



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:17 AM GMT

PDB ID : 3HKZ  
Title : The X-ray crystal structure of RNA polymerase from Archaea  
Authors : Murakami, K.S.  
Deposited on : 2009-05-26  
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

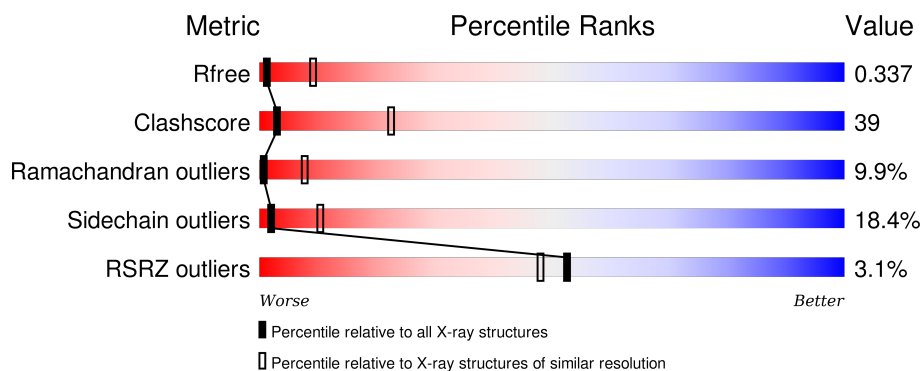
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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))
$R_{free}$	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	880	<div> <div>33%</div> <div>46%</div> <div>14%</div> <div>• 5%</div> </div>
1	I	880	<div> <div>32%</div> <div>48%</div> <div>14%</div> <div>• 5%</div> </div>
2	C	395	<div> <div>32%</div> <div>43%</div> <div>16%</div> <div>• 6%</div> </div>
2	M	395	<div> <div>27%</div> <div>44%</div> <div>19%</div> <div>• 6%</div> </div>
3	B	1124	<div> <div>32%</div> <div>48%</div> <div>15%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
3	J	1124	
4	D	265	
4	O	265	
5	E	180	
5	Q	180	
6	F	113	
6	R	113	
7	G	132	
7	S	132	
8	H	84	
8	T	84	
9	K	95	
9	U	95	
10	L	92	
10	V	92	
11	N	66	
11	W	66	
12	P	48	
12	X	48	
13	Y	104	
13	Z	104	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	ZN	B	2001	-	-	X	-
14	ZN	J	2001	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	F3S	O	1001	-	-	X	-

## 2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 53072 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	836	Total	C	N	O	S	0	0	0
			6673	4248	1178	1221	26			
1	I	836	Total	C	N	O	S	0	0	0
			6673	4248	1178	1221	26			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	370	Total	C	N	O	S	0	0	0
			2868	1818	490	551	9			
2	M	370	Total	C	N	O	S	0	0	0
			2868	1818	490	551	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	EXPRESSION TAG	UNP P58192
C	2	GLU	-	EXPRESSION TAG	UNP P58192
C	3	GLY	-	EXPRESSION TAG	UNP P58192
M	1	MET	-	EXPRESSION TAG	UNP P58192
M	2	GLU	-	EXPRESSION TAG	UNP P58192
M	3	GLY	-	EXPRESSION TAG	UNP P58192

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	1090	Total	C	N	O	S	0	0	0
			8645	5483	1529	1602	31			
3	J	1090	Total	C	N	O	S	0	0	0
			8645	5483	1529	1602	31			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	264	Total	C	N	O	S	0	0	0
			2114	1355	342	403	14			
4	O	264	Total	C	N	O	S	0	0	0
			2114	1355	342	403	14			

- Molecule 5 is a protein called DNA-directed RNA polymerase, subunit E' (RpoE1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	176	Total	C	N	O	S	0	0	0
			1402	903	236	259	4			
5	Q	176	Total	C	N	O	S	0	0	0
			1402	903	236	259	4			

- Molecule 6 is a protein called DNA-directed RNA polymerase, subunit F (RpoF).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	89	Total	C	N	O	S	0	0	0
			694	433	115	142	4			
6	R	89	Total	C	N	O	S	0	0	0
			694	433	115	142	4			

- Molecule 7 is a protein called DNA-directed RNA polymerase, subunit G (RpoG).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	113	Total	C	N	O	S	0	0	0
			884	556	149	174	5			
7	S	113	Total	C	N	O	S	0	0	0
			884	556	149	174	5			

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	74	Total	C	N	O		0	0	0
			611	397	109	105				
8	T	74	Total	C	N	O		0	0	0
			611	397	109	105				

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	82	Total	C	N	O	S	0	0	0
			658	420	121	116	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	U	82	Total	C	N	O	S	0	0	0
			658	420	121	116	1			

- Molecule 10 is a protein called DNA-directed RNA polymerase subunit L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	92	Total	C	N	O	S	0	0	0
			723	459	121	141	2			
10	V	92	Total	C	N	O	S	0	0	0
			723	459	121	141	2			

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	N	64	Total	C	N	O	S	0	0	0
			514	326	94	88	6			
11	W	64	Total	C	N	O	S	0	0	0
			514	326	94	88	6			

- Molecule 12 is a protein called DNA-directed RNA polymerase subunit P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	P	43	Total	C	N	O	S	0	0	0
			346	230	58	53	5			
12	X	43	Total	C	N	O	S	0	0	0
			346	230	58	53	5			

- Molecule 13 is a protein called DNA-directed RNA polymerase subunit 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	Y	45	Total	C	N	O	S	0	0	0
			391	245	68	77	1			
13	Z	45	Total	C	N	O	S	0	0	0
			391	245	68	77	1			

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	P	1	Total	Zn	0	0
			1	1		
14	J	1	Total	Zn	0	0
			1	1		

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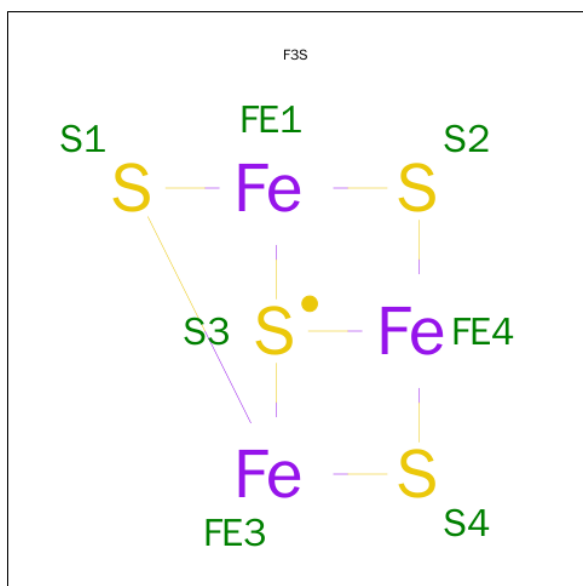
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	B	1	Total	Zn	0	0
			1	1		
14	I	2	Total	Zn	0	0
			2	2		
14	W	1	Total	Zn	0	0
			1	1		
14	A	2	Total	Zn	0	0
			2	2		
14	N	1	Total	Zn	0	0
			1	1		
14	X	1	Total	Zn	0	0
			1	1		

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	I	1	Total	Mg	0	0
			1	1		
15	A	1	Total	Mg	0	0
			1	1		

- Molecule 16 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe<sub>3</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	D	1	Total	Fe	S	0	0
			7	3	4		

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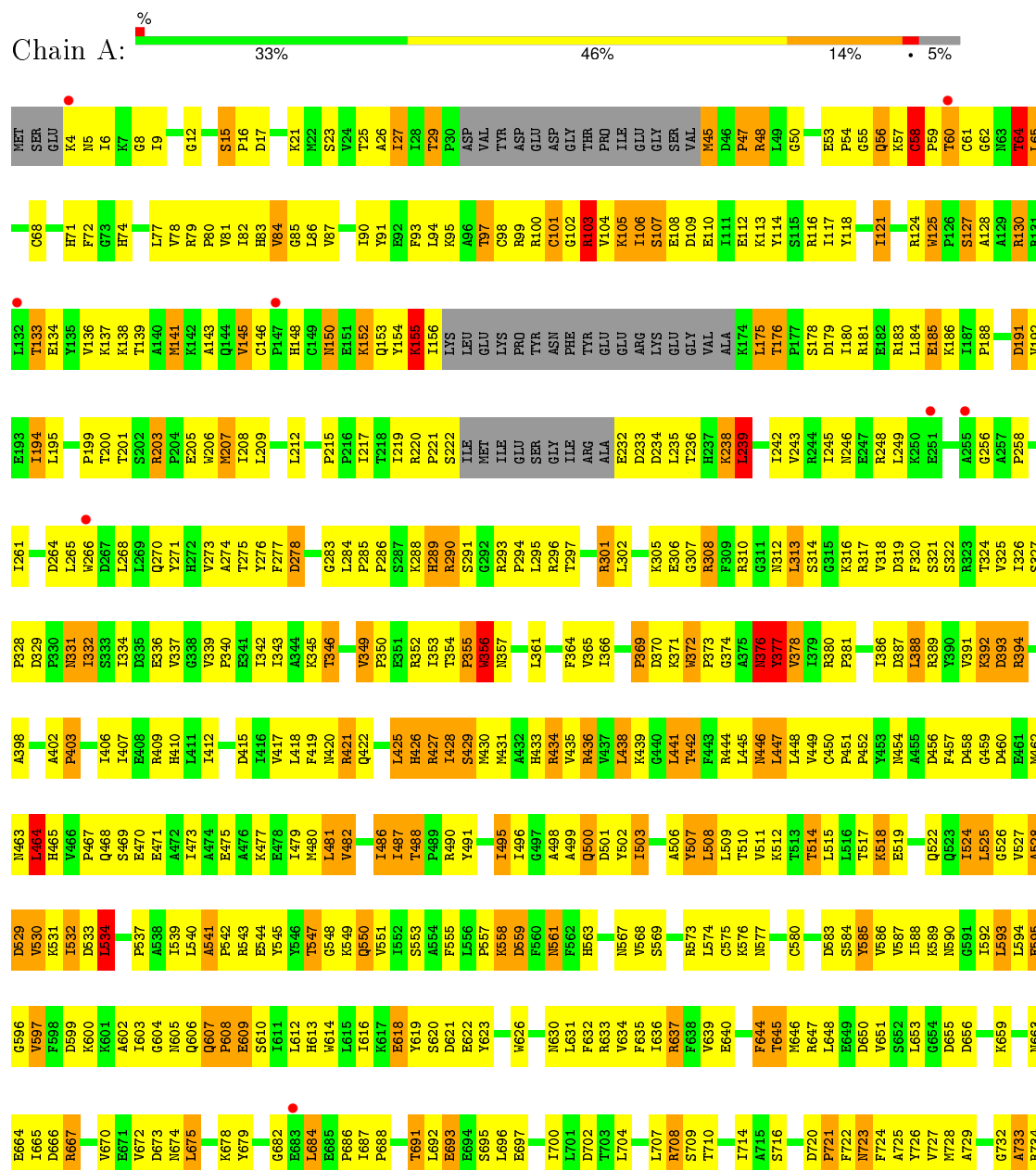
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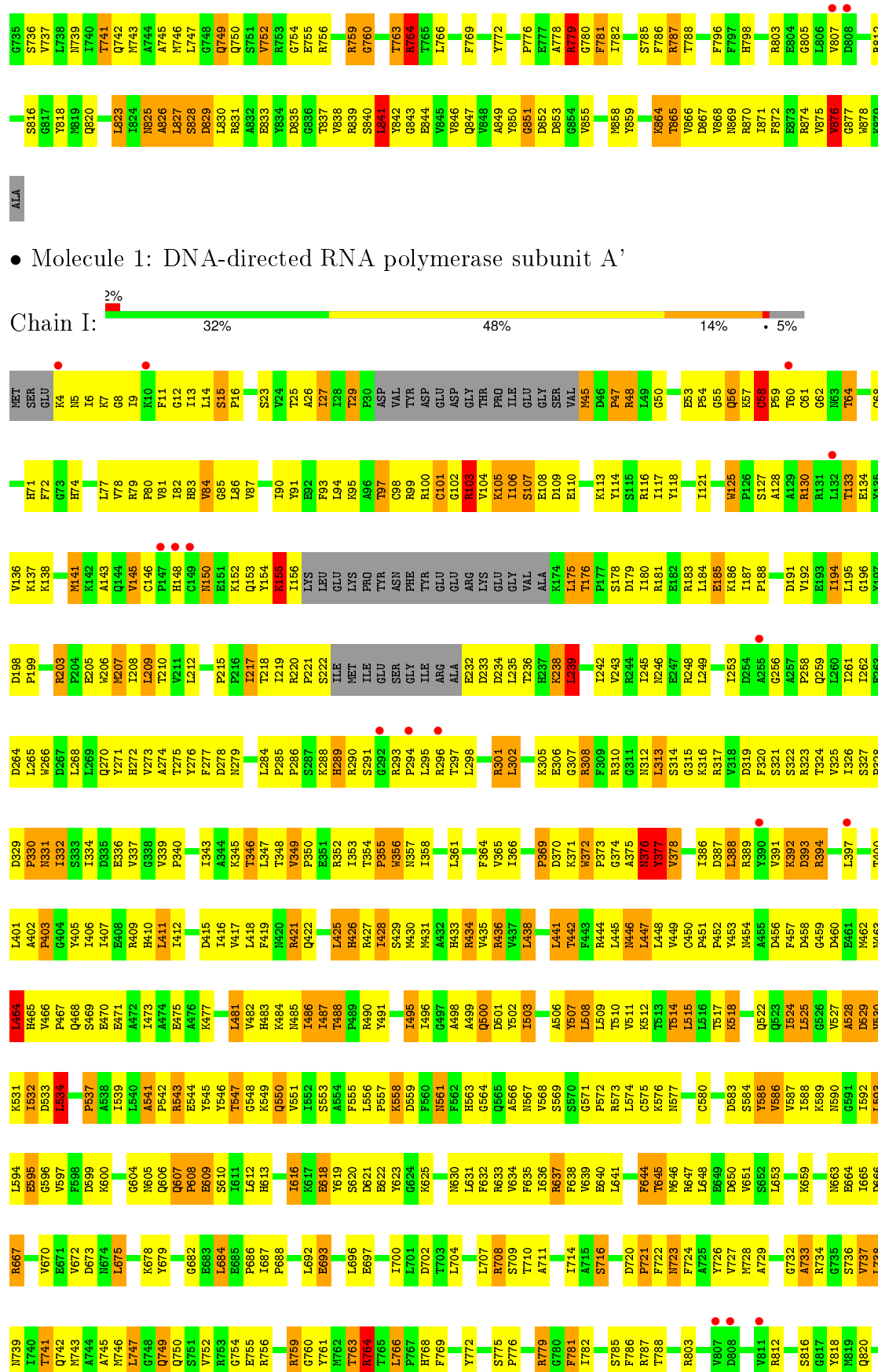
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
16	O	1	7	3	4	0	0

### 3 Residue-property plots

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

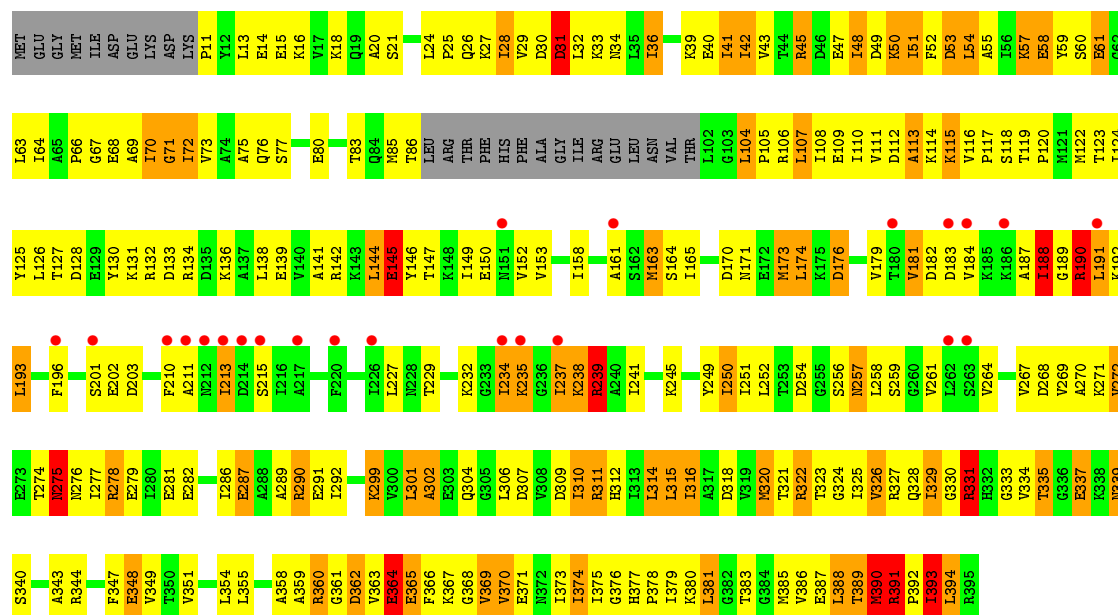
- Molecule 1: DNA-directed RNA polymerase subunit A'



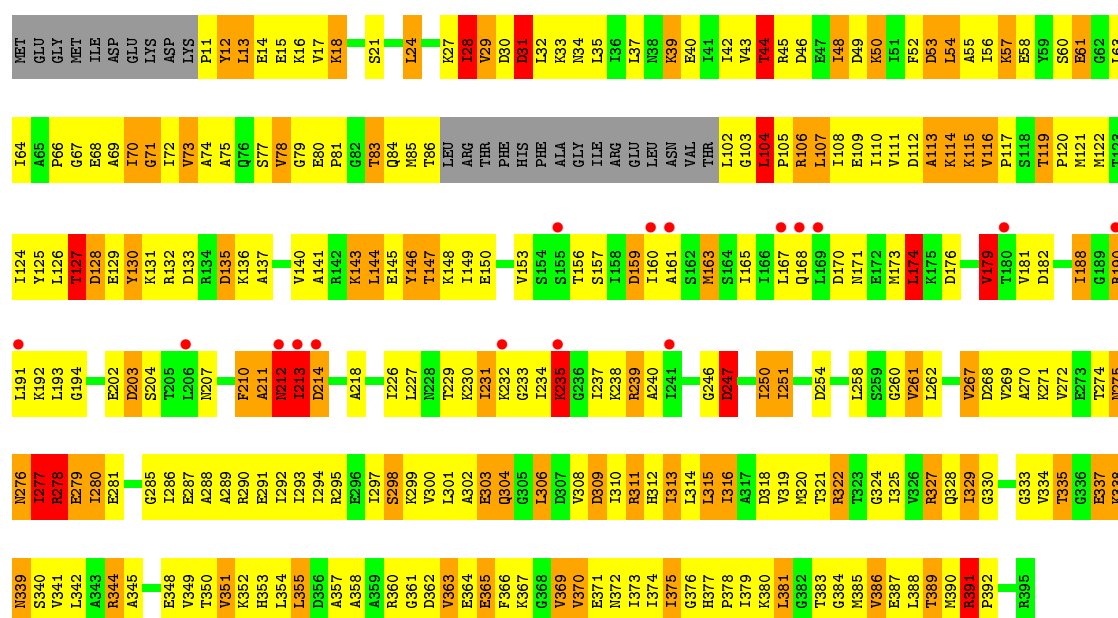




• Molecule 2: DNA-directed RNA polymerase subunit A"



• Molecule 2: DNA-directed RNA polymerase subunit A"



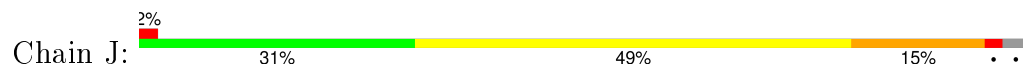
• Molecule 3: DNA-directed RNA polymerase subunit B



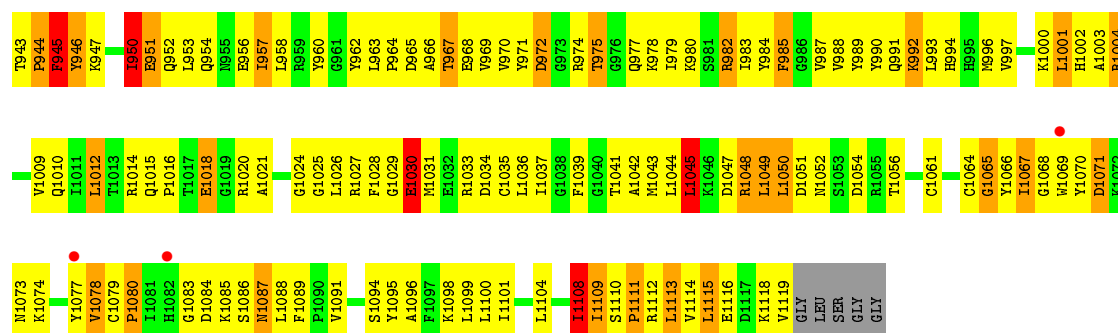


G1083	D1084	K1085	S1086	N1087	L1088	F1089	V1090	V1091	S1094	Y1095	A1096	F1097	K1098	L1099	L1100	L1101	Q1102	E1103	M1105	S1106	M1107	I1108	I1109	S1110	P1111	R1112	L1113	V1114	L1115	E1116	D1117	K1118	V1119	GLY	LEU	SER	GLY	GLY
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-----	-----	-----	-----	-----

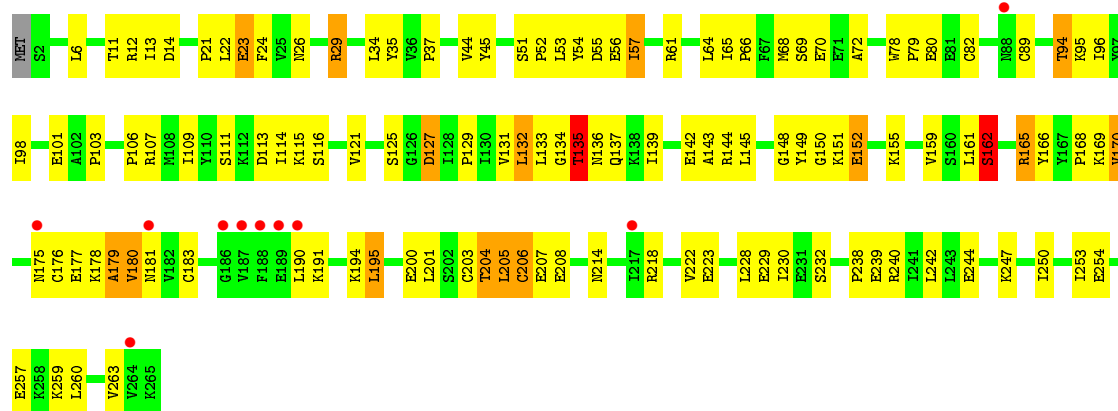
● Molecule 3: DNA-directed RNA polymerase subunit B



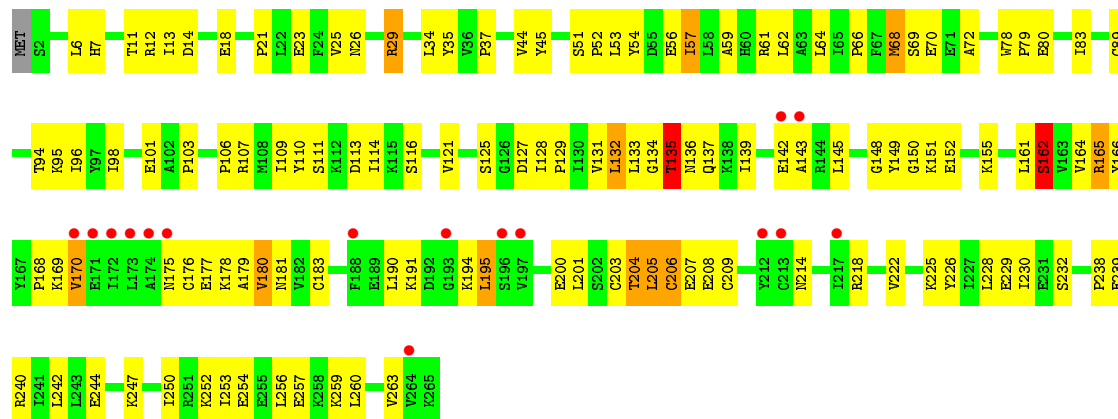
T873	G812	S744	G678	Y615	D551	R483	W419	A346	F271	V200	I130	R67
I874	R813	V745	L679	L616	E552	V484	L420	D348	S421	E203	S131	P68
G875	W814	E746	Y680	D617	V553	V486	V482	G349	S421	E203	Q132	R69
D876	S815	R747	N683	A618	N554	E486	M422	F350	H425	K306	T134	R71
F878	P817	W748	Y684	B520	G556	T488	R428	A351	L426	D207	L135	E72
R881	R818	W750	Q685	B521	H557	L489	R428	S352	L426	G208	D136	I7
	P819	E822	L686	B522	L558	Y490	R428	S352	L426	G208	K137	D8
G886	L819	S752	R687	N623	V559	V495	R428	L353	R428	F210	L138	E9
E887	GLN	T753	T688	A624	T600	V495	V429	V356	V429	F210	I139	R10
I888	GLU	T760	D689	V625	D561	P496	I430	K359	I430	F214	E140	R11
P889	P818	R756	T690	V626	F562	V497	S431	E360	A289	P215	I141	S81
	G889	L757	L757	W628	F562	V497	S431	A360	Q290	A216	I141	P82
M890	GLU	W758	E691	A627	L563	E498	S432	F361	Q291	A216	G142	R82
L891	LEU	S759	A692	L628	N564	E498	L433	R434	L433	P218	E143	R83
V895	SER	T760	P698	B629	E565	T501	A434	R435	L292	P218	E143	B84
	PRD	T761	Q699	P630	V566	T501	R435	R435	T293	P218	D147	A85
P898	GLU	E762	R700	L633	H567	ARG	Q437	T366	D294	I221	P148	F18
	GLN	E763	R701	L633	H567	ARG	Q437	T366	D294	I221	P148	R86
R899	A831	R764	F702	T634	N569	THR	Q437	Q368	Y296	P222	L87	S20
	T900	R832	R764	P635	C570	THR	Q437	Q368	Y296	P222	L87	R88
G902	R833	W766	W703	P635	D571	GLY	M439	K370	F297	F223	V154	K21
K903	D834	T766	W703	P635	D571	GLY	M439	K370	L298	I225	L90	G22
G903	T635	G767	G704	T638	S572	GLY	R443	S372	P299	M227	G156	T91
	G903	T635	G767	T638	S572	GLY	R443	S372	P299	M227	G156	T91
V904	S836	Q769	R706	H639	R574	ASP	D444	S372	B300	R228	E158	R25
D907	I837	Q769	R706	H639	R574	ASP	D444	S372	B300	R228	E158	R25
	W838	D771	Q769	H639	R574	ASP	D444	S372	B300	R228	E158	R25
I908	T839	K772	D709	N643	R576	ASN	H446	R378	A312	A229	R159	Q26
I909	R840	I773	W710	S644	R578	GLY	G447	R378	A312	A229	R159	Q26
L910	E843	W778	T711	P645	L579	TYR	Q449	R381	V313	L230	V160	H27
	N911	N911	T713	L647	L580	L515	Q449	R381	V313	L230	V160	H27
P912	R844	G779	T714	L648	L581	L515	Q449	R381	V313	L230	V160	H27
R913	G845	W780	W715	N649	V582	L515	Q449	R381	V313	L230	V160	H27
A914	L846	R781	W716	L650	N586	L521	F456	R386	L319	V239	A168	V103
L915	W847	G782	R716	L651	L587	L521	F456	R386	L319	V239	A168	V103
P916	D848	R783	G719	L652	L588	L522	E457	D388	S320	A241	P169	E104
S917	L849	G784	W720	S653	L589	L523	E457	D388	S320	A241	P169	E104
R918	R850	W785	W721	L654	L590	L524	T458	R389	V322	V242	R171	M106
M919	L851	G785	W722	L654	L591	G524	T458	R389	V322	V242	R171	M106
T920	T852	W788	W723	L655	L592	L526	G461	T391	E324	S243	W172	I107
L921	T853	R789	W724	L656	E593	L526	G461	T391	E324	S243	W172	I107
G922	E854	W790	W725	L657	D593	L527	M463	R393	L326	D245	V174	A109
Q923	T855	R790	W726	L658	L594	G528	S464	R394	L327	P246	D175	E110
R924	T856	L791	W727	E595	L595	G529	S464	R395	L327	P246	D175	E110
M925	R856	W792	W728	L660	K596	L529	G465	R395	L327	P246	D175	E110
G926	G858	D794	W729	N661	L597	Q531	L466	A399	R330	V248	T179	E112
R927	L859	W794	W730	D662	L598	Q531	L466	A399	R330	V248	T179	E112
I928	T860	G797	W731	S663	S599	G533	L466	A399	R330	V248	T179	E112
A929	L861	W798	W732	P664	G600	G534	L466	A399	R330	V248	T179	E112
G930	R862	S799	W733	L665	A601	E535	L466	A399	R330	V248	T179	E112
K931	T863	P800	W734	L666	T602	L536	L470	T400	R331	N250	V114	T51
Y932	W864	E801	W735	L667	T603	L536	L470	T400	R331	N250	V114	T51
A933	R865	R902	W736	L668	F604	A537	L470	T400	R331	N250	V114	T51
R934	T866	E803	W737	D669	D605	H538	L470	T400	R331	N250	V114	T51
L935	R867	W804	W738	L670	D606	K539	L470	T400	R331	N250	V114	T51
S936	D868	R739	W739	L671	L607	L540	L470	T400	R331	N250	V114	T51
W940	L869	G806	W740	L672	V608	R544	L470	T400	R331	N250	V114	T51
	D941	T870	W741	L673	L608	R544	L470	T400	R331	N250	V114	T51
R942	R871	L914	W742	L674	L609	R544	L470	T400	R331	N250	V114	T51
G946	T872	S743	W743	L675	L610	R544	L470	T400	R331	N250	V114	T51
	R947	W744	W744	L676	L611	R544	L470	T400	R331	N250	V114	T51
R948	L873	L914	W745	L677	L612	R544	L470	T400	R331	N250	V114	T51
	T874	S744	W746	L678	L613	R544	L470	T400	R331	N250	V114	T51
G949	R875	W747	W747	L679	L614	R544	L470	T400	R331	N250	V114	T51
	T876	S745	W748	L680	L615	R544	L470	T400	R331	N250	V114	T51
R950	L877	L915	W749	L681	L616	R544	L470	T400	R331	N250	V114	T51
	T878	S746	W749	L682	L617	R544	L470	T400	R331	N250	V114	T51
G951	R879	W750	W750	L683	L618	R544	L470	T400	R331	N250	V114	T51
	T879	S747	W751	L684	L619	R544	L470	T400	R331	N250	V114	T51
R952	L880	L916	W752	L685	L620	R544	L470	T400	R331	N250	V114	T51
	T880	S748	W753	L686	L621	R544	L470	T400	R331	N250	V114	T51
G953	R881	W754	W754	L687	L622	R544	L470	T400	R331	N250	V114	T51
	T881	S749	W755	L688	L623	R544	L470	T400	R331	N250	V114	T51
R954	L882	L917	W756	L689	L624	R544	L470	T400	R331	N250	V114	T51
	T882	S750	W757	L690	L625	R544	L470	T400	R331	N250	V114	T51
G955	R883	W758	W758	L691	L626	R544	L470	T400	R331	N250	V114	T51
	T883	S751	W759	L692	L627	R544	L470	T400	R331	N250	V114	T51
R956	L884	L918	W759	L693	L628	R544	L470	T400	R331	N250	V114	T51
	T884	S752	W760	L694	L629	R544	L470	T400	R331	N250	V114	T51
G957	R885	W761	W761	L695	L629	R544	L470	T400	R331	N250	V114	T51
	T885	S753	W762	L696	L630	R544	L470	T400	R331	N250	V114	T51
R958	L886	L919	W762	L697	L630	R544	L470	T400	R331	N250	V114	T51
	T886	S754	W763	L698	L631	R544	L470	T400	R331	N250	V114	T51
G959	R887	W764	W764	L699	L632	R544	L470	T400	R331	N250	V114	T51
	T887	S755	W765	L700	L633	R544	L470	T400	R331	N250	V114	T51
R960	L888	L920	W765	L701	L634	R544	L470	T400	R331	N250	V114	T51
	T888	S756	W766	L702	L635	R544	L470	T400	R331	N250	V114	T51
G961	R889	W767	W767	L703	L635	R544	L470	T400	R331	N250	V114	T51
	T889	S757	W768	L704	L636	R544	L470	T400	R331	N250	V114	T51
R962	L890	L921	W768	L705	L636	R544	L470	T400	R331	N250	V114	T51
	T890	S758	W769	L706	L637	R544	L470	T400	R331	N250	V114	T51
G963	R891	W769	W769	L707	L637	R544	L470	T400	R331	N250	V114	T51
	T891	S759	W770	L708	L638	R544	L470	T400	R331	N250	V114	T51
R964	L892	L922	W770	L709	L638	R544	L470	T400	R331	N250	V114	T51
	T892	S760	W771	L710	L639	R544	L470	T400	R331	N250	V114	T51
G965	R893	W771	W771	L711	L639	R544	L470	T400	R331	N250	V114	T51
	T893	S761	W772	L712	L640	R544	L470	T400	R331	N250	V114	T51
R966	L894	L923	W772	L713	L640	R544	L470	T400	R331	N250	V114	T51
	T894	S762	W773	L714	L641	R544	L470	T400	R331	N250	V114	T51
G967	R895	W773	W773	L715	L641	R544	L470	T400	R331	N250	V114	T51
	T895	S763	W774	L716	L642	R544	L470	T400	R331	N250	V114	T51
R968	L896	L924	W774	L717	L642	R544	L470	T400	R331	N250	V114	T51
	T896	S764	W775	L718	L643	R544	L470	T400	R331	N250	V114	T51
G969	R897	W775	W775	L719	L643	R544	L470	T400	R331	N250	V114	T51
	T897	S765	W776	L720	L644	R544	L470	T400	R331	N250	V114	T51
R970	L898	L925	W776	L721	L644	R544	L470	T400	R331	N250	V114	T51
	T898	S766	W777	L722	L645	R544	L470	T400	R331	N250	V114	T51
G971	R899	W777	W777	L723	L645	R544	L470	T400	R331	N250	V114	T51
	T899	S767	W778	L724	L646	R544	L470	T400	R331	N250	V114	T51
R972	L899	L926	W778	L725	L646	R544	L470	T400	R331	N250	V114	T51
	T899	S768	W779	L726	L647	R544	L470	T400	R331	N250	V114	T51
G973	R900	W779	W779	L727	L647	R544	L470	T400	R331	N250	V114	T51
	T900	S769	W780	L728	L648	R544	L470	T400	R331	N250	V114	T51
R974	L900	L927	W780	L729	L648	R544	L470	T400	R331	N250	V114	T51
	T901	S770	W781	L730	L649	R544	L470	T400	R331	N250	V114	T51
G975	R901	W781	W781	L731	L649	R544	L470	T400	R331	N250		



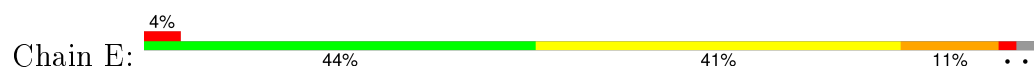
• Molecule 4: DNA-directed RNA polymerase subunit D

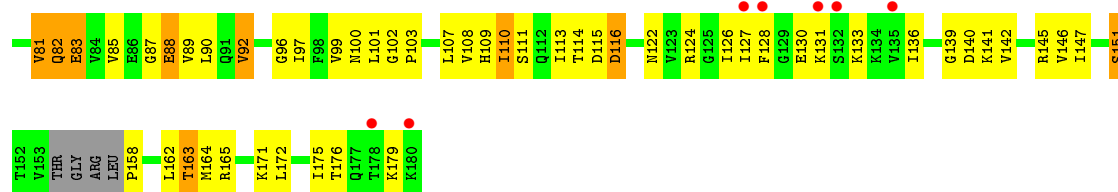


• Molecule 4: DNA-directed RNA polymerase subunit D

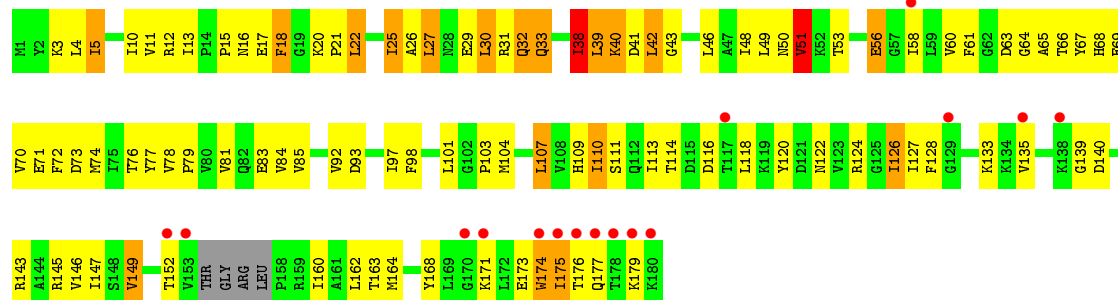


• Molecule 5: DNA-directed RNA polymerase, subunit E' (RpoE1)

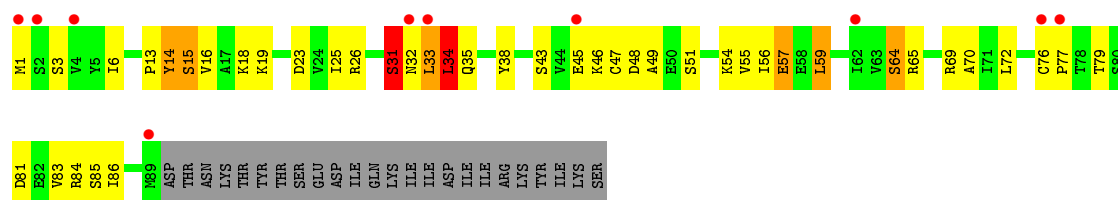
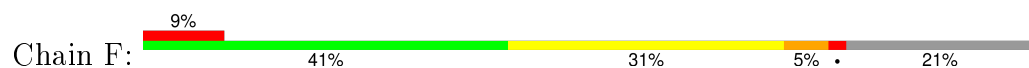




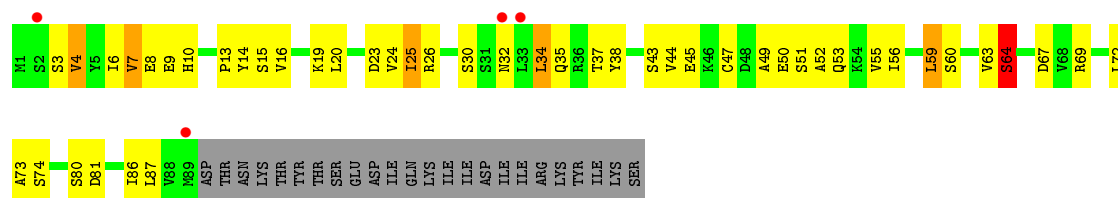
- Molecule 5: DNA-directed RNA polymerase, subunit E' (RpoE1)



- Molecule 6: DNA-directed RNA polymerase, subunit F (RpoF)



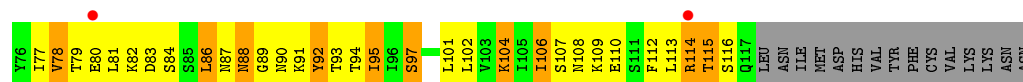
- Molecule 6: DNA-directed RNA polymerase, subunit F (RpoF)



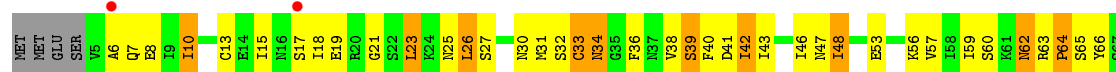
- Molecule 7: DNA-directed RNA polymerase, subunit G (RpoG)







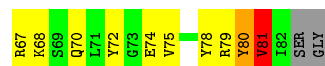
• Molecule 7: DNA-directed RNA polymerase, subunit G (RpoG)



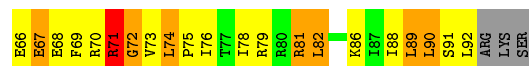
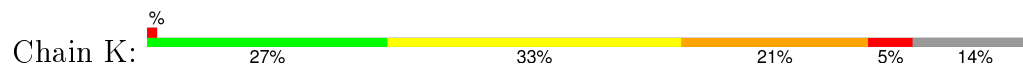
• Molecule 8: DNA-directed RNA polymerase subunit H



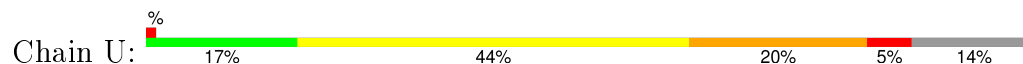
• Molecule 8: DNA-directed RNA polymerase subunit H

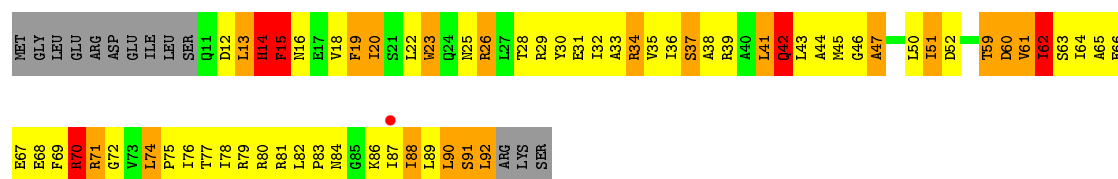


• Molecule 9: DNA-directed RNA polymerase subunit K

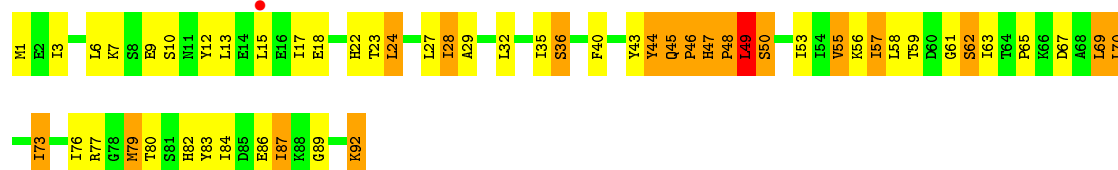


• Molecule 9: DNA-directed RNA polymerase subunit K

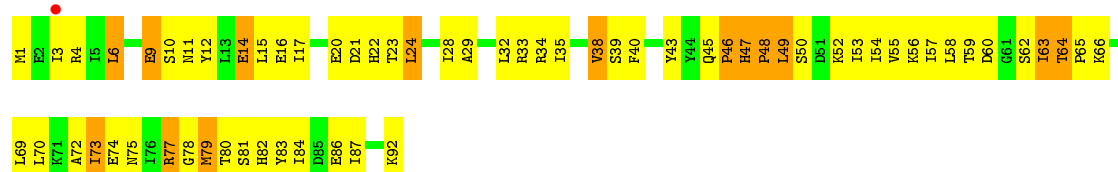




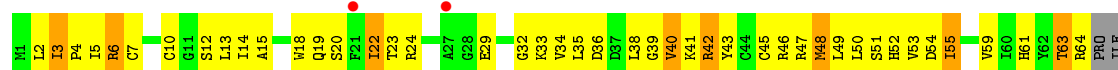
• Molecule 10: DNA-directed RNA polymerase subunit L



• Molecule 10: DNA-directed RNA polymerase subunit L



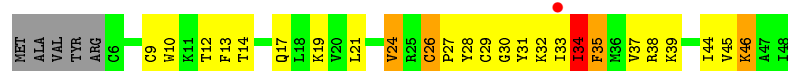
• Molecule 11: DNA-directed RNA polymerase subunit N



• Molecule 11: DNA-directed RNA polymerase subunit N



• Molecule 12: DNA-directed RNA polymerase subunit P

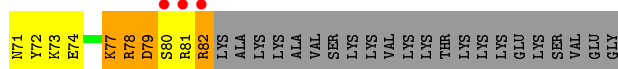
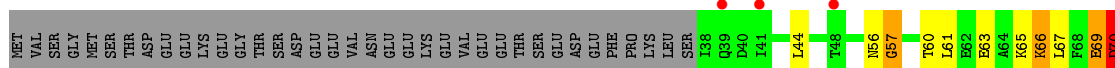
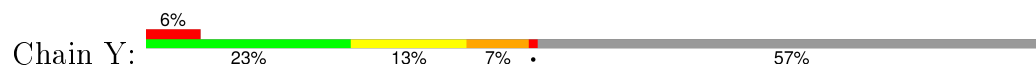


• Molecule 12: DNA-directed RNA polymerase subunit P

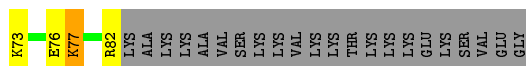
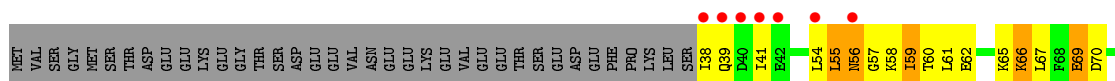
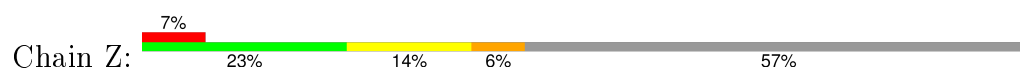




- Molecule 13: DNA-directed RNA polymerase subunit 13



- Molecule 13: DNA-directed RNA polymerase subunit 13



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.82Å 201.24Å 196.05Å 90.00° 100.92° 90.00°	Depositor
Resolution (Å)	40.00 – 3.40 39.79 – 3.40	Depositor EDS
% Data completeness (in resolution range)	80.3 (40.00-3.40) 80.3 (39.79-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.265 , 0.341 0.264 , 0.337	Depositor DCC
$R_{free}$ test set	5323 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	76.2	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 71.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 105618 reflections	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	53072	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, F3S, MG

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	0.60	0/6815	0.76	4/9219 (0.0%)
1	I	0.62	0/6815	0.77	5/9219 (0.1%)
2	C	0.64	0/2892	0.85	1/3891 (0.0%)
2	M	0.66	0/2892	0.84	2/3891 (0.1%)
3	B	0.60	0/8810	0.78	7/11921 (0.1%)
3	J	0.60	0/8810	0.79	6/11921 (0.1%)
4	D	0.49	0/2152	0.66	0/2911
4	O	0.52	0/2152	0.66	0/2911
5	E	0.53	0/1423	0.72	0/1919
5	Q	0.52	0/1423	0.72	0/1919
6	F	0.50	0/701	0.66	1/949 (0.1%)
6	R	0.52	0/701	0.70	0/949
7	G	0.63	0/895	0.78	0/1203
7	S	0.68	0/895	0.75	1/1203 (0.1%)
8	H	0.54	0/625	0.77	0/848
8	T	0.61	0/625	0.83	1/848 (0.1%)
9	K	0.61	0/667	0.87	0/903
9	U	0.70	0/667	0.95	1/903 (0.1%)
10	L	0.51	0/733	0.71	1/986 (0.1%)
10	V	0.57	0/733	0.74	0/986
11	N	0.51	0/523	0.74	0/705
11	W	0.52	0/523	0.74	0/705
12	P	0.63	0/354	0.73	0/475
12	X	0.65	0/354	0.70	0/475
13	Y	0.71	0/395	0.73	0/527
13	Z	0.67	0/395	0.75	0/527
All	All	0.60	0/53970	0.77	30/72914 (0.0%)

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

of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	M	0	1
3	B	0	1
3	J	0	1
7	G	0	1
9	K	0	1
9	U	0	1
All	All	0	6

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	464	LEU	CA-CB-CG	6.85	131.04	115.30
1	I	239	LEU	CA-CB-CG	6.55	130.36	115.30
8	T	42	LEU	CA-CB-CG	6.31	129.80	115.30
1	A	239	LEU	CA-CB-CG	6.30	129.79	115.30
1	I	464	LEU	CA-CB-CG	6.19	129.55	115.30
2	C	54	LEU	CA-CB-CG	6.15	129.45	115.30
3	B	1045	LEU	CA-CB-CG	6.04	129.20	115.30
3	J	23	LEU	CA-CB-CG	6.02	129.14	115.30
3	J	5	LEU	CA-CB-CG	5.89	128.85	115.30
3	B	571	ASP	N-CA-C	5.87	126.86	111.00
1	I	534	LEU	CA-CB-CG	5.86	128.77	115.30
3	B	5	LEU	CA-CB-CG	5.85	128.76	115.30
3	J	571	ASP	N-CA-C	5.84	126.77	111.00
3	J	1045	LEU	CA-CB-CG	5.82	128.68	115.30
1	I	827	LEU	CA-CB-CG	5.80	128.64	115.30
3	J	522	LEU	CA-CB-CG	5.72	128.45	115.30
3	B	522	LEU	CA-CB-CG	5.70	128.42	115.30
3	B	23	LEU	CA-CB-CG	5.59	128.15	115.30
1	A	534	LEU	CA-CB-CG	5.55	128.06	115.30
2	M	174	LEU	CA-CB-CG	5.51	127.98	115.30
3	B	436	GLY	N-CA-C	-5.43	99.52	113.10
1	A	827	LEU	CA-CB-CG	5.40	127.72	115.30
2	M	37	LEU	CA-CB-CG	5.28	127.44	115.30
10	L	49	LEU	CA-CB-CG	5.12	127.08	115.30
1	I	302	LEU	CA-CB-CG	5.10	127.03	115.30
9	U	60	ASP	N-CA-C	5.07	124.69	111.00
3	B	963	LEU	CA-CB-CG	-5.05	103.69	115.30
6	F	34	LEU	CA-CB-CG	5.05	126.91	115.30
7	S	26	LEU	CA-CB-CG	5.04	126.88	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	792	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	945	PHE	Peptide
7	G	40	PHE	Peptide
3	J	945	PHE	Peptide
9	K	26	ARG	Peptide
2	M	27	LYS	Peptide
9	U	59	THR	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6673	0	6763	612	0
1	I	6673	0	6763	619	0
2	C	2868	0	3035	277	0
2	M	2868	0	3035	331	0
3	B	8645	0	8780	817	0
3	J	8645	0	8780	862	0
4	D	2114	0	2146	120	0
4	O	2114	0	2146	122	0
5	E	1402	0	1467	80	0
5	Q	1402	0	1467	97	0
6	F	694	0	705	37	0
6	R	694	0	705	29	0
7	G	884	0	888	91	0
7	S	884	0	888	86	0
8	H	611	0	641	49	0
8	T	611	0	641	51	0
9	K	658	0	692	81	0
9	U	658	0	692	92	0
10	L	723	0	749	54	0
10	V	723	0	749	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	N	514	0	528	66	0
11	W	514	0	528	69	0
12	P	346	0	375	28	0
12	X	346	0	375	28	0
13	Y	391	0	389	27	0
13	Z	391	0	389	13	0
14	A	2	0	0	0	0
14	B	1	0	0	2	0
14	I	2	0	0	0	0
14	J	1	0	0	2	0
14	N	1	0	0	0	0
14	P	1	0	0	0	0
14	W	1	0	0	0	0
14	X	1	0	0	0	0
15	A	1	0	0	0	0
15	I	1	0	0	0	0
16	D	7	0	0	1	0
16	O	7	0	0	6	0
All	All	53072	0	54316	4172	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

All (4172) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:29:TYR:OH	13:Y:67:LEU:HD22	1.31	1.25
4:D:183:CYS:SG	16:D:1001:F3S:S2	2.42	1.17
6:R:72:LEU:HD21	6:R:86:ILE:HD12	1.30	1.14
5:Q:147:ILE:HD11	5:Q:163:THR:HB	1.21	1.14
4:D:250:ILE:HD11	10:L:84:ILE:HD11	1.31	1.13
3:B:581:ILE:HD11	3:B:614:GLU:HB2	1.16	1.13
3:B:353:LEU:HA	3:B:404:VAL:HG11	1.21	1.13
3:J:353:LEU:HA	3:J:404:VAL:HG11	1.18	1.12
2:M:389:THR:HG23	9:U:77:THR:HB	1.30	1.11
3:J:759:SER:HB2	3:J:862:VAL:O	1.51	1.11
1:A:760:GLY:HA3	3:B:447:GLY:HA3	1.24	1.10
3:B:88:ARG:HD3	3:B:853:THR:HG21	1.10	1.10
5:Q:53:THR:HB	5:Q:71:GLU:H	1.09	1.09
3:J:922:GLY:HA2	3:J:925:MET:HB2	1.26	1.09
3:J:581:ILE:HD11	3:J:614:GLU:CB	1.83	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:90:LEU:HD23	9:K:90:LEU:H	1.09	1.09
1:I:647:ARG:HH11	3:J:965:ASP:HB2	0.96	1.09
3:J:88:ARG:HD3	3:J:853:THR:HG21	1.09	1.08
2:C:340:SER:HB3	2:C:371:GLU:HG2	1.14	1.08
2:M:146:TYR:HD2	2:M:233:GLY:O	1.35	1.08
1:I:308:ARG:HH21	3:J:1099:LEU:HD13	1.16	1.08
1:A:647:ARG:HH11	3:B:965:ASP:HB2	0.99	1.08
5:E:36:GLU:HG2	6:F:34:LEU:HD11	1.37	1.07
3:J:26:GLN:O	3:J:345:LEU:HD23	1.55	1.06
5:E:39:LEU:HD11	6:F:1:MET:HA	1.35	1.06
2:C:55:ALA:HA	2:C:58:GLU:HG3	1.38	1.06
3:B:26:GLN:O	3:B:345:LEU:HD23	1.56	1.06
1:A:418:LEU:HD21	3:B:1044:LEU:HD21	1.35	1.06
1:I:68:CYS:SG	1:I:71:HIS:NE2	2.28	1.05
1:A:532:ILE:HD11	10:L:56:LYS:HD3	1.39	1.05
3:J:581:ILE:HD11	3:J:614:GLU:HB2	1.05	1.04
1:A:541:ALA:HB1	1:A:542:PRO:HD3	1.36	1.04
1:I:760:GLY:HA3	3:J:447:GLY:HA3	1.09	1.04
3:B:579:LEU:HD12	3:B:616:LEU:HD12	1.38	1.04
3:B:1033:ARG:NH1	3:B:1034:ASP:OD2	1.92	1.03
3:J:672:MET:HG2	3:J:993:LEU:HD21	1.37	1.03
2:M:28:ILE:HG21	9:U:14:HIS:CE1	1.93	1.02
2:C:55:ALA:HA	2:C:58:GLU:CG	1.89	1.02
4:O:175:ASN:HA	4:O:195:LEU:HD11	1.39	1.02
1:A:308:ARG:HH21	3:B:1099:LEU:HD13	1.14	1.02
3:B:922:GLY:HA2	3:B:925:MET:HB2	1.39	1.01
2:M:340:SER:CB	2:M:371:GLU:HG2	1.90	1.01
9:U:61:VAL:HG12	9:U:62:ILE:H	1.25	1.01
3:B:38:LYS:HG3	3:B:39:LEU:H	1.18	1.00
3:J:38:LYS:HG3	3:J:39:LEU:H	1.23	1.00
2:C:146:TYR:HB2	2:C:238:LYS:HD3	1.43	1.00
8:H:40:GLU:OE1	13:Y:66:LYS:HE2	1.61	1.00
3:J:1113:LEU:HD12	3:J:1113:LEU:H	1.24	1.00
3:J:702:LEU:HD22	3:J:933:ALA:HB1	1.39	1.00
3:J:569:ASN:HB3	3:J:574:ARG:HH22	1.22	1.00
5:Q:53:THR:O	5:Q:70:VAL:HG13	1.62	1.00
3:J:650:ILE:HD13	3:J:650:ILE:H	1.25	0.99
3:B:445:LEU:HD21	3:B:455:PRO:HA	1.45	0.99
7:S:63:ARG:HG3	7:S:114:ARG:HH22	1.25	0.99
1:I:647:ARG:NH1	3:J:965:ASP:HB2	1.76	0.98
1:A:877:GLY:C	3:J:377:ARG:HH12	1.65	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:458:THR:HG21	3:J:465:GLY:H	1.28	0.98
2:C:391:ARG:HH11	2:C:391:ARG:HG2	1.26	0.98
1:A:376:ASN:O	1:A:377:TYR:HB2	1.62	0.98
12:P:26:CYS:HB2	12:P:27:PRO:HD2	1.43	0.98
12:X:26:CYS:SG	12:X:29:CYS:HB2	2.02	0.98
1:A:558:LYS:HG3	3:J:104:GLU:HB2	1.42	0.98
2:C:109:GLU:O	2:C:113:ALA:HA	1.63	0.98
2:M:274:THR:HG22	2:M:275:ASN:H	1.27	0.97
12:P:46:LYS:HD2	12:P:46:LYS:H	1.29	0.97
1:A:647:ARG:NH1	3:B:965:ASP:HB2	1.78	0.97
2:M:340:SER:HB3	2:M:371:GLU:CG	1.94	0.97
1:I:331:ASN:O	1:I:332:ILE:HB	1.62	0.97
2:C:340:SER:HB3	2:C:371:GLU:CG	1.94	0.97
1:I:376:ASN:O	1:I:377:TYR:HB2	1.65	0.97
2:M:55:ALA:HA	2:M:58:GLU:HB2	1.47	0.97
2:M:340:SER:HB3	2:M:371:GLU:HG2	0.98	0.97
9:K:45:MET:CE	9:K:45:MET:HA	1.95	0.97
2:C:329:ILE:HA	2:C:334:VAL:HG12	1.46	0.97
2:C:276:ASN:HD22	2:C:279:GLU:HB2	1.29	0.97
4:D:175:ASN:HA	4:D:195:LEU:HD11	1.43	0.96
6:R:72:LEU:CD2	6:R:86:ILE:HD12	1.94	0.96
1:A:541:ALA:HB1	1:A:542:PRO:CD	1.94	0.96
1:I:541:ALA:HB1	1:I:542:PRO:HD3	1.44	0.96
2:C:126:LEU:HB2	2:C:131:LYS:HG3	1.46	0.96
3:B:581:ILE:HD11	3:B:614:GLU:CB	1.94	0.96
8:H:43:PRO:O	8:H:44:TRP:HB2	1.63	0.96
3:B:702:LEU:HD22	3:B:933:ALA:HB1	1.45	0.96
3:B:702:LEU:H	3:B:721:ASN:HD21	0.98	0.96
1:I:426:HIS:CE1	1:I:428:ILE:HG22	2.00	0.96
3:J:579:LEU:HD12	3:J:616:LEU:HD12	1.45	0.96
3:B:88:ARG:CD	3:B:853:THR:HG21	1.96	0.95
3:J:88:ARG:CD	3:J:853:THR:HG21	1.95	0.95
3:J:339:ALA:HB2	3:J:618:ALA:HB3	1.45	0.95
5:Q:27:LEU:HB2	5:Q:51:VAL:HG11	1.48	0.95
1:I:109:ASP:O	1:I:113:LYS:HG3	1.64	0.95
9:U:69:PHE:HA	9:U:74:LEU:HD11	1.47	0.95
3:J:450:TRP:HZ2	3:J:641:GLU:OE1	1.50	0.94
3:J:104:GLU:O	3:J:105:ASN:HB2	1.63	0.94
3:J:748:GLY:HA2	3:J:751:ARG:HD2	1.47	0.94
3:B:82:PRO:HG2	3:B:143:GLU:OE1	1.67	0.94
3:B:1113:LEU:HD12	3:B:1113:LEU:H	1.28	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:26:CYS:SG	12:P:29:CYS:HB2	2.07	0.94
3:J:1033:ARG:NH1	3:J:1034:ASP:OD2	2.00	0.94
3:B:855:THR:HB	3:B:857:GLU:HG2	1.47	0.94
4:O:98:ILE:HD11	4:O:114:ILE:HG13	1.50	0.94
3:B:650:ILE:H	3:B:650:ILE:HD13	1.32	0.94
1:A:830:LEU:HD23	1:A:840:SER:HB3	1.47	0.94
3:J:445:LEU:HD21	3:J:455:PRO:HA	1.49	0.94
2:C:237:ILE:HG13	2:C:238:LYS:N	1.82	0.93
2:C:40:GLU:O	2:C:45:ARG:HG2	1.68	0.93
3:J:88:ARG:HD3	3:J:853:THR:CG2	1.98	0.93
2:M:126:LEU:HB2	2:M:131:LYS:HG3	1.50	0.93
9:K:82:LEU:H	9:K:82:LEU:HD23	1.32	0.93
1:A:124:ARG:HH21	13:Y:81:ARG:HH12	1.17	0.93
2:M:70:ILE:CD1	2:M:70:ILE:H	1.82	0.93
3:J:764:LYS:HE2	3:J:813:LYS:HE2	1.51	0.93
3:J:702:LEU:H	3:J:721:ASN:HD21	0.94	0.93
1:A:317:ARG:HA	3:B:1027:ARG:HA	1.51	0.93
2:C:391:ARG:HH11	2:C:391:ARG:CG	1.82	0.92
12:X:46:LYS:H	12:X:46:LYS:HD2	1.32	0.92
3:J:855:THR:HB	3:J:857:GLU:HG2	1.51	0.92
3:J:881:ARG:HH11	3:J:989:TYR:HB3	1.34	0.92
1:A:595:GLU:HB2	7:G:91:LYS:HE2	1.52	0.92
1:I:760:GLY:HA3	3:J:447:GLY:CA	1.97	0.92
3:J:854:GLU:HA	3:J:859:ASN:O	1.69	0.91
3:B:88:ARG:HD3	3:B:853:THR:CG2	1.97	0.91
7:S:7:GLN:HG2	7:S:8:GLU:H	1.33	0.91
1:I:541:ALA:HB1	1:I:542:PRO:CD	1.98	0.91
9:K:50:LEU:HD23	9:K:74:LEU:HA	1.52	0.91
1:I:317:ARG:HA	3:J:1027:ARG:HA	1.51	0.91
3:B:672:MET:HG2	3:B:993:LEU:HD21	1.52	0.91
7:G:86:LEU:HD11	7:G:89:GLY:O	1.70	0.91
9:K:34:ARG:O	9:K:37:SER:HB2	1.71	0.91
1:A:365:VAL:HG23	1:A:388:LEU:HD11	1.51	0.91
2:C:340:SER:CB	2:C:371:GLU:HG2	2.01	0.90
1:A:541:ALA:HB2	7:G:72:CYS:H	1.36	0.90
1:A:308:ARG:NH2	3:B:1099:LEU:HD13	1.86	0.90
1:A:853:ASP:HB2	2:C:311:ARG:HH12	1.36	0.90
3:B:104:GLU:O	3:B:105:ASN:HB2	1.71	0.90
3:B:640:LEU:HD22	3:B:641:GLU:H	1.35	0.90
3:B:687:ARG:HG3	3:B:687:ARG:HH11	1.34	0.90
1:I:594:LEU:HA	7:S:86:LEU:HD22	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:830:LEU:HD23	1:I:840:SER:HB3	1.50	0.90
2:M:28:ILE:HG21	9:U:14:HIS:HE1	1.36	0.90
3:B:854:GLU:HA	3:B:859:ASN:O	1.72	0.90
1:A:590:ASN:ND2	3:J:377:ARG:HB2	1.87	0.89
4:D:96:ILE:HG22	4:D:116:SER:HA	1.54	0.89
9:K:45:MET:HA	9:K:45:MET:HE2	1.55	0.89
2:M:392:PRO:HB2	5:Q:22:LEU:HD11	1.51	0.89
3:J:418:ASN:HD21	3:J:421:SER:H	1.20	0.89
1:A:872:PHE:HA	1:A:876:VAL:HB	1.55	0.89
4:O:96:ILE:HG22	4:O:116:SER:HA	1.54	0.89
3:J:98:LEU:HD11	3:J:100:MET:HG3	1.54	0.89
1:I:647:ARG:HH11	3:J:965:ASP:CB	1.85	0.88
3:B:638:THR:HB	3:B:639:HIS:CD2	2.08	0.88
2:C:390:MET:O	2:C:391:ARG:HB3	1.72	0.88
3:B:569:ASN:HB3	3:B:574:ARG:HH22	1.39	0.88
4:D:98:ILE:HD11	4:D:114:ILE:HG13	1.55	0.88
12:X:26:CYS:HB2	12:X:27:PRO:HD2	1.54	0.88
3:B:339:ALA:HB2	3:B:618:ALA:HB3	1.54	0.88
1:A:109:ASP:O	1:A:113:LYS:HG3	1.74	0.88
3:B:640:LEU:CD2	3:B:641:GLU:H	1.86	0.88
3:B:418:ASN:ND2	3:B:421:SER:H	1.71	0.88
3:B:702:LEU:H	3:B:721:ASN:ND2	1.72	0.87
3:J:418:ASN:ND2	3:J:421:SER:H	1.72	0.87
4:D:111:SER:HA	4:D:114:ILE:HD13	1.54	0.87
3:J:82:PRO:HG2	3:J:143:GLU:OE1	1.74	0.87
1:A:541:ALA:CB	1:A:542:PRO:CD	2.52	0.87
3:J:638:THR:HB	3:J:639:HIS:CD2	2.10	0.87
3:B:242:VAL:HA	3:B:316:ALA:HB1	1.55	0.87
1:A:512:LYS:HE2	7:G:91:LYS:HE3	1.56	0.87
3:B:759:SER:HB2	3:B:862:VAL:O	1.74	0.87
3:B:910:LEU:HD22	3:B:911:ASN:N	1.89	0.87
3:J:560:THR:HG22	3:J:562:PHE:H	1.38	0.87
3:J:1064:CYS:SG	14:J:2001:ZN:ZN	1.62	0.87
3:J:242:VAL:HA	3:J:316:ALA:HB1	1.57	0.87
5:Q:53:THR:HB	5:Q:71:GLU:N	1.88	0.87
1:I:823:LEU:HD13	2:M:75:ALA:HB1	1.56	0.87
2:C:241:ILE:O	2:C:251:ILE:HG13	1.73	0.87
1:A:369:PRO:HB3	1:A:376:ASN:HB3	1.56	0.87
1:I:632:PHE:HA	1:I:635:PHE:CD1	2.10	0.87
3:J:314:TYR:HE2	3:J:526:LEU:H	1.23	0.87
3:B:579:LEU:HD12	3:B:616:LEU:CD1	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:209:CYS:HG	16:O:1001:F3S:FE1	0.56	0.86
1:A:589:LYS:O	1:A:592:ILE:HG12	1.73	0.86
3:B:560:THR:HG22	3:B:562:PHE:H	1.40	0.86
4:D:250:ILE:HD11	10:L:84:ILE:CD1	2.03	0.86
3:B:595:GLU:HA	3:B:599:SER:HB3	1.56	0.86
9:K:90:LEU:N	9:K:90:LEU:HD23	1.90	0.86
3:B:314:TYR:HE2	3:B:526:LEU:H	1.21	0.86
1:I:308:ARG:NH2	3:J:1099:LEU:HD13	1.91	0.86
2:M:289:ALA:O	2:M:292:ILE:HG22	1.74	0.86
3:B:47:GLY:HA2	3:B:58:VAL:O	1.76	0.86
3:J:650:ILE:CD1	3:J:650:ILE:H	1.89	0.86
3:J:902:LYS:HB3	11:W:42:ARG:HD3	1.55	0.86
3:B:98:LEU:HD11	3:B:100:MET:HG3	1.56	0.86
3:J:851:LEU:HA	12:X:35:PHE:HB3	1.58	0.86
3:J:662:GLN:HG2	3:J:664:PRO:HD2	1.58	0.85
1:I:875:VAL:O	1:I:877:GLY:N	2.08	0.85
1:A:841:LEU:O	1:A:843:GLY:N	2.10	0.85
8:T:42:LEU:HB2	8:T:43:PRO:HD2	1.55	0.85
3:B:418:ASN:HD21	3:B:421:SER:H	1.16	0.85
1:I:365:VAL:HG23	1:I:388:LEU:HD11	1.58	0.85
3:B:183:ILE:HD13	3:B:183:ILE:O	1.76	0.85
3:J:47:GLY:HA2	3:J:58:VAL:O	1.76	0.85
4:O:111:SER:HA	4:O:114:ILE:HD13	1.55	0.85
3:J:640:LEU:HD22	3:J:641:GLU:H	1.42	0.85
1:I:589:LYS:O	1:I:592:ILE:HG12	1.77	0.85
3:J:687:ARG:HH11	3:J:687:ARG:HG3	1.40	0.85
3:J:529:TYR:O	3:J:530:TYR:HB3	1.76	0.85
3:J:702:LEU:H	3:J:721:ASN:ND2	1.73	0.85
3:B:451:GLY:HA3	3:B:577:ARG:HH11	1.42	0.85
3:B:748:GLY:HA2	3:B:751:ARG:HD2	1.58	0.85
2:C:340:SER:HA	2:C:364:GLU:HG2	1.59	0.85
1:I:672:VAL:HG13	1:I:700:ILE:HD12	1.58	0.85
3:B:662:GLN:HG2	3:B:664:PRO:HD2	1.57	0.85
3:J:958:LEU:HD12	3:J:964:PRO:HG3	1.59	0.84
2:M:391:ARG:HH22	9:U:39:ARG:HH11	1.20	0.84
3:B:427:ARG:HH11	3:B:650:ILE:HD12	1.42	0.84
1:A:426:HIS:CE1	1:A:428:ILE:HG22	2.11	0.84
3:B:497:VAL:HG23	3:B:528:GLY:HA2	1.60	0.84
1:A:331:ASN:O	1:A:332:ILE:HB	1.76	0.84
3:B:557:HIS:N	3:B:623:ASN:HD21	1.75	0.84
3:J:595:GLU:HA	3:J:599:SER:HB3	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:72:CYS:SG	7:G:114:ARG:HD3	2.17	0.84
3:J:702:LEU:N	3:J:721:ASN:HD21	1.74	0.84
1:A:875:VAL:O	1:A:877:GLY:N	2.10	0.84
5:E:50:ASN:HB2	5:E:73:ASP:OD2	1.76	0.84
1:I:426:HIS:CD2	1:I:490:ARG:HH12	1.96	0.84
2:C:388:LEU:HD11	9:K:34:ARG:HG3	1.59	0.84
1:I:667:ARG:O	1:I:670:VAL:HG22	1.77	0.84
1:I:547:THR:O	1:I:550:GLN:HB3	1.78	0.84
3:B:764:LYS:HE2	3:B:813:LYS:HE2	1.60	0.84
2:M:72:ILE:N	2:M:72:ILE:HD12	1.91	0.84
13:Z:57:GLY:HA2	13:Z:61:LEU:HG	1.59	0.84
3:J:702:LEU:CD2	3:J:933:ALA:HB1	2.07	0.83
1:I:418:LEU:HD21	3:J:1044:LEU:HD21	1.60	0.83
1:I:412:ILE:O	1:I:415:ASP:HB2	1.78	0.83
1:I:369:PRO:HB3	1:I:376:ASN:HB3	1.60	0.83
1:A:672:VAL:HG13	1:A:700:ILE:HD12	1.57	0.83
1:A:647:ARG:HH11	3:B:965:ASP:CB	1.89	0.83
4:O:13:ILE:HD11	4:O:238:PRO:HB2	1.61	0.83
2:M:146:TYR:CD2	2:M:233:GLY:O	2.26	0.83
3:B:958:LEU:HD12	3:B:964:PRO:HG3	1.59	0.83
3:B:253:PHE:H	3:B:254:PRO:HD2	1.42	0.83
3:J:90:LEU:HD11	3:J:856:ALA:H	1.43	0.83
3:J:451:GLY:HA3	3:J:577:ARG:HH11	1.41	0.83
1:I:220:ARG:NH1	1:I:236:THR:HG23	1.93	0.83
4:O:209:CYS:SG	16:O:1001:F3S:FE1	1.69	0.83
3:B:557:HIS:H	3:B:623:ASN:HD21	1.27	0.83
3:J:544:ARG:HH11	3:J:544:ARG:HG3	1.42	0.83
1:I:541:ALA:CB	1:I:542:PRO:CD	2.57	0.83
1:A:324:THR:HG22	1:A:325:VAL:H	1.43	0.83
3:B:870:ARG:NH1	3:B:996:MET:HB2	1.93	0.82
1:I:872:PHE:HA	1:I:876:VAL:HB	1.61	0.82
5:E:53:THR:HG23	5:E:55:GLU:HG3	1.60	0.82
4:O:13:ILE:CD1	4:O:238:PRO:HB2	2.10	0.82
3:B:881:ARG:HH11	3:B:989:TYR:HB3	1.45	0.82
3:B:851:LEU:HA	12:P:35:PHE:HB3	1.59	0.82
3:B:458:THR:HG21	3:B:465:GLY:H	1.44	0.82
3:B:450:TRP:HZ2	3:B:641:GLU:OE1	1.60	0.82
3:B:702:LEU:N	3:B:721:ASN:HD21	1.77	0.82
3:B:138:LEU:HA	3:B:141:ILE:HD12	1.59	0.82
3:J:890:MET:HE2	3:J:891:LEU:H	1.44	0.82
1:A:733:ALA:HB1	3:B:913:HIS:CE1	2.15	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:390:MET:HG3	5:Q:56:GLU:HG2	1.60	0.82
3:J:738:ILE:HD11	3:J:908:ILE:HG23	1.62	0.82
5:E:15:PRO:HG2	9:K:45:MET:HB3	1.60	0.81
3:B:529:TYR:O	3:B:530:TYR:HB3	1.79	0.81
9:K:71:ARG:O	9:K:73:VAL:HG13	1.80	0.81
1:I:90:ILE:HD11	1:I:207:MET:HB2	1.61	0.81
3:B:203:GLU:HA	3:B:203:GLU:OE1	1.76	0.81
1:A:412:ILE:O	1:A:415:ASP:HB2	1.80	0.81
3:J:800:PRO:O	3:J:802:VAL:N	2.14	0.81
9:K:28:THR:OG1	9:K:31:GLU:HG3	1.79	0.81
5:Q:97:ILE:HD12	5:Q:113:ILE:HD11	1.62	0.81
1:A:760:GLY:HA3	3:B:447:GLY:CA	2.10	0.81
5:E:36:GLU:HG2	6:F:34:LEU:CD1	2.10	0.81
1:A:491:TYR:HB2	1:A:607:GLN:OE1	1.81	0.81
1:A:220:ARG:NH1	1:A:236:THR:HG23	1.94	0.81
2:C:55:ALA:HA	2:C:58:GLU:CB	2.09	0.81
3:J:579:LEU:HD12	3:J:616:LEU:CD1	2.10	0.81
2:M:170:ASP:O	2:M:174:LEU:HD11	1.81	0.81
3:J:569:ASN:HB3	3:J:574:ARG:NH2	1.95	0.81
3:J:935:LEU:HD12	3:J:957:ILE:HG22	1.63	0.81
2:M:329:ILE:HA	2:M:334:VAL:HG12	1.60	0.81
5:Q:15:PRO:HG2	9:U:45:MET:HB3	1.63	0.81
5:E:39:LEU:HD13	5:E:42:LEU:H	1.46	0.81
3:J:138:LEU:HA	3:J:141:ILE:HD12	1.62	0.81
2:C:179:VAL:HG21	2:C:232:LYS:HZ2	1.44	0.81
2:M:48:ILE:HG12	2:M:50:LYS:HE3	1.63	0.81
6:F:35:GLN:HA	6:F:38:TYR:CD1	2.16	0.80
3:J:771:ASP:HB2	3:J:816:PRO:HD3	1.63	0.80
4:D:13:ILE:HD11	4:D:238:PRO:HB2	1.64	0.80
3:J:458:THR:CG2	3:J:465:GLY:H	1.95	0.80
3:J:253:PHE:H	3:J:254:PRO:HD2	1.47	0.80
1:I:79:ARG:HB2	1:I:266:TRP:CE3	2.17	0.80
1:I:336:GLU:HA	1:I:434:ARG:O	1.82	0.80
2:M:114:LYS:O	2:M:116:VAL:N	2.13	0.80
3:J:910:LEU:HD22	3:J:911:ASN:N	1.97	0.80
3:B:687:ARG:CG	3:B:687:ARG:HH11	1.94	0.80
1:I:853:ASP:OD2	1:I:864:LYS:HB3	1.82	0.80
3:J:813:LYS:H	3:J:836:SER:HB3	1.45	0.80
1:A:647:ARG:HH21	3:B:982:ARG:HH12	1.26	0.80
2:C:55:ALA:HA	2:C:58:GLU:HB2	1.64	0.80
3:B:90:LEU:HD11	3:B:856:ALA:H	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:29:ARG:HG3	4:D:162:SER:HB3	1.63	0.80
4:O:259:LYS:O	4:O:263:VAL:HG23	1.82	0.80
5:E:89:VAL:HG11	5:E:92:VAL:HG22	1.64	0.79
8:H:29:TYR:HA	8:H:32:LEU:HD12	1.61	0.79
1:A:549:LYS:HE2	7:G:89:GLY:HA2	1.64	0.79
1:I:331:ASN:O	1:I:332:ILE:CB	2.30	0.79
3:J:450:TRP:CZ2	3:J:641:GLU:OE1	2.36	0.79
1:A:733:ALA:HB1	3:B:913:HIS:HE1	1.47	0.79
1:A:547:THR:O	1:A:550:GLN:HB3	1.83	0.79
1:A:426:HIS:CD2	1:A:490:ARG:HH12	1.99	0.79
6:R:35:GLN:HA	6:R:38:TYR:CD1	2.17	0.79
5:E:87:GLY:O	5:E:88:GLU:HB2	1.81	0.79
3:J:773:ILE:HG12	3:J:813:LYS:HG2	1.64	0.79
3:B:539:LYS:O	3:B:543:ARG:HG3	1.83	0.79
2:M:61:GLU:O	2:M:64:ILE:HD12	1.83	0.79
2:M:110:ILE:HD11	2:M:277:ILE:HD11	1.64	0.79
3:J:665:ARG:HG3	3:J:920:THR:CG2	2.13	0.79
3:J:183:ILE:HG12	3:J:206:LYS:HB3	1.65	0.79
3:J:203:GLU:HA	3:J:203:GLU:OE1	1.82	0.79
8:H:29:TYR:HH	13:Y:67:LEU:HD22	1.48	0.79
1:I:491:TYR:HB2	1:I:607:GLN:OE1	1.83	0.79
1:A:79:ARG:HB2	1:A:266:TRP:CE3	2.17	0.79
4:D:109:ILE:HD11	4:D:133:LEU:HD12	1.65	0.79
9:U:91:SER:O	9:U:92:LEU:HB2	1.82	0.79
1:I:134:GLU:HA	1:I:137:LYS:HD2	1.64	0.78
1:I:353:ILE:HG13	1:I:361:LEU:HD23	1.65	0.78
1:A:525:LEU:HD11	1:A:530:VAL:HG11	1.65	0.78
1:I:541:ALA:HB2	7:S:72:CYS:H	1.46	0.78
3:B:702:LEU:CD2	3:B:933:ALA:HB1	2.12	0.78
1:A:61:CYS:SG	3:B:1070:TYR:HB3	2.23	0.78
1:A:206:TRP:O	1:A:208:ILE:N	2.16	0.78
7:G:72:CYS:SG	7:G:114:ARG:HB3	2.22	0.78
3:B:850:VAL:O	12:P:35:PHE:HB2	1.84	0.78
1:A:58:CYS:HB2	1:A:59:PRO:HD3	1.64	0.78
3:J:497:VAL:HG23	3:J:528:GLY:HA2	1.63	0.78
8:T:39:PRO:HB2	8:T:80:TYR:HE2	1.48	0.78
1:I:313:LEU:HB3	2:M:374:ILE:HG13	1.65	0.78
1:I:853:ASP:HB2	2:M:311:ARG:HH12	1.49	0.78
1:A:353:ILE:HG13	1:A:361:LEU:HD23	1.64	0.78
1:A:853:ASP:OD2	1:A:864:LYS:HB3	1.83	0.78
2:C:70:ILE:HA	2:C:73:VAL:HG22	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:ALA:CB	7:G:72:CYS:H	1.96	0.78
1:I:721:PRO:HA	1:I:726:TYR:HD1	1.49	0.78
7:S:63:ARG:HG3	7:S:114:ARG:NH2	1.99	0.78
4:D:13:ILE:CD1	4:D:238:PRO:HB2	2.13	0.78
1:I:324:THR:HG22	1:I:325:VAL:H	1.47	0.78
3:J:557:HIS:N	3:J:623:ASN:HD21	1.82	0.78
3:J:451:GLY:H	3:J:647:ILE:HG23	1.47	0.77
3:B:38:LYS:HG3	3:B:39:LEU:N	1.98	0.77
3:J:554:ASN:HD21	3:J:576:ARG:HH21	1.32	0.77
2:C:41:ILE:HB	2:C:42:ILE:HD12	1.64	0.77
2:C:173:MET:HA	2:C:176:ASP:HB2	1.65	0.77
7:G:55:VAL:HG23	7:G:116:SER:O	1.84	0.77
1:A:301:ARG:O	1:A:302:LEU:HG	1.84	0.77
2:C:391:ARG:NH2	9:K:42:GLN:HG2	1.98	0.77
1:A:507:TYR:O	1:A:508:LEU:HB2	1.83	0.77
2:M:345:ALA:HB1	2:M:350:THR:HG23	1.66	0.77
8:T:24:ASN:O	8:T:27:GLU:HG2	1.84	0.77
2:M:168:GLN:HA	2:M:204:SER:HA	1.67	0.77
1:I:647:ARG:HH21	3:J:982:ARG:HH12	1.33	0.77
3:J:853:THR:HG22	3:J:854:GLU:H	1.48	0.77
1:A:530:VAL:O	1:A:532:ILE:HG12	1.84	0.77
3:B:771:ASP:HB2	3:B:816:PRO:HD3	1.64	0.77
9:K:90:LEU:CD2	9:K:90:LEU:H	1.89	0.77
3:J:317:TYR:CD2	3:J:526:LEU:HD13	2.20	0.77
3:B:935:LEU:HD12	3:B:957:ILE:HG22	1.66	0.77
1:I:823:LEU:HB3	2:M:329:ILE:HD13	1.66	0.77
3:B:962:TYR:OH	11:N:42:ARG:HD2	1.83	0.77
2:C:63:LEU:HD23	2:C:63:LEU:O	1.84	0.77
1:A:667:ARG:O	1:A:670:VAL:HG22	1.85	0.77
3:B:1064:CYS:SG	14:B:2001:ZN:ZN	1.74	0.77
8:H:25:ILE:HD11	8:H:61:ASP:OD1	1.85	0.77
3:B:853:THR:HG22	3:B:854:GLU:H	1.49	0.77
10:V:40:PHE:HB3	10:V:58:LEU:HB3	1.66	0.77
1:A:447:LEU:HD13	3:B:734:MET:SD	2.25	0.77
3:J:88:ARG:NH1	3:J:854:GLU:O	2.18	0.77
2:C:391:ARG:H	2:C:392:PRO:HD3	1.49	0.77
1:A:336:GLU:HA	1:A:434:ARG:O	1.85	0.77
3:B:813:LYS:H	3:B:836:SER:HB3	1.49	0.77
1:I:378:VAL:O	1:I:378:VAL:HG22	1.85	0.77
12:X:17:GLN:HB3	12:X:19:LYS:HG3	1.64	0.77
3:J:758:TYR:O	3:J:759:SER:HB3	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:329:ILE:HA	2:C:334:VAL:CG1	2.15	0.76
1:A:812:ARG:HE	2:C:86:THR:HG23	1.48	0.76
4:O:29:ARG:HG3	4:O:162:SER:HB3	1.68	0.76
1:I:841:LEU:O	1:I:843:GLY:N	2.18	0.76
1:A:697:GLU:OE1	1:A:756:ARG:HD3	1.85	0.76
3:J:473:MET:SD	3:J:474:ALA:N	2.58	0.76
1:I:308:ARG:HH21	3:J:1099:LEU:CD1	1.97	0.76
3:J:911:ASN:HD22	3:J:913:HIS:H	1.33	0.76
3:B:630:PRO:O	3:B:633:LEU:HB3	1.84	0.76
3:J:640:LEU:CD2	3:J:641:GLU:H	1.98	0.76
1:I:58:CYS:HB2	1:I:59:PRO:HD3	1.66	0.76
1:A:134:GLU:HA	1:A:137:LYS:HD2	1.67	0.76
1:I:760:GLY:CA	3:J:447:GLY:HA3	2.04	0.76
1:I:507:TYR:O	1:I:508:LEU:HB2	1.84	0.76
4:O:44:VAL:HA	4:O:143:ALA:HA	1.67	0.76
1:I:530:VAL:O	1:I:532:ILE:HG12	1.86	0.76
2:M:35:LEU:O	2:M:39:LYS:HE3	1.85	0.76
3:J:992:LYS:HE3	3:J:996:MET:SD	2.25	0.76
3:J:870:ARG:NH1	3:J:996:MET:HB2	2.00	0.76
1:A:595:GLU:CB	7:G:91:LYS:HE2	2.15	0.76
3:J:249:GLN:HG3	3:J:250:ASN:H	1.50	0.76
8:H:29:TYR:O	8:H:33:LYS:HG3	1.86	0.76
3:J:922:GLY:HA2	3:J:925:MET:CB	2.13	0.76
3:J:569:ASN:CB	3:J:574:ARG:HH22	1.98	0.76
12:P:26:CYS:HB2	12:P:27:PRO:CD	2.14	0.76
2:M:179:VAL:HG11	2:M:232:LYS:HZ2	1.50	0.75
9:K:92:LEU:O	9:K:92:LEU:HD23	1.86	0.75
10:L:13:LEU:HB3	10:L:57:ILE:HD12	1.68	0.75
3:J:873:THR:HG22	3:J:874:ILE:N	2.01	0.75
3:B:588:LEU:HD13	3:B:612:LYS:HB3	1.67	0.75
3:B:730:THR:HB	3:B:732:TYR:HD1	1.51	0.75
2:M:60:SER:O	2:M:63:LEU:HB3	1.87	0.75
3:J:650:ILE:N	3:J:650:ILE:HD13	2.01	0.75
7:G:109:LYS:HZ3	3:J:378:LYS:HE3	1.51	0.75
2:M:115:LYS:HD3	2:M:278:ARG:HB3	1.68	0.75
1:I:541:ALA:CB	7:S:72:CYS:H	1.98	0.75
3:B:317:TYR:CD2	3:B:526:LEU:HD13	2.22	0.75
10:V:59:THR:HG21	10:V:65:PRO:HD3	1.68	0.75
1:A:742:GLN:HB2	3:B:919:MET:HE3	1.69	0.75
1:A:308:ARG:HH21	3:B:1099:LEU:CD1	1.94	0.75
3:B:650:ILE:H	3:B:650:ILE:CD1	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ARG:HB3	1:A:195:LEU:O	1.87	0.75
3:B:773:ILE:HG12	3:B:813:LYS:HG2	1.69	0.75
1:A:293:ARG:HH11	1:A:296:ARG:NH2	1.85	0.75
1:A:15:SER:HA	1:A:203:ARG:HH22	1.51	0.75
2:M:146:TYR:CE2	2:M:235:LYS:HB2	2.22	0.75
1:I:220:ARG:HH11	1:I:236:THR:HG23	1.50	0.75
2:C:377:HIS:ND1	2:C:378:PRO:HD2	2.02	0.75
1:I:326:ILE:HG21	1:I:462:MET:HG3	1.69	0.75
1:I:324:THR:HG22	1:I:325:VAL:N	2.02	0.75
3:J:874:ILE:HD12	3:J:874:ILE:H	1.52	0.75
3:J:539:LYS:O	3:J:543:ARG:HG3	1.87	0.75
1:A:525:LEU:HD12	10:L:56:LYS:HE3	1.69	0.74
3:J:38:LYS:HG3	3:J:39:LEU:N	2.01	0.74
1:I:234:ASP:OD2	1:I:296:ARG:HD3	1.85	0.74
3:J:427:ARG:HH11	3:J:650:ILE:HD12	1.53	0.74
3:B:249:GLN:HG3	3:B:250:ASN:H	1.50	0.74
3:B:851:LEU:HD12	12:P:35:PHE:HD2	1.50	0.74
3:B:591:ILE:HG12	3:B:612:LYS:NZ	2.02	0.74
1:A:525:LEU:CD1	1:A:530:VAL:HG11	2.17	0.74
2:C:389:THR:HG21	9:K:79:ARG:HH11	1.52	0.74
3:B:870:ARG:CZ	3:B:996:MET:SD	2.75	0.74
3:B:800:PRO:O	3:B:802:VAL:N	2.20	0.74
3:B:874:ILE:H	3:B:874:ILE:HD12	1.53	0.74
1:A:833:GLU:OE2	1:A:839:ARG:HB2	1.88	0.74
1:A:632:PHE:HA	1:A:635:PHE:CD1	2.22	0.74
2:M:30:ASP:O	2:M:31:ASP:HB3	1.87	0.74
3:B:763:VAL:HG22	3:B:770:GLU:HG3	1.68	0.74
10:V:3:ILE:CG2	10:V:15:LEU:HD21	2.17	0.74
3:J:972:ASP:OD2	3:J:974:ARG:HG2	1.87	0.74
7:G:80:GLU:HG2	7:G:81:LEU:H	1.52	0.74
3:J:581:ILE:CD1	3:J:614:GLU:HB2	2.01	0.74
1:A:490:ARG:HA	2:C:312:HIS:HE1	1.51	0.74
3:J:557:HIS:H	3:J:623:ASN:HD21	1.35	0.74
1:I:206:TRP:O	1:I:208:ILE:N	2.20	0.74
3:B:1000:LYS:O	3:B:1001:LEU:HB2	1.86	0.74
1:I:470:GLU:O	1:I:473:ILE:HG12	1.88	0.74
2:C:60:SER:O	2:C:63:LEU:N	2.20	0.74
2:C:55:ALA:O	2:C:58:GLU:HB2	1.88	0.74
1:A:324:THR:HG22	1:A:325:VAL:N	2.02	0.74
3:B:738:ILE:HD11	3:B:908:ILE:HG23	1.70	0.74
5:Q:84:VAL:HG21	6:R:86:ILE:HG12	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:LEU:HA	7:G:86:LEU:HD22	1.69	0.73
8:T:65:ILE:HD11	8:T:79:ARG:HG2	1.68	0.73
3:J:473:MET:SD	3:J:475:GLN:N	2.61	0.73
3:B:1054:ASP:HB3	3:B:1095:TYR:H	1.53	0.73
1:I:331:ASN:HD22	10:V:47:HIS:HB2	1.53	0.73
1:I:499:ALA:HB3	3:J:734:MET:CE	2.18	0.73
2:M:70:ILE:CD1	2:M:70:ILE:N	2.49	0.73
1:A:541:ALA:HB2	7:G:72:CYS:N	2.04	0.73
2:M:103:GLY:C	2:M:105:PRO:HD2	2.09	0.73
3:J:763:VAL:HG22	3:J:770:GLU:HG3	1.69	0.73
1:A:256:GLY:O	1:A:258:PRO:HD3	1.88	0.73
8:T:29:TYR:HA	8:T:32:LEU:HD12	1.70	0.73
3:B:451:GLY:H	3:B:647:ILE:HG23	1.53	0.73
3:J:687:ARG:HH11	3:J:687:ARG:CG	2.00	0.73
1:A:721:PRO:HA	1:A:726:TYR:HD1	1.51	0.73
1:I:567:ASN:N	1:I:599:ASP:OD2	2.22	0.73
3:J:708:LEU:HD13	3:J:713:TYR:HB3	1.69	0.73
7:G:30:ASN:O	7:G:31:MET:HG3	1.87	0.73
3:B:700:ARG:O	11:N:51:SER:HB2	1.88	0.73
2:M:70:ILE:HD12	2:M:70:ILE:H	1.52	0.73
1:A:859:TYR:HB2	2:C:64:ILE:HG12	1.71	0.73
3:J:461:GLY:O	3:J:464:SER:HB3	1.89	0.73
1:A:98:CYS:HA	1:A:146:CYS:SG	2.28	0.73
3:J:345:LEU:HD11	3:J:476:ILE:HG13	1.69	0.73
3:J:700:ARG:O	11:W:51:SER:HB2	1.89	0.73
11:N:7:CYS:SG	11:N:48:MET:HG3	2.29	0.73
3:B:911:ASN:HD22	3:B:913:HIS:H	1.36	0.73
7:G:83:ASP:O	7:G:93:THR:HA	1.89	0.73
1:I:245:ILE:HD13	1:I:268:LEU:HB3	1.71	0.73
3:B:353:LEU:HA	3:B:404:VAL:CG1	2.11	0.73
1:I:50:GLY:HA2	1:I:68:CYS:SG	2.29	0.73
1:A:846:VAL:HA	2:C:322:ARG:HE	1.54	0.73
1:I:828:SER:C	1:I:830:LEU:H	1.93	0.73
5:E:179:LYS:HE2	6:F:81:ASP:HB2	1.70	0.73
1:I:301:ARG:O	1:I:302:LEU:HG	1.89	0.72
3:J:726:VAL:HG12	3:J:912:PRO:HG3	1.69	0.72
3:B:210:PHE:HZ	3:B:323:ILE:HG22	1.54	0.72
9:U:50:LEU:HD22	9:U:75:PRO:HD3	1.71	0.72
3:J:1067:ILE:HG13	3:J:1068:GLY:N	2.03	0.72
3:J:353:LEU:HA	3:J:404:VAL:CG1	2.10	0.72
2:M:63:LEU:HD12	9:U:22:LEU:HD22	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:15:SER:HA	1:I:203:ARG:HH22	1.54	0.72
2:C:322:ARG:N	2:C:322:ARG:HH11	1.88	0.72
1:A:721:PRO:HA	1:A:726:TYR:CD1	2.24	0.72
3:J:1047:ASP:HA	3:J:1051:ASP:HB2	1.71	0.72
3:J:161:ILE:HG21	3:J:346:ALA:HA	1.71	0.72
3:B:88:ARG:NH1	3:B:854:GLU:O	2.22	0.72
3:B:687:ARG:NH1	3:B:687:ARG:HG3	2.04	0.72
1:I:632:PHE:HA	1:I:635:PHE:HD1	1.53	0.72
3:B:665:ARG:HG3	3:B:920:THR:CG2	2.19	0.72
2:M:70:ILE:HD13	2:M:70:ILE:N	2.03	0.72
3:B:758:TYR:O	3:B:759:SER:HB3	1.88	0.72
1:A:220:ARG:HH11	1:A:236:THR:HG23	1.53	0.72
1:A:507:TYR:HB3	1:A:597:VAL:HG13	1.71	0.72
1:A:90:ILE:HD11	1:A:207:MET:HB2	1.70	0.72
8:T:30:LYS:O	8:T:33:LYS:HB2	1.90	0.72
7:S:7:GLN:HG2	7:S:8:GLU:N	2.04	0.72
5:Q:84:VAL:HG22	5:Q:145:ARG:HH11	1.54	0.72
3:J:458:THR:HG21	3:J:465:GLY:N	2.04	0.72
3:B:902:LYS:HB3	11:N:42:ARG:HD3	1.69	0.72
5:E:53:THR:HB	5:E:71:GLU:H	1.55	0.72
2:M:179:VAL:HG11	2:M:232:LYS:NZ	2.04	0.72
4:O:11:THR:O	4:O:238:PRO:HB3	1.90	0.72
3:J:805:LYS:HG3	3:J:844:MET:HB2	1.71	0.72
2:C:343:ALA:HB2	2:C:371:GLU:HG3	1.71	0.72
2:C:237:ILE:HG22	2:C:257:ASN:HB2	1.72	0.72
3:B:890:MET:HE2	3:B:891:LEU:H	1.55	0.72
2:C:55:ALA:CA	2:C:58:GLU:HG3	2.19	0.72
7:G:63:ARG:HG3	7:G:114:ARG:HH22	1.55	0.72
1:A:558:LYS:HZ3	3:J:108:GLU:HG2	1.53	0.72
5:E:26:ALA:O	5:E:30:LEU:HB2	1.89	0.72
2:M:179:VAL:HG23	2:M:182:ASP:H	1.55	0.71
3:J:873:THR:CG2	3:J:874:ILE:N	2.53	0.71
3:B:522:LEU:O	3:B:525:ARG:HB3	1.90	0.71
2:M:391:ARG:NH2	9:U:39:ARG:HH11	1.88	0.71
1:I:525:LEU:CD1	1:I:530:VAL:HG11	2.20	0.71
4:O:254:GLU:HG2	10:V:77:ARG:HH12	1.54	0.71
7:S:30:ASN:HA	7:S:39:SER:HB3	1.73	0.71
1:A:502:TYR:CE1	1:A:636:ILE:HD11	2.24	0.71
2:M:391:ARG:HH22	9:U:39:ARG:HD2	1.55	0.71
3:J:890:MET:HA	3:J:890:MET:HE3	1.72	0.71
1:A:567:ASN:N	1:A:599:ASP:OD2	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ASN:ND2	3:J:377:ARG:CB	2.53	0.71
1:I:220:ARG:HA	1:I:233:ASP:OD1	1.91	0.71
1:I:90:ILE:HD11	1:I:207:MET:CB	2.20	0.71
3:B:690:THR:HG22	3:B:691:ARG:HG3	1.71	0.71
3:J:730:THR:HB	3:J:732:TYR:HD1	1.55	0.71
5:Q:64:GLY:H	9:U:41:LEU:HD22	1.55	0.71
1:A:446:ASN:ND2	1:A:448:LEU:H	1.89	0.71
9:K:60:ASP:O	9:K:61:VAL:O	2.08	0.71
1:I:666:ASP:O	1:I:670:VAL:HG13	1.91	0.71
3:J:739:ILE:CG2	3:J:909:ILE:HB	2.21	0.71
3:B:1070:TYR:O	3:B:1071:ASP:O	2.08	0.71
3:J:803:GLU:HB3	3:J:805:LYS:NZ	2.05	0.71
5:Q:135:VAL:H	5:Q:174:TRP:HZ2	1.36	0.71
10:V:4:ARG:HG2	10:V:4:ARG:HH11	1.56	0.71
1:A:846:VAL:O	2:C:322:ARG:NH2	2.23	0.71
2:M:54:LEU:O	2:M:58:GLU:HG3	1.90	0.71
2:C:327:ARG:HG3	2:C:334:VAL:HB	1.71	0.71
12:X:46:LYS:N	12:X:46:LYS:HD2	2.06	0.71
1:A:853:ASP:HB2	2:C:311:ARG:NH1	2.05	0.71
1:I:106:ILE:HG22	1:I:107:SER:H	1.56	0.71
1:I:155:LYS:H	1:I:155:LYS:HZ1	1.37	0.71
1:I:595:GLU:CB	7:S:91:LYS:HE2	2.21	0.71
1:A:446:ASN:HD22	1:A:446:ASN:C	1.94	0.71
3:B:805:LYS:HG3	3:B:844:MET:HB2	1.71	0.71
1:A:468:GLN:HG3	3:B:1052:ASN:HD21	1.54	0.71
2:M:69:ALA:HB2	2:M:381:LEU:HD13	1.72	0.71
1:A:532:ILE:CD1	10:L:56:LYS:HD3	2.20	0.71
3:B:554:ASN:HD21	3:B:576:ARG:HH21	1.39	0.71
1:A:234:ASP:OD2	1:A:296:ARG:HD3	1.91	0.71
1:I:697:GLU:OE1	1:I:756:ARG:HD3	1.91	0.71
2:C:354:LEU:HD13	3:B:1104:LEU:HD21	1.73	0.71
12:P:17:GLN:HB3	12:P:19:LYS:HG3	1.73	0.71
8:T:39:PRO:HB2	8:T:80:TYR:CE2	2.25	0.70
1:A:331:ASN:O	1:A:332:ILE:CB	2.39	0.70
1:I:238:LYS:HD3	1:I:276:TYR:HA	1.73	0.70
8:H:46:ARG:HH22	13:Y:78:ARG:HH11	1.39	0.70
7:G:87:ASN:C	7:G:89:GLY:H	1.93	0.70
1:A:828:SER:C	1:A:830:LEU:H	1.94	0.70
3:B:183:ILE:HB	3:B:207:ASP:C	2.11	0.70
3:J:1000:LYS:O	3:J:1001:LEU:HB2	1.90	0.70
5:E:179:LYS:CE	6:F:81:ASP:HB2	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:57:GLY:CA	13:Z:61:LEU:HG	2.21	0.70
8:H:29:TYR:OH	13:Y:67:LEU:CD2	2.25	0.70
1:I:589:LYS:HG2	1:I:877:GLY:HA2	1.73	0.70
3:B:458:THR:CG2	3:B:465:GLY:H	2.03	0.70
3:J:724:LEU:HD12	3:J:908:ILE:HG22	1.73	0.70
9:U:90:LEU:N	9:U:90:LEU:HD23	2.07	0.70
3:B:28:LEU:HG	3:B:122:MET:HE1	1.72	0.70
2:M:301:LEU:HA	2:M:304:GLN:HG3	1.71	0.70
3:J:1070:TYR:O	3:J:1071:ASP:O	2.09	0.70
1:A:828:SER:O	1:A:830:LEU:N	2.22	0.70
3:B:1004:ARG:HH11	3:B:1025:GLY:H	1.39	0.70
1:I:742:GLN:HB3	3:J:919:MET:HE1	1.73	0.70
1:I:604:GLY:C	1:I:606:GLN:H	1.93	0.70
7:S:72:CYS:SG	7:S:114:ARG:HB3	2.31	0.70
12:P:46:LYS:HD2	12:P:46:LYS:N	2.04	0.70
3:J:1095:TYR:CE1	3:J:1098:LYS:HD2	2.26	0.70
1:I:525:LEU:HD11	1:I:530:VAL:HG11	1.71	0.70
10:L:24:LEU:O	10:L:28:ILE:HG12	1.90	0.70
2:M:377:HIS:ND1	2:M:378:PRO:HD2	2.07	0.70
3:B:1067:ILE:HG13	3:B:1068:GLY:N	2.07	0.70
1:I:704:LEU:HD22	1:I:781:PHE:CE1	2.26	0.70
1:I:733:ALA:HB1	3:J:913:HIS:CE1	2.27	0.70
1:I:316:LYS:HE2	3:J:1054:ASP:OD2	1.91	0.70
2:M:277:ILE:O	2:M:279:GLU:N	2.24	0.70
1:I:827:LEU:HD11	2:M:315:LEU:HD13	1.73	0.70
1:A:604:GLY:C	1:A:606:GLN:H	1.93	0.70
2:C:276:ASN:HD22	2:C:279:GLU:CB	2.05	0.70
1:I:9:ILE:O	2:M:363:VAL:O	2.10	0.70
1:A:50:GLY:HA2	1:A:68:CYS:SG	2.31	0.70
9:K:23:TRP:CE3	9:K:23:TRP:HA	2.27	0.70
1:I:594:LEU:CA	7:S:86:LEU:HD22	2.21	0.70
5:Q:18:PHE:CE2	9:U:42:GLN:HG2	2.27	0.70
3:B:848:ASP:HB2	3:B:867:ARG:H	1.55	0.70
1:I:468:GLN:HG3	3:J:1052:ASN:HD21	1.56	0.70
3:J:210:PHE:HZ	3:J:323:ILE:HG22	1.56	0.70
2:C:269:VAL:HA	2:C:272:VAL:HG23	1.74	0.69
11:W:22:ILE:HD13	11:W:23:THR:H	1.56	0.69
1:I:541:ALA:HB1	7:S:71:PHE:HA	1.73	0.69
7:G:109:LYS:NZ	3:J:378:LYS:HE3	2.07	0.69
3:J:1004:ARG:HH11	3:J:1025:GLY:H	1.38	0.69
1:I:293:ARG:HH11	1:I:296:ARG:NH2	1.88	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ARG:HD2	1:A:150:ASN:H	1.58	0.69
9:K:38:ALA:HB1	9:K:42:GLN:HE22	1.56	0.69
2:M:70:ILE:HD13	2:M:70:ILE:H	1.57	0.69
2:C:69:ALA:HB2	2:C:381:LEU:HD22	1.73	0.69
3:B:480:ILE:HG22	3:B:481:ASN:N	2.07	0.69
5:E:83:GLU:H	5:E:145:ARG:HG3	1.55	0.69
1:A:541:ALA:HB1	7:G:71:PHE:HA	1.75	0.69
2:M:86:THR:HA	2:M:104:LEU:HD12	1.74	0.69
3:J:591:ILE:CG1	3:J:612:LYS:HZ3	2.06	0.69
3:J:812:GLY:HA2	3:J:836:SER:HB3	1.74	0.69
3:J:70:VAL:HG11	3:J:90:LEU:HD23	1.75	0.69
3:J:881:ARG:NH1	3:J:989:TYR:HB3	2.06	0.69
3:J:930:GLY:HA2	11:W:47:ARG:HH22	1.58	0.69
1:A:470:GLU:O	1:A:473:ILE:HG12	1.91	0.69
4:D:111:SER:HA	4:D:114:ILE:CD1	2.22	0.69
3:B:800:PRO:HD3	3:B:850:VAL:HG23	1.74	0.69
3:J:181:SER:HB3	3:J:183:ILE:HD12	1.72	0.69
1:I:4:LYS:HD2	3:J:1089:PHE:HB3	1.74	0.69
1:A:313:LEU:HG	2:C:374:ILE:HG23	1.73	0.69
3:B:974:ARG:HB2	10:L:22:HIS:CD2	2.27	0.69
2:C:54:LEU:O	2:C:58:GLU:N	2.25	0.69
1:A:510:THR:O	1:A:549:LYS:HG3	1.93	0.69
1:A:364:PHE:CE1	1:A:409:ARG:HD2	2.28	0.69
1:I:502:TYR:CE1	1:I:636:ILE:HD11	2.27	0.69
3:J:10:ARG:HB2	3:J:642:ILE:O	1.91	0.69
3:J:1015:GLN:NE2	3:J:1096:ALA:HB2	2.08	0.69
1:I:594:LEU:HA	7:S:86:LEU:CD2	2.22	0.69
2:M:390:MET:HB2	5:Q:56:GLU:CG	2.23	0.69
1:I:293:ARG:HH11	1:I:296:ARG:HH22	1.39	0.69
3:B:890:MET:HE3	3:B:890:MET:HA	1.73	0.69
6:F:81:ASP:O	6:F:84:ARG:HG2	1.92	0.69
3:J:1067:ILE:HG13	3:J:1068:GLY:H	1.57	0.69
2:C:237:ILE:HG13	2:C:238:LYS:H	1.57	0.69
3:J:933:ALA:HB3	11:W:47:ARG:HH12	1.58	0.69
1:I:541:ALA:HB2	7:S:72:CYS:N	2.08	0.69
7:S:43:ILE:O	7:S:46:ILE:HG22	1.93	0.69
3:B:602:ILE:CG2	3:B:603:THR:H	2.05	0.69
10:V:83:TYR:O	10:V:87:ILE:HB	1.92	0.69
3:B:479:GLY:HA2	3:B:552:GLU:HB3	1.75	0.69
1:I:696:LEU:O	1:I:700:ILE:HG12	1.93	0.69
2:C:70:ILE:N	2:C:70:ILE:HD13	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ASN:HD22	1:A:448:LEU:H	1.38	0.69
7:G:67:SER:O	7:G:69:ASP:N	2.26	0.69
3:B:10:ARG:HB2	3:B:642:ILE:O	1.92	0.68
3:J:17:TYR:OH	3:J:474:ALA:HA	1.93	0.68
2:M:315:LEU:O	2:M:319:VAL:HG23	1.93	0.68
3:J:851:LEU:HD12	12:X:35:PHE:HD2	1.56	0.68
3:B:81:SER:HB3	3:B:84:GLU:HG3	1.74	0.68
1:I:637:ARG:HD3	1:I:640:GLU:CD	2.13	0.68
1:I:852:ASP:HB3	8:T:75:VAL:HG21	1.76	0.68
6:R:47:CYS:HB2	6:R:52:ALA:HB2	1.76	0.68
1:I:110:GLU:HG2	1:I:113:LYS:HD2	1.75	0.68
3:B:708:LEU:HD13	3:B:713:TYR:HB3	1.75	0.68
1:A:293:ARG:HH11	1:A:296:ARG:HH22	1.39	0.68
1:A:245:ILE:HD13	1:A:268:LEU:HB3	1.75	0.68
11:N:18:TRP:HD1	11:N:49:LEU:HD22	1.57	0.68
2:M:366:PHE:CZ	2:M:375:ILE:HD12	2.28	0.68
1:I:11:PHE:HB2	2:M:361:GLY:O	1.93	0.68
2:M:386:VAL:HG13	9:U:34:ARG:HG2	1.74	0.68
3:B:445:LEU:HD11	3:B:455:PRO:CB	2.23	0.68
11:N:7:CYS:HB3	11:N:45:CYS:SG	2.33	0.68
1:A:491:TYR:HD1	1:A:607:GLN:NE2	1.92	0.68
3:B:253:PHE:N	3:B:254:PRO:HD2	2.08	0.68
2:C:190:ARG:HD3	2:C:191:LEU:H	1.58	0.68
2:M:111:VAL:HG12	2:M:329:ILE:HB	1.75	0.68
5:E:179:LYS:NZ	6:F:79:THR:HB	2.09	0.68
3:B:361:PHE:HE1	3:B:385:VAL:HG13	1.57	0.68
1:I:68:CYS:SG	1:I:71:HIS:CE1	2.86	0.68
1:I:826:ALA:H	2:M:335:THR:CG2	2.07	0.68
1:I:99:ARG:HD2	1:I:150:ASN:H	1.56	0.68
3:J:555:VAL:O	3:J:620:GLU:HG3	1.93	0.68
4:D:230:ILE:HG13	4:D:242:LEU:HD21	1.75	0.68
3:J:602:ILE:CG2	3:J:603:THR:H	2.06	0.68
1:I:733:ALA:HB1	3:J:913:HIS:HE1	1.59	0.68
3:J:20:SER:O	3:J:25:ARG:NH2	2.24	0.68
1:I:325:VAL:O	1:I:442:THR:HB	1.94	0.68
3:B:763:VAL:HA	3:B:770:GLU:HG3	1.75	0.68
3:B:17:TYR:OH	3:B:474:ALA:HA	1.94	0.68
1:A:595:GLU:HB3	7:G:86:LEU:HD13	1.76	0.68
8:H:40:GLU:OE1	13:Y:66:LYS:CE	2.39	0.68
1:I:491:TYR:HD1	1:I:607:GLN:NE2	1.91	0.68
3:J:630:PRO:O	3:J:633:LEU:HB3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ASN:ND2	3:B:732:TYR:OH	2.27	0.68
13:Z:58:LYS:O	13:Z:59:ILE:HB	1.94	0.68
3:J:591:ILE:HG12	3:J:612:LYS:NZ	2.09	0.68
2:M:117:PRO:O	2:M:120:PRO:HG3	1.92	0.68
1:I:575:CYS:HG	1:I:580:CYS:CB	2.06	0.68
1:I:721:PRO:HA	1:I:726:TYR:CD1	2.27	0.68
3:J:926:GLU:HB3	3:J:988:VAL:HG22	1.76	0.68
1:A:549:LYS:HG2	1:A:593:LEU:HD13	1.75	0.68
1:I:130:ARG:HB3	1:I:195:LEU:O	1.93	0.68
2:M:277:ILE:C	2:M:279:GLU:H	1.97	0.68
2:M:392:PRO:HD3	5:Q:56:GLU:HG3	1.75	0.68
9:K:82:LEU:CD2	9:K:82:LEU:H	2.07	0.67
1:I:828:SER:O	1:I:830:LEU:N	2.27	0.67
1:I:839:ARG:NH1	8:T:37:ILE:HG23	2.09	0.67
1:I:141:MET:HG3	1:I:148:HIS:HA	1.76	0.67
2:M:55:ALA:CA	2:M:58:GLU:HB2	2.22	0.67
3:B:881:ARG:HD2	3:B:989:TYR:HD2	1.59	0.67
1:I:256:GLY:O	1:I:258:PRO:HD3	1.94	0.67
1:I:328:PRO:HG3	1:I:457:PHE:CD1	2.30	0.67
3:J:28:LEU:HG	3:J:122:MET:HE1	1.75	0.67
3:J:759:SER:HB3	3:J:863:LYS:HA	1.76	0.67
4:O:111:SER:HA	4:O:114:ILE:CD1	2.24	0.67
1:A:90:ILE:HD11	1:A:207:MET:CB	2.24	0.67
3:B:544:ARG:HH11	3:B:544:ARG:HG3	1.59	0.67
2:M:109:GLU:O	2:M:113:ALA:N	2.28	0.67
1:A:499:ALA:HB3	3:B:734:MET:CE	2.25	0.67
4:D:250:ILE:HA	4:D:253:ILE:HG22	1.77	0.67
2:M:373:ILE:HG13	3:J:1049:LEU:HD13	1.75	0.67
3:J:64:ARG:HG2	3:J:97:TRP:CD1	2.29	0.67
3:J:851:LEU:HD12	12:X:35:PHE:CD2	2.30	0.67
3:B:851:LEU:HD12	12:P:35:PHE:CD2	2.28	0.67
3:J:537:ALA:HB2	3:J:557:HIS:NE2	2.09	0.67
2:C:237:ILE:HG22	2:C:257:ASN:CB	2.25	0.67
11:W:18:TRP:HD1	11:W:49:LEU:HD22	1.58	0.67
2:M:391:ARG:H	2:M:392:PRO:HD3	1.60	0.67
1:A:490:ARG:HG2	1:A:491:TYR:CD2	2.30	0.67
2:M:355:LEU:HD22	3:J:1109:ILE:HD11	1.76	0.67
3:B:161:ILE:HG21	3:B:346:ALA:HA	1.77	0.67
1:I:426:HIS:CE1	1:I:428:ILE:CG2	2.77	0.67
5:Q:27:LEU:HB2	5:Q:51:VAL:CG1	2.22	0.67
11:N:22:ILE:HD13	11:N:23:THR:H	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:237:ILE:HG13	2:M:238:LYS:N	2.10	0.67
9:U:61:VAL:HG12	9:U:62:ILE:N	2.06	0.67
2:M:55:ALA:HA	2:M:58:GLU:CB	2.21	0.67
4:D:11:THR:O	4:D:238:PRO:HB3	1.94	0.67
2:M:231:ILE:HB	2:M:234:ILE:HG12	1.75	0.67
1:A:532:ILE:HD11	10:L:56:LYS:CD	2.22	0.67
3:J:38:LYS:HA	3:J:41:GLU:HG3	1.76	0.67
3:B:933:ALA:HB3	11:N:47:ARG:HH12	1.58	0.67
3:J:848:ASP:HB2	3:J:867:ARG:H	1.60	0.67
3:B:291:GLN:HB3	3:B:295:LYS:HE2	1.77	0.67
1:A:589:LYS:HG2	1:A:877:GLY:HA2	1.77	0.67
3:J:850:VAL:O	12:X:35:PHE:HB2	1.95	0.67
3:B:602:ILE:HG23	3:B:603:THR:H	1.59	0.67
6:R:51:SER:O	6:R:55:VAL:HG23	1.94	0.67
3:J:962:TYR:OH	11:W:42:ARG:HD2	1.95	0.66
3:J:665:ARG:HG3	3:J:920:THR:HG21	1.76	0.66
3:B:602:ILE:CG2	3:B:603:THR:N	2.58	0.66
1:I:826:ALA:HB2	2:M:335:THR:HG23	1.77	0.66
5:Q:64:GLY:N	9:U:41:LEU:HD22	2.09	0.66
3:J:451:GLY:CA	3:J:577:ARG:HH11	2.08	0.66
3:B:451:GLY:CA	3:B:577:ARG:HH11	2.08	0.66
3:B:934:ALA:O	11:N:46:ARG:HD3	1.95	0.66
2:M:391:ARG:HH22	9:U:39:ARG:NH1	1.93	0.66
2:M:159:ASP:HB3	2:M:163:MET:HB2	1.77	0.66
3:B:457:GLU:HG2	3:B:469:ASN:OD1	1.96	0.66
2:M:104:LEU:HB3	2:M:105:PRO:HD3	1.76	0.66
2:M:309:ASP:OD2	2:M:311:ARG:N	2.29	0.66
2:M:390:MET:CG	5:Q:56:GLU:HG2	2.25	0.66
3:J:253:PHE:N	3:J:254:PRO:HD2	2.09	0.66
2:C:104:LEU:HB3	2:C:105:PRO:HD3	1.77	0.66
1:A:666:ASP:O	1:A:670:VAL:HG13	1.94	0.66
2:M:261:VAL:O	2:M:261:VAL:HG12	1.96	0.66
1:A:326:ILE:HG21	1:A:462:MET:HG3	1.77	0.66
3:B:20:SER:O	3:B:25:ARG:NH2	2.28	0.66
3:B:806:GLY:O	3:B:839:THR:HB	1.95	0.66
1:A:569:SER:HB2	1:A:584:SER:OG	1.95	0.66
7:S:86:LEU:HD12	7:S:91:LYS:CG	2.26	0.66
1:A:104:VAL:HG12	1:A:104:VAL:O	1.96	0.66
4:O:250:ILE:HA	4:O:253:ILE:HG22	1.78	0.66
1:I:4:LYS:HD3	3:J:1091:VAL:HB	1.78	0.66
1:I:722:PHE:HZ	7:S:23:LEU:HG	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:33:LEU:O	6:F:34:LEU:HD23	1.96	0.66
3:B:26:GLN:O	3:B:345:LEU:CD2	2.40	0.66
3:J:702:LEU:HD12	11:W:51:SER:HB3	1.76	0.66
4:D:111:SER:CA	4:D:114:ILE:HD13	2.24	0.66
3:J:602:ILE:HG23	3:J:603:THR:H	1.61	0.66
4:O:109:ILE:HD11	4:O:133:LEU:HD12	1.77	0.66
3:J:1012:LEU:O	3:J:1095:TYR:HE2	1.79	0.66
2:M:298:SER:O	2:M:302:ALA:HB2	1.96	0.66
3:B:450:TRP:CZ2	3:B:641:GLU:OE1	2.47	0.66
1:A:549:LYS:CE	7:G:89:GLY:HA2	2.25	0.66
3:J:448:THR:C	3:J:450:TRP:H	1.99	0.66
1:I:549:LYS:CE	7:S:89:GLY:HA2	2.26	0.66
2:M:72:ILE:HD12	2:M:72:ILE:H	1.58	0.66
3:J:291:GLN:HB3	3:J:295:LYS:HE2	1.77	0.66
7:S:13:CYS:HA	7:S:33:CYS:HA	1.77	0.66
1:I:534:LEU:HB2	10:V:39:SER:OG	1.96	0.66
3:J:522:LEU:O	3:J:525:ARG:HB3	1.95	0.66
4:O:190:LEU:CD2	4:O:195:LEU:HA	2.26	0.66
4:D:190:LEU:CD2	4:D:195:LEU:HA	2.25	0.66
1:A:575:CYS:HG	1:A:580:CYS:CB	2.09	0.66
5:Q:43:GLY:HA3	5:Q:78:VAL:HG23	1.78	0.66
1:A:818:TYR:OH	2:C:348:GLU:OE2	2.12	0.66
4:D:259:LYS:O	4:D:263:VAL:HG23	1.96	0.66
3:B:1095:TYR:CE1	3:B:1098:LYS:HD2	2.30	0.65
3:J:902:LYS:HB3	11:W:42:ARG:CD	2.25	0.65
1:I:345:LYS:HA	1:I:410:HIS:CD2	2.30	0.65
1:I:353:ILE:HD11	1:I:407:ILE:HG23	1.78	0.65
2:M:168:GLN:HG2	2:M:204:SER:HB3	1.78	0.65
5:E:113:ILE:O	5:E:164:MET:HB2	1.96	0.65
3:J:690:THR:HG22	3:J:691:ARG:HG3	1.77	0.65
3:B:1015:GLN:NE2	3:B:1096:ALA:HB2	2.11	0.65
1:A:239:LEU:HD22	1:A:276:TYR:CE1	2.31	0.65
1:A:106:ILE:HG22	1:A:107:SER:H	1.59	0.65
1:A:647:ARG:NH2	3:B:982:ARG:HH12	1.94	0.65
4:D:44:VAL:HA	4:D:143:ALA:HA	1.77	0.65
3:B:569:ASN:HB3	3:B:574:ARG:NH2	2.09	0.65
2:M:354:LEU:HD22	3:J:1104:LEU:HD21	1.77	0.65
3:B:448:THR:C	3:B:450:TRP:H	1.99	0.65
3:B:591:ILE:CG1	3:B:612:LYS:HZ3	2.08	0.65
1:I:308:ARG:HG3	1:I:312:ASN:HD22	1.61	0.65
3:B:345:LEU:HD11	3:B:476:ILE:HG13	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:515:LEU:HD13	7:S:43:ILE:HD12	1.78	0.65
1:A:696:LEU:O	1:A:700:ILE:HG12	1.95	0.65
12:P:24:VAL:O	12:P:24:VAL:HG13	1.96	0.65
1:I:27:ILE:HG23	1:I:45:MET:HA	1.78	0.65
3:J:781:ARG:HD3	3:J:782:GLY:H	1.61	0.65
1:A:837:THR:HG22	1:A:838:VAL:H	1.62	0.65
1:A:590:ASN:HD21	3:J:377:ARG:HD2	1.61	0.65
3:J:587:PRO:O	3:J:588:LEU:HD23	1.96	0.65
5:E:127:ILE:HB	5:E:136:ILE:HB	1.78	0.65
1:I:841:LEU:HD11	2:M:339:ASN:HB3	1.78	0.65
1:A:141:MET:HG3	1:A:148:HIS:HA	1.78	0.65
2:M:390:MET:CB	5:Q:56:GLU:HG2	2.26	0.65
1:A:421:ARG:HB2	1:A:462:MET:HE3	1.78	0.65
10:L:67:ASP:HA	10:L:70:LEU:HB2	1.77	0.65
5:Q:26:ALA:O	5:Q:30:LEU:HB2	1.97	0.65
7:S:60:SER:OG	7:S:64:PRO:HD3	1.95	0.65
3:B:739:ILE:CG2	3:B:909:ILE:HB	2.27	0.65
2:M:288:ALA:HB2	8:T:17:VAL:HB	1.77	0.65
3:J:162:VAL:HG11	3:J:412:GLN:NE2	2.10	0.65
3:J:588:LEU:HD13	3:J:612:LYS:HB3	1.79	0.65
1:I:635:PHE:O	1:I:639:VAL:HG23	1.97	0.65
1:A:827:LEU:HD11	2:C:315:LEU:HD12	1.79	0.65
3:B:1047:ASP:HA	3:B:1051:ASP:HB2	1.79	0.65
3:J:147:ASP:OD2	3:J:148:PRO:HD2	1.97	0.65
1:A:749:GLN:H	1:A:781:PHE:HA	1.61	0.65
3:B:245:ASP:N	3:B:246:PRO:HD3	2.12	0.65
9:U:91:SER:O	9:U:92:LEU:CB	2.44	0.65
3:B:724:LEU:HD12	3:B:908:ILE:HG22	1.78	0.65
3:J:602:ILE:CG2	3:J:603:THR:N	2.60	0.65
1:A:512:LYS:HE2	7:G:91:LYS:CE	2.26	0.65
12:X:26:CYS:HB2	12:X:27:PRO:CD	2.26	0.65
3:B:552:GLU:HA	3:B:576:ARG:HH22	1.62	0.65
7:G:15:ILE:HD13	7:G:53:GLU:HB3	1.78	0.65
1:I:764:ARG:HH11	1:I:764:ARG:CB	2.09	0.65
2:M:192:LYS:C	2:M:194:GLY:H	2.00	0.65
5:E:39:LEU:O	5:E:40:LYS:HB2	1.96	0.64
9:U:61:VAL:CG1	9:U:62:ILE:H	2.05	0.64
2:C:390:MET:O	2:C:391:ARG:CB	2.45	0.64
1:I:507:TYR:HB3	1:I:597:VAL:HG13	1.79	0.64
1:I:549:LYS:HG2	1:I:593:LEU:HD13	1.79	0.64
1:A:378:VAL:HG22	1:A:378:VAL:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:VAL:HG23	1:A:407:ILE:HG22	1.80	0.64
2:C:299:LYS:HA	2:C:302:ALA:HB3	1.78	0.64
3:J:840:ARG:HH11	3:J:1021:ALA:HB2	1.62	0.64
1:I:750:GLN:HG3	1:I:782:ILE:CD1	2.27	0.64
7:G:41:ASP:HB2	7:G:90:ASN:HB3	1.79	0.64
1:I:354:THR:HB	1:I:355:PRO:HD2	1.78	0.64
1:A:345:LYS:HA	1:A:410:HIS:CD2	2.32	0.64
1:A:558:LYS:NZ	3:J:108:GLU:HG2	2.12	0.64
3:J:1064:CYS:HG	14:J:2001:ZN:ZN	1.08	0.64
2:C:69:ALA:CB	2:C:381:LEU:HD22	2.27	0.64
2:C:104:LEU:O	2:C:108:ILE:HG12	1.96	0.64
4:O:133:LEU:HD21	4:O:139:ILE:HG13	1.78	0.64
7:S:83:ASP:O	7:S:93:THR:HA	1.98	0.64
1:A:4:LYS:HD2	3:B:1089:PHE:HB3	1.79	0.64
3:B:764:LYS:HZ3	3:B:814:VAL:H	1.44	0.64
3:B:577:ARG:HE	3:B:578:PRO:HD2	1.63	0.64
3:B:881:ARG:HD2	3:B:989:TYR:CD2	2.32	0.64
1:I:196:GLY:O	2:M:360:ARG:HG2	1.97	0.64
8:H:78:TYR:O	8:H:79:ARG:HG2	1.98	0.64
10:V:32:LEU:O	10:V:32:LEU:HD13	1.98	0.64
4:D:247:LYS:HA	4:D:250:ILE:HD12	1.78	0.64
3:J:336:ASP:HA	3:J:341:LYS:HE3	1.79	0.64
2:M:328:GLN:O	2:M:333:GLY:HA3	1.98	0.64
3:B:28:LEU:HG	3:B:122:MET:CE	2.28	0.64
8:H:42:LEU:HB2	8:H:43:PRO:HD2	1.78	0.64
5:Q:15:PRO:HG2	9:U:45:MET:CB	2.28	0.64
2:C:50:LYS:HA	2:C:53:ASP:HB2	1.79	0.64
2:M:68:GLU:HB3	9:U:30:TYR:HE1	1.62	0.64
12:X:24:VAL:HG13	12:X:24:VAL:O	1.97	0.64
1:I:647:ARG:O	1:I:650:ASP:HB2	1.96	0.64
3:B:900:THR:HG22	3:B:970:VAL:HG12	1.79	0.64
3:B:416:ARG:NH1	3:B:687:ARG:NH2	2.46	0.64
1:I:830:LEU:CD2	1:I:840:SER:HB3	2.24	0.64
2:M:391:ARG:HH21	9:U:42:GLN:CG	2.11	0.64
3:J:890:MET:CE	3:J:891:LEU:H	2.08	0.64
2:M:150:GLU:HG3	2:M:227:LEU:HD22	1.78	0.64
3:J:318:ALA:O	3:J:321:LYS:HB2	1.97	0.64
6:F:1:MET:SD	6:F:6:ILE:HG12	2.37	0.64
3:B:569:ASN:CB	3:B:574:ARG:HH22	2.10	0.64
3:B:64:ARG:O	3:B:97:TRP:HB2	1.98	0.64
7:G:101:LEU:HD12	7:G:104:LYS:NZ	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:657:TYR:O	3:B:660:HIS:HB2	1.97	0.64
1:A:678:LYS:HD2	1:A:684:LEU:HG	1.79	0.64
3:J:246:PRO:C	3:J:248:VAL:H	2.02	0.64
3:B:972:ASP:OD2	3:B:974:ARG:HG2	1.97	0.64
1:A:27:ILE:HG23	1:A:45:MET:HA	1.79	0.64
1:I:490:ARG:HG2	1:I:491:TYR:CD2	2.33	0.64
8:T:42:LEU:O	8:T:44:TRP:N	2.30	0.64
1:I:549:LYS:HE2	7:S:89:GLY:HA2	1.80	0.64
3:B:239:VAL:HA	3:B:253:PHE:HE2	1.63	0.64
3:B:116:ILE:HG22	3:B:390:VAL:HG21	1.79	0.64
3:J:480:ILE:HG22	3:J:481:ASN:N	2.13	0.64
9:U:61:VAL:C	9:U:63:SER:H	2.00	0.63
3:B:930:GLY:HA2	11:N:47:ARG:HH22	1.62	0.63
3:J:591:ILE:HG12	3:J:612:LYS:HZ3	1.63	0.63
2:C:311:ARG:HD3	2:C:311:ARG:N	2.14	0.63
2:C:60:SER:O	2:C:63:LEU:HB3	1.98	0.63
10:V:59:THR:CG2	10:V:65:PRO:HD3	2.28	0.63
2:M:68:GLU:HB3	9:U:30:TYR:CE1	2.33	0.63
6:R:23:ASP:O	6:R:26:ARG:HB2	1.97	0.63
1:I:647:ARG:NH2	3:J:982:ARG:HH12	1.97	0.63
3:J:591:ILE:HD12	3:J:591:ILE:H	1.61	0.63
3:J:702:LEU:HB2	3:J:721:ASN:ND2	2.14	0.63
9:K:41:LEU:O	9:K:42:GLN:C	2.36	0.63
8:H:11:PRO:O	8:H:13:ILE:N	2.29	0.63
3:B:246:PRO:C	3:B:248:VAL:H	2.02	0.63
3:B:537:ALA:HB2	3:B:557:HIS:NE2	2.13	0.63
1:A:353:ILE:HG13	1:A:361:LEU:CD2	2.29	0.63
1:A:133:THR:HB	1:A:137:LYS:HZ2	1.63	0.63
4:D:131:VAL:HG22	4:D:132:LEU:N	2.13	0.63
1:A:156:ILE:HD11	1:A:270:GLN:HG2	1.80	0.63
3:B:99:THR:HG22	3:B:99:THR:O	1.98	0.63
2:C:321:THR:C	2:C:322:ARG:HH11	2.02	0.63
3:J:638:THR:HB	3:J:639:HIS:HD2	1.62	0.63
1:I:364:PHE:CE1	1:I:409:ARG:HD2	2.34	0.63
3:J:739:ILE:HG12	3:J:890:MET:O	1.98	0.63
3:J:325:LEU:HD13	3:J:330:ARG:H	1.62	0.63
3:B:840:ARG:HH11	3:B:1021:ALA:HB2	1.62	0.63
2:C:33:LYS:O	2:C:36:ILE:HG22	1.99	0.63
9:K:74:LEU:N	9:K:74:LEU:HD12	2.14	0.63
2:M:106:ARG:O	2:M:109:GLU:N	2.31	0.63
1:I:750:GLN:HG3	1:I:782:ILE:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:361:PHE:HE1	3:J:385:VAL:HG13	1.62	0.63
8:T:65:ILE:HD11	8:T:79:ARG:CG	2.28	0.63
1:I:512:LYS:HE2	7:S:91:LYS:CE	2.29	0.63
5:Q:109:HIS:CD2	5:Q:111:SER:H	2.17	0.63
1:I:191:ASP:HA	1:I:194:ILE:HD11	1.81	0.63
3:B:922:GLY:O	3:B:926:GLU:HB2	1.99	0.63
1:I:503:ILE:HD11	1:I:733:ALA:N	2.12	0.63
1:I:595:GLU:HB2	7:S:91:LYS:HE2	1.80	0.63
3:J:64:ARG:HG2	3:J:97:TRP:CG	2.33	0.63
3:J:245:ASP:N	3:J:246:PRO:HD3	2.13	0.63
1:I:12:GLY:HA2	2:M:358:ALA:O	1.99	0.63
3:J:922:GLY:CA	3:J:925:MET:HB2	2.17	0.63
1:I:327:SER:HB2	1:I:444:ARG:HD3	1.80	0.63
7:S:86:LEU:HD12	7:S:91:LYS:HG2	1.81	0.63
1:A:110:GLU:HG2	1:A:113:LYS:HD2	1.81	0.63
3:J:239:VAL:HA	3:J:253:PHE:HE2	1.63	0.63
3:B:683:ASN:O	3:B:685:GLN:N	2.32	0.63
2:C:183:ASP:O	2:C:187:ALA:HB2	1.98	0.63
3:B:249:GLN:HG3	3:B:250:ASN:N	2.14	0.63
6:R:34:LEU:HD22	6:R:38:TYR:CE2	2.34	0.63
3:B:356:VAL:HG11	3:B:404:VAL:HG12	1.81	0.62
1:A:316:LYS:HD2	3:B:1049:LEU:O	1.99	0.62
12:X:37:VAL:HG22	12:X:38:ARG:H	1.63	0.62
2:M:150:GLU:HG3	2:M:227:LEU:CD2	2.29	0.62
3:J:296:TYR:O	3:J:297:PHE:HB2	1.99	0.62
6:F:23:ASP:O	6:F:26:ARG:HB2	1.99	0.62
1:I:475:GLU:CD	2:M:383:THR:HG21	2.19	0.62
3:B:591:ILE:HG12	3:B:612:LYS:HZ3	1.64	0.62
1:I:823:LEU:HD13	2:M:75:ALA:CB	2.27	0.62
2:M:391:ARG:HH21	9:U:42:GLN:HG2	1.64	0.62
12:P:37:VAL:HG22	12:P:38:ARG:H	1.63	0.62
5:E:179:LYS:HZ3	6:F:79:THR:HB	1.64	0.62
3:B:1067:ILE:HG13	3:B:1068:GLY:H	1.64	0.62
1:A:587:VAL:HB	1:A:594:LEU:O	1.99	0.62
1:A:555:PHE:CD2	1:A:631:LEU:HD13	2.34	0.62
3:B:700:ARG:N	11:N:51:SER:O	2.31	0.62
3:J:738:ILE:CD1	3:J:908:ILE:HG23	2.29	0.62
3:B:1085:LYS:O	3:B:1086:SER:OG	2.17	0.62
2:M:389:THR:CG2	9:U:77:THR:HB	2.17	0.62
8:H:25:ILE:HA	8:H:28:ALA:HB3	1.81	0.62
1:I:421:ARG:HB2	1:I:462:MET:HE3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:890:MET:CE	3:B:891:LEU:H	2.13	0.62
1:I:833:GLU:HG3	1:I:839:ARG:HG3	1.81	0.62
3:B:469:ASN:HD22	3:B:469:ASN:N	1.98	0.62
2:M:338:LYS:HA	2:M:338:LYS:HE2	1.80	0.62
7:S:104:LYS:HB3	7:S:104:LYS:NZ	2.14	0.62
3:B:1033:ARG:HD2	3:B:1037:ILE:HD11	1.80	0.62
3:B:1045:LEU:O	3:B:1049:LEU:HB3	1.99	0.62
1:A:877:GLY:C	3:J:377:ARG:NH1	2.47	0.62
3:J:81:SER:HB3	3:J:84:GLU:HG3	1.82	0.62
6:R:50:GLU:HA	6:R:53:GLN:HB2	1.79	0.62
3:J:794:ASP:N	3:J:794:ASP:OD1	2.32	0.62
1:I:483:HIS:CD2	1:I:625:LYS:HG3	2.35	0.62
5:Q:143:ARG:CZ	5:Q:168:TYR:O	2.48	0.62
5:Q:83:GLU:O	5:Q:145:ARG:HA	1.99	0.62
3:B:1012:LEU:O	3:B:1095:TYR:HE2	1.82	0.62
3:J:1033:ARG:HD2	3:J:1037:ILE:HD11	1.80	0.62
3:B:60:LEU:HD22	3:B:98:LEU:HD21	1.80	0.62
1:A:865:THR:HG21	1:A:870:ARG:NH1	2.14	0.62
3:J:931:LYS:HE2	3:J:985:PHE:O	1.98	0.62
8:T:12:ARG:HH12	8:T:55:ILE:HB	1.65	0.62
3:B:356:VAL:HG22	3:B:393:ARG:HH12	1.65	0.62
3:J:963:LEU:HD22	4:O:208:GLU:HG3	1.82	0.62
3:B:473:MET:SD	3:B:475:GLN:N	2.72	0.62
7:G:66:TYR:HD1	7:G:114:ARG:NH1	1.98	0.62
4:O:175:ASN:HA	4:O:195:LEU:CD1	2.22	0.62
11:W:22:ILE:HD13	11:W:23:THR:N	2.14	0.62
3:B:650:ILE:HD13	3:B:650:ILE:N	2.11	0.62
2:C:139:GLU:HA	2:C:142:ARG:HB2	1.80	0.62
7:S:101:LEU:C	7:S:103:VAL:H	2.02	0.62
1:I:834:TYR:CE1	9:U:80:ARG:HD3	2.34	0.62
3:J:881:ARG:HH11	3:J:989:TYR:CB	2.12	0.62
2:C:124:ILE:HG23	2:C:272:VAL:HG22	1.82	0.62
2:C:125:TYR:HD1	2:C:271:LYS:HB3	1.64	0.62
1:A:336:GLU:OE1	1:A:436:ARG:NH1	2.33	0.62
2:C:31:ASP:O	2:C:34:ASN:N	2.33	0.62
1:I:93:PHE:HB3	1:I:184:LEU:HD21	1.80	0.62
1:I:376:ASN:O	1:I:377:TYR:CB	2.46	0.62
2:C:276:ASN:ND2	2:C:279:GLU:HB2	2.09	0.62
5:Q:31:ARG:C	5:Q:33:GLN:H	2.01	0.62
1:I:864:LYS:HG3	2:M:32:LEU:HD11	1.81	0.62
4:D:137:GLN:HE21	11:N:63:THR:HG22	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:GLU:CD	2:C:383:THR:HG21	2.20	0.62
3:J:707:ALA:O	3:J:711:ILE:HG13	1.99	0.62
1:A:418:LEU:HD21	3:B:1044:LEU:CD2	2.20	0.62
1:I:104:VAL:HG12	1:I:104:VAL:O	2.00	0.62
4:O:247:LYS:HA	4:O:250:ILE:HD12	1.81	0.62
1:I:11:PHE:HA	3:J:1110:SER:O	2.00	0.62
1:I:98:CYS:HA	1:I:146:CYS:SG	2.40	0.62
3:B:296:TYR:O	3:B:297:PHE:HB2	1.99	0.62
8:H:29:TYR:HA	8:H:32:LEU:CD1	2.30	0.61
3:B:702:LEU:HD12	11:N:51:SER:HB3	1.79	0.61
1:I:502:TYR:HE1	1:I:636:ILE:HD11	1.65	0.61
9:K:82:LEU:HD23	9:K:82:LEU:N	2.10	0.61
3:J:881:ARG:HD2	3:J:989:TYR:HD2	1.64	0.61
3:J:806:GLY:O	3:J:839:THR:HB	2.00	0.61
7:S:15:ILE:HD13	7:S:53:GLU:HB3	1.80	0.61
1:A:866:VAL:HG12	1:A:869:ASN:H	1.65	0.61
1:A:289:HIS:HB2	1:A:295:LEU:HD21	1.81	0.61
5:Q:110:ILE:HD13	5:Q:113:ILE:HG21	1.82	0.61
3:B:587:PRO:O	3:B:588:LEU:HD23	2.00	0.61
3:B:21:LYS:HE2	3:B:475:GLN:OE1	2.00	0.61
2:C:390:MET:HG3	5:E:57:GLY:N	2.16	0.61
2:C:125:TYR:CD1	2:C:271:LYS:HB3	2.36	0.61
2:M:49:ASP:O	2:M:52:PHE:N	2.32	0.61
3:J:289:ALA:O	3:J:293:ILE:HG12	2.00	0.61
4:O:131:VAL:HA	11:W:2:LEU:HD11	1.81	0.61
1:A:710:THR:O	1:A:714:ILE:HG12	2.00	0.61
3:J:679:LEU:HD23	3:J:716:ARG:HG2	1.81	0.61
1:A:506:ALA:HA	1:A:635:PHE:CE2	2.36	0.61
3:J:764:LYS:HZ1	3:J:814:VAL:H	1.47	0.61
1:A:812:ARG:NE	2:C:86:THR:HG23	2.14	0.61
1:A:833:GLU:HG3	1:A:839:ARG:HG3	1.82	0.61
10:V:3:ILE:HG23	10:V:15:LEU:HD21	1.82	0.61
3:J:763:VAL:HA	3:J:770:GLU:HG3	1.83	0.61
1:I:239:LEU:HD22	1:I:276:TYR:CE1	2.35	0.61
3:J:484:ILE:H	3:J:484:ILE:HD12	1.65	0.61
3:B:356:VAL:CG1	3:B:404:VAL:HG12	2.31	0.61
7:G:63:ARG:HA	7:G:114:ARG:NH2	2.16	0.61
1:I:426:HIS:HD2	1:I:490:ARG:HH12	1.45	0.61
3:B:683:ASN:C	3:B:685:GLN:H	2.04	0.61
3:B:448:THR:O	3:B:450:TRP:N	2.33	0.61
7:G:87:ASN:C	7:G:89:GLY:N	2.53	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:391:ARG:NH1	2:C:391:ARG:CG	2.50	0.61
9:K:50:LEU:HD23	9:K:75:PRO:HD3	1.83	0.61
2:C:107:LEU:O	2:C:110:ILE:HG22	2.00	0.61
1:I:501:ASP:OD2	3:J:913:HIS:CD2	2.54	0.61
2:M:309:ASP:OD2	2:M:310:ILE:N	2.34	0.61
1:I:371:LYS:NZ	1:I:373:PRO:HD3	2.16	0.61
1:A:238:LYS:HD3	1:A:276:TYR:HA	1.81	0.61
1:A:827:LEU:HD11	2:C:315:LEU:CD1	2.30	0.61
2:M:127:THR:OG1	2:M:130:TYR:O	2.19	0.61
3:J:965:ASP:O	3:J:967:THR:N	2.33	0.61
3:J:934:ALA:O	11:W:46:ARG:HD3	1.99	0.61
2:M:274:THR:HG22	2:M:275:ASN:N	2.09	0.61
2:C:270:ALA:HA	8:H:14:HIS:ND1	2.15	0.61
3:B:557:HIS:H	3:B:623:ASN:ND2	1.97	0.61
3:B:739:ILE:HG23	3:B:909:ILE:HB	1.81	0.61
3:J:28:LEU:HG	3:J:122:MET:CE	2.30	0.61
2:M:269:VAL:HA	2:M:272:VAL:HG23	1.81	0.61
1:A:85:GLY:HA3	2:C:355:LEU:CD1	2.31	0.61
3:J:450:TRP:HZ3	3:J:621:GLU:OE2	1.84	0.61
2:C:311:ARG:HD3	2:C:311:ARG:H	1.66	0.61
1:I:632:PHE:HA	1:I:635:PHE:CE1	2.35	0.61
4:D:106:PRO:HA	4:D:134:GLY:HA2	1.81	0.61
10:V:74:GLU:HA	10:V:77:ARG:HE	1.65	0.61
3:J:291:GLN:C	3:J:293:ILE:H	2.04	0.61
6:F:19:LYS:HG3	6:F:49:ALA:HB2	1.83	0.61
4:O:23:GLU:OE1	10:V:34:ARG:NH2	2.34	0.61
1:I:720:ASP:O	1:I:722:PHE:N	2.33	0.61
6:F:14:TYR:HD1	6:F:14:TYR:N	1.98	0.61
2:C:16:LYS:O	2:C:20:ALA:HB3	2.01	0.61
1:A:105:LYS:NZ	1:A:108:GLU:HB2	2.16	0.61
3:B:6:THR:HG22	3:B:7:ILE:H	1.66	0.61
11:W:7:CYS:SG	11:W:48:MET:HG3	2.41	0.61
4:O:111:SER:CA	4:O:114:ILE:HD13	2.27	0.61
9:K:71:ARG:O	9:K:72:GLY:C	2.37	0.61
6:F:14:TYR:CD1	6:F:14:TYR:N	2.69	0.61
3:J:686:LEU:H	3:J:686:LEU:HD12	1.64	0.61
10:L:7:LYS:HE3	10:L:12:TYR:HE2	1.65	0.61
8:H:49:ASP:OD2	8:H:50:PRO:HD2	2.01	0.61
1:I:856:PHE:CE2	2:M:73:VAL:HG21	2.35	0.61
1:I:595:GLU:HB3	7:S:91:LYS:HE2	1.82	0.61
3:J:495:VAL:O	3:J:528:GLY:HA3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:70:ILE:N	2:C:70:ILE:CD1	2.64	0.61
1:A:637:ARG:HD3	1:A:640:GLU:CD	2.20	0.61
8:T:12:ARG:NH1	8:T:55:ILE:HB	2.15	0.61
1:I:866:VAL:HG12	1:I:869:ASN:H	1.65	0.61
1:A:176:THR:O	1:A:180:ILE:HG13	2.00	0.61
1:A:191:ASP:HA	1:A:194:ILE:HD11	1.81	0.61
2:M:237:ILE:HG13	2:M:238:LYS:H	1.66	0.60
1:A:121:ILE:HG21	13:Y:66:LYS:HE3	1.81	0.60
1:I:329:ASP:CG	1:I:332:ILE:HD12	2.21	0.60
2:M:104:LEU:HB3	2:M:105:PRO:CD	2.30	0.60
1:I:856:PHE:HE2	2:M:73:VAL:HG21	1.65	0.60
3:J:881:ARG:HD2	3:J:989:TYR:CD2	2.36	0.60
3:B:458:THR:HG21	3:B:465:GLY:N	2.15	0.60
3:J:249:GLN:HG3	3:J:250:ASN:N	2.15	0.60
3:J:163:THR:HG23	3:J:428:ARG:O	2.01	0.60
5:Q:13:ILE:HG23	5:Q:25:ILE:HG21	1.83	0.60
1:A:506:ALA:HA	1:A:635:PHE:CD2	2.36	0.60
1:A:853:ASP:CB	2:C:311:ARG:HH12	2.12	0.60
3:J:81:SER:O	3:J:84:GLU:HB2	2.01	0.60
1:I:155:LYS:H	1:I:155:LYS:NZ	1.99	0.60
1:I:734:ARG:HG3	3:J:917:SER:HB3	1.82	0.60
1:A:531:LYS:O	1:A:532:ILE:HB	2.00	0.60
3:J:298:LEU:C	3:J:300:HIS:H	2.05	0.60
3:B:759:SER:HB3	3:B:863:LYS:HA	1.81	0.60
1:I:58:CYS:CB	1:I:59:PRO:HD3	2.31	0.60
3:B:873:THR:HG22	3:B:874:ILE:N	2.14	0.60
1:A:640:GLU:OE1	3:B:974:ARG:NH1	2.34	0.60
1:A:328:PRO:HG3	1:A:457:PHE:CD1	2.36	0.60
5:Q:110:ILE:O	5:Q:113:ILE:HG22	2.00	0.60
3:J:958:LEU:HD21	4:O:181:ASN:O	2.01	0.60
3:J:60:LEU:HD22	3:J:98:LEU:HD21	1.82	0.60
3:J:87:LEU:HD23	3:J:688:THR:CG2	2.31	0.60
1:A:798:HIS:HE2	3:B:663:SER:H	1.50	0.60
3:B:803:GLU:HB3	3:B:805:LYS:NZ	2.16	0.60
2:M:303:GLU:O	2:M:304:GLN:HG2	2.01	0.60
8:H:23:LEU:HB2	8:H:62:ILE:O	2.01	0.60
3:B:160:VAL:O	3:B:411:SER:HA	2.02	0.60
9:U:87:ILE:HG22	9:U:87:ILE:O	2.01	0.60
3:J:356:VAL:HG22	3:J:393:ARG:HH12	1.65	0.60
9:K:41:LEU:O	9:K:43:LEU:N	2.34	0.60
3:J:1004:ARG:NH1	3:J:1024:GLY:HA2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:781:ARG:HD3	3:B:782:GLY:H	1.67	0.60
3:B:707:ALA:O	3:B:711:ILE:HG13	2.01	0.60
3:J:902:LYS:HB2	11:W:42:ARG:NH1	2.15	0.60
2:C:392:PRO:HG3	5:E:66:THR:HG21	1.82	0.60
3:B:727:MET:HE1	3:B:898:PRO:CG	2.31	0.60
1:I:531:LYS:O	1:I:532:ILE:HB	2.00	0.60
7:S:80:GLU:CG	7:S:81:LEU:H	2.14	0.60
3:B:197:ARG:HB2	3:B:199:PRO:HD3	1.84	0.60
3:B:741:ASN:OD1	3:B:743:SER:N	2.34	0.60
2:M:286:ILE:HD12	8:T:45:ILE:HG13	1.84	0.60
1:A:859:TYR:CB	2:C:64:ILE:HG12	2.32	0.60
1:A:81:VAL:HG12	1:A:270:GLN:HG3	1.84	0.60
3:B:163:THR:HG23	3:B:428:ARG:O	2.02	0.60
3:J:367:TYR:CD2	3:J:367:TYR:C	2.75	0.60
1:I:847:GLN:HG2	2:M:318:ASP:OD1	2.02	0.60
3:B:298:LEU:C	3:B:300:HIS:H	2.04	0.60
1:A:491:TYR:CB	1:A:607:GLN:OE1	2.50	0.60
3:J:183:ILE:HB	3:J:207:ASP:C	2.22	0.60
1:A:71:HIS:ND1	3:B:1070:TYR:HE2	1.98	0.60
7:G:80:GLU:O	7:G:81:LEU:HD12	2.00	0.60
1:A:155:LYS:NZ	1:A:155:LYS:H	1.99	0.60
3:B:40:GLN:HE22	3:B:62:LYS:HA	1.66	0.60
3:J:971:TYR:CZ	4:O:165:ARG:HA	2.37	0.60
1:A:632:PHE:HA	1:A:635:PHE:HD1	1.63	0.60
3:B:38:LYS:HA	3:B:41:GLU:HG3	1.84	0.60
5:E:66:THR:CG2	5:E:68:HIS:NE2	2.64	0.60
1:A:376:ASN:O	1:A:377:TYR:CB	2.43	0.60
9:U:41:LEU:O	9:U:45:MET:HG2	2.01	0.60
3:B:555:VAL:O	3:B:620:GLU:HG3	2.00	0.60
3:J:197:ARG:HB2	3:J:199:PRO:HD3	1.83	0.60
1:A:868:VAL:HG22	2:C:39:LYS:NZ	2.17	0.60
3:B:686:LEU:H	3:B:686:LEU:HD12	1.67	0.60
9:K:90:LEU:N	9:K:90:LEU:CD2	2.57	0.60
1:I:447:LEU:HD13	3:J:734:MET:SD	2.42	0.60
1:I:510:THR:O	1:I:549:LYS:HG3	2.02	0.60
3:J:83:MET:HG3	3:J:142:GLY:O	2.01	0.60
2:M:133:ASP:HB2	2:M:136:LYS:HG2	1.84	0.60
10:L:1:MET:HA	10:L:18:GLU:O	2.01	0.60
1:I:446:ASN:C	1:I:446:ASN:HD22	2.05	0.59
1:I:317:ARG:NH1	3:J:1018:GLU:HG3	2.17	0.59
2:M:390:MET:CB	5:Q:56:GLU:CG	2.80	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ARG:HA	1:A:233:ASP:OD1	2.02	0.59
1:I:839:ARG:HH12	8:T:37:ILE:HG23	1.65	0.59
1:A:93:PHE:HB3	1:A:184:LEU:HD21	1.84	0.59
7:G:87:ASN:O	7:G:89:GLY:N	2.35	0.59
2:M:318:ASP:O	2:M:322:ARG:CD	2.50	0.59
1:A:329:ASP:CG	1:A:332:ILE:HD12	2.22	0.59
3:B:881:ARG:HH11	3:B:989:TYR:CB	2.15	0.59
1:A:354:THR:HB	1:A:355:PRO:HD2	1.84	0.59
1:A:133:THR:HB	1:A:137:LYS:NZ	2.16	0.59
1:I:355:PRO:O	1:I:356:TRP:CD1	2.55	0.59
3:J:75:ARG:H	3:J:75:ARG:HE	1.47	0.59
10:V:72:ALA:HA	10:V:75:ASN:HB2	1.82	0.59
1:I:849:ALA:HB2	9:U:15:PHE:CD1	2.37	0.59
3:J:230:LEU:HD13	3:J:312:ALA:HA	1.82	0.59
9:U:19:PHE:O	9:U:20:ILE:C	2.40	0.59
3:B:484:ILE:H	3:B:484:ILE:HD12	1.67	0.59
3:J:902:LYS:HE2	11:W:41:LYS:HB3	1.83	0.59
3:J:479:GLY:HA2	3:J:552:GLU:HB3	1.84	0.59
2:M:330:GLY:O	2:M:335:THR:OG1	2.20	0.59
3:J:183:ILE:HD13	3:J:183:ILE:O	2.03	0.59
1:I:720:ASP:C	1:I:722:PHE:H	2.04	0.59
1:I:290:ARG:HD2	1:I:291:SER:N	2.16	0.59
1:I:678:LYS:HD2	1:I:684:LEU:HG	1.84	0.59
1:I:84:VAL:HG11	1:I:274:ALA:HB1	1.83	0.59
1:A:450:CYS:HB2	1:A:451:PRO:HD3	1.84	0.59
1:A:284:LEU:N	1:A:285:PRO:HD2	2.17	0.59
4:O:183:CYS:SG	16:O:1001:F3S:S1	3.00	0.59
2:M:144:LEU:HA	2:M:146:TYR:CE2	2.37	0.59
3:J:577:ARG:HE	3:J:578:PRO:HD2	1.66	0.59
3:J:1113:LEU:CD1	3:J:1113:LEU:H	2.03	0.59
3:J:448:THR:O	3:J:450:TRP:N	2.35	0.59
3:J:1004:ARG:HH12	3:J:1016:PRO:HB3	1.67	0.59
3:B:799:SER:O	3:B:800:PRO:O	2.19	0.59
3:B:735:GLU:O	3:B:736:ASP:C	2.40	0.59
5:Q:110:ILE:HG23	5:Q:118:LEU:HB3	1.84	0.59
5:Q:53:THR:OG1	5:Q:71:GLU:HB2	2.03	0.59
3:B:473:MET:SD	3:B:474:ALA:N	2.76	0.59
2:C:390:MET:HB2	5:E:56:GLU:HG2	1.85	0.59
1:A:558:LYS:HG3	3:J:104:GLU:CB	2.26	0.59
1:I:491:TYR:CB	1:I:607:GLN:OE1	2.49	0.59
2:M:78:VAL:O	2:M:81:PRO:HD2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:309:ASP:C	2:M:309:ASP:OD2	2.41	0.59
1:A:58:CYS:CB	1:A:59:PRO:HD3	2.29	0.59
3:J:99:THR:O	3:J:99:THR:HG22	2.02	0.59
3:J:315:LEU:O	3:J:319:ILE:HG12	2.02	0.59
3:B:75:ARG:H	3:B:75:ARG:HE	1.50	0.59
2:M:389:THR:HG21	9:U:79:ARG:HH11	1.67	0.59
1:A:502:TYR:HE1	1:A:636:ILE:HD11	1.66	0.59
1:A:316:LYS:HE2	3:B:1054:ASP:OD2	2.03	0.59
2:C:321:THR:HG22	2:C:321:THR:O	2.02	0.59
3:J:700:ARG:N	11:W:51:SER:O	2.36	0.59
9:K:45:MET:HE3	9:K:45:MET:HA	1.82	0.59
9:K:74:LEU:H	9:K:74:LEU:HD12	1.65	0.59
6:R:30:SER:OG	6:R:34:LEU:HB3	2.02	0.59
4:D:69:SER:HA	4:D:72:ALA:HB3	1.84	0.59
9:K:54:ASN:HD21	9:K:58:SER:HB2	1.67	0.59
1:I:518:LYS:HE2	1:I:544:GLU:HB2	1.83	0.59
3:B:68:PRO:HD3	3:B:129:PRO:HG2	1.85	0.59
1:A:878:TRP:N	3:J:377:ARG:HH12	2.00	0.59
9:K:50:LEU:CD2	9:K:75:PRO:HD3	2.33	0.59
1:I:847:GLN:OE1	1:I:850:TYR:HA	2.02	0.59
1:A:249:LEU:HB3	1:A:266:TRP:CH2	2.38	0.59
4:D:131:VAL:HA	11:N:2:LEU:HD11	1.84	0.59
1:A:720:ASP:O	1:A:722:PHE:N	2.33	0.59
1:I:659:LYS:O	1:I:663:ASN:HB2	2.02	0.59
11:W:18:TRP:CD1	11:W:49:LEU:HD22	2.38	0.59
1:I:812:ARG:HE	2:M:86:THR:HG23	1.68	0.59
1:I:522:GLN:HG2	10:V:40:PHE:CE1	2.37	0.59
5:E:141:LYS:HB2	5:E:172:LEU:HG	1.85	0.59
1:A:644:PHE:HA	1:A:724:PHE:CE2	2.37	0.59
1:A:530:VAL:HG13	1:A:530:VAL:O	2.02	0.59
3:J:900:THR:HG22	3:J:970:VAL:HG12	1.84	0.59
1:I:826:ALA:H	2:M:335:THR:HG22	1.66	0.59
1:A:97:THR:HG22	1:A:99:ARG:H	1.67	0.59
1:A:321:SER:O	1:A:322:SER:HB2	2.03	0.59
1:A:750:GLN:HG3	1:A:782:ILE:CD1	2.32	0.59
3:B:123:LEU:O	3:B:125:SER:N	2.36	0.59
7:G:40:PHE:HA	7:G:92:TYR:HD1	1.68	0.59
13:Y:67:LEU:O	13:Y:71:ASN:ND2	2.36	0.59
2:C:55:ALA:CA	2:C:58:GLU:HB2	2.31	0.59
8:T:59:PRO:HA	8:T:81:VAL:HB	1.84	0.59
1:I:508:LEU:O	1:I:514:THR:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:730:THR:HB	3:B:732:TYR:CD1	2.36	0.59
4:O:259:LYS:O	4:O:263:VAL:CG2	2.51	0.59
3:J:325:LEU:HD11	3:J:331:GLU:H	1.67	0.59
1:A:569:SER:HB2	1:A:584:SER:HG	1.67	0.59
4:D:51:SER:HB2	4:D:52:PRO:HD2	1.85	0.59
2:M:188:ILE:HG23	2:M:190:ARG:H	1.68	0.59
5:Q:64:GLY:H	9:U:41:LEU:CD2	2.16	0.58
3:B:171:ARG:HH22	3:B:569:ASN:HD21	1.49	0.58
3:J:416:ARG:NH1	3:J:687:ARG:NH2	2.51	0.58
8:H:31:ILE:HD11	9:K:13:LEU:HG	1.84	0.58
10:V:6:LEU:HB2	10:V:14:GLU:O	2.03	0.58
1:A:752:VAL:C	1:A:754:GLY:H	2.06	0.58
1:I:816:SER:OG	2:M:83:THR:HG22	2.02	0.58
2:M:202:GLU:O	2:M:203:ASP:HB2	2.03	0.58
2:C:359:ALA:C	2:C:361:GLY:H	2.06	0.58
4:O:180:VAL:HG21	4:O:190:LEU:HG	1.85	0.58
2:C:268:ASP:OD1	2:C:270:ALA:HB3	2.03	0.58
3:B:183:ILE:HG12	3:B:206:LYS:HB3	1.84	0.58
3:B:1069:TRP:CD1	3:B:1088:LEU:HD22	2.38	0.58
1:I:530:VAL:HG13	1:I:530:VAL:O	2.02	0.58
3:J:325:LEU:HD22	3:J:330:ARG:HG3	1.85	0.58
1:A:704:LEU:HD22	1:A:781:PHE:CE1	2.38	0.58
3:J:193:THR:HG21	3:J:197:ARG:H	1.68	0.58
3:J:12:ARG:HH11	3:J:596:LYS:HG2	1.68	0.58
2:C:373:ILE:HG12	3:B:1049:LEU:HD13	1.85	0.58
2:M:112:ASP:HA	2:M:328:GLN:HB3	1.86	0.58
1:I:575:CYS:HG	1:I:580:CYS:HG	0.80	0.58
1:I:549:LYS:NZ	7:S:89:GLY:HA2	2.17	0.58
1:I:512:LYS:HE2	7:S:91:LYS:HE3	1.85	0.58
3:B:569:ASN:HB3	3:B:574:ARG:HH12	1.68	0.58
1:A:491:TYR:HD1	1:A:607:GLN:HE22	1.49	0.58
1:I:749:GLN:H	1:I:781:PHE:HA	1.69	0.58
3:J:325:LEU:CD1	3:J:331:GLU:H	2.16	0.58
4:O:131:VAL:HG22	4:O:132:LEU:N	2.18	0.58
1:A:720:ASP:C	1:A:722:PHE:H	2.06	0.58
6:F:13:PRO:HG2	6:F:16:VAL:HG23	1.85	0.58
3:B:419:TRP:CZ3	3:B:712:GLY:HA3	2.38	0.58
1:I:345:LYS:NZ	1:I:370:ASP:O	2.35	0.58
2:M:70:ILE:O	2:M:71:GLY:C	2.41	0.58
3:J:87:LEU:HD23	3:J:688:THR:HG21	1.86	0.58
1:A:48:ARG:HB2	1:A:59:PRO:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U:90:LEU:HD23	9:U:90:LEU:H	1.68	0.58
3:J:707:ALA:C	3:J:709:ASP:H	2.07	0.58
4:O:69:SER:HA	4:O:72:ALA:HB3	1.85	0.58
1:I:569:SER:HB2	1:I:584:SER:OG	2.02	0.58
2:C:15:GLU:HG3	2:C:18:LYS:HD2	1.85	0.58
5:Q:147:ILE:CD1	5:Q:163:THR:HB	2.15	0.58
1:A:301:ARG:HH12	1:A:312:ASN:HD21	1.52	0.58
1:A:830:LEU:CD2	1:A:840:SER:HB3	2.26	0.58
1:I:825:ASN:O	1:I:826:ALA:C	2.41	0.58
3:B:183:ILE:CG1	3:B:206:LYS:HB3	2.33	0.58
1:I:106:ILE:HG22	1:I:107:SER:N	2.17	0.58
4:O:239:GLU:HA	4:O:242:LEU:HD12	1.85	0.58
3:J:160:VAL:O	3:J:411:SER:HA	2.03	0.58
3:B:518:SER:HB3	3:B:564:ASN:ND2	2.19	0.58
1:I:859:TYR:HB2	2:M:64:ILE:CG2	2.33	0.58
2:M:104:LEU:O	2:M:108:ILE:HG12	2.03	0.58
1:I:83:HIS:HB3	1:I:86:LEU:HB2	1.86	0.58
5:E:97:ILE:HD13	5:E:136:ILE:HG21	1.85	0.58
3:J:557:HIS:H	3:J:623:ASN:ND2	2.01	0.58
3:J:992:LYS:CE	3:J:996:MET:SD	2.91	0.58
3:B:739:ILE:HG12	3:B:890:MET:O	2.03	0.58
1:A:155:LYS:HZ1	1:A:155:LYS:H	1.52	0.58
1:A:509:LEU:O	1:A:548:GLY:HA3	2.03	0.58
1:A:392:LYS:O	1:A:394:ARG:HB2	2.04	0.58
2:C:115:LYS:HG3	2:C:115:LYS:O	2.03	0.58
12:X:26:CYS:HG	12:X:29:CYS:HB2	1.67	0.58
2:M:277:ILE:C	2:M:279:GLU:N	2.57	0.58
2:M:310:ILE:HG22	2:M:314:LEU:CD2	2.32	0.58
3:J:762:GLU:O	3:J:764:LYS:HG3	2.03	0.58
1:I:353:ILE:HG13	1:I:361:LEU:CD2	2.32	0.58
3:B:873:THR:CG2	3:B:874:ILE:N	2.65	0.58
8:H:46:ARG:NH2	13:Y:78:ARG:HH11	2.00	0.58
3:B:227:MET:HE1	3:B:232:ILE:HG13	1.85	0.58
6:R:3:SER:OG	6:R:4:VAL:N	2.36	0.58
1:I:803:ARG:HG2	3:J:444:ASP:HA	1.86	0.58
1:I:301:ARG:HH12	1:I:312:ASN:HD21	1.52	0.58
3:B:445:LEU:HD11	3:B:455:PRO:HB3	1.86	0.58
4:O:98:ILE:CD1	4:O:114:ILE:HG13	2.30	0.58
2:M:295:ARG:HA	2:M:298:SER:HB2	1.86	0.58
5:Q:3:LYS:HB2	6:R:10:HIS:O	2.04	0.58
3:B:794:ASP:N	3:B:794:ASP:OD1	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:785:SER:H	1:I:788:THR:HB	1.68	0.58
2:M:373:ILE:O	3:J:1049:LEU:HD11	2.04	0.58
2:M:392:PRO:HG3	5:Q:68:HIS:HE1	1.69	0.58
1:I:387:ASP:OD2	1:I:388:LEU:N	2.34	0.58
3:J:1119:VAL:HG22	5:Q:10:ILE:HD13	1.85	0.58
5:E:108:VAL:HG22	5:E:162:LEU:HB2	1.85	0.58
3:B:489:LEU:HD11	3:B:568:VAL:HG21	1.84	0.58
11:W:7:CYS:HB3	11:W:45:CYS:SG	2.44	0.58
1:A:589:LYS:O	1:A:592:ILE:CG1	2.49	0.58
3:J:376:GLY:O	3:J:377:ARG:HB3	2.02	0.58
2:C:389:THR:HG21	9:K:79:ARG:NH1	2.18	0.58
3:J:1045:LEU:O	3:J:1049:LEU:HB3	2.04	0.58
1:I:524:ILE:CG2	1:I:634:VAL:HG13	2.34	0.58
1:I:97:THR:HG22	1:I:99:ARG:H	1.69	0.58
9:U:82:LEU:HD12	9:U:86:LYS:HB3	1.85	0.58
3:B:895:VAL:HG11	4:D:34:LEU:HD21	1.86	0.58
3:J:1031:MET:O	3:J:1034:ASP:HB2	2.04	0.57
2:M:103:GLY:HA2	2:M:106:ARG:CB	2.34	0.57
3:J:881:ARG:NH1	3:J:989:TYR:CB	2.67	0.57
3:B:738:ILE:HG23	3:B:888:ILE:HA	1.86	0.57
3:J:489:LEU:HD11	3:J:568:VAL:HG21	1.85	0.57
4:O:230:ILE:HG13	4:O:242:LEU:HD21	1.85	0.57
8:T:19:LYS:HD2	8:T:19:LYS:H	1.69	0.57
3:B:87:LEU:HD23	3:B:688:THR:CG2	2.34	0.57
3:J:40:GLN:HE22	3:J:62:LYS:HA	1.69	0.57
3:J:457:GLU:HG2	3:J:469:ASN:OD1	2.04	0.57
1:I:289:HIS:HB2	1:I:295:LEU:HD21	1.86	0.57
2:C:49:ASP:O	2:C:52:PHE:N	2.36	0.57
2:C:391:ARG:HB3	9:K:75:PRO:O	2.03	0.57
1:A:355:PRO:O	1:A:356:TRP:CD1	2.57	0.57
1:I:742:GLN:HB2	3:J:919:MET:HE3	1.86	0.57
3:J:324:GLU:O	3:J:325:LEU:HB2	2.04	0.57
1:I:4:LYS:HD2	3:J:1089:PHE:CB	2.35	0.57
3:J:922:GLY:O	3:J:926:GLU:HB2	2.02	0.57
1:I:865:THR:HG21	1:I:870:ARG:NH1	2.19	0.57
2:C:234:ILE:O	2:C:235:LYS:HG3	2.04	0.57
2:M:21:SER:O	2:M:33:LYS:HE3	2.04	0.57
1:I:587:VAL:HB	1:I:594:LEU:O	2.05	0.57
2:C:270:ALA:HA	8:H:14:HIS:CG	2.39	0.57
3:J:801:GLU:HG3	12:X:38:ARG:NH2	2.19	0.57
1:I:249:LEU:HB3	1:I:266:TRP:CH2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ASP:HB2	3:B:1052:ASN:HB3	1.86	0.57
1:I:477:LYS:O	1:I:481:LEU:HB2	2.03	0.57
3:B:853:THR:HG23	12:P:32:LYS:O	2.04	0.57
3:B:14:ILE:HG13	3:B:18:PHE:CE2	2.40	0.57
1:A:594:LEU:CA	7:G:86:LEU:HD22	2.33	0.57
1:A:503:ILE:HD11	1:A:733:ALA:N	2.19	0.57
3:J:662:GLN:O	3:J:663:SER:C	2.43	0.57
3:B:812:GLY:HA2	3:B:836:SER:HB3	1.85	0.57
9:K:91:SER:O	9:K:92:LEU:CB	2.51	0.57
3:B:348:ASP:OD2	3:B:348:ASP:N	2.38	0.57
1:A:785:SER:H	1:A:788:THR:HB	1.70	0.57
3:B:119:LEU:HD12	3:B:120:PRO:HD2	1.86	0.57
1:A:555:PHE:HD2	1:A:631:LEU:HD13	1.69	0.57
2:M:392:PRO:CD	5:Q:56:GLU:HG3	2.34	0.57
3:B:64:ARG:HG2	3:B:97:TRP:CD1	2.39	0.57
1:A:488:THR:HB	1:A:495:ILE:HB	1.86	0.57
1:I:637:ARG:NH1	3:J:974:ARG:HH22	2.02	0.57
3:J:210:PHE:CZ	3:J:323:ILE:HG22	2.39	0.57
3:B:289:ALA:O	3:B:293:ILE:HG12	2.05	0.57
3:B:658:PRO:O	3:B:660:HIS:N	2.35	0.57
1:A:327:SER:HB2	1:A:444:ARG:HD3	1.85	0.57
3:J:119:LEU:HD12	3:J:120:PRO:HD2	1.85	0.57
3:B:172:VAL:HG22	3:B:189:ILE:HD11	1.85	0.57
1:A:477:LYS:O	1:A:481:LEU:HB2	2.05	0.57
2:C:340:SER:HA	2:C:364:GLU:CG	2.34	0.57
3:J:451:GLY:CA	3:J:577:ARG:NH1	2.68	0.57
2:M:61:GLU:C	2:M:63:LEU:H	2.06	0.57
5:Q:18:PHE:HE2	9:U:42:GLN:HG2	1.70	0.57
1:A:607:GLN:O	1:A:608:PRO:C	2.43	0.57
3:B:495:VAL:O	3:B:528:GLY:HA3	2.04	0.57
8:H:63:ILE:CG2	8:H:64:ARG:N	2.67	0.57
3:J:6:THR:HG22	3:J:7:ILE:H	1.69	0.57
3:B:402:ASN:HB2	3:B:410:VAL:CG2	2.34	0.57
3:J:943:THR:HG22	3:J:944:PRO:HD2	1.87	0.57
3:B:159:ARG:HD3	3:B:399:ALA:HA	1.86	0.57
3:B:43:ILE:HG22	3:B:43:ILE:O	2.04	0.57
3:J:702:LEU:HD22	3:J:933:ALA:CB	2.27	0.57
2:M:53:ASP:C	2:M:55:ALA:H	2.07	0.57
1:A:490:ARG:HG3	2:C:77:SER:HB3	1.86	0.57
1:I:249:LEU:HD22	1:I:266:TRP:CE2	2.40	0.57
2:C:70:ILE:HA	2:C:73:VAL:CG2	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:833:GLU:OE2	1:I:839:ARG:HB2	2.05	0.57
3:B:68:PRO:HA	3:B:93:ALA:O	2.05	0.57
11:W:6:ARG:HG2	11:W:11:GLY:O	2.05	0.57
3:J:26:GLN:O	3:J:345:LEU:CD2	2.42	0.57
3:B:727:MET:CE	3:B:898:PRO:HG3	2.35	0.57
1:I:426:HIS:O	1:I:429:SER:HB2	2.04	0.57
2:M:107:LEU:O	2:M:111:VAL:HG23	2.04	0.57
1:A:426:HIS:CE1	1:A:428:ILE:CG2	2.85	0.57
3:B:367:TYR:CD2	3:B:367:TYR:C	2.77	0.57
3:B:315:LEU:O	3:B:319:ILE:HG12	2.04	0.57
3:B:376:GLY:O	3:B:377:ARG:HB3	2.05	0.57
2:C:373:ILE:HD13	3:B:1033:ARG:HD3	1.87	0.57
3:J:338:TYR:HB2	3:J:448:THR:HG21	1.87	0.57
3:J:1054:ASP:HB3	3:J:1095:TYR:H	1.69	0.57
3:J:82:PRO:HG3	3:J:130:ILE:CD1	2.35	0.57
3:B:64:ARG:HG2	3:B:97:TRP:CG	2.39	0.57
1:A:575:CYS:HG	1:A:580:CYS:HB3	1.70	0.57
5:E:88:GLU:H	5:E:99:VAL:HG13	1.68	0.57
1:I:133:THR:HB	1:I:137:LYS:HZ2	1.70	0.57
7:G:80:GLU:HG2	7:G:81:LEU:N	2.20	0.57
1:A:98:CYS:O	1:A:99:ARG:HB2	2.05	0.57
1:I:6:ILE:HD11	3:J:1091:VAL:HG11	1.86	0.57
3:B:116:ILE:HD12	3:B:361:PHE:CZ	2.40	0.57
3:J:683:ASN:O	3:J:685:GLN:N	2.38	0.57
3:B:291:GLN:C	3:B:293:ILE:H	2.08	0.57
5:Q:30:LEU:HD21	5:Q:72:PHE:CE1	2.40	0.57
3:J:116:ILE:HG22	3:J:390:VAL:HG21	1.85	0.57
6:F:15:SER:HA	6:F:18:LYS:NZ	2.19	0.57
3:J:197:ARG:HH22	3:J:359:LYS:HG2	1.70	0.57
1:I:352:ARG:HA	1:I:406:ILE:HA	1.86	0.57
1:A:803:ARG:HG2	3:B:444:ASP:HA	1.86	0.57
1:A:734:ARG:HG3	3:B:917:SER:HB3	1.85	0.57
3:J:445:LEU:HD11	3:J:455:PRO:CB	2.34	0.57
2:M:103:GLY:HA3	2:M:300:VAL:HG13	1.87	0.57
4:D:134:GLY:N	4:D:137:GLN:OE1	2.23	0.57
3:B:291:GLN:O	3:B:295:LYS:HG2	2.05	0.57
1:A:106:ILE:HG22	1:A:107:SER:N	2.20	0.57
2:C:355:LEU:CD2	3:B:1109:ILE:HD11	2.35	0.57
1:A:594:LEU:HA	7:G:86:LEU:CD2	2.33	0.56
1:A:764:ARG:CB	1:A:764:ARG:HH11	2.18	0.56
1:A:825:ASN:O	1:A:826:ALA:C	2.44	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:110:ILE:HD11	2:C:277:ILE:HD11	1.86	0.56
3:B:699:GLN:HB2	3:B:720:ASN:HA	1.87	0.56
4:D:101:GLU:O	4:D:107:ARG:NH1	2.36	0.56
3:J:870:ARG:CZ	3:J:996:MET:SD	2.93	0.56
1:I:764:ARG:HB2	1:I:764:ARG:HH11	1.69	0.56
4:D:53:LEU:HD22	4:D:57:ILE:CG2	2.35	0.56
2:C:139:GLU:HG2	2:C:142:ARG:HD2	1.86	0.56
5:Q:42:LEU:HD23	5:Q:42:LEU:H	1.69	0.56
7:S:17:SER:HB2	7:S:19:GLU:HG3	1.86	0.56
1:I:176:THR:O	1:I:180:ILE:HG13	2.04	0.56
1:A:369:PRO:HA	1:A:410:HIS:HE1	1.70	0.56
1:I:446:ASN:ND2	1:I:448:LEU:H	2.03	0.56
1:I:853:ASP:HB2	2:M:311:ARG:NH1	2.20	0.56
3:J:64:ARG:O	3:J:97:TRP:HB2	2.05	0.56
3:J:739:ILE:HG23	3:J:909:ILE:HB	1.86	0.56
3:J:181:SER:O	3:J:182:ASN:HB2	2.06	0.56
3:J:183:ILE:CD1	3:J:183:ILE:O	2.53	0.56
4:D:133:LEU:HD21	4:D:139:ILE:HG13	1.87	0.56
3:B:193:THR:HG21	3:B:197:ARG:H	1.70	0.56
7:S:18:ILE:O	7:S:18:ILE:HG22	2.05	0.56
3:B:591:ILE:H	3:B:591:ILE:HD12	1.70	0.56
1:I:870:ARG:NH2	2:M:57:LYS:O	2.38	0.56
3:J:171:ARG:HH22	3:J:569:ASN:HD21	1.53	0.56
2:C:390:MET:HE1	5:E:66:THR:HA	1.87	0.56
1:I:116:ARG:HE	1:I:117:ILE:HG12	1.71	0.56
1:I:512:LYS:HE2	7:S:91:LYS:NZ	2.19	0.56
7:S:87:ASN:C	7:S:89:GLY:H	2.09	0.56
2:M:390:MET:HB2	5:Q:56:GLU:HG2	1.87	0.56
4:O:96:ILE:CG1	4:O:143:ALA:HB3	2.36	0.56
3:B:910:LEU:CD2	3:B:911:ASN:N	2.66	0.56
3:B:662:GLN:O	3:B:663:SER:C	2.44	0.56
3:B:457:GLU:OE1	3:B:652:ALA:HB2	2.06	0.56
1:A:749:GLN:N	1:A:781:PHE:HA	2.21	0.56
2:M:262:LEU:HD23	2:M:269:VAL:HG11	1.86	0.56
3:B:419:TRP:HZ3	3:B:712:GLY:HA3	1.70	0.56
1:I:392:LYS:O	1:I:394:ARG:HB2	2.06	0.56
3:B:157:SER:O	3:B:158:GLU:HB2	2.04	0.56
4:D:94:THR:OG1	4:D:95:LYS:N	2.39	0.56
4:O:51:SER:HB2	4:O:52:PRO:HD2	1.87	0.56
3:J:710:ILE:H	3:J:710:ILE:HD13	1.69	0.56
5:Q:124:ARG:HE	5:Q:126:ILE:HD13	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:710:THR:O	1:I:714:ILE:HG12	2.06	0.56
5:Q:113:ILE:O	5:Q:164:MET:HB2	2.05	0.56
1:A:220:ARG:N	1:A:221:PRO:HD3	2.20	0.56
5:E:179:LYS:NZ	6:F:81:ASP:HB2	2.20	0.56
1:I:81:VAL:HG23	1:I:209:LEU:HB2	1.87	0.56
9:K:23:TRP:HE3	9:K:23:TRP:HA	1.69	0.56
1:I:569:SER:HB2	1:I:584:SER:HG	1.69	0.56
3:B:1036:LEU:HD22	3:B:1041:THR:HG21	1.87	0.56
1:I:557:PRO:HD3	1:I:623:TYR:OH	2.05	0.56
7:G:82:LYS:HB2	7:G:95:ILE:HG13	1.86	0.56
3:B:451:GLY:CA	3:B:577:ARG:NH1	2.68	0.56
1:A:345:LYS:HG2	1:A:410:HIS:CD2	2.41	0.56
1:A:816:SER:OG	2:C:83:THR:HA	2.06	0.56
3:B:81:SER:O	3:B:84:GLU:HB2	2.06	0.56
9:K:35:VAL:HG22	9:K:36:ILE:HD13	1.88	0.56
11:N:22:ILE:HD13	11:N:23:THR:N	2.20	0.56
3:B:230:LEU:HD13	3:B:312:ALA:HA	1.88	0.56
2:C:376:GLY:HA2	3:B:1049:LEU:HD21	1.87	0.56
8:H:40:GLU:HG2	8:H:41:GLN:N	2.20	0.56
1:I:727:VAL:O	1:I:729:ALA:O	2.23	0.56
7:G:79:THR:HG22	7:G:80:GLU:H	1.70	0.56
8:T:29:TYR:OH	13:Z:67:LEU:HD13	2.05	0.56
4:O:253:ILE:HG13	10:V:73:ILE:HD13	1.88	0.56
3:B:544:ARG:HB2	3:B:549:ILE:HG22	1.88	0.56
3:J:943:THR:CG2	3:J:944:PRO:HD2	2.35	0.56
1:A:518:LYS:HE2	1:A:544:GLU:HB2	1.87	0.56
3:J:68:PRO:HD3	3:J:129:PRO:HG2	1.87	0.56
3:J:946:TYR:HD2	3:J:947:LYS:H	1.54	0.56
3:J:765:TYR:CG	3:J:766:PRO:HD2	2.41	0.56
3:J:227:MET:HE1	3:J:232:ILE:HG13	1.86	0.56
11:N:3:ILE:HG22	11:N:4:PRO:HD2	1.88	0.56
3:B:1004:ARG:HH12	3:B:1016:PRO:HB3	1.70	0.56
1:I:575:CYS:CB	1:I:580:CYS:HG	2.18	0.56
3:B:719:GLY:O	3:B:989:TYR:CE1	2.59	0.56
1:A:4:LYS:HD3	3:B:1091:VAL:HB	1.88	0.56
3:B:83:MET:O	3:B:87:LEU:HD12	2.06	0.56
3:J:741:ASN:OD1	3:J:743:SER:N	2.39	0.56
1:A:563:HIS:HB2	1:A:872:PHE:HE2	1.70	0.56
2:M:24:LEU:HD13	2:M:33:LYS:HA	1.88	0.56
2:M:80:GLU:HB3	2:M:81:PRO:HD3	1.87	0.56
2:M:72:ILE:N	2:M:72:ILE:CD1	2.63	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:220:ARG:N	1:I:221:PRO:HD3	2.21	0.56
10:V:80:THR:O	10:V:84:ILE:HG12	2.05	0.56
2:C:383:THR:HG22	3:B:1040:GLY:O	2.05	0.56
1:I:55:GLY:O	1:I:57:LYS:N	2.39	0.56
3:J:381:LEU:C	3:J:383:ALA:H	2.09	0.56
2:M:14:GLU:O	2:M:17:VAL:HG12	2.05	0.56
5:Q:11:VAL:HG12	5:Q:12:ARG:H	1.70	0.56
3:J:402:ASN:HB2	3:J:410:VAL:CG2	2.36	0.56
2:C:387:GLU:OE1	9:K:81:ARG:HD2	2.06	0.56
9:U:33:ALA:O	9:U:35:VAL:N	2.39	0.56
3:J:1071:ASP:C	3:J:1073:ASN:H	2.09	0.56
2:C:238:LYS:HB2	2:C:239:ARG:CZ	2.36	0.56
3:J:365:LEU:O	3:J:369:LEU:HB2	2.06	0.56
3:J:687:ARG:NH1	3:J:687:ARG:HG3	2.11	0.56
2:C:386:VAL:HG11	9:K:31:GLU:HA	1.88	0.56
1:A:15:SER:HA	1:A:203:ARG:NH2	2.19	0.56
2:C:70:ILE:H	2:C:70:ILE:CD1	2.19	0.56
2:M:159:ASP:HB3	2:M:163:MET:CB	2.35	0.56
1:A:91:TYR:OH	1:A:153:GLN:O	2.12	0.56
2:C:30:ASP:O	2:C:31:ASP:HB3	2.05	0.56
4:D:34:LEU:HA	4:D:150:GLY:HA3	1.88	0.56
3:B:43:ILE:HG13	3:B:63:ILE:CD1	2.36	0.56
1:A:288:LYS:HG2	1:A:294:PRO:HA	1.88	0.56
1:I:509:LEU:O	1:I:548:GLY:HA3	2.05	0.56
13:Y:63:GLU:O	13:Y:67:LEU:HD13	2.06	0.56
1:I:345:LYS:HG2	1:I:410:HIS:CD2	2.41	0.56
1:I:491:TYR:HD1	1:I:607:GLN:HE22	1.53	0.56
1:I:317:ARG:HB2	3:J:1016:PRO:HB2	1.87	0.56
3:J:82:PRO:HG3	3:J:130:ILE:HD11	1.88	0.56
1:I:155:LYS:CB	1:I:156:ILE:HA	2.35	0.56
3:J:683:ASN:C	3:J:685:GLN:H	2.09	0.56
2:C:286:ILE:O	2:C:289:ALA:HB3	2.05	0.56
1:A:155:LYS:CB	1:A:156:ILE:HA	2.35	0.56
3:B:12:ARG:HH11	3:B:596:LYS:HG2	1.70	0.56
4:D:129:PRO:HG2	11:N:15:ALA:HB1	1.88	0.56
1:I:610:SER:O	1:I:613:HIS:HB3	2.06	0.56
1:I:831:ARG:NH2	2:M:385:MET:HG3	2.20	0.56
2:C:146:TYR:CE1	2:C:237:ILE:HG12	2.41	0.55
3:J:934:ALA:HB2	11:W:47:ARG:HD3	1.87	0.55
2:M:53:ASP:C	2:M:55:ALA:N	2.59	0.55
1:I:563:HIS:HB2	1:I:872:PHE:HE2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:GLN:HB3	3:B:919:MET:HE1	1.88	0.55
1:A:742:GLN:CB	3:B:919:MET:HE3	2.35	0.55
1:I:156:ILE:HD11	1:I:270:GLN:HG2	1.88	0.55
1:I:98:CYS:O	1:I:99:ARG:HB2	2.06	0.55
3:B:1100:LEU:O	3:B:1101:ILE:C	2.44	0.55
1:I:215:PRO:HB2	1:I:219:ILE:HD11	1.88	0.55
3:B:325:LEU:HD13	3:B:330:ARG:H	1.70	0.55
3:J:24:VAL:HG21	3:J:426:LEU:HD13	1.87	0.55
3:J:922:GLY:O	3:J:926:GLU:N	2.34	0.55
5:E:39:LEU:HD22	5:E:41:ASP:H	1.69	0.55
3:J:727:MET:HE3	3:J:898:PRO:HG3	1.87	0.55
3:J:902:LYS:CB	11:W:42:ARG:NH1	2.69	0.55
3:B:760:THR:OG1	3:B:813:LYS:HD2	2.06	0.55
1:A:249:LEU:HD13	1:A:266:TRP:CE3	2.41	0.55
3:B:210:PHE:CZ	3:B:323:ILE:HG22	2.38	0.55
1:I:81:VAL:HG12	1:I:270:GLN:HG3	1.87	0.55
3:B:848:ASP:OD1	3:B:865:ARG:CZ	2.54	0.55
3:B:197:ARG:HH22	3:B:359:LYS:HG2	1.71	0.55
1:I:94:LEU:HD11	1:I:180:ILE:HG23	1.88	0.55
3:B:318:ALA:O	3:B:321:LYS:HB2	2.06	0.55
1:A:650:ASP:HB3	1:A:723:ASN:ND2	2.21	0.55
3:J:552:GLU:HA	3:J:576:ARG:HH22	1.71	0.55
2:M:285:GLY:HA2	8:T:49:ASP:OD2	2.06	0.55
3:B:762:GLU:O	3:B:764:LYS:HG3	2.06	0.55
4:O:137:GLN:HE21	11:W:63:THR:HG22	1.71	0.55
1:A:610:SER:O	1:A:613:HIS:HB3	2.05	0.55
2:M:384:GLY:HA2	5:Q:61:PHE:CZ	2.41	0.55
6:R:14:TYR:N	6:R:14:TYR:CD1	2.74	0.55
2:M:28:ILE:HG13	9:U:18:VAL:HG21	1.89	0.55
3:J:727:MET:HE3	3:J:898:PRO:CG	2.37	0.55
3:J:730:THR:HB	3:J:732:TYR:CD1	2.38	0.55
1:I:293:ARG:HD3	1:I:296:ARG:HH22	1.71	0.55
3:B:390:VAL:O	3:B:394:ILE:HB	2.06	0.55
1:I:25:THR:HG22	1:I:27:ILE:H	1.71	0.55
1:I:849:ALA:HB2	9:U:15:PHE:CG	2.40	0.55
3:J:1074:LYS:HE2	3:J:1074:LYS:HA	1.88	0.55
1:I:752:VAL:C	1:I:754:GLY:H	2.10	0.55
3:J:1009:VAL:HB	3:J:1014:ARG:O	2.06	0.55
1:I:305:LYS:HA	1:I:310:ARG:HD2	1.88	0.55
4:O:34:LEU:HD22	4:O:151:LYS:HB2	1.87	0.55
1:A:549:LYS:HB2	7:G:88:ASN:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1031:MET:O	3:B:1034:ASP:HB2	2.07	0.55
3:J:106:ASN:O	3:J:108:GLU:HG3	2.07	0.55
3:J:910:LEU:HD22	3:J:911:ASN:H	1.70	0.55
3:J:582:VAL:HG13	3:J:586:ASN:N	2.21	0.55
1:A:113:LYS:HA	1:A:116:ARG:HB3	1.88	0.55
1:A:426:HIS:HD2	1:A:490:ARG:HH12	1.51	0.55
3:J:745:VAL:HG21	3:J:891:LEU:HD11	1.88	0.55
10:V:59:THR:HG21	10:V:65:PRO:CD	2.35	0.55
4:D:239:GLU:HA	4:D:242:LEU:HD12	1.89	0.55
1:A:81:VAL:HG23	1:A:209:LEU:HB2	1.86	0.55
3:B:950:ILE:O	3:B:952:GLN:N	2.39	0.55
1:I:26:ALA:HA	1:I:74:HIS:CE1	2.41	0.55
2:C:366:PHE:O	2:C:368:GLY:N	2.39	0.55
4:D:253:ILE:HD11	10:L:76:ILE:HD12	1.88	0.55
1:A:532:ILE:HG23	10:L:40:PHE:CG	2.41	0.55
2:C:318:ASP:O	2:C:322:ARG:CZ	2.54	0.55
2:M:390:MET:O	2:M:391:ARG:HB3	2.04	0.55
1:A:58:CYS:HB2	1:A:59:PRO:CD	2.36	0.55
7:G:79:THR:HG22	7:G:80:GLU:N	2.20	0.55
1:I:604:GLY:C	1:I:606:GLN:N	2.58	0.55
1:I:704:LEU:HD13	1:I:781:PHE:HD1	1.72	0.55
1:I:337:VAL:HG21	1:I:419:PHE:CD1	2.41	0.55
7:S:6:ALA:HB1	7:S:62:ASN:OD1	2.07	0.55
8:T:46:ARG:HD2	8:T:48:SER:HB2	1.87	0.55
5:Q:97:ILE:CD1	5:Q:113:ILE:HD11	2.34	0.55
7:G:86:LEU:HD12	7:G:91:LYS:HG3	1.88	0.55
2:C:146:TYR:HD1	2:C:238:LYS:H	1.55	0.55
3:B:560:THR:HG22	3:B:562:PHE:N	2.17	0.55
1:A:25:THR:HG22	1:A:27:ILE:H	1.71	0.55
3:J:43:ILE:O	3:J:43:ILE:HG22	2.06	0.55
5:Q:46:LEU:HD11	5:Q:77:TYR:HB2	1.88	0.55
2:C:213:ILE:O	2:C:213:ILE:HG22	2.07	0.55
3:J:963:LEU:HD21	4:O:206:CYS:SG	2.47	0.55
11:W:3:ILE:HG22	11:W:4:PRO:HD2	1.88	0.55
11:N:42:ARG:CG	11:N:43:TYR:H	2.19	0.55
3:B:1113:LEU:CD1	3:B:1113:LEU:H	2.07	0.55
2:M:369:VAL:HG21	3:J:1037:ILE:HG21	1.87	0.55
3:J:764:LYS:NZ	3:J:772:LYS:O	2.40	0.55
1:I:595:GLU:HB3	7:S:86:LEU:HD13	1.89	0.55
3:B:726:VAL:HG12	3:B:912:PRO:HG3	1.88	0.55
10:V:38:VAL:HG13	10:V:58:LEU:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:742:GLN:CB	3:J:919:MET:CE	2.85	0.55
1:I:84:VAL:CG1	1:I:274:ALA:HB1	2.36	0.55
3:J:657:TYR:O	3:J:660:HIS:HB2	2.06	0.55
13:Z:76:GLU:O	13:Z:77:LYS:HB3	2.07	0.55
1:A:595:GLU:N	7:G:86:LEU:HD22	2.22	0.55
2:C:257:ASN:OD1	2:C:259:SER:HB2	2.07	0.55
11:N:7:CYS:CB	11:N:45:CYS:SG	2.95	0.55
4:O:106:PRO:HA	4:O:134:GLY:HA2	1.87	0.55
3:B:946:TYR:HD2	3:B:947:LYS:H	1.55	0.55
4:O:21:PRO:HG3	10:V:79:MET:SD	2.47	0.55
3:B:765:TYR:CG	3:B:766:PRO:HD2	2.42	0.55
1:A:763:THR:CG2	1:A:772:TYR:HA	2.37	0.55
1:A:828:SER:C	1:A:830:LEU:N	2.61	0.55
1:A:387:ASP:OD2	1:A:388:LEU:N	2.35	0.55
1:A:501:ASP:OD2	3:B:913:HIS:CD2	2.60	0.55
1:I:589:LYS:O	1:I:592:ILE:CG1	2.54	0.55
1:A:249:LEU:HD22	1:A:266:TRP:CE2	2.42	0.55
3:B:139:ILE:HD13	11:N:61:HIS:CD2	2.42	0.55
2:M:124:ILE:HG21	2:M:267:VAL:HG13	1.89	0.55
10:L:59:THR:CG2	10:L:65:PRO:HD3	2.35	0.55
3:B:346:ALA:O	3:B:350:PHE:N	2.36	0.54
1:A:540:LEU:HB3	7:G:66:TYR:OH	2.06	0.54
3:J:672:MET:HA	3:J:675:GLN:HB2	1.88	0.54
11:N:35:LEU:CD2	11:N:40:VAL:HG21	2.37	0.54
1:I:608:PRO:C	1:I:609:GLU:HG2	2.27	0.54
3:J:616:LEU:HD11	3:J:639:HIS:CE1	2.41	0.54
2:M:311:ARG:H	2:M:311:ARG:HD3	1.72	0.54
3:J:799:SER:O	3:J:800:PRO:O	2.25	0.54
5:E:27:LEU:HB2	5:E:51:VAL:HG11	1.89	0.54
1:I:555:PHE:CD2	1:I:631:LEU:HD13	2.42	0.54
1:I:203:ARG:HG3	1:I:205:GLU:HB2	1.88	0.54
4:O:134:GLY:N	4:O:137:GLN:OE1	2.23	0.54
3:B:147:ASP:OD2	3:B:148:PRO:HD2	2.07	0.54
3:B:727:MET:CE	3:B:898:PRO:CG	2.85	0.54
3:B:70:VAL:HG11	3:B:90:LEU:HD23	1.90	0.54
3:J:98:LEU:C	3:J:98:LEU:HD13	2.27	0.54
3:J:365:LEU:HG	3:J:369:LEU:HD12	1.90	0.54
3:J:157:SER:O	3:J:158:GLU:HB2	2.07	0.54
3:B:800:PRO:HB2	12:P:38:ARG:HA	1.87	0.54
3:B:729:PHE:C	3:B:731:GLY:H	2.11	0.54
4:O:254:GLU:CG	10:V:77:ARG:HH12	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U:82:LEU:HD11	9:U:88:ILE:HD11	1.88	0.54
3:J:159:ARG:HD3	3:J:399:ALA:HA	1.89	0.54
3:B:1010:GLN:HA	3:B:1010:GLN:OE1	2.07	0.54
11:W:35:LEU:CD2	11:W:40:VAL:HG21	2.37	0.54
1:I:868:VAL:O	1:I:871:ILE:HG22	2.06	0.54
5:Q:29:GLU:O	5:Q:33:GLN:HG3	2.07	0.54
3:B:365:LEU:O	3:B:369:LEU:HB2	2.07	0.54
1:I:249:LEU:HD13	1:I:266:TRP:CE3	2.42	0.54
1:A:742:GLN:CB	3:B:919:MET:CE	2.86	0.54
3:J:172:VAL:HG22	3:J:189:ILE:HD11	1.89	0.54
3:B:588:LEU:CD1	3:B:612:LYS:HB3	2.37	0.54
2:M:146:TYR:HB2	2:M:238:LYS:HD3	1.90	0.54
3:J:582:VAL:HG13	3:J:586:ASN:H	1.73	0.54
5:Q:66:THR:HG22	5:Q:68:HIS:NE2	2.21	0.54
1:A:116:ARG:HE	1:A:117:ILE:HG12	1.73	0.54
1:A:448:LEU:HD23	1:A:498:ALA:HA	1.88	0.54
6:F:55:VAL:O	6:F:59:LEU:HB2	2.08	0.54
2:M:291:GLU:HA	2:M:294:ILE:HD12	1.90	0.54
2:M:63:LEU:HD21	9:U:23:TRP:HZ3	1.72	0.54
1:A:470:GLU:HB2	9:K:41:LEU:HD12	1.89	0.54
2:C:107:LEU:O	2:C:111:VAL:HG23	2.07	0.54
3:B:904:VAL:HG21	11:N:42:ARG:HE	1.72	0.54
1:I:446:ASN:HD22	1:I:447:LEU:N	2.05	0.54
3:J:812:GLY:HA2	3:J:836:SER:CB	2.36	0.54
3:B:910:LEU:HD22	3:B:911:ASN:H	1.68	0.54
2:M:52:PHE:O	2:M:56:ILE:HG12	2.08	0.54
1:A:507:TYR:O	1:A:508:LEU:CB	2.56	0.54
1:A:84:VAL:HG11	1:A:274:ALA:HB1	1.88	0.54
1:A:84:VAL:CG1	1:A:274:ALA:HB1	2.37	0.54
3:J:457:GLU:OE1	3:J:652:ALA:HB2	2.08	0.54
3:J:518:SER:HB3	3:J:564:ASN:ND2	2.22	0.54
1:A:345:LYS:NZ	1:A:370:ASP:O	2.35	0.54
4:O:96:ILE:HG13	4:O:143:ALA:HB3	1.89	0.54
9:K:31:GLU:O	9:K:35:VAL:HG13	2.07	0.54
1:A:508:LEU:O	1:A:514:THR:HG23	2.08	0.54
1:I:764:ARG:NH1	1:I:769:PHE:O	2.40	0.54
3:B:707:ALA:C	3:B:709:ASP:H	2.10	0.54
3:J:368:GLN:O	3:J:372:SER:HB3	2.07	0.54
2:M:11:PRO:C	2:M:13:LEU:H	2.10	0.54
10:L:46:PRO:HD2	10:L:53:ILE:HA	1.90	0.54
3:B:463:ASN:HB3	3:B:467:VAL:CG1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:65:ARG:O	6:F:69:ARG:HG3	2.07	0.54
1:A:102:GLY:H	1:A:103:ARG:HE	1.54	0.54
3:B:200:VAL:O	3:B:200:VAL:HG13	2.08	0.54
1:A:563:HIS:HB2	1:A:872:PHE:CE2	2.42	0.54
4:D:175:ASN:HA	4:D:195:LEU:CD1	2.26	0.54
2:M:309:ASP:OD2	2:M:311:ARG:HD3	2.08	0.54
7:S:86:LEU:HD12	7:S:91:LYS:HG3	1.90	0.54
1:A:239:LEU:CD2	1:A:276:TYR:HE1	2.20	0.54
3:B:139:ILE:HG21	11:N:61:HIS:HD2	1.72	0.54
10:V:1:MET:HB3	10:V:20:GLU:OE1	2.08	0.54
4:O:209:CYS:SG	16:O:1001:F3S:S2	3.06	0.54
2:C:322:ARG:HD2	2:C:322:ARG:H	1.73	0.54
3:J:560:THR:HG22	3:J:562:PHE:N	2.16	0.54
1:A:608:PRO:C	1:A:609:GLU:HG2	2.27	0.54
3:B:1071:ASP:C	3:B:1073:ASN:H	2.11	0.54
3:J:803:GLU:HB3	3:J:805:LYS:HZ1	1.72	0.54
2:C:134:ARG:O	2:C:138:LEU:HG	2.08	0.54
1:A:352:ARG:HA	1:A:406:ILE:HA	1.90	0.54
7:S:56:LYS:O	7:S:115:THR:HA	2.06	0.54
6:F:56:ILE:HD11	6:F:70:ALA:HA	1.90	0.54
3:B:926:GLU:HB3	3:B:988:VAL:HG22	1.89	0.54
1:I:448:LEU:HD23	1:I:498:ALA:HA	1.89	0.54
3:J:800:PRO:HD3	3:J:850:VAL:HG23	1.88	0.54
1:I:15:SER:HA	1:I:203:ARG:NH2	2.21	0.54
3:J:803:GLU:HB3	3:J:805:LYS:HZ2	1.68	0.54
1:A:12:GLY:HA2	2:C:358:ALA:O	2.08	0.54
4:D:205:LEU:O	4:D:207:GLU:N	2.40	0.54
4:O:176:CYS:H	4:O:195:LEU:HD21	1.73	0.54
3:J:699:GLN:HB2	3:J:720:ASN:HA	1.90	0.54
3:J:680:TYR:HE1	3:J:687:ARG:HH12	1.56	0.54
6:R:56:ILE:HG23	6:R:69:ARG:HD2	1.90	0.54
2:M:337:GLU:OE1	2:M:337:GLU:N	2.41	0.54
2:M:388:LEU:HD21	9:U:35:VAL:HG12	1.90	0.54
8:H:24:ASN:O	8:H:26:ASP:N	2.41	0.54
3:J:228:ARG:NH2	3:J:233:LEU:O	2.41	0.54
3:B:381:LEU:C	3:B:383:ALA:H	2.11	0.54
3:J:356:VAL:HG11	3:J:404:VAL:HG12	1.91	0.53
3:B:582:VAL:HG13	3:B:586:ASN:N	2.23	0.53
11:W:42:ARG:CG	11:W:43:TYR:H	2.21	0.53
2:M:290:ARG:HB2	2:M:321:THR:HG21	1.90	0.53
1:I:828:SER:C	1:I:830:LEU:N	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:116:SER:OG	4:D:121:VAL:O	2.20	0.53
1:I:133:THR:HB	1:I:137:LYS:NZ	2.23	0.53
3:J:356:VAL:CG1	3:J:404:VAL:HG12	2.38	0.53
1:A:644:PHE:HA	1:A:724:PHE:HE2	1.73	0.53
4:O:190:LEU:HD22	4:O:195:LEU:HA	1.89	0.53
4:O:180:VAL:CG2	4:O:190:LEU:HG	2.38	0.53
1:A:558:LYS:CG	3:J:104:GLU:HB2	2.28	0.53
2:M:373:ILE:HD12	3:J:1049:LEU:HD22	1.90	0.53
3:B:669:GLN:NE2	3:B:881:ARG:HA	2.23	0.53
1:I:91:TYR:OH	1:I:153:GLN:O	2.18	0.53
2:M:301:LEU:O	2:M:304:GLN:HB2	2.09	0.53
1:A:637:ARG:NH1	3:B:974:ARG:HH22	2.06	0.53
1:A:827:LEU:HG	2:C:75:ALA:HB2	1.89	0.53
3:J:367:TYR:HD2	3:J:367:TYR:C	2.10	0.53
1:A:95:LYS:NZ	1:A:152:LYS:HB3	2.23	0.53
3:J:932:TYR:CD2	3:J:932:TYR:O	2.61	0.53
3:B:922:GLY:HA2	3:B:925:MET:CB	2.26	0.53
1:I:369:PRO:HG3	1:I:389:ARG:HA	1.89	0.53
5:E:88:GLU:H	5:E:99:VAL:CG1	2.22	0.53
3:J:346:ALA:O	3:J:350:PHE:N	2.42	0.53
1:A:350:PRO:HG3	1:A:468:GLN:NE2	2.23	0.53
3:J:895:VAL:HG21	4:O:34:LEU:HD21	1.90	0.53
1:A:337:VAL:HG23	1:A:433:HIS:ND1	2.23	0.53
3:B:103:VAL:HG12	3:B:103:VAL:O	2.08	0.53
1:A:647:ARG:HB2	1:A:650:ASP:CG	2.29	0.53
1:A:595:GLU:HB2	7:G:91:LYS:CE	2.31	0.53
2:C:145:GLU:HA	2:C:239:ARG:H	1.73	0.53
3:J:727:MET:CE	3:J:898:PRO:HG3	2.39	0.53
11:W:44:CYS:SG	11:W:45:CYS:N	2.81	0.53
1:I:637:ARG:HH11	3:J:974:ARG:HH22	1.56	0.53
1:I:743:MET:HG3	3:J:919:MET:HE2	1.90	0.53
3:J:321:LYS:HA	3:J:324:GLU:HB3	1.90	0.53
3:B:946:TYR:HD2	3:B:947:LYS:N	2.06	0.53
1:A:750:GLN:HG3	1:A:782:ILE:HD11	1.89	0.53
3:B:321:LYS:HA	3:B:324:GLU:HB3	1.90	0.53
7:S:85:SER:HB3	7:S:92:TYR:HB2	1.90	0.53
3:J:490:TYR:HE1	3:J:527:ILE:CG2	2.21	0.53
3:J:1069:TRP:CD1	3:J:1088:LEU:HD22	2.43	0.53
1:A:764:ARG:NH1	1:A:769:PHE:O	2.42	0.53
3:J:663:SER:HB3	3:J:664:PRO:HD3	1.89	0.53
3:B:1077:TYR:HD1	3:B:1077:TYR:O	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1069:TRP:HE1	3:B:1088:LEU:HB3	1.73	0.53
3:J:27:HIS:HD2	3:J:346:ALA:HB2	1.74	0.53
2:C:299:LYS:CA	2:C:302:ALA:HB3	2.38	0.53
5:Q:109:HIS:HD2	5:Q:111:SER:H	1.56	0.53
7:G:40:PHE:CE2	7:G:113:LEU:HD21	2.44	0.53
3:B:87:LEU:HD23	3:B:688:THR:HG21	1.91	0.53
3:B:94:ALA:O	3:B:119:LEU:N	2.39	0.53
3:J:946:TYR:HD2	3:J:947:LYS:N	2.06	0.53
6:R:14:TYR:N	6:R:14:TYR:HD1	2.06	0.53
6:F:48:ASP:H	6:F:51:SER:HG	1.56	0.53
3:B:578:PRO:HB3	3:B:615:TYR:CE1	2.44	0.53
1:I:607:GLN:O	1:I:608:PRO:C	2.47	0.53
3:J:760:THR:OG1	3:J:813:LYS:HD2	2.08	0.53
1:I:584:SER:OG	1:I:585:TYR:N	2.40	0.53
3:B:943:THR:CG2	3:B:944:PRO:HD2	2.38	0.53
1:A:127:SER:HB2	2:C:360:ARG:NH1	2.23	0.53
1:I:61:CYS:SG	3:J:1070:TYR:HB3	2.48	0.53
8:T:45:ILE:HG22	8:T:81:VAL:N	2.24	0.53
3:J:764:LYS:NZ	3:J:814:VAL:O	2.35	0.53
1:A:58:CYS:CB	1:A:59:PRO:CD	2.86	0.53
3:J:390:VAL:O	3:J:394:ILE:HB	2.08	0.53
1:A:94:LEU:HD11	1:A:180:ILE:HG23	1.90	0.53
3:B:937:GLY:HA2	11:N:50:LEU:HD11	1.90	0.53
6:F:54:LYS:HA	6:F:57:GLU:HB2	1.91	0.53
3:B:368:GLN:O	3:B:372:SER:HB3	2.08	0.53
3:J:971:TYR:CE2	3:J:978:LYS:HB3	2.44	0.53
3:B:474:ALA:HB2	3:B:578:PRO:HG3	1.91	0.53
7:S:21:GLY:HA3	7:S:26:LEU:HD12	1.90	0.53
3:J:54:PRO:O	3:J:56:LEU:N	2.42	0.53
2:C:328:GLN:O	2:C:333:GLY:HA3	2.09	0.53
1:I:874:ARG:HE	2:M:53:ASP:CB	2.21	0.53
2:M:119:THR:N	2:M:120:PRO:HD3	2.24	0.53
2:M:329:ILE:HA	2:M:334:VAL:CG1	2.35	0.53
2:C:190:ARG:CD	2:C:191:LEU:H	2.21	0.53
9:U:82:LEU:HB2	9:U:84:ASN:HB2	1.91	0.53
2:C:76:GLN:O	2:C:80:GLU:N	2.37	0.53
2:M:212:ASN:HD22	2:M:213:ILE:N	2.07	0.53
1:A:26:ALA:HA	1:A:74:HIS:CE1	2.44	0.53
1:A:199:PRO:O	1:A:200:THR:OG1	2.23	0.53
5:E:17:GLU:OE2	5:E:20:LYS:NZ	2.24	0.53
1:I:644:PHE:HA	1:I:724:PHE:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1069:TRP:HE1	3:J:1088:LEU:HB3	1.73	0.53
1:I:541:ALA:N	7:S:72:CYS:O	2.42	0.53
2:M:122:MET:HG2	2:M:274:THR:HG23	1.90	0.53
4:D:190:LEU:HD22	4:D:195:LEU:HA	1.91	0.53
2:M:370:VAL:O	2:M:373:ILE:HG22	2.09	0.53
1:I:827:LEU:HD13	2:M:319:VAL:HG21	1.90	0.53
2:M:391:ARG:H	2:M:392:PRO:CD	2.22	0.53
1:A:113:LYS:HG2	1:A:116:ARG:CZ	2.38	0.53
1:I:209:LEU:HD13	1:I:273:VAL:HG11	1.91	0.53
4:O:34:LEU:HA	4:O:150:GLY:HA3	1.91	0.53
3:J:43:ILE:HG13	3:J:63:ILE:CD1	2.39	0.53
1:A:215:PRO:HB2	1:A:219:ILE:HD11	1.91	0.53
1:A:647:ARG:HB2	1:A:650:ASP:OD1	2.09	0.53
3:B:954:GLN:HA	3:B:957:ILE:HD11	1.90	0.53
2:M:289:ALA:O	2:M:290:ARG:C	2.48	0.53
3:J:1004:ARG:NH1	3:J:1025:GLY:H	2.05	0.53
3:B:560:THR:HG22	3:B:561:ASP:N	2.24	0.53
2:M:190:ARG:CZ	2:M:191:LEU:HG	2.39	0.53
2:M:212:ASN:C	2:M:214:ASP:H	2.12	0.53
1:A:458:ASP:HA	3:B:886:GLY:HA2	1.90	0.53
1:I:458:ASP:HA	3:J:886:GLY:HA2	1.91	0.53
1:A:290:ARG:HD2	1:A:291:SER:N	2.24	0.53
1:I:450:CYS:N	1:I:451:PRO:CD	2.72	0.53
1:I:336:GLU:OE1	1:I:436:ARG:NH1	2.43	0.52
1:I:501:ASP:HB2	3:J:734:MET:SD	2.49	0.52
3:J:83:MET:O	3:J:87:LEU:HD12	2.09	0.52
3:B:762:GLU:HG2	3:B:772:LYS:HA	1.91	0.52
1:I:364:PHE:HD2	1:I:373:PRO:O	1.93	0.52
1:I:378:VAL:HG23	1:I:407:ILE:HG22	1.91	0.52
1:I:268:LEU:HD23	1:I:271:TYR:HD1	1.74	0.52
11:N:18:TRP:CD1	11:N:49:LEU:HD22	2.39	0.52
8:T:11:PRO:HD2	8:T:12:ARG:HD3	1.90	0.52
3:B:367:TYR:HD2	3:B:367:TYR:C	2.13	0.52
2:M:13:LEU:HD23	2:M:16:LYS:NZ	2.24	0.52
1:I:775:SER:OG	1:I:776:PRO:HD2	2.10	0.52
4:D:253:ILE:CD1	10:L:76:ILE:HD12	2.39	0.52
3:B:591:ILE:O	3:B:594:ILE:HG12	2.09	0.52
3:B:702:LEU:HD13	11:N:47:ARG:HD2	1.91	0.52
1:A:851:GLY:C	1:A:853:ASP:H	2.11	0.52
3:B:602:ILE:HG22	3:B:603:THR:N	2.24	0.52
1:A:417:VAL:HG13	1:A:464:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:679:TYR:OH	1:I:693:GLU:HG2	2.08	0.52
5:E:130:GLU:HA	5:E:133:LYS:HE2	1.90	0.52
5:E:66:THR:HG23	5:E:68:HIS:CE1	2.44	0.52
3:J:834:ASP:O	3:J:836:SER:N	2.38	0.52
3:B:48:GLU:HG2	3:B:58:VAL:HB	1.91	0.52
3:B:461:GLY:O	3:B:464:SER:HB3	2.09	0.52
3:B:1069:TRP:CH2	3:B:1077:TYR:HB2	2.44	0.52
4:O:29:ARG:HG3	4:O:162:SER:O	2.10	0.52
1:I:781:PHE:C	1:I:781:PHE:CD2	2.83	0.52
3:B:425:HIS:HA	3:B:428:ARG:HD3	1.91	0.52
3:B:895:VAL:HG21	4:D:34:LEU:HD21	1.92	0.52
3:J:533:GLY:O	3:J:535:GLU:N	2.41	0.52
3:J:474:ALA:HB2	3:J:578:PRO:HG3	1.90	0.52
2:C:237:ILE:CG1	2:C:238:LYS:N	2.63	0.52
3:B:971:TYR:CE2	3:B:978:LYS:HB3	2.45	0.52
1:A:490:ARG:HA	2:C:312:HIS:CE1	2.39	0.52
1:I:349:VAL:HG21	1:I:409:ARG:NH2	2.24	0.52
5:E:51:VAL:O	5:E:53:THR:N	2.41	0.52
1:I:742:GLN:HB3	3:J:919:MET:CE	2.39	0.52
1:I:750:GLN:CG	1:I:782:ILE:CD1	2.88	0.52
4:O:129:PRO:HG2	11:W:15:ALA:HB1	1.90	0.52
2:C:153:VAL:O	2:C:153:VAL:HG13	2.09	0.52
12:P:9:CYS:HB3	12:P:12:THR:O	2.10	0.52
13:Y:71:ASN:HA	13:Y:74:GLU:CD	2.29	0.52
1:A:647:ARG:O	1:A:650:ASP:HB2	2.08	0.52
3:J:21:LYS:HE2	3:J:475:GLN:OE1	2.09	0.52
11:W:4:PRO:HG2	11:W:48:MET:HE2	1.92	0.52
2:C:392:PRO:HG2	5:E:22:LEU:HD21	1.91	0.52
1:I:426:HIS:ND1	1:I:428:ILE:HG22	2.24	0.52
1:I:448:LEU:O	1:I:496:ILE:HG23	2.10	0.52
3:B:82:PRO:CG	3:B:143:GLU:OE1	2.48	0.52
2:M:112:ASP:O	2:M:113:ALA:CB	2.58	0.52
9:U:38:ALA:HB1	9:U:42:GLN:HE22	1.75	0.52
2:C:124:ILE:O	2:C:251:ILE:HG22	2.10	0.52
3:B:677:LEU:HD12	3:B:992:LYS:HD3	1.90	0.52
1:I:563:HIS:HB2	1:I:872:PHE:CE2	2.44	0.52
2:M:372:ASN:O	2:M:375:ILE:HG22	2.09	0.52
1:A:239:LEU:CD2	1:A:276:TYR:CE1	2.92	0.52
3:B:435:ARG:HB3	3:B:437:GLN:HB2	1.90	0.52
11:W:43:TYR:HA	11:W:46:ARG:HB2	1.91	0.52
1:I:488:THR:HG23	1:I:490:ARG:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:825:ASN:O	1:I:827:LEU:N	2.43	0.52
5:Q:18:PHE:CD2	9:U:47:ALA:HB1	2.45	0.52
1:A:446:ASN:O	1:A:448:LEU:N	2.42	0.52
1:I:457:PHE:HB2	3:J:737:SER:HB2	1.91	0.52
10:L:69:LEU:O	10:L:73:ILE:N	2.36	0.52
2:C:355:LEU:HD23	3:B:1109:ILE:HD11	1.91	0.52
3:J:368:GLN:NE2	3:J:386:ARG:HE	2.08	0.52
3:B:162:VAL:HG11	3:B:412:GLN:NE2	2.25	0.52
3:B:582:VAL:HG11	3:B:633:LEU:HD11	1.91	0.52
1:A:369:PRO:HG3	1:A:389:ARG:HA	1.91	0.52
3:B:902:LYS:HE2	11:N:41:LYS:HB3	1.91	0.52
4:D:96:ILE:HG13	4:D:143:ALA:HB3	1.91	0.52
3:J:130:ILE:HA	3:J:133:TYR:CE1	2.45	0.52
3:B:369:LEU:HG	3:B:384:LEU:HD13	1.91	0.52
3:J:369:LEU:HG	3:J:384:LEU:HD13	1.91	0.52
1:I:378:VAL:O	1:I:378:VAL:CG2	2.55	0.52
2:C:70:ILE:O	2:C:71:GLY:C	2.48	0.52
2:M:153:VAL:HG23	2:M:168:GLN:O	2.10	0.52
1:A:743:MET:HG3	3:B:919:MET:HE2	1.91	0.52
3:J:849:LEU:HB3	3:J:865:ARG:HB3	1.91	0.52
4:D:131:VAL:HG22	4:D:132:LEU:H	1.73	0.52
1:A:868:VAL:HG22	2:C:39:LYS:HZ1	1.75	0.52
3:J:96:LEU:HB2	3:J:117:GLY:H	1.75	0.52
1:A:215:PRO:HB3	3:B:1106:SER:HB3	1.90	0.52
2:C:261:VAL:HG12	2:C:261:VAL:O	2.10	0.52
4:O:101:GLU:O	4:O:107:ARG:NH1	2.43	0.52
3:B:682:ALA:O	11:N:59:VAL:HG13	2.10	0.52
3:J:215:PRO:O	3:J:216:ALA:HB3	2.10	0.52
1:I:664:GLU:OE1	1:I:707:LEU:HD22	2.09	0.52
3:J:1061:CYS:HA	3:J:1088:LEU:HD23	1.92	0.52
7:G:71:PHE:O	7:G:114:ARG:HA	2.10	0.52
3:J:902:LYS:HB2	11:W:42:ARG:HH11	1.75	0.52
4:D:180:VAL:HG21	4:D:190:LEU:HG	1.92	0.52
1:I:761:TYR:OH	3:J:621:GLU:OE1	2.20	0.52
2:M:103:GLY:HA2	2:M:106:ARG:HB3	1.90	0.52
1:A:855:VAL:HG22	2:C:64:ILE:HB	1.92	0.52
3:B:850:VAL:O	12:P:35:PHE:CB	2.57	0.52
1:A:353:ILE:CG1	1:A:361:LEU:HD23	2.37	0.52
3:J:848:ASP:OD1	3:J:865:ARG:CZ	2.57	0.52
3:J:193:THR:HG21	3:J:197:ARG:N	2.25	0.52
4:D:21:PRO:HG3	10:L:79:MET:SD	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:81:VAL:O	5:E:82:GLN:HB2	2.09	0.52
1:A:632:PHE:HA	1:A:635:PHE:CE1	2.45	0.52
9:K:69:PHE:HA	9:K:74:LEU:HD11	1.92	0.52
3:J:911:ASN:HD21	3:J:913:HIS:HD2	1.57	0.52
9:K:86:LYS:HD2	9:K:86:LYS:N	2.25	0.52
1:I:507:TYR:HB2	1:I:511:VAL:HG13	1.92	0.52
4:D:96:ILE:CG1	4:D:143:ALA:HB3	2.40	0.52
1:A:495:ILE:O	1:A:495:ILE:HG13	2.10	0.52
12:X:17:GLN:C	12:X:19:LYS:H	2.12	0.52
1:A:155:LYS:HA	1:A:156:ILE:O	2.10	0.52
1:A:868:VAL:HG13	2:C:39:LYS:HE2	1.92	0.52
3:B:367:TYR:HD2	3:B:367:TYR:O	1.93	0.52
1:I:337:VAL:HG12	1:I:339:VAL:HG23	1.91	0.52
1:I:763:THR:CG2	1:I:772:TYR:HA	2.40	0.52
2:M:344:ARG:HB3	2:M:353:HIS:CD2	2.44	0.52
3:B:471:ALA:O	3:B:473:MET:HG3	2.10	0.52
1:I:71:HIS:ND1	3:J:1070:TYR:HE2	2.07	0.52
7:S:42:ILE:HD12	7:S:46:ILE:HG21	1.91	0.52
4:D:176:CYS:H	4:D:195:LEU:HD21	1.74	0.52
1:I:506:ALA:O	1:I:510:THR:HG23	2.10	0.52
9:U:43:LEU:C	9:U:45:MET:H	2.13	0.52
3:J:560:THR:HG22	3:J:561:ASP:N	2.25	0.52
1:I:441:LEU:HD12	3:J:873:THR:HG21	1.92	0.52
10:L:32:LEU:HD11	10:L:69:LEU:HD12	1.92	0.52
3:B:943:THR:HG22	3:B:944:PRO:HD2	1.91	0.52
3:B:368:GLN:HE22	3:B:386:ARG:HH21	1.57	0.52
2:M:145:GLU:O	2:M:147:THR:N	2.43	0.52
3:B:789:TYR:O	3:B:791:LEU:N	2.43	0.52
4:D:204:THR:O	4:D:206:CYS:N	2.43	0.51
3:B:27:HIS:HD2	3:B:346:ALA:HB2	1.75	0.51
3:B:579:LEU:O	3:B:613:ILE:HG23	2.09	0.51
1:A:557:PRO:HD3	1:A:623:TYR:OH	2.10	0.51
3:B:727:MET:HE1	3:B:898:PRO:HG3	1.92	0.51
1:I:728:MET:CE	3:J:913:HIS:HA	2.40	0.51
3:J:800:PRO:HB2	12:X:38:ARG:HA	1.92	0.51
1:A:507:TYR:OH	1:A:727:VAL:HG13	2.09	0.51
1:A:83:HIS:HB3	1:A:86:LEU:HB2	1.92	0.51
3:B:685:GLN:HE22	3:B:867:ARG:HH22	1.58	0.51
3:J:602:ILE:HG22	3:J:603:THR:N	2.25	0.51
8:H:63:ILE:HG22	8:H:64:ARG:N	2.25	0.51
7:G:29:VAL:HB	7:G:40:PHE:HD1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:94:ALA:O	3:J:119:LEU:N	2.37	0.51
1:I:95:LYS:HB3	1:I:138:LYS:HG3	1.92	0.51
1:I:837:THR:HG22	1:I:838:VAL:H	1.75	0.51
4:D:250:ILE:CD1	10:L:84:ILE:CD1	2.83	0.51
7:G:86:LEU:HD12	7:G:91:LYS:CG	2.39	0.51
1:A:541:ALA:CA	7:G:72:CYS:H	2.23	0.51
3:J:624:ALA:HB1	3:J:639:HIS:CD2	2.45	0.51
5:Q:31:ARG:O	5:Q:33:GLN:N	2.42	0.51
3:B:855:THR:O	3:B:856:ALA:C	2.48	0.51
4:O:134:GLY:O	4:O:135:THR:O	2.28	0.51
3:J:419:TRP:CZ3	3:J:712:GLY:HA3	2.45	0.51
1:I:737:VAL:HG23	1:I:738:LEU:HD22	1.93	0.51
1:A:541:ALA:CB	7:G:71:PHE:HA	2.40	0.51
11:W:42:ARG:HG3	11:W:43:TYR:H	1.74	0.51
2:C:391:ARG:H	2:C:392:PRO:CD	2.22	0.51
1:I:486:ILE:HG12	1:I:496:ILE:HB	1.93	0.51
1:I:594:LEU:O	1:I:595:GLU:HG2	2.10	0.51
1:A:446:ASN:HD22	1:A:447:LEU:N	2.08	0.51
3:B:745:VAL:HG21	3:B:891:LEU:HD11	1.91	0.51
3:B:738:ILE:CD1	3:B:908:ILE:HG23	2.39	0.51
3:J:116:ILE:HD12	3:J:361:PHE:CZ	2.46	0.51
2:M:388:LEU:HD21	9:U:35:VAL:CG1	2.39	0.51
9:U:12:ASP:O	9:U:13:LEU:C	2.47	0.51
5:Q:79:PRO:HG2	5:Q:149:VAL:HG21	1.92	0.51
3:J:963:LEU:HD22	3:J:982:ARG:NH2	2.26	0.51
2:M:146:TYR:CZ	2:M:235:LYS:HB2	2.45	0.51
3:J:569:ASN:HB3	3:J:574:ARG:HH12	1.76	0.51
2:C:392:PRO:HB2	5:E:22:LEU:HD11	1.93	0.51
5:E:64:GLY:O	9:K:42:GLN:OE1	2.28	0.51
1:A:558:LYS:H	1:A:558:LYS:CD	2.23	0.51
2:M:55:ALA:CB	2:M:58:GLU:OE2	2.58	0.51
2:M:55:ALA:O	2:M:58:GLU:HB2	2.10	0.51
1:I:105:LYS:NZ	1:I:108:GLU:HB2	2.25	0.51
2:M:376:GLY:HA2	3:J:1049:LEU:HD21	1.91	0.51
3:J:92:TYR:O	3:J:92:TYR:CD2	2.63	0.51
3:B:921:LEU:C	3:B:923:GLN:H	2.13	0.51
3:J:367:TYR:HD2	3:J:367:TYR:O	1.93	0.51
3:J:735:GLU:O	3:J:736:ASP:C	2.49	0.51
7:G:46:ILE:O	7:G:46:ILE:CG2	2.58	0.51
1:A:612:LEU:C	1:A:612:LEU:HD23	2.31	0.51
3:J:978:LYS:HG2	4:O:166:TYR:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:970:VAL:HG22	3:J:979:ILE:HG12	1.92	0.51
1:I:438:LEU:HD21	1:I:444:ARG:CZ	2.40	0.51
3:B:170:ASN:HB3	3:B:300:HIS:HE1	1.76	0.51
1:A:238:LYS:HE2	1:A:297:THR:HG22	1.92	0.51
3:J:741:ASN:C	3:J:741:ASN:OD1	2.49	0.51
2:C:278:ARG:HD2	2:C:278:ARG:O	2.11	0.51
1:I:7:LYS:HE2	2:M:365:GLU:OE2	2.11	0.51
3:J:644:SER:C	3:J:646:ALA:H	2.14	0.51
7:G:17:SER:HB2	7:G:19:GLU:HG2	1.92	0.51
3:B:517:TRP:HD1	3:B:531:GLN:H	1.59	0.51
3:B:356:VAL:HG22	3:B:393:ARG:NH1	2.25	0.51
1:A:557:PRO:HA	1:A:558:LYS:HZ2	1.75	0.51
1:A:317:ARG:NH1	3:B:1018:GLU:HG3	2.26	0.51
2:M:149:ILE:HB	2:M:227:LEU:HA	1.92	0.51
3:B:665:ARG:HG3	3:B:920:THR:HG21	1.91	0.51
1:I:98:CYS:HB3	1:I:101:CYS:H	1.76	0.51
4:O:137:GLN:NE2	11:W:63:THR:HG22	2.26	0.51
3:J:469:ASN:N	3:J:469:ASN:HD22	2.07	0.51
3:B:1074:LYS:HE2	3:B:1074:LYS:HA	1.93	0.51
9:K:19:PHE:O	9:K:20:ILE:C	2.49	0.51
1:A:528:ALA:HB3	1:A:630:ASN:HD21	1.74	0.51
2:M:369:VAL:O	2:M:373:ILE:HB	2.11	0.51
1:I:853:ASP:HB3	1:I:855:VAL:H	1.76	0.51
3:B:1004:ARG:NH1	3:B:1024:GLY:HA2	2.25	0.51
5:Q:15:PRO:HB2	9:U:45:MET:O	2.10	0.51
5:E:87:GLY:O	5:E:88:GLU:CB	2.55	0.51
1:A:209:LEU:HD13	1:A:273:VAL:HG11	1.92	0.51
1:I:290:ARG:NH1	1:I:291:SER:HB2	2.25	0.51
3:B:330:ARG:HA	3:B:563:ILE:HD11	1.93	0.51
2:M:384:GLY:HA2	5:Q:61:PHE:HZ	1.75	0.51
1:A:290:ARG:NH1	1:A:291:SER:HB2	2.25	0.51
8:H:69:SER:HB2	8:H:75:VAL:HG22	1.93	0.51
5:Q:120:TYR:CZ	5:Q:122:ASN:HA	2.46	0.51
2:C:11:PRO:O	2:C:14:GLU:HG3	2.11	0.51
1:A:659:LYS:O	1:A:663:ASN:HB2	2.09	0.51
3:J:435:ARG:HB3	3:J:437:GLN:HB2	1.93	0.51
3:B:1009:VAL:HB	3:B:1014:ARG:O	2.09	0.51
1:I:859:TYR:HB2	2:M:64:ILE:HG23	1.93	0.51
3:J:904:VAL:HG22	11:W:44:CYS:HB3	1.93	0.51
1:A:371:LYS:NZ	1:A:373:PRO:HD3	2.26	0.51
2:M:121:MET:H	2:M:275:ASN:ND2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:286:ILE:HG13	8:T:49:ASP:OD2	2.11	0.51
3:J:560:THR:CG2	3:J:561:ASP:N	2.74	0.51
1:I:532:ILE:HG23	10:V:40:PHE:CD2	2.46	0.51
9:K:91:SER:O	9:K:92:LEU:HB3	2.11	0.51
9:K:61:VAL:O	9:K:62:ILE:HB	2.11	0.51
6:R:13:PRO:HB3	6:R:73:ALA:HB3	1.92	0.51
2:C:301:LEU:O	2:C:304:GLN:N	2.44	0.51
3:B:931:LYS:HE2	3:B:985:PHE:O	2.10	0.51
1:A:539:ILE:HB	1:A:545:TYR:HB2	1.93	0.51
6:F:77:PRO:HG3	6:F:83:VAL:HG22	1.93	0.51
3:J:14:ILE:HG13	3:J:18:PHE:CE2	2.46	0.51
2:C:49:ASP:O	2:C:51:ILE:N	2.44	0.51
3:B:497:VAL:HG12	3:B:498:GLU:N	2.26	0.51
3:B:834:ASP:O	3:B:836:SER:N	2.39	0.51
1:I:749:GLN:N	1:I:781:PHE:HA	2.25	0.51
1:A:604:GLY:C	1:A:606:GLN:N	2.62	0.51
9:K:54:ASN:HD21	9:K:58:SER:CB	2.24	0.51
3:J:232:ILE:HG23	3:J:237:ASP:HB3	1.92	0.51
6:F:64:SER:H	6:F:69:ARG:HH21	1.59	0.51
2:C:72:ILE:CG2	2:C:76:GLN:OE1	2.59	0.51
3:B:710:ILE:HD13	3:B:710:ILE:H	1.76	0.51
5:Q:50:ASN:HB2	5:Q:73:ASP:OD2	2.11	0.51
1:I:465:HIS:CD2	3:J:1048:ARG:HD2	2.46	0.51
2:M:24:LEU:HD11	2:M:58:GLU:OE1	2.12	0.51
3:B:932:TYR:CD2	3:B:932:TYR:O	2.64	0.51
3:B:699:GLN:HA	11:N:51:SER:O	2.11	0.51
3:J:729:PHE:O	3:J:731:GLY:N	2.43	0.51
2:M:286:ILE:HG12	2:M:324:GLY:O	2.10	0.51
1:A:324:THR:CG2	1:A:325:VAL:N	2.73	0.51
1:A:293:ARG:HD3	1:A:296:ARG:HH22	1.76	0.51
3:J:975:THR:OG1	3:J:977:GLN:HG2	2.11	0.51
5:E:110:ILE:O	5:E:113:ILE:HG22	2.11	0.51
1:I:290:ARG:HD2	1:I:291:SER:H	1.76	0.51
3:B:67:LYS:HB3	3:B:68:PRO:HD2	1.93	0.51
1:A:305:LYS:HA	1:A:310:ARG:HD2	1.91	0.51
3:B:875:GLY:HA2	3:B:887:VAL:HG13	1.93	0.51
3:J:950:ILE:O	3:J:952:GLN:N	2.45	0.51
10:V:82:HIS:O	10:V:86:GLU:N	2.43	0.51
3:B:582:VAL:HG13	3:B:586:ASN:H	1.76	0.50
1:A:525:LEU:HG	10:L:40:PHE:HZ	1.75	0.50
3:J:699:GLN:HA	11:W:51:SER:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:45:ILE:O	8:T:81:VAL:HA	2.12	0.50
3:J:762:GLU:HG2	3:J:772:LYS:HA	1.93	0.50
3:B:870:ARG:HH11	3:B:996:MET:HB2	1.74	0.50
1:I:78:VAL:HG23	1:I:266:TRP:HZ3	1.75	0.50
3:J:291:GLN:O	3:J:295:LYS:HG2	2.10	0.50
8:H:65:ILE:HD11	8:H:79:ARG:HG2	1.92	0.50
4:D:131:VAL:CG2	4:D:132:LEU:H	2.24	0.50
3:B:68:PRO:CD	3:B:129:PRO:HG2	2.40	0.50
3:B:325:LEU:HD11	3:B:331:GLU:H	1.76	0.50
4:D:250:ILE:CD1	10:L:84:ILE:HD11	2.21	0.50
2:C:52:PHE:HA	2:C:55:ALA:HB3	1.93	0.50
1:A:549:LYS:CB	7:G:88:ASN:O	2.60	0.50
1:A:549:LYS:HB2	1:A:549:LYS:HZ3	1.75	0.50
3:B:579:LEU:CD1	3:B:616:LEU:HD12	2.26	0.50
8:T:42:LEU:CB	8:T:43:PRO:HD2	2.31	0.50
1:I:506:ALA:HA	1:I:635:PHE:CE2	2.46	0.50
7:G:37:ASN:O	7:G:94:THR:HA	2.10	0.50
3:B:849:LEU:HB3	3:B:865:ARG:HB3	1.94	0.50
7:G:40:PHE:CZ	7:G:115:THR:HG21	2.46	0.50
4:O:12:ARG:HA	4:O:230:ILE:O	2.11	0.50
2:C:150:GLU:HB2	2:C:227:LEU:HB3	1.93	0.50
3:B:154:VAL:O	3:B:155:ASN:C	2.50	0.50
1:I:320:PHE:HE2	1:I:348:THR:HG1	1.58	0.50
1:I:644:PHE:HA	1:I:724:PHE:HE2	1.77	0.50
10:L:40:PHE:HB3	10:L:58:LEU:HB3	1.93	0.50
1:I:859:TYR:HB3	2:M:64:ILE:HG12	1.93	0.50
1:A:317:ARG:HB2	3:B:1016:PRO:HB2	1.93	0.50
1:A:353:ILE:HD11	1:A:407:ILE:HG23	1.92	0.50
1:I:324:THR:CG2	1:I:325:VAL:H	2.22	0.50
1:I:524:ILE:O	1:I:525:LEU:HD22	2.11	0.50
3:B:729:PHE:O	3:B:731:GLY:N	2.44	0.50
3:B:763:VAL:HA	3:B:770:GLU:CG	2.41	0.50
1:I:239:LEU:CD2	1:I:276:TYR:CE1	2.94	0.50
1:I:238:LYS:HE2	1:I:297:THR:HG22	1.94	0.50
6:F:15:SER:HA	6:F:18:LYS:HZ1	1.76	0.50
1:A:450:CYS:N	1:A:451:PRO:CD	2.74	0.50
3:B:325:LEU:HD22	3:B:330:ARG:HG3	1.93	0.50
7:S:57:VAL:HG13	7:S:115:THR:HG22	1.92	0.50
3:J:921:LEU:C	3:J:923:GLN:H	2.13	0.50
3:J:517:TRP:HD1	3:J:531:GLN:H	1.59	0.50
3:J:103:VAL:O	3:J:103:VAL:HG12	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:448:THR:HG22	3:J:452:ARG:HD2	1.93	0.50
9:U:41:LEU:O	9:U:43:LEU:N	2.44	0.50
3:B:361:PHE:CE1	3:B:385:VAL:HG13	2.44	0.50
13:Z:76:GLU:O	13:Z:77:LYS:CB	2.58	0.50
1:A:337:VAL:HG21	1:A:419:PHE:CD1	2.46	0.50
1:I:288:LYS:HG2	1:I:294:PRO:HA	1.92	0.50
3:J:377:ARG:O	3:J:378:LYS:HB2	2.12	0.50
3:B:900:THR:OG1	3:B:904:VAL:HB	2.12	0.50
1:I:446:ASN:HD22	1:I:448:LEU:H	1.59	0.50
1:A:728:MET:CE	3:B:913:HIS:HA	2.41	0.50
3:J:497:VAL:HG12	3:J:498:GLU:N	2.25	0.50
8:H:58:LYS:HB2	8:H:61:ASP:HB2	1.93	0.50
1:A:486:ILE:O	1:A:486:ILE:HD13	2.11	0.50
2:M:339:ASN:N	2:M:339:ASN:OD1	2.42	0.50
1:A:742:GLN:HB3	3:B:919:MET:CE	2.41	0.50
3:J:330:ARG:NH2	3:J:565:GLU:OE1	2.44	0.50
4:D:131:VAL:CG2	4:D:132:LEU:N	2.74	0.50
7:S:80:GLU:HG3	7:S:81:LEU:H	1.76	0.50
2:C:11:PRO:HB2	2:C:14:GLU:OE1	2.10	0.50
4:O:228:LEU:O	4:O:229:GLU:HG3	2.11	0.50
3:B:533:GLY:O	3:B:535:GLU:N	2.45	0.50
3:J:453:MET:HG2	3:J:468:LYS:HD2	1.92	0.50
1:A:653:LEU:HD11	1:A:745:ALA:HB2	1.94	0.50
2:M:238:LYS:HB2	2:M:239:ARG:NH1	2.27	0.50
3:J:1069:TRP:CH2	3:J:1077:TYR:HB2	2.46	0.50
7:G:66:TYR:HB2	7:G:70:ASP:OD1	2.12	0.50
3:J:34:PHE:HE1	3:J:351:ALA:HA	1.75	0.50
3:B:934:ALA:HB2	11:N:47:ARG:HD3	1.92	0.50
1:I:507:TYR:O	1:I:508:LEU:CB	2.57	0.50
3:B:813:LYS:O	3:B:814:VAL:HG23	2.12	0.50
3:J:557:HIS:CE1	3:J:566:VAL:HG13	2.47	0.50
10:V:15:LEU:HB3	10:V:55:VAL:CG2	2.41	0.50
3:B:226:LEU:O	3:B:230:LEU:HD12	2.12	0.50
2:M:349:VAL:CG2	2:M:352:LYS:HB2	2.42	0.50
1:I:465:HIS:NE2	3:J:1028:PHE:HD1	2.10	0.50
1:I:284:LEU:N	1:I:285:PRO:HD2	2.27	0.50
1:I:653:LEU:HD11	1:I:745:ALA:HB2	1.94	0.50
3:J:473:MET:HA	3:J:577:ARG:NH2	2.27	0.50
1:I:369:PRO:HA	1:I:410:HIS:HE1	1.77	0.50
1:I:547:THR:HG21	7:S:89:GLY:HA3	1.93	0.50
3:J:738:ILE:HG23	3:J:888:ILE:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:239:VAL:HA	3:J:253:PHE:CE2	2.46	0.50
1:I:640:GLU:OE1	3:J:974:ARG:NH1	2.45	0.50
1:A:468:GLN:HB2	3:B:1047:ASP:OD2	2.12	0.50
3:B:1067:ILE:CG2	3:B:1080:PRO:HG2	2.41	0.50
8:T:17:VAL:HG21	8:T:51:VAL:HG21	1.92	0.50
5:Q:168:TYR:O	5:Q:175:ILE:HD13	2.11	0.50
7:G:40:PHE:HZ	7:G:115:THR:HG21	1.77	0.50
10:L:45:GLN:O	10:L:46:PRO:O	2.30	0.50
5:E:29:GLU:O	5:E:33:GLN:HG3	2.11	0.50
2:C:122:MET:SD	2:C:256:SER:HA	2.52	0.50
3:J:747:ARG:NH1	11:W:8:PHE:O	2.44	0.50
3:B:579:LEU:CD1	3:B:616:LEU:CD1	2.85	0.50
2:C:145:GLU:HG2	2:C:239:ARG:HA	1.94	0.50
1:A:372:TRP:O	1:A:374:GLY:N	2.45	0.50
10:V:46:PRO:O	10:V:47:HIS:HB3	2.10	0.50
4:D:180:VAL:CG2	4:D:190:LEU:HG	2.42	0.50
1:I:826:ALA:HB1	2:M:334:VAL:HG13	1.94	0.50
3:J:855:THR:O	3:J:856:ALA:C	2.48	0.50
3:B:171:ARG:HB3	3:B:524:GLY:HA3	1.94	0.50
3:B:560:THR:CG2	3:B:561:ASP:N	2.74	0.50
3:B:762:GLU:HG3	3:B:773:ILE:HG13	1.93	0.50
1:I:532:ILE:HG13	10:V:12:TYR:OH	2.12	0.50
1:I:532:ILE:HG22	10:V:58:LEU:HD22	1.93	0.50
8:H:45:ILE:N	8:H:79:ARG:HB3	2.27	0.50
3:B:125:SER:O	3:B:131:SER:HB2	2.12	0.50
2:C:133:ASP:HB2	2:C:136:LYS:HG2	1.92	0.50
4:O:37:PRO:HA	4:O:148:GLY:O	2.12	0.50
5:Q:113:ILE:HG23	5:Q:114:THR:N	2.27	0.50
3:B:345:LEU:N	3:B:345:LEU:HD12	2.27	0.50
3:B:624:ALA:HB1	3:B:639:HIS:CD2	2.47	0.50
2:M:276:ASN:O	2:M:279:GLU:HB3	2.12	0.50
1:I:220:ARG:HH11	1:I:236:THR:CG2	2.22	0.50
3:J:740:MET:O	3:J:891:LEU:HA	2.11	0.50
2:M:168:GLN:HG2	2:M:204:SER:CB	2.42	0.50
8:H:25:ILE:HA	8:H:28:ALA:CB	2.42	0.50
1:I:58:CYS:CB	1:I:59:PRO:CD	2.89	0.50
3:J:769:GLN:O	3:J:770:GLU:HB3	2.11	0.50
3:J:603:THR:O	3:J:604:PHE:C	2.49	0.50
1:A:4:LYS:HD2	3:B:1089:PHE:CB	2.42	0.50
1:A:188:PRO:O	1:A:192:VAL:HG23	2.12	0.50
3:B:432:SER:HB3	3:B:435:ARG:HH21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:348:ASP:N	3:J:348:ASP:OD2	2.45	0.50
9:K:26:ARG:HB3	9:K:27:LEU:HD12	1.94	0.50
3:B:214:PHE:CD1	3:B:215:PRO:HD2	2.47	0.50
2:C:393:ILE:HG22	2:C:394:LEU:H	1.76	0.50
3:B:221:ILE:N	3:B:221:ILE:HD13	2.26	0.50
1:I:259:GLN:HA	1:I:262:ILE:HG22	1.94	0.50
4:O:191:LYS:HB2	4:O:194:LYS:HD2	1.94	0.50
4:O:125:SER:O	4:O:127:ASP:N	2.45	0.49
3:J:128:ASP:OD1	3:J:130:ILE:HB	2.12	0.49
1:I:409:ARG:NH2	1:I:415:ASP:OD2	2.45	0.49
3:J:544:ARG:NH1	3:J:544:ARG:HG3	2.17	0.49
3:B:654:ILE:HG13	3:B:708:LEU:HD21	1.93	0.49
1:I:716:SER:CB	1:I:726:TYR:OH	2.60	0.49
3:B:769:GLN:O	3:B:770:GLU:HB3	2.10	0.49
3:B:740:MET:O	3:B:891:LEU:HA	2.12	0.49
3:B:803:GLU:HB3	3:B:805:LYS:HZ1	1.76	0.49
2:M:386:VAL:HB	9:U:31:GLU:HG2	1.94	0.49
5:E:109:HIS:CD2	5:E:111:SER:H	2.29	0.49
4:O:35:TYR:O	4:O:149:TYR:HD2	1.95	0.49
2:M:238:LYS:HB2	2:M:239:ARG:CZ	2.42	0.49
3:J:475:GLN:HG2	3:J:476:ILE:H	1.77	0.49
1:A:525:LEU:C	1:A:527:VAL:H	2.16	0.49
2:C:126:LEU:HG	2:C:249:TYR:O	2.12	0.49
3:J:314:TYR:HE2	3:J:526:LEU:N	2.02	0.49
1:A:425:LEU:O	1:A:426:HIS:HB2	2.11	0.49
7:G:79:THR:CG2	7:G:80:GLU:H	2.25	0.49
1:A:831:ARG:NH2	2:C:385:MET:HG3	2.27	0.49
1:I:417:VAL:HG13	1:I:464:LEU:HD13	1.94	0.49
3:J:759:SER:CB	3:J:862:VAL:O	2.42	0.49
3:J:904:VAL:HG21	11:W:42:ARG:HG2	1.94	0.49
1:A:325:VAL:O	1:A:442:THR:HB	2.11	0.49
3:B:655:ILE:HG12	3:B:669:GLN:HG2	1.94	0.49
1:I:353:ILE:CG1	1:I:361:LEU:HD23	2.39	0.49
2:C:122:MET:HG2	2:C:274:THR:HG23	1.95	0.49
2:M:357:ALA:O	2:M:362:ASP:HB2	2.13	0.49
4:O:257:GLU:O	4:O:260:LEU:HB3	2.12	0.49
10:V:21:ASP:OD1	10:V:22:HIS:N	2.45	0.49
3:B:338:TYR:CZ	3:B:341:LYS:NZ	2.81	0.49
3:J:477:ALA:HB3	3:J:574:ARG:CG	2.42	0.49
1:I:331:ASN:ND2	3:J:732:TYR:OH	2.45	0.49
3:J:729:PHE:C	3:J:731:GLY:H	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:ASP:OD2	3:B:913:HIS:HD2	1.95	0.49
3:B:764:LYS:NZ	3:B:772:LYS:O	2.45	0.49
2:C:179:VAL:HG23	2:C:182:ASP:H	1.77	0.49
1:I:48:ARG:HB2	1:I:59:PRO:HB3	1.93	0.49
1:I:781:PHE:HD2	1:I:781:PHE:C	2.14	0.49
1:A:6:ILE:HD11	3:B:1091:VAL:HG11	1.93	0.49
7:S:31:MET:N	7:S:38:VAL:O	2.45	0.49
10:V:69:LEU:O	10:V:72:ALA:N	2.45	0.49
10:V:14:GLU:OE1	10:V:56:LYS:HG2	2.12	0.49
3:B:430:ILE:HG22	3:B:431:SER:O	2.12	0.49
2:M:349:VAL:HG21	2:M:352:LYS:HB2	1.93	0.49
1:A:23:SER:HA	1:A:72:PHE:O	2.11	0.49
3:B:753:THR:HG23	3:B:868:ASP:H	1.77	0.49
3:B:588:LEU:HD22	3:B:612:LYS:HG2	1.95	0.49
3:J:969:VAL:HG21	4:O:205:LEU:HB3	1.95	0.49
3:B:965:ASP:O	3:B:967:THR:N	2.46	0.49
3:J:677:LEU:HD21	3:J:994:HIS:HB3	1.94	0.49
3:J:927:GLY:HA2	3:J:987:VAL:O	2.12	0.49
11:W:7:CYS:CB	11:W:45:CYS:SG	3.01	0.49
2:C:327:ARG:HH21	2:C:337:GLU:HG3	1.77	0.49
2:M:376:GLY:HA3	3:J:1050:LEU:HD13	1.94	0.49
2:M:75:ALA:O	2:M:79:GLY:N	2.29	0.49
1:I:506:ALA:HA	1:I:635:PHE:CD2	2.48	0.49
2:M:390:MET:HB3	2:M:392:PRO:HD3	1.95	0.49
1:A:324:THR:CG2	1:A:325:VAL:H	2.21	0.49
1:I:528:ALA:HB3	1:I:630:ASN:HD21	1.78	0.49
2:M:39:LYS:O	2:M:43:VAL:HG23	2.12	0.49
3:B:690:THR:O	3:B:691:ARG:C	2.50	0.49
1:I:239:LEU:CD2	1:I:276:TYR:HE1	2.24	0.49
1:I:319:ASP:HB2	3:J:1052:ASN:HB3	1.93	0.49
3:J:325:LEU:HD12	3:J:328:GLY:HA2	1.95	0.49
1:A:188:PRO:HD2	1:A:191:ASP:HB2	1.95	0.49
2:C:359:ALA:C	2:C:361:GLY:N	2.66	0.49
1:A:337:VAL:HG12	1:A:339:VAL:HG23	1.95	0.49
1:A:449:VAL:HG12	1:A:449:VAL:O	2.12	0.49
3:B:551:ASP:OD2	3:B:551:ASP:N	2.44	0.49
1:I:487:ILE:O	1:I:858:MET:HG3	2.13	0.49
3:J:790:ARG:HH22	12:X:39:LYS:HE3	1.77	0.49
3:J:790:ARG:NH2	12:X:39:LYS:HE3	2.27	0.49
4:O:169:LYS:HG2	4:O:222:VAL:HG22	1.94	0.49
11:N:38:LEU:HD23	11:N:39:GLY:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:86:LEU:CD1	7:G:91:LYS:HG3	2.42	0.49
2:C:322:ARG:HD2	2:C:322:ARG:N	2.27	0.49
1:I:372:TRP:O	1:I:374:GLY:N	2.45	0.49
1:A:826:ALA:HB1	2:C:334:VAL:HG13	1.94	0.49
7:S:87:ASN:C	7:S:89:GLY:N	2.65	0.49
1:A:488:THR:HG23	1:A:490:ARG:H	1.77	0.49
3:B:881:ARG:NH1	3:B:989:TYR:CB	2.75	0.49
1:I:353:ILE:HA	1:I:357:ASN:HD21	1.77	0.49
5:E:83:GLU:N	5:E:145:ARG:HG3	2.25	0.49
1:A:752:VAL:C	1:A:754:GLY:N	2.66	0.49
9:K:27:LEU:HD21	9:K:78:ILE:HD13	1.95	0.49
2:C:120:PRO:HA	2:C:275:ASN:ND2	2.27	0.49
3:B:520:VAL:HG12	3:B:527:ILE:HB	1.95	0.49
3:J:789:TYR:O	3:J:791:LEU:N	2.45	0.49
4:D:228:LEU:O	4:D:229:GLU:HG3	2.13	0.49
4:O:176:CYS:H	4:O:195:LEU:CD2	2.26	0.49
3:J:574:ARG:O	3:J:574:ARG:HG3	2.12	0.49
1:A:853:ASP:HB3	1:A:855:VAL:H	1.76	0.49
1:A:607:GLN:HB2	1:A:608:PRO:CD	2.43	0.49
2:M:72:ILE:H	2:M:72:ILE:CD1	2.24	0.49
1:A:575:CYS:CB	1:A:580:CYS:SG	3.01	0.49
5:E:92:VAL:HG13	5:E:97:ILE:HG23	1.94	0.49
1:A:203:ARG:HG3	1:A:205:GLU:HB2	1.94	0.49
2:C:61:GLU:C	2:C:63:LEU:H	2.16	0.49
3:B:480:ILE:CG2	3:B:481:ASN:N	2.75	0.49
6:F:18:LYS:HZ3	6:F:45:GLU:HG2	1.77	0.49
8:H:12:ARG:HH22	8:H:55:ILE:HD12	1.77	0.49
3:J:578:PRO:HB3	3:J:615:TYR:CE1	2.47	0.49
2:M:28:ILE:HG21	9:U:14:HIS:ND1	2.26	0.49
1:A:308:ARG:HG3	1:A:312:ASN:HD22	1.78	0.49
9:U:63:SER:HA	9:U:66:GLU:HG3	1.95	0.49
2:C:237:ILE:CG1	2:C:238:LYS:H	2.25	0.49
3:J:910:LEU:CD2	3:J:911:ASN:N	2.73	0.49
8:T:42:LEU:HB2	8:T:43:PRO:CD	2.38	0.49
1:I:529:ASP:O	1:I:529:ASP:CG	2.51	0.49
3:J:853:THR:HG23	12:X:32:LYS:O	2.12	0.49
2:C:321:THR:C	2:C:322:ARG:NH1	2.66	0.49
1:I:728:MET:HE3	3:J:913:HIS:HA	1.94	0.49
1:I:471:GLU:OE1	9:U:41:LEU:HD13	2.13	0.49
1:I:525:LEU:HA	1:I:527:VAL:HG23	1.94	0.49
1:I:527:VAL:HB	1:I:530:VAL:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:972:ASP:O	3:J:975:THR:HG23	2.13	0.49
3:J:975:THR:O	4:O:26:ASN:ND2	2.46	0.49
3:B:193:THR:HG21	3:B:197:ARG:N	2.28	0.49
5:E:82:GLN:H	5:E:146:VAL:HB	1.77	0.49
1:A:55:GLY:O	1:A:57:LYS:N	2.46	0.49
4:D:169:LYS:HG2	4:D:222:VAL:HG22	1.94	0.49
6:R:72:LEU:HD23	6:R:86:ILE:HD12	1.90	0.49
1:A:374:GLY:C	1:A:410:HIS:ND1	2.66	0.49
1:I:446:ASN:O	1:I:448:LEU:N	2.46	0.49
1:I:501:ASP:OD2	3:J:913:HIS:HD2	1.94	0.49
1:I:847:GLN:HE22	2:M:314:LEU:HB3	1.78	0.49
1:I:549:LYS:HB2	7:S:88:ASN:O	2.13	0.49
2:M:342:LEU:CD2	2:M:374:ILE:HG21	2.43	0.49
1:A:486:ILE:HG12	1:A:496:ILE:HB	1.93	0.49
1:A:486:ILE:HG12	1:A:496:ILE:HD12	1.94	0.49
7:G:8:GLU:O	7:G:9:ILE:HG13	2.12	0.49
1:A:584:SER:OG	1:A:585:TYR:N	2.43	0.49
1:A:704:LEU:HD13	1:A:781:PHE:HD1	1.77	0.49
1:A:4:LYS:NZ	3:B:1115:LEU:HB3	2.27	0.49
1:A:868:VAL:O	1:A:871:ILE:HG22	2.12	0.49
3:J:419:TRP:HZ3	3:J:712:GLY:HA3	1.77	0.49
3:J:644:SER:N	3:J:645:PRO:CD	2.76	0.49
3:J:749:MET:CE	3:J:907:ASP:HB3	2.43	0.49
1:A:847:GLN:OE1	1:A:850:TYR:HA	2.12	0.49
2:C:390:MET:HG3	5:E:57:GLY:H	1.78	0.48
3:B:971:TYR:CZ	4:D:165:ARG:HA	2.48	0.48
2:M:392:PRO:HG3	5:Q:68:HIS:CE1	2.47	0.48
2:C:312:HIS:O	2:C:316:ILE:HG12	2.13	0.48
3:B:958:LEU:HD21	4:D:181:ASN:O	2.13	0.48
3:B:1061:CYS:HA	3:B:1088:LEU:HD23	1.95	0.48
1:A:16:PRO:HD3	1:A:206:TRP:CD1	2.48	0.48
1:A:353:ILE:HA	1:A:357:ASN:HD21	1.77	0.48
1:A:402:ALA:O	1:A:403:PRO:C	2.50	0.48
7:S:101:LEU:C	7:S:103:VAL:N	2.66	0.48
1:I:8:GLY:HA2	2:M:365:GLU:HA	1.94	0.48
1:A:831:ARG:HH21	2:C:385:MET:HB2	1.77	0.48
7:S:69:ASP:N	7:S:69:ASP:OD2	2.45	0.48
7:G:60:SER:O	7:G:112:PHE:HD1	1.96	0.48
3:B:644:SER:C	3:B:646:ALA:H	2.17	0.48
1:I:543:ARG:HH11	1:I:545:TYR:HE1	1.61	0.48
3:B:699:GLN:NE2	11:N:48:MET:HE2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:617:ASP:O	3:J:618:ALA:HB2	2.13	0.48
3:B:1004:ARG:NH1	3:B:1025:GLY:H	2.07	0.48
3:J:669:GLN:NE2	3:J:881:ARG:HA	2.28	0.48
4:D:111:SER:O	4:D:114:ILE:HD13	2.13	0.48
1:A:78:VAL:HG23	1:A:266:TRP:HZ3	1.77	0.48
2:M:35:LEU:O	2:M:39:LYS:CG	2.61	0.48
2:M:337:GLU:CD	2:M:338:LYS:H	2.16	0.48
1:I:337:VAL:HG23	1:I:433:HIS:ND1	2.28	0.48
1:A:831:ARG:HH21	2:C:385:MET:CG	2.26	0.48
1:I:145:VAL:HG22	1:I:145:VAL:O	2.12	0.48
1:A:422:GLN:NE2	1:A:463:ASN:HD21	2.10	0.48
2:M:313:ILE:HA	2:M:316:ILE:HG13	1.94	0.48
3:J:446:HIS:O	3:J:447:GLY:C	2.50	0.48
2:C:146:TYR:HE1	2:C:237:ILE:HG12	1.76	0.48
2:C:390:MET:HB2	5:E:56:GLU:CG	2.43	0.48
2:M:55:ALA:HA	2:M:58:GLU:CG	2.43	0.48
1:A:124:ARG:HH21	13:Y:81:ARG:NH1	1.98	0.48
1:I:353:ILE:CD1	1:I:407:ILE:HG23	2.42	0.48
3:B:1069:TRP:HE1	3:B:1088:LEU:CB	2.25	0.48
1:A:837:THR:HG22	1:A:838:VAL:N	2.28	0.48
3:B:840:ARG:NH1	3:B:1021:ALA:HB2	2.28	0.48
1:A:620:SER:C	1:A:622:GLU:H	2.15	0.48
10:L:80:THR:O	10:L:83:TYR:HB3	2.13	0.48
3:J:17:TYR:HH	3:J:474:ALA:HA	1.77	0.48
3:B:475:GLN:HG2	3:B:476:ILE:H	1.78	0.48
2:M:28:ILE:CG1	9:U:18:VAL:HG21	2.43	0.48
3:J:191:SER:HB3	3:J:300:HIS:NE2	2.29	0.48
2:C:112:ASP:O	2:C:113:ALA:CB	2.60	0.48
3:J:579:LEU:O	3:J:613:ILE:HG23	2.13	0.48
1:I:575:CYS:CB	1:I:580:CYS:SG	3.02	0.48
3:J:654:ILE:CG2	3:J:881:ARG:HG2	2.43	0.48
4:O:116:SER:OG	4:O:121:VAL:O	2.21	0.48
3:B:249:GLN:CG	3:B:250:ASN:H	2.23	0.48
1:A:357:ASN:HD22	1:A:361:LEU:HD22	1.78	0.48
1:I:637:ARG:HH11	3:J:974:ARG:NH2	2.11	0.48
1:A:268:LEU:HD23	1:A:271:TYR:HD1	1.78	0.48
3:J:75:ARG:N	3:J:75:ARG:HE	2.11	0.48
3:J:67:LYS:HB3	3:J:68:PRO:HD2	1.94	0.48
3:J:368:GLN:HE22	3:J:386:ARG:HH21	1.61	0.48
6:F:69:ARG:HA	6:F:72:LEU:HD12	1.94	0.48
4:O:66:PRO:HG2	11:W:13:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:34:PHE:HE1	3:B:351:ALA:HA	1.78	0.48
3:B:450:TRP:HZ3	3:B:621:GLU:OE2	1.97	0.48
1:I:645:THR:OG1	1:I:646:MET:N	2.46	0.48
4:O:205:LEU:O	4:O:207:GLU:N	2.46	0.48
2:C:144:LEU:O	2:C:145:GLU:C	2.51	0.48
11:W:20:SER:O	11:W:24:ARG:HG3	2.14	0.48
3:J:702:LEU:HD13	11:W:47:ARG:HD2	1.96	0.48
3:B:680:TYR:HE1	3:B:687:ARG:HH12	1.60	0.48
1:I:824:ILE:O	1:I:828:SER:HB3	2.13	0.48
9:K:28:THR:OG1	9:K:31:GLU:CG	2.58	0.48
3:J:555:VAL:HA	3:J:567:HIS:O	2.12	0.48
8:T:18:PRO:HB2	8:T:67:ARG:HA	1.95	0.48
5:Q:38:ILE:O	5:Q:39:LEU:CB	2.61	0.48
1:A:95:LYS:HB3	1:A:138:LYS:HG3	1.95	0.48
7:S:59:ILE:O	7:S:59:ILE:HG22	2.13	0.48
11:N:33:LYS:HA	11:N:36:ASP:HB2	1.96	0.48
2:C:27:LYS:O	2:C:29:VAL:HG23	2.13	0.48
4:D:257:GLU:O	4:D:260:LEU:HB3	2.13	0.48
3:J:551:ASP:N	3:J:551:ASP:OD2	2.47	0.48
3:B:644:SER:N	3:B:645:PRO:CD	2.76	0.48
1:A:512:LYS:N	1:A:583:ASP:OD2	2.46	0.48
7:G:66:TYR:HD1	7:G:114:ARG:HH11	1.62	0.48
1:I:428:ILE:HD11	1:I:485:ASN:HB3	1.95	0.48
1:I:116:ARG:O	1:I:130:ARG:NH2	2.46	0.48
3:J:591:ILE:O	3:J:594:ILE:HG12	2.13	0.48
8:T:44:TRP:O	8:T:79:ARG:HD3	2.13	0.48
9:K:61:VAL:HG12	9:K:62:ILE:H	1.77	0.48
3:B:657:TYR:HE2	3:B:946:TYR:CZ	2.30	0.48
6:R:20:LEU:O	6:R:23:ASP:HB2	2.13	0.48
3:J:227:MET:CE	3:J:232:ILE:HG13	2.43	0.48
1:A:57:LYS:HB3	1:A:62:GLY:HA2	1.94	0.48
3:B:106:ASN:O	3:B:108:GLU:HG3	2.12	0.48
1:I:102:GLY:H	1:I:103:ARG:HE	1.60	0.48
2:M:270:ALA:HA	8:T:14:HIS:ND1	2.28	0.48
4:D:240:ARG:O	4:D:244:GLU:HG2	2.13	0.48
5:E:163:THR:HG23	5:E:165:ARG:H	1.77	0.48
2:C:55:ALA:C	2:C:58:GLU:HB2	2.33	0.48
3:B:473:MET:HA	3:B:577:ARG:NH2	2.29	0.48
3:J:102:PRO:HD2	3:J:109:ALA:HB3	1.95	0.48
4:D:178:LYS:O	4:D:180:VAL:N	2.46	0.48
3:B:181:SER:O	3:B:182:ASN:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:CYS:SG	3:B:1070:TYR:CB	3.00	0.48
13:Z:59:ILE:HA	13:Z:62:GLU:CD	2.34	0.48
4:O:131:VAL:HG22	4:O:132:LEU:H	1.79	0.48
6:F:46:LYS:HD3	6:F:76:CYS:HB2	1.96	0.48
3:B:336:ASP:HA	3:B:341:LYS:HE3	1.94	0.48
3:B:448:THR:C	3:B:450:TRP:N	2.67	0.48
1:A:826:ALA:HB2	2:C:335:THR:HG23	1.95	0.48
3:J:654:ILE:HG22	3:J:881:ARG:HG2	1.95	0.48
3:B:191:SER:HB3	3:B:300:HIS:NE2	2.28	0.48
3:B:240:TYR:HD2	3:B:244:LEU:HD23	1.79	0.48
3:J:330:ARG:HA	3:J:563:ILE:HD11	1.95	0.48
3:B:540:ILE:HG21	3:B:555:VAL:HG21	1.94	0.48
1:I:392:LYS:O	1:I:393:ASP:C	2.52	0.48
1:I:57:LYS:HB3	1:I:62:GLY:HA2	1.95	0.48
3:B:325:LEU:CD1	3:B:331:GLU:H	2.25	0.48
1:I:752:VAL:C	1:I:754:GLY:N	2.66	0.48
8:T:78:TYR:OH	9:U:12:ASP:HB3	2.14	0.48
8:T:68:LYS:HA	8:T:74:GLU:HA	1.96	0.48
3:J:139:ILE:HG21	11:W:61:HIS:HD2	1.79	0.48
1:I:647:ARG:HB2	1:I:650:ASP:OD1	2.13	0.48
2:C:322:ARG:HA	8:H:43:PRO:O	2.13	0.48
1:I:500:GLN:HB2	3:J:913:HIS:ND1	2.28	0.48
2:M:286:ILE:O	2:M:289:ALA:HB3	2.13	0.48
8:T:45:ILE:HB	8:T:79:ARG:HB3	1.96	0.48
1:A:116:ARG:O	1:A:130:ARG:NH2	2.47	0.48
1:I:203:ARG:CZ	1:I:206:TRP:HB2	2.43	0.48
1:A:99:ARG:HG2	1:A:183:ARG:NH1	2.29	0.48
1:I:87:VAL:HG21	1:I:156:ILE:O	2.14	0.48
3:J:425:HIS:HA	3:J:428:ARG:HD3	1.96	0.48
5:E:140:ASP:HB3	5:E:171:LYS:HG3	1.95	0.48
5:Q:39:LEU:HD23	5:Q:41:ASP:H	1.79	0.48
4:D:22:LEU:C	4:D:24:PHE:H	2.16	0.48
3:B:550:SER:HB3	3:B:553:VAL:HG23	1.95	0.48
3:B:749:MET:CE	3:B:907:ASP:HB3	2.43	0.48
3:B:294:ASP:O	3:B:303:THR:HG23	2.13	0.48
2:M:61:GLU:C	2:M:63:LEU:N	2.68	0.48
3:J:900:THR:OG1	3:J:904:VAL:HB	2.14	0.48
1:I:539:ILE:HB	1:I:545:TYR:HB2	1.94	0.48
3:J:1029:GLY:O	3:J:1031:MET:N	2.47	0.48
2:M:103:GLY:CA	2:M:106:ARG:HB3	2.44	0.48
3:J:813:LYS:O	3:J:814:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:111:SER:C	4:D:114:ILE:HD13	2.34	0.48
7:G:80:GLU:CG	7:G:81:LEU:N	2.77	0.48
2:C:354:LEU:HD13	3:B:1104:LEU:CD2	2.43	0.48
3:B:480:ILE:HG22	3:B:481:ASN:H	1.77	0.48
1:I:354:THR:HB	1:I:355:PRO:CD	2.44	0.48
1:I:93:PHE:HB3	1:I:184:LEU:CD2	2.44	0.48
3:B:1036:LEU:HD22	3:B:1041:THR:CG2	2.43	0.48
1:A:831:ARG:HH21	2:C:385:MET:CB	2.27	0.48
1:I:620:SER:C	1:I:622:GLU:H	2.18	0.48
3:J:904:VAL:CG2	11:W:42:ARG:HG2	2.44	0.47
1:I:332:ILE:HA	1:I:436:ARG:HH12	1.78	0.47
1:I:353:ILE:HD11	1:I:407:ILE:CG2	2.45	0.47
1:A:446:ASN:C	1:A:446:ASN:ND2	2.65	0.47
3:B:683:ASN:C	3:B:685:GLN:N	2.64	0.47
9:U:28:THR:OG1	9:U:31:GLU:HG3	2.15	0.47
4:O:134:GLY:O	4:O:135:THR:C	2.52	0.47
8:H:80:TYR:CD1	8:H:81:VAL:O	2.67	0.47
3:J:520:VAL:HG12	3:J:527:ILE:HB	1.94	0.47
4:D:55:ASP:HB3	12:P:45:VAL:HG21	1.96	0.47
3:J:86:ARG:HG3	3:J:153:ILE:HD13	1.96	0.47
3:B:634:THR:N	3:B:635:PRO:HD3	2.29	0.47
1:A:524:ILE:O	1:A:525:LEU:HD22	2.14	0.47
3:J:727:MET:CE	3:J:898:PRO:CG	2.92	0.47
3:J:904:VAL:HG21	11:W:42:ARG:HE	1.78	0.47
9:K:38:ALA:C	9:K:42:GLN:NE2	2.67	0.47
2:M:289:ALA:O	2:M:292:ILE:CG2	2.56	0.47
1:I:830:LEU:HD22	1:I:846:VAL:HG21	1.96	0.47
10:V:12:TYR:CD1	10:V:57:ILE:O	2.68	0.47
3:J:443:ARG:NH2	3:J:462:PRO:O	2.47	0.47
10:V:73:ILE:HG22	10:V:74:GLU:N	2.29	0.47
3:J:325:LEU:HA	3:J:329:ARG:H	1.79	0.47
5:E:96:GLY:HA2	5:E:110:ILE:HG12	1.96	0.47
1:A:194:ILE:H	1:A:194:ILE:HG13	1.34	0.47
5:Q:38:ILE:O	5:Q:39:LEU:HB2	2.14	0.47
5:Q:12:ARG:HG3	5:Q:67:TYR:CZ	2.49	0.47
10:L:45:GLN:HE22	10:L:48:PRO:HD3	1.78	0.47
7:S:68:HIS:ND1	7:S:68:HIS:N	2.46	0.47
3:J:1083:GLY:C	3:J:1085:LYS:H	2.16	0.47
1:A:420:ASN:HB2	1:A:430:MET:HG2	1.96	0.47
1:I:23:SER:HA	1:I:72:PHE:O	2.14	0.47
2:C:376:GLY:HA3	3:B:1050:LEU:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:42:ARG:HG3	11:N:43:TYR:H	1.80	0.47
3:B:1113:LEU:N	3:B:1113:LEU:HD12	2.11	0.47
3:J:813:LYS:N	3:J:836:SER:HB3	2.20	0.47
3:B:617:ASP:O	3:B:618:ALA:HB2	2.14	0.47
3:J:48:GLU:HG3	3:J:365:LEU:HD23	1.95	0.47
1:A:490:ARG:HD3	2:C:77:SER:HA	1.97	0.47
3:J:954:GLN:HA	3:J:957:ILE:HD11	1.95	0.47
2:M:48:ILE:HG22	2:M:49:ASP:H	1.78	0.47
1:I:104:VAL:HG12	1:I:137:LYS:HA	1.97	0.47
1:I:524:ILE:O	1:I:525:LEU:CD2	2.62	0.47
7:G:31:MET:HB2	7:G:38:VAL:O	2.14	0.47
1:I:742:GLN:HB2	3:J:919:MET:CE	2.44	0.47
8:H:78:TYR:C	8:H:79:ARG:HG2	2.35	0.47
4:O:131:VAL:CG2	4:O:132:LEU:N	2.78	0.47
1:A:457:PHE:HB2	3:B:737:SER:HB2	1.96	0.47
2:C:15:GLU:O	2:C:18:LYS:N	2.47	0.47
1:I:467:PRO:HA	3:J:1048:ARG:NH2	2.29	0.47
3:B:1117:ASP:O	3:B:1118:LYS:HB3	2.14	0.47
1:A:691:THR:O	1:A:695:SER:OG	2.30	0.47
3:J:294:ASP:O	3:J:303:THR:HG23	2.14	0.47
4:O:240:ARG:O	4:O:244:GLU:HG2	2.14	0.47
5:E:72:PHE:HE1	5:E:74:MET:SD	2.37	0.47
1:I:541:ALA:CA	7:S:72:CYS:H	2.26	0.47
1:A:559:ASP:OD2	3:J:109:ALA:HA	2.15	0.47
11:N:3:ILE:HG22	11:N:4:PRO:CD	2.43	0.47
3:B:855:THR:CB	3:B:857:GLU:HG2	2.31	0.47
2:M:35:LEU:O	2:M:39:LYS:HG2	2.15	0.47
1:A:833:GLU:CG	1:A:839:ARG:HG3	2.44	0.47
1:A:99:ARG:HG2	1:A:183:ARG:HH12	1.79	0.47
3:B:603:THR:O	3:B:604:PHE:C	2.52	0.47
1:A:105:LYS:HZ3	1:A:108:GLU:HB2	1.79	0.47
1:A:750:GLN:CG	1:A:782:ILE:CD1	2.92	0.47
10:L:3:ILE:HG13	10:L:17:ILE:HD13	1.96	0.47
1:I:14:LEU:HB3	3:J:1108:ILE:HG23	1.96	0.47
3:J:200:VAL:HG13	3:J:200:VAL:O	2.13	0.47
10:L:76:ILE:O	10:L:77:ARG:C	2.53	0.47
3:J:356:VAL:HG22	3:J:393:ARG:NH1	2.29	0.47
3:B:902:LYS:HB3	11:N:42:ARG:CD	2.42	0.47
1:I:490:ARG:NH1	2:M:80:GLU:HG3	2.29	0.47
1:I:113:LYS:HA	1:I:116:ARG:HB3	1.95	0.47
3:J:1054:ASP:HB2	3:J:1094:SER:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:191:SER:HB3	3:B:300:HIS:CD2	2.49	0.47
1:A:425:LEU:HD22	2:C:83:THR:HG21	1.96	0.47
1:A:98:CYS:HB3	1:A:101:CYS:H	1.79	0.47
3:J:289:ALA:O	3:J:293:ILE:CG1	2.62	0.47
6:R:16:VAL:HG22	6:R:53:GLN:HE21	1.79	0.47
10:V:35:ILE:HD13	10:V:75:ASN:OD1	2.14	0.47
3:B:232:ILE:HG23	3:B:237:ASP:HB3	1.94	0.47
3:B:377:ARG:O	3:B:378:LYS:HB2	2.13	0.47
3:J:320:SER:OG	3:J:320:SER:O	2.32	0.47
2:C:123:THR:HG22	2:C:252:LEU:HD23	1.96	0.47
2:M:15:GLU:HA	2:M:18:LYS:HE3	1.95	0.47
3:J:804:VAL:HG11	3:J:810:LEU:HD21	1.97	0.47
13:Z:69:GLU:O	13:Z:73:LYS:NZ	2.35	0.47
3:J:1069:TRP:HE1	3:J:1088:LEU:CB	2.28	0.47
2:M:28:ILE:CG2	9:U:14:HIS:HE1	2.18	0.47
4:D:176:CYS:H	4:D:195:LEU:CD2	2.28	0.47
1:A:728:MET:HE3	3:B:913:HIS:HA	1.95	0.47
3:J:48:GLU:HG2	3:J:58:VAL:HB	1.95	0.47
3:B:813:LYS:N	3:B:836:SER:HB3	2.25	0.47
3:B:881:ARG:NH1	3:B:989:TYR:HB3	2.22	0.47
2:M:355:LEU:N	2:M:355:LEU:HD23	2.29	0.47
3:B:324:GLU:O	3:B:325:LEU:HB2	2.14	0.47
11:W:33:LYS:HA	11:W:36:ASP:HB2	1.96	0.47
3:B:92:TYR:O	3:B:92:TYR:CD2	2.68	0.47
1:I:77:LEU:HD12	1:I:210:THR:C	2.35	0.47
1:A:664:GLU:OE1	1:A:707:LEU:HD22	2.14	0.47
3:B:679:LEU:HD23	3:B:716:ARG:HG2	1.97	0.47
3:B:594:ILE:HB	3:B:599:SER:HB2	1.97	0.47
3:J:971:TYR:CE2	4:O:165:ARG:HA	2.49	0.47
11:W:35:LEU:HD22	11:W:40:VAL:HG21	1.97	0.47
1:I:438:LEU:HD12	10:V:47:HIS:NE2	2.30	0.47
3:B:702:LEU:HD22	3:B:933:ALA:CB	2.32	0.47
3:B:898:PRO:HA	3:B:971:TYR:O	2.14	0.47
3:B:930:GLY:HA3	3:B:987:VAL:HB	1.97	0.47
9:K:82:LEU:HD23	9:K:86:LYS:O	2.15	0.47
2:M:106:ARG:O	2:M:107:LEU:C	2.52	0.47
8:T:42:LEU:HD13	8:T:79:ARG:O	2.14	0.47
3:B:54:PRO:O	3:B:56:LEU:N	2.48	0.47
3:J:64:ARG:H	3:J:97:TRP:HB2	1.80	0.47
3:B:663:SER:HB3	3:B:664:PRO:HD3	1.96	0.47
3:B:557:HIS:N	3:B:623:ASN:ND2	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:70:ARG:C	9:K:72:GLY:H	2.16	0.47
1:A:99:ARG:HE	1:A:183:ARG:NH2	2.12	0.47
1:A:319:ASP:O	1:A:320:PHE:HB2	2.15	0.47
3:B:972:ASP:HB3	3:B:975:THR:HG23	1.97	0.47
3:J:291:GLN:HB3	3:J:295:LYS:CE	2.44	0.47
3:B:950:ILE:C	3:B:952:GLN:N	2.67	0.47
1:I:433:HIS:HE2	1:I:453:TYR:HH	1.57	0.47
3:J:368:GLN:HE22	3:J:386:ARG:HE	1.62	0.47
2:M:13:LEU:HD23	2:M:16:LYS:HZ2	1.78	0.47
1:I:763:THR:HG23	1:I:779:ARG:HH12	1.80	0.47
2:C:393:ILE:HG13	2:C:393:ILE:H	1.56	0.47
5:Q:128:PHE:HE2	5:Q:133:LYS:HD3	1.80	0.47
3:J:463:ASN:HB3	3:J:467:VAL:CG1	2.44	0.47
1:I:321:SER:O	1:I:322:SER:HB2	2.14	0.47
12:X:12:THR:O	12:X:14:THR:N	2.37	0.47
8:T:25:ILE:HA	8:T:28:ALA:HB3	1.97	0.47
1:A:590:ASN:CG	3:J:377:ARG:HB2	2.34	0.47
1:A:349:VAL:HG21	1:A:415:ASP:OD2	2.15	0.47
10:V:46:PRO:HD2	10:V:52:LYS:O	2.15	0.47
3:B:130:ILE:HA	3:B:133:TYR:CE1	2.50	0.47
1:I:845:VAL:O	8:T:43:PRO:HD3	2.15	0.47
1:A:727:VAL:O	1:A:729:ALA:O	2.32	0.47
1:I:841:LEU:HB3	1:I:842:TYR:H	1.54	0.47
4:O:256:LEU:HD13	10:V:3:ILE:HD12	1.97	0.47
3:J:972:ASP:OD2	3:J:974:ARG:CG	2.59	0.47
1:I:533:ASP:O	1:I:534:LEU:C	2.52	0.47
3:J:412:GLN:HG3	3:J:425:HIS:NE2	2.30	0.47
4:O:94:THR:O	4:O:95:LYS:HG3	2.15	0.47
5:Q:179:LYS:HD3	6:R:81:ASP:HB2	1.97	0.47
5:Q:110:ILE:CG2	5:Q:118:LEU:HB3	2.45	0.47
3:J:926:GLU:HB3	3:J:988:VAL:CG2	2.43	0.47
3:J:902:LYS:CB	11:W:42:ARG:HH11	2.27	0.47
2:C:390:MET:C	2:C:391:ARG:CD	2.83	0.47
9:K:42:GLN:O	9:K:45:MET:HB2	2.15	0.47
9:K:82:LEU:CD2	9:K:82:LEU:N	2.72	0.47
1:I:568:VAL:HG21	1:I:597:VAL:HG11	1.96	0.47
7:S:41:ASP:HB2	7:S:91:LYS:H	1.80	0.47
3:B:239:VAL:HA	3:B:253:PHE:CE2	2.48	0.47
3:B:946:TYR:CD2	3:B:947:LYS:N	2.82	0.47
3:J:401:GLY:O	3:J:402:ASN:O	2.32	0.47
1:A:763:THR:HG21	1:A:772:TYR:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:49:LEU:O	10:L:50:SER:HB3	2.15	0.47
3:B:96:LEU:O	3:B:115:TYR:HA	2.15	0.47
3:B:591:ILE:CG1	3:B:612:LYS:NZ	2.71	0.47
1:A:524:ILE:O	1:A:525:LEU:CD2	2.63	0.47
3:J:930:GLY:O	11:W:47:ARG:NH1	2.48	0.47
11:W:10:CYS:HB3	11:W:44:CYS:SG	2.55	0.47
2:M:55:ALA:C	2:M:58:GLU:HB2	2.35	0.47
3:J:1012:LEU:O	3:J:1095:TYR:CE2	2.64	0.47
1:I:595:GLU:HB2	7:S:91:LYS:CE	2.45	0.47
3:B:298:LEU:O	3:B:300:HIS:N	2.48	0.47
3:B:574:ARG:O	3:B:574:ARG:HG3	2.14	0.47
3:B:98:LEU:HD11	3:B:100:MET:CG	2.38	0.47
3:B:677:LEU:HD21	3:B:994:HIS:HB3	1.97	0.47
9:K:67:GLU:CD	9:K:70:ARG:HH21	2.17	0.47
7:G:15:ILE:HG22	7:G:51:GLN:O	2.15	0.47
2:C:189:GLY:O	2:C:190:ARG:HB2	2.15	0.47
3:B:391:THR:O	3:B:394:ILE:HG22	2.15	0.47
1:I:833:GLU:CG	1:I:839:ARG:HG3	2.45	0.47
1:I:85:GLY:HA3	2:M:355:LEU:HD12	1.96	0.47
3:J:683:ASN:C	3:J:685:GLN:N	2.68	0.47
1:A:870:ARG:NH2	2:C:57:LYS:O	2.48	0.47
3:B:781:ARG:HB2	3:B:831:ALA:N	2.30	0.47
3:B:437:GLN:OE1	3:B:438:PRO:HD2	2.15	0.47
3:J:1085:LYS:O	3:J:1086:SER:OG	2.30	0.47
4:D:37:PRO:HA	4:D:148:GLY:O	2.14	0.47
5:E:13:ILE:HG23	5:E:25:ILE:HG21	1.97	0.47
5:E:18:PHE:CD2	9:K:47:ALA:HB2	2.50	0.47
1:A:8:GLY:HA2	2:C:365:GLU:HA	1.96	0.47
3:B:963:LEU:HD22	3:B:982:ARG:NH2	2.30	0.46
1:A:594:LEU:O	1:A:595:GLU:HG2	2.15	0.46
1:I:874:ARG:HE	2:M:53:ASP:HB3	1.79	0.46
5:Q:31:ARG:C	5:Q:33:GLN:N	2.68	0.46
3:B:855:THR:C	3:B:857:GLU:N	2.66	0.46
1:A:16:PRO:HD3	1:A:206:TRP:HD1	1.80	0.46
3:B:921:LEU:O	3:B:923:GLN:N	2.46	0.46
1:I:87:VAL:O	1:I:91:TYR:HB2	2.15	0.46
3:J:840:ARG:NH1	3:J:1021:ALA:HB2	2.29	0.46
4:O:53:LEU:HD22	4:O:57:ILE:CG2	2.44	0.46
3:J:946:TYR:CD2	3:J:947:LYS:N	2.83	0.46
11:N:38:LEU:HD23	11:N:39:GLY:H	1.80	0.46
4:D:45:TYR:HB2	4:D:142:GLU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:X:25:ARG:HD2	12:X:30:GLY:HA2	1.96	0.46
3:B:88:ARG:HG2	12:P:33:ILE:HD11	1.97	0.46
2:C:337:GLU:N	2:C:337:GLU:OE1	2.47	0.46
1:I:428:ILE:HG23	1:I:452:PRO:HB2	1.96	0.46
3:J:582:VAL:HG11	3:J:633:LEU:HD11	1.95	0.46
2:M:318:ASP:O	2:M:322:ARG:HD2	2.15	0.46
2:M:287:GLU:OE2	8:T:79:ARG:CZ	2.63	0.46
3:J:881:ARG:CD	3:J:989:TYR:HD2	2.27	0.46
3:J:249:GLN:CG	3:J:250:ASN:H	2.24	0.46
4:D:134:GLY:O	4:D:135:THR:O	2.33	0.46
3:J:1067:ILE:CG2	3:J:1080:PRO:HG2	2.45	0.46
5:E:113:ILE:HG23	5:E:114:THR:N	2.30	0.46
2:C:152:VAL:O	2:C:152:VAL:HG22	2.14	0.46
2:M:140:VAL:O	2:M:143:LYS:HB2	2.16	0.46
2:C:163:MET:N	2:C:164:SER:HA	2.28	0.46
1:I:537:PRO:O	7:S:74:HIS:NE2	2.47	0.46
4:D:254:GLU:HG2	10:L:77:ARG:NH1	2.31	0.46
4:O:206:CYS:O	4:O:207:GLU:HB2	2.15	0.46
3:J:170:ASN:O	3:J:171:ARG:O	2.34	0.46
3:J:191:SER:HB3	3:J:300:HIS:CD2	2.51	0.46
3:B:953:LEU:O	3:B:957:ILE:HG12	2.14	0.46
4:D:137:GLN:NE2	11:N:63:THR:HG22	2.30	0.46
1:I:525:LEU:C	1:I:527:VAL:H	2.18	0.46
3:J:873:THR:CG2	3:J:874:ILE:H	2.26	0.46
2:M:295:ARG:O	2:M:299:LYS:HB2	2.16	0.46
4:D:53:LEU:HD22	4:D:57:ILE:HG21	1.97	0.46
3:B:227:MET:CE	3:B:232:ILE:HG13	2.46	0.46
4:O:64:LEU:O	11:W:6:ARG:HD2	2.15	0.46
1:I:217:ILE:C	1:I:219:ILE:H	2.18	0.46
1:A:759:ARG:NH2	1:A:763:THR:OG1	2.48	0.46
4:D:170:VAL:HG23	4:D:200:GLU:HG3	1.96	0.46
9:U:70:ARG:HB3	9:U:70:ARG:CZ	2.46	0.46
3:B:698:PRO:HG2	11:N:55:ILE:HD12	1.96	0.46
3:J:1010:GLN:HA	3:J:1010:GLN:OE1	2.15	0.46
4:O:208:GLU:N	16:O:1001:F3S:S2	2.88	0.46
3:B:1029:GLY:O	3:B:1030:GLU:C	2.53	0.46
2:C:321:THR:O	2:C:321:THR:CG2	2.63	0.46
3:J:170:ASN:HB3	3:J:300:HIS:HE1	1.80	0.46
3:J:569:ASN:HB3	3:J:574:ARG:CZ	2.45	0.46
2:C:390:MET:O	2:C:391:ARG:HD2	2.15	0.46
2:C:277:ILE:C	2:C:279:GLU:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U:39:ARG:HE	9:U:68:GLU:CD	2.18	0.46
1:A:425:LEU:HD12	1:A:425:LEU:H	1.80	0.46
1:A:672:VAL:HG11	1:A:776:PRO:HD3	1.98	0.46
4:D:29:ARG:HG3	4:D:162:SER:O	2.16	0.46
3:J:248:VAL:HG21	3:J:329:ARG:HH22	1.80	0.46
3:J:116:ILE:HG23	3:J:361:PHE:CZ	2.50	0.46
2:M:341:VAL:HG11	2:M:357:ALA:HB1	1.97	0.46
2:M:268:ASP:OD1	2:M:270:ALA:HB3	2.15	0.46
2:C:68:GLU:HB3	9:K:30:TYR:CZ	2.50	0.46
1:A:9:ILE:O	2:C:363:VAL:O	2.33	0.46
3:J:343:LEU:HD22	3:J:575:VAL:HG22	1.98	0.46
3:B:721:ASN:HB3	11:N:47:ARG:HE	1.80	0.46
1:I:486:ILE:HG12	1:I:496:ILE:HD12	1.97	0.46
1:A:830:LEU:HD23	1:A:840:SER:CB	2.34	0.46
9:U:41:LEU:O	9:U:42:GLN:C	2.54	0.46
3:B:910:LEU:CD2	3:B:911:ASN:H	2.25	0.46
3:B:870:ARG:NE	3:B:996:MET:SD	2.88	0.46
3:B:1077:TYR:O	3:B:1077:TYR:CD1	2.69	0.46
1:I:631:LEU:O	1:I:634:VAL:HB	2.15	0.46
1:I:58:CYS:HB2	1:I:59:PRO:CD	2.39	0.46
1:A:599:ASP:H	1:A:602:ALA:HB3	1.80	0.46
1:I:741:THR:O	1:I:742:GLN:C	2.54	0.46
2:M:231:ILE:H	2:M:231:ILE:HD12	1.81	0.46
3:J:848:ASP:HB2	3:J:867:ARG:HB2	1.98	0.46
3:J:162:VAL:HG11	3:J:412:GLN:HE21	1.80	0.46
1:I:433:HIS:NE2	1:I:453:TYR:OH	2.43	0.46
3:B:937:GLY:HA3	11:N:32:GLY:CA	2.46	0.46
2:C:72:ILE:HG23	2:C:76:GLN:OE1	2.15	0.46
5:Q:79:PRO:HG3	5:Q:160:ILE:HG12	1.98	0.46
3:J:723:ILE:HG12	3:J:907:ASP:OD2	2.16	0.46
13:Y:57:GLY:HA2	13:Y:61:LEU:HD21	1.97	0.46
4:D:254:GLU:HG2	10:L:77:ARG:HH12	1.80	0.46
3:B:640:LEU:CD2	3:B:641:GLU:N	2.67	0.46
3:J:971:TYR:CZ	3:J:978:LYS:HB3	2.50	0.46
3:J:11:TRP:O	3:J:14:ILE:HG22	2.16	0.46
5:E:39:LEU:HD12	5:E:42:LEU:HG	1.96	0.46
1:A:764:ARG:HB2	1:A:764:ARG:HH11	1.80	0.46
2:C:391:ARG:HB2	9:K:75:PRO:HB2	1.96	0.46
1:I:316:LYS:HD2	3:J:1049:LEU:O	2.15	0.46
9:K:86:LYS:HD2	9:K:86:LYS:H	1.81	0.46
2:M:86:THR:HA	2:M:104:LEU:CD1	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:45:ILE:HG22	8:T:81:VAL:H	1.79	0.46
3:B:246:PRO:C	3:B:248:VAL:N	2.68	0.46
3:J:663:SER:CB	3:J:664:PRO:HD3	2.46	0.46
3:J:158:GLU:OE2	3:J:416:ARG:NH1	2.45	0.46
3:B:992:LYS:HE3	3:B:996:MET:SD	2.55	0.46
1:I:13:ILE:HG13	1:I:207:MET:HG2	1.97	0.46
2:M:48:ILE:HG22	2:M:49:ASP:N	2.31	0.46
6:R:59:LEU:HD22	6:R:69:ARG:HD3	1.97	0.46
3:J:781:ARG:CD	3:J:782:GLY:H	2.26	0.46
1:I:187:ILE:HA	1:I:188:PRO:HD3	1.70	0.46
3:B:402:ASN:HB2	3:B:410:VAL:HB	1.97	0.46
3:B:330:ARG:NH2	3:B:565:GLU:OE1	2.48	0.46
3:J:24:VAL:HG21	3:J:426:LEU:CD1	2.46	0.46
3:J:214:PHE:CD1	3:J:215:PRO:HD2	2.51	0.46
4:O:252:LYS:HD2	10:V:24:LEU:HD23	1.97	0.46
1:I:723:ASN:O	1:I:724:PHE:C	2.51	0.46
2:C:51:ILE:HG13	2:C:51:ILE:H	1.34	0.46
3:J:586:ASN:HA	3:J:587:PRO:HD3	1.82	0.46
3:B:133:TYR:HD2	3:B:137:LYS:HB3	1.80	0.46
3:J:855:THR:CB	3:J:857:GLU:HG2	2.34	0.46
9:U:39:ARG:O	9:U:39:ARG:HG3	2.16	0.46
2:C:269:VAL:O	8:H:14:HIS:HB3	2.15	0.46
3:B:848:ASP:HB2	3:B:867:ARG:HB2	1.97	0.46
3:J:691:ARG:NH1	3:J:756:ARG:NH2	2.64	0.46
6:F:18:LYS:NZ	6:F:45:GLU:HG2	2.29	0.46
5:E:142:VAL:HA	5:E:171:LYS:HA	1.98	0.46
8:T:46:ARG:HD3	8:T:48:SER:H	1.80	0.46
3:B:260:SER:C	3:B:262:ILE:H	2.19	0.46
3:J:797:VAL:HG12	3:J:798:VAL:N	2.31	0.46
1:I:495:ILE:O	1:I:495:ILE:HG13	2.16	0.46
3:J:448:THR:C	3:J:450:TRP:N	2.67	0.46
3:J:751:ARG:HG2	3:J:871:ILE:HG23	1.97	0.46
3:J:762:GLU:HG3	3:J:773:ILE:HG13	1.96	0.46
1:I:371:LYS:HZ3	1:I:373:PRO:HD3	1.80	0.46
3:B:655:ILE:HG23	3:B:881:ARG:O	2.16	0.46
2:C:179:VAL:CG2	2:C:232:LYS:HZ2	2.21	0.46
3:B:289:ALA:O	3:B:293:ILE:CG1	2.64	0.46
5:Q:43:GLY:CA	5:Q:78:VAL:HG23	2.46	0.46
3:J:533:GLY:C	3:J:535:GLU:H	2.19	0.46
10:V:9:GLU:O	10:V:11:ASN:N	2.49	0.46
4:O:80:GLU:HA	4:O:83:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:115:ASP:O	5:E:116:ASP:HB2	2.16	0.46
11:N:20:SER:O	11:N:24:ARG:HG3	2.16	0.46
1:A:145:VAL:O	1:A:145:VAL:HG22	2.16	0.46
13:Y:71:ASN:O	13:Y:74:GLU:HB2	2.15	0.46
1:I:851:GLY:C	1:I:853:ASP:H	2.19	0.46
8:T:80:TYR:O	8:T:81:VAL:HG23	2.16	0.46
3:B:248:VAL:HG21	3:B:329:ARG:HH22	1.80	0.46
2:C:179:VAL:HG21	2:C:232:LYS:NZ	2.25	0.46
7:G:9:ILE:HD13	7:G:104:LYS:HB2	1.98	0.46
3:J:325:LEU:HD21	3:J:332:PRO:HD3	1.97	0.46
9:U:34:ARG:C	9:U:37:SER:HB2	2.36	0.46
9:U:82:LEU:HB3	9:U:83:PRO:HD2	1.97	0.46
7:S:103:VAL:HG13	7:S:103:VAL:O	2.16	0.46
4:O:131:VAL:CG2	4:O:132:LEU:H	2.29	0.46
7:G:84:SER:HA	7:G:92:TYR:O	2.16	0.46
3:J:402:ASN:HB2	3:J:410:VAL:HB	1.98	0.46
10:L:47:HIS:O	10:L:49:LEU:N	2.49	0.46
1:I:445:LEU:HD21	1:I:450:CYS:HA	1.97	0.46
3:J:950:ILE:C	3:J:952:GLN:N	2.70	0.46
2:C:281:GLU:OE1	2:C:326:VAL:HG12	2.15	0.46
5:E:124:ARG:HG3	5:E:126:ILE:CG1	2.46	0.46
1:A:532:ILE:HG23	10:L:40:PHE:CD2	2.51	0.46
3:B:638:THR:HB	3:B:639:HIS:HD2	1.68	0.46
12:P:26:CYS:CB	12:P:27:PRO:HD2	2.30	0.46
3:B:170:ASN:O	3:B:171:ARG:O	2.34	0.46
3:J:81:SER:OG	3:J:141:ILE:CG2	2.64	0.46
3:B:48:GLU:HG3	3:B:365:LEU:HD23	1.97	0.46
1:A:329:ASP:CB	1:A:332:ILE:HD12	2.45	0.46
3:J:738:ILE:HD12	3:J:739:ILE:H	1.81	0.46
4:D:134:GLY:O	4:D:135:THR:C	2.54	0.46
4:D:133:LEU:HD22	4:D:137:GLN:HB3	1.98	0.46
9:U:50:LEU:H	9:U:50:LEU:HD12	1.79	0.46
1:I:209:LEU:HD11	1:I:277:PHE:HE2	1.80	0.46
2:M:297:ILE:O	2:M:298:SER:C	2.55	0.46
1:I:475:GLU:OE2	3:J:1043:MET:HB2	2.16	0.46
3:B:895:VAL:HG11	4:D:34:LEU:CD2	2.46	0.46
3:J:658:PRO:O	3:J:660:HIS:N	2.44	0.46
3:B:174:VAL:HG12	3:B:175:ASP:N	2.31	0.46
3:J:661:ASN:ND2	3:J:921:LEU:O	2.48	0.46
12:X:9:CYS:HB3	12:X:12:THR:O	2.16	0.46
1:A:487:ILE:O	1:A:858:MET:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1054:ASP:HB2	3:B:1094:SER:HA	1.98	0.45
1:A:553:SER:OG	1:A:592:ILE:HA	2.15	0.45
3:J:54:PRO:O	3:J:55:GLY:C	2.54	0.45
1:I:434:ARG:HE	1:I:434:ARG:HB3	1.40	0.45
3:J:338:TYR:CZ	3:J:341:LYS:NZ	2.84	0.45
9:K:82:LEU:HD21	9:K:88:ILE:HG12	1.98	0.45
2:M:322:ARG:HD2	2:M:322:ARG:N	2.32	0.45
3:J:1004:ARG:NH1	3:J:1016:PRO:HB3	2.30	0.45
3:B:557:HIS:CE1	3:B:566:VAL:HG13	2.52	0.45
3:B:881:ARG:CD	3:B:989:TYR:HD2	2.27	0.45
1:I:181:ARG:HG3	1:I:208:ILE:HB	1.98	0.45
7:G:94:THR:HG21	7:G:101:LEU:HD11	1.98	0.45
1:I:722:PHE:CZ	7:S:23:LEU:HG	2.45	0.45
1:A:45:MET:O	1:A:47:PRO:HD3	2.15	0.45
6:F:14:TYR:O	6:F:18:LYS:HE3	2.16	0.45
3:B:200:VAL:O	3:B:200:VAL:CG1	2.64	0.45
3:J:437:GLN:OE1	3:J:438:PRO:HD2	2.17	0.45
3:B:96:LEU:HB2	3:B:117:GLY:H	1.80	0.45
4:D:191:LYS:HB2	4:D:194:LYS:HD2	1.97	0.45
3:B:23:LEU:HB3	3:B:24:VAL:H	1.52	0.45
3:J:430:ILE:HG22	3:J:431:SER:O	2.16	0.45
10:L:82:HIS:O	10:L:86:GLU:N	2.48	0.45
11:N:6:ARG:HA	11:N:12:SER:O	2.15	0.45
3:B:633:LEU:HD13	3:B:640:LEU:HG	1.99	0.45
1:A:723:ASN:O	1:A:724:PHE:C	2.54	0.45
3:B:472:LEU:HD12	3:B:646:ALA:HA	1.99	0.45
3:J:672:MET:CG	3:J:993:LEU:HD21	2.27	0.45
9:U:61:VAL:O	9:U:63:SER:N	2.42	0.45
11:W:35:LEU:HD22	11:W:46:ARG:HG3	1.99	0.45
9:K:50:LEU:CD2	9:K:74:LEU:HA	2.36	0.45
1:A:342:ILE:O	1:A:345:LYS:N	2.49	0.45
2:M:290:ARG:HG3	2:M:321:THR:HG21	1.98	0.45
2:M:70:ILE:HA	2:M:73:VAL:HG22	1.97	0.45
3:J:246:PRO:O	3:J:248:VAL:N	2.44	0.45
3:J:110:GLU:HA	3:J:111:PRO:HA	1.51	0.45
1:I:518:LYS:H	1:I:518:LYS:HG2	1.61	0.45
8:H:69:SER:HB2	8:H:75:VAL:CG2	2.46	0.45
13:Y:57:GLY:HA2	13:Y:61:LEU:CD2	2.46	0.45
2:C:339:ASN:N	2:C:339:ASN:OD1	2.32	0.45
3:B:570:CYS:HB3	3:B:571:ASP:H	1.59	0.45
3:J:1036:LEU:HD22	3:J:1041:THR:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:708:ARG:O	1:I:711:ALA:HB3	2.17	0.45
1:I:618:GLU:O	1:I:619:TYR:CG	2.69	0.45
3:J:983:ILE:HG22	3:J:984:TYR:O	2.17	0.45
7:G:75:GLY:HA3	7:G:86:LEU:O	2.16	0.45
5:Q:27:LEU:HD21	5:Q:31:ARG:NH2	2.31	0.45
1:A:234:ASP:C	1:A:236:THR:H	2.19	0.45
3:J:182:ASN:N	3:J:182:ASN:HD22	2.14	0.45
3:J:346:ALA:O	3:J:350:PHE:HB2	2.16	0.45
3:B:691:ARG:NH1	3:B:756:ARG:NH2	2.65	0.45
10:L:7:LYS:HE3	10:L:12:TYR:CE2	2.48	0.45
3:J:921:LEU:O	3:J:923:GLN:N	2.48	0.45
7:S:66:TYR:N	7:S:66:TYR:CD1	2.83	0.45
3:J:123:LEU:O	3:J:125:SER:N	2.49	0.45
3:J:264:ASN:H	3:J:267:ASP:HB2	1.81	0.45
3:J:343:LEU:HB2	3:J:476:ILE:HG21	1.99	0.45
3:J:633:LEU:HD13	3:J:640:LEU:HG	1.98	0.45
7:S:86:LEU:HG	7:S:87:ASN:N	2.31	0.45
1:I:371:LYS:HZ2	1:I:373:PRO:HD3	1.81	0.45
3:J:544:ARG:HB2	3:J:549:ILE:HG22	1.99	0.45
12:P:37:VAL:HG22	12:P:38:ARG:N	2.31	0.45
1:A:71:HIS:ND1	3:B:1070:TYR:CE2	2.82	0.45
9:U:31:GLU:CD	9:U:78:ILE:HG21	2.37	0.45
1:I:839:ARG:NH1	8:T:37:ILE:CG2	2.78	0.45
3:J:685:GLN:HE22	3:J:867:ARG:HH22	1.64	0.45
6:R:24:VAL:C	6:R:26:ARG:H	2.20	0.45
3:J:96:LEU:HD21	3:J:119:LEU:HB2	1.98	0.45
9:K:30:TYR:CD1	9:K:30:TYR:N	2.85	0.45
1:I:346:THR:HG21	3:J:1003:ALA:HB1	1.97	0.45
3:B:591:ILE:HG12	3:B:612:LYS:HZ2	1.77	0.45
1:A:525:LEU:HA	1:A:527:VAL:HG23	1.97	0.45
3:B:702:LEU:HB2	3:B:721:ASN:ND2	2.32	0.45
1:I:486:ILE:HA	1:I:496:ILE:HD12	1.99	0.45
3:B:298:LEU:C	3:B:300:HIS:N	2.70	0.45
3:J:133:TYR:HD2	3:J:137:LYS:HB3	1.81	0.45
3:B:314:TYR:HE2	3:B:526:LEU:N	2.02	0.45
13:Z:61:LEU:O	13:Z:65:LYS:HB2	2.16	0.45
3:B:661:ASN:ND2	3:B:921:LEU:O	2.48	0.45
1:I:155:LYS:HA	1:I:156:ILE:O	2.17	0.45
3:B:544:ARG:NH2	3:B:620:GLU:OE2	2.50	0.45
3:J:691:ARG:NH1	3:J:756:ARG:HH21	2.15	0.45
4:D:53:LEU:HD11	11:N:2:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:PHE:HB3	1:A:184:LEU:CD2	2.46	0.45
2:C:359:ALA:O	2:C:361:GLY:N	2.49	0.45
1:A:392:LYS:O	1:A:393:ASP:C	2.54	0.45
3:B:215:PRO:O	3:B:216:ALA:HB3	2.17	0.45
1:I:759:ARG:HE	1:I:759:ARG:HB3	1.57	0.45
1:A:527:VAL:HB	1:A:530:VAL:HB	1.98	0.45
3:B:930:GLY:CA	11:N:47:ARG:HH22	2.29	0.45
1:I:512:LYS:N	1:I:583:ASP:OD2	2.50	0.45
5:Q:15:PRO:HG3	5:Q:64:GLY:O	2.15	0.45
3:B:569:ASN:HB3	3:B:574:ARG:NH1	2.29	0.45
3:B:554:ASN:ND2	3:B:576:ARG:HH21	2.11	0.45
8:H:13:ILE:HG23	8:H:14:HIS:CE1	2.51	0.45
3:B:98:LEU:CD1	3:B:100:MET:HG3	2.37	0.45
4:O:11:THR:HG22	4:O:232:SER:HB3	1.98	0.45
5:E:51:VAL:C	5:E:53:THR:H	2.19	0.45
1:A:446:ASN:O	1:A:447:LEU:C	2.55	0.45
1:I:16:PRO:HD3	1:I:206:TRP:CD1	2.52	0.45
3:J:768:GLY:O	3:J:769:GLN:HB2	2.15	0.45
10:V:84:ILE:O	10:V:87:ILE:HG22	2.17	0.45
4:D:34:LEU:HD22	4:D:151:LYS:HB2	1.99	0.45
1:I:279:ASN:ND2	1:I:295:LEU:O	2.49	0.45
5:Q:101:LEU:HD21	5:Q:162:LEU:HD11	1.99	0.45
13:Y:71:ASN:HA	13:Y:74:GLU:OE1	2.16	0.45
3:B:1012:LEU:O	3:B:1095:TYR:CE2	2.68	0.45
2:M:28:ILE:HG12	2:M:28:ILE:H	1.60	0.45
3:J:900:THR:HG21	3:J:968:GLU:OE2	2.16	0.45
11:W:18:TRP:CZ2	11:W:22:ILE:HG13	2.52	0.45
11:N:35:LEU:HD23	11:N:40:VAL:HG21	1.98	0.45
11:N:4:PRO:HG2	11:N:48:MET:HE1	1.99	0.45
1:I:827:LEU:HD12	2:M:71:GLY:HA2	1.99	0.45
1:A:728:MET:HE1	3:B:912:PRO:O	2.17	0.45
3:B:1069:TRP:NE1	3:B:1088:LEU:HD13	2.32	0.45
1:A:354:THR:HB	1:A:355:PRO:CD	2.46	0.45
1:A:86:LEU:HD22	1:A:207:MET:HE3	1.99	0.45
10:V:4:ARG:CG	10:V:4:ARG:HH11	2.27	0.45
3:B:555:VAL:HA	3:B:567:HIS:O	2.17	0.45
1:A:5:ASN:O	3:B:1116:GLU:N	2.50	0.45
3:B:123:LEU:C	3:B:125:SER:H	2.20	0.45
2:M:210:PHE:HB3	2:M:211:ALA:H	1.54	0.45
3:J:240:TYR:HD2	3:J:244:LEU:HD23	1.82	0.45
3:J:758:TYR:O	3:J:759:SER:CB	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:VAL:HG12	1:A:635:PHE:N	2.32	0.45
3:J:34:PHE:HA	3:J:38:LYS:HB3	1.98	0.45
3:J:930:GLY:CA	11:W:47:ARG:HH22	2.27	0.45
2:M:55:ALA:HB2	2:M:58:GLU:OE2	2.17	0.45
11:N:35:LEU:HD22	11:N:40:VAL:HG21	1.98	0.45
1:I:447:LEU:HD11	3:J:731:GLY:O	2.16	0.45
3:B:97:TRP:O	3:B:98:LEU:HB3	2.17	0.45
2:M:226:ILE:HB	2:M:227:LEU:HD12	1.97	0.45
3:J:555:VAL:HG22	3:J:568:VAL:HA	1.99	0.45
1:I:556:LEU:HA	1:I:557:PRO:HD3	1.90	0.45
10:L:49:LEU:H	10:L:49:LEU:HD22	1.82	0.45
3:J:454:CYS:HB2	3:J:649:GLY:N	2.32	0.45
3:J:778:ALA:HA	3:J:783:TYR:CE1	2.51	0.45
1:I:430:MET:O	1:I:431:MET:HG3	2.16	0.45
2:C:171:ASN:HA	2:C:174:LEU:HB3	1.98	0.45
10:L:87:ILE:HD13	10:L:87:ILE:HA	1.79	0.45
3:J:21:LYS:HA	3:J:25:ARG:CZ	2.47	0.45
3:J:298:LEU:O	3:J:300:HIS:N	2.50	0.45
5:E:66:THR:CG2	5:E:68:HIS:CE1	2.99	0.45
1:I:327:SER:HB2	1:I:444:ARG:CD	2.47	0.45
1:A:206:TRP:C	1:A:208:ILE:H	2.20	0.45
9:U:84:ASN:HB3	9:U:86:LYS:HB2	1.99	0.45
3:J:781:ARG:HB2	3:J:831:ALA:N	2.32	0.45
3:B:657:TYR:HB3	3:B:660:HIS:CD2	2.52	0.45
1:I:483:HIS:HD2	1:I:625:LYS:HG3	1.79	0.45
3:J:226:LEU:O	3:J:230:LEU:HD12	2.17	0.45
3:B:148:PRO:HG3	3:B:422:MET:CE	2.47	0.45
3:J:221:ILE:HD13	3:J:221:ILE:N	2.31	0.45
10:L:92:LYS:HE3	10:L:92:LYS:HA	1.98	0.45
3:B:5:LEU:O	3:B:5:LEU:HD22	2.17	0.45
4:O:170:VAL:HG23	4:O:200:GLU:HG3	1.99	0.45
4:D:125:SER:OG	4:D:127:ASP:HB3	2.16	0.45
4:D:78:TRP:O	4:D:80:GLU:N	2.50	0.45
3:J:956:GLU:O	3:J:960:TYR:HD1	2.00	0.45
1:A:456:ASP:OD1	1:A:460:ASP:OD2	2.35	0.45
3:J:260:SER:C	3:J:262:ILE:H	2.20	0.45
3:B:353:LEU:CA	3:B:404:VAL:HG11	2.16	0.45
4:O:178:LYS:O	4:O:180:VAL:N	2.50	0.45
3:J:554:ASN:O	3:J:569:ASN:N	2.48	0.45
3:J:569:ASN:HB3	3:J:574:ARG:NH1	2.32	0.45
1:I:607:GLN:HB2	1:I:608:PRO:CD	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:106:ARG:O	2:M:109:GLU:HB2	2.16	0.45
3:B:687:ARG:NH1	3:B:689:ASP:OD1	2.49	0.45
1:I:508:LEU:HB3	1:I:638:PHE:HE2	1.81	0.45
7:S:87:ASN:O	7:S:89:GLY:N	2.50	0.45
1:A:332:ILE:HA	1:A:436:ARG:HH12	1.82	0.45
1:I:371:LYS:HZ2	1:I:373:PRO:CD	2.30	0.45
1:A:575:CYS:CB	1:A:580:CYS:HG	2.30	0.45
1:I:181:ARG:O	1:I:185:GLU:HG3	2.17	0.45
3:B:291:GLN:HB3	3:B:295:LYS:CE	2.44	0.45
1:A:820:GLN:O	1:A:823:LEU:HD12	2.17	0.45
2:C:282:GLU:O	8:H:50:PRO:HG3	2.17	0.45
2:M:388:LEU:CD2	9:U:35:VAL:HG12	2.47	0.45
2:C:170:ASP:OD1	2:C:171:ASN:N	2.46	0.45
1:I:564:GLY:O	1:I:586:VAL:N	2.47	0.45
3:B:792:LEU:HD21	3:B:809:VAL:HG12	1.98	0.45
1:A:586:VAL:HA	1:A:596:GLY:HA3	1.99	0.45
1:I:647:ARG:HB2	1:I:650:ASP:CG	2.37	0.44
9:K:39:ARG:HD3	9:K:74:LEU:HD23	1.98	0.44
2:C:258:LEU:HD22	2:C:279:GLU:HG2	1.99	0.44
2:M:289:ALA:HA	2:M:292:ILE:HG22	1.99	0.44
2:M:322:ARG:C	2:M:324:GLY:H	2.21	0.44
3:J:814:VAL:HG22	3:J:833:ARG:O	2.17	0.44
3:B:239:VAL:HG22	3:B:253:PHE:HD2	1.82	0.44
1:I:528:ALA:O	1:I:530:VAL:HG12	2.16	0.44
2:C:347:PHE:CE2	2:C:348:GLU:HG3	2.53	0.44
1:I:764:ARG:NH1	1:I:764:ARG:HB2	2.33	0.44
1:A:283:GLY:C	1:A:285:PRO:HD2	2.37	0.44
3:B:936:SER:HA	3:B:960:TYR:CE2	2.53	0.44
3:B:108:GLU:O	3:B:110:GLU:N	2.51	0.44
4:O:78:TRP:CD1	4:O:78:TRP:N	2.85	0.44
5:E:2:TYR:N	5:E:2:TYR:CD1	2.85	0.44
1:I:641:LEU:O	3:J:980:LYS:HB2	2.17	0.44
7:G:64:PRO:O	7:G:114:ARG:HD2	2.18	0.44
2:C:318:ASP:OD2	2:C:322:ARG:NH2	2.51	0.44
1:I:452:PRO:HG3	1:I:496:ILE:HG12	2.00	0.44
3:J:634:THR:N	3:J:635:PRO:HD3	2.33	0.44
3:J:855:THR:C	3:J:857:GLU:N	2.70	0.44
3:B:243:SER:O	3:B:249:GLN:OE1	2.35	0.44
1:I:16:PRO:HD3	1:I:206:TRP:HD1	1.83	0.44
6:F:23:ASP:HA	6:F:26:ARG:HD2	2.00	0.44
3:J:402:ASN:O	3:J:403:TRP:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:325:LEU:HD12	3:B:328:GLY:HA2	1.98	0.44
3:B:490:TYR:HE1	3:B:527:ILE:CG2	2.30	0.44
3:B:86:ARG:HG3	3:B:153:ILE:HD13	1.98	0.44
1:A:648:LEU:HB2	3:B:924:ILE:HG21	1.99	0.44
7:S:10:ILE:HD12	7:S:10:ILE:H	1.81	0.44
7:G:75:GLY:HA3	7:G:87:ASN:HA	1.98	0.44
7:S:42:ILE:HD13	7:S:42:ILE:HA	1.85	0.44
2:M:314:LEU:O	2:M:315:LEU:C	2.53	0.44
9:U:38:ALA:O	9:U:41:LEU:N	2.50	0.44
3:B:554:ASN:O	3:B:569:ASN:N	2.49	0.44
1:A:500:GLN:HG3	1:A:501:ASP:H	1.82	0.44
1:A:665:ILE:HG13	1:A:666:ASP:N	2.32	0.44
1:A:441:LEU:HD12	3:B:873:THR:HG21	2.00	0.44
1:A:346:THR:O	3:B:1005:ALA:HB2	2.17	0.44
12:P:17:GLN:C	12:P:19:LYS:H	2.19	0.44
3:J:246:PRO:C	3:J:248:VAL:N	2.68	0.44
3:J:1104:LEU:HB3	3:J:1109:ILE:HB	1.99	0.44
2:M:192:LYS:C	2:M:194:GLY:N	2.69	0.44
4:D:34:LEU:O	4:D:150:GLY:N	2.49	0.44
3:J:68:PRO:HA	3:J:93:ALA:O	2.16	0.44
3:J:657:TYR:HE2	3:J:946:TYR:CZ	2.35	0.44
1:I:561:ASN:HD22	1:I:590:ASN:H	1.65	0.44
1:I:347:LEU:HD13	1:I:466:VAL:CG2	2.47	0.44
3:B:595:GLU:CA	3:B:599:SER:HB3	2.39	0.44
1:A:647:ARG:HD3	3:B:965:ASP:HB3	1.99	0.44
3:B:343:LEU:HB2	3:B:476:ILE:HG21	2.00	0.44
3:J:1069:TRP:HE3	3:J:1070:TYR:N	2.14	0.44
7:S:72:CYS:HA	7:S:114:ARG:HA	1.99	0.44
1:A:878:TRP:NE1	3:J:377:ARG:HD3	2.31	0.44
3:B:971:TYR:CZ	3:B:978:LYS:HB3	2.52	0.44
3:B:82:PRO:HG3	3:B:130:ILE:CD1	2.47	0.44
2:M:70:ILE:HG12	2:M:315:LEU:HD11	2.00	0.44
8:T:80:TYR:CD1	8:T:81:VAL:O	2.70	0.44
3:J:655:ILE:HG23	3:J:881:ARG:O	2.17	0.44
3:B:249:GLN:HB2	3:B:253:PHE:CZ	2.52	0.44
2:M:149:ILE:O	2:M:153:VAL:HG12	2.18	0.44
3:B:975:THR:OG1	3:B:977:GLN:HG2	2.17	0.44
1:A:827:LEU:CD2	2:C:75:ALA:HB2	2.47	0.44
2:C:32:LEU:O	2:C:36:ILE:HB	2.17	0.44
8:H:62:ILE:HG22	8:H:80:TYR:HA	1.99	0.44
3:B:419:TRP:HZ3	3:B:712:GLY:CA	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:368:GLN:NE2	3:B:386:ARG:HE	2.16	0.44
2:M:135:ASP:C	2:M:137:ALA:H	2.20	0.44
4:D:35:TYR:O	4:D:149:TYR:HD2	2.01	0.44
3:J:753:THR:HG23	3:J:868:ASP:H	1.82	0.44
2:C:310:ILE:O	2:C:314:LEU:HD23	2.16	0.44
8:H:82:ILE:HA	8:H:82:ILE:HD13	1.87	0.44
3:B:963:LEU:HD22	4:D:208:GLU:HG3	2.00	0.44
3:J:554:ASN:ND2	3:J:576:ARG:HH21	2.06	0.44
3:J:108:GLU:HB2	3:J:109:ALA:H	1.65	0.44
1:I:425:LEU:H	1:I:425:LEU:HD12	1.81	0.44
3:J:668:TYR:O	3:J:671:ALA:HB3	2.17	0.44
3:B:911:ASN:HD21	3:B:913:HIS:HD2	1.65	0.44
1:I:249:LEU:HD21	1:I:265:LEU:HB2	1.99	0.44
1:A:181:ARG:O	1:A:185:GLU:HG3	2.17	0.44
1:I:747:LEU:HD22	1:I:786:PHE:CE1	2.53	0.44
2:C:188:ILE:HB	2:C:189:GLY:H	1.65	0.44
3:J:480:ILE:HG22	3:J:481:ASN:H	1.83	0.44
1:A:209:LEU:HD11	1:A:277:PHE:HE2	1.82	0.44
3:J:484:ILE:H	3:J:484:ILE:CD1	2.27	0.44
3:B:12:ARG:HB2	3:B:592:GLU:OE2	2.17	0.44
2:M:141:ALA:HB2	2:M:251:ILE:HD11	1.99	0.44
1:A:275:THR:HA	1:A:278:ASP:O	2.18	0.44
3:B:804:VAL:HG11	3:B:810:LEU:HD21	1.99	0.44
1:A:723:ASN:ND2	1:A:725:ALA:H	2.15	0.44
1:A:874:ARG:HG3	2:C:54:LEU:HB2	1.99	0.44
1:A:506:ALA:O	1:A:510:THR:HG23	2.18	0.44
1:I:870:ARG:CZ	2:M:57:LYS:O	2.66	0.44
1:A:409:ARG:NH2	1:A:415:ASP:OD2	2.49	0.44
1:I:728:MET:HE1	3:J:912:PRO:O	2.17	0.44
1:I:864:LYS:NZ	2:M:29:VAL:HA	2.33	0.44
2:M:109:GLU:OE2	2:M:117:PRO:HA	2.16	0.44
3:B:183:ILE:HG22	3:B:209:THR:N	2.33	0.44
3:J:557:HIS:N	3:J:623:ASN:ND2	2.57	0.44
1:A:448:LEU:O	1:A:496:ILE:HG23	2.17	0.44
1:A:498:ALA:HB3	1:A:603:ILE:O	2.18	0.44
7:G:101:LEU:HD12	7:G:104:LYS:HZ3	1.80	0.44
3:J:291:GLN:C	3:J:293:ILE:N	2.71	0.44
2:M:383:THR:HG22	3:J:1042:ALA:H	1.82	0.44
1:I:184:LEU:O	1:I:186:LYS:N	2.50	0.44
3:J:111:PRO:O	3:J:112:GLU:CB	2.64	0.44
3:B:75:ARG:N	3:B:75:ARG:HE	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:658:PRO:HB2	3:J:666:ASN:ND2	2.33	0.44
3:B:139:ILE:HD13	11:N:61:HIS:HD2	1.80	0.44
1:I:763:THR:HG21	1:I:772:TYR:HA	1.99	0.44
8:H:72:TYR:C	8:H:74:GLU:H	2.21	0.44
3:B:24:VAL:HG21	3:B:426:LEU:HD13	2.00	0.44
1:I:586:VAL:HA	1:I:596:GLY:HA3	1.99	0.44
11:W:38:LEU:HD23	11:W:39:GLY:N	2.32	0.44
1:I:402:ALA:O	1:I:403:PRO:C	2.54	0.44
1:A:526:GLY:HA2	10:L:44:TYR:CD1	2.53	0.44
2:M:125:TYR:HD2	2:M:250:ILE:HG23	1.82	0.44
3:J:965:ASP:C	3:J:967:THR:H	2.21	0.44
11:W:3:ILE:HG22	11:W:4:PRO:CD	2.48	0.44
2:C:113:ALA:HB3	2:C:328:GLN:NE2	2.32	0.44
3:J:910:LEU:CD2	3:J:911:ASN:H	2.30	0.44
3:B:759:SER:CB	3:B:862:VAL:O	2.56	0.44
3:B:244:LEU:C	3:B:246:PRO:HD3	2.38	0.44
3:B:1001:LEU:O	3:B:1020:ARG:HD3	2.17	0.44
7:G:30:ASN:C	7:G:31:MET:HG3	2.38	0.44
3:J:325:LEU:O	3:J:326:TYR:C	2.56	0.44
1:I:5:ASN:O	3:J:1116:GLU:N	2.51	0.44
1:I:416:ILE:HD11	1:I:477:LYS:HG3	2.00	0.44
8:T:46:ARG:CD	8:T:48:SER:HB2	2.47	0.44
3:J:932:TYR:CD2	3:J:953:LEU:HD22	2.52	0.44
1:A:337:VAL:HG23	1:A:433:HIS:CG	2.52	0.44
2:M:352:LYS:O	2:M:353:HIS:C	2.56	0.44
1:A:524:ILE:CG2	1:A:634:VAL:HG13	2.48	0.44
7:G:66:TYR:CD1	7:G:114:ARG:NH1	2.82	0.44
7:S:64:PRO:C	7:S:114:ARG:HH11	2.21	0.44
1:A:364:PHE:HD2	1:A:373:PRO:O	2.00	0.44
3:B:970:VAL:HG22	3:B:979:ILE:HG12	2.00	0.44
1:A:829:ASP:HA	2:C:369:VAL:HG13	1.99	0.44
8:T:44:TRP:HA	8:T:80:TYR:HB3	2.00	0.44
5:Q:56:GLU:HA	5:Q:68:HIS:ND1	2.33	0.44
3:B:812:GLY:HA2	3:B:836:SER:CB	2.47	0.44
1:I:528:ALA:C	1:I:530:VAL:H	2.21	0.44
2:M:115:LYS:HD3	2:M:278:ARG:HD2	2.00	0.44
1:I:4:LYS:NZ	3:J:1115:LEU:HB3	2.32	0.44
11:N:22:ILE:HD12	11:N:22:ILE:H	1.82	0.44
1:A:175:LEU:HD23	1:A:176:THR:H	1.82	0.44
5:E:107:LEU:O	5:E:162:LEU:N	2.50	0.44
3:J:68:PRO:CD	3:J:129:PRO:HG2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:936:SER:HA	3:J:960:TYR:CE2	2.53	0.44
3:J:785:GLY:HA3	3:J:788:TYR:HE2	1.82	0.44
13:Z:38:ILE:O	13:Z:39:GLN:HB2	2.17	0.44
3:J:705:THR:HG22	3:J:706:ARG:H	1.83	0.44
1:I:456:ASP:OD1	1:I:460:ASP:OD2	2.35	0.44
1:A:679:TYR:OH	1:A:693:GLU:HG2	2.17	0.44
13:Y:67:LEU:HA	13:Y:70:ASP:HB2	2.00	0.44
13:Y:69:GLU:O	13:Y:73:LYS:HG2	2.18	0.44
3:B:586:ASN:HA	3:B:587:PRO:HD3	1.80	0.44
1:I:650:ASP:HB3	1:I:723:ASN:ND2	2.32	0.44
3:J:720:ASN:N	3:J:720:ASN:HD22	2.16	0.44
1:A:588:ILE:HA	1:A:592:ILE:O	2.17	0.44
5:E:15:PRO:CG	9:K:45:MET:HB3	2.41	0.44
5:Q:27:LEU:HD21	5:Q:31:ARG:CZ	2.48	0.44
2:M:286:ILE:CD1	8:T:45:ILE:HG13	2.48	0.44
3:J:134:THR:O	3:J:138:LEU:HD12	2.18	0.44
1:A:500:GLN:HB2	3:B:913:HIS:CG	2.53	0.44
3:J:249:GLN:HB2	3:J:253:PHE:CZ	2.53	0.44
1:A:747:LEU:HD23	1:A:747:LEU:N	2.33	0.44
1:A:637:ARG:HH11	3:B:974:ARG:HH22	1.66	0.44
1:A:4:LYS:HG2	1:A:5:ASN:N	2.32	0.44
1:A:105:LYS:HZ2	1:A:108:GLU:HB2	1.81	0.44
10:V:72:ALA:O	10:V:75:ASN:HB2	2.18	0.44
4:D:64:LEU:O	11:N:6:ARG:HD2	2.18	0.44
10:V:63:ILE:HG22	10:V:64:THR:H	1.83	0.44
7:G:26:LEU:HD13	7:G:27:SER:N	2.32	0.44
4:D:168:PRO:HG3	4:D:203:CYS:O	2.18	0.44
3:B:446:HIS:O	3:B:447:GLY:C	2.56	0.43
1:I:859:TYR:HB2	2:M:64:ILE:HG21	2.00	0.43
3:J:50:PRO:C	3:J:52:GLU:H	2.21	0.43
1:I:874:ARG:HD3	1:I:874:ARG:HA	1.76	0.43
2:M:391:ARG:NH2	9:U:39:ARG:HD2	2.27	0.43
1:A:426:HIS:O	1:A:429:SER:HB2	2.18	0.43
3:B:814:VAL:HG22	3:B:833:ARG:O	2.18	0.43
3:B:253:PHE:N	3:B:254:PRO:CD	2.79	0.43
1:A:781:PHE:CD2	1:A:781:PHE:C	2.91	0.43
3:B:741:ASN:C	3:B:741:ASN:OD1	2.56	0.43
10:L:47:HIS:O	10:L:48:PRO:C	2.56	0.43
3:J:432:SER:HB3	3:J:435:ARG:HH21	1.81	0.43
4:O:59:ALA:O	4:O:62:LEU:HB2	2.18	0.43
1:I:600:LYS:HB2	1:I:732:GLY:HA3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:482:GLU:O	3:B:483:ARG:C	2.56	0.43
1:A:723:ASN:C	1:A:723:ASN:ND2	2.72	0.43
1:A:549:LYS:NZ	7:G:89:GLY:HA2	2.33	0.43
3:J:721:ASN:HB3	11:W:47:ARG:HE	1.82	0.43
10:V:45:GLN:HG3	10:V:45:GLN:O	2.19	0.43
11:N:35:LEU:HD22	11:N:46:ARG:HG3	2.00	0.43
4:D:44:VAL:HG13	4:D:143:ALA:HB2	2.00	0.43
1:I:665:ILE:HG13	1:I:666:ASP:N	2.33	0.43
1:A:672:VAL:O	1:A:673:ASP:C	2.56	0.43
5:Q:171:LYS:HE2	5:Q:173:GLU:HB2	1.99	0.43
1:A:239:LEU:HD23	1:A:276:TYR:HE1	1.83	0.43
1:A:4:LYS:HZ2	3:B:1115:LEU:HB3	1.82	0.43
3:J:361:PHE:CE1	3:J:385:VAL:HG13	2.50	0.43
7:G:57:VAL:HG12	7:G:57:VAL:O	2.18	0.43
3:J:895:VAL:HG11	4:O:34:LEU:HD21	2.00	0.43
3:B:154:VAL:O	3:B:156:GLY:N	2.52	0.43
3:J:139:ILE:HD13	11:W:61:HIS:CD2	2.53	0.43
3:B:92:TYR:OH	3:B:128:ASP:OD2	2.35	0.43
4:O:45:TYR:HB2	4:O:142:GLU:O	2.18	0.43
6:R:7:VAL:HG12	6:R:8:GLU:N	2.33	0.43
5:Q:98:PHE:CE1	5:Q:107:LEU:HD13	2.53	0.43
3:B:6:THR:HB	3:B:9:GLU:CB	2.48	0.43
3:J:971:TYR:CD2	4:O:164:VAL:O	2.72	0.43
11:W:35:LEU:HD23	11:W:40:VAL:HG21	1.99	0.43
3:B:898:PRO:HB2	3:B:970:VAL:HG21	2.00	0.43
3:B:899:TYR:CE1	3:B:971:TYR:HB2	2.53	0.43
1:A:828:SER:OG	1:A:829:ASP:N	2.51	0.43
2:M:391:ARG:NH2	9:U:39:ARG:NH1	2.58	0.43
1:I:588:ILE:HA	1:I:592:ILE:O	2.18	0.43
5:E:27:LEU:HD21	5:E:31:ARG:NH1	2.33	0.43
3:B:134:THR:O	3:B:138:LEU:HD12	2.18	0.43
9:K:71:ARG:HB2	9:K:71:ARG:HH11	1.83	0.43
3:J:183:ILE:HG22	3:J:209:THR:N	2.33	0.43
2:C:287:GLU:OE2	8:H:79:ARG:CZ	2.66	0.43
2:C:286:ILE:HD12	8:H:45:ILE:HG13	1.99	0.43
1:I:194:ILE:H	1:I:194:ILE:HG13	1.42	0.43
1:I:475:GLU:OE1	3:J:1043:MET:N	2.48	0.43
3:B:123:LEU:C	3:B:125:SER:N	2.71	0.43
11:W:6:ARG:HA	11:W:12:SER:O	2.18	0.43
5:Q:11:VAL:HG12	5:Q:12:ARG:N	2.31	0.43
1:I:397:LEU:HA	1:I:400:THR:OG1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:15:SER:O	6:R:19:LYS:HG2	2.18	0.43
10:V:48:PRO:C	10:V:50:SER:H	2.21	0.43
10:L:15:LEU:HB3	10:L:55:VAL:HG23	2.01	0.43
8:T:40:GLU:OE1	13:Z:66:LYS:NZ	2.46	0.43
1:I:272:HIS:HA	1:I:275:THR:HB	2.00	0.43
3:B:580:ILE:HG13	3:B:642:ILE:HD13	2.00	0.43
3:B:629:GLU:HB3	3:B:630:PRO:HD2	2.00	0.43
5:E:42:LEU:HD13	5:E:74:MET:HE1	1.99	0.43
1:A:541:ALA:HB3	1:A:542:PRO:CD	2.44	0.43
2:C:111:VAL:HG12	2:C:329:ILE:HB	1.99	0.43
11:N:43:TYR:HA	11:N:46:ARG:HB2	1.99	0.43
3:J:594:ILE:HB	3:J:599:SER:HB2	2.00	0.43
3:B:672:MET:HA	3:B:675:GLN:HB2	2.00	0.43
3:B:55:GLY:O	3:B:105:ASN:N	2.51	0.43
1:I:90:ILE:CD1	1:I:207:MET:HB2	2.41	0.43
1:A:786:PHE:CD1	3:B:919:MET:HE1	2.53	0.43
7:G:101:LEU:HD12	7:G:104:LYS:HZ1	1.80	0.43
3:J:803:GLU:HG2	3:J:846:ILE:HG13	1.99	0.43
3:B:1083:GLY:C	3:B:1085:LYS:H	2.22	0.43
1:A:438:LEU:HD21	1:A:444:ARG:CZ	2.47	0.43
3:B:43:ILE:HG13	3:B:63:ILE:HD12	2.00	0.43
3:J:136:ASP:HA	3:J:139:ILE:HD12	2.01	0.43
1:I:323:ARG:H	3:J:1002:HIS:HB2	1.82	0.43
2:M:246:GLY:O	2:M:247:ASP:C	2.57	0.43
3:J:1100:LEU:O	3:J:1101:ILE:C	2.56	0.43
5:E:36:GLU:CG	6:F:34:LEU:HD11	2.27	0.43
3:B:445:LEU:HD11	3:B:455:PRO:HB2	2.00	0.43
2:M:274:THR:CG2	2:M:275:ASN:H	2.07	0.43
1:A:112:GLU:O	1:A:116:ARG:HB2	2.18	0.43
3:B:757:LEU:HD21	3:B:863:LYS:HB3	2.01	0.43
3:B:183:ILE:HG12	3:B:207:ASP:N	2.33	0.43
3:J:890:MET:HG3	3:J:891:LEU:N	2.32	0.43
6:F:84:ARG:HG3	6:F:85:SER:N	2.32	0.43
9:K:61:VAL:HG12	9:K:62:ILE:N	2.33	0.43
5:Q:171:LYS:HB3	5:Q:174:TRP:CD1	2.54	0.43
6:R:64:SER:H	6:R:69:ARG:HH21	1.66	0.43
3:J:148:PRO:HG3	3:J:422:MET:CE	2.47	0.43
3:J:296:TYR:CD1	3:J:296:TYR:N	2.87	0.43
3:B:296:TYR:CD1	3:B:296:TYR:N	2.87	0.43
3:B:597:LEU:O	3:B:598:GLU:HB2	2.19	0.43
10:V:78:GLY:O	10:V:81:SER:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:ASP:O	1:A:534:LEU:C	2.56	0.43
1:A:849:ALA:HB2	9:K:15:PHE:CD1	2.54	0.43
1:A:64:THR:HB	1:A:65:LEU:H	1.48	0.43
5:E:175:ILE:HG22	5:E:175:ILE:O	2.18	0.43
3:J:1087:ASN:C	3:J:1088:LEU:HG	2.39	0.43
3:J:675:GLN:HG2	3:J:994:HIS:NE2	2.33	0.43
2:C:238:LYS:O	2:C:239:ARG:HB2	2.18	0.43
9:K:50:LEU:O	9:K:51:ILE:C	2.56	0.43
3:B:191:SER:CB	3:B:300:HIS:CD2	3.01	0.43
1:A:353:ILE:CD1	1:A:407:ILE:HG23	2.47	0.43
3:B:873:THR:HG23	3:B:874:ILE:HD12	2.00	0.43
3:J:848:ASP:CG	3:J:867:ARG:HH11	2.20	0.43
2:C:24:LEU:HD13	2:C:33:LYS:HA	2.01	0.43
1:I:188:PRO:O	1:I:192:VAL:HG23	2.19	0.43
1:A:457:PHE:C	1:A:459:GLY:H	2.21	0.43
6:F:64:SER:N	6:F:69:ARG:HH21	2.16	0.43
2:M:145:GLU:HG3	2:M:240:ALA:HB3	2.00	0.43
3:B:875:GLY:HA2	3:B:887:VAL:CG1	2.48	0.43
11:N:53:VAL:HG23	11:N:55:ILE:HG23	2.01	0.43
1:I:347:LEU:HB2	1:I:411:LEU:HD22	2.01	0.43
5:Q:146:VAL:HG12	5:Q:147:ILE:N	2.34	0.43
3:J:1077:TYR:HD1	3:J:1077:TYR:O	2.02	0.43
1:A:635:PHE:O	1:A:639:VAL:HG23	2.19	0.43
2:C:146:TYR:HD1	2:C:238:LYS:N	2.17	0.43
3:J:108:GLU:OE2	3:J:108:GLU:C	2.56	0.43
11:N:48:MET:HA	11:N:48:MET:HE2	2.00	0.43
1:I:853:ASP:CB	2:M:311:ARG:HH12	2.26	0.43
3:B:1004:ARG:NH1	3:B:1016:PRO:HB3	2.34	0.43
3:B:687:ARG:HH11	3:B:687:ARG:CB	2.31	0.43
3:B:654:ILE:HG22	3:B:881:ARG:HG2	2.01	0.43
3:B:81:SER:OG	3:B:141:ILE:CG2	2.67	0.43
1:A:249:LEU:HD21	1:A:265:LEU:HB2	2.01	0.43
3:J:763:VAL:HA	3:J:770:GLU:CG	2.48	0.43
3:B:685:GLN:NE2	3:B:867:ARG:HH22	2.17	0.43
3:B:361:PHE:C	3:B:361:PHE:CD2	2.92	0.43
5:E:20:LYS:HA	5:E:21:PRO:HD2	1.68	0.43
1:A:835:ASP:HA	9:K:20:ILE:CD1	2.49	0.43
3:J:1083:GLY:O	3:J:1084:ASP:HB2	2.18	0.43
1:I:571:GLY:HA3	1:I:572:PRO:HD2	1.91	0.43
4:D:6:LEU:HB3	4:D:14:ASP:HB2	2.00	0.43
1:A:517:THR:HG22	1:A:519:GLU:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:698:PRO:HB2	11:W:53:VAL:CG2	2.47	0.43
3:J:217:VAL:HA	3:J:218:PRO:HD3	1.90	0.43
2:C:330:GLY:O	2:C:331:ARG:C	2.57	0.43
3:J:5:LEU:O	3:J:5:LEU:HD22	2.18	0.43
3:J:1069:TRP:HB2	3:J:1078:VAL:O	2.18	0.43
1:A:631:LEU:O	1:A:634:VAL:HB	2.19	0.43
8:H:41:GLN:O	8:H:42:LEU:HB3	2.19	0.43
9:K:68:GLU:HG3	9:K:74:LEU:HG	2.00	0.43
3:B:935:LEU:O	11:N:46:ARG:NH1	2.51	0.43
1:I:812:ARG:NE	2:M:86:THR:HG23	2.31	0.43
3:J:764:LYS:HZ2	3:J:772:LYS:C	2.22	0.43
3:J:764:LYS:NZ	3:J:814:VAL:H	2.14	0.43
1:I:365:VAL:HG11	1:I:401:LEU:HD11	2.01	0.43
3:J:253:PHE:N	3:J:254:PRO:CD	2.80	0.43
3:J:665:ARG:HH21	3:J:918:ARG:NE	2.15	0.43
4:O:133:LEU:HD22	4:O:137:GLN:HB3	2.01	0.43
4:D:94:THR:CG2	4:D:145:LEU:HB2	2.49	0.43
3:J:402:ASN:O	3:J:403:TRP:CB	2.66	0.43
3:B:1074:LYS:HB3	3:B:1076:LYS:HE2	2.01	0.43
9:K:89:LEU:HG	9:K:89:LEU:H	1.77	0.43
8:T:20:HIS:O	8:T:21:GLU:HG3	2.19	0.43
11:N:52:HIS:CE1	11:N:54:ASP:H	2.36	0.43
7:S:90:ASN:N	7:S:90:ASN:OD1	2.41	0.43
3:B:88:ARG:CD	3:B:853:THR:CG2	2.77	0.43
3:J:14:ILE:O	3:J:17:TYR:HB3	2.18	0.43
1:I:541:ALA:CB	7:S:71:PHE:HA	2.46	0.43
7:G:109:LYS:NZ	3:J:378:LYS:CE	2.78	0.43
1:A:349:VAL:HG21	1:A:409:ARG:NH2	2.33	0.43
1:A:415:ASP:H	1:A:435:VAL:HG12	1.84	0.43
2:M:21:SER:O	2:M:33:LYS:CE	2.67	0.43
3:J:871:ILE:H	3:J:871:ILE:HG13	1.62	0.43
1:A:426:HIS:ND1	1:A:428:ILE:HG22	2.30	0.43
3:J:181:SER:O	3:J:182:ASN:CB	2.67	0.43
1:A:98:CYS:CA	1:A:146:CYS:SG	3.05	0.43
3:B:848:ASP:CG	3:B:867:ARG:HH11	2.22	0.43
3:J:246:PRO:HD2	3:J:247:GLU:H	1.84	0.43
3:B:549:ILE:HD13	3:B:549:ILE:HA	1.75	0.43
2:M:148:LYS:HE3	2:M:231:ILE:HG23	2.00	0.43
3:J:522:LEU:HD13	3:J:523:ASN:HB2	2.01	0.43
3:J:480:ILE:CG2	3:J:481:ASN:N	2.80	0.43
1:I:259:GLN:HA	1:I:262:ILE:CG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:38:ARG:HB3	8:T:40:GLU:HG2	2.00	0.43
1:A:529:ASP:O	1:A:529:ASP:CG	2.57	0.43
13:Y:77:LYS:HB3	13:Y:77:LYS:NZ	2.34	0.43
10:L:35:ILE:O	10:L:36:SER:C	2.57	0.43
13:Y:82:ARG:HA	13:Y:82:ARG:HE	1.83	0.43
4:D:61:ARG:HG2	4:D:61:ARG:HH11	1.82	0.43
2:M:237:ILE:C	2:M:238:LYS:HG2	2.40	0.43
1:I:71:HIS:ND1	3:J:1070:TYR:CE2	2.86	0.43
1:A:502:TYR:CD1	1:A:632:PHE:HB3	2.53	0.43
3:B:1054:ASP:HB3	3:B:1095:TYR:N	2.26	0.43
1:A:796:PHE:CZ	3:B:445:LEU:HD13	2.54	0.43
3:J:55:GLY:O	3:J:105:ASN:N	2.51	0.43
1:I:375:ALA:O	1:I:377:TYR:N	2.52	0.43
2:M:373:ILE:CD1	3:J:1049:LEU:HD22	2.49	0.43
3:J:445:LEU:HD11	3:J:455:PRO:HB3	2.01	0.43
1:I:507:TYR:HA	1:I:510:THR:H	1.84	0.43
3:J:416:ARG:NH1	3:J:687:ARG:HH21	2.17	0.43
1:I:672:VAL:O	1:I:675:LEU:N	2.51	0.43
1:I:234:ASP:C	1:I:236:THR:H	2.22	0.43
1:A:353:ILE:O	1:A:403:PRO:HA	2.19	0.43
3:J:461:GLY:HA3	3:J:462:PRO:HD3	1.91	0.43
3:B:600:GLY:C	3:B:602:ILE:H	2.22	0.43
13:Z:59:ILE:HA	13:Z:62:GLU:OE2	2.19	0.43
7:S:33:CYS:HB2	7:S:36:PHE:O	2.19	0.43
3:B:735:GLU:OE2	3:B:735:GLU:HA	2.18	0.43
6:F:13:PRO:HG2	6:F:16:VAL:CG2	2.48	0.43
3:B:402:ASN:O	3:B:403:TRP:CB	2.67	0.43
5:Q:38:ILE:HB	5:Q:39:LEU:H	1.43	0.43
2:C:11:PRO:O	2:C:14:GLU:CG	2.67	0.43
3:J:388:ASP:HB3	3:J:391:THR:HB	2.01	0.43
2:C:181:VAL:O	2:C:184:VAL:HG12	2.19	0.43
3:B:9:GLU:O	3:B:10:ARG:C	2.58	0.42
3:B:345:LEU:O	3:B:346:ALA:C	2.57	0.42
1:A:528:ALA:C	1:A:530:VAL:H	2.22	0.42
7:G:86:LEU:HG	7:G:87:ASN:N	2.34	0.42
4:O:178:LYS:HE2	4:O:178:LYS:HB2	1.89	0.42
3:J:970:VAL:O	3:J:979:ILE:HG13	2.19	0.42
3:J:171:ARG:HB3	3:J:524:GLY:HA3	2.00	0.42
1:A:875:VAL:HB	1:A:876:VAL:H	1.71	0.42
2:M:117:PRO:HD3	2:M:276:ASN:ND2	2.34	0.42
2:M:292:ILE:HG23	2:M:293:ILE:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:X:37:VAL:HG22	12:X:38:ARG:N	2.32	0.42
3:B:663:SER:CB	3:B:664:PRO:HD3	2.48	0.42
2:C:60:SER:O	2:C:63:LEU:CB	2.64	0.42
3:B:690:THR:CG2	3:B:691:ARG:HG3	2.46	0.42
3:J:174:VAL:HG12	3:J:175:ASP:N	2.34	0.42
5:E:83:GLU:O	5:E:145:ARG:HA	2.19	0.42
1:A:87:VAL:O	1:A:91:TYR:HB2	2.18	0.42
1:I:517:THR:HG22	1:I:518:LYS:N	2.34	0.42
2:C:361:GLY:O	2:C:362:ASP:O	2.37	0.42
3:J:96:LEU:O	3:J:115:TYR:HA	2.19	0.42
12:P:12:THR:O	12:P:14:THR:N	2.39	0.42
3:J:123:LEU:C	3:J:125:SER:N	2.72	0.42
3:J:132:GLN:HA	3:J:132:GLN:OE1	2.19	0.42
11:W:52:HIS:NE2	11:W:54:ASP:HB2	2.34	0.42
1:A:340:PRO:HB2	1:A:343:ILE:HG12	2.00	0.42
1:I:723:ASN:ND2	1:I:723:ASN:C	2.72	0.42
12:X:33:ILE:HD13	12:X:33:ILE:HA	1.90	0.42
3:J:191:SER:CB	3:J:300:HIS:CD2	3.01	0.42
3:J:617:ASP:O	3:J:618:ALA:CB	2.66	0.42
1:I:826:ALA:H	2:M:335:THR:HG23	1.83	0.42
9:U:46:GLY:O	9:U:47:ALA:O	2.38	0.42
2:C:271:LYS:O	2:C:272:VAL:C	2.57	0.42
3:B:246:PRO:O	3:B:248:VAL:N	2.47	0.42
1:I:349:VAL:HG21	1:I:415:ASP:OD2	2.18	0.42
2:M:174:LEU:HB2	2:M:179:VAL:HG13	2.00	0.42
1:I:357:ASN:HD22	1:I:361:LEU:HD22	1.83	0.42
1:I:555:PHE:HD2	1:I:631:LEU:HD13	1.81	0.42
3:J:750:TYR:OH	3:J:990:TYR:O	2.27	0.42
3:B:544:ARG:HB2	3:B:549:ILE:CG2	2.48	0.42
1:A:84:VAL:O	1:A:87:VAL:HG12	2.19	0.42
2:C:31:ASP:C	2:C:33:LYS:N	2.71	0.42
1:A:763:THR:HG23	1:A:779:ARG:HH12	1.85	0.42
10:L:59:THR:HG22	10:L:65:PRO:HD3	1.99	0.42
3:B:110:GLU:HA	3:B:111:PRO:HA	1.57	0.42
4:D:64:LEU:HD22	11:N:6:ARG:HD3	2.01	0.42
1:I:558:LYS:HA	1:I:590:ASN:O	2.19	0.42
3:B:797:VAL:HG12	3:B:798:VAL:N	2.33	0.42
1:I:879:LYS:NZ	2:M:44:THR:HB	2.34	0.42
3:J:759:SER:CB	3:J:863:LYS:HA	2.47	0.42
3:B:446:HIS:HD2	3:B:448:THR:OG1	2.02	0.42
2:M:146:TYR:O	2:M:238:LYS:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:391:ARG:HH22	9:K:42:GLN:HG2	1.82	0.42
3:J:418:ASN:HD21	3:J:421:SER:N	2.00	0.42
3:B:94:ALA:O	3:B:118:ASP:HA	2.19	0.42
3:J:657:TYR:HB3	3:J:660:HIS:CD2	2.55	0.42
7:G:42:ILE:HD13	7:G:46:ILE:HG21	2.00	0.42
4:O:110:TYR:HA	4:O:128:ILE:O	2.19	0.42
4:O:128:ILE:CG1	11:W:16:ASP:HB3	2.49	0.42
3:J:597:LEU:O	3:J:598:GLU:HB2	2.19	0.42
4:O:68:MET:CE	4:O:68:MET:HA	2.49	0.42
13:Y:65:LYS:C	13:Y:67:LEU:H	2.23	0.42
3:J:930:GLY:HA3	3:J:987:VAL:HB	2.01	0.42
10:V:45:GLN:HA	10:V:46:PRO:HD2	1.73	0.42
1:I:490:ARG:HG3	2:M:77:SER:HB3	2.01	0.42
3:J:579:LEU:CD1	3:J:616:LEU:CD1	2.91	0.42
1:I:507:TYR:OH	1:I:727:VAL:HG13	2.19	0.42
4:D:115:LYS:O	4:D:116:SER:HB3	2.18	0.42
5:E:31:ARG:O	5:E:35:GLN:HB2	2.19	0.42
1:I:716:SER:HB3	1:I:726:TYR:OH	2.19	0.42
7:G:83:ASP:HB3	7:G:94:THR:HB	2.02	0.42
1:I:155:LYS:HB3	1:I:156:ILE:HA	2.02	0.42
1:A:637:ARG:HH11	3:B:974:ARG:HH12	1.68	0.42
7:S:33:CYS:HB3	7:S:34:ASN:H	1.62	0.42
10:L:70:LEU:HA	10:L:73:ILE:HB	2.01	0.42
3:B:781:ARG:HD3	3:B:832:LYS:O	2.20	0.42
1:A:722:PHE:CD2	7:G:24:LYS:HG3	2.55	0.42
7:G:57:VAL:O	7:G:59:ILE:HG13	2.19	0.42
1:I:175:LEU:HD23	1:I:176:THR:H	1.84	0.42
3:B:435:ARG:CB	3:B:439:ASN:HD21	2.32	0.42
4:O:78:TRP:O	4:O:80:GLU:N	2.53	0.42
1:I:648:LEU:HB2	3:J:924:ILE:HG21	2.01	0.42
4:O:25:VAL:HG21	4:O:226:TYR:HD1	1.84	0.42
1:A:17:ASP:O	1:A:21:LYS:HG3	2.19	0.42
3:B:624:ALA:HB1	3:B:639:HIS:HD2	1.84	0.42
3:B:616:LEU:HD11	3:B:639:HIS:CE1	2.54	0.42
9:U:61:VAL:C	9:U:63:SER:N	2.69	0.42
3:J:624:ALA:HB1	3:J:639:HIS:HD2	1.84	0.42
2:M:318:ASP:O	2:M:322:ARG:NE	2.53	0.42
3:B:181:SER:HB3	3:B:183:ILE:CD1	2.50	0.42
1:I:313:LEU:HA	1:I:313:LEU:HD12	1.90	0.42
2:C:70:ILE:HD13	2:C:71:GLY:H	1.83	0.42
1:A:452:PRO:HG3	1:A:496:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:738:ILE:HD12	3:B:739:ILE:H	1.84	0.42
4:D:12:ARG:HA	4:D:230:ILE:O	2.19	0.42
4:D:259:LYS:O	4:D:263:VAL:CG2	2.64	0.42
3:B:657:TYR:O	3:B:658:PRO:C	2.56	0.42
7:S:15:ILE:HG13	7:S:31:MET:HE2	2.00	0.42
3:B:741:ASN:OD1	3:B:744:SER:N	2.44	0.42
2:C:11:PRO:HB2	2:C:14:GLU:CD	2.40	0.42
1:A:57:LYS:HD2	1:A:60:THR:HA	2.01	0.42
3:B:196:TYR:CE1	3:B:303:THR:HB	2.54	0.42
3:J:264:ASN:HB2	3:J:267:ASP:H	1.84	0.42
3:J:501:ILE:N	3:J:501:ILE:HD12	2.35	0.42
3:B:173:LEU:HA	3:B:333:ASP:OD2	2.19	0.42
1:I:340:PRO:HB2	1:I:343:ILE:HG12	2.00	0.42
8:H:30:LYS:HA	8:H:33:LYS:HE2	2.01	0.42
3:B:6:THR:HB	3:B:9:GLU:H	1.85	0.42
3:B:644:SER:O	3:B:647:ILE:HG13	2.20	0.42
2:M:63:LEU:HD12	9:U:22:LEU:CD2	2.43	0.42
9:U:18:VAL:HG12	9:U:22:LEU:HD12	2.01	0.42
2:C:146:TYR:CE2	2:C:235:LYS:HB2	2.54	0.42
9:K:41:LEU:C	9:K:43:LEU:N	2.73	0.42
2:C:126:LEU:CD1	2:C:249:TYR:HB2	2.50	0.42
3:J:588:LEU:HD22	3:J:612:LYS:HG2	2.01	0.42
4:O:111:SER:OG	4:O:125:SER:O	2.35	0.42
2:M:322:ARG:HG3	8:T:43:PRO:HA	2.01	0.42
3:B:958:LEU:C	3:B:958:LEU:HD23	2.39	0.42
2:C:179:VAL:HG23	2:C:182:ASP:HB2	2.01	0.42
3:J:243:SER:O	3:J:249:GLN:OE1	2.37	0.42
1:A:499:ALA:HB3	3:B:734:MET:HE1	2.01	0.42
3:J:174:VAL:HG11	3:J:325:LEU:HD23	2.02	0.42
11:N:22:ILE:CD1	11:N:22:ILE:N	2.83	0.42
3:B:1015:GLN:HE21	3:B:1096:ALA:HB2	1.80	0.42
3:J:657:TYR:O	3:J:658:PRO:C	2.57	0.42
1:I:217:ILE:C	1:I:219:ILE:N	2.73	0.42
3:J:435:ARG:CB	3:J:439:ASN:HD21	2.32	0.42
5:Q:128:PHE:CE2	5:Q:133:LYS:HD3	2.55	0.42
1:A:648:LEU:O	1:A:651:VAL:HG12	2.19	0.42
3:B:338:TYR:HB2	3:B:448:THR:HG21	2.02	0.42
3:J:382:LYS:O	3:J:382:LYS:HG2	2.19	0.42
4:O:178:LYS:H	4:O:178:LYS:HZ3	1.67	0.42
9:U:63:SER:C	9:U:65:ALA:H	2.22	0.42
7:S:42:ILE:HD11	7:S:71:PHE:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:871:ILE:HG13	2:M:54:LEU:HD11	2.01	0.42
1:I:549:LYS:HZ3	1:I:549:LYS:HB2	1.84	0.42
2:M:392:PRO:HG2	5:Q:22:LEU:HD21	2.01	0.42
3:J:92:TYR:OH	3:J:128:ASP:OD2	2.36	0.42
3:B:365:LEU:HG	3:B:369:LEU:HD12	2.02	0.42
1:I:220:ARG:NH1	1:I:236:THR:CG2	2.74	0.42
3:B:768:GLY:O	3:B:769:GLN:HB2	2.19	0.42
10:V:3:ILE:HD13	10:V:17:ILE:HG23	2.01	0.42
7:G:79:THR:CG2	7:G:80:GLU:N	2.82	0.42
3:J:793:GLU:HB3	3:J:794:ASP:H	1.72	0.42
1:I:612:LEU:C	1:I:612:LEU:HD23	2.39	0.42
3:B:778:ALA:HA	3:B:783:TYR:CE1	2.55	0.42
1:A:618:GLU:O	1:A:619:TYR:CG	2.72	0.42
2:C:21:SER:O	2:C:25:PRO:HD3	2.19	0.42
4:D:206:CYS:O	4:D:207:GLU:HB2	2.20	0.42
2:C:389:THR:O	2:C:390:MET:O	2.37	0.42
12:X:28:TYR:O	12:X:29:CYS:C	2.57	0.42
1:I:488:THR:HB	1:I:495:ILE:HB	2.02	0.42
4:D:107:ARG:N	4:D:133:LEU:O	2.51	0.42
3:B:1069:TRP:HE3	3:B:1070:TYR:N	2.18	0.42
1:A:427:ARG:NH1	2:C:73:VAL:HG11	2.34	0.42
3:J:537:ALA:HB2	3:J:557:HIS:CD2	2.55	0.42
1:A:104:VAL:HG12	1:A:137:LYS:HA	2.02	0.42
1:A:320:PHE:CE2	3:B:1005:ALA:HB1	2.55	0.42
1:A:827:LEU:CG	2:C:75:ALA:HB2	2.49	0.42
1:A:394:ARG:O	1:A:398:ALA:HB2	2.20	0.42
3:B:136:ASP:HA	3:B:139:ILE:HD12	2.01	0.42
3:B:386:ARG:HB3	3:B:389:ILE:HD11	2.02	0.42
2:C:149:ILE:O	2:C:153:VAL:HG12	2.19	0.42
4:D:21:PRO:O	4:D:24:PHE:HB3	2.20	0.42
4:O:128:ILE:HG12	11:W:16:ASP:HB3	2.01	0.42
7:G:18:ILE:HG22	7:G:18:ILE:O	2.18	0.42
2:C:106:ARG:HH21	2:C:117:PRO:HB3	1.85	0.42
1:A:380:ARG:HB3	1:A:381:PRO:HD2	2.01	0.42
2:M:239:ARG:HE	2:M:239:ARG:HB2	1.71	0.42
3:B:1029:GLY:O	3:B:1031:MET:N	2.52	0.42
7:S:42:ILE:HD11	7:S:71:PHE:CE1	2.55	0.42
2:M:258:LEU:HB2	2:M:279:GLU:HG2	2.01	0.42
3:J:418:ASN:C	3:J:418:ASN:ND2	2.73	0.42
3:B:298:LEU:N	3:B:299:PRO:HD3	2.35	0.42
3:B:418:ASN:HD21	3:B:420:LEU:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:458:THR:CG2	3:B:464:SER:HA	2.49	0.42
3:J:928:ILE:HD13	3:J:954:GLN:HE21	1.84	0.42
2:C:190:ARG:HD3	2:C:191:LEU:N	2.31	0.42
3:B:388:ASP:HB3	3:B:391:THR:HB	2.01	0.42
11:N:22:ILE:CD1	11:N:22:ILE:H	2.33	0.42
1:A:85:GLY:HA3	2:C:355:LEU:HD12	2.01	0.42
1:I:861:ALA:CB	1:I:866:VAL:HG23	2.49	0.42
1:A:548:GLY:O	1:A:551:VAL:HG12	2.20	0.42
1:A:835:ASP:HA	9:K:20:ILE:HD13	2.02	0.42
3:J:435:ARG:HB3	3:J:439:ASN:HD21	1.84	0.42
3:B:111:PRO:O	3:B:112:GLU:CB	2.68	0.42
11:N:24:ARG:HD2	11:N:34:VAL:HG13	2.02	0.42
3:B:24:VAL:HG11	3:B:426:LEU:HD13	2.01	0.42
3:J:752:SER:OG	3:J:753:THR:N	2.53	0.42
3:B:205:LEU:HD23	3:B:212:VAL:HG22	2.01	0.42
2:C:202:GLU:O	2:C:203:ASP:HB2	2.20	0.42
10:V:60:ASP:C	10:V:62:SER:H	2.22	0.42
3:J:173:LEU:HA	3:J:333:ASP:OD2	2.19	0.42
13:Y:65:LYS:C	13:Y:67:LEU:N	2.73	0.42
3:B:1099:LEU:O	3:B:1102:GLN:HB2	2.20	0.42
2:C:109:GLU:O	2:C:113:ALA:CA	2.51	0.42
3:J:580:ILE:HA	3:J:613:ILE:HD13	2.01	0.42
3:J:633:LEU:C	3:J:635:PRO:CD	2.88	0.42
3:J:669:GLN:C	3:J:671:ALA:H	2.23	0.42
7:S:75:GLY:HA3	7:S:87:ASN:HA	2.02	0.42
1:I:550:GLN:NE2	7:S:88:ASN:ND2	2.68	0.42
3:J:87:LEU:HD22	3:J:851:LEU:HD13	2.02	0.42
1:I:553:SER:OG	1:I:592:ILE:HA	2.20	0.42
1:A:672:VAL:O	1:A:675:LEU:N	2.52	0.42
3:B:1064:CYS:SG	3:B:1081:ILE:HD12	2.60	0.42
3:J:540:ILE:HG21	3:J:555:VAL:HG21	2.01	0.42
3:B:469:ASN:ND2	3:B:469:ASN:N	2.67	0.42
10:L:29:ALA:HA	10:L:32:LEU:HB2	2.02	0.42
1:A:823:LEU:HD13	2:C:75:ALA:O	2.18	0.42
1:I:188:PRO:HD2	1:I:191:ASP:HB2	2.00	0.42
4:O:53:LEU:HD11	11:W:2:LEU:HD12	2.01	0.42
7:G:57:VAL:HG13	7:G:115:THR:HG22	2.02	0.42
10:L:3:ILE:H	10:L:3:ILE:HD12	1.85	0.42
1:I:212:LEU:CD2	1:I:242:ILE:HD13	2.49	0.42
3:B:264:ASN:H	3:B:267:ASP:HB2	1.85	0.42
1:A:655:ASP:HB3	1:A:656:ASP:H	1.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:644:PHE:HB3	3:J:728:SER:OG	2.20	0.41
4:O:204:THR:O	4:O:206:CYS:N	2.53	0.41
5:E:38:ILE:O	5:E:39:LEU:HB2	2.20	0.41
3:J:898:PRO:HB2	3:J:970:VAL:HG21	2.02	0.41
11:W:48:MET:HE3	11:W:48:MET:HA	2.02	0.41
9:K:74:LEU:HD22	9:K:76:ILE:HD12	2.01	0.41
1:A:425:LEU:CD2	2:C:83:THR:HG21	2.50	0.41
1:I:349:VAL:HA	1:I:350:PRO:HD2	1.80	0.41
1:I:364:PHE:CD2	1:I:373:PRO:O	2.73	0.41
1:A:181:ARG:HG3	1:A:208:ILE:HB	2.00	0.41
1:A:355:PRO:O	1:A:357:ASN:OD1	2.37	0.41
3:J:750:TYR:O	3:J:992:LYS:NZ	2.52	0.41
3:B:874:ILE:H	3:B:874:ILE:CD1	2.17	0.41
3:B:975:THR:O	4:D:26:ASN:ND2	2.53	0.41
3:B:116:ILE:HD12	3:B:361:PHE:HZ	1.83	0.41
3:B:388:ASP:OD1	3:B:391:THR:OG1	2.25	0.41
8:H:64:ARG:HG3	8:H:78:TYR:HE2	1.84	0.41
3:J:6:THR:HB	3:J:9:GLU:CB	2.50	0.41
4:D:144:ARG:C	4:D:145:LEU:HD12	2.41	0.41
1:I:548:GLY:HA2	1:I:551:VAL:HG12	2.02	0.41
3:B:430:ILE:HG22	3:B:431:SER:N	2.35	0.41
1:A:439:LYS:H	1:A:439:LYS:HG3	1.57	0.41
1:I:449:VAL:HG12	1:I:449:VAL:O	2.20	0.41
3:B:785:GLY:HA3	3:B:788:TYR:HE2	1.84	0.41
3:B:454:CYS:HB2	3:B:649:GLY:N	2.35	0.41
3:B:587:PRO:C	3:B:588:LEU:HG	2.40	0.41
1:I:486:ILE:HD12	1:I:616:ILE:HD13	2.02	0.41
1:I:485:ASN:HD21	3:J:1039:PHE:HE2	1.67	0.41
3:J:764:LYS:HD3	3:J:815:SER:HB3	2.02	0.41
3:J:811:ILE:HB	3:J:837:ILE:HB	2.02	0.41
1:A:609:GLU:HB3	1:A:614:TRP:CZ2	2.55	0.41
3:J:738:ILE:HD12	3:J:739:ILE:N	2.34	0.41
1:I:839:ARG:NH2	9:U:83:PRO:HG3	2.35	0.41
2:M:234:ILE:HG13	2:M:234:ILE:H	1.65	0.41
1:I:45:MET:O	1:I:47:PRO:HD3	2.20	0.41
1:A:781:PHE:HD2	1:A:781:PHE:C	2.23	0.41
1:A:445:LEU:HD21	1:A:450:CYS:HA	2.02	0.41
1:A:327:SER:HB2	1:A:444:ARG:CD	2.47	0.41
4:D:94:THR:O	4:D:95:LYS:HG3	2.20	0.41
10:L:59:THR:HG21	10:L:65:PRO:HD3	2.02	0.41
3:B:148:PRO:HG3	3:B:422:MET:HE1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:723:ILE:HG12	3:B:907:ASP:OD2	2.19	0.41
4:D:45:TYR:CD1	12:P:44:ILE:HG12	2.54	0.41
1:I:708:ARG:HG3	1:I:709:SER:N	2.35	0.41
10:L:87:ILE:C	10:L:89:GLY:N	2.74	0.41
4:D:125:SER:O	4:D:127:ASP:N	2.52	0.41
3:J:1065:GLY:O	3:J:1112:ARG:HA	2.20	0.41
3:J:366:THR:O	3:J:370:GLU:HG3	2.19	0.41
13:Z:55:LEU:HB3	13:Z:56:ASN:H	1.63	0.41
2:M:389:THR:HG21	9:U:79:ARG:NH1	2.34	0.41
3:B:633:LEU:C	3:B:635:PRO:CD	2.89	0.41
3:J:88:ARG:HG2	12:X:33:ILE:HD11	2.02	0.41
9:U:60:ASP:O	9:U:61:VAL:O	2.38	0.41
12:P:26:CYS:CB	12:P:27:PRO:CD	2.87	0.41
10:V:45:GLN:HB3	10:V:53:ILE:HG22	2.01	0.41
1:I:874:ARG:HE	2:M:53:ASP:HB2	1.85	0.41
2:C:320:MET:HA	2:C:327:ARG:HG2	2.02	0.41
1:I:500:GLN:HG3	1:I:501:ASP:H	1.85	0.41
2:M:80:GLU:CB	2:M:81:PRO:HD3	2.50	0.41
3:B:54:PRO:O	3:B:55:GLY:C	2.58	0.41
3:J:138:LEU:HA	3:J:141:ILE:CD1	2.43	0.41
3:J:549:ILE:HD13	3:J:549:ILE:HA	1.80	0.41
4:O:256:LEU:CD1	10:V:3:ILE:HD12	2.50	0.41
1:I:153:GLN:HG2	1:I:154:TYR:H	1.85	0.41
1:I:742:GLN:HG2	1:I:747:LEU:HA	2.02	0.41
3:J:603:THR:C	3:J:605:ASP:N	2.73	0.41
1:A:153:GLN:HG2	1:A:154:TYR:H	1.85	0.41
7:S:104:LYS:O	7:S:106:ILE:N	2.54	0.41
2:C:57:LYS:HA	2:C:57:LYS:HE3	2.02	0.41
1:I:352:ARG:HD3	1:I:406:ILE:HG12	2.02	0.41
3:B:157:SER:O	3:B:158:GLU:CB	2.67	0.41
1:A:95:LYS:HZ3	1:A:152:LYS:HB3	1.84	0.41
5:Q:20:LYS:HA	5:Q:21:PRO:HD2	1.80	0.41
3:B:256:LEU:C	3:B:258:GLN:H	2.24	0.41
9:U:61:VAL:C	9:U:62:ILE:HG12	2.41	0.41
1:I:541:ALA:CB	1:I:542:PRO:HD2	2.46	0.41
1:I:329:ASP:CB	1:I:332:ILE:HD12	2.49	0.41
1:I:374:GLY:C	1:I:410:HIS:ND1	2.74	0.41
3:J:1015:GLN:HE21	3:J:1096:ALA:HB2	1.81	0.41
3:J:654:ILE:HG13	3:J:708:LEU:HD21	2.03	0.41
3:J:719:GLY:O	3:J:989:TYR:CE1	2.74	0.41
2:C:309:ASP:OD2	2:C:311:ARG:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:64:ARG:CG	3:J:97:TRP:CD1	3.01	0.41
3:J:97:TRP:O	3:J:98:LEU:HB3	2.20	0.41
3:J:133:TYR:CD2	3:J:141:ILE:HD11	2.56	0.41
3:J:800:PRO:HG2	12:X:37:VAL:HA	2.02	0.41
3:B:972:ASP:O	3:B:975:THR:HG23	2.20	0.41
7:S:36:PHE:CD2	7:S:96:ILE:HD11	2.54	0.41
3:B:402:ASN:O	3:B:403:TRP:HB2	2.21	0.41
3:J:659:GLU:O	3:J:660:HIS:CD2	2.72	0.41
1:A:290:ARG:HD2	1:A:291:SER:H	1.84	0.41
1:I:600:LYS:HE3	1:I:732:GLY:HA2	2.00	0.41
1:I:879:LYS:HA	1:I:879:LYS:HD3	1.90	0.41
1:A:778:ALA:O	1:A:780:GLY:N	2.53	0.41
1:A:212:LEU:CD2	1:A:242:ILE:HD13	2.50	0.41
10:L:61:GLY:O	10:L:62:SER:C	2.58	0.41
3:J:154:VAL:O	3:J:155:ASN:C	2.59	0.41
3:B:963:LEU:HD21	4:D:206:CYS:SG	2.60	0.41
1:I:870:ARG:HH21	2:M:61:GLU:H	1.69	0.41
10:V:47:HIS:O	10:V:49:LEU:N	2.53	0.41
4:D:178:LYS:O	4:D:179:ALA:C	2.59	0.41
1:I:768:HIS:NE2	3:J:450:TRP:CZ2	2.79	0.41
2:C:40:GLU:HG2	2:C:40:GLU:H	1.62	0.41
3:B:617:ASP:O	3:B:618:ALA:CB	2.67	0.41
3:B:751:ARG:HG2	3:B:871:ILE:HG23	2.01	0.41
3:B:764:LYS:HZ1	3:B:772:LYS:C	2.23	0.41
3:B:654:ILE:CG2	3:B:881:ARG:HG2	2.51	0.41
1:A:220:ARG:HH11	1:A:236:THR:CG2	2.27	0.41
1:I:239:LEU:HD23	1:I:276:TYR:HE1	1.85	0.41
3:B:291:GLN:C	3:B:293:ILE:N	2.74	0.41
6:R:55:VAL:HG12	6:R:59:LEU:HD12	2.02	0.41
2:M:261:VAL:O	2:M:261:VAL:CG1	2.67	0.41
7:S:34:ASN:OD1	7:S:34:ASN:N	2.53	0.41
1:A:155:LYS:HB3	1:A:156:ILE:HA	2.01	0.41
1:A:87:VAL:HG21	1:A:156:ILE:O	2.20	0.41
3:B:589:VAL:O	3:B:592:GLU:N	2.54	0.41
10:L:59:THR:HG21	10:L:63:ILE:O	2.19	0.41
1:A:125:TRP:CZ3	8:H:82:ILE:HG21	2.56	0.41
4:O:6:LEU:HB3	4:O:14:ASP:HB2	2.02	0.41
1:A:465:HIS:NE2	3:B:1028:PHE:HD1	2.19	0.41
4:D:65:ILE:HA	4:D:66:PRO:HD3	1.95	0.41
5:E:102:GLY:HA3	5:E:103:PRO:HD3	1.95	0.41
1:I:422:GLN:NE2	1:I:463:ASN:HD21	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:THR:OG1	1:A:646:MET:N	2.54	0.41
4:O:178:LYS:H	4:O:178:LYS:NZ	2.18	0.41
11:W:18:TRP:O	11:W:20:SER:N	2.50	0.41
7:S:26:LEU:HD22	7:S:42:ILE:O	2.21	0.41
9:K:39:ARG:HB3	9:K:65:ALA:HB1	2.03	0.41
3:J:52:GLU:HB2	3:J:56:LEU:HB3	2.02	0.41
4:D:178:LYS:HB2	4:D:178:LYS:HE2	1.92	0.41
3:B:987:VAL:HG11	11:N:47:ARG:NE	2.36	0.41
3:J:587:PRO:C	3:J:588:LEU:HG	2.40	0.41
1:I:820:GLN:O	1:I:823:LEU:HD12	2.19	0.41
2:M:258:LEU:HB2	2:M:279:GLU:CG	2.49	0.41
9:U:43:LEU:C	9:U:45:MET:N	2.73	0.41
3:J:130:ILE:HA	3:J:133:TYR:CD1	2.54	0.41
4:D:11:THR:HG22	4:D:232:SER:HB3	2.03	0.41
3:J:918:ARG:O	3:J:920:THR:HG23	2.21	0.41
1:A:568:VAL:HG21	1:A:597:VAL:HG11	2.01	0.41
2:C:28:ILE:HG23	2:C:30:ASP:CG	2.41	0.41
7:S:104:LYS:HZ2	7:S:104:LYS:HB3	1.84	0.41
1:A:831:ARG:NH2	2:C:385:MET:CG	2.83	0.41
2:M:312:HIS:O	2:M:316:ILE:HG12	2.20	0.41
9:U:70:ARG:O	9:U:72:GLY:N	2.53	0.41
4:D:223:GLU:H	4:D:223:GLU:HG3	1.69	0.41
1:I:198:ASP:HA	1:I:199:PRO:HD2	1.99	0.41
1:A:708:ARG:HG3	1:A:709:SER:N	2.34	0.41
1:A:805:GLY:C	1:A:807:VAL:H	2.24	0.41
13:Y:79:ASP:HB3	13:Y:80:SER:H	1.72	0.41
3:B:440:PHE:C	3:B:442:ALA:H	2.23	0.41
7:S:76:TYR:CZ	7:S:110:GLU:HG3	2.56	0.41
3:B:448:THR:HG22	3:B:452:ARG:HD2	2.03	0.41
3:B:1033:ARG:HG3	3:B:1033:ARG:HH11	1.85	0.41
2:C:390:MET:HE2	5:E:66:THR:OG1	2.21	0.41
1:I:425:LEU:O	1:I:426:HIS:HB2	2.20	0.41
5:Q:66:THR:CG2	5:Q:68:HIS:NE2	2.84	0.41
3:J:81:SER:OG	3:J:141:ILE:HG23	2.20	0.41
3:J:92:TYR:O	3:J:92:TYR:HD2	2.02	0.41
1:I:563:HIS:ND1	1:I:876:VAL:HG13	2.36	0.41
3:B:1069:TRP:HB2	3:B:1078:VAL:O	2.20	0.41
1:A:741:THR:O	1:A:742:GLN:C	2.59	0.41
1:A:747:LEU:HD22	1:A:786:PHE:CE1	2.56	0.41
3:J:919:MET:HE2	3:J:919:MET:HB3	1.88	0.41
3:B:867:ARG:NH2	4:D:54:TYR:CE2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:LEU:HD12	1:A:313:LEU:HA	1.93	0.41
3:J:1109:ILE:O	3:J:1111:PRO:HD3	2.21	0.41
1:A:326:ILE:HG21	1:A:462:MET:CG	2.48	0.41
1:A:421:ARG:HB2	1:A:462:MET:CE	2.49	0.41
3:B:1085:LYS:HG2	3:B:1086:SER:N	2.36	0.41
4:D:34:LEU:O	4:D:150:GLY:HA3	2.21	0.41
1:A:785:SER:C	1:A:787:ARG:N	2.73	0.41
2:M:12:TYR:C	2:M:13:LEU:HG	2.41	0.41
3:J:490:TYR:CE1	3:J:527:ILE:CG2	3.03	0.41
8:H:69:SER:HB3	8:H:72:TYR:H	1.85	0.41
1:I:77:LEU:HD23	1:I:246:ASN:HD21	1.85	0.41
9:K:47:ALA:HA	9:K:48:PRO:HD2	1.95	0.41
4:D:35:TYR:HE2	10:L:23:THR:HG21	1.86	0.41
1:I:402:ALA:O	1:I:405:TYR:HD1	2.03	0.41
2:M:125:TYR:HD1	2:M:271:LYS:HB2	1.85	0.41
2:M:320:MET:O	2:M:327:ARG:HG2	2.21	0.41
1:A:77:LEU:HD23	1:A:246:ASN:HD21	1.84	0.41
5:Q:103:PRO:HD3	6:R:37:THR:HG23	2.03	0.41
3:B:790:ARG:HH22	12:P:39:LYS:HE3	1.85	0.41
2:C:158:ILE:HD11	2:C:165:ILE:HG23	2.02	0.41
3:J:167:LEU:HB2	3:J:168:ALA:H	1.74	0.41
13:Y:69:GLU:HB3	13:Y:73:LYS:NZ	2.36	0.41
12:P:33:ILE:O	12:P:34:ILE:C	2.59	0.41
1:A:541:ALA:CB	1:A:542:PRO:HD2	2.45	0.41
11:W:22:ILE:HD12	11:W:22:ILE:H	1.86	0.41
1:A:561:ASN:HA	1:A:588:ILE:O	2.20	0.41
2:M:31:ASP:C	2:M:33:LYS:N	2.72	0.41
2:C:276:ASN:O	2:C:279:GLU:HB3	2.20	0.41
3:J:1029:GLY:O	3:J:1030:GLU:C	2.59	0.41
4:O:111:SER:C	4:O:114:ILE:HD13	2.41	0.41
3:J:816:PRO:HA	3:J:817:PRO:HD3	1.85	0.41
4:D:159:VAL:HG23	4:D:232:SER:HA	2.03	0.41
1:A:507:TYR:HB2	1:A:511:VAL:HG13	2.01	0.41
3:B:661:ASN:HD22	3:B:920:THR:HA	1.86	0.41
3:J:997:VAL:O	3:J:1000:LYS:O	2.39	0.41
3:B:838:VAL:CG1	3:B:839:THR:N	2.83	0.41
1:I:29:THR:HG1	1:I:45:MET:N	2.19	0.41
4:O:21:PRO:HB3	10:V:34:ARG:HH21	1.84	0.41
3:J:223:PHE:CD2	3:J:256:LEU:HD22	2.56	0.41
5:E:171:LYS:HG2	5:E:172:LEU:H	1.85	0.41
3:B:419:TRP:HZ3	3:B:712:GLY:C	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:763:THR:HG22	1:A:772:TYR:HA	2.01	0.41
1:A:199:PRO:C	1:A:201:THR:H	2.24	0.41
3:B:533:GLY:C	3:B:535:GLU:H	2.23	0.41
4:O:35:TYR:HE2	10:V:23:THR:HG21	1.85	0.41
1:A:430:MET:O	1:A:431:MET:HG3	2.21	0.41
1:A:431:MET:CE	1:A:482:VAL:HG13	2.50	0.41
3:J:123:LEU:C	3:J:125:SER:H	2.24	0.41
1:A:125:TRP:HD1	1:A:128:ALA:HB3	1.85	0.41
3:B:264:ASN:HB2	3:B:267:ASP:H	1.85	0.41
5:Q:5:ILE:O	5:Q:74:MET:N	2.53	0.41
3:B:892:ILE:HA	3:B:893:PRO:HD3	1.96	0.41
9:K:63:SER:HA	9:K:66:GLU:HG3	2.03	0.41
2:C:323:THR:O	2:C:325:ILE:N	2.54	0.41
3:J:49:ILE:HG13	3:J:49:ILE:H	1.65	0.41
5:Q:110:ILE:O	5:Q:118:LEU:HD22	2.21	0.41
5:Q:163:THR:O	5:Q:164:MET:HG3	2.21	0.41
3:B:580:ILE:HB	3:B:640:LEU:HB3	2.03	0.41
3:J:978:LYS:HZ3	4:O:205:LEU:HD22	1.85	0.41
2:M:146:TYR:O	2:M:238:LYS:CD	2.69	0.41
3:J:471:ALA:O	3:J:473:MET:HG3	2.21	0.41
3:B:14:ILE:O	3:B:17:TYR:HB3	2.21	0.41
1:I:859:TYR:CB	2:M:64:ILE:HG12	2.50	0.41
7:G:107:SER:O	7:G:109:LYS:N	2.37	0.41
1:A:371:LYS:HZ2	1:A:373:PRO:HD3	1.84	0.41
1:I:329:ASP:HA	1:I:330:PRO:HD3	1.74	0.41
2:C:126:LEU:HD11	2:C:249:TYR:HB2	2.03	0.41
3:J:580:ILE:HG13	3:J:642:ILE:HD13	2.03	0.41
3:B:82:PRO:HG3	3:B:130:ILE:HD11	2.02	0.41
2:C:125:TYR:HD1	2:C:271:LYS:CB	2.30	0.41
1:A:575:CYS:O	1:A:577:ASN:N	2.54	0.41
1:I:86:LEU:HD13	1:I:207:MET:HG2	2.02	0.41
2:M:174:LEU:CB	2:M:179:VAL:HG13	2.50	0.41
1:A:378:VAL:CG2	1:A:378:VAL:O	2.67	0.41
1:A:670:VAL:O	1:A:674:ASN:ND2	2.54	0.41
7:G:80:GLU:C	7:G:81:LEU:HD12	2.41	0.41
7:G:15:ILE:HG13	7:G:31:MET:HE2	2.03	0.41
3:J:321:LYS:CA	3:J:324:GLU:HB3	2.51	0.41
1:I:4:LYS:HG2	1:I:5:ASN:N	2.36	0.41
7:S:83:ASP:N	7:S:94:THR:O	2.49	0.41
2:M:130:TYR:HD2	2:M:130:TYR:HA	1.77	0.41
3:J:99:THR:HG23	3:J:111:PRO:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:793:GLU:HB3	3:B:794:ASP:H	1.72	0.41
3:J:402:ASN:HB3	3:J:403:TRP:H	1.46	0.41
3:B:950:ILE:C	3:B:952:GLN:H	2.24	0.41
3:J:419:TRP:HZ3	3:J:712:GLY:CA	2.34	0.41
3:B:34:PHE:CE1	3:B:351:ALA:HA	2.56	0.41
1:I:537:PRO:HA	1:I:546:TYR:CD2	2.55	0.41
11:N:14:ILE:HD13	11:N:14:ILE:HA	1.93	0.41
3:J:589:VAL:O	3:J:592:GLU:N	2.54	0.41
2:C:245:LYS:HB2	2:C:250:ILE:HD11	2.03	0.41
3:B:78:ARG:HH22	12:P:30:GLY:HA3	1.85	0.41
4:O:168:PRO:HG3	4:O:203:CYS:O	2.21	0.41
9:U:32:ILE:O	9:U:36:ILE:HG12	2.20	0.41
4:O:61:ARG:HH11	4:O:61:ARG:HG2	1.86	0.41
3:B:102:PRO:HD2	3:B:109:ALA:HB3	2.01	0.41
3:B:228:ARG:NH2	3:B:233:LEU:O	2.50	0.41
7:G:102:LEU:HA	7:G:106:ILE:HG21	2.03	0.41
3:J:88:ARG:CD	3:J:853:THR:CG2	2.78	0.41
1:A:764:ARG:NH2	3:B:624:ALA:O	2.54	0.41
9:U:18:VAL:HG12	9:U:22:LEU:CD1	2.50	0.41
9:U:61:VAL:CG1	9:U:62:ILE:N	2.76	0.41
3:J:1113:LEU:HD12	3:J:1113:LEU:N	2.08	0.41
1:A:371:LYS:HD3	1:A:372:TRP:N	2.36	0.41
3:B:978:LYS:HG2	4:D:166:TYR:CE2	2.56	0.41
2:M:258:LEU:HA	2:M:258:LEU:HD12	1.90	0.41
9:U:42:GLN:HB2	9:U:42:GLN:HE21	1.78	0.41
4:O:44:VAL:HG13	4:O:143:ALA:HB2	2.03	0.41
1:I:716:SER:HB2	1:I:726:TYR:OH	2.22	0.41
10:V:4:ARG:HG2	10:V:4:ARG:NH1	2.29	0.41
3:J:867:ARG:NH2	4:O:54:TYR:CE2	2.89	0.41
12:P:24:VAL:O	12:P:24:VAL:CG1	2.67	0.41
8:H:39:PRO:HB2	8:H:80:TYR:CE2	2.56	0.41
1:A:184:LEU:O	1:A:186:LYS:N	2.54	0.41
5:Q:3:LYS:HE3	5:Q:3:LYS:HB2	1.60	0.41
4:D:78:TRP:CD1	4:D:78:TRP:N	2.86	0.41
1:I:561:ASN:ND2	1:I:590:ASN:H	2.18	0.41
3:B:304:SER:OG	3:B:307:ASP:OD2	2.39	0.41
1:A:467:PRO:HA	3:B:1048:ARG:NH2	2.36	0.41
1:A:114:TYR:O	1:A:118:TYR:HB2	2.20	0.41
3:B:446:HIS:H	3:B:449:GLN:NE2	2.19	0.40
4:O:183:CYS:HB2	16:O:1001:F3S:S1	2.61	0.40
12:X:33:ILE:O	12:X:34:ILE:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:49:ASP:CG	3:J:382:LYS:HE2	2.41	0.40
9:U:23:TRP:HA	9:U:23:TRP:CE3	2.56	0.40
11:W:3:ILE:HD11	11:W:18:TRP:CE3	2.56	0.40
3:B:932:TYR:CD2	3:B:953:LEU:HD22	2.56	0.40
1:I:499:ALA:H	1:I:502:TYR:HD2	1.69	0.40
1:I:608:PRO:HA	1:I:862:HIS:CE1	2.56	0.40
2:M:103:GLY:HA2	2:M:106:ARG:HB2	2.02	0.40
3:J:157:SER:O	3:J:158:GLU:CB	2.68	0.40
3:B:138:LEU:HA	3:B:141:ILE:CD1	2.41	0.40
3:B:81:SER:OG	3:B:141:ILE:HG23	2.21	0.40
1:A:447:LEU:HD11	3:B:731:GLY:O	2.20	0.40
3:B:691:ARG:NH1	3:B:756:ARG:HH21	2.18	0.40
1:I:651:VAL:HG21	1:I:743:MET:HB3	2.02	0.40
1:I:99:ARG:HG2	1:I:183:ARG:NH1	2.35	0.40
4:O:131:VAL:HA	11:W:2:LEU:CD1	2.49	0.40
3:J:256:LEU:C	3:J:258:GLN:H	2.24	0.40
3:B:489:LEU:HA	3:B:489:LEU:HD23	1.87	0.40
3:J:658:PRO:HB2	3:J:666:ASN:HD21	1.86	0.40
2:M:344:ARG:HB3	2:M:353:HIS:NE2	2.36	0.40
3:J:644:SER:C	3:J:646:ALA:N	2.74	0.40
3:B:221:ILE:HA	3:B:222:PRO:HD3	1.95	0.40
1:A:53:GLU:O	1:A:55:GLY:N	2.54	0.40
1:A:8:GLY:O	3:B:1114:VAL:HG22	2.21	0.40
3:J:125:SER:O	3:J:126:ALA:C	2.59	0.40
1:I:114:TYR:O	1:I:118:TYR:HB2	2.20	0.40
4:D:23:GLU:O	10:L:27:LEU:HD13	2.21	0.40
1:I:125:TRP:HD1	1:I:128:ALA:HB3	1.86	0.40
3:B:443:ARG:NH2	3:B:462:PRO:O	2.54	0.40
5:E:44:LEU:HD12	5:E:44:LEU:C	2.41	0.40
5:Q:110:ILE:HD12	5:Q:118:LEU:HA	2.04	0.40
1:A:522:GLN:HG2	10:L:40:PHE:CE1	2.56	0.40
4:O:176:CYS:N	4:O:195:LEU:HD21	2.37	0.40
2:C:141:ALA:O	2:C:145:GLU:HB2	2.21	0.40
3:J:298:LEU:C	3:J:300:HIS:N	2.71	0.40
1:I:500:GLN:HB2	3:J:913:HIS:CG	2.56	0.40
1:I:575:CYS:O	1:I:577:ASN:N	2.52	0.40
3:J:655:ILE:HG12	3:J:669:GLN:HG2	2.03	0.40
1:I:471:GLU:OE1	9:U:41:LEU:CD1	2.70	0.40
3:J:680:TYR:CE2	3:J:692:ALA:HB1	2.56	0.40
1:A:203:ARG:CZ	1:A:206:TRP:HB2	2.50	0.40
1:A:58:CYS:SG	1:A:59:PRO:CD	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1001:LEU:O	3:J:1020:ARG:HD3	2.21	0.40
2:M:298:SER:O	2:M:301:LEU:HD12	2.22	0.40
7:S:36:PHE:CG	7:S:96:ILE:HD11	2.56	0.40
8:T:17:VAL:HA	8:T:18:PRO:HD3	1.83	0.40
3:B:1083:GLY:O	3:B:1084:ASP:HB2	2.21	0.40
3:J:707:ALA:O	3:J:709:ASP:N	2.54	0.40
3:B:174:VAL:HG11	3:B:325:LEU:HD23	2.03	0.40
3:B:936:SER:O	11:N:32:GLY:HA3	2.21	0.40
3:B:752:SER:OG	3:B:753:THR:N	2.55	0.40
9:K:63:SER:O	9:K:66:GLU:HB2	2.21	0.40
11:W:21:PHE:O	11:W:25:VAL:HG23	2.21	0.40
6:F:31:SER:HB2	6:F:32:ASN:H	1.70	0.40
3:J:876:ASP:HB2	3:J:878:PHE:HE1	1.86	0.40
5:E:90:LEU:HD12	5:E:100:ASN:HB2	2.01	0.40
2:M:167:LEU:HD12	2:M:207:ASN:HD21	1.87	0.40
13:Y:69:GLU:O	13:Y:70:ASP:C	2.60	0.40
3:B:353:LEU:HD12	3:B:404:VAL:HG13	2.03	0.40
1:A:634:VAL:O	1:A:635:PHE:C	2.60	0.40
2:C:391:ARG:HG3	2:C:391:ARG:NH1	2.33	0.40
2:M:53:ASP:O	2:M:55:ALA:N	2.54	0.40
3:B:902:LYS:HB2	11:N:42:ARG:NH1	2.37	0.40
1:I:105:LYS:HB3	1:I:109:ASP:OD1	2.21	0.40
3:J:1015:GLN:HG2	3:J:1054:ASP:OD1	2.21	0.40
5:Q:64:GLY:O	9:U:42:GLN:HG3	2.21	0.40
3:B:245:ASP:N	3:B:246:PRO:CD	2.83	0.40
1:I:672:VAL:O	1:I:673:ASP:C	2.60	0.40
3:B:249:GLN:O	3:B:253:PHE:CD1	2.74	0.40
3:B:669:GLN:C	3:B:671:ALA:H	2.25	0.40
1:I:326:ILE:HG21	1:I:462:MET:CG	2.47	0.40
1:I:704:LEU:HD22	1:I:781:PHE:CD1	2.55	0.40
3:J:323:ILE:HG13	3:J:324:GLU:N	2.35	0.40
1:I:457:PHE:C	1:I:459:GLY:H	2.24	0.40
2:M:148:LYS:HG2	2:M:230:LYS:O	2.21	0.40
1:A:29:THR:HG1	1:A:45:MET:N	2.19	0.40
1:A:81:VAL:O	1:A:209:LEU:N	2.54	0.40
3:J:361:PHE:C	3:J:361:PHE:CD2	2.95	0.40
5:Q:39:LEU:HD13	5:Q:42:LEU:HD21	2.02	0.40
6:R:63:VAL:HG12	6:R:63:VAL:O	2.21	0.40
1:A:480:MET:HG2	3:B:1039:PHE:CE1	2.56	0.40
1:I:818:TYR:OH	2:M:348:GLU:OE2	2.25	0.40
5:Q:63:ASP:C	5:Q:65:ALA:H	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:151:SER:HB3	5:E:158:PRO:N	2.36	0.40
6:R:72:LEU:C	6:R:74:SER:H	2.25	0.40
1:I:645:THR:HG22	1:I:724:PHE:CZ	2.55	0.40
3:J:963:LEU:HA	3:J:964:PRO:HD3	1.96	0.40
1:I:312:ASN:HA	1:I:315:GLY:O	2.21	0.40
3:J:554:ASN:HD22	3:J:574:ARG:HH11	1.69	0.40
4:D:178:LYS:C	4:D:180:VAL:N	2.75	0.40
3:J:165:GLU:OE2	3:J:338:TYR:OH	2.39	0.40
3:J:811:ILE:O	3:J:836:SER:HB2	2.21	0.40
1:A:732:GLY:O	1:A:733:ALA:C	2.60	0.40
3:B:811:ILE:O	3:B:836:SER:HB2	2.21	0.40
1:I:566:ALA:HB1	1:I:599:ASP:OD2	2.21	0.40
3:J:707:ALA:C	3:J:709:ASP:N	2.73	0.40
1:A:866:VAL:O	1:A:867:ASP:C	2.60	0.40
3:B:781:ARG:CD	3:B:782:GLY:H	2.33	0.40
1:A:318:VAL:HG23	1:A:321:SER:HB2	2.03	0.40
3:B:234:THR:O	3:B:237:ASP:HB2	2.22	0.40
4:D:151:LYS:O	4:D:152:GLU:C	2.60	0.40
1:A:288:LYS:HG2	1:A:294:PRO:CA	2.52	0.40
1:I:217:ILE:O	1:I:219:ILE:N	2.54	0.40
1:A:217:ILE:C	1:A:219:ILE:H	2.24	0.40
4:O:94:THR:CG2	4:O:145:LEU:HB2	2.52	0.40
3:J:1066:TYR:CE1	3:J:1112:ARG:HD3	2.55	0.40
4:O:18:GLU:HB2	4:O:225:LYS:HE3	2.02	0.40
3:B:320:SER:OG	3:B:320:SER:O	2.33	0.40
3:J:853:THR:O	3:J:861:LEU:N	2.55	0.40
3:J:676:ALA:O	3:J:677:LEU:HD23	2.21	0.40
2:C:290:ARG:HG3	2:C:321:THR:HG21	2.04	0.40
1:I:539:ILE:HG21	7:S:46:ILE:HD11	2.04	0.40
3:B:904:VAL:HG21	11:N:42:ARG:HG2	2.03	0.40
1:A:130:ARG:HB3	1:A:195:LEU:C	2.42	0.40
1:A:600:LYS:HB2	1:A:732:GLY:HA3	2.03	0.40
1:A:733:ALA:CB	3:B:913:HIS:HE1	2.26	0.40
3:B:329:ARG:HD2	3:B:562:PHE:HB3	2.04	0.40
1:I:415:ASP:H	1:I:435:VAL:HG12	1.85	0.40
3:J:725:ALA:O	3:J:909:ILE:HG23	2.21	0.40
1:I:253:ILE:HG12	1:I:266:TRP:HZ2	1.87	0.40
1:I:353:ILE:HG21	1:I:358:ILE:HD12	2.04	0.40
3:B:1064:CYS:HG	14:B:2001:ZN:ZN	1.29	0.40
1:I:206:TRP:C	1:I:208:ILE:H	2.25	0.40
2:C:370:VAL:O	2:C:374:ILE:HD12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:600:GLY:C	3:J:602:ILE:H	2.24	0.40
2:C:48:ILE:H	2:C:50:LYS:HG3	1.87	0.40
2:C:26:GLN:C	2:C:28:ILE:N	2.74	0.40
3:J:116:ILE:HD12	3:J:361:PHE:HZ	1.86	0.40
3:J:223:PHE:CE1	3:J:319:ILE:HG13	2.57	0.40
1:I:53:GLU:O	1:I:55:GLY:N	2.55	0.40
3:J:895:VAL:HG11	4:O:34:LEU:CG	2.52	0.40
3:B:430:ILE:HD13	3:B:467:VAL:HB	2.02	0.40
3:B:463:ASN:HB3	3:B:467:VAL:HG12	2.02	0.40
4:D:22:LEU:C	4:D:24:PHE:N	2.74	0.40
3:J:419:TRP:HZ3	3:J:712:GLY:C	2.24	0.40
5:E:147:ILE:HD11	5:E:163:THR:HG22	2.03	0.40
13:Y:57:GLY:CA	13:Y:61:LEU:HD21	2.51	0.40
10:V:29:ALA:O	10:V:33:ARG:HG3	2.21	0.40
5:Q:92:VAL:HG12	5:Q:93:ASP:H	1.85	0.40
1:I:766:LEU:HD22	1:I:766:LEU:HA	2.01	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	828/880 (94%)	597 (72%)	154 (19%)	77 (9%)	1	9
1	I	828/880 (94%)	594 (72%)	157 (19%)	77 (9%)	1	9
2	C	366/395 (93%)	225 (62%)	92 (25%)	49 (13%)	0	4
2	M	366/395 (93%)	232 (63%)	84 (23%)	50 (14%)	0	3
3	B	1084/1124 (96%)	752 (69%)	215 (20%)	117 (11%)	0	6
3	J	1084/1124 (96%)	752 (69%)	217 (20%)	115 (11%)	0	6
4	D	262/265 (99%)	199 (76%)	50 (19%)	13 (5%)	3	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	O	262/265 (99%)	198 (76%)	53 (20%)	11 (4%)	3	29
5	E	172/180 (96%)	125 (73%)	35 (20%)	12 (7%)	1	15
5	Q	172/180 (96%)	128 (74%)	34 (20%)	10 (6%)	2	20
6	F	87/113 (77%)	57 (66%)	25 (29%)	5 (6%)	2	20
6	R	87/113 (77%)	59 (68%)	19 (22%)	9 (10%)	1	7
7	G	111/132 (84%)	82 (74%)	22 (20%)	7 (6%)	2	18
7	S	111/132 (84%)	84 (76%)	16 (14%)	11 (10%)	1	8
8	H	72/84 (86%)	46 (64%)	12 (17%)	14 (19%)	0	1
8	T	72/84 (86%)	39 (54%)	20 (28%)	13 (18%)	0	1
9	K	80/95 (84%)	50 (62%)	21 (26%)	9 (11%)	0	6
9	U	80/95 (84%)	43 (54%)	18 (22%)	19 (24%)	0	1
10	L	90/92 (98%)	66 (73%)	16 (18%)	8 (9%)	1	9
10	V	90/92 (98%)	58 (64%)	28 (31%)	4 (4%)	3	28
11	N	62/66 (94%)	41 (66%)	17 (27%)	4 (6%)	1	17
11	W	62/66 (94%)	43 (69%)	15 (24%)	4 (6%)	1	17
12	P	41/48 (85%)	29 (71%)	8 (20%)	4 (10%)	1	8
12	X	41/48 (85%)	28 (68%)	8 (20%)	5 (12%)	0	5
13	Y	43/104 (41%)	26 (60%)	13 (30%)	4 (9%)	1	9
13	Z	43/104 (41%)	30 (70%)	11 (26%)	2 (5%)	3	26
All	All	6596/7156 (92%)	4583 (70%)	1360 (21%)	653 (10%)	1	8

All (653) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	PRO
1	A	56	GLN
1	A	58	CYS
1	A	64	THR
1	A	145	VAL
1	A	207	MET
1	A	332	ILE
1	A	376	ASN
1	A	377	TYR
1	A	426	HIS
1	A	508	LEU

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Mol	Chain	Res	Type
1	A	528	ALA
1	A	532	ILE
1	A	541	ALA
1	A	585	TYR
1	A	608	PRO
1	A	746	MET
1	A	829	ASP
1	A	842	TYR
1	A	865	THR
1	A	876	VAL
2	C	28	ILE
2	C	31	ASP
2	C	48	ILE
2	C	50	LYS
2	C	66	PRO
2	C	104	LEU
2	C	113	ALA
2	C	127	THR
2	C	188	ILE
2	C	191	LEU
2	C	193	LEU
2	C	211	ALA
2	C	275	ASN
2	C	306	LEU
2	C	324	GLY
2	C	362	ASP
2	C	364	GLU
2	C	365	GLU
2	C	390	MET
2	C	391	ARG
3	B	23	LEU
3	B	97	TRP
3	B	124	LYS
3	B	171	ARG
3	B	297	PHE
3	B	300	HIS
3	B	325	LEU
3	B	347	GLY
3	B	372	SER
3	B	378	LYS
3	B	382	LYS
3	B	402	ASN

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Mol	Chain	Res	Type
3	B	403	TRP
3	B	448	THR
3	B	473	MET
3	B	483	ARG
3	B	571	ASP
3	B	602	ILE
3	B	659	GLU
3	B	663	SER
3	B	730	THR
3	B	790	ARG
3	B	800	PRO
3	B	801	GLU
3	B	945	PHE
3	B	966	ALA
3	B	1030	GLU
3	B	1056	THR
3	B	1071	ASP
3	B	1114	VAL
3	B	1118	LYS
4	D	135	THR
4	D	152	GLU
4	D	205	LEU
5	E	39	LEU
5	E	88	GLU
5	E	116	ASP
6	F	3	SER
7	G	68	HIS
7	G	88	ASN
7	G	108	ASN
8	H	12	ARG
8	H	25	ILE
8	H	28	ALA
8	H	43	PRO
9	K	42	GLN
9	K	51	ILE
9	K	61	VAL
9	K	62	ILE
9	K	72	GLY
10	L	10	SER
10	L	36	SER
10	L	46	PRO
10	L	48	PRO

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Mol	Chain	Res	Type
11	N	29	GLU
12	P	26	CYS
12	P	34	ILE
1	I	47	PRO
1	I	56	GLN
1	I	58	CYS
1	I	64	THR
1	I	145	VAL
1	I	207	MET
1	I	332	ILE
1	I	377	TYR
1	I	426	HIS
1	I	508	LEU
1	I	528	ALA
1	I	532	ILE
1	I	541	ALA
1	I	585	TYR
1	I	595	GLU
1	I	607	GLN
1	I	608	PRO
1	I	721	PRO
1	I	733	ALA
1	I	746	MET
1	I	825	ASN
1	I	826	ALA
1	I	829	ASP
1	I	842	TYR
1	I	865	THR
1	I	876	VAL
2	M	28	ILE
2	M	31	ASP
2	M	48	ILE
2	M	54	LEU
2	M	66	PRO
2	M	104	LEU
2	M	113	ALA
2	M	115	LYS
2	M	127	THR
2	M	146	TYR
2	M	213	ILE
2	M	306	LEU
2	M	365	GLU

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Mol	Chain	Res	Type
2	M	391	ARG
3	J	23	LEU
3	J	97	TRP
3	J	112	GLU
3	J	124	LYS
3	J	171	ARG
3	J	297	PHE
3	J	300	HIS
3	J	325	LEU
3	J	372	SER
3	J	378	LYS
3	J	402	ASN
3	J	403	TRP
3	J	448	THR
3	J	473	MET
3	J	483	ARG
3	J	530	TYR
3	J	571	ASP
3	J	602	ILE
3	J	659	GLU
3	J	663	SER
3	J	730	THR
3	J	790	ARG
3	J	800	PRO
3	J	801	GLU
3	J	945	PHE
3	J	966	ALA
3	J	1030	GLU
3	J	1056	THR
3	J	1071	ASP
3	J	1111	PRO
3	J	1114	VAL
3	J	1118	LYS
4	O	135	THR
4	O	152	GLU
4	O	205	LEU
5	Q	32	GLN
5	Q	39	LEU
5	Q	40	LYS
6	R	7	VAL
6	R	32	ASN
6	R	64	SER

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Mol	Chain	Res	Type
7	S	65	SER
7	S	88	ASN
7	S	108	ASN
8	T	15	TYR
8	T	21	GLU
8	T	43	PRO
9	U	14	HIS
9	U	15	PHE
9	U	20	ILE
9	U	26	ARG
9	U	34	ARG
9	U	42	GLN
9	U	47	ALA
9	U	51	ILE
9	U	59	THR
9	U	61	VAL
11	W	29	GLU
12	X	26	CYS
12	X	34	ILE
13	Z	59	ILE
13	Z	77	LYS
1	A	27	ILE
1	A	150	ASN
1	A	155	LYS
1	A	185	GLU
1	A	307	GLY
1	A	355	PRO
1	A	378	VAL
1	A	392	LYS
1	A	393	ASP
1	A	447	LEU
1	A	529	ASP
1	A	534	LEU
1	A	576	LYS
1	A	595	GLU
1	A	607	GLN
1	A	621	ASP
1	A	682	GLY
1	A	721	PRO
1	A	733	ALA
1	A	749	GLN
1	A	763	THR

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Mol	Chain	Res	Type
1	A	764	ARG
1	A	825	ASN
1	A	826	ALA
1	A	841	LEU
2	C	115	LYS
2	C	190	ARG
2	C	210	PHE
2	C	264	VAL
2	C	299	LYS
2	C	331	ARG
2	C	360	ARG
2	C	367	LYS
3	B	30	SER
3	B	47	GLY
3	B	50	PRO
3	B	55	GLY
3	B	74	ASP
3	B	105	ASN
3	B	109	ALA
3	B	112	GLU
3	B	158	GLU
3	B	167	LEU
3	B	246	PRO
3	B	292	ILE
3	B	404	VAL
3	B	418	ASN
3	B	482	GLU
3	B	530	TYR
3	B	534	GLY
3	B	574	ARG
3	B	587	PRO
3	B	604	PHE
3	B	605	ASP
3	B	618	ALA
3	B	684	TYR
3	B	691	ARG
3	B	708	LEU
3	B	736	ASP
3	B	806	GLY
3	B	933	ALA
3	B	951	GLU
3	B	1001	LEU

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Mol	Chain	Res	Type
3	B	1065	GLY
3	B	1111	PRO
4	D	103	PRO
4	D	206	CYS
5	E	40	LYS
5	E	65	ALA
5	E	82	GLN
5	E	122	ASN
5	E	139	GLY
7	G	97	SER
8	H	56	ASN
8	H	74	GLU
8	H	80	TYR
8	H	81	VAL
9	K	47	ALA
10	L	50	SER
10	L	62	SER
11	N	63	THR
13	Y	66	LYS
1	I	27	ILE
1	I	80	PRO
1	I	150	ASN
1	I	155	LYS
1	I	185	GLU
1	I	307	GLY
1	I	372	TRP
1	I	376	ASN
1	I	378	VAL
1	I	392	LYS
1	I	393	ASP
1	I	447	LEU
1	I	454	ASN
1	I	482	VAL
1	I	529	ASP
1	I	534	LEU
1	I	576	LYS
1	I	621	ASP
1	I	682	GLY
1	I	741	THR
1	I	749	GLN
1	I	764	ARG
1	I	841	LEU

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Mol	Chain	Res	Type
2	M	44	THR
2	M	128	ASP
2	M	211	ALA
2	M	212	ASN
2	M	235	LYS
2	M	247	ASP
2	M	280	ILE
2	M	281	GLU
2	M	304	GLN
2	M	351	VAL
3	J	30	SER
3	J	50	PRO
3	J	51	THR
3	J	55	GLY
3	J	74	ASP
3	J	105	ASN
3	J	109	ALA
3	J	158	GLU
3	J	167	LEU
3	J	246	PRO
3	J	292	ILE
3	J	347	GLY
3	J	382	LYS
3	J	404	VAL
3	J	418	ASN
3	J	457	GLU
3	J	482	GLU
3	J	534	GLY
3	J	574	ARG
3	J	587	PRO
3	J	604	PHE
3	J	605	ASP
3	J	618	ALA
3	J	684	TYR
3	J	708	LEU
3	J	736	ASP
3	J	806	GLY
3	J	933	ALA
3	J	951	GLU
3	J	972	ASP
3	J	1001	LEU
3	J	1065	GLY

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Mol	Chain	Res	Type
4	O	162	SER
4	O	179	ALA
6	R	49	ALA
7	S	80	GLU
7	S	97	SER
7	S	105	ILE
8	T	28	ALA
8	T	29	TYR
9	U	25	ASN
9	U	71	ARG
10	V	28	ILE
10	V	66	LYS
11	W	63	THR
1	A	80	PRO
1	A	106	ILE
1	A	121	ILE
1	A	286	PRO
1	A	356	TRP
1	A	372	TRP
1	A	454	ASN
1	A	514	THR
1	A	688	PRO
1	A	741	THR
1	A	852	ASP
2	C	58	GLU
2	C	145	GLU
2	C	192	LYS
2	C	196	PHE
2	C	235	LYS
2	C	272	VAL
2	C	290	ARG
2	C	302	ALA
3	B	51	THR
3	B	75	ARG
3	B	110	GLU
3	B	155	ASN
3	B	170	ASN
3	B	182	ASN
3	B	184	THR
3	B	247	GLU
3	B	276	VAL
3	B	449	GLN

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Mol	Chain	Res	Type
3	B	559	VAL
3	B	660	HIS
3	B	769	GLN
3	B	901	VAL
3	B	921	LEU
3	B	1080	PRO
4	D	23	GLU
4	D	70	GLU
4	D	179	ALA
5	E	52	LYS
6	F	43	SER
7	G	48	ILE
8	H	44	TRP
9	K	26	ARG
9	K	27	LEU
9	K	71	ARG
12	P	13	PHE
13	Y	56	ASN
13	Y	70	ASP
1	I	97	THR
1	I	106	ILE
1	I	235	LEU
1	I	356	TRP
1	I	514	THR
1	I	688	PRO
1	I	763	THR
1	I	864	LYS
2	M	50	LYS
2	M	71	GLY
2	M	114	LYS
2	M	278	ARG
2	M	279	GLU
2	M	337	GLU
2	M	367	LYS
3	J	47	GLY
3	J	75	ARG
3	J	110	GLU
3	J	170	ASN
3	J	182	ASN
3	J	184	THR
3	J	231	GLY
3	J	247	GLU

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Mol	Chain	Res	Type
3	J	276	VAL
3	J	332	PRO
3	J	449	GLN
3	J	559	VAL
3	J	657	TYR
3	J	660	HIS
3	J	691	ARG
3	J	759	SER
3	J	769	GLN
3	J	888	ILE
3	J	921	LEU
3	J	1080	PRO
4	O	103	PRO
4	O	206	CYS
5	Q	16	ASN
5	Q	56	GLU
5	Q	116	ASP
7	S	47	ASN
7	S	102	LEU
8	T	19	LYS
8	T	20	HIS
8	T	54	SER
8	T	81	VAL
9	U	13	LEU
9	U	16	ASN
9	U	44	ALA
12	X	13	PHE
12	X	28	TYR
1	A	54	PRO
1	A	97	THR
1	A	103	ARG
1	A	235	LEU
1	A	524	ILE
1	A	626	TRP
1	A	645	THR
1	A	686	PRO
2	C	45	ARG
2	C	67	GLY
2	C	238	LYS
3	B	111	PRO
3	B	210	PHE
3	B	223	PHE

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Mol	Chain	Res	Type
3	B	231	GLY
3	B	331	GLU
3	B	338	TYR
3	B	376	GLY
3	B	657	TYR
3	B	759	SER
3	B	860	LYS
3	B	1048	ARG
3	B	1087	ASN
4	D	162	SER
4	D	177	GLU
5	E	131	LYS
6	F	34	LEU
6	F	57	GLU
8	H	10	ASP
8	H	15	TYR
8	H	29	TYR
8	H	79	ARG
10	L	6	LEU
11	N	19	GLN
12	P	28	TYR
1	I	103	ARG
1	I	218	THR
1	I	286	PRO
1	I	355	PRO
1	I	537	PRO
1	I	686	PRO
1	I	852	ASP
2	M	12	TYR
2	M	144	LEU
2	M	193	LEU
2	M	210	PHE
2	M	218	ALA
3	J	98	LEU
3	J	111	PRO
3	J	113	GLU
3	J	331	GLU
3	J	338	TYR
3	J	486	GLU
3	J	901	VAL
4	O	7	HIS
4	O	70	GLU

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Mol	Chain	Res	Type
5	Q	81	VAL
5	Q	139	GLY
6	R	25	ILE
6	R	43	SER
6	R	80	SER
7	S	48	ILE
7	S	99	TYR
8	T	12	ARG
9	U	19	PHE
11	W	6	ARG
11	W	19	GLN
1	A	391	VAL
1	A	403	PRO
1	A	482	VAL
1	A	537	PRO
1	A	543	ARG
1	A	779	ARG
2	C	144	LEU
2	C	161	ALA
2	C	213	ILE
2	C	239	ARG
2	C	348	GLU
3	B	98	LEU
3	B	103	VAL
3	B	194	ALA
3	B	441	GLU
3	B	635	PRO
3	B	915	LEU
3	B	1034	ASP
4	D	127	ASP
6	F	31	SER
11	N	6	ARG
1	I	54	PRO
1	I	143	ALA
1	I	524	ILE
1	I	543	ARG
1	I	645	THR
2	M	74	ALA
2	M	298	SER
3	J	103	VAL
3	J	194	ALA
3	J	210	PHE

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Mol	Chain	Res	Type
3	J	376	GLY
3	J	598	GLU
3	J	635	PRO
3	J	770	GLU
3	J	781	ARG
3	J	915	LEU
4	O	177	GLU
5	Q	38	ILE
8	T	80	TYR
1	A	143	ALA
2	C	114	LYS
2	C	128	ASP
3	B	332	PRO
3	B	377	ARG
3	B	438	PRO
3	B	598	GLU
3	B	703	VAL
3	B	770	GLU
3	B	779	GLY
3	B	972	ASP
4	D	79	PRO
4	D	94	THR
5	E	51	VAL
1	I	334	ILE
1	I	391	VAL
1	I	403	PRO
1	I	851	GLY
2	M	161	ALA
2	M	203	ASP
2	M	363	VAL
2	M	364	GLU
3	J	223	PHE
3	J	377	ARG
3	J	438	PRO
3	J	703	VAL
3	J	779	GLY
3	J	793	GLU
3	J	1048	ARG
3	J	1087	ASN
6	R	60	SER
8	T	11	PRO
9	U	70	ARG

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Mol	Chain	Res	Type
12	X	18	LEU
1	A	530	VAL
1	A	851	GLY
2	C	71	GLY
3	B	299	PRO
3	B	328	GLY
3	B	591	ILE
3	B	814	VAL
3	B	944	PRO
3	B	950	ILE
8	H	59	PRO
1	I	121	ILE
2	M	24	LEU
2	M	67	GLY
2	M	119	THR
2	M	179	VAL
2	M	181	VAL
3	J	299	PRO
3	J	903	GLY
3	J	950	ILE
3	J	1108	ILE
3	B	767	GLY
3	B	1108	ILE
10	L	28	ILE
1	I	530	VAL
2	M	277	ILE
6	R	4	VAL
7	S	64	PRO
8	T	10	ASP
1	A	334	ILE
1	A	369	PRO
2	C	393	ILE
3	B	253	PHE
7	G	64	PRO
7	G	78	VAL
13	Y	57	GLY
2	M	260	GLY
2	M	261	VAL
3	J	645	PRO
3	J	944	PRO
5	Q	51	VAL
9	U	64	ILE

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Mol	Chain	Res	Type
10	V	48	PRO
2	C	181	VAL
3	B	645	PRO
3	B	888	ILE
5	E	25	ILE
1	I	330	PRO
1	I	369	PRO
3	J	591	ILE
9	U	62	ILE
10	V	46	PRO
1	A	760	GLY
4	O	79	PRO

### 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	729/766 (95%)	601 (82%)	128 (18%)	2	12
1	I	729/766 (95%)	604 (83%)	125 (17%)	2	14
2	C	318/340 (94%)	241 (76%)	77 (24%)	1	4
2	M	318/340 (94%)	226 (71%)	92 (29%)	0	2
3	B	937/965 (97%)	772 (82%)	165 (18%)	2	12
3	J	937/965 (97%)	771 (82%)	166 (18%)	2	12
4	D	241/242 (100%)	220 (91%)	21 (9%)	13	47
4	O	241/242 (100%)	221 (92%)	20 (8%)	14	49
5	E	156/159 (98%)	128 (82%)	28 (18%)	2	11
5	Q	156/159 (98%)	123 (79%)	33 (21%)	1	6
6	F	82/106 (77%)	72 (88%)	10 (12%)	6	28
6	R	82/106 (77%)	72 (88%)	10 (12%)	6	28
7	G	105/125 (84%)	87 (83%)	18 (17%)	2	14
7	S	105/125 (84%)	82 (78%)	23 (22%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	67/75 (89%)	49 (73%)	18 (27%)	0	3
8	T	67/75 (89%)	54 (81%)	13 (19%)	2	8
9	K	72/84 (86%)	48 (67%)	24 (33%)	0	2
9	U	72/84 (86%)	50 (69%)	22 (31%)	0	2
10	L	81/81 (100%)	66 (82%)	15 (18%)	2	10
10	V	81/81 (100%)	63 (78%)	18 (22%)	1	5
11	N	58/60 (97%)	48 (83%)	10 (17%)	2	13
11	W	58/60 (97%)	48 (83%)	10 (17%)	2	13
12	P	39/43 (91%)	32 (82%)	7 (18%)	2	11
12	X	39/43 (91%)	32 (82%)	7 (18%)	2	11
13	Y	43/97 (44%)	34 (79%)	9 (21%)	1	6
13	Z	43/97 (44%)	34 (79%)	9 (21%)	1	6
All	All	5856/6286 (93%)	4778 (82%)	1078 (18%)	2	10

All (1078) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	29	THR
1	A	45	MET
1	A	48	ARG
1	A	56	GLN
1	A	58	CYS
1	A	60	THR
1	A	64	THR
1	A	65	LEU
1	A	82	ILE
1	A	84	VAL
1	A	100	ARG
1	A	101	CYS
1	A	103	ARG
1	A	105	LYS
1	A	107	SER
1	A	125	TRP
1	A	127	SER
1	A	130	ARG
1	A	133	THR
1	A	136	VAL

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Mol	Chain	Res	Type
1	A	139	THR
1	A	141	MET
1	A	152	LYS
1	A	155	LYS
1	A	175	LEU
1	A	176	THR
1	A	178	SER
1	A	179	ASP
1	A	191	ASP
1	A	194	ILE
1	A	203	ARG
1	A	222	SER
1	A	232	GLU
1	A	238	LYS
1	A	239	LEU
1	A	243	VAL
1	A	248	ARG
1	A	261	ILE
1	A	264	ASP
1	A	278	ASP
1	A	289	HIS
1	A	290	ARG
1	A	301	ARG
1	A	306	GLU
1	A	308	ARG
1	A	313	LEU
1	A	314	SER
1	A	331	ASN
1	A	346	THR
1	A	349	VAL
1	A	356	TRP
1	A	366	ILE
1	A	376	ASN
1	A	377	TYR
1	A	386	ILE
1	A	388	LEU
1	A	394	ARG
1	A	421	ARG
1	A	425	LEU
1	A	427	ARG
1	A	428	ILE
1	A	429	SER

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Mol	Chain	Res	Type
1	A	434	ARG
1	A	436	ARG
1	A	438	LEU
1	A	441	LEU
1	A	442	THR
1	A	446	ASN
1	A	464	LEU
1	A	469	SER
1	A	471	GLU
1	A	479	ILE
1	A	481	LEU
1	A	486	ILE
1	A	487	ILE
1	A	488	THR
1	A	495	ILE
1	A	500	GLN
1	A	503	ILE
1	A	507	TYR
1	A	515	LEU
1	A	518	LYS
1	A	525	LEU
1	A	547	THR
1	A	550	GLN
1	A	558	LYS
1	A	559	ASP
1	A	561	ASN
1	A	573	ARG
1	A	574	LEU
1	A	593	LEU
1	A	597	VAL
1	A	605	ASN
1	A	609	GLU
1	A	616	ILE
1	A	618	GLU
1	A	633	ARG
1	A	637	ARG
1	A	644	PHE
1	A	667	ARG
1	A	675	LEU
1	A	684	LEU
1	A	687	ILE
1	A	691	THR

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Mol	Chain	Res	Type
1	A	692	LEU
1	A	693	GLU
1	A	702	ASP
1	A	708	ARG
1	A	716	SER
1	A	723	ASN
1	A	736	SER
1	A	737	VAL
1	A	739	ASN
1	A	752	VAL
1	A	755	GLU
1	A	759	ARG
1	A	764	ARG
1	A	766	LEU
1	A	779	ARG
1	A	781	PHE
1	A	787	ARG
1	A	823	LEU
1	A	828	SER
1	A	841	LEU
1	A	844	GLU
1	A	864	LYS
1	A	876	VAL
2	C	13	LEU
2	C	31	ASP
2	C	36	ILE
2	C	41	ILE
2	C	42	ILE
2	C	43	VAL
2	C	47	GLU
2	C	51	ILE
2	C	53	ASP
2	C	57	LYS
2	C	59	TYR
2	C	61	GLU
2	C	70	ILE
2	C	72	ILE
2	C	85	MET
2	C	107	LEU
2	C	116	VAL
2	C	118	SER
2	C	119	THR

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Mol	Chain	Res	Type
2	C	130	TYR
2	C	132	ARG
2	C	145	GLU
2	C	147	THR
2	C	163	MET
2	C	173	MET
2	C	174	LEU
2	C	176	ASP
2	C	188	ILE
2	C	190	ARG
2	C	193	LEU
2	C	201	SER
2	C	215	SER
2	C	229	THR
2	C	234	ILE
2	C	237	ILE
2	C	239	ARG
2	C	250	ILE
2	C	254	ASP
2	C	257	ASN
2	C	267	VAL
2	C	275	ASN
2	C	278	ARG
2	C	287	GLU
2	C	291	GLU
2	C	292	ILE
2	C	301	LEU
2	C	307	ASP
2	C	310	ILE
2	C	311	ARG
2	C	314	LEU
2	C	315	LEU
2	C	316	ILE
2	C	320	MET
2	C	322	ARG
2	C	326	VAL
2	C	329	ILE
2	C	331	ARG
2	C	335	THR
2	C	337	GLU
2	C	339	ASN
2	C	344	ARG

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Mol	Chain	Res	Type
2	C	349	VAL
2	C	351	VAL
2	C	364	GLU
2	C	369	VAL
2	C	370	VAL
2	C	374	ILE
2	C	375	ILE
2	C	379	ILE
2	C	380	LYS
2	C	381	LEU
2	C	388	LEU
2	C	389	THR
2	C	390	MET
2	C	391	ARG
2	C	393	ILE
2	C	394	LEU
3	B	5	LEU
3	B	6	THR
3	B	8	ASP
3	B	20	SER
3	B	23	LEU
3	B	30	SER
3	B	33	ASP
3	B	34	PHE
3	B	51	THR
3	B	56	LEU
3	B	64	ARG
3	B	65	ILE
3	B	70	VAL
3	B	72	GLU
3	B	75	ARG
3	B	80	ILE
3	B	90	LEU
3	B	105	ASN
3	B	108	GLU
3	B	113	GLU
3	B	118	ASP
3	B	137	LYS
3	B	155	ASN
3	B	159	ARG
3	B	163	THR
3	B	182	ASN

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Mol	Chain	Res	Type
3	B	183	ILE
3	B	193	THR
3	B	203	GLU
3	B	207	ASP
3	B	221	ILE
3	B	227	MET
3	B	234	THR
3	B	245	ASP
3	B	282	ARG
3	B	296	TYR
3	B	322	VAL
3	B	327	LEU
3	B	335	LYS
3	B	348	ASP
3	B	361	PHE
3	B	367	TYR
3	B	369	LEU
3	B	371	LYS
3	B	374	VAL
3	B	378	LYS
3	B	391	THR
3	B	395	ARG
3	B	402	ASN
3	B	404	VAL
3	B	407	ARG
3	B	416	ARG
3	B	418	ASN
3	B	421	SER
3	B	432	SER
3	B	444	ASP
3	B	448	THR
3	B	453	MET
3	B	457	GLU
3	B	467	VAL
3	B	468	LYS
3	B	469	ASN
3	B	476	ILE
3	B	478	VAL
3	B	484	ILE
3	B	486	GLU
3	B	488	THR
3	B	497	VAL

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Mol	Chain	Res	Type
3	B	498	GLU
3	B	518	SER
3	B	530	TYR
3	B	531	GLN
3	B	544	ARG
3	B	549	ILE
3	B	551	ASP
3	B	564	ASN
3	B	570	CYS
3	B	572	SER
3	B	576	ARG
3	B	588	LEU
3	B	594	ILE
3	B	603	THR
3	B	606	ASP
3	B	607	LEU
3	B	608	VAL
3	B	626	VAL
3	B	628	LEU
3	B	634	THR
3	B	638	THR
3	B	640	LEU
3	B	643	TRP
3	B	650	ILE
3	B	655	ILE
3	B	659	GLU
3	B	669	GLN
3	B	685	GLN
3	B	686	LEU
3	B	687	ARG
3	B	688	THR
3	B	689	ASP
3	B	691	ARG
3	B	702	LEU
3	B	705	THR
3	B	708	LEU
3	B	710	ILE
3	B	714	THR
3	B	720	ASN
3	B	739	ILE
3	B	741	ASN
3	B	757	LEU

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Mol	Chain	Res	Type
3	B	765	TYR
3	B	770	GLU
3	B	780	VAL
3	B	781	ARG
3	B	787	GLU
3	B	789	TYR
3	B	794	ASP
3	B	800	PRO
3	B	814	VAL
3	B	843	GLU
3	B	846	ILE
3	B	850	VAL
3	B	855	THR
3	B	867	ARG
3	B	871	ILE
3	B	887	VAL
3	B	890	MET
3	B	895	VAL
3	B	910	LEU
3	B	911	ASN
3	B	915	LEU
3	B	919	MET
3	B	924	ILE
3	B	926	GLU
3	B	931	LYS
3	B	940	VAL
3	B	941	ASP
3	B	945	PHE
3	B	946	TYR
3	B	950	ILE
3	B	951	GLU
3	B	957	ILE
3	B	967	THR
3	B	975	THR
3	B	982	ARG
3	B	985	PHE
3	B	991	GLN
3	B	992	LYS
3	B	1004	ARG
3	B	1012	LEU
3	B	1016	PRO
3	B	1018	GLU

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Mol	Chain	Res	Type
3	B	1026	LEU
3	B	1030	GLU
3	B	1035	CYS
3	B	1045	LEU
3	B	1049	LEU
3	B	1050	LEU
3	B	1067	ILE
3	B	1078	VAL
3	B	1079	CYS
3	B	1108	ILE
3	B	1109	ILE
3	B	1113	LEU
3	B	1115	LEU
4	D	29	ARG
4	D	56	GLU
4	D	57	ILE
4	D	68	MET
4	D	82	CYS
4	D	89	CYS
4	D	113	ASP
4	D	132	LEU
4	D	135	THR
4	D	136	ASN
4	D	155	LYS
4	D	161	LEU
4	D	162	SER
4	D	165	ARG
4	D	170	VAL
4	D	180	VAL
4	D	195	LEU
4	D	201	LEU
4	D	204	THR
4	D	214	ASN
4	D	218	ARG
5	E	12	ARG
5	E	18	PHE
5	E	22	LEU
5	E	27	LEU
5	E	30	LEU
5	E	33	GLN
5	E	38	ILE
5	E	39	LEU

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Mol	Chain	Res	Type
5	E	40	LYS
5	E	41	ASP
5	E	44	LEU
5	E	51	VAL
5	E	58	ILE
5	E	59	LEU
5	E	66	THR
5	E	67	TYR
5	E	69	GLU
5	E	76	THR
5	E	81	VAL
5	E	83	GLU
5	E	85	VAL
5	E	92	VAL
5	E	101	LEU
5	E	110	ILE
5	E	128	PHE
5	E	151	SER
5	E	163	THR
5	E	176	THR
6	F	14	TYR
6	F	15	SER
6	F	25	ILE
6	F	31	SER
6	F	33	LEU
6	F	34	LEU
6	F	47	CYS
6	F	59	LEU
6	F	64	SER
6	F	86	ILE
7	G	5	VAL
7	G	10	ILE
7	G	19	GLU
7	G	25	ASN
7	G	42	ILE
7	G	46	ILE
7	G	65	SER
7	G	77	ILE
7	G	78	VAL
7	G	86	LEU
7	G	92	TYR
7	G	95	ILE

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Mol	Chain	Res	Type
7	G	97	SER
7	G	104	LYS
7	G	106	ILE
7	G	110	GLU
7	G	114	ARG
7	G	115	THR
8	H	12	ARG
8	H	13	ILE
8	H	19	LYS
8	H	22	VAL
8	H	31	ILE
8	H	37	ILE
8	H	38	ARG
8	H	43	PRO
8	H	44	TRP
8	H	45	ILE
8	H	46	ARG
8	H	48	SER
8	H	64	ARG
8	H	65	ILE
8	H	74	GLU
8	H	75	VAL
8	H	76	VAL
8	H	82	ILE
9	K	15	PHE
9	K	18	VAL
9	K	19	PHE
9	K	20	ILE
9	K	22	LEU
9	K	23	TRP
9	K	29	ARG
9	K	35	VAL
9	K	36	ILE
9	K	37	SER
9	K	41	LEU
9	K	42	GLN
9	K	45	MET
9	K	50	LEU
9	K	51	ILE
9	K	52	ASP
9	K	61	VAL
9	K	67	GLU

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Mol	Chain	Res	Type
9	K	71	ARG
9	K	74	LEU
9	K	81	ARG
9	K	82	LEU
9	K	89	LEU
9	K	90	LEU
10	L	9	GLU
10	L	24	LEU
10	L	43	TYR
10	L	44	TYR
10	L	45	GLN
10	L	47	HIS
10	L	49	LEU
10	L	55	VAL
10	L	57	ILE
10	L	69	LEU
10	L	70	LEU
10	L	73	ILE
10	L	79	MET
10	L	87	ILE
10	L	92	LYS
11	N	3	ILE
11	N	5	ILE
11	N	10	CYS
11	N	13	LEU
11	N	22	ILE
11	N	40	VAL
11	N	42	ARG
11	N	48	MET
11	N	55	ILE
11	N	64	ARG
12	P	10	TRP
12	P	21	LEU
12	P	24	VAL
12	P	31	TYR
12	P	34	ILE
12	P	35	PHE
12	P	46	LYS
13	Y	44	LEU
13	Y	60	THR
13	Y	69	GLU
13	Y	70	ASP

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Mol	Chain	Res	Type
13	Y	72	TYR
13	Y	77	LYS
13	Y	78	ARG
13	Y	79	ASP
13	Y	82	ARG
1	I	15	SER
1	I	29	THR
1	I	45	MET
1	I	48	ARG
1	I	56	GLN
1	I	58	CYS
1	I	60	THR
1	I	64	THR
1	I	82	ILE
1	I	84	VAL
1	I	100	ARG
1	I	101	CYS
1	I	103	ARG
1	I	105	LYS
1	I	107	SER
1	I	125	TRP
1	I	127	SER
1	I	130	ARG
1	I	133	THR
1	I	136	VAL
1	I	141	MET
1	I	152	LYS
1	I	155	LYS
1	I	175	LEU
1	I	176	THR
1	I	178	SER
1	I	179	ASP
1	I	194	ILE
1	I	203	ARG
1	I	209	LEU
1	I	217	ILE
1	I	222	SER
1	I	232	GLU
1	I	238	LYS
1	I	239	LEU
1	I	243	VAL
1	I	248	ARG

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Mol	Chain	Res	Type
1	I	261	ILE
1	I	264	ASP
1	I	278	ASP
1	I	289	HIS
1	I	298	LEU
1	I	301	ARG
1	I	306	GLU
1	I	308	ARG
1	I	313	LEU
1	I	314	SER
1	I	331	ASN
1	I	346	THR
1	I	349	VAL
1	I	366	ILE
1	I	376	ASN
1	I	377	TYR
1	I	386	ILE
1	I	388	LEU
1	I	394	ARG
1	I	411	LEU
1	I	421	ARG
1	I	425	LEU
1	I	427	ARG
1	I	428	ILE
1	I	434	ARG
1	I	436	ARG
1	I	438	LEU
1	I	441	LEU
1	I	442	THR
1	I	446	ASN
1	I	464	LEU
1	I	469	SER
1	I	481	LEU
1	I	484	LYS
1	I	486	ILE
1	I	487	ILE
1	I	488	THR
1	I	495	ILE
1	I	500	GLN
1	I	503	ILE
1	I	507	TYR
1	I	515	LEU

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Mol	Chain	Res	Type
1	I	518	LYS
1	I	525	LEU
1	I	547	THR
1	I	550	GLN
1	I	558	LYS
1	I	559	ASP
1	I	561	ASN
1	I	573	ARG
1	I	574	LEU
1	I	586	VAL
1	I	593	LEU
1	I	605	ASN
1	I	609	GLU
1	I	616	ILE
1	I	618	GLU
1	I	633	ARG
1	I	637	ARG
1	I	644	PHE
1	I	667	ARG
1	I	675	LEU
1	I	684	LEU
1	I	687	ILE
1	I	692	LEU
1	I	693	GLU
1	I	702	ASP
1	I	708	ARG
1	I	716	SER
1	I	723	ASN
1	I	736	SER
1	I	737	VAL
1	I	738	LEU
1	I	739	ASN
1	I	747	LEU
1	I	755	GLU
1	I	759	ARG
1	I	764	ARG
1	I	766	LEU
1	I	779	ARG
1	I	781	PHE
1	I	787	ARG
1	I	823	LEU
1	I	831	ARG

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Mol	Chain	Res	Type
1	I	841	LEU
1	I	844	GLU
1	I	864	LYS
1	I	876	VAL
2	M	13	LEU
2	M	18	LYS
2	M	28	ILE
2	M	29	VAL
2	M	31	ASP
2	M	34	ASN
2	M	39	LYS
2	M	40	GLU
2	M	42	ILE
2	M	44	THR
2	M	45	ARG
2	M	46	ASP
2	M	53	ASP
2	M	57	LYS
2	M	61	GLU
2	M	70	ILE
2	M	73	VAL
2	M	78	VAL
2	M	83	THR
2	M	84	GLN
2	M	85	MET
2	M	102	LEU
2	M	104	LEU
2	M	106	ARG
2	M	107	LEU
2	M	116	VAL
2	M	127	THR
2	M	128	ASP
2	M	129	GLU
2	M	130	TYR
2	M	132	ARG
2	M	135	ASP
2	M	143	LYS
2	M	147	THR
2	M	156	THR
2	M	157	SER
2	M	159	ASP
2	M	160	ILE

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Mol	Chain	Res	Type
2	M	163	MET
2	M	165	ILE
2	M	171	ASN
2	M	173	MET
2	M	174	LEU
2	M	176	ASP
2	M	179	VAL
2	M	188	ILE
2	M	190	ARG
2	M	212	ASN
2	M	213	ILE
2	M	214	ASP
2	M	229	THR
2	M	231	ILE
2	M	235	LYS
2	M	239	ARG
2	M	247	ASP
2	M	250	ILE
2	M	251	ILE
2	M	254	ASP
2	M	267	VAL
2	M	275	ASN
2	M	276	ASN
2	M	277	ILE
2	M	278	ARG
2	M	280	ILE
2	M	303	GLU
2	M	306	LEU
2	M	308	VAL
2	M	309	ASP
2	M	311	ARG
2	M	313	ILE
2	M	315	LEU
2	M	316	ILE
2	M	322	ARG
2	M	325	ILE
2	M	327	ARG
2	M	329	ILE
2	M	335	THR
2	M	338	LYS
2	M	339	ASN
2	M	344	ARG

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Mol	Chain	Res	Type
2	M	351	VAL
2	M	355	LEU
2	M	369	VAL
2	M	370	VAL
2	M	375	ILE
2	M	379	ILE
2	M	380	LYS
2	M	381	LEU
2	M	386	VAL
2	M	387	GLU
2	M	389	THR
2	M	391	ARG
3	J	5	LEU
3	J	6	THR
3	J	8	ASP
3	J	20	SER
3	J	23	LEU
3	J	30	SER
3	J	33	ASP
3	J	51	THR
3	J	56	LEU
3	J	64	ARG
3	J	65	ILE
3	J	70	VAL
3	J	72	GLU
3	J	75	ARG
3	J	80	ILE
3	J	105	ASN
3	J	108	GLU
3	J	113	GLU
3	J	118	ASP
3	J	155	ASN
3	J	159	ARG
3	J	163	THR
3	J	179	THR
3	J	182	ASN
3	J	183	ILE
3	J	193	THR
3	J	196	TYR
3	J	203	GLU
3	J	207	ASP
3	J	221	ILE

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Mol	Chain	Res	Type
3	J	227	MET
3	J	234	THR
3	J	245	ASP
3	J	282	ARG
3	J	296	TYR
3	J	322	VAL
3	J	327	LEU
3	J	335	LYS
3	J	348	ASP
3	J	361	PHE
3	J	367	TYR
3	J	369	LEU
3	J	371	LYS
3	J	378	LYS
3	J	391	THR
3	J	394	ILE
3	J	395	ARG
3	J	402	ASN
3	J	404	VAL
3	J	407	ARG
3	J	416	ARG
3	J	418	ASN
3	J	421	SER
3	J	432	SER
3	J	444	ASP
3	J	448	THR
3	J	453	MET
3	J	457	GLU
3	J	467	VAL
3	J	468	LYS
3	J	469	ASN
3	J	476	ILE
3	J	478	VAL
3	J	484	ILE
3	J	486	GLU
3	J	488	THR
3	J	497	VAL
3	J	498	GLU
3	J	518	SER
3	J	530	TYR
3	J	531	GLN
3	J	544	ARG

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Mol	Chain	Res	Type
3	J	549	ILE
3	J	551	ASP
3	J	564	ASN
3	J	570	CYS
3	J	572	SER
3	J	576	ARG
3	J	588	LEU
3	J	594	ILE
3	J	603	THR
3	J	606	ASP
3	J	607	LEU
3	J	608	VAL
3	J	626	VAL
3	J	628	LEU
3	J	634	THR
3	J	638	THR
3	J	640	LEU
3	J	643	TRP
3	J	650	ILE
3	J	655	ILE
3	J	659	GLU
3	J	669	GLN
3	J	685	GLN
3	J	686	LEU
3	J	687	ARG
3	J	688	THR
3	J	689	ASP
3	J	691	ARG
3	J	702	LEU
3	J	705	THR
3	J	708	LEU
3	J	710	ILE
3	J	714	THR
3	J	720	ASN
3	J	727	MET
3	J	739	ILE
3	J	741	ASN
3	J	752	SER
3	J	757	LEU
3	J	765	TYR
3	J	770	GLU
3	J	780	VAL

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Mol	Chain	Res	Type
3	J	781	ARG
3	J	789	TYR
3	J	794	ASP
3	J	800	PRO
3	J	814	VAL
3	J	839	THR
3	J	843	GLU
3	J	846	ILE
3	J	855	THR
3	J	867	ARG
3	J	871	ILE
3	J	887	VAL
3	J	890	MET
3	J	891	LEU
3	J	895	VAL
3	J	910	LEU
3	J	911	ASN
3	J	915	LEU
3	J	919	MET
3	J	923	GLN
3	J	924	ILE
3	J	926	GLU
3	J	931	LYS
3	J	940	VAL
3	J	941	ASP
3	J	945	PHE
3	J	946	TYR
3	J	950	ILE
3	J	951	GLU
3	J	957	ILE
3	J	967	THR
3	J	975	THR
3	J	982	ARG
3	J	985	PHE
3	J	991	GLN
3	J	992	LYS
3	J	1004	ARG
3	J	1012	LEU
3	J	1018	GLU
3	J	1026	LEU
3	J	1030	GLU
3	J	1035	CYS

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Mol	Chain	Res	Type
3	J	1045	LEU
3	J	1049	LEU
3	J	1050	LEU
3	J	1067	ILE
3	J	1078	VAL
3	J	1079	CYS
3	J	1108	ILE
3	J	1109	ILE
3	J	1113	LEU
3	J	1115	LEU
4	O	29	ARG
4	O	56	GLU
4	O	57	ILE
4	O	68	MET
4	O	89	CYS
4	O	113	ASP
4	O	132	LEU
4	O	135	THR
4	O	136	ASN
4	O	155	LYS
4	O	161	LEU
4	O	162	SER
4	O	165	ARG
4	O	170	VAL
4	O	180	VAL
4	O	195	LEU
4	O	201	LEU
4	O	204	THR
4	O	214	ASN
4	O	218	ARG
5	Q	4	LEU
5	Q	5	ILE
5	Q	17	GLU
5	Q	18	PHE
5	Q	22	LEU
5	Q	25	ILE
5	Q	27	LEU
5	Q	30	LEU
5	Q	32	GLN
5	Q	33	GLN
5	Q	38	ILE
5	Q	40	LYS

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Mol	Chain	Res	Type
5	Q	42	LEU
5	Q	48	ILE
5	Q	49	LEU
5	Q	51	VAL
5	Q	58	ILE
5	Q	60	VAL
5	Q	69	GLU
5	Q	76	THR
5	Q	85	VAL
5	Q	104	MET
5	Q	107	LEU
5	Q	110	ILE
5	Q	126	ILE
5	Q	127	ILE
5	Q	140	ASP
5	Q	149	VAL
5	Q	152	THR
5	Q	174	TRP
5	Q	175	ILE
5	Q	176	THR
5	Q	177	GLN
6	R	6	ILE
6	R	9	GLU
6	R	25	ILE
6	R	34	LEU
6	R	44	VAL
6	R	45	GLU
6	R	59	LEU
6	R	64	SER
6	R	67	ASP
6	R	87	LEU
7	S	10	ILE
7	S	23	LEU
7	S	25	ASN
7	S	27	SER
7	S	32	SER
7	S	33	CYS
7	S	34	ASN
7	S	39	SER
7	S	40	PHE
7	S	42	ILE
7	S	48	ILE

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Mol	Chain	Res	Type
7	S	62	ASN
7	S	68	HIS
7	S	69	ASP
7	S	77	ILE
7	S	79	THR
7	S	86	LEU
7	S	90	ASN
7	S	95	ILE
7	S	102	LEU
7	S	104	LYS
7	S	110	GLU
7	S	116	SER
8	T	12	ARG
8	T	19	LYS
8	T	25	ILE
8	T	30	LYS
8	T	37	ILE
8	T	38	ARG
8	T	42	LEU
8	T	44	TRP
8	T	46	ARG
8	T	62	ILE
8	T	70	GLN
8	T	72	TYR
8	T	81	VAL
9	U	14	HIS
9	U	15	PHE
9	U	23	TRP
9	U	26	ARG
9	U	29	ARG
9	U	37	SER
9	U	41	LEU
9	U	42	GLN
9	U	51	ILE
9	U	52	ASP
9	U	62	ILE
9	U	67	GLU
9	U	70	ARG
9	U	71	ARG
9	U	74	LEU
9	U	76	ILE
9	U	81	ARG

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Mol	Chain	Res	Type
9	U	88	ILE
9	U	89	LEU
9	U	90	LEU
9	U	91	SER
9	U	92	LEU
10	V	6	LEU
10	V	9	GLU
10	V	10	SER
10	V	14	GLU
10	V	16	GLU
10	V	24	LEU
10	V	38	VAL
10	V	43	TYR
10	V	47	HIS
10	V	49	LEU
10	V	54	ILE
10	V	63	ILE
10	V	64	THR
10	V	70	LEU
10	V	73	ILE
10	V	77	ARG
10	V	79	MET
10	V	92	LYS
11	W	3	ILE
11	W	5	ILE
11	W	10	CYS
11	W	13	LEU
11	W	22	ILE
11	W	40	VAL
11	W	42	ARG
11	W	48	MET
11	W	55	ILE
11	W	64	ARG
12	X	10	TRP
12	X	21	LEU
12	X	24	VAL
12	X	31	TYR
12	X	34	ILE
12	X	35	PHE
12	X	46	LYS
13	Z	41	ILE
13	Z	54	LEU

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Mol	Chain	Res	Type
13	Z	55	LEU
13	Z	56	ASN
13	Z	60	THR
13	Z	66	LYS
13	Z	69	GLU
13	Z	70	ASP
13	Z	82	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (134) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	63	ASN
1	A	119	ASN
1	A	259	GLN
1	A	312	ASN
1	A	331	ASN
1	A	367	ASN
1	A	420	ASN
1	A	422	GLN
1	A	446	ASN
1	A	465	HIS
1	A	483	HIS
1	A	485	ASN
1	A	561	ASN
1	A	567	ASN
1	A	590	ASN
1	A	677	GLN
1	A	723	ASN
2	C	38	ASN
2	C	207	ASN
2	C	209	ASN
2	C	275	ASN
2	C	276	ASN
2	C	328	GLN
3	B	27	HIS
3	B	40	GLN
3	B	164	GLN
3	B	182	ASN
3	B	300	HIS
3	B	368	GLN
3	B	412	GLN

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Mol	Chain	Res	Type
3	B	418	ASN
3	B	439	ASN
3	B	446	HIS
3	B	449	GLN
3	B	554	ASN
3	B	569	ASN
3	B	610	GLN
3	B	623	ASN
3	B	637	HIS
3	B	639	HIS
3	B	660	HIS
3	B	669	GLN
3	B	685	GLN
3	B	715	ASN
3	B	721	ASN
3	B	911	ASN
3	B	913	HIS
3	B	991	GLN
3	B	1015	GLN
3	B	1052	ASN
3	B	1087	ASN
5	E	16	ASN
5	E	33	GLN
5	E	109	HIS
5	E	112	GLN
6	F	61	ASN
7	G	88	ASN
8	H	20	HIS
9	K	42	GLN
9	K	54	ASN
10	L	22	HIS
11	N	19	GLN
11	N	57	ASN
1	I	5	ASN
1	I	56	GLN
1	I	63	ASN
1	I	119	ASN
1	I	259	GLN
1	I	312	ASN
1	I	331	ASN
1	I	367	ASN
1	I	420	ASN

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Mol	Chain	Res	Type
1	I	422	GLN
1	I	426	HIS
1	I	446	ASN
1	I	483	HIS
1	I	485	ASN
1	I	522	GLN
1	I	561	ASN
1	I	567	ASN
1	I	677	GLN
1	I	723	ASN
2	M	38	ASN
2	M	207	ASN
2	M	209	ASN
2	M	212	ASN
2	M	276	ASN
2	M	328	GLN
3	J	27	HIS
3	J	40	GLN
3	J	106	ASN
3	J	182	ASN
3	J	300	HIS
3	J	368	GLN
3	J	412	GLN
3	J	418	ASN
3	J	439	ASN
3	J	446	HIS
3	J	449	GLN
3	J	531	GLN
3	J	554	ASN
3	J	567	HIS
3	J	569	ASN
3	J	610	GLN
3	J	623	ASN
3	J	637	HIS
3	J	639	HIS
3	J	660	HIS
3	J	669	GLN
3	J	685	GLN
3	J	715	ASN
3	J	720	ASN
3	J	721	ASN
3	J	911	ASN

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Mol	Chain	Res	Type
3	J	913	HIS
3	J	954	GLN
3	J	1015	GLN
3	J	1052	ASN
5	Q	33	GLN
5	Q	109	HIS
5	Q	112	GLN
5	Q	177	GLN
6	R	53	GLN
7	S	88	ASN
7	S	117	GLN
8	T	20	HIS
8	T	70	GLN
9	U	14	HIS
9	U	42	GLN
9	U	54	ASN
9	U	84	ASN
11	W	19	GLN
11	W	57	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
16	F3S	D	1001	4	0,9,9	0.00	-	0,15,15	0.00	-
16	F3S	O	1001	-	0,9,9	0.00	-	0,15,15	0.00	-

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
16	F3S	D	1001	4	-	0/0/24/24	0/0/3/3
16	F3S	O	1001	-	-	0/0/24/24	0/0/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	D	1001	F3S	1	0
16	O	1001	F3S	6	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	836/880 (95%)	-0.14	10 (1%) 81 75	28, 71, 105, 133	0
1	I	836/880 (95%)	-0.15	16 (1%) 70 64	28, 71, 106, 133	0
2	C	370/395 (93%)	0.21	23 (6%) 24 22	37, 78, 130, 138	0
2	M	370/395 (93%)	0.09	16 (4%) 39 34	38, 79, 130, 138	0
3	B	1090/1124 (96%)	-0.12	21 (1%) 70 64	33, 66, 117, 149	0
3	J	1090/1124 (96%)	-0.11	24 (2%) 65 60	33, 67, 117, 149	0
4	D	264/265 (99%)	0.11	10 (3%) 44 39	57, 86, 121, 139	0
4	O	264/265 (99%)	0.22	16 (6%) 25 23	57, 86, 121, 139	0
5	E	176/180 (97%)	0.20	7 (3%) 42 37	58, 98, 140, 143	0
5	Q	176/180 (97%)	0.26	16 (9%) 11 11	58, 98, 139, 142	0
6	F	89/113 (78%)	0.27	10 (11%) 7 7	100, 127, 132, 133	0
6	R	89/113 (78%)	0.24	4 (4%) 37 33	100, 127, 132, 133	0
7	G	113/132 (85%)	0.19	4 (3%) 48 42	65, 88, 108, 112	0
7	S	113/132 (85%)	0.12	4 (3%) 48 42	66, 88, 108, 112	0
8	H	74/84 (88%)	-0.11	0 100 100	66, 81, 99, 102	0
8	T	74/84 (88%)	-0.16	1 (1%) 78 73	66, 81, 99, 102	0
9	K	82/95 (86%)	-0.39	1 (1%) 81 75	41, 57, 86, 94	0
9	U	82/95 (86%)	-0.31	1 (1%) 81 75	43, 58, 87, 93	0
10	L	92/92 (100%)	-0.10	1 (1%) 82 77	53, 73, 103, 107	0
10	V	92/92 (100%)	-0.00	1 (1%) 82 77	54, 73, 103, 107	0
11	N	64/66 (96%)	-0.10	2 (3%) 52 48	62, 80, 103, 124	0
11	W	64/66 (96%)	-0.04	1 (1%) 74 69	62, 80, 103, 124	0
12	P	43/48 (89%)	0.10	1 (2%) 64 58	66, 89, 103, 110	0
12	X	43/48 (89%)	-0.08	2 (4%) 35 32	66, 89, 103, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	Y	45/104 (43%)	0.63	6 (13%) 4 4	98, 108, 124, 125	0
13	Z	45/104 (43%)	0.79	7 (15%) 3 3	98, 108, 124, 124	0
All	All	6676/7156 (93%)	-0.03	205 (3%) 52 48	28, 76, 127, 149	0

All (205) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	278	ILE	7.4
6	R	89	MET	5.5
2	C	213	ILE	5.2
3	B	434	ALA	5.0
13	Y	82	ARG	4.9
5	E	135	VAL	4.9
1	A	60	THR	4.8
5	E	131	LYS	4.7
4	O	188	PHE	4.6
3	B	1069	TRP	4.6
5	Q	153	VAL	4.5
5	E	180	LYS	4.5
5	E	128	PHE	4.5
2	C	214	ASP	4.4
7	G	5	VAL	4.2
2	M	213	ILE	4.1
1	I	148	HIS	4.0
3	J	279	GLY	4.0
2	C	235	LYS	4.0
13	Y	81	ARG	4.0
3	J	244	LEU	4.0
4	O	217	ILE	3.9
2	C	180	THR	3.8
1	A	132	LEU	3.7
3	B	600	GLY	3.7
1	I	147	PRO	3.7
2	M	180	THR	3.7
2	C	234	ILE	3.7
4	O	171	GLU	3.6
3	J	194	ALA	3.6
5	Q	178	THR	3.6
1	I	294	PRO	3.6
3	J	831	ALA	3.5
4	D	217	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
3	J	277	ALA	3.5
3	J	434	ALA	3.5
13	Z	38	ILE	3.5
1	I	149	CYS	3.5
4	O	197	VAL	3.4
2	M	235	LYS	3.4
3	B	625	TYR	3.4
9	K	51	ILE	3.4
4	D	190	LEU	3.4
4	O	172	ILE	3.4
3	J	781	ARG	3.4
5	Q	175	ILE	3.3
4	O	175	ASN	3.3
5	Q	177	GLN	3.3
7	S	6	ALA	3.3
5	Q	152	THR	3.3
6	F	45	GLU	3.3
3	J	1077	TYR	3.3
2	C	211	ALA	3.3
6	R	2	SER	3.2
2	M	190	ARG	3.2
5	Q	179	LYS	3.2
5	E	132	SER	3.2
1	A	147	PRO	3.2
4	O	193	GLY	3.2
3	J	600	GLY	3.1
1	I	390	TYR	3.1
4	O	173	LEU	3.1
3	J	557	HIS	3.1
3	J	601	ALA	3.1
1	A	255	ALA	3.1
5	Q	135	VAL	3.1
4	O	170	VAL	3.1
3	J	271	PHE	3.0
4	D	175	ASN	3.0
2	C	220	PHE	3.0
2	C	262	LEU	3.0
3	J	1069	TRP	3.0
3	B	557	HIS	3.0
1	A	266	TRP	3.0
1	I	132	LEU	3.0
5	Q	170	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
3	B	264	ASN	2.9
2	M	160	ILE	2.9
7	S	73	GLY	2.9
3	J	771	ASP	2.9
2	C	212	ASN	2.9
8	T	57	ALA	2.9
1	I	4	LYS	2.9
2	M	191	LEU	2.9
4	O	264	VAL	2.9
6	F	62	ILE	2.9
1	I	808	ASP	2.9
3	B	597	LEU	2.9
1	I	255	ALA	2.9
3	J	597	LEU	2.9
2	M	169	LEU	2.9
4	D	188	PHE	2.9
3	B	634	THR	2.9
1	I	60	THR	2.8
1	I	811	VAL	2.8
1	A	4	LYS	2.8
4	D	187	VAL	2.7
4	D	181	ASN	2.7
6	F	1	MET	2.7
7	S	80	GLU	2.7
5	E	127	ILE	2.7
2	C	191	LEU	2.7
5	Q	58	ILE	2.7
2	M	168	GLN	2.7
11	W	21	PHE	2.7
3	J	596	LYS	2.7
2	M	206	LEU	2.6
5	Q	180	LYS	2.6
1	I	807	VAL	2.6
2	C	151	ASN	2.6
3	J	602	ILE	2.6
6	F	2	SER	2.6
2	C	237	ILE	2.6
11	N	27	ALA	2.6
13	Y	41	ILE	2.6
3	B	1078	VAL	2.6
13	Z	41	ILE	2.6
1	A	808	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
5	Q	129	GLY	2.5
7	G	80	GLU	2.5
3	B	279	GLY	2.5
13	Z	39	GLN	2.5
2	C	196	PHE	2.5
2	C	201	SER	2.5
1	A	251	GLU	2.5
2	C	161	ALA	2.5
4	O	174	ALA	2.5
1	I	10	LYS	2.5
2	C	210	PHE	2.4
2	C	263	SER	2.4
2	C	217	ALA	2.4
4	O	213	CYS	2.4
5	E	178	THR	2.4
5	Q	117	THR	2.4
13	Y	48	THR	2.4
13	Y	80	SER	2.4
4	D	189	GLU	2.4
12	X	34	ILE	2.4
5	Q	171	LYS	2.4
12	X	30	GLY	2.4
2	M	167	LEU	2.4
7	G	114	ARG	2.3
10	V	3	ILE	2.3
6	F	89	MET	2.3
5	Q	174	TRP	2.3
3	J	792	LEU	2.3
7	G	6	ALA	2.3
3	B	766	PRO	2.3
3	B	948	THR	2.3
4	D	88	ASN	2.3
1	I	296	ARG	2.3
3	J	280	GLN	2.3
1	A	807	VAL	2.3
4	D	186	GLY	2.3
3	B	182	ASN	2.3
13	Z	56	ASN	2.3
4	O	212	TYR	2.3
2	M	161	ALA	2.2
3	B	592	GLU	2.2
4	O	142	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
13	Y	39	GLN	2.2
6	F	33	LEU	2.2
10	L	15	LEU	2.2
1	A	683	GLU	2.2
4	O	196	SER	2.2
3	B	54	PRO	2.2
2	M	232	LYS	2.2
1	I	292	GLY	2.2
3	J	207	ASP	2.2
3	J	224	VAL	2.2
12	P	33	ILE	2.2
13	Z	42	GLU	2.2
2	M	214	ASP	2.2
6	F	76	CYS	2.2
6	F	77	PRO	2.2
3	J	245	ASP	2.2
3	J	1082	HIS	2.2
2	C	184	VAL	2.1
2	C	183	ASP	2.1
2	M	241	ILE	2.1
2	M	155	SER	2.1
2	C	226	ILE	2.1
2	M	212	ASN	2.1
4	D	264	VAL	2.1
2	C	215	SER	2.1
3	B	1071	ASP	2.1
6	F	4	VAL	2.1
2	C	186	LYS	2.1
3	B	193	THR	2.1
6	R	32	ASN	2.1
13	Z	40	ASP	2.1
9	U	87	ILE	2.1
11	N	21	PHE	2.1
3	B	49	ILE	2.1
5	Q	176	THR	2.1
7	S	17	SER	2.0
3	B	367	TYR	2.0
6	F	32	ASN	2.0
3	B	53	ILE	2.0
3	B	317	TYR	2.0
5	Q	138	LYS	2.0
4	O	143	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	397	LEU	2.0
6	R	33	LEU	2.0
13	Z	54	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
14	ZN	I	1001	1/1	0.99	0.12	-1.27	57,57,57,57	0
14	ZN	A	1002	1/1	0.98	0.06	-1.37	69,69,69,69	0
16	F3S	D	1001	7/7	0.99	0.10	-1.39	79,81,82,84	0
14	ZN	X	1001	1/1	0.98	0.09	-1.40	54,54,54,54	0
16	F3S	O	1001	7/7	0.99	0.07	-1.41	104,105,106,106	0
14	ZN	A	1001	1/1	0.98	0.04	-1.81	46,46,46,46	0
14	ZN	I	1002	1/1	0.96	0.06	-1.91	78,78,78,78	0
14	ZN	N	1001	1/1	0.99	0.07	-1.95	56,56,56,56	0
14	ZN	P	1001	1/1	0.98	0.05	-1.98	33,33,33,33	0
14	ZN	B	2001	1/1	0.98	0.03	-2.19	66,66,66,66	0
14	ZN	J	2001	1/1	0.99	0.03	-2.35	124,124,124,124	0
14	ZN	W	1001	1/1	0.99	0.11	-4.74	63,63,63,63	0
15	MG	A	1003	1/1	0.98	0.05	-	2,2,2,2	0
15	MG	I	1003	1/1	0.99	0.03	-	2,2,2,2	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.