA:HB3	1:G:455:TRP:HD1	1.77	0.49
2:D:325:ASP:HA	2:D:512:ARG:NH1	2.17	0.49
2:J:499:ARG:CG	2:J:499:ARG:NH1	2.76	0.49
1:E:467:ARG:HE	1:E:630:ARG:HG3	1.77	0.49
1:A:396:ILE:HD12	1:A:396:ILE:N	2.28	0.49
2:D:347:LEU:HD12	2:D:352:VAL:HG21	1.95	0.49
2:D:149:MET:CE	2:D:189:VAL:HG11	2.43	0.49
2:J:43:ARG:HH11	2:J:43:ARG:CG	2.26	0.49
2:H:227:GLY:O	2:H:231:VAL:HG23	2.13	0.49
2:H:235:THR:HG22	2:H:237:GLU:HB2	1.94	0.49
1:C:283:ILE:HG22	1:C:386:GLN:HG2	1.95	0.49
1:K:367:VAL:HG12	1:K:368:ASP:N	2.28	0.49
2:H:195:MET:SD	2:H:271:VAL:HG21	2.52	0.49
1:A:348:LEU:O	1:A:348:LEU:HD23	2.12	0.48
1:G:309:ASP:OD1	1:G:312:THR:CG2	2.50	0.48
1:K:156:LEU:HD13	1:K:163:PHE:HB2	1.94	0.48
1:E:455:TRP:CG	1:E:456:ALA:N	2.81	0.48
1:G:523:ARG:HB3	1:G:590:MET:CE	2.39	0.48
1:I:275:LEU:HD23	1:I:276:CYS:H	1.76	0.48
1:K:195:TYR:O	1:K:259:PHE:HA	2.12	0.48
2:J:398:LEU:HD12	2:J:399:PRO:HD2	1.95	0.48
2:F:122:PHE:CD1	2:F:141:ILE:HG23	2.48	0.48
2:B:376:ARG:NH1	2:J:410:LYS:NZ	2.60	0.48
2:F:49:GLY:C	2:F:51:GLY:H	2.15	0.48
1:E:400:LEU:HD21	1:E:482:LEU:CD1	2.42	0.48
1:E:435:VAL:HG22	1:E:436:TYR:H	1.77	0.48
1:E:118:ASN:C	1:E:119:GLN:HG3	2.34	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:156:LEU:HD13	1:E:163:PHE:HB2	1.94	0.48
1:G:443:MET:SD	1:G:444:TYR:CE1	3.06	0.48
1:K:653:LYS:H	1:K:653:LYS:CD	2.12	0.48
1:I:123:VAL:HG12	1:I:126:LYS:H	1.79	0.48
1:C:517:LEU:CD2	1:C:517:LEU:H	2.17	0.48
1:C:83:ARG:CZ	1:C:83:ARG:HB3	2.43	0.48
2:F:61:ARG:HB2	2:F:63:LYS:HG3	1.95	0.48
1:C:283:ILE:HB	1:C:386:GLN:CD	2.33	0.48
1:G:304:PRO:HD2	1:G:394:TRP:CE2	2.48	0.48
1:E:376:VAL:C	1:E:378:ALA:H	2.15	0.48
1:E:515:VAL:HB	1:E:631:GLY:C	2.33	0.48
1:E:400:LEU:HD13	1:E:449:ILE:CD1	2.25	0.48
1:C:99:GLN:HB2	1:C:436:TYR:OH	2.13	0.48
1:E:670:ILE:HD12	1:E:712:ALA:HB1	1.94	0.48
1:K:467:ARG:HE	1:K:630:ARG:CG	2.26	0.48
1:A:358:HIS:N	1:A:359:PRO:CD	2.76	0.48
1:I:455:TRP:CG	1:I:456:ALA:N	2.80	0.48
1:A:626:ARG:C	1:A:627:ILE:HD12	2.33	0.48
1:K:112:ILE:O	1:K:120:SER:HA	2.12	0.48
2:B:417:TYR:HB2	2:J:210:MET:HE2	1.94	0.48
1:E:596:TRP:CG	1:E:597:THR:N	2.81	0.48
1:G:630:ARG:C	1:G:632:ALA:N	2.65	0.48
1:I:625:PHE:HB2	1:I:627:ILE:CD1	2.43	0.48
2:D:492:ASN:HB2	2:D:493:PRO:CD	2.43	0.48
1:A:334:THR:CG2	1:A:351:ASN:HB2	2.43	0.48
2:B:227:GLY:O	2:B:231:VAL:HG23	2.14	0.48
1:A:515:VAL:CG2	1:A:631:GLY:HA3	2.44	0.48
2:D:69:ARG:HA	2:D:268:LEU:HD11	1.94	0.48
2:J:469:THR:HG23	2:J:482:HIS:HB3	1.95	0.48
1:E:295:ARG:O	1:E:296:ASN:HB2	2.13	0.48
2:F:232:LYS:O	2:F:236:ASN:N	2.42	0.48
2:D:317:LYS:HG3	2:D:341:ILE:HD13	1.95	0.48
1:G:480:HIS:HD2	1:G:482:LEU:H	1.62	0.48
1:I:316:MET:CE	1:I:337:PHE:CD1	2.95	0.48
1:C:400:LEU:HD11	1:C:482:LEU:CD1	2.44	0.48
1:C:619:ILE:HD11	1:C:626:ARG:HB2	1.95	0.48
1:A:414:ILE:HD11	1:A:443:MET:N	2.28	0.48
1:C:66:ILE:HG22	1:C:137:GLN:HG3	1.95	0.48
1:E:457:PRO:HG2	1:E:458:THR:N	2.20	0.48
1:K:518:PRO:O	1:K:521:ASP:HB2	2.12	0.48
1:K:563:LEU:CD2	1:K:636:VAL:HG22	2.43	0.48
1:I:292:ILE:HD13	1:I:300:VAL:O	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:334:THR:CG2	1:G:351:ASN:HB2	2.44	0.48
2:B:462:VAL:HG21	2:J:169:GLY:HA2	1.95	0.48
1:A:69:ALA:HB3	1:A:141:PRO:HA	1.96	0.48
1:A:283:ILE:HD12	1:A:389:VAL:CG2	2.43	0.48
1:G:150:SER:O	1:G:153:ALA:N	2.47	0.48
1:K:646:LEU:HD12	2:L:72:LEU:HD21	1.94	0.48
1:A:675:VAL:CG1	1:A:707:VAL:HG21	2.43	0.48
1:K:405:PRO:CG	1:K:481:ASN:HA	2.44	0.48
1:E:146:LEU:HD23	1:E:152:PHE:CG	2.49	0.48
1:C:77:ARG:NH1	1:C:370:VAL:HG21	2.28	0.48
1:I:124:ILE:HG23	1:I:152:PHE:HD2	1.77	0.48
1:A:131:ILE:CG2	1:A:136:ALA:HB2	2.38	0.48
1:E:528:ALA:HB1	1:E:605:LEU:HD22	1.95	0.48
2:H:499:ARG:CG	2:H:499:ARG:NH1	2.77	0.48
1:A:467:ARG:NH1	1:A:467:ARG:HB3	2.24	0.48
1:A:528:ALA:HB1	1:A:605:LEU:CD2	2.43	0.48
1:C:504:ILE:CG2	1:C:505:ALA:N	2.77	0.48
2:D:207:SER:HB3	2:D:208:PRO:CD	2.41	0.48
1:A:273:GLN:O	1:A:285:LEU:HD12	2.14	0.48
2:L:337:ALA:HB1	2:L:370:SER:HA	1.96	0.48
1:I:537:GLU:HG3	1:I:553:ARG:HH21	1.78	0.48
2:F:474:ARG:HD3	2:F:474:ARG:HA	1.63	0.48
2:F:376:ARG:HH11	2:H:410:LYS:HZ2	1.62	0.48
2:J:69:ARG:HA	2:J:268:LEU:HD11	1.95	0.48
1:E:150:SER:O	1:E:151:LYS:C	2.51	0.48
1:I:71:ARG:O	1:I:75:ALA:CB	2.62	0.48
1:E:617:GLY:O	1:E:625:PHE:CB	2.50	0.48
1:I:393:GLY:HA3	1:I:455:TRP:CZ3	2.49	0.48
2:J:325:ASP:C	2:J:327:GLY:H	2.17	0.48
1:G:517:LEU:HD21	1:G:632:ALA:HB1	1.96	0.48
1:G:517:LEU:H	1:G:564:GLN:HE22	1.60	0.48
2:F:149:MET:CE	2:F:189:VAL:HG11	2.43	0.48
2:L:58:GLN:CD	2:L:63:LYS:HE3	2.32	0.48
1:C:283:ILE:HD12	1:C:389:VAL:CG2	2.44	0.48
2:H:58:GLN:OE1	2:H:63:LYS:HE3	2.13	0.48
2:B:43:ARG:HG2	2:B:43:ARG:NH1	2.28	0.48
2:H:501:PHE:N	2:H:501:PHE:CD2	2.78	0.48
1:A:167:PRO:O	1:A:169:GLY:N	2.47	0.48
1:C:168:LYS:HA	1:C:171:ILE:HD12	1.96	0.48
1:I:400:LEU:HD13	1:I:449:ILE:CD1	2.24	0.48
1:C:308:LEU:HD12	1:C:308:LEU:O	2.13	0.48
1:E:93:TYR:HA	1:E:121:TYR:OH	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:378:ALA:O	1:C:379:GLY:C	2.51	0.48
1:K:417:LEU:HD21	1:K:478:ILE:CD1	2.39	0.48
2:H:432:ARG:HG2	2:H:433:LYS:N	2.28	0.48
2:H:432:ARG:O	2:H:458:ALA:HA	2.13	0.48
2:J:346:ARG:HH11	2:J:346:ARG:HG3	1.78	0.48
1:I:189:VAL:CG2	1:I:323:LEU:HB2	2.44	0.48
2:J:436:GLY:O	2:J:439:TYR:HB3	2.13	0.48
1:K:411:LEU:HB2	1:K:682:GLN:HG3	1.95	0.48
1:K:270:ILE:HG12	1:K:289:GLU:HG3	1.95	0.48
2:B:309:ASN:HD21	2:B:311:ASN:HB2	1.79	0.48
2:J:188:GLY:HA2	2:J:384:PHE:CE2	2.49	0.48
1:A:78:VAL:CG1	1:A:79:ILE:N	2.77	0.48
1:E:95:ASP:OD2	1:E:114:PRO:HA	2.14	0.48
1:K:400:LEU:HD21	1:K:482:LEU:CD1	2.44	0.48
1:E:132:ARG:HD3	1:E:159:GLU:OE1	2.14	0.48
1:G:136:ALA:HB1	1:G:161:VAL:CG1	2.38	0.48
1:I:517:LEU:HD22	1:I:517:LEU:N	2.22	0.48
1:G:518:PRO:O	1:G:521:ASP:HB2	2.14	0.48
1:E:583:PHE:CZ	1:E:590:MET:HE3	2.48	0.48
1:C:419:ARG:HB2	1:C:476:GLU:HB2	1.95	0.48
2:F:42:ARG:O	2:F:45:ALA:HB3	2.13	0.48
2:L:296:ASP:O	2:L:298:ILE:HD12	2.14	0.48
2:F:109:THR:HG22	2:F:122:PHE:HB2	1.95	0.48
1:G:411:LEU:HG	1:G:412:PRO:O	2.13	0.48
2:F:376:ARG:NH1	2:H:410:LYS:NZ	2.62	0.48
2:L:160:ASP:OD1	2:L:198:GLY:HA3	2.14	0.48
1:K:671:VAL:CG2	1:K:691:GLU:HB2	2.44	0.48
1:E:441:ILE:HD12	1:E:478:ILE:HD13	1.95	0.48
1:G:292:ILE:HG23	1:G:503:PHE:CD2	2.48	0.48
1:K:131:ILE:CG2	1:K:136:ALA:HB2	2.32	0.48
1:I:164:VAL:HG23	1:I:373:MET:O	2.14	0.48
1:G:155:ALA:O	1:G:159:GLU:HG2	2.14	0.48
2:B:90:CYS:HB2	2:B:168:GLU:OE2	2.14	0.48
1:I:64:ASN:H	1:I:137:GLN:HG2	1.79	0.48
1:C:390:LYS:HD3	1:C:391:LEU:H	1.75	0.48
2:J:91:THR:HG22	2:J:98:GLN:HG2	1.96	0.48
2:F:476(A):LEU:C	2:F:476(C):ASP:H	2.16	0.48
1:K:283:ILE:CG2	1:K:386:GLN:HG2	2.44	0.48
2:B:492:ASN:ND2	2:B:494:PHE:H	2.11	0.48
2:H:193:ILE:HD13	2:H:274:LEU:HD23	1.95	0.48
1:A:403:GLU:O	1:A:405:PRO:HD3	2.14	0.48
1:G:553:ARG:NH1	2:H:115:ASN:OD1	2.47	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:J:351:THR:HG22	2:J:386:ILE:HG23	1.96	0.48
1:G:367:VAL:HG12	1:G:368:ASP:N	2.29	0.48
1:E:339:VAL:HG22	1:E:345:PHE:HB3	1.95	0.48
1:C:473:PHE:O	1:C:615:LYS:NZ	2.33	0.48
1:K:422:PRO:HG3	1:K:473:PHE:CZ	2.49	0.48
1:K:358:HIS:CD2	1:K:362:GLU:OE1	2.67	0.48
2:J:117:ARG:HB3	2:J:280:LEU:HD21	1.94	0.48
1:A:156:LEU:HD13	1:A:163:PHE:HB2	1.95	0.48
1:A:518:PRO:O	1:A:521:ASP:HB2	2.13	0.48
1:K:74:ILE:HG23	1:K:75:ALA:N	2.29	0.48
1:G:627:ILE:N	1:G:627:ILE:HD12	2.29	0.48
2:D:476(C):ASP:HB3	2:D:478:LYS:HG3	1.96	0.48
1:C:596:TRP:CG	1:C:597:THR:N	2.82	0.48
2:D:348:GLU:O	2:D:350:ARG:HD2	2.14	0.48
2:H:312:THR:HG22	2:H:313:PRO:O	2.14	0.48
2:H:235:THR:HG22	2:H:237:GLU:CB	2.44	0.48
2:H:339:ASN:HD21	2:H:370:SER:HB3	1.79	0.48
2:D:178:GLU:HB3	2:D:182:ARG:NH1	2.29	0.48
1:I:454:THR:HG21	1:I:466:MET:HA	1.95	0.48
1:E:683:GLU:HB2	1:E:704:LYS:HG3	1.94	0.48
1:I:267:PRO:O	1:I:501:THR:HG23	2.14	0.48
1:K:433:THR:HG22	1:K:434:GLY:N	2.29	0.47
1:I:443:MET:HG3	1:I:444:TYR:CE1	2.49	0.47
1:C:78:VAL:HA	1:C:370:VAL:HG11	1.96	0.47
1:E:712:ALA:HA	1:E:716:ASN:ND2	2.28	0.47
1:K:139:VAL:O	1:K:164:VAL:HG12	2.14	0.47
1:E:393:GLY:HA2	1:E:457:PRO:O	2.14	0.47
1:I:457:PRO:CG	1:I:458:THR:H	2.24	0.47
1:A:124:ILE:O	1:A:128:MET:HB2	2.14	0.47
1:A:136:ALA:HB1	1:A:161:VAL:CG1	2.35	0.47
1:G:670:ILE:HD12	1:G:712:ALA:HB1	1.95	0.47
1:A:325:LYS:O	1:A:327:VAL:N	2.46	0.47
2:J:492:ASN:HB2	2:J:493:PRO:CD	2.43	0.47
1:E:634:LEU:N	1:E:634:LEU:CD2	2.76	0.47
2:H:339:ASN:HB3	2:H:361:VAL:HG12	1.96	0.47
2:H:339:ASN:ND2	2:H:370:SER:HB3	2.29	0.47
2:L:492:ASN:HD22	2:L:494:PHE:H	1.61	0.47
1:A:401:TYR:CD2	1:A:448:MET:HA	2.49	0.47
1:E:376:VAL:C	1:E:378:ALA:N	2.66	0.47
2:B:339:ASN:ND2	2:B:370:SER:HB3	2.29	0.47
1:A:347:PHE:CD1	1:A:347:PHE:O	2.67	0.47
2:H:300:PRO:HA	2:H:509:ARG:NH1	2.28	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:446:ASP:OD1	1:G:447:PRO:HD2	2.14	0.47
1:K:308:LEU:HA	1:K:343:LYS:HE3	1.95	0.47
1:G:289:GLU:OE1	1:G:305:SER:OG	2.31	0.47
1:E:653:LYS:CD	1:E:653:LYS:N	2.75	0.47
1:K:162:ILE:HD13	1:K:377:ALA:O	2.14	0.47
1:K:292:ILE:HG23	1:K:503:PHE:CD2	2.49	0.47
1:C:162:ILE:O	1:C:164:VAL:N	2.47	0.47
2:F:210:MET:HE1	2:H:417:TYR:N	2.29	0.47
1:G:626:ARG:NE	1:G:628:ARG:HD2	2.28	0.47
1:K:293:GLN:HB3	1:K:298:LYS:HA	1.96	0.47
2:D:476(C):ASP:C	2:D:477:GLU:H	2.17	0.47
1:G:283:ILE:HB	1:G:386:GLN:CD	2.35	0.47
1:E:107:ASP:C	1:E:108:GLU:HG3	2.34	0.47
2:J:356:ALA:CB	2:J:391:LEU:HB2	2.44	0.47
2:D:394:VAL:HG23	2:D:395:PRO:HD2	1.97	0.47
2:D:419:TYR:CE1	2:D:443:SER:HB2	2.48	0.47
1:I:416:ARG:HG3	1:I:439:GLY:O	2.13	0.47
1:I:522:LEU:HD22	1:I:563:LEU:HD13	1.96	0.47
1:A:163:PHE:C	1:A:163:PHE:CD1	2.87	0.47
1:C:139:VAL:HG11	1:C:156:LEU:HD21	1.96	0.47
1:C:718:LEU:HD23	1:C:718:LEU:H	1.76	0.47
1:I:517:LEU:H	1:I:517:LEU:CD2	2.20	0.47
2:B:368:ILE:CG1	2:B:408:VAL:HG13	2.43	0.47
1:I:206:VAL:HG13	1:I:235:ASP:CB	2.44	0.47
2:J:126:PHE:HB2	2:J:160:ASP:OD2	2.13	0.47
1:G:83:ARG:HH11	1:G:83:ARG:CG	2.27	0.47
1:G:492:PRO:HA	1:G:495:ILE:HD12	1.95	0.47
1:A:401:TYR:CE2	1:A:448:MET:HB2	2.49	0.47
2:H:522:LEU:HD23	2:J:151:ASN:HD21	1.79	0.47
1:A:367:VAL:HG12	1:A:368:ASP:N	2.29	0.47
2:D:148:ALA:HB1	2:D:153:ALA:O	2.14	0.47
1:I:400:LEU:HD11	1:I:482:LEU:CD1	2.43	0.47
1:I:433:THR:HG23	1:I:449:ILE:O	2.14	0.47
1:G:309:ASP:OD2	1:G:343:LYS:HE2	2.14	0.47
1:E:163:PHE:CD1	1:E:163:PHE:C	2.87	0.47
1:K:358:HIS:HD2	1:K:362:GLU:OE1	1.97	0.47
1:A:467:ARG:HE	1:A:630:ARG:HG3	1.79	0.47
1:G:317:GLY:O	1:G:321:VAL:HG12	2.14	0.47
1:G:283:ILE:HG22	1:G:386:GLN:HG2	1.96	0.47
2:D:138:SER:OG	2:D:139:LYS:N	2.47	0.47
1:C:67:LEU:HG	1:C:68:ILE:H	1.79	0.47
2:J:355:VAL:O	2:J:390:THR:HA	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:65:LYS:HE2	1:E:134:THR:O	2.14	0.47
1:E:319:GLN:NE2	1:E:345:PHE:CE1	2.83	0.47
1:C:309:ASP:OD2	1:C:343:LYS:HE2	2.15	0.47
1:G:78:VAL:CG1	1:G:79:ILE:N	2.78	0.47
1:I:178:ILE:CD1	1:I:178:ILE:H	2.08	0.47
1:K:390:LYS:HD3	1:K:391:LEU:H	1.75	0.47
1:C:518:PRO:HD2	1:C:521:ASP:OD1	2.15	0.47
2:B:420:GLY:HA3	2:J:184:ILE:CD1	2.37	0.47
1:K:140:HIS:ND1	1:K:141:PRO:N	2.62	0.47
2:D:298:ILE:N	2:D:298:ILE:HD12	2.29	0.47
1:C:401:TYR:CD2	1:C:448:MET:HA	2.50	0.47
2:B:58:GLN:HA	2:B:61:ARG:HH21	1.80	0.47
2:J:141:ILE:O	2:J:145:MET:HG3	2.14	0.47
1:A:484:PHE:O	1:A:487:ALA:HB3	2.14	0.47
1:E:670:ILE:HD11	1:E:718:LEU:HD11	1.96	0.47
1:A:146:LEU:HD23	1:A:152:PHE:CD2	2.50	0.47
1:G:614:LEU:HD22	1:G:627:ILE:HG21	1.95	0.47
1:A:285:LEU:N	1:A:285:LEU:HD12	2.29	0.47
1:I:231:ILE:N	1:I:231:ILE:HD12	2.27	0.47
1:G:195:TYR:O	1:G:259:PHE:HA	2.15	0.47
2:J:298:ILE:HG23	2:J:509:ARG:HB2	1.96	0.47
2:F:108:VAL:O	2:F:122:PHE:HA	2.14	0.47
2:H:309:ASN:HD21	2:H:311:ASN:HB2	1.80	0.47
1:G:515:VAL:CG2	1:G:631:GLY:HA3	2.45	0.47
1:A:400:LEU:HD11	1:A:482:LEU:CD1	2.45	0.47
1:C:400:LEU:HD23	1:C:481:ASN:OD1	2.15	0.47
1:E:117:ALA:C	1:E:119:GLN:N	2.68	0.47
1:I:115:PRO:HG2	1:I:444:TYR:CE2	2.50	0.47
1:E:358:HIS:CG	1:E:359:PRO:HD3	2.49	0.47
1:K:152:PHE:CE1	1:K:156:LEU:HD11	2.49	0.47
1:K:163:PHE:CD1	1:K:163:PHE:C	2.88	0.47
1:K:630:ARG:C	1:K:632:ALA:H	2.17	0.47
1:C:358:HIS:N	1:C:359:PRO:CD	2.77	0.47
1:A:617:GLY:O	1:A:625:PHE:CB	2.53	0.47
1:G:663:LEU:O	1:G:665:PRO:HD3	2.15	0.47
1:I:517:LEU:HB3	1:I:521:ASP:HB3	1.96	0.47
2:B:522:LEU:HA	2:F:151:ASN:ND2	2.30	0.47
1:C:658:THR:CB	1:C:703:LYS:HD3	2.40	0.47
2:B:403:GLN:O	2:B:408:VAL:HG22	2.15	0.47
1:K:275:LEU:HD23	1:K:276:CYS:H	1.80	0.47
2:J:58:GLN:CD	2:J:63:LYS:HE3	2.34	0.47
2:J:121:VAL:CG2	2:J:122:PHE:N	2.76	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:186:GLU:C	1:K:188:ASN:N	2.68	0.47
2:H:229:ASP:N	2:H:229:ASP:OD1	2.47	0.47
1:G:140:HIS:ND1	1:G:141:PRO:HD2	2.30	0.47
2:L:492:ASN:HB2	2:L:493:PRO:HD2	1.95	0.47
1:I:515:VAL:HG21	1:I:631:GLY:HA3	1.97	0.47
2:B:193:ILE:CD1	2:B:274:LEU:HD23	2.45	0.47
2:H:299:GLU:O	2:H:509:ARG:HA	2.15	0.47
1:G:720:VAL:HG22	1:G:721:ASP:H	1.80	0.47
2:J:261:PHE:CD1	2:J:267:ALA:HA	2.49	0.47
1:I:63:PHE:N	1:I:63:PHE:CD1	2.82	0.47
2:B:484:ALA:O	2:B:488:GLU:OE1	2.33	0.47
1:A:289:GLU:OE1	1:A:306:PRO:HD2	2.15	0.47
1:C:66:ILE:HD13	1:C:88:SER:O	2.14	0.47
1:G:551:HIS:HE1	2:L:348:GLU:OE2	1.97	0.47
1:I:229:MET:HG3	1:I:229:MET:O	2.15	0.47
2:H:307:PRO:HG3	2:H:312:THR:HG22	1.97	0.47
2:H:458:ALA:HB3	2:H:493:PRO:HB3	1.97	0.47
1:G:184:ALA:HB1	1:G:189:VAL:HB	1.96	0.47
1:G:71:ARG:O	1:G:75:ALA:CB	2.63	0.47
1:C:78:VAL:HG23	1:C:370:VAL:CG1	2.45	0.47
2:J:476(D):PRO:HA	2:J:479:ILE:HD11	1.97	0.47
2:B:379:ARG:NH2	2:J:535:ASP:OD2	2.47	0.47
1:C:517:LEU:HD21	1:C:632:ALA:CB	2.45	0.47
1:I:518:PRO:O	1:I:521:ASP:HB2	2.15	0.47
2:D:434:ALA:HB3	2:D:460:VAL:HG12	1.97	0.47
1:G:235:ASP:OD1	1:G:235:ASP:N	2.46	0.47
2:F:432:ARG:HG2	2:F:433:LYS:N	2.30	0.47
1:A:415:GLY:C	1:A:440:GLU:HG3	2.34	0.47
2:F:202:GLY:O	2:F:205:VAL:HG22	2.14	0.47
1:I:626:ARG:NE	1:I:628:ARG:HD2	2.30	0.47
1:G:107:ASP:O	1:G:108:GLU:HG3	2.15	0.47
2:F:124:GLN:HE21	2:F:137:HIS:CE1	2.32	0.47
1:A:436:TYR:HE1	1:A:439:GLY:CA	2.28	0.47
1:G:436:TYR:HE1	1:G:439:GLY:CA	2.28	0.47
1:K:625:PHE:CD1	1:K:627:ILE:HD11	2.49	0.47
1:K:630:ARG:C	1:K:632:ALA:N	2.69	0.47
1:I:136:ALA:HB1	1:I:161:VAL:CG1	2.34	0.47
2:L:479:ILE:HD12	2:L:479:ILE:C	2.33	0.47
1:A:658:THR:HG22	1:A:659:SER:O	2.14	0.47
2:F:170:VAL:HG11	2:H:460:VAL:HG23	1.96	0.47
2:F:390:THR:CG2	2:F:419:TYR:OH	2.63	0.47
1:I:537:GLU:HG3	1:I:553:ARG:NH2	2.30	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:390:THR:CG2	2:L:419:TYR:OH	2.63	0.47
1:I:394:TRP:CE3	1:I:459:ARG:HG3	2.50	0.47
2:D:501:PHE:CE1	2:L:174:ALA:HB2	2.49	0.47
1:E:683:GLU:H	1:E:704:LYS:HG2	1.78	0.47
2:H:95:MET:HE3	2:H:95:MET:HA	1.97	0.47
1:G:63:PHE:N	1:G:63:PHE:CD1	2.83	0.47
1:K:515:VAL:HG21	1:K:631:GLY:HA3	1.97	0.47
2:H:80:GLU:HB2	2:L:517:ARG:NH2	2.30	0.47
2:L:48:LEU:HA	2:L:48:LEU:HD23	1.63	0.47
2:B:355:VAL:O	2:B:390:THR:HA	2.14	0.47
2:L:469:THR:HG23	2:L:482:HIS:HB3	1.96	0.47
2:B:195:MET:SD	2:B:271:VAL:HG21	2.54	0.47
1:A:117:ALA:CB	1:A:121:TYR:HB2	2.43	0.46
1:K:444:TYR:N	1:K:444:TYR:CD1	2.83	0.46
1:C:292:ILE:HG23	1:C:503:PHE:CD2	2.50	0.46
1:G:71:ARG:CA	1:G:75:ALA:HB2	2.45	0.46
1:A:354:LEU:HD11	1:A:358:HIS:ND1	2.31	0.46
1:E:292:ILE:H	1:E:292:ILE:CD1	2.07	0.46
1:I:467:ARG:HH21	1:I:630:ARG:NE	2.14	0.46
1:G:625:PHE:CD1	1:G:627:ILE:HD11	2.50	0.46
2:J:291:PHE:CE1	2:J:348:GLU:HA	2.51	0.46
1:C:396:ILE:HG12	1:C:463:ILE:CD1	2.40	0.46
2:J:432:ARG:HG2	2:J:433:LYS:N	2.31	0.46
1:A:583:PHE:CZ	1:A:590:MET:HE3	2.51	0.46
1:K:283:ILE:HB	1:K:386:GLN:CD	2.36	0.46
1:A:279:HIS:NE2	1:A:380:GLU:N	2.62	0.46
2:B:432:ARG:HG2	2:B:433:LYS:N	2.29	0.46
2:J:382:ASP:HA	2:J:424:VAL:CG1	2.45	0.46
2:H:196:ILE:HG22	2:H:221:SER:HB2	1.97	0.46
1:K:515:VAL:CG2	1:K:631:GLY:HA3	2.45	0.46
2:J:309:ASN:HD21	2:J:311:ASN:HB2	1.80	0.46
2:F:192:GLN:O	2:F:211:THR:HB	2.15	0.46
1:C:627:ILE:HD12	1:C:627:ILE:N	2.30	0.46
1:G:164:VAL:HG23	1:G:377:ALA:CB	2.44	0.46
1:I:543:VAL:HG12	1:I:544:SER:N	2.31	0.46
1:A:164:VAL:HG23	1:A:373:MET:O	2.16	0.46
2:B:210:MET:HE1	2:J:416:LEU:HG	1.97	0.46
1:I:285:LEU:HB3	1:I:365:THR:HG21	1.97	0.46
1:A:321:VAL:O	1:A:324:ALA:CB	2.60	0.46
2:F:336:PHE:O	2:F:373:LYS:NZ	2.40	0.46
1:G:419:ARG:HB2	1:G:476:GLU:HB2	1.97	0.46
2:J:307:PRO:HG3	2:J:312:THR:HG22	1.95	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:91:THR:O	2:L:98:GLN:NE2	2.45	0.46
1:C:190:SER:N	1:C:319:GLN:OE1	2.36	0.46
1:A:189:VAL:CG2	1:A:323:LEU:HB2	2.45	0.46
2:L:458:ALA:HB3	2:L:493:PRO:HB3	1.97	0.46
1:K:287:GLU:OE2	1:K:305:SER:N	2.44	0.46
1:I:649:LEU:HD13	2:J:59:HIS:CD2	2.50	0.46
2:D:229:ASP:O	2:D:233:THR:HG23	2.16	0.46
1:C:515:VAL:CG2	1:C:631:GLY:HA3	2.44	0.46
1:I:316:MET:HE3	1:I:337:PHE:CD1	2.42	0.46
1:C:316:MET:HE3	1:C:337:PHE:HD1	1.79	0.46
1:E:400:LEU:HD11	1:E:482:LEU:CD1	2.45	0.46
1:I:78:VAL:CG1	1:I:79:ILE:N	2.77	0.46
1:C:73:GLU:HG3	1:C:74:ILE:H	1.80	0.46
1:E:619:ILE:HD11	1:E:626:ARG:HB2	1.98	0.46
1:A:670:ILE:CD1	1:A:718:LEU:HD21	2.46	0.46
1:G:543:VAL:HG12	1:G:544:SER:N	2.29	0.46
1:C:146:LEU:HD23	1:C:152:PHE:CG	2.51	0.46
1:G:390:LYS:HD3	1:G:390:LYS:C	2.34	0.46
1:A:517:LEU:HD21	1:A:632:ALA:HB1	1.97	0.46
1:A:327:VAL:HG22	1:A:327:VAL:O	2.15	0.46
1:E:614:LEU:HD22	1:E:627:ILE:HG21	1.96	0.46
2:H:235:THR:HG22	2:H:235:THR:O	2.15	0.46
1:C:83:ARG:CG	1:C:83:ARG:HH11	2.26	0.46
2:J:346:ARG:NH1	2:J:346:ARG:HG3	2.30	0.46
1:G:319:GLN:NE2	1:G:345:PHE:CE1	2.83	0.46
1:K:541:THR:HG22	1:K:541:THR:O	2.14	0.46
1:A:411:LEU:HB2	1:A:682:GLN:HG3	1.96	0.46
1:I:675:VAL:HG12	1:I:707:VAL:HG21	1.96	0.46
1:A:675:VAL:HG12	1:A:707:VAL:HG21	1.98	0.46
2:D:378:VAL:HG13	2:D:388:LEU:CD1	2.45	0.46
2:L:215:PHE:HD2	2:L:259:ALA:HB3	1.81	0.46
1:E:664:CYS:HB2	1:E:724:ILE:HD11	1.96	0.46
2:L:232:LYS:O	2:L:236:ASN:N	2.42	0.46
2:H:94:ASN:HA	2:H:98:GLN:OE1	2.16	0.46
2:F:69:ARG:HA	2:F:268:LEU:HD11	1.97	0.46
2:L:200:CYS:HB3	2:L:223:MET:HB3	1.96	0.46
2:J:239:VAL:HG22	2:J:243:GLU:HB2	1.97	0.46
1:E:348:LEU:HD23	1:E:348:LEU:O	2.16	0.46
1:A:74:ILE:HG23	1:A:75:ALA:N	2.30	0.46
1:C:626:ARG:NE	1:C:628:ARG:HD2	2.30	0.46
1:E:78:VAL:HA	1:E:370:VAL:HG11	1.98	0.46
1:K:334:THR:CG2	1:K:351:ASN:HB2	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:149:MET:SD	2:B:186:ALA:HB2	2.56	0.46
2:F:89:ARG:NH2	2:J:135:GLU:OE1	2.48	0.46
1:A:528:ALA:CB	1:A:605:LEU:HD22	2.43	0.46
2:D:135:GLU:OE1	2:H:89:ARG:NH2	2.48	0.46
1:E:563:LEU:HB3	1:E:564:GLN:H	1.38	0.46
2:F:460:VAL:HG23	2:H:170:VAL:HG11	1.97	0.46
2:F:339:ASN:HB3	2:F:361:VAL:HG12	1.96	0.46
1:K:401:TYR:CD2	1:K:448:MET:HA	2.49	0.46
1:I:195:TYR:CD2	1:I:208:ILE:HD13	2.51	0.46
2:H:458:ALA:O	2:H:493:PRO:HD3	2.15	0.46
1:I:401:TYR:HD2	1:I:448:MET:HA	1.80	0.46
1:E:83:ARG:HH11	1:E:83:ARG:CG	2.26	0.46
2:L:329:PHE:HE1	2:L:343:GLY:HA3	1.77	0.46
2:F:382:ASP:HA	2:F:424:VAL:CG1	2.46	0.46
2:D:119:VAL:HG13	2:D:156:ILE:HD13	1.96	0.46
2:H:108:VAL:O	2:H:122:PHE:HA	2.14	0.46
2:B:469:THR:CG2	2:B:482:HIS:HB3	2.46	0.46
1:I:563:LEU:O	1:I:565:GLY:N	2.48	0.46
2:F:252:ARG:NH2	2:F:335:GLU:HG3	2.31	0.46
1:K:539:ARG:NH2	2:L:326:GLU:OE2	2.49	0.46
1:G:273:GLN:O	1:G:285:LEU:HD12	2.16	0.46
1:I:539:ARG:NH2	2:J:326:GLU:OE2	2.49	0.46
1:C:547:MET:O	1:C:548:ASP:C	2.52	0.46
2:F:314:TYR:CE1	2:F:359:PRO:HG2	2.50	0.46
1:E:316:MET:O	1:E:320:ALA:HB2	2.15	0.46
1:E:114:PRO:HB2	1:E:115:PRO:HD2	1.97	0.46
1:I:93:TYR:HA	1:I:121:TYR:OH	2.15	0.46
1:E:139:VAL:HG11	1:E:156:LEU:HD21	1.98	0.46
1:K:164:VAL:HG23	1:K:373:MET:O	2.15	0.46
1:C:457:PRO:HG2	1:C:458:THR:N	2.18	0.46
1:I:419:ARG:HD2	1:I:601:GLN:OE1	2.15	0.46
1:G:517:LEU:HA	1:G:518:PRO:HD3	1.58	0.46
1:K:283:ILE:HD12	1:K:389:VAL:CG2	2.44	0.46
1:K:436:TYR:HE1	1:K:439:GLY:CA	2.28	0.46
1:E:515:VAL:HG21	1:E:631:GLY:HA3	1.97	0.46
2:L:52:GLN:OE1	2:L:52:GLN:O	2.34	0.46
2:H:138:SER:OG	2:H:139:LYS:N	2.47	0.46
1:I:690:ILE:CD1	1:I:699:LEU:HD11	2.46	0.46
2:H:469:THR:HG23	2:H:482:HIS:HB3	1.96	0.46
1:A:308:LEU:CD2	1:A:316:MET:SD	2.97	0.46
1:C:602:LEU:HD12	1:C:614:LEU:O	2.15	0.46
1:A:93:TYR:HD1	1:A:94:SER:O	1.99	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:518:PRO:O	1:K:521:ASP:N	2.36	0.46
1:E:596:TRP:CH2	1:E:600:ASP:O	2.67	0.46
2:F:299:GLU:HB2	2:F:302:LEU:CD1	2.45	0.46
2:F:299:GLU:O	2:F:509:ARG:HA	2.15	0.46
1:I:658:THR:HG22	1:I:659:SER:O	2.16	0.46
2:L:340:ILE:HG23	2:L:373:LYS:HD3	1.97	0.46
2:L:108:VAL:O	2:L:122:PHE:HA	2.15	0.46
1:G:186:GLU:C	1:G:188:ASN:N	2.68	0.46
1:E:140:HIS:ND1	1:E:141:PRO:N	2.64	0.46
1:E:264:VAL:HG13	1:E:340:ASP:HB3	1.97	0.46
2:B:492:ASN:ND2	2:B:494:PHE:HB2	2.31	0.46
1:A:541:THR:HG22	1:A:541:THR:O	2.15	0.46
2:F:376:ARG:HH11	2:H:410:LYS:NZ	2.13	0.46
1:G:515:VAL:HG21	1:G:631:GLY:HA3	1.96	0.46
1:C:93:TYR:HD1	1:C:94:SER:O	1.98	0.46
1:A:414:ILE:HD12	1:A:441:ILE:O	2.15	0.46
1:I:363:LEU:HD13	1:I:455:TRP:HB3	1.96	0.46
1:K:528:ALA:CB	1:K:605:LEU:HD22	2.45	0.46
1:G:457:PRO:CG	1:G:458:THR:N	2.78	0.46
1:A:268:ARG:NH2	1:A:497:GLY:O	2.43	0.46
1:A:596:TRP:CG	1:A:597:THR:N	2.83	0.46
1:A:140:HIS:ND1	1:A:141:PRO:N	2.63	0.46
1:C:530:ALA:HB2	1:C:561:VAL:HG21	1.97	0.46
1:A:640:THR:OG1	1:A:643:GLN:HB2	2.15	0.46
1:C:68:ILE:CG2	1:C:70:ASN:H	2.29	0.46
2:B:49:GLY:C	2:B:51:GLY:H	2.18	0.46
1:E:547:MET:O	1:E:548:ASP:C	2.52	0.46
2:J:50:GLY:HA3	2:J:127:THR:O	2.15	0.46
1:G:539:ARG:NH2	2:H:326:GLU:OE2	2.48	0.46
2:B:423:THR:O	2:B:525:LYS:HE2	2.16	0.46
2:H:474:ARG:HD3	2:H:474:ARG:HA	1.65	0.46
1:I:70:ASN:ND2	1:I:145:PHE:CD1	2.84	0.46
1:C:85:MET:O	1:C:86:GLY:C	2.53	0.46
1:I:162:ILE:O	1:I:164:VAL:N	2.49	0.46
1:K:65:LYS:HA	1:K:88:SER:O	2.16	0.46
2:J:416:LEU:HB2	2:J:441:VAL:HG22	1.96	0.46
1:A:517:LEU:HA	1:A:518:PRO:HD3	1.59	0.46
1:G:396:ILE:N	1:G:396:ILE:HD12	2.30	0.46
1:I:661:MET:HG3	1:I:723:VAL:HG13	1.98	0.46
1:G:93:TYR:HA	1:G:121:TYR:OH	2.15	0.46
2:B:235:THR:O	2:B:235:THR:HG22	2.16	0.46
1:A:186:GLU:C	1:A:188:ASN:N	2.69	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:491:HIS:CE1	1:C:493:LYS:HB2	2.51	0.46
1:E:150:SER:O	1:E:153:ALA:N	2.48	0.46
1:E:724:ILE:HG22	1:E:725:MET:HG3	1.98	0.46
2:H:192:GLN:O	2:H:211:THR:HB	2.16	0.46
1:A:577:ASP:HB2	1:A:591:ARG:NH2	2.31	0.46
1:C:414:ILE:HD12	1:C:441:ILE:O	2.16	0.46
1:E:444:TYR:O	1:E:445:TYR:CG	2.69	0.46
1:I:334:THR:CG2	1:I:351:ASN:HB2	2.46	0.46
1:C:132:ARG:HD3	1:C:159:GLU:OE1	2.15	0.46
2:H:476(C):ASP:C	2:H:477:GLU:H	2.19	0.46
1:C:583:PHE:HZ	1:C:590:MET:HE3	1.80	0.46
2:J:227:GLY:O	2:J:231:VAL:HG23	2.16	0.46
2:L:45:ALA:O	2:L:48:LEU:HB2	2.16	0.46
1:G:285:LEU:HD12	1:G:285:LEU:N	2.31	0.46
2:L:199:PRO:HB3	2:L:222:TYR:CZ	2.51	0.46
1:C:415:GLY:C	1:C:440:GLU:HG3	2.36	0.46
1:C:167:PRO:O	1:C:169:GLY:N	2.49	0.46
1:G:295:ARG:O	1:G:296:ASN:HB2	2.16	0.46
1:C:457:PRO:CG	1:C:458:THR:N	2.79	0.46
1:G:156:LEU:HD13	1:G:163:PHE:HB2	1.95	0.46
1:G:92:ILE:CG1	1:G:112:ILE:HD13	2.46	0.46
1:K:229:MET:O	1:K:230:ARG:HB2	2.13	0.46
1:A:658:THR:CB	1:A:703:LYS:HD3	2.46	0.46
2:L:325:ASP:C	2:L:327:GLY:N	2.70	0.46
1:C:189:VAL:CG2	1:C:323:LEU:HB2	2.45	0.46
1:K:690:ILE:CD1	1:K:699:LEU:HD11	2.45	0.46
2:L:474:ARG:HA	2:L:474:ARG:HD3	1.60	0.46
1:K:713:SER:O	1:K:714:ALA:C	2.55	0.46
2:F:195:MET:SD	2:F:271:VAL:HG21	2.56	0.46
1:A:170:ALA:O	1:A:173:ALA:HB3	2.16	0.46
2:J:124:GLN:HE21	2:J:137:HIS:CE1	2.34	0.46
2:D:232:LYS:O	2:D:236:ASN:N	2.42	0.46
1:K:265:THR:HG21	1:K:342:GLN:NE2	2.31	0.45
1:E:162:ILE:O	1:E:164:VAL:N	2.49	0.45
1:I:334:THR:HG22	1:I:351:ASN:HB2	1.98	0.45
1:G:396:ILE:CG1	1:G:463:ILE:HD13	2.38	0.45
1:K:78:VAL:HA	1:K:370:VAL:HG11	1.97	0.45
1:C:293:GLN:HB3	1:C:298:LYS:HA	1.97	0.45
1:C:112:ILE:O	1:C:120:SER:HA	2.16	0.45
1:E:304:PRO:HD2	1:E:394:TRP:CE2	2.51	0.45
2:F:88:HIS:C	2:F:88:HIS:CD2	2.89	0.45
2:F:307:PRO:HG3	2:F:312:THR:O	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:419:TYR:CE1	2:H:443:SER:HB2	2.51	0.45
2:B:43:ARG:HG2	2:B:43:ARG:HH11	1.80	0.45
2:L:295:PRO:O	2:L:513:LYS:HA	2.16	0.45
1:A:150:SER:O	1:A:151:LYS:C	2.55	0.45
2:H:394:VAL:HG23	2:H:395:PRO:HD2	1.98	0.45
2:H:66:ALA:HB2	2:H:125:ASP:HA	1.98	0.45
1:E:347:PHE:CD1	1:E:347:PHE:O	2.69	0.45
1:I:68:ILE:HG12	1:I:78:VAL:HG11	1.97	0.45
1:E:358:HIS:N	1:E:359:PRO:CD	2.79	0.45
1:E:718:LEU:H	1:E:718:LEU:HD23	1.80	0.45
1:K:517:LEU:HD21	1:K:632:ALA:HB2	1.97	0.45
1:I:124:ILE:HG22	1:I:128:MET:CE	2.46	0.45
1:G:365:THR:HG22	1:G:391:LEU:HD22	1.98	0.45
1:K:71:ARG:CA	1:K:75:ALA:HB2	2.46	0.45
2:D:476(C):ASP:N	2:D:476(D):PRO:HD3	2.31	0.45
2:J:348:GLU:OE2	1:K:551:HIS:HE1	2.00	0.45
1:I:190:SER:N	1:I:319:GLN:OE1	2.36	0.45
1:G:646:LEU:HD13	2:H:64:LEU:HD13	1.97	0.45
1:E:690:ILE:CD1	1:E:699:LEU:HD11	2.46	0.45
1:K:265:THR:HB	1:K:341:GLY:N	2.30	0.45
1:E:92:ILE:HG13	1:E:112:ILE:HD13	1.98	0.45
1:K:136:ALA:HB1	1:K:161:VAL:CG1	2.36	0.45
1:I:139:VAL:O	1:I:164:VAL:HG12	2.16	0.45
1:G:124:ILE:HG22	1:G:128:MET:CE	2.46	0.45
1:C:537:GLU:HG3	1:C:553:ARG:NH2	2.32	0.45
2:B:476(C):ASP:C	2:B:477:GLU:H	2.19	0.45
1:G:497:GLY:O	1:G:499:MET:HG2	2.16	0.45
1:I:484:PHE:HZ	1:I:504:ILE:HD11	1.80	0.45
1:I:317:GLY:O	1:I:321:VAL:HG12	2.17	0.45
1:A:395:ALA:C	1:A:396:ILE:HD12	2.37	0.45
1:C:112:ILE:HD12	1:C:120:SER:O	2.16	0.45
1:I:411:LEU:HD22	1:I:682:GLN:HG3	1.99	0.45
2:B:119:VAL:HG13	2:B:156:ILE:HD13	1.98	0.45
2:B:134:SER:H	2:B:137:HIS:HB3	1.81	0.45
1:C:272:ILE:HG22	1:C:274:VAL:HG13	1.98	0.45
2:H:337:ALA:HB3	2:H:373:LYS:CD	2.46	0.45
2:H:43:ARG:CG	2:H:43:ARG:HH11	2.30	0.45
2:J:522:LEU:HD23	2:L:151:ASN:ND2	2.30	0.45
2:B:298:ILE:HG23	2:B:509:ARG:HB2	1.98	0.45
1:I:353:ARG:HG3	1:I:353:ARG:HH11	1.82	0.45
1:E:598:PRO:HD2	2:F:292:PHE:CE1	2.50	0.45
1:E:316:MET:CE	1:E:337:PHE:HD1	2.29	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:320:ALA:HB1	1:K:335:VAL:HG21	1.98	0.45
1:A:443:MET:HG3	1:A:444:TYR:CE1	2.52	0.45
2:D:117:ARG:HH21	2:D:280:LEU:HG	1.81	0.45
1:C:146:LEU:HD23	1:C:152:PHE:CD2	2.51	0.45
2:B:208:PRO:O	2:B:214:ILE:HD11	2.16	0.45
1:I:517:LEU:H	1:I:564:GLN:HE22	1.65	0.45
2:J:337:ALA:HB1	2:J:370:SER:HA	1.99	0.45
2:L:460:VAL:O	2:L:460:VAL:HG23	2.16	0.45
1:I:396:ILE:HG12	1:I:463:ILE:CD1	2.44	0.45
2:H:149:MET:CE	2:H:186:ALA:HA	2.45	0.45
1:I:83:ARG:NH1	1:I:83:ARG:CG	2.79	0.45
1:G:189:VAL:CG2	1:G:323:LEU:HB2	2.47	0.45
1:I:683:GLU:H	1:I:704:LYS:HG2	1.82	0.45
1:K:279:HIS:HD2	1:K:380:GLU:O	1.99	0.45
1:E:367:VAL:HG12	1:E:368:ASP:N	2.31	0.45
2:L:273:ARG:HD2	2:L:330:TYR:CD1	2.52	0.45
2:D:390:THR:CG2	2:D:419:TYR:OH	2.65	0.45
1:C:515:VAL:HB	1:C:631:GLY:C	2.36	0.45
1:K:650:MET:HA	1:K:651:PRO:HD3	1.86	0.45
1:C:287:GLU:OE1	1:C:313:ARG:CD	2.64	0.45
2:B:242:GLU:OE2	2:B:246:GLY:HA3	2.17	0.45
1:A:348:LEU:O	1:A:349:GLU:HB3	2.16	0.45
1:A:482:LEU:N	1:A:483:PRO:HD2	2.32	0.45
1:K:308:LEU:HD12	1:K:308:LEU:O	2.16	0.45
1:E:128:MET:SD	1:E:131:ILE:HD12	2.56	0.45
1:G:73:GLU:HG3	1:G:74:ILE:H	1.82	0.45
1:C:455:TRP:C	1:C:455:TRP:CD1	2.87	0.45
2:B:149:MET:CE	2:B:189:VAL:CG1	2.95	0.45
2:B:189:VAL:HG23	2:J:532:LYS:HE2	1.98	0.45
2:L:180:PHE:O	2:L:184:ILE:HG13	2.17	0.45
1:A:285:LEU:HB3	1:A:365:THR:HG21	1.99	0.45
2:D:347:LEU:O	2:D:348:GLU:C	2.54	0.45
2:D:291:PHE:CZ	2:D:348:GLU:HA	2.51	0.45
2:D:145:MET:HE1	2:D:183:ASN:ND2	2.31	0.45
2:B:126:PHE:HB2	2:B:160:ASP:OD2	2.17	0.45
2:J:398:LEU:HA	2:J:399:PRO:HD3	1.80	0.45
2:H:228:PRO:HB3	2:H:239:VAL:O	2.17	0.45
1:C:675:VAL:HG12	1:C:707:VAL:HG21	1.98	0.45
2:H:299:GLU:HG3	2:H:322:LYS:HB3	1.98	0.45
1:G:512:PHE:CZ	1:G:515:VAL:HG23	2.51	0.45
2:J:228:PRO:HB3	2:J:239:VAL:O	2.17	0.45
2:B:474:ARG:HD3	2:B:474:ARG:HA	1.66	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:335:GLU:HA	2:D:338:LYS:HE2	1.98	0.45
1:C:170:ALA:O	1:C:173:ALA:HB3	2.17	0.45
1:G:65:LYS:HE2	1:G:134:THR:O	2.16	0.45
1:G:287:GLU:OE1	1:G:287:GLU:N	2.47	0.45
1:G:354:LEU:HD11	1:G:358:HIS:CE1	2.52	0.45
1:A:178:ILE:CD1	1:A:178:ILE:H	2.10	0.45
1:I:369:LEU:O	1:I:373:MET:HB2	2.16	0.45
1:K:614:LEU:HD22	1:K:627:ILE:HG21	1.96	0.45
1:K:627:ILE:HD12	1:K:627:ILE:N	2.31	0.45
1:E:516:ASN:CB	1:E:564:GLN:NE2	2.76	0.45
1:K:504:ILE:CG2	1:K:505:ALA:N	2.80	0.45
2:J:149:MET:CE	2:J:189:VAL:CG1	2.95	0.45
1:C:646:LEU:HD12	2:D:72:LEU:HD11	1.98	0.45
2:D:61:ARG:HB2	2:D:63:LYS:HG3	1.98	0.45
2:J:460:VAL:CG2	2:J:496:ALA:HB2	2.47	0.45
2:L:156:ILE:N	2:L:156:ILE:CD1	2.80	0.45
2:L:390:THR:HG23	2:L:419:TYR:OH	2.17	0.45
2:B:492:ASN:HB2	2:B:493:PRO:CD	2.46	0.45
1:G:491:HIS:CE1	1:G:493:LYS:HB2	2.52	0.45
2:H:58:GLN:CD	2:H:63:LYS:HE3	2.37	0.45
1:E:675:VAL:HG12	1:E:707:VAL:HG21	1.97	0.45
2:J:355:VAL:HB	2:J:390:THR:HG23	1.98	0.45
2:H:514:ARG:HD2	2:H:514:ARG:HA	1.68	0.45
2:F:84:MET:O	2:F:84:MET:HG2	2.15	0.45
2:D:126:PHE:O	2:D:130:GLY:HA2	2.16	0.45
2:D:410:LYS:NZ	2:L:376:ARG:NH1	2.63	0.45
1:G:433:THR:HG21	1:G:435:VAL:HG12	1.94	0.45
1:A:71:ARG:CA	1:A:75:ALA:HB2	2.47	0.45
1:C:625:PHE:CD1	1:C:625:PHE:N	2.85	0.45
1:K:376:VAL:HG23	1:K:377:ALA:N	2.31	0.45
1:G:164:VAL:HG23	1:G:373:MET:O	2.17	0.45
1:I:543:VAL:CG1	2:J:117:ARG:HD2	2.45	0.45
1:A:517:LEU:HB3	1:A:521:ASP:HB3	1.98	0.45
2:F:337:ALA:HB3	2:F:373:LYS:CD	2.43	0.45
2:J:88:HIS:CD2	2:J:88:HIS:C	2.90	0.45
2:F:476(C):ASP:O	2:F:478:LYS:N	2.44	0.45
1:E:165:GLY:HA2	1:E:331:SER:OG	2.16	0.45
2:L:235:THR:HG22	2:L:237:GLU:HB2	1.99	0.45
1:E:83:ARG:CZ	1:E:83:ARG:HB3	2.47	0.45
1:I:272:ILE:HB	1:I:335:VAL:HG23	1.99	0.45
1:E:267:PRO:O	1:E:501:THR:HG23	2.17	0.45
1:I:302:GLU:OE2	1:I:394:TRP:HZ3	2.00	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:407:ARG:HH11	1:G:407:ARG:HG2	1.81	0.45
2:J:154:PRO:HG3	2:J:191:PRO:HD2	1.99	0.45
1:E:537:GLU:HG3	1:E:553:ARG:HH21	1.82	0.45
1:E:537:GLU:HG3	1:E:553:ARG:NH2	2.31	0.45
1:I:642:ARG:HH11	2:J:71:ASP:HB3	1.82	0.45
1:I:339:VAL:HG22	1:I:345:PHE:HB3	1.99	0.45
1:I:342:GLN:O	1:I:343:LYS:HB2	2.17	0.45
2:D:423:THR:O	2:D:525:LYS:HE2	2.17	0.45
1:K:316:MET:HE3	1:K:337:PHE:HD1	1.82	0.45
1:E:436:TYR:HE1	1:E:439:GLY:CA	2.29	0.45
1:C:436:TYR:HE1	1:C:439:GLY:CA	2.30	0.45
1:A:653:LYS:N	1:A:653:LYS:CD	2.75	0.45
2:F:417:TYR:N	2:H:210:MET:HE1	2.32	0.45
1:C:467:ARG:CB	1:C:467:ARG:HH11	2.28	0.45
1:C:670:ILE:CG1	1:C:718:LEU:HD21	2.42	0.45
2:F:509:ARG:HB3	2:F:509:ARG:HH11	1.81	0.45
1:G:598:PRO:HD2	2:H:292:PHE:CD1	2.52	0.45
2:J:367:ASP:O	2:J:368:ILE:C	2.55	0.45
1:K:214:TYR:HB2	1:K:215:PRO:HA	1.99	0.45
1:A:491:HIS:CE1	1:A:493:LYS:HB2	2.51	0.45
2:F:121:VAL:HG22	2:F:122:PHE:N	2.31	0.45
2:H:356:ALA:HB2	2:H:391:LEU:HB2	1.97	0.45
1:I:642:ARG:NH1	2:J:71:ASP:OD2	2.50	0.45
2:B:514:ARG:HA	2:B:514:ARG:HD2	1.72	0.45
1:C:150:SER:O	1:C:151:LYS:C	2.55	0.45
2:B:66:ALA:HB2	2:B:125:ASP:HA	1.97	0.45
2:D:340:ILE:HD13	2:D:374:ALA:HB2	1.99	0.45
2:B:67:ARG:NH1	2:B:67:ARG:HG2	2.31	0.45
1:E:272:ILE:HG22	1:E:274:VAL:HG13	1.99	0.45
1:C:342:GLN:O	1:C:343:LYS:HB2	2.15	0.45
1:I:414:ILE:HD12	1:I:441:ILE:O	2.17	0.45
1:C:468:ILE:O	1:C:471:ASP:HB2	2.17	0.45
1:A:369:LEU:O	1:A:373:MET:HB2	2.17	0.45
1:G:393:GLY:HA3	1:G:455:TRP:CZ3	2.52	0.45
2:F:180:PHE:O	2:F:183:ASN:HB2	2.17	0.45
2:B:151:ASN:ND2	2:D:522:LEU:HA	2.32	0.45
1:K:596:TRP:CH2	1:K:600:ASP:O	2.69	0.45
1:I:666:MET:O	1:I:668:GLY:N	2.50	0.45
1:I:619:ILE:HD12	1:I:625:PHE:C	2.37	0.45
1:C:395:ALA:C	1:C:396:ILE:HD12	2.37	0.45
2:H:495:VAL:HG13	2:H:496:ALA:N	2.32	0.45
1:K:83:ARG:HH11	1:K:83:ARG:CG	2.28	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:J:300:PRO:HA	2:J:509:ARG:NH1	2.31	0.45
1:K:245:SER:C	1:K:247:ASN:N	2.70	0.45
2:J:484:ALA:O	2:J:488:GLU:OE1	2.35	0.45
1:I:720:VAL:HG22	1:I:721:ASP:H	1.82	0.45
2:J:164:ALA:HB2	2:J:176:TYR:HE2	1.82	0.45
1:C:414:ILE:HD11	1:C:442:SER:C	2.37	0.45
1:A:435:VAL:HG22	1:A:436:TYR:H	1.80	0.45
1:A:71:ARG:O	1:A:75:ALA:HB2	2.17	0.45
1:G:376:VAL:HG23	1:G:377:ALA:N	2.31	0.45
1:A:122:ILE:HA	1:A:146:LEU:CD1	2.45	0.45
1:G:396:ILE:HD13	1:G:462:ALA:CB	2.47	0.45
1:A:494:PHE:HD2	1:A:499:MET:HE1	1.82	0.45
2:B:83:ASP:HB3	2:B:86:VAL:HG23	1.97	0.45
2:L:460:VAL:HG21	2:L:496:ALA:CB	2.44	0.45
1:C:92:ILE:HD12	1:C:112:ILE:HD13	1.99	0.45
1:E:165:GLY:CA	1:E:331:SER:OG	2.65	0.45
2:L:476(A):LEU:C	2:L:476(C):ASP:H	2.20	0.45
2:D:235:THR:HG22	2:D:237:GLU:HB2	1.99	0.45
1:K:598:PRO:HD2	2:L:292:PHE:CD1	2.51	0.45
2:D:121:VAL:O	2:D:144:ILE:HD13	2.17	0.45
1:A:537:GLU:HG3	1:A:553:ARG:HH21	1.82	0.45
1:A:270:ILE:HG12	1:A:289:GLU:HG3	1.98	0.45
1:C:515:VAL:HG21	1:C:631:GLY:HA3	1.99	0.45
1:A:98:LYS:O	1:A:98:LYS:HG3	2.17	0.45
2:F:66:ALA:HB2	2:F:125:ASP:HA	1.98	0.45
1:E:99:GLN:HB2	1:E:436:TYR:OH	2.16	0.44
1:E:405:PRO:CG	1:E:481:ASN:HA	2.45	0.44
1:E:390:LYS:HD3	1:E:391:LEU:H	1.78	0.44
1:K:627:ILE:HD13	1:K:636:VAL:HB	1.98	0.44
1:G:124:ILE:O	1:G:128:MET:HB2	2.17	0.44
1:C:537:GLU:HG3	1:C:553:ARG:HH21	1.82	0.44
1:A:517:LEU:HD21	1:A:632:ALA:HB2	1.98	0.44
2:L:504:GLU:HG3	2:L:505:VAL:H	1.77	0.44
2:H:89:ARG:NH1	2:L:499:ARG:HH21	2.13	0.44
1:I:517:LEU:HA	1:I:518:PRO:HD3	1.57	0.44
2:B:460:VAL:O	2:B:460:VAL:HG23	2.18	0.44
1:I:596:TRP:CH2	1:I:600:ASP:O	2.70	0.44
2:F:149:MET:SD	2:F:186:ALA:HB2	2.57	0.44
1:G:283:ILE:CG2	1:G:386:GLN:HG2	2.47	0.44
2:D:509:ARG:HH11	2:D:509:ARG:HB3	1.82	0.44
2:D:50:GLY:HA3	2:D:127:THR:O	2.17	0.44
2:H:109:THR:HG22	2:H:122:PHE:CB	2.47	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:347:PHE:CD1	1:G:347:PHE:C	2.90	0.44
1:K:305:SER:HA	1:K:306:PRO:HD3	1.81	0.44
2:D:474:ARG:HD3	2:D:474:ARG:HA	1.63	0.44
1:A:347:PHE:C	1:A:347:PHE:CD1	2.90	0.44
2:J:537:ILE:HG13	2:J:538:PRO:HD2	1.99	0.44
1:K:118:ASN:HD21	1:K:119:GLN:HE21	1.65	0.44
1:K:443:MET:HG3	1:K:444:TYR:CE1	2.52	0.44
1:I:93:TYR:HD1	1:I:94:SER:O	2.00	0.44
1:C:456:ALA:CB	1:C:457:PRO:CD	2.94	0.44
1:A:292:ILE:HG23	1:A:503:PHE:CD2	2.52	0.44
1:G:494:PHE:HA	1:G:499:MET:CE	2.40	0.44
1:E:518:PRO:O	1:E:519:GLU:C	2.55	0.44
2:D:204:ALA:O	2:D:205:VAL:C	2.54	0.44
1:I:627:ILE:N	1:I:627:ILE:HD12	2.33	0.44
1:I:229:MET:O	1:I:230:ARG:HB2	2.18	0.44
1:I:69:ALA:HB3	1:I:141:PRO:HA	1.99	0.44
2:B:329:PHE:HD1	2:B:345:ILE:HG22	1.83	0.44
2:B:436:GLY:HA2	2:J:173:LEU:HD21	1.99	0.44
1:I:704:LYS:H	1:I:704:LYS:HG3	1.58	0.44
1:G:612:LEU:HD12	1:G:612:LEU:C	2.37	0.44
2:B:229:ASP:N	2:B:229:ASP:OD1	2.49	0.44
1:A:288:ARG:HD3	1:A:361:THR:OG1	2.17	0.44
2:J:335:GLU:HA	2:J:338:LYS:HE2	1.99	0.44
1:E:74:ILE:HG23	1:E:75:ALA:N	2.32	0.44
1:I:68:ILE:HG12	1:I:78:VAL:CG1	2.47	0.44
1:K:653:LYS:CD	1:K:653:LYS:N	2.78	0.44
1:I:256:ASP:N	1:I:256:ASP:OD1	2.50	0.44
1:C:661:MET:CE	1:C:726:GLU:HB3	2.46	0.44
2:H:361:VAL:C	2:H:363:ALA:N	2.71	0.44
2:D:139:LYS:HE2	2:D:139:LYS:HB3	1.74	0.44
1:K:491:HIS:CE1	1:K:493:LYS:HB2	2.52	0.44
1:G:150:SER:O	1:G:151:LYS:C	2.56	0.44
1:E:347:PHE:CD1	1:E:347:PHE:C	2.90	0.44
2:B:67:ARG:HH11	2:B:67:ARG:HG2	1.82	0.44
2:D:196:ILE:HD13	2:D:214:ILE:HG23	1.99	0.44
1:G:664:CYS:HB2	1:G:724:ILE:HD11	2.00	0.44
1:C:683:GLU:H	1:C:704:LYS:HG2	1.82	0.44
1:C:400:LEU:HD13	1:C:449:ILE:CD1	2.25	0.44
1:A:115:PRO:HG2	1:A:444:TYR:CE2	2.52	0.44
1:I:77:ARG:HE	1:I:430:ARG:HH22	1.66	0.44
1:C:71:ARG:CA	1:C:75:ALA:HB2	2.48	0.44
2:D:325:ASP:C	2:D:327:GLY:H	2.21	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:563:LEU:HB3	1:C:564:GLN:H	1.33	0.44
1:A:419:ARG:HD2	1:A:601:GLN:OE1	2.17	0.44
1:A:325:LYS:O	1:A:328:GLY:N	2.41	0.44
1:G:517:LEU:N	1:G:517:LEU:HD22	2.23	0.44
1:I:83:ARG:CZ	1:I:83:ARG:HB3	2.47	0.44
1:C:177:LYS:HB3	1:C:181:LYS:HZ1	1.81	0.44
1:I:302:GLU:OE2	1:I:394:TRP:CZ3	2.70	0.44
1:A:405:PRO:CG	1:A:481:ASN:HA	2.47	0.44
1:C:107:ASP:C	1:C:108:GLU:HG3	2.38	0.44
1:C:271:GLU:O	1:C:287:GLU:HB2	2.18	0.44
2:L:69:ARG:HA	2:L:268:LEU:HD11	1.98	0.44
2:D:447:LEU:O	2:D:448:ARG:HB2	2.16	0.44
1:E:414:ILE:HD11	1:E:442:SER:C	2.37	0.44
1:E:93:TYR:HD1	1:E:94:SER:O	2.01	0.44
1:K:139:VAL:HG11	1:K:156:LEU:CD2	2.48	0.44
1:E:457:PRO:CG	1:E:458:THR:N	2.80	0.44
1:A:164:VAL:HG23	1:A:377:ALA:CB	2.48	0.44
1:I:122:ILE:HA	1:I:146:LEU:CD1	2.46	0.44
1:I:388:ASP:O	1:I:390:LYS:N	2.51	0.44
2:D:425:PRO:HB3	2:D:522:LEU:HB3	2.00	0.44
1:K:285:LEU:N	1:K:285:LEU:HD12	2.32	0.44
1:G:321:VAL:O	1:G:324:ALA:CB	2.60	0.44
1:E:563:LEU:O	1:E:565:GLY:N	2.50	0.44
2:B:368:ILE:HG23	2:B:411:HIS:CG	2.53	0.44
1:C:165:GLY:CA	1:C:331:SER:OG	2.66	0.44
2:B:156:ILE:CD1	2:B:156:ILE:N	2.81	0.44
2:F:355:VAL:O	2:F:390:THR:HA	2.16	0.44
1:C:401:TYR:HD2	1:C:448:MET:HA	1.83	0.44
1:E:264:VAL:HG12	1:E:340:ASP:HB3	2.00	0.44
2:B:297:ARG:NH1	2:B:297:ARG:HG2	2.32	0.44
2:F:121:VAL:O	2:F:144:ILE:HD13	2.18	0.44
2:D:410:LYS:HZ2	2:L:376:ARG:HH11	1.65	0.44
2:B:258:ASP:O	2:B:259:ALA:HB2	2.18	0.44
1:G:99:GLN:O	1:G:100:ALA:O	2.36	0.44
1:K:115:PRO:HG2	1:K:444:TYR:CE2	2.52	0.44
1:E:273:GLN:O	1:E:285:LEU:HD12	2.18	0.44
1:I:354:LEU:HD13	1:I:355:GLN:O	2.17	0.44
1:G:156:LEU:HD22	1:G:161:VAL:HB	1.99	0.44
1:C:467:ARG:HE	1:C:630:ARG:CG	2.29	0.44
1:C:516:ASN:CB	1:C:564:GLN:NE2	2.76	0.44
1:K:71:ARG:O	1:K:75:ALA:HB2	2.17	0.44
1:I:92:ILE:CG1	1:I:112:ILE:HD13	2.48	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:92:ILE:HG13	1:I:112:ILE:HD13	1.98	0.44
1:G:626:ARG:C	1:G:627:ILE:HD12	2.38	0.44
2:F:401:THR:CG2	2:F:402:SER:N	2.80	0.44
1:E:275:LEU:HD23	1:E:276:CYS:H	1.81	0.44
1:A:275:LEU:HD23	1:A:276:CYS:H	1.82	0.44
1:I:177:LYS:HE3	1:I:181:LYS:HZ1	1.83	0.44
1:E:491:HIS:O	1:E:495:ILE:HG13	2.17	0.44
1:G:704:LYS:HG3	1:G:704:LYS:H	1.63	0.44
1:G:534:ARG:NH1	1:G:534:ARG:HG3	2.33	0.44
2:F:196:ILE:N	2:F:196:ILE:HD12	2.33	0.44
2:F:174:ALA:HB2	2:H:501:PHE:CE1	2.53	0.44
2:J:95:MET:HE3	2:J:95:MET:HA	1.99	0.44
2:J:474:ARG:O	2:J:476:ASP:N	2.47	0.44
1:G:662:LEU:HD22	1:G:687:LEU:HD12	2.00	0.44
1:A:400:LEU:HD21	1:A:482:LEU:CD1	2.48	0.44
1:K:272:ILE:HG22	1:K:274:VAL:HG13	2.00	0.44
1:C:347:PHE:HD1	1:C:347:PHE:O	2.00	0.44
1:I:393:GLY:HA2	1:I:457:PRO:O	2.17	0.44
1:C:629:THR:HB	1:C:630:ARG:H	1.71	0.44
1:A:421:ARG:O	1:A:421:ARG:CD	2.66	0.44
1:I:421:ARG:C	1:I:421:ARG:HD3	2.38	0.44
1:K:212:ILE:HD12	1:K:260:ILE:CG2	2.47	0.44
2:D:303:ASP:OD1	2:D:508:PRO:HB2	2.18	0.44
1:C:182:LYS:HA	1:C:185:GLN:HG3	2.00	0.44
2:B:58:GLN:NE2	2:B:63:LYS:HE3	2.32	0.44
1:E:615:LYS:HB2	1:E:628:ARG:HB2	2.00	0.44
2:F:501:PHE:CE1	2:H:174:ALA:HB2	2.53	0.44
2:L:258:ASP:O	2:L:259:ALA:HB2	2.17	0.44
2:B:229:ASP:O	2:B:233:THR:HG23	2.18	0.44
2:J:95:MET:HE2	2:J:95:MET:HB3	1.89	0.44
1:E:168:LYS:O	1:E:172:GLU:OE1	2.36	0.44
2:L:356:ALA:HB2	2:L:391:LEU:HB2	1.99	0.44
2:F:447:LEU:O	2:F:448:ARG:HB2	2.17	0.44
2:J:206:TYR:O	2:J:209:ALA:HB3	2.17	0.44
2:H:378:VAL:HG13	2:H:388:LEU:CD1	2.47	0.44
1:A:414:ILE:CD1	1:A:441:ILE:O	2.64	0.44
1:A:441:ILE:HD12	1:A:478:ILE:HD13	1.99	0.44
1:G:653:LYS:N	1:G:653:LYS:CD	2.78	0.44
1:I:156:LEU:HD13	1:I:163:PHE:HB2	1.96	0.44
2:B:184:ILE:CD1	2:J:417:TYR:HA	2.44	0.44
1:K:388:ASP:O	1:K:390:LYS:N	2.51	0.44
1:E:640:THR:OG1	1:E:643:GLN:HB2	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:J:498:GLU:HG2	2:L:87:THR:HG23	2.00	0.44
2:D:312:THR:HG22	2:D:313:PRO:O	2.17	0.44
1:C:186:GLU:OE2	1:C:187:ALA:N	2.51	0.44
2:F:45:ALA:O	2:F:48:LEU:HB2	2.18	0.44
1:K:651:PRO:CG	2:L:62:GLY:HA3	2.48	0.44
1:I:209:SER:O	1:I:212:ILE:N	2.51	0.44
1:K:199:ILE:HD13	1:K:205:ALA:HA	1.99	0.44
1:E:539:ARG:NH2	2:F:326:GLU:OE2	2.51	0.44
2:H:440:VAL:O	2:H:444:SER:HB3	2.18	0.44
2:D:94:ASN:HA	2:D:98:GLN:OE1	2.18	0.44
1:I:684:GLY:N	1:I:701:ALA:O	2.48	0.44
2:H:374:ALA:HB3	2:H:415:LEU:HD13	1.99	0.44
2:L:514:ARG:HD2	2:L:514:ARG:HA	1.67	0.44
1:I:271:GLU:O	1:I:287:GLU:HB2	2.18	0.44
1:E:112:ILE:O	1:E:120:SER:HA	2.18	0.44
1:K:93:TYR:HD1	1:K:94:SER:O	2.01	0.44
1:I:71:ARG:NH1	1:I:445:TYR:CG	2.86	0.44
1:G:70:ASN:OD1	1:G:74:ILE:HG21	2.17	0.44
1:K:334:THR:HG21	1:K:355:GLN:CG	2.47	0.44
1:C:455:TRP:CG	1:C:456:ALA:N	2.82	0.44
1:C:376:VAL:HG23	1:C:377:ALA:N	2.33	0.44
1:C:518:PRO:O	1:C:521:ASP:HB2	2.17	0.44
1:I:276:CYS:HB2	1:I:277:ASP:H	1.44	0.44
2:J:109:THR:HG22	2:J:122:PHE:CB	2.47	0.44
1:E:411:LEU:HD22	1:E:682:GLN:CB	2.46	0.44
1:I:140:HIS:ND1	1:I:141:PRO:N	2.66	0.44
1:C:634:LEU:H	1:C:634:LEU:HD23	1.83	0.44
2:J:374:ALA:HB3	2:J:415:LEU:HD13	1.99	0.44
2:B:356:ALA:HB2	2:B:391:LEU:HB2	1.99	0.44
2:F:366:LEU:HA	2:F:366:LEU:HD23	1.81	0.44
1:I:150:SER:O	1:I:153:ALA:N	2.51	0.44
1:E:117:ALA:HA	1:E:121:TYR:H	1.82	0.43
1:I:71:ARG:O	1:I:75:ALA:HB2	2.18	0.43
1:E:139:VAL:O	1:E:164:VAL:HG12	2.18	0.43
1:C:157:GLU:C	1:C:159:GLU:N	2.72	0.43
2:B:325:ASP:C	2:B:327:GLY:H	2.20	0.43
2:B:205:VAL:HB	2:J:409:ILE:HG23	2.00	0.43
1:G:92:ILE:HG13	1:G:112:ILE:HD13	1.99	0.43
1:G:615:LYS:HB2	1:G:628:ARG:HB2	2.00	0.43
2:D:479:ILE:C	2:D:479:ILE:HD12	2.39	0.43
2:F:492:ASN:HB2	2:F:493:PRO:CD	2.46	0.43
1:E:411:LEU:HB2	1:E:682:GLN:HG3	1.99	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:272:ILE:HG22	1:I:274:VAL:HG13	2.00	0.43
1:I:279:HIS:HD2	1:I:380:GLU:O	2.00	0.43
1:I:598:PRO:HD2	2:J:292:PHE:CD1	2.53	0.43
2:B:339:ASN:HB3	2:B:361:VAL:HG12	2.00	0.43
1:G:422:PRO:HA	1:G:422(A):PRO:HD3	1.82	0.43
3:A:801:BTI:H63	2:B:399:PRO:HD3	2.00	0.43
1:K:107:ASP:O	1:K:108:GLU:HG3	2.19	0.43
1:I:446:ASP:OD1	1:I:447:PRO:HD2	2.17	0.43
1:C:552:GLU:H	1:C:552:GLU:CD	2.20	0.43
1:A:287:GLU:HG3	1:A:308:LEU:HD21	2.00	0.43
1:C:482:LEU:N	1:C:483:PRO:HD2	2.32	0.43
1:I:117:ALA:C	1:I:119:GLN:N	2.71	0.43
1:E:285:LEU:HD12	1:E:285:LEU:N	2.33	0.43
1:K:164:VAL:HG23	1:K:377:ALA:HB2	1.99	0.43
1:K:619:ILE:HD11	1:K:626:ARG:HB2	2.00	0.43
2:H:180:PHE:O	2:H:183:ASN:HB2	2.18	0.43
1:G:532:MET:O	1:G:535:VAL:HB	2.18	0.43
1:I:92:ILE:HD12	1:I:112:ILE:HD13	1.99	0.43
1:C:583:PHE:CD1	1:C:583:PHE:N	2.86	0.43
1:E:467:ARG:HH11	1:E:467:ARG:CB	2.27	0.43
1:E:658:THR:CB	1:E:703:LYS:HD3	2.43	0.43
1:G:596:TRP:CH2	1:G:600:ASP:O	2.71	0.43
1:C:179:THR:HG22	1:C:183:ILE:CD1	2.46	0.43
2:H:460:VAL:CG2	2:H:460:VAL:O	2.66	0.43
1:G:258:ILE:HG22	1:G:259:PHE:N	2.33	0.43
1:C:283:ILE:CG2	1:C:386:GLN:HG2	2.48	0.43
1:G:167:PRO:C	1:G:169:GLY:H	2.21	0.43
2:L:298:ILE:HD12	2:L:298:ILE:N	2.33	0.43
1:C:279:HIS:CD2	1:C:380:GLU:O	2.71	0.43
1:A:492:PRO:HA	1:A:495:ILE:HD12	2.00	0.43
1:G:272:ILE:HB	1:G:335:VAL:CG2	2.48	0.43
1:G:682:GLN:OE1	1:G:682:GLN:HA	2.19	0.43
2:F:134:SER:H	2:F:137:HIS:HB3	1.82	0.43
1:A:150:SER:O	1:A:153:ALA:N	2.51	0.43
2:J:514:ARG:HA	2:J:514:ARG:HD2	1.74	0.43
1:I:100:ALA:HB3	1:I:103:VAL:HG23	1.99	0.43
1:A:418:THR:O	1:A:437:GLU:HG3	2.18	0.43
1:G:245:SER:C	1:G:247:ASN:N	2.72	0.43
2:L:196:ILE:HD12	2:L:196:ILE:N	2.33	0.43
2:F:372:ARG:NH2	2:H:539:LEU:OXT	2.50	0.43
1:I:287:GLU:OE2	1:I:305:SER:N	2.45	0.43
1:I:308:LEU:C	1:I:308:LEU:HD12	2.38	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:414:ILE:CD1	1:E:441:ILE:O	2.66	0.43
1:A:93:TYR:HA	1:A:121:TYR:OH	2.17	0.43
1:K:124:ILE:HG22	1:K:128:MET:CE	2.48	0.43
1:A:162:ILE:O	1:A:164:VAL:N	2.51	0.43
2:H:180:PHE:O	2:H:184:ILE:HG13	2.18	0.43
2:B:88:HIS:C	2:B:88:HIS:CD2	2.91	0.43
1:C:285:LEU:HD12	1:C:285:LEU:N	2.33	0.43
1:G:563:LEU:HD23	1:G:636:VAL:HG22	2.00	0.43
2:D:460:VAL:CG2	2:D:496:ALA:HB2	2.43	0.43
1:G:188:ASN:OD1	1:G:188:ASN:O	2.36	0.43
1:K:675:VAL:HG11	1:K:707:VAL:HG21	1.98	0.43
2:L:196:ILE:HD13	2:L:214:ILE:HG23	1.99	0.43
1:I:552:GLU:H	1:I:552:GLU:CD	2.21	0.43
2:F:423:THR:O	2:F:525:LYS:HE2	2.18	0.43
1:I:289:GLU:OE1	1:I:306:PRO:HD2	2.18	0.43
2:L:351:THR:HG22	2:L:386:ILE:HG23	2.00	0.43
1:I:245:SER:C	1:I:247:ASN:H	2.20	0.43
2:B:394:VAL:HG23	2:B:395:PRO:HD2	2.00	0.43
2:B:164:ALA:HB2	2:B:176:TYR:HE2	1.83	0.43
1:C:480:HIS:HD2	1:C:482:LEU:H	1.66	0.43
1:E:285:LEU:HB3	1:E:365:THR:HG21	2.00	0.43
1:G:70:ASN:ND2	1:G:145:PHE:CE1	2.86	0.43
1:K:369:LEU:O	1:K:373:MET:HB2	2.17	0.43
1:I:376:VAL:HG23	1:I:377:ALA:N	2.33	0.43
1:C:273:GLN:HG2	1:C:369:LEU:HD11	2.00	0.43
2:B:145:MET:CE	2:B:183:ASN:ND2	2.81	0.43
1:K:325:LYS:O	1:K:327:VAL:N	2.52	0.43
1:C:327:VAL:HG22	1:C:327:VAL:O	2.18	0.43
1:E:467:ARG:HD2	1:E:467:ARG:O	2.19	0.43
2:D:476(D):PRO:HA	2:D:479:ILE:HD11	2.00	0.43
1:G:256:ASP:OD1	1:G:256:ASP:N	2.52	0.43
1:G:229:MET:O	1:G:230:ARG:HB2	2.17	0.43
1:G:206:VAL:HG13	1:G:235:ASP:CB	2.49	0.43
1:G:417:LEU:HD21	1:G:478:ILE:CD1	2.46	0.43
1:A:70:ASN:ND2	1:A:145:PHE:CE1	2.87	0.43
2:L:126:PHE:HB2	2:L:160:ASP:OD2	2.18	0.43
2:F:258:ASP:O	2:F:259:ALA:HB2	2.17	0.43
2:B:80:GLU:HB2	2:D:517:ARG:NH2	2.33	0.43
1:A:316:MET:HE2	1:A:337:PHE:CD1	2.54	0.43
1:A:99:GLN:O	1:A:100:ALA:O	2.36	0.43
1:I:347:PHE:CD1	1:I:347:PHE:C	2.91	0.43
1:G:348:LEU:O	1:G:348:LEU:HD23	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:164:VAL:HG23	1:E:377:ALA:CB	2.47	0.43
1:E:421:ARG:HD3	1:E:421:ARG:O	2.19	0.43
1:K:354:LEU:HD13	1:K:355:GLN:O	2.17	0.43
2:F:117:ARG:NH2	2:F:280:LEU:HG	2.33	0.43
1:G:393:GLY:HA2	1:G:457:PRO:O	2.19	0.43
1:E:518:PRO:HD2	1:E:521:ASP:OD1	2.18	0.43
1:E:327:VAL:O	1:E:327:VAL:HG22	2.19	0.43
1:G:625:PHE:HB2	1:G:627:ILE:CD1	2.48	0.43
2:D:476(A):LEU:C	2:D:476(C):ASP:H	2.20	0.43
2:D:458:ALA:O	2:D:492:ASN:HA	2.19	0.43
1:K:401:TYR:HD2	1:K:448:MET:HA	1.84	0.43
2:J:251:THR:HG21	2:J:260:ALA:CB	2.46	0.43
1:C:421:ARG:O	1:C:421:ARG:CD	2.67	0.43
1:I:396:ILE:HD13	1:I:462:ALA:CB	2.49	0.43
2:D:149:MET:SD	2:D:186:ALA:HB2	2.59	0.43
1:G:634:LEU:H	1:G:634:LEU:HD23	1.82	0.43
2:D:145:MET:HE3	2:D:183:ASN:ND2	2.34	0.43
2:H:401:THR:CG2	2:H:402:SER:N	2.80	0.43
1:E:401:TYR:CD2	1:E:448:MET:HA	2.53	0.43
2:L:126:PHE:O	2:L:130:GLY:HA2	2.19	0.43
2:L:200:CYS:O	2:L:223:MET:HA	2.18	0.43
1:G:245:SER:C	1:G:247:ASN:H	2.20	0.43
1:I:245:SER:C	1:I:247:ASN:N	2.72	0.43
1:C:650:MET:HA	1:C:651:PRO:HD3	1.87	0.43
2:D:202:GLY:HA2	2:D:225:VAL:O	2.18	0.43
1:G:435:VAL:HG22	1:G:436:TYR:N	2.34	0.43
1:G:287:GLU:OE2	1:G:305:SER:N	2.48	0.43
1:C:617:GLY:O	1:C:625:PHE:CB	2.55	0.43
1:E:93:TYR:O	1:E:112:ILE:HG12	2.19	0.43
1:I:157:GLU:OE1	1:I:168:LYS:NZ	2.52	0.43
1:G:85:MET:O	1:G:86:GLY:C	2.57	0.43
1:G:388:ASP:O	1:G:390:LYS:N	2.52	0.43
1:C:517:LEU:HD21	1:C:632:ALA:HB1	2.00	0.43
1:G:325:LYS:O	1:G:327:VAL:N	2.51	0.43
2:D:210:MET:HE3	2:L:416:LEU:HD23	2.00	0.43
2:F:531:TRP:CG	2:F:532:LYS:N	2.86	0.43
2:H:367:ASP:O	2:H:368:ILE:C	2.57	0.43
2:L:235:THR:HG22	2:L:235:THR:O	2.18	0.43
1:I:231:ILE:HG22	1:I:232:ALA:N	2.33	0.43
1:A:283:ILE:HG22	1:A:386:GLN:HG2	2.01	0.43
1:K:675:VAL:HG12	1:K:707:VAL:HG21	1.99	0.43
1:C:367:VAL:HG12	1:C:368:ASP:N	2.34	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:515:VAL:HB	1:A:631:GLY:C	2.39	0.43
1:I:515:VAL:HB	1:I:631:GLY:C	2.39	0.43
1:C:287:GLU:OE1	1:C:313:ARG:HD2	2.19	0.43
1:C:693:MET:O	1:C:694:LYS:HB2	2.18	0.43
2:D:74:LEU:HD13	2:D:112:GLY:HA3	2.00	0.43
1:G:271:GLU:O	1:G:287:GLU:HB2	2.18	0.43
1:I:70:ASN:ND2	1:I:145:PHE:CE1	2.87	0.43
1:I:71:ARG:CA	1:I:75:ALA:HB2	2.48	0.43
1:E:162:ILE:HD13	1:E:377:ALA:O	2.19	0.43
1:G:68:ILE:CG1	1:G:78:VAL:HG11	2.49	0.43
1:K:354:LEU:HD11	1:K:358:HIS:ND1	2.33	0.43
1:K:517:LEU:HA	1:K:518:PRO:HD3	1.62	0.43
1:K:563:LEU:HB3	1:K:564:GLN:H	1.37	0.43
2:B:121:VAL:CG2	2:B:122:PHE:N	2.81	0.43
1:G:563:LEU:HB3	1:G:564:GLN:H	1.30	0.43
2:D:492:ASN:ND2	2:D:494:PHE:HB2	2.33	0.43
2:F:346:ARG:CG	2:F:346:ARG:HH11	2.28	0.43
2:D:460:VAL:HG23	2:D:460:VAL:O	2.19	0.43
1:I:411:LEU:HD22	1:I:682:GLN:CG	2.49	0.43
1:A:704:LYS:HG3	1:A:704:LYS:H	1.64	0.43
1:A:401:TYR:HD2	1:A:448:MET:HA	1.84	0.43
2:B:339:ASN:HD21	2:B:370:SER:HB3	1.83	0.43
1:G:546:ARG:HG2	1:G:546:ARG:H	1.54	0.43
2:J:392:ILE:HD12	2:J:428:THR:CG2	2.48	0.43
1:A:308:LEU:HD11	1:A:313:ARG:HD3	2.00	0.43
1:C:270:ILE:HG21	1:C:308:LEU:HD21	2.01	0.43
1:C:405:PRO:CG	1:C:481:ASN:HA	2.49	0.43
1:C:605:LEU:CD1	1:C:614:LEU:HD12	2.49	0.43
1:K:481:ASN:O	1:K:482:LEU:C	2.56	0.43
1:G:292:ILE:N	1:G:292:ILE:HD12	2.11	0.43
1:K:354:LEU:HD13	1:K:355:GLN:N	2.34	0.43
1:A:164:VAL:HA	1:A:377:ALA:HB1	2.00	0.43
1:I:124:ILE:HG22	1:I:128:MET:HE3	2.01	0.43
1:A:563:LEU:HB3	1:A:564:GLN:H	1.25	0.43
1:C:110:VAL:HG21	1:C:130:ALA:CB	2.46	0.43
1:A:504:ILE:CG2	1:A:505:ALA:N	2.81	0.43
2:B:291:PHE:CZ	2:B:348:GLU:HA	2.54	0.43
2:J:498:GLU:HA	2:L:86:VAL:HA	1.99	0.43
1:K:231:ILE:HD12	1:K:231:ILE:N	2.32	0.43
2:L:155:VAL:C	2:L:156:ILE:HD12	2.39	0.43
1:K:245:SER:O	1:K:247:ASN:N	2.52	0.43
1:G:675:VAL:HG11	1:G:707:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:196:ILE:HG22	2:D:221:SER:HB2	2.01	0.43
2:L:356:ALA:CB	2:L:391:LEU:HB2	2.49	0.43
2:H:297:ARG:HG2	2:H:297:ARG:HH11	1.83	0.43
1:C:690:ILE:CD1	1:C:699:LEU:HD11	2.48	0.43
1:E:679:GLN:O	1:E:706:VAL:HG13	2.19	0.43
1:G:348:LEU:O	1:G:349:GLU:HB3	2.19	0.43
1:K:443:MET:SD	1:K:444:TYR:CE1	3.11	0.43
1:C:74:ILE:HG23	1:C:75:ALA:N	2.33	0.43
1:A:358:HIS:CG	1:A:359:PRO:HD3	2.54	0.43
2:F:325:ASP:C	2:F:327:GLY:H	2.21	0.43
1:K:64:ASN:H	1:K:137:GLN:HG2	1.83	0.43
1:C:670:ILE:HD12	1:C:712:ALA:HB1	2.01	0.43
2:B:531:TRP:CG	2:B:532:LYS:N	2.87	0.43
1:E:661:MET:HG3	1:E:723:VAL:HG13	2.00	0.43
2:D:300:PRO:HB3	2:D:509:ARG:HH12	1.83	0.43
2:D:54:ARG:HH11	2:D:54:ARG:HG2	1.82	0.43
1:E:102:HIS:CG	1:E:103:VAL:N	2.87	0.43
1:K:664:CYS:HB2	1:K:724:ILE:HD11	2.00	0.43
2:J:196:ILE:HD13	2:J:214:ILE:HG23	2.00	0.43
2:L:297:ARG:HG2	2:L:297:ARG:HH11	1.84	0.43
2:B:128:VAL:O	2:B:129:LEU:C	2.55	0.43
1:E:308:LEU:HD12	1:E:308:LEU:C	2.38	0.43
1:E:316:MET:HG2	1:E:345:PHE:CD2	2.54	0.43
1:A:712:ALA:HA	1:A:716:ASN:ND2	2.34	0.43
1:I:456:ALA:CB	1:I:457:PRO:CD	2.95	0.43
2:H:117:ARG:HH21	2:H:280:LEU:HG	1.84	0.43
1:K:85:MET:O	1:K:86:GLY:C	2.58	0.43
2:B:109:THR:HG22	2:B:122:PHE:HB2	2.00	0.43
2:B:183:ASN:OD1	2:B:207:SER:OG	2.26	0.43
2:H:476(D):PRO:HA	2:H:479:ILE:HD11	2.00	0.43
2:F:235:THR:O	2:F:235:THR:HG22	2.18	0.43
2:H:434:ALA:HB3	2:H:460:VAL:HG12	2.01	0.43
2:J:222:TYR:C	2:J:222:TYR:CD1	2.93	0.43
2:B:501:PHE:HD2	2:B:501:PHE:N	2.13	0.43
2:H:303:ASP:OD2	2:H:509:ARG:HD2	2.19	0.43
1:K:693:MET:O	1:K:694:LYS:HB2	2.19	0.43
2:F:75:ASP:OD1	2:F:272:ARG:NH2	2.48	0.43
1:C:664:CYS:HB2	1:C:724:ILE:HD11	2.01	0.43
2:H:468:ALA:O	2:H:472:ILE:HG13	2.18	0.43
1:E:309:ASP:OD2	1:E:343:LYS:HE2	2.19	0.42
1:C:71:ARG:O	1:C:75:ALA:CB	2.67	0.42
1:K:459:ARG:O	1:K:463:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:293:ASP:OD2	2:F:294:ASP:N	2.52	0.42
1:E:543:VAL:CG1	2:F:117:ARG:HD2	2.49	0.42
2:H:499:ARG:HD3	2:H:499:ARG:HA	1.88	0.42
1:K:78:VAL:CG1	1:K:79:ILE:N	2.82	0.42
2:L:251:THR:HG21	2:L:260:ALA:CB	2.43	0.42
1:A:388:ASP:O	1:A:390:LYS:N	2.52	0.42
2:D:460:VAL:HG21	2:D:496:ALA:CB	2.47	0.42
1:K:319:GLN:NE2	1:K:345:PHE:HE1	2.16	0.42
2:L:340:ILE:CG2	2:L:373:LYS:HD3	2.49	0.42
2:F:58:GLN:HA	2:F:61:ARG:HH21	1.84	0.42
2:F:403:GLN:O	2:F:408:VAL:HG22	2.19	0.42
1:A:187:ALA:O	1:A:188:ASN:CG	2.58	0.42
1:G:212:ILE:HD12	1:G:260:ILE:HG22	2.01	0.42
1:G:231:ILE:N	1:G:231:ILE:HD12	2.31	0.42
2:H:392:ILE:HG12	2:H:442:MET:HB3	2.01	0.42
1:K:454:THR:HG21	1:K:466:MET:HA	2.00	0.42
2:F:206:TYR:O	2:F:209:ALA:HB3	2.18	0.42
1:I:266:GLN:HB3	1:I:500:THR:HG22	2.01	0.42
1:C:452:LEU:O	1:C:466:MET:CE	2.67	0.42
1:E:68:ILE:HG12	1:E:78:VAL:HG11	2.01	0.42
1:I:118:ASN:HD21	1:I:119:GLN:HE21	1.67	0.42
1:G:75:ALA:O	1:G:79:ILE:HG13	2.18	0.42
1:E:421:ARG:HD3	1:E:421:ARG:C	2.39	0.42
1:K:396:ILE:HG12	1:K:463:ILE:CD1	2.45	0.42
1:K:625:PHE:N	1:K:625:PHE:CD1	2.87	0.42
1:E:176:ASP:OD1	1:E:178:ILE:HD13	2.19	0.42
1:A:317:GLY:O	1:A:321:VAL:HG12	2.19	0.42
1:C:130:ALA:HA	1:C:133:ALA:CB	2.45	0.42
2:F:355:VAL:HB	2:F:390:THR:HG23	2.01	0.42
1:C:319:GLN:NE2	1:C:345:PHE:CE1	2.87	0.42
2:L:382:ASP:HA	2:L:424:VAL:CG1	2.50	0.42
2:B:376:ARG:NH1	2:J:410:LYS:HZ2	2.16	0.42
2:H:50:GLY:HA3	2:H:127:THR:O	2.19	0.42
1:G:411:LEU:HB2	1:G:682:GLN:HG3	2.00	0.42
1:E:553:ARG:NH1	2:F:115:ASN:OD1	2.52	0.42
1:K:649:LEU:HD13	2:L:59:HIS:CD2	2.54	0.42
1:K:191:THR:O	1:K:193:PRO:HD3	2.18	0.42
1:C:118:ASN:O	1:C:119:GLN:HG3	2.19	0.42
1:K:272:ILE:HB	1:K:335:VAL:CG2	2.49	0.42
1:G:68:ILE:HG12	1:G:78:VAL:CG1	2.50	0.42
1:K:273:GLN:HG2	1:K:369:LEU:HD11	2.01	0.42
1:G:354:LEU:C	1:G:354:LEU:HD13	2.40	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:518:PRO:HD2	1:K:521:ASP:OD1	2.20	0.42
1:K:617:GLY:O	1:K:625:PHE:CB	2.52	0.42
1:K:66:ILE:HD13	1:K:88:SER:O	2.19	0.42
1:E:66:ILE:HG22	1:E:137:GLN:HG3	2.01	0.42
2:J:479:ILE:C	2:J:479:ILE:HD12	2.37	0.42
1:I:85:MET:O	1:I:86:GLY:C	2.57	0.42
2:L:416:LEU:HD13	2:L:441:VAL:HG22	2.01	0.42
1:I:464:GLU:OE2	1:I:464:GLU:HA	2.19	0.42
2:H:460:VAL:CG2	2:H:496:ALA:HB2	2.46	0.42
1:C:323:LEU:O	1:C:326:ALA:HB3	2.19	0.42
1:C:186:GLU:CD	1:C:186:GLU:N	2.72	0.42
2:B:303:ASP:OD2	2:B:509:ARG:HD2	2.19	0.42
1:I:628:ARG:HG3	1:I:633:ASP:HA	2.01	0.42
1:A:353:ARG:HH11	1:A:353:ARG:HG3	1.83	0.42
2:D:252:ARG:HE	2:D:252:ARG:HB2	1.68	0.42
2:B:52:GLN:OE1	2:B:52:GLN:O	2.37	0.42
2:J:84:MET:SD	2:J:85:PHE:CE1	3.13	0.42
2:B:533:LYS:HD2	2:J:385:GLU:OE2	2.18	0.42
1:G:191:THR:O	1:G:193:PRO:HD3	2.19	0.42
2:F:138:SER:O	2:F:139:LYS:C	2.57	0.42
1:G:71:ARG:HA	1:G:75:ALA:HB2	2.01	0.42
1:A:156:LEU:HD22	1:A:161:VAL:HB	2.02	0.42
1:A:625:PHE:CD1	1:A:627:ILE:HD11	2.54	0.42
1:A:292:ILE:HD13	1:A:300:VAL:O	2.19	0.42
1:C:285:LEU:HB3	1:C:365:THR:HG21	2.02	0.42
1:I:629:THR:H	1:I:632:ALA:HB3	1.84	0.42
1:E:325:LYS:O	1:E:328:GLY:N	2.45	0.42
1:K:421:ARG:O	1:K:421:ARG:CD	2.67	0.42
1:I:419:ARG:HB2	1:I:476:GLU:HB2	2.00	0.42
1:G:467:ARG:HD2	1:G:467:ARG:O	2.19	0.42
1:A:388:ASP:N	1:A:388:ASP:OD2	2.52	0.42
1:I:130:ALA:HA	1:I:133:ALA:CB	2.43	0.42
2:D:200:CYS:O	2:D:223:MET:HA	2.20	0.42
2:B:234:VAL:CG2	3:I:801:BTI:H83	2.50	0.42
2:J:447:LEU:HD23	2:J:447:LEU:HA	1.75	0.42
2:D:355:VAL:O	2:D:390:THR:HA	2.19	0.42
1:C:690:ILE:HD12	1:C:699:LEU:HD11	2.01	0.42
2:B:410:LYS:NZ	2:J:376:ARG:HH11	2.17	0.42
1:I:651:PRO:CG	2:J:62:GLY:HA3	2.50	0.42
2:D:66:ALA:HB2	2:D:125:ASP:HA	2.02	0.42
2:L:398:LEU:HD12	2:L:399:PRO:HD2	2.00	0.42
1:A:107:ASP:O	1:A:108:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:316:MET:HE2	1:C:337:PHE:HD1	1.84	0.42
1:C:532:MET:O	1:C:535:VAL:HB	2.20	0.42
1:G:74:ILE:CD1	1:G:143:TYR:CE2	2.99	0.42
1:K:455:TRP:CG	1:K:456:ALA:N	2.85	0.42
2:B:476(C):ASP:O	2:B:478:LYS:N	2.44	0.42
1:C:563:LEU:O	1:C:565:GLY:N	2.52	0.42
1:C:321:VAL:O	1:C:324:ALA:CB	2.61	0.42
1:A:596:TRP:CH2	1:A:600:ASP:O	2.72	0.42
2:F:347:LEU:O	2:F:348:GLU:C	2.58	0.42
2:D:149:MET:CE	2:D:186:ALA:HA	2.50	0.42
1:A:583:PHE:CD1	1:A:583:PHE:N	2.88	0.42
1:I:214:TYR:HB2	1:I:215:PRO:HA	2.00	0.42
1:A:186:GLU:OE2	1:A:187:ALA:N	2.52	0.42
1:A:411:LEU:HD22	1:A:682:GLN:CB	2.49	0.42
1:A:283:ILE:HB	1:A:386:GLN:CD	2.40	0.42
2:H:436:GLY:O	2:H:439:TYR:HB3	2.18	0.42
1:C:642:ARG:NH1	2:D:71:ASP:OD2	2.53	0.42
1:E:65:LYS:HA	1:E:88:SER:O	2.19	0.42
1:E:347:PHE:CZ	1:E:349:GLU:HA	2.54	0.42
2:H:182:ARG:HH11	2:H:182:ARG:HG3	1.84	0.42
2:B:48:LEU:HD23	2:B:48:LEU:HA	1.61	0.42
2:L:315:ASP:C	2:L:315:ASP:OD1	2.58	0.42
1:G:671:VAL:CG2	1:G:691:GLU:HB2	2.49	0.42
1:G:690:ILE:CD1	1:G:699:LEU:HD11	2.49	0.42
2:D:471:ILE:HG21	2:L:166:ILE:HG13	2.02	0.42
1:I:218:ILE:CD1	1:I:260:ILE:HG12	2.49	0.42
1:I:654:LEU:HA	1:I:654:LEU:HD23	1.89	0.42
1:I:422:PRO:HA	1:I:422(A):PRO:HD3	1.85	0.42
1:C:347:PHE:CZ	1:C:349:GLU:HA	2.55	0.42
1:I:414:ILE:HD11	1:I:442:SER:C	2.40	0.42
1:A:157:GLU:C	1:A:159:GLU:N	2.72	0.42
2:L:499:ARG:CG	2:L:499:ARG:NH1	2.80	0.42
1:C:325:LYS:O	1:C:327:VAL:N	2.52	0.42
1:K:195:TYR:CD2	1:K:208:ILE:HD13	2.54	0.42
1:E:627:ILE:N	1:E:627:ILE:HD12	2.34	0.42
1:A:140:HIS:ND1	1:A:141:PRO:CD	2.82	0.42
1:I:188:ASN:O	1:I:188:ASN:OD1	2.38	0.42
1:I:380:GLU:HG2	1:I:381:PRO:HD2	2.01	0.42
1:E:283:ILE:HD12	1:E:389:VAL:CG2	2.50	0.42
1:G:530:ALA:HB2	1:G:561:VAL:HG21	2.01	0.42
1:K:515:VAL:HB	1:K:631:GLY:C	2.39	0.42
2:H:118:VAL:CG1	2:H:119:VAL:N	2.83	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:48:LEU:HD23	2:H:48:LEU:HA	1.69	0.42
2:D:351:THR:HG22	2:D:386:ILE:HG23	2.02	0.42
2:L:536:ASN:O	2:L:537:ILE:C	2.58	0.42
1:E:695:MET:SD	2:F:313:PRO:HG3	2.59	0.42
1:A:99:GLN:HG3	1:A:100:ALA:H	1.84	0.42
1:I:287:GLU:HG3	1:I:308:LEU:HD21	2.02	0.42
1:E:718:LEU:N	1:E:718:LEU:CD2	2.69	0.42
1:K:146:LEU:HD23	1:K:152:PHE:CD2	2.54	0.42
1:G:384:ILE:HB	1:G:388:ASP:HB2	2.01	0.42
2:B:109:THR:HG22	2:B:122:PHE:HB3	2.01	0.42
2:B:180:PHE:O	2:B:183:ASN:HB2	2.19	0.42
1:K:390:LYS:C	1:K:390:LYS:HD3	2.39	0.42
1:I:421:ARG:CD	1:I:421:ARG:O	2.68	0.42
1:C:463:ILE:HD12	1:C:494:PHE:CE1	2.54	0.42
1:E:276:CYS:HB2	1:E:277:ASP:H	1.41	0.42
2:F:442:MET:O	2:F:443:SER:C	2.58	0.42
1:I:187:ALA:O	1:I:188:ASN:CG	2.58	0.42
1:G:301:GLU:OE2	1:G:397:GLU:OE1	2.37	0.42
2:L:355:VAL:O	2:L:390:THR:HA	2.20	0.42
2:B:69:ARG:HH12	2:B:160:ASP:CB	2.33	0.42
1:I:304:PRO:HD2	1:I:394:TRP:CE2	2.55	0.42
2:L:196:ILE:HG22	2:L:221:SER:HB2	2.02	0.42
1:I:650:MET:HA	1:I:651:PRO:HD3	1.90	0.42
1:G:583:PHE:N	1:G:583:PHE:CD1	2.87	0.42
1:A:274:VAL:HA	1:A:284:TYR:HA	2.02	0.42
2:D:301:SER:HB2	2:D:322:LYS:NZ	2.35	0.42
2:J:193:ILE:CD1	2:J:274:LEU:HD23	2.50	0.42
2:F:315:ASP:OD1	2:F:317:LYS:HB2	2.19	0.42
1:E:480:HIS:HD2	1:E:482:LEU:HB2	1.82	0.42
1:K:93:TYR:HA	1:K:121:TYR:OH	2.19	0.42
1:I:67:LEU:HG	1:I:68:ILE:N	2.32	0.42
1:K:157:GLU:C	1:K:159:GLU:N	2.72	0.42
1:E:666:MET:HG2	1:E:666:MET:O	2.18	0.42
1:K:292:ILE:HD12	1:K:292:ILE:N	2.14	0.42
1:I:457:PRO:HG2	1:I:458:THR:N	2.27	0.42
1:A:85:MET:O	1:A:86:GLY:C	2.58	0.42
1:E:85:MET:HB2	1:E:87:ILE:HD11	2.02	0.42
1:G:92:ILE:HD12	1:G:112:ILE:CD1	2.50	0.42
1:I:504:ILE:CG2	1:I:505:ALA:N	2.82	0.42
1:I:625:PHE:HB2	1:I:627:ILE:HD12	2.02	0.42
1:I:541:THR:O	1:I:541:THR:HG22	2.20	0.42
2:L:524:ASN:O	2:L:525:LYS:C	2.58	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:371:GLU:O	1:G:372:GLN:C	2.58	0.42
2:D:141:ILE:O	2:D:145:MET:HG3	2.19	0.42
1:E:279:HIS:CD2	1:E:380:GLU:O	2.71	0.42
1:G:675:VAL:HG12	1:G:707:VAL:HG21	2.01	0.42
2:J:536:ASN:O	2:J:537:ILE:C	2.58	0.42
2:D:299:GLU:HG3	2:D:322:LYS:HB3	2.02	0.42
1:K:446:ASP:HA	1:K:447:PRO:HD2	1.87	0.42
2:D:539:LEU:OXT	2:L:372:ARG:NH2	2.52	0.42
2:B:285:LYS:HB3	2:B:286:PRO:HD2	2.01	0.42
1:I:347:PHE:CD1	1:I:347:PHE:O	2.72	0.42
1:E:71:ARG:O	1:E:75:ALA:CB	2.68	0.42
1:I:78:VAL:HA	1:I:370:VAL:HG11	2.02	0.42
1:E:358:HIS:CE1	1:E:359:PRO:HD3	2.55	0.42
1:G:279:HIS:NE2	1:G:379:GLY:HA2	2.35	0.42
1:G:64:ASN:H	1:G:137:GLN:HG2	1.85	0.42
1:C:354:LEU:HD11	1:C:358:HIS:ND1	2.35	0.42
1:G:455:TRP:C	1:G:455:TRP:CD1	2.87	0.42
2:H:325:ASP:O	2:H:327:GLY:N	2.53	0.42
1:A:302:GLU:OE2	1:A:394:TRP:CZ3	2.73	0.42
1:K:665:PRO:HG2	1:K:666:MET:HE2	1.96	0.42
2:H:476(C):ASP:N	2:H:476(D):PRO:HD3	2.35	0.42
1:G:670:ILE:HD11	1:G:718:LEU:HD11	2.02	0.42
1:C:583:PHE:CZ	1:C:590:MET:CE	3.02	0.42
1:A:661:MET:HG3	1:A:723:VAL:HG13	2.02	0.42
1:K:140:HIS:ND1	1:K:141:PRO:CD	2.82	0.42
1:I:235:ASP:N	1:I:235:ASP:OD1	2.47	0.42
1:C:140:HIS:ND1	1:C:141:PRO:HD2	2.35	0.42
1:G:186:GLU:N	1:G:186:GLU:CD	2.74	0.42
1:C:266:GLN:HG2	1:C:341:GLY:HA2	2.02	0.42
1:I:283:ILE:HD12	1:I:389:VAL:CG2	2.49	0.42
1:E:515:VAL:HB	1:E:631:GLY:HA3	2.02	0.42
2:B:319:LEU:CD2	2:B:391:LEU:HD13	2.50	0.42
2:J:354:VAL:HA	2:J:389:LEU:O	2.20	0.42
2:D:537:ILE:HA	2:D:538:PRO:HD3	1.91	0.42
1:A:371:GLU:O	1:A:374:ILE:HG12	2.20	0.42
2:F:126:PHE:O	2:F:130:GLY:HA2	2.20	0.42
1:E:400:LEU:HD23	1:E:400:LEU:HA	1.74	0.42
1:E:85:MET:O	1:E:86:GLY:C	2.58	0.42
2:J:205:VAL:O	2:J:208:PRO:HD2	2.20	0.42
2:J:42:ARG:CG	2:J:42:ARG:HH11	2.18	0.42
1:C:524:ARG:HA	1:C:590:MET:SD	2.60	0.42
1:E:325:LYS:O	1:E:327:VAL:N	2.53	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:518:PRO:O	1:G:519:GLU:C	2.58	0.42
1:G:504:ILE:CG2	1:G:505:ALA:N	2.82	0.42
1:K:583:PHE:CD1	1:K:583:PHE:N	2.88	0.42
1:A:111:HIS:O	1:A:112:ILE:HG23	2.19	0.42
2:B:50:GLY:HA3	2:B:127:THR:O	2.19	0.42
2:B:367:ASP:O	2:B:368:ILE:C	2.58	0.42
1:K:140:HIS:CE1	1:K:142:GLY:N	2.84	0.42
1:C:69:ALA:HB3	1:C:141:PRO:HA	2.01	0.42
1:I:682:GLN:HA	1:I:682:GLN:OE1	2.20	0.42
2:D:141:ILE:O	2:D:144:ILE:HG13	2.20	0.42
1:G:304:PRO:HD2	1:G:394:TRP:CD2	2.55	0.42
1:K:724:ILE:HG22	1:K:725:MET:HG3	2.01	0.42
1:G:422(A):PRO:O	1:G:422(B):ALA:HB2	2.19	0.42
2:H:222:TYR:HB2	2:H:245:GLY:O	2.20	0.42
1:E:482:LEU:N	1:E:483:PRO:HD2	2.35	0.41
1:E:68:ILE:CG2	1:E:70:ASN:H	2.33	0.41
1:E:75:ALA:O	1:E:79:ILE:HG13	2.20	0.41
1:K:482:LEU:N	1:K:483:PRO:HD2	2.35	0.41
1:I:77:ARG:NH1	1:I:370:VAL:CG2	2.80	0.41
1:I:68:ILE:CG1	1:I:78:VAL:HG11	2.50	0.41
1:G:78:VAL:HG23	1:G:370:VAL:HG11	2.01	0.41
1:K:394:TRP:O	1:K:455:TRP:HA	2.20	0.41
1:K:456:ALA:CB	1:K:457:PRO:HD2	2.34	0.41
1:I:358:HIS:CG	1:I:359:PRO:HD3	2.55	0.41
1:A:146:LEU:HD23	1:A:152:PHE:CG	2.55	0.41
2:B:205:VAL:HG23	2:B:206:TYR:N	2.34	0.41
2:D:425:PRO:HB3	2:D:522:LEU:HD13	2.01	0.41
1:I:518:PRO:HD2	1:I:521:ASP:OD1	2.20	0.41
1:I:663:LEU:O	1:I:665:PRO:HD3	2.20	0.41
2:B:454:ALA:O	2:B:505:VAL:HA	2.20	0.41
2:L:183:ASN:HD22	2:L:183:ASN:HA	1.67	0.41
1:A:165:GLY:CA	1:A:331:SER:OG	2.68	0.41
1:K:186:GLU:OE2	1:K:187:ALA:N	2.53	0.41
1:I:140:HIS:CE1	1:I:142:GLY:N	2.88	0.41
2:H:202:GLY:O	2:H:205:VAL:HG22	2.20	0.41
1:A:279:HIS:HD2	1:A:380:GLU:O	2.03	0.41
2:L:239:VAL:CG2	2:L:243:GLU:HB2	2.50	0.41
1:E:515:VAL:HB	1:E:631:GLY:CA	2.50	0.41
2:B:319:LEU:HD23	2:B:391:LEU:HD13	2.02	0.41
2:H:522:LEU:HA	2:J:151:ASN:ND2	2.34	0.41
2:L:138:SER:OG	2:L:139:LYS:N	2.53	0.41
1:E:312:THR:HG21	1:E:343:LYS:HD3	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:128:MET:O	1:G:131:ILE:N	2.53	0.41
1:A:136:ALA:O	1:A:137:GLN:CB	2.69	0.41
1:A:304:PRO:HD2	1:A:394:TRP:CE2	2.56	0.41
2:F:180:PHE:O	2:F:184:ILE:HG13	2.19	0.41
1:C:711:ASN:O	1:C:712:ALA:HB2	2.20	0.41
2:J:149:MET:HE1	2:J:189:VAL:HG11	2.00	0.41
1:G:485:LEU:O	1:G:486:SER:C	2.57	0.41
2:F:462:VAL:HG22	2:H:169:GLY:CA	2.50	0.41
2:H:83:ASP:HB3	2:H:86:VAL:HG23	2.00	0.41
1:G:167:PRO:C	1:G:169:GLY:N	2.73	0.41
1:G:394:TRP:CE3	1:G:459:ARG:HG3	2.55	0.41
1:K:534:ARG:NH1	1:K:534:ARG:HG3	2.35	0.41
1:I:150:SER:O	1:I:151:LYS:C	2.58	0.41
1:I:546:ARG:HG2	1:I:546:ARG:H	1.55	0.41
1:E:710:ILE:HG22	1:E:711:ASN:N	2.35	0.41
1:C:570:VAL:HG22	1:C:581:VAL:HG12	2.02	0.41
1:C:65:LYS:HE2	1:C:134:THR:O	2.19	0.41
1:A:271:GLU:O	1:A:287:GLU:HB2	2.21	0.41
1:I:270:ILE:HG21	1:I:308:LEU:HD21	2.02	0.41
1:K:156:LEU:HD22	1:K:161:VAL:HB	2.03	0.41
1:C:428(L):ALA:HB3	1:C:455:TRP:CD1	2.49	0.41
1:I:156:LEU:HD22	1:I:161:VAL:HB	2.02	0.41
1:I:364:ILE:HG22	1:I:392:THR:O	2.20	0.41
1:A:619:ILE:O	1:A:620:SER:C	2.59	0.41
1:E:490:ASP:OD2	1:E:630:ARG:NH1	2.53	0.41
1:E:517:LEU:HA	1:E:518:PRO:HD3	1.62	0.41
1:I:325:LYS:O	1:I:327:VAL:N	2.53	0.41
2:D:210:MET:HE1	2:L:416:LEU:HG	2.02	0.41
1:G:293:GLN:O	1:G:504:ILE:CG2	2.64	0.41
1:G:334:THR:HG21	1:G:355:GLN:CG	2.50	0.41
1:G:234:ASN:O	1:G:237:GLU:HB3	2.19	0.41
1:I:195:TYR:O	1:I:259:PHE:HA	2.21	0.41
1:G:695:MET:HG3	2:H:313:PRO:HG3	2.01	0.41
1:C:140:HIS:ND1	1:C:141:PRO:N	2.68	0.41
1:K:83:ARG:CZ	1:K:83:ARG:HB3	2.50	0.41
1:G:195:TYR:CD2	1:G:208:ILE:HD13	2.56	0.41
2:D:138:SER:O	2:D:141:ILE:N	2.53	0.41
2:L:432:ARG:O	2:L:459:GLU:N	2.54	0.41
2:H:442:MET:O	2:H:443:SER:C	2.58	0.41
1:K:436:TYR:CD1	1:K:436:TYR:C	2.93	0.41
1:C:724:ILE:HG22	1:C:725:MET:HG3	2.02	0.41
2:D:48:LEU:HA	2:D:48:LEU:HD23	1.63	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:447:LEU:HD23	2:L:447:LEU:HA	1.78	0.41
1:C:407:ARG:HH11	1:C:407:ARG:HG2	1.85	0.41
1:C:314:ARG:O	1:C:318:GLU:HG3	2.19	0.41
1:E:268:ARG:NH2	1:E:497:GLY:O	2.45	0.41
2:J:248:THR:O	2:J:252:ARG:HG2	2.20	0.41
2:L:309:ASN:HD21	2:L:311:ASN:HB2	1.86	0.41
1:C:446:ASP:OD1	1:C:447:PRO:HD2	2.19	0.41
1:C:338:ILE:N	1:C:338:ILE:CD1	2.82	0.41
1:A:118:ASN:HD21	1:A:119:GLN:HE21	1.68	0.41
1:E:670:ILE:CD1	1:E:718:LEU:HD21	2.50	0.41
1:E:456:ALA:CB	1:E:457:PRO:HD2	2.35	0.41
1:C:363:LEU:O	1:C:455:TRP:CE3	2.73	0.41
1:A:376:VAL:CG2	1:A:377:ALA:N	2.83	0.41
1:C:358:HIS:CG	1:C:359:PRO:HD3	2.54	0.41
2:L:88:HIS:CD2	2:L:88:HIS:C	2.94	0.41
1:E:302:GLU:OE2	1:E:394:TRP:CZ3	2.73	0.41
1:C:275:LEU:HD23	1:C:276:CYS:H	1.85	0.41
2:J:229:ASP:N	2:J:229:ASP:OD1	2.52	0.41
2:B:401:THR:CG2	2:B:402:SER:N	2.83	0.41
1:G:541:THR:O	1:G:541:THR:HG22	2.21	0.41
1:A:634:LEU:N	1:A:634:LEU:CD2	2.82	0.41
2:B:248:THR:O	2:B:252:ARG:HG2	2.20	0.41
2:J:145:MET:HE3	2:J:183:ASN:HD21	1.85	0.41
1:K:191:THR:O	1:K:193:PRO:CD	2.69	0.41
1:K:295:ARG:O	1:K:296:ASN:HB2	2.20	0.41
2:D:206:TYR:O	2:D:209:ALA:HB3	2.20	0.41
1:I:90:VAL:HG12	1:I:91:ALA:N	2.35	0.41
1:C:174:MET:HA	1:C:180:SER:OG	2.20	0.41
1:A:398:ASN:HB3	1:A:485:LEU:HD13	2.02	0.41
1:K:274:VAL:HA	1:K:284:TYR:HA	2.02	0.41
1:A:114:PRO:HB2	1:A:115:PRO:HD2	2.02	0.41
1:K:358:HIS:O	1:K:361:THR:N	2.54	0.41
1:K:543:VAL:HG12	1:K:544:SER:N	2.35	0.41
2:L:117:ARG:NH2	2:L:280:LEU:HG	2.33	0.41
2:F:417:TYR:N	2:H:210:MET:CE	2.83	0.41
1:A:428(L):ALA:HB3	1:A:455:TRP:CD1	2.44	0.41
2:H:479:ILE:HD12	2:H:479:ILE:C	2.39	0.41
1:K:285:LEU:HB3	1:K:365:THR:HG21	2.02	0.41
2:B:476(C):ASP:N	2:B:476(D):PRO:HD3	2.35	0.41
1:C:357:GLU:CD	1:C:357:GLU:H	2.23	0.41
2:J:293:ASP:OD1	2:J:325:ASP:O	2.38	0.41
1:E:563:LEU:CD2	1:E:636:VAL:HG22	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:563:LEU:CD2	1:G:636:VAL:HG22	2.50	0.41
1:C:396:ILE:HD12	1:C:396:ILE:N	2.36	0.41
1:E:107:ASP:O	1:E:108:GLU:CG	2.68	0.41
2:B:509:ARG:HH11	2:B:509:ARG:HB3	1.86	0.41
2:D:134:SER:H	2:D:137:HIS:HB3	1.85	0.41
2:B:356:ALA:HA	2:B:391:LEU:O	2.19	0.41
2:H:375:ALA:HA	2:H:415:LEU:HD12	2.03	0.41
2:F:67:ARG:HG2	2:F:67:ARG:HH11	1.84	0.41
1:C:114:PRO:CB	1:C:115:PRO:HD2	2.50	0.41
1:K:342:GLN:O	1:K:343:LYS:HB2	2.21	0.41
1:I:482:LEU:N	1:I:483:PRO:HD2	2.35	0.41
1:I:347:PHE:CZ	1:I:349:GLU:HA	2.56	0.41
1:G:316:MET:HB3	1:G:337:PHE:CE1	2.55	0.41
1:K:114:PRO:HB2	1:K:115:PRO:HD2	2.03	0.41
1:I:116:PRO:HG3	1:I:444:TYR:CE2	2.55	0.41
1:K:164:VAL:HA	1:K:377:ALA:CB	2.51	0.41
1:A:394:TRP:O	1:A:455:TRP:HA	2.21	0.41
2:D:90:CYS:HB2	2:D:168:GLU:OE2	2.21	0.41
2:F:347:LEU:HA	2:F:347:LEU:HD23	1.86	0.41
1:C:396:ILE:HD13	1:C:462:ALA:CB	2.51	0.41
2:J:312:THR:HG22	2:J:313:PRO:O	2.21	0.41
2:D:347:LEU:HD23	2:D:347:LEU:HA	1.84	0.41
1:A:140:HIS:CE1	1:A:142:GLY:N	2.85	0.41
2:J:121:VAL:HG22	2:J:122:PHE:H	1.84	0.41
1:E:83:ARG:NH1	1:E:83:ARG:CG	2.83	0.41
1:I:177:LYS:HB3	1:I:181:LYS:HZ1	1.82	0.41
1:I:186:GLU:CD	1:I:186:GLU:N	2.73	0.41
2:F:182:ARG:NH1	2:F:182:ARG:HG3	2.36	0.41
1:I:675:VAL:HG11	1:I:707:VAL:HG21	2.02	0.41
2:D:182:ARG:NH1	2:D:182:ARG:HG3	2.35	0.41
2:H:199:PRO:HB3	2:H:222:TYR:CZ	2.56	0.41
2:D:244:LEU:HA	2:D:244:LEU:HD12	1.85	0.41
1:K:720:VAL:HG22	1:K:721:ASP:H	1.85	0.41
2:D:295:PRO:O	2:D:513:LYS:HA	2.20	0.41
1:A:168:LYS:O	1:A:172:GLU:OE1	2.38	0.41
2:L:192:GLN:O	2:L:211:THR:HB	2.20	0.41
1:I:422:PRO:HG3	1:I:473:PHE:CZ	2.56	0.41
1:C:348:LEU:O	1:C:349:GLU:HB3	2.21	0.41
1:E:71:ARG:NH1	1:E:445:TYR:CG	2.89	0.41
1:I:74:ILE:HG23	1:I:75:ALA:N	2.35	0.41
1:E:273:GLN:HG2	1:E:369:LEU:HD11	2.03	0.41
1:E:455:TRP:CD1	1:E:455:TRP:C	2.91	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:458:THR:O	1:C:461:ALA:HB3	2.20	0.41
1:K:602:LEU:HD12	1:K:614:LEU:O	2.19	0.41
1:K:627:ILE:HD13	1:K:636:VAL:CG2	2.51	0.41
1:C:537:GLU:HA	1:C:540:ARG:HG3	2.01	0.41
1:C:139:VAL:O	1:C:164:VAL:HG12	2.20	0.41
2:J:479:ILE:HD12	2:J:480:ALA:H	1.79	0.41
1:K:77:ARG:HH11	1:K:77:ARG:HG3	1.85	0.41
2:B:495:VAL:HG13	2:B:496:ALA:N	2.36	0.41
1:C:596:TRP:CH2	1:C:600:ASP:O	2.73	0.41
1:C:421:ARG:HD3	1:C:421:ARG:O	2.21	0.41
1:A:111:HIS:O	1:A:112:ILE:CG2	2.69	0.41
1:A:112:ILE:O	1:A:120:SER:HA	2.19	0.41
1:E:658:THR:HG22	1:E:659:SER:O	2.20	0.41
1:C:165:GLY:HA2	1:C:331:SER:OG	2.21	0.41
2:D:300:PRO:O	2:D:303:ASP:HB2	2.20	0.41
2:B:382:ASP:HA	2:B:424:VAL:CG1	2.51	0.41
2:F:393:ASP:CG	2:F:432:ARG:HB3	2.41	0.41
1:I:140:HIS:ND1	1:I:141:PRO:CD	2.84	0.41
1:E:140:HIS:ND1	1:E:141:PRO:CD	2.84	0.41
2:B:69:ARG:HA	2:B:268:LEU:CD1	2.51	0.41
2:B:300:PRO:HB3	2:B:509:ARG:NH1	2.35	0.41
1:A:553:ARG:NH1	2:B:115:ASN:OD1	2.53	0.41
2:B:252:ARG:NH2	2:B:335:GLU:HG3	2.35	0.41
2:B:64:LEU:HA	2:B:64:LEU:HD23	1.83	0.41
1:C:446:ASP:HA	1:C:447:PRO:HD2	1.91	0.41
1:A:422:PRO:HA	1:A:422(A):PRO:HD3	1.86	0.41
1:A:610:ALA:HA	1:A:611:PRO:HD3	1.78	0.41
2:B:372:ARG:NH2	2:J:539:LEU:OXT	2.52	0.41
1:E:316:MET:HB3	1:E:337:PHE:CE1	2.56	0.41
1:E:99:GLN:O	1:E:100:ALA:C	2.59	0.41
2:H:167:GLN:NE2	2:H:167:GLN:N	2.37	0.41
1:I:121:TYR:HE2	1:I:445:TYR:OH	2.04	0.41
1:I:70:ASN:OD1	1:I:74:ILE:HG21	2.20	0.41
1:K:467:ARG:HD2	1:K:467:ARG:O	2.21	0.41
1:I:124:ILE:CG2	1:I:128:MET:CE	2.99	0.41
1:I:455:TRP:CD2	1:I:456:ALA:N	2.89	0.41
1:E:64:ASN:H	1:E:137:GLN:HG2	1.85	0.41
1:G:390:LYS:HD3	1:G:391:LEU:H	1.77	0.41
2:F:135:GLU:OE1	2:J:89:ARG:NH2	2.54	0.41
1:K:663:LEU:O	1:K:665:PRO:HD3	2.21	0.41
1:C:517:LEU:HD11	1:C:632:ALA:HB2	2.02	0.41
1:I:325:LYS:H	1:I:325:LYS:HG3	1.74	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:583:PHE:CZ	1:K:590:MET:HE3	2.56	0.41
2:F:149:MET:CE	2:F:189:VAL:CG1	2.99	0.41
1:G:118:ASN:HD21	1:G:119:GLN:HE21	1.69	0.41
1:K:339:VAL:HG22	1:K:345:PHE:HB3	2.02	0.41
2:L:145:MET:CE	2:L:183:ASN:ND2	2.84	0.41
2:H:361:VAL:O	2:H:363:ALA:N	2.53	0.41
2:L:303:ASP:OD2	2:L:509:ARG:HD2	2.20	0.41
2:D:222:TYR:C	2:D:222:TYR:CD1	2.94	0.41
1:G:207:LYS:O	1:G:207:LYS:HD3	2.20	0.41
1:K:416:ARG:HG3	1:K:439:GLY:O	2.21	0.41
2:H:252:ARG:NH2	2:H:335:GLU:HG3	2.36	0.41
1:A:266:GLN:H	1:A:266:GLN:HG2	1.49	0.41
1:E:270:ILE:HG21	1:E:308:LEU:HD21	2.03	0.41
1:A:316:MET:HE3	1:A:337:PHE:HD1	1.85	0.41
1:G:99:GLN:HG3	1:G:100:ALA:H	1.86	0.41
1:G:270:ILE:HG21	1:G:308:LEU:HD21	2.02	0.41
1:E:68:ILE:CG1	1:E:78:VAL:HG11	2.50	0.41
1:G:73:GLU:OE1	1:G:451:LYS:NZ	2.51	0.41
1:K:162:ILE:O	1:K:164:VAL:N	2.54	0.41
1:I:718:LEU:H	1:I:718:LEU:HD23	1.79	0.41
1:C:461:ALA:O	1:C:464:GLU:HB3	2.21	0.41
1:I:334:THR:HG21	1:I:355:GLN:CG	2.51	0.41
1:K:517:LEU:HB3	1:K:521:ASP:HB3	2.03	0.41
1:K:626:ARG:C	1:K:627:ILE:HD12	2.40	0.41
1:I:157:GLU:C	1:I:159:GLU:N	2.73	0.41
1:K:340:ASP:OD1	1:K:344:ASN:HB2	2.21	0.41
1:G:340:ASP:OD1	1:G:344:ASN:HB2	2.21	0.41
2:B:205:VAL:HB	2:J:409:ILE:HD13	2.02	0.41
1:C:390:LYS:HD3	1:C:390:LYS:C	2.40	0.41
2:H:476(A):LEU:C	2:H:476(C):ASP:H	2.22	0.41
2:D:417:TYR:N	2:L:210:MET:HE1	2.36	0.41
2:J:98:GLN:N	2:J:98:GLN:OE1	2.50	0.41
1:G:713:SER:H	1:G:716:ASN:CG	2.24	0.41
1:I:467:ARG:HH21	1:I:630:ARG:HE	1.68	0.41
1:E:504:ILE:CG2	1:E:505:ALA:H	2.32	0.41
1:I:327:VAL:HG22	1:I:327:VAL:O	2.20	0.41
1:A:543:VAL:HG12	1:A:544:SER:N	2.36	0.41
1:K:293:GLN:HA	1:K:299:VAL:HG23	2.02	0.41
2:D:205:VAL:HB	2:L:409:ILE:HD13	2.03	0.41
2:D:205:VAL:O	2:D:208:PRO:HD2	2.21	0.41
2:D:207:SER:O	2:D:208:PRO:C	2.59	0.41
1:A:384:ILE:HB	1:A:388:ASP:HB2	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:347:LEU:O	2:B:348:GLU:C	2.58	0.41
1:G:658:THR:HG22	1:G:659:SER:O	2.20	0.41
1:E:396:ILE:CG1	1:E:463:ILE:HD13	2.46	0.41
1:C:276:CYS:HB2	1:C:277:ASP:H	1.42	0.41
1:C:331:SER:HB3	1:C:332:ALA:H	1.61	0.41
1:A:83:ARG:CG	1:A:83:ARG:NH1	2.80	0.41
1:E:485:LEU:O	1:E:486:SER:C	2.59	0.41
2:F:392:ILE:HG22	2:F:393:ASP:N	2.35	0.41
2:D:156:ILE:N	2:D:156:ILE:CD1	2.82	0.41
2:J:476(C):ASP:C	2:J:477:GLU:H	2.24	0.41
2:F:173:LEU:HD13	2:H:439:TYR:CD2	2.56	0.41
1:K:552:GLU:N	1:K:552:GLU:CD	2.73	0.41
1:G:69:ALA:HB3	1:G:141:PRO:HA	2.02	0.41
1:I:283:ILE:HG22	1:I:386:GLN:CG	2.51	0.41
1:K:436:TYR:C	1:K:436:TYR:HD1	2.24	0.41
2:J:145:MET:CE	2:J:183:ASN:ND2	2.83	0.41
1:I:690:ILE:HD12	1:I:699:LEU:HD11	2.02	0.41
2:L:294:ASP:HA	2:L:295:PRO:HD2	1.94	0.41
2:J:48:LEU:HA	2:J:48:LEU:HD23	1.71	0.41
2:L:182:ARG:HG3	2:L:182:ARG:HH11	1.86	0.41
2:H:244:LEU:HA	2:H:244:LEU:HD12	1.83	0.41
2:J:347:LEU:HD23	2:J:347:LEU:HA	1.87	0.41
1:K:660:LYS:O	1:K:727:PHE:N	2.51	0.41
1:C:90:VAL:HG12	1:C:91:ALA:N	2.36	0.41
1:G:274:VAL:HA	1:G:284:TYR:HA	2.03	0.41
1:A:191:THR:O	1:A:193:PRO:HD3	2.21	0.41
2:B:456:PRO:HD3	2:B:506:ILE:O	2.21	0.41
2:H:366:LEU:HA	2:H:366:LEU:HD23	1.79	0.41
2:B:366:LEU:HA	2:B:366:LEU:HD23	1.87	0.41
2:F:273:ARG:HD2	2:F:330:TYR:HD1	1.86	0.41
2:L:314:TYR:CE1	2:L:359:PRO:HG2	2.56	0.41
2:F:471:ILE:HG21	2:H:166:ILE:HG13	2.03	0.41
2:B:254:SER:O	2:B:255:SER:CB	2.68	0.41
2:F:118:VAL:HG12	2:F:119:VAL:N	2.36	0.41
2:D:250:HIS:HA	2:D:254:SER:OG	2.20	0.41
1:K:309:ASP:OD2	1:K:343:LYS:HE2	2.20	0.41
1:K:272:ILE:HB	1:K:335:VAL:HG23	2.03	0.41
1:I:77:ARG:O	1:I:77:ARG:NH1	2.50	0.41
1:K:288:ARG:HD3	1:K:361:THR:OG1	2.21	0.41
1:G:378:ALA:O	1:G:379:GLY:O	2.38	0.41
1:I:292:ILE:CD1	1:I:292:ILE:H	2.01	0.41
1:G:543:VAL:CG1	2:H:117:ARG:HD2	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:626:ARG:NE	1:A:628:ARG:HD2	2.36	0.41
2:B:122:PHE:CD1	2:B:141:ILE:HG23	2.56	0.41
2:B:476(D):PRO:O	2:B:480:ALA:HB2	2.20	0.41
1:C:517:LEU:HB3	1:C:521:ASP:HB3	2.02	0.41
1:G:713:SER:O	1:G:714:ALA:C	2.59	0.41
2:H:346:ARG:HH11	2:H:346:ARG:CG	2.32	0.41
1:A:661:MET:CE	1:A:726:GLU:HB3	2.50	0.41
1:C:634:LEU:CD2	1:C:634:LEU:N	2.82	0.41
1:A:598:PRO:HD2	2:B:292:PHE:CD1	2.55	0.41
1:G:272:ILE:HB	1:G:335:VAL:HG23	2.03	0.41
1:E:283:ILE:HG22	1:E:386:GLN:CG	2.49	0.41
1:I:512:PHE:CZ	1:I:515:VAL:HG23	2.56	0.41
2:D:120:TYR:CD1	2:D:148:ALA:HA	2.56	0.41
2:D:410:LYS:HZ2	2:L:376:ARG:NH1	2.18	0.41
1:G:353:ARG:HG3	1:G:353:ARG:HH11	1.86	0.41
1:I:592:VAL:HG13	1:I:607:VAL:HG22	2.03	0.41
1:I:99:GLN:HB2	1:I:436:TYR:OH	2.21	0.41
1:C:118:ASN:C	1:C:119:GLN:HG3	2.41	0.40
1:E:78:VAL:HG23	1:E:370:VAL:HG11	2.02	0.40
1:E:157:GLU:C	1:E:159:GLU:N	2.74	0.40
1:G:71:ARG:O	1:G:75:ALA:HB2	2.21	0.40
1:G:74:ILE:CG2	1:G:75:ALA:N	2.84	0.40
1:C:164:VAL:HG23	1:C:377:ALA:CB	2.51	0.40
2:B:205:VAL:O	2:B:208:PRO:HD2	2.21	0.40
1:C:301:GLU:HG2	1:C:357:GLU:HB3	2.03	0.40
1:E:292:ILE:HD12	1:E:292:ILE:N	2.25	0.40
1:K:321:VAL:O	1:K:324:ALA:CB	2.61	0.40
1:I:517:LEU:HD21	1:I:632:ALA:HB2	2.02	0.40
1:I:630:ARG:O	1:I:632:ALA:N	2.54	0.40
1:C:572:ILE:HG22	1:C:573:ALA:N	2.36	0.40
2:D:499:ARG:HA	2:D:499:ARG:HD3	1.92	0.40
1:E:583:PHE:CD1	1:E:583:PHE:N	2.88	0.40
2:F:298:ILE:HG23	2:F:509:ARG:HB2	2.03	0.40
1:I:497:GLY:O	1:I:499:MET:HG2	2.21	0.40
1:E:468:ILE:O	1:E:471:ASP:HB2	2.20	0.40
1:G:118:ASN:C	1:G:119:GLN:HG3	2.41	0.40
2:J:368:ILE:HG23	2:J:411:HIS:CG	2.56	0.40
2:D:336:PHE:O	2:D:337:ALA:C	2.58	0.40
1:C:140:HIS:CE1	1:C:142:GLY:N	2.85	0.40
1:C:525:VAL:O	1:C:526:ALA:C	2.57	0.40
1:A:68:ILE:CG2	1:A:70:ASN:H	2.34	0.40
1:C:415:GLY:O	1:C:440:GLU:HG3	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:514:ARG:HD2	2:F:514:ARG:HA	1.73	0.40
2:B:374:ALA:HB3	2:B:415:LEU:HD13	2.03	0.40
2:D:366:LEU:HD23	2:D:366:LEU:HA	1.97	0.40
1:A:433:THR:CG2	1:A:434:GLY:N	2.83	0.40
1:G:405:PRO:CG	1:G:481:ASN:HA	2.51	0.40
1:E:124:ILE:HG22	1:E:128:MET:CE	2.51	0.40
1:G:68:ILE:HG12	1:G:78:VAL:HG11	2.03	0.40
1:G:114:PRO:HB2	1:G:115:PRO:HD2	2.03	0.40
1:K:139:VAL:HG11	1:K:156:LEU:HD21	2.02	0.40
1:I:273:GLN:HG2	1:I:369:LEU:HD11	2.04	0.40
1:C:139:VAL:HG11	1:C:156:LEU:CD2	2.51	0.40
1:G:455:TRP:CD2	1:G:456:ALA:N	2.89	0.40
1:I:137:GLN:O	1:I:138:ALA:CB	2.69	0.40
2:J:325:ASP:HA	2:J:512:ARG:NH1	2.25	0.40
1:A:92:ILE:CD1	1:A:112:ILE:HD13	2.49	0.40
1:G:597:THR:OG1	2:H:292:PHE:CG	2.74	0.40
1:E:186:GLU:N	1:E:186:GLU:CD	2.75	0.40
2:F:390:THR:HG21	2:F:419:TYR:OH	2.21	0.40
2:H:120:TYR:CD1	2:H:148:ALA:HA	2.56	0.40
1:A:67:LEU:HG	1:A:68:ILE:N	2.35	0.40
2:D:537:ILE:HG13	2:D:538:PRO:HD2	2.03	0.40
2:H:315:ASP:C	2:H:315:ASP:OD1	2.60	0.40
2:L:195:MET:SD	2:L:271:VAL:HG21	2.61	0.40
1:E:384:ILE:HB	1:E:388:ASP:HB2	2.04	0.40
2:B:273:ARG:HD2	2:B:330:TYR:CD1	2.57	0.40
1:I:710:ILE:HG12	1:I:725:MET:HG2	2.02	0.40
1:E:78:VAL:CG1	1:E:79:ILE:H	2.33	0.40
1:E:92:ILE:CG1	1:E:112:ILE:HD13	2.50	0.40
1:A:444:TYR:HD1	1:A:444:TYR:H	1.69	0.40
1:I:71:ARG:HD3	1:I:445:TYR:CD2	2.56	0.40
1:C:71:ARG:CG	1:C:72:GLY:N	2.85	0.40
1:K:494:PHE:HA	1:K:499:MET:HE1	2.03	0.40
1:C:392:THR:O	1:C:455:TRP:CZ3	2.71	0.40
1:G:152:PHE:CE1	1:G:156:LEU:HD11	2.56	0.40
1:C:369:LEU:O	1:C:373:MET:HB2	2.21	0.40
1:G:461:ALA:O	1:G:464:GLU:HB3	2.22	0.40
1:C:666:MET:O	1:C:668:GLY:N	2.54	0.40
2:L:413:ALA:O	2:L:416:LEU:HB3	2.21	0.40
1:E:329:TYR:HE2	1:E:352:THR:HA	1.86	0.40
1:G:319:GLN:NE2	1:G:345:PHE:CZ	2.89	0.40
2:D:121:VAL:CG2	2:D:122:PHE:N	2.83	0.40
1:A:491:HIS:HA	1:A:492:PRO:HD2	1.92	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:69:ARG:HH12	2:B:160:ASP:CG	2.25	0.40
2:D:225:VAL:N	2:L:404:GLU:OE2	2.52	0.40
2:J:139:LYS:HE2	2:J:139:LYS:HB3	1.85	0.40
1:G:610:ALA:HA	1:G:611:PRO:HD3	1.89	0.40
1:G:168:LYS:O	1:G:172:GLU:OE1	2.39	0.40
1:C:192:VAL:O	1:C:193:PRO:C	2.59	0.40
1:G:654:LEU:O	1:G:655:PRO:O	2.38	0.40
2:B:294:ASP:HA	2:B:295:PRO:HD2	1.92	0.40
1:G:400:LEU:HD23	1:G:400:LEU:HA	1.68	0.40
1:C:416:ARG:HG3	1:C:439:GLY:O	2.21	0.40
1:C:435:VAL:HG22	1:C:436:TYR:H	1.87	0.40
1:C:625:PHE:CD1	1:C:627:ILE:HD11	2.56	0.40
1:I:68:ILE:CG2	1:I:70:ASN:H	2.34	0.40
1:E:456:ALA:CB	1:E:457:PRO:CD	2.94	0.40
2:J:499:ARG:NH2	2:L:89:ARG:HH11	2.04	0.40
2:H:476(C):ASP:CG	2:H:478:LYS:HG2	2.42	0.40
1:K:384:ILE:HB	1:K:388:ASP:HB2	2.03	0.40
1:G:463:ILE:HD12	1:G:494:PHE:CE1	2.56	0.40
1:E:583:PHE:HZ	1:E:590:MET:HE3	1.86	0.40
2:L:445:LYS:HE3	2:L:503:ASP:OD1	2.22	0.40
2:H:329:PHE:CZ	2:H:343:GLY:HA3	2.55	0.40
2:F:476(C):ASP:N	2:F:476(D):PRO:HD3	2.35	0.40
1:K:319:GLN:NE2	1:K:345:PHE:CZ	2.89	0.40
2:D:298:ILE:CG2	2:D:509:ARG:HB2	2.51	0.40
2:B:114:ILE:O	2:B:115:ASN:HB2	2.21	0.40
1:K:713:SER:O	1:K:714:ALA:O	2.38	0.40
1:K:720:VAL:O	1:K:722:ASP:N	2.54	0.40
1:I:257:ARG:HB2	1:I:257:ARG:HE	1.58	0.40
2:B:196:ILE:HG22	2:B:221:SER:HB2	2.02	0.40
1:G:710:ILE:HG22	1:G:711:ASN:N	2.37	0.40
1:C:422:PRO:HA	1:C:422(A):PRO:HD3	1.85	0.40
1:G:650:MET:SD	2:H:263:ASN:HB2	2.62	0.40
2:F:78:SER:O	2:F:112:GLY:HA2	2.20	0.40
2:D:132:SER:HA	2:D:163:GLY:O	2.20	0.40
1:G:312:THR:O	1:G:315:ALA:HB3	2.22	0.40
1:A:490:ASP:OD2	1:A:630:ARG:NH1	2.55	0.40
1:K:77:ARG:NH1	1:K:77:ARG:O	2.53	0.40
1:G:619:ILE:HD11	1:G:626:ARG:HB2	2.03	0.40
1:E:110:VAL:HG21	1:E:130:ALA:CB	2.46	0.40
1:A:396:ILE:HG12	1:A:463:ILE:CD1	2.45	0.40
2:D:75:ASP:OD2	2:D:115:ASN:N	2.55	0.40
1:A:334:THR:HG21	1:A:355:GLN:CG	2.51	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:231:ILE:HG22	1:K:232:ALA:N	2.37	0.40
1:G:185:GLN:O	1:G:188:ASN:N	2.49	0.40
1:G:186:GLU:OE2	1:G:187:ALA:N	2.54	0.40
1:A:319:GLN:NE2	1:A:345:PHE:CE1	2.89	0.40
1:C:534:ARG:NH1	1:C:534:ARG:HG3	2.37	0.40
1:G:107:ASP:C	1:G:108:GLU:HG3	2.41	0.40
2:H:474:ARG:O	2:H:476:ASP:N	2.51	0.40
1:I:107:ASP:O	1:I:108:GLU:HG3	2.21	0.40
1:A:720:VAL:HG22	1:A:721:ASP:H	1.87	0.40
2:L:394:VAL:HG23	2:L:395:PRO:HD2	2.03	0.40
1:C:677:VAL:CG1	1:C:708:ALA:O	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	585/681 (86%)	451 (77%)	99 (17%)	35 (6%)	2	20
1	C	585/681 (86%)	456 (78%)	94 (16%)	35 (6%)	2	20
1	E	585/681 (86%)	449 (77%)	98 (17%)	38 (6%)	2	17
1	G	638/681 (94%)	502 (79%)	100 (16%)	36 (6%)	3	23
1	I	638/681 (94%)	504 (79%)	94 (15%)	40 (6%)	2	18
1	K	638/681 (94%)	505 (79%)	92 (14%)	41 (6%)	2	17
2	B	504/531 (95%)	444 (88%)	49 (10%)	11 (2%)	10	53
2	D	504/531 (95%)	445 (88%)	47 (9%)	12 (2%)	9	51
2	F	504/531 (95%)	451 (90%)	43 (8%)	10 (2%)	11	56
2	H	504/531 (95%)	451 (90%)	43 (8%)	10 (2%)	11	56
2	J	504/531 (95%)	452 (90%)	43 (8%)	9 (2%)	13	60
2	L	504/531 (95%)	455 (90%)	39 (8%)	10 (2%)	11	56
All	All	6693/7272 (92%)	5565 (83%)	841 (13%)	287 (4%)	4	30

All (287) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	ALA
1	A	137	GLN
1	A	138	ALA
1	A	277	ASP
1	A	331	SER
1	A	389	VAL
2	B	218	LYS
2	B	325	ASP
2	B	476(D)	PRO
1	C	64	ASN
1	C	100	ALA
1	C	137	GLN
1	C	138	ALA
1	C	265	THR
1	C	331	SER
1	C	389	VAL
2	D	218	LYS
2	D	325	ASP
2	D	476(D)	PRO
1	E	64	ASN
1	E	100	ALA
1	E	137	GLN
1	E	138	ALA
1	E	193	PRO
1	E	265	THR
1	E	277	ASP
1	E	331	SER
1	E	389	VAL
1	E	564	GLN
2	F	218	LYS
2	F	325	ASP
2	F	476(D)	PRO
1	G	100	ALA
1	G	137	GLN
1	G	138	ALA
1	G	331	SER
1	G	389	VAL
1	G	409	PHE
1	G	456	ALA
2	H	218	LYS
2	H	325	ASP
2	H	476(D)	PRO

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Mol	Chain	Res	Type
1	I	100	ALA
1	I	137	GLN
1	I	138	ALA
1	I	331	SER
1	I	389	VAL
2	J	218	LYS
2	J	325	ASP
2	J	476(D)	PRO
1	K	100	ALA
1	K	137	GLN
1	K	138	ALA
1	K	277	ASP
1	K	331	SER
1	K	389	VAL
1	K	456	ALA
1	K	564	GLN
2	L	218	LYS
2	L	325	ASP
2	L	476(D)	PRO
1	A	64	ASN
1	A	65	LYS
1	A	72	GLY
1	A	163	PHE
1	A	168	LYS
1	A	265	THR
1	A	326	ALA
1	A	379	GLY
1	A	393	GLY
1	A	596	TRP
2	B	476	ASP
1	C	65	LYS
1	C	162	ILE
1	C	163	PHE
1	C	185	GLN
1	C	277	ASP
1	C	324	ALA
1	C	326	ALA
1	C	379	GLY
1	C	393	GLY
1	C	457	PRO
1	C	564	GLN
1	C	721	ASP

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Mol	Chain	Res	Type
2	D	476	ASP
1	E	65	LYS
1	E	72	GLY
1	E	88	SER
1	E	163	PHE
1	E	168	LYS
1	E	324	ALA
1	E	326	ALA
1	E	379	GLY
1	E	393	GLY
1	E	457	PRO
2	F	476	ASP
1	G	64	ASN
1	G	65	LYS
1	G	163	PHE
1	G	168	LYS
1	G	230	ARG
1	G	265	THR
1	G	277	ASP
1	G	324	ALA
1	G	326	ALA
1	G	379	GLY
1	G	393	GLY
1	G	457	PRO
1	G	564	GLN
1	G	655	PRO
1	G	721	ASP
2	H	476	ASP
1	I	64	ASN
1	I	65	LYS
1	I	162	ILE
1	I	163	PHE
1	I	168	LYS
1	I	185	GLN
1	I	230	ARG
1	I	277	ASP
1	I	324	ALA
1	I	326	ALA
1	I	379	GLY
1	I	393	GLY
1	I	409	PHE
1	I	456	ALA

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Mol	Chain	Res	Type
1	I	457	PRO
1	I	564	GLN
1	I	721	ASP
2	J	476	ASP
1	K	64	ASN
1	K	65	LYS
1	K	163	PHE
1	K	168	LYS
1	K	185	GLN
1	K	230	ARG
1	K	324	ALA
1	K	326	ALA
1	K	379	GLY
1	K	409	PHE
1	K	457	PRO
1	K	596	TRP
1	K	721	ASP
2	L	476	ASP
1	A	112	ILE
1	A	185	GLN
1	A	324	ALA
1	A	457	PRO
1	A	721	ASP
2	B	78	SER
2	B	362	LEU
2	B	393	ASP
2	B	442	MET
1	C	72	GLY
1	C	88	SER
1	C	168	LYS
1	C	630	ARG
1	C	655	PRO
1	E	112	ILE
1	E	162	ILE
1	E	185	GLN
1	E	422(A)	PRO
1	E	519	GLU
1	E	596	TRP
1	E	633	ASP
1	E	655	PRO
1	E	721	ASP
2	F	338	LYS

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Mol	Chain	Res	Type
2	F	393	ASP
1	G	72	GLY
1	G	185	GLN
1	G	630	ARG
2	H	338	LYS
1	I	88	SER
1	I	265	THR
1	I	422(A)	PRO
1	I	655	PRO
2	J	338	LYS
2	J	362	LEU
2	J	393	ASP
1	K	88	SER
1	K	136	ALA
1	K	393	GLY
1	K	422(A)	PRO
1	K	655	PRO
1	K	714	ALA
2	L	393	ASP
2	L	466	LYS
1	A	136	ALA
1	A	193	PRO
1	A	633	ASP
1	C	86	GLY
1	C	94	SER
1	C	112	ILE
1	C	135	GLY
1	C	422(A)	PRO
1	C	456	ALA
1	C	596	TRP
1	C	633	ASP
2	D	78	SER
2	D	393	ASP
1	E	456	ALA
2	F	76	GLU
1	G	112	ILE
1	G	135	GLY
1	G	422(A)	PRO
2	H	393	ASP
2	H	442	MET
2	H	466	LYS
1	I	72	GLY

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Mol	Chain	Res	Type
1	I	97	ASP
1	I	112	ILE
1	I	596	TRP
1	I	609	GLY
1	K	112	ILE
1	K	162	ILE
1	K	200	GLU
1	K	246	LYS
1	K	265	THR
1	K	586	ASP
1	K	630	ARG
1	K	692	ALA
2	L	326	GLU
2	L	368	ILE
1	A	135	GLY
1	A	162	ILE
1	A	266	GLN
1	A	422(A)	PRO
1	A	456	ALA
1	A	630	ARG
1	A	655	PRO
1	A	714	ALA
2	B	77	GLY
2	B	338	LYS
1	C	609	GLY
2	D	76	GLU
1	E	135	GLY
1	E	136	ALA
1	E	190	SER
1	G	88	SER
1	G	136	ALA
1	G	162	ILE
1	G	422(B)	ALA
1	G	586	ASP
2	H	303	ASP
1	I	86	GLY
1	I	633	ASP
1	I	692	ALA
2	J	466	LYS
1	K	71	ARG
1	K	72	GLY
1	K	135	GLY

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Mol	Chain	Res	Type
1	A	123	VAL
1	C	71	ARG
2	F	368	ILE
1	G	94	SER
1	G	97	ASP
1	I	94	SER
1	I	135	GLY
1	I	422(B)	ALA
1	K	123	VAL
1	K	609	GLY
1	A	86	GLY
2	D	50	GLY
2	D	368	ILE
1	E	86	GLY
1	E	123	VAL
1	G	86	GLY
2	D	77	GLY
1	E	447	PRO
2	J	368	ILE
1	K	86	GLY
1	E	609	GLY
2	H	368	ILE
1	I	123	VAL
1	I	127	VAL
1	I	667	PRO
1	A	609	GLY
1	C	123	VAL
2	D	395	PRO
2	D	475	GLY
2	F	154	PRO
2	F	395	PRO
2	L	77	GLY
2	L	537	ILE
2	B	50	GLY
1	E	280	GLY

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	474/540 (88%)	417 (88%)	57 (12%)	7	32
1	C	474/540 (88%)	420 (89%)	54 (11%)	8	35
1	E	474/540 (88%)	418 (88%)	56 (12%)	8	33
1	G	520/540 (96%)	461 (89%)	59 (11%)	9	36
1	I	520/540 (96%)	461 (89%)	59 (11%)	9	36
1	K	520/540 (96%)	460 (88%)	60 (12%)	8	35
2	B	415/437 (95%)	392 (94%)	23 (6%)	30	75
2	D	415/437 (95%)	392 (94%)	23 (6%)	30	75
2	F	415/437 (95%)	394 (95%)	21 (5%)	33	77
2	H	415/437 (95%)	390 (94%)	25 (6%)	27	72
2	J	415/437 (95%)	385 (93%)	30 (7%)	21	63
2	L	415/437 (95%)	392 (94%)	23 (6%)	30	75
All	All	5472/5862 (93%)	4982 (91%)	490 (9%)	14	49

All (490) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	PHE
1	A	66	ILE
1	A	67	LEU
1	A	70	ASN
1	A	89	THR
1	A	97	ASP
1	A	99	GLN
1	A	163	PHE
1	A	168	LYS
1	A	182	LYS
1	A	186	GLU
1	A	265	THR
1	A	266	GLN
1	A	275	LEU
1	A	285	LEU
1	A	292	ILE
1	A	344	ASN
1	A	347	PHE
1	A	360	VAL
1	A	375	ARG
1	A	388	ASP
1	A	400	LEU

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Mol	Chain	Res	Type
1	A	416	ARG
1	A	419	ARG
1	A	421	ARG
1	A	436	TYR
1	A	443	MET
1	A	444	TYR
1	A	449	ILE
1	A	455	TRP
1	A	467	ARG
1	A	488	VAL
1	A	517	LEU
1	A	539	ARG
1	A	548	ASP
1	A	553	ARG
1	A	554	ARG
1	A	570	VAL
1	A	571	THR
1	A	577	ASP
1	A	582	SER
1	A	593	THR
1	A	625	PHE
1	A	630	ARG
1	A	634	LEU
1	A	643	GLN
1	A	652	GLU
1	A	653	LYS
1	A	661	MET
1	A	666	MET
1	A	674	ASP
1	A	677	VAL
1	A	683	GLU
1	A	700	ARG
1	A	702	GLU
1	A	711	ASN
1	A	718	LEU
2	B	42	ARG
2	B	43	ARG
2	B	52	GLN
2	B	91	THR
2	B	138	SER
2	B	147	MET
2	B	167	GLN

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Mol	Chain	Res	Type
2	B	224	PHE
2	B	238	GLN
2	B	273	ARG
2	B	288	VAL
2	B	301	SER
2	B	325	ASP
2	B	401	THR
2	B	408	VAL
2	B	448	ARG
2	B	462	VAL
2	B	476	ASP
2	B	476(D)	PRO
2	B	499	ARG
2	B	504	GLU
2	B	509	ARG
2	B	514	ARG
1	C	63	PHE
1	C	66	ILE
1	C	70	ASN
1	C	73	GLU
1	C	89	THR
1	C	97	ASP
1	C	99	GLN
1	C	163	PHE
1	C	168	LYS
1	C	182	LYS
1	C	186	GLU
1	C	275	LEU
1	C	276	CYS
1	C	285	LEU
1	C	292	ILE
1	C	344	ASN
1	C	347	PHE
1	C	360	VAL
1	C	375	ARG
1	C	400	LEU
1	C	416	ARG
1	C	419	ARG
1	C	421	ARG
1	C	436	TYR
1	C	444	TYR
1	C	455	TRP

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Mol	Chain	Res	Type
1	C	467	ARG
1	C	473	PHE
1	C	517	LEU
1	C	520	THR
1	C	539	ARG
1	C	548	ASP
1	C	553	ARG
1	C	554	ARG
1	C	570	VAL
1	C	571	THR
1	C	577	ASP
1	C	582	SER
1	C	593	THR
1	C	625	PHE
1	C	630	ARG
1	C	634	LEU
1	C	643	GLN
1	C	652	GLU
1	C	653	LYS
1	C	661	MET
1	C	666	MET
1	C	674	ASP
1	C	677	VAL
1	C	683	GLU
1	C	700	ARG
1	C	702	GLU
1	C	711	ASN
1	C	718	LEU
2	D	42	ARG
2	D	43	ARG
2	D	52	GLN
2	D	138	SER
2	D	147	MET
2	D	167	GLN
2	D	194	SER
2	D	224	PHE
2	D	273	ARG
2	D	288	VAL
2	D	301	SER
2	D	325	ASP
2	D	401	THR
2	D	408	VAL

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Mol	Chain	Res	Type
2	D	448	ARG
2	D	462	VAL
2	D	476	ASP
2	D	476(D)	PRO
2	D	488	GLU
2	D	493	PRO
2	D	504	GLU
2	D	509	ARG
2	D	514	ARG
1	E	63	PHE
1	E	66	ILE
1	E	70	ASN
1	E	89	THR
1	E	97	ASP
1	E	99	GLN
1	E	163	PHE
1	E	168	LYS
1	E	182	LYS
1	E	186	GLU
1	E	276	CYS
1	E	285	LEU
1	E	292	ILE
1	E	344	ASN
1	E	347	PHE
1	E	360	VAL
1	E	375	ARG
1	E	400	LEU
1	E	416	ARG
1	E	419	ARG
1	E	421	ARG
1	E	435	VAL
1	E	436	TYR
1	E	449	ILE
1	E	455	TRP
1	E	467	ARG
1	E	473	PHE
1	E	488	VAL
1	E	517	LEU
1	E	520	THR
1	E	539	ARG
1	E	548	ASP
1	E	553	ARG

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Mol	Chain	Res	Type
1	E	554	ARG
1	E	570	VAL
1	E	571	THR
1	E	577	ASP
1	E	582	SER
1	E	593	THR
1	E	598	PRO
1	E	625	PHE
1	E	629	THR
1	E	630	ARG
1	E	634	LEU
1	E	643	GLN
1	E	652	GLU
1	E	653	LYS
1	E	661	MET
1	E	666	MET
1	E	674	ASP
1	E	677	VAL
1	E	683	GLU
1	E	700	ARG
1	E	702	GLU
1	E	711	ASN
1	E	718	LEU
2	F	42	ARG
2	F	43	ARG
2	F	52	GLN
2	F	138	SER
2	F	147	MET
2	F	167	GLN
2	F	194	SER
2	F	238	GLN
2	F	273	ARG
2	F	288	VAL
2	F	301	SER
2	F	338	LYS
2	F	401	THR
2	F	408	VAL
2	F	448	ARG
2	F	462	VAL
2	F	476	ASP
2	F	476(D)	PRO
2	F	499	ARG

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Mol	Chain	Res	Type
2	F	509	ARG
2	F	514	ARG
1	G	63	PHE
1	G	66	ILE
1	G	70	ASN
1	G	73	GLU
1	G	89	THR
1	G	97	ASP
1	G	99	GLN
1	G	145	PHE
1	G	163	PHE
1	G	168	LYS
1	G	182	LYS
1	G	186	GLU
1	G	207	LYS
1	G	211	GLN
1	G	230	ARG
1	G	243	GLN
1	G	247	ASN
1	G	256	ASP
1	G	275	LEU
1	G	285	LEU
1	G	292	ILE
1	G	312	THR
1	G	347	PHE
1	G	360	VAL
1	G	375	ARG
1	G	400	LEU
1	G	416	ARG
1	G	419	ARG
1	G	421	ARG
1	G	436	TYR
1	G	455	TRP
1	G	467	ARG
1	G	473	PHE
1	G	488	VAL
1	G	517	LEU
1	G	539	ARG
1	G	542	ARG
1	G	548	ASP
1	G	553	ARG
1	G	554	ARG

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Mol	Chain	Res	Type
1	G	570	VAL
1	G	571	THR
1	G	582	SER
1	G	593	THR
1	G	625	PHE
1	G	629	THR
1	G	630	ARG
1	G	634	LEU
1	G	643	GLN
1	G	652	GLU
1	G	653	LYS
1	G	661	MET
1	G	666	MET
1	G	674	ASP
1	G	683	GLU
1	G	700	ARG
1	G	702	GLU
1	G	711	ASN
1	G	718	LEU
2	H	42	ARG
2	H	43	ARG
2	H	52	GLN
2	H	71	ASP
2	H	119	VAL
2	H	138	SER
2	H	147	MET
2	H	167	GLN
2	H	194	SER
2	H	238	GLN
2	H	273	ARG
2	H	288	VAL
2	H	301	SER
2	H	325	ASP
2	H	390	THR
2	H	401	THR
2	H	408	VAL
2	H	462	VAL
2	H	476	ASP
2	H	476(D)	PRO
2	H	499	ARG
2	H	504	GLU
2	H	509	ARG

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Mol	Chain	Res	Type
2	H	514	ARG
2	H	536	ASN
1	I	63	PHE
1	I	66	ILE
1	I	67	LEU
1	I	70	ASN
1	I	73	GLU
1	I	89	THR
1	I	97	ASP
1	I	99	GLN
1	I	163	PHE
1	I	168	LYS
1	I	182	LYS
1	I	186	GLU
1	I	207	LYS
1	I	230	ARG
1	I	243	GLN
1	I	247	ASN
1	I	256	ASP
1	I	257	ARG
1	I	285	LEU
1	I	292	ILE
1	I	312	THR
1	I	347	PHE
1	I	360	VAL
1	I	375	ARG
1	I	400	LEU
1	I	416	ARG
1	I	419	ARG
1	I	421	ARG
1	I	436	TYR
1	I	444	TYR
1	I	455	TRP
1	I	467	ARG
1	I	488	VAL
1	I	517	LEU
1	I	539	ARG
1	I	548	ASP
1	I	553	ARG
1	I	554	ARG
1	I	570	VAL
1	I	571	THR

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Mol	Chain	Res	Type
1	I	577	ASP
1	I	582	SER
1	I	593	THR
1	I	625	PHE
1	I	629	THR
1	I	630	ARG
1	I	634	LEU
1	I	643	GLN
1	I	652	GLU
1	I	653	LYS
1	I	661	MET
1	I	666	MET
1	I	674	ASP
1	I	677	VAL
1	I	683	GLU
1	I	700	ARG
1	I	702	GLU
1	I	711	ASN
1	I	718	LEU
2	J	42	ARG
2	J	43	ARG
2	J	52	GLN
2	J	71	ASP
2	J	91	THR
2	J	98	GLN
2	J	138	SER
2	J	147	MET
2	J	167	GLN
2	J	194	SER
2	J	273	ARG
2	J	288	VAL
2	J	301	SER
2	J	325	ASP
2	J	354	VAL
2	J	365	CYS
2	J	390	THR
2	J	401	THR
2	J	408	VAL
2	J	448	ARG
2	J	460	VAL
2	J	462	VAL
2	J	476	ASP

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Mol	Chain	Res	Type
2	J	476(D)	PRO
2	J	488	GLU
2	J	493	PRO
2	J	499	ARG
2	J	504	GLU
2	J	509	ARG
2	J	514	ARG
1	K	63	PHE
1	K	66	ILE
1	K	70	ASN
1	K	73	GLU
1	K	89	THR
1	K	97	ASP
1	K	99	GLN
1	K	163	PHE
1	K	168	LYS
1	K	182	LYS
1	K	186	GLU
1	K	211	GLN
1	K	230	ARG
1	K	243	GLN
1	K	247	ASN
1	K	257	ARG
1	K	276	CYS
1	K	285	LEU
1	K	292	ILE
1	K	312	THR
1	K	347	PHE
1	K	360	VAL
1	K	375	ARG
1	K	400	LEU
1	K	416	ARG
1	K	419	ARG
1	K	421	ARG
1	K	436	TYR
1	K	449	ILE
1	K	455	TRP
1	K	467	ARG
1	K	473	PHE
1	K	488	VAL
1	K	517	LEU
1	K	520	THR

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Mol	Chain	Res	Type
1	K	539	ARG
1	K	548	ASP
1	K	553	ARG
1	K	554	ARG
1	K	570	VAL
1	K	571	THR
1	K	577	ASP
1	K	582	SER
1	K	593	THR
1	K	625	PHE
1	K	629	THR
1	K	630	ARG
1	K	634	LEU
1	K	643	GLN
1	K	652	GLU
1	K	653	LYS
1	K	661	MET
1	K	666	MET
1	K	674	ASP
1	K	677	VAL
1	K	683	GLU
1	K	700	ARG
1	K	702	GLU
1	K	711	ASN
1	K	718	LEU
2	L	42	ARG
2	L	43	ARG
2	L	71	ASP
2	L	147	MET
2	L	167	GLN
2	L	194	SER
2	L	238	GLN
2	L	273	ARG
2	L	288	VAL
2	L	301	SER
2	L	365	CYS
2	L	390	THR
2	L	401	THR
2	L	408	VAL
2	L	448	ARG
2	L	462	VAL
2	L	476	ASP

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Mol	Chain	Res	Type
2	L	476(D)	PRO
2	L	488	GLU
2	L	499	ARG
2	L	504	GLU
2	L	509	ARG
2	L	514	ARG

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

Mol	Chain	Res	Type
1	A	70	ASN
1	A	102	HIS
1	A	119	GLN
1	A	188	ASN
1	A	480	HIS
1	A	550	ASN
1	A	551	HIS
1	A	564	GLN
2	B	52	GLN
2	B	58	GLN
2	B	88	HIS
2	B	100	GLN
2	B	124	GLN
2	B	137	HIS
2	B	151	ASN
2	B	167	GLN
2	B	183	ASN
2	B	309	ASN
2	B	482	HIS
2	B	492	ASN
2	B	536	ASN
1	C	70	ASN
1	C	102	HIS
1	C	119	GLN
1	C	137	GLN
1	C	188	ASN
1	C	351	ASN
1	C	480	HIS
1	C	551	HIS
1	C	564	GLN
1	C	716	ASN
2	D	52	GLN

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Mol	Chain	Res	Type
2	D	58	GLN
2	D	88	HIS
2	D	100	GLN
2	D	151	ASN
2	D	167	GLN
2	D	183	ASN
2	D	309	ASN
2	D	482	HIS
2	D	492	ASN
2	D	536	ASN
1	E	70	ASN
1	E	102	HIS
1	E	119	GLN
1	E	137	GLN
1	E	188	ASN
1	E	351	ASN
1	E	386	GLN
1	E	480	HIS
1	E	551	HIS
1	E	564	GLN
2	F	52	GLN
2	F	58	GLN
2	F	88	HIS
2	F	100	GLN
2	F	151	ASN
2	F	167	GLN
2	F	238	GLN
2	F	309	ASN
2	F	482	HIS
2	F	492	ASN
2	F	536	ASN
1	G	70	ASN
1	G	102	HIS
1	G	119	GLN
1	G	188	ASN
1	G	351	ASN
1	G	386	GLN
1	G	480	HIS
1	G	551	HIS
1	G	564	GLN
2	H	52	GLN
2	H	58	GLN

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Mol	Chain	Res	Type
2	H	88	HIS
2	H	100	GLN
2	H	151	ASN
2	H	167	GLN
2	H	183	ASN
2	H	238	GLN
2	H	309	ASN
2	H	446	HIS
2	H	482	HIS
2	H	492	ASN
2	H	536	ASN
1	I	70	ASN
1	I	102	HIS
1	I	119	GLN
1	I	188	ASN
1	I	386	GLN
1	I	480	HIS
1	I	551	HIS
1	I	564	GLN
1	I	716	ASN
2	J	58	GLN
2	J	88	HIS
2	J	100	GLN
2	J	151	ASN
2	J	167	GLN
2	J	183	ASN
2	J	309	ASN
2	J	482	HIS
2	J	492	ASN
2	J	528	GLN
2	J	536	ASN
1	K	70	ASN
1	K	102	HIS
1	K	119	GLN
1	K	137	GLN
1	K	188	ASN
1	K	342	GLN
1	K	386	GLN
1	K	480	HIS
1	K	551	HIS
1	K	564	GLN
2	L	58	GLN

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Mol	Chain	Res	Type
2	L	88	HIS
2	L	100	GLN
2	L	151	ASN
2	L	167	GLN
2	L	238	GLN
2	L	309	ASN
2	L	482	HIS
2	L	536	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BTI	A	801	1	16,16,16	1.62	1 (6%)	21,21,21	2.28	6 (28%)
3	BTI	C	801	1	16,16,16	1.61	1 (6%)	21,21,21	2.49	6 (28%)
3	BTI	E	801	1	16,16,16	1.67	1 (6%)	21,21,21	2.54	6 (28%)
3	BTI	G	801	1	16,16,16	1.76	1 (6%)	21,21,21	2.70	7 (33%)
3	BTI	I	801	1	16,16,16	1.67	1 (6%)	21,21,21	2.44	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BTI	K	801	1	16,16,16	1.67	1 (6%)	21,21,21	2.41	6 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BTI	A	801	1	-	0/6/27/27	0/0/2/2
3	BTI	C	801	1	-	0/6/27/27	0/0/2/2
3	BTI	E	801	1	-	0/6/27/27	0/0/2/2
3	BTI	G	801	1	-	0/6/27/27	0/0/2/2
3	BTI	I	801	1	-	0/6/27/27	0/0/2/2
3	BTI	K	801	1	-	0/6/27/27	0/0/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	801	BTI	O3-C3	6.06	1.37	1.23
3	I	801	BTI	O3-C3	5.82	1.36	1.23
3	E	801	BTI	O3-C3	5.81	1.36	1.23
3	K	801	BTI	O3-C3	5.76	1.36	1.23
3	C	801	BTI	O3-C3	5.68	1.36	1.23
3	A	801	BTI	O3-C3	5.64	1.36	1.23

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	801	BTI	N2-C3-N3	6.88	113.13	108.99
3	G	801	BTI	N2-C3-N3	6.80	113.08	108.99
3	E	801	BTI	N2-C3-N3	6.63	112.98	108.99
3	K	801	BTI	N2-C3-N3	6.36	112.82	108.99
3	I	801	BTI	N2-C3-N3	6.20	112.72	108.99
3	A	801	BTI	N2-C3-N3	6.00	112.60	108.99
3	G	801	BTI	C4-N2-C3	-5.92	107.49	112.54
3	E	801	BTI	C4-N2-C3	-5.76	107.62	112.54
3	C	801	BTI	C4-N2-C3	-5.72	107.66	112.54
3	I	801	BTI	C4-N2-C3	-5.40	107.93	112.54
3	K	801	BTI	C4-N2-C3	-5.39	107.94	112.54
3	G	801	BTI	C5-N3-C3	-4.95	106.64	112.35
3	A	801	BTI	C4-N2-C3	-4.48	108.72	112.54
3	I	801	BTI	C5-N3-C3	-4.08	107.64	112.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	801	BTI	C5-N3-C3	-3.73	108.06	112.35
3	E	801	BTI	C4-C2-S1	-3.72	100.63	105.29
3	C	801	BTI	C5-N3-C3	-3.50	108.31	112.35
3	A	801	BTI	C5-N3-C3	-3.44	108.39	112.35
3	I	801	BTI	C6-S1-C2	3.34	98.37	90.94
3	E	801	BTI	C5-N3-C3	-3.31	108.53	112.35
3	G	801	BTI	C6-S1-C2	3.22	98.09	90.94
3	A	801	BTI	C6-S1-C2	3.14	97.91	90.94
3	K	801	BTI	C6-S1-C2	3.00	97.60	90.94
3	G	801	BTI	C6-C5-N3	-2.82	107.34	112.56
3	C	801	BTI	C6-S1-C2	2.74	97.02	90.94
3	G	801	BTI	C4-C5-N3	-2.64	100.00	102.51
3	E	801	BTI	C6-C5-N3	-2.61	107.72	112.56
3	I	801	BTI	C4-C5-N3	-2.60	100.04	102.51
3	C	801	BTI	C6-C5-N3	-2.43	108.06	112.56
3	K	801	BTI	C6-C5-N3	-2.42	108.08	112.56
3	I	801	BTI	C6-C5-N3	-2.40	108.11	112.56
3	E	801	BTI	C6-S1-C2	2.36	96.19	90.94
3	A	801	BTI	C6-C5-N3	-2.30	108.29	112.56
3	A	801	BTI	C6-C5-C4	2.18	112.84	108.20
3	C	801	BTI	C4-C2-S1	-2.13	102.62	105.29
3	G	801	BTI	C4-C2-S1	-2.10	102.66	105.29
3	K	801	BTI	C4-C5-N3	-2.10	100.51	102.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	591/681 (86%)	-0.24	0 100 100	17, 65, 113, 128	0
1	C	591/681 (86%)	-0.21	0 100 100	17, 65, 113, 128	0
1	E	591/681 (86%)	-0.19	1 (0%) 93 66	17, 66, 113, 128	0
1	G	646/681 (94%)	-0.23	0 100 100	15, 67, 112, 128	0
1	I	646/681 (94%)	-0.18	0 100 100	16, 67, 112, 127	0
1	K	646/681 (94%)	-0.20	1 (0%) 93 66	16, 68, 112, 128	0
2	B	506/531 (95%)	-0.57	1 (0%) 93 66	10, 26, 57, 101	0
2	D	506/531 (95%)	-0.56	1 (0%) 93 66	11, 26, 58, 101	0
2	F	506/531 (95%)	-0.57	1 (0%) 93 66	12, 27, 58, 100	0
2	H	506/531 (95%)	-0.58	0 100 100	10, 26, 58, 101	0
2	J	506/531 (95%)	-0.57	0 100 100	11, 26, 58, 100	0
2	L	506/531 (95%)	-0.57	0 100 100	11, 26, 57, 100	0
All	All	6747/7272 (92%)	-0.37	5 (0%) 93 74	10, 43, 108, 128	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	476(A)	LEU	2.3
1	E	329	TYR	2.3
2	D	476(A)	LEU	2.3
2	F	476(A)	LEU	2.3
1	K	159	GLU	2.1

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	BTI	G	801	15/15	0.19	-	43,49,56,60	0
3	BTI	A	801	15/15	0.16	-	30,42,56,62	0
3	BTI	C	801	15/15	0.13	-	30,38,46,47	0
3	BTI	I	801	15/15	0.20	-	57,65,68,69	0
3	BTI	K	801	15/15	0.17	-	39,50,57,62	0
3	BTI	E	801	15/15	0.17	-	31,39,49,50	0

6.5 Other polymers

There are no such residues in this entry.