



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:41 PM GMT

PDB ID : 4FSX  
Title : crystal structure of Se-substituted Zea mays ZMET2 in complex with SAH  
Authors : Du, J.; Patel, D.J.  
Deposited on : 2012-06-27  
Resolution : 3.20 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

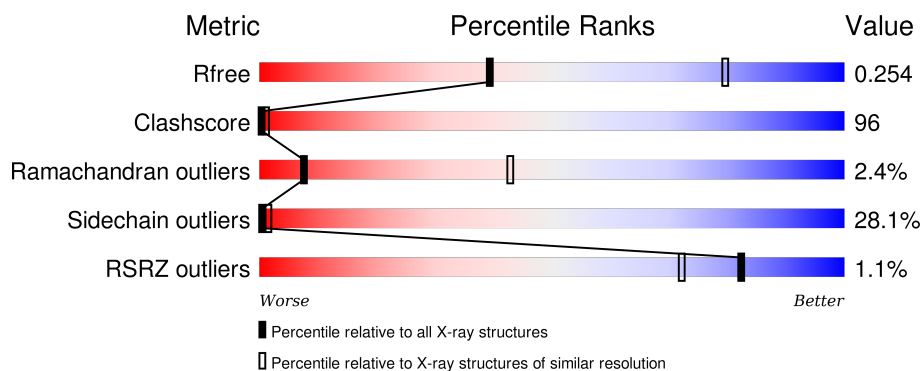
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	784	<div> <div></div> <div>21% 47% 17% • 13%</div> </div>
1	B	784	<div> <div></div> <div>19% 48% 18% • 14%</div> </div>

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
2	SAH	A	1000	-	-	-	X

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 10631 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.

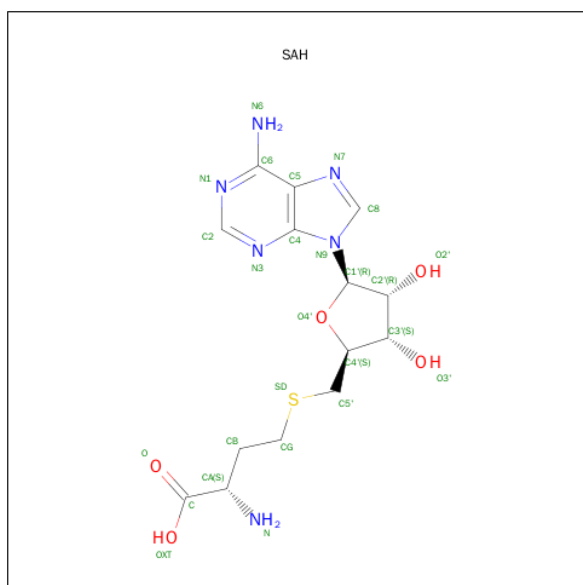
- Molecule 1 is a protein called DNA (cytosine-5)-methyltransferase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	680	Total	C	N	O	S	Se	0	0	0
			5331	3401	904	993	18	15			
1	B	675	Total	C	N	O	S	Se	0	0	0
			5248	3346	893	976	18	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	SER	-	EXPRESSION TAG	UNP Q9AXT8
B	129	SER	-	EXPRESSION TAG	UNP Q9AXT8

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula:  $C_{14}H_{20}N_6O_5S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

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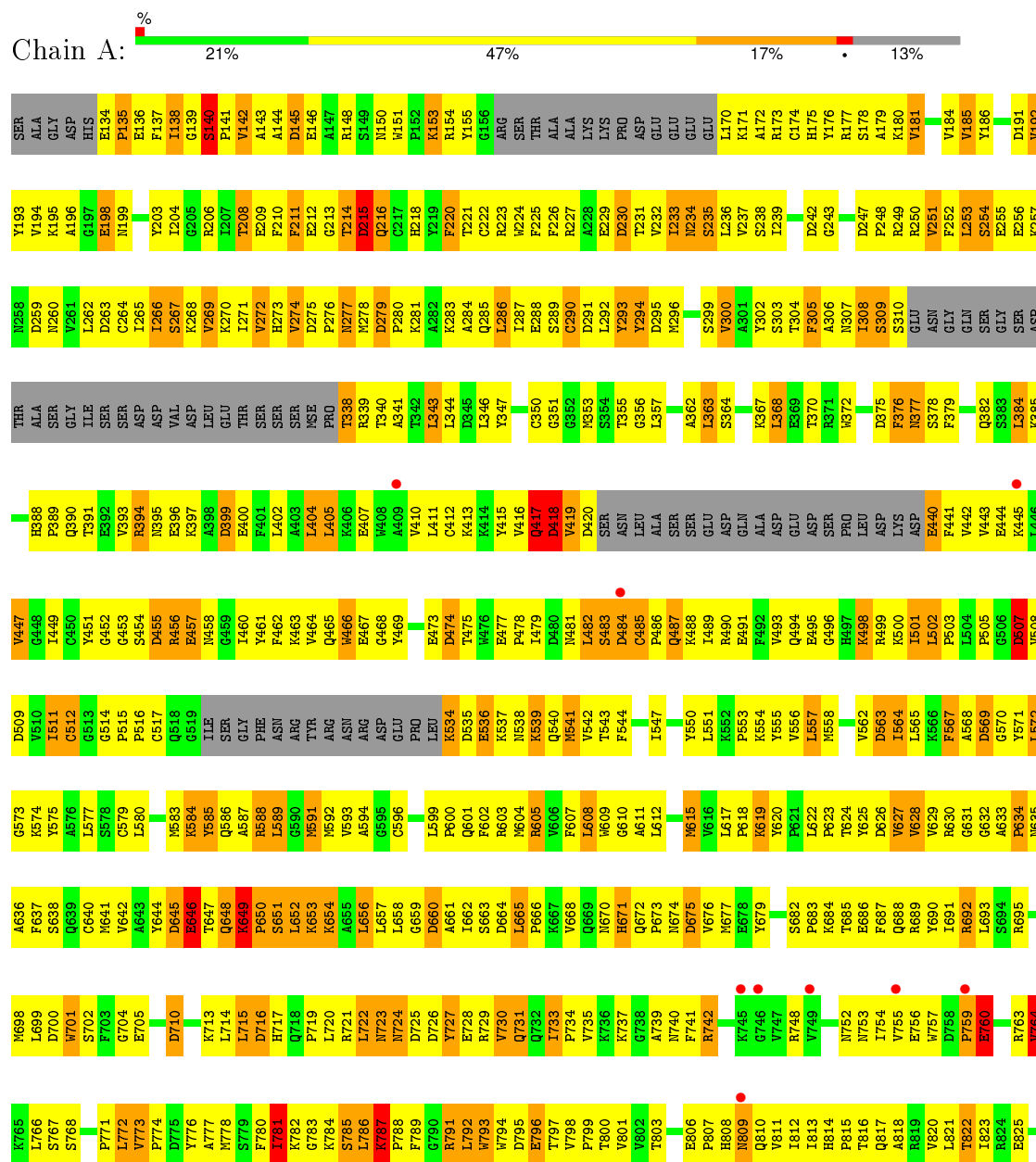
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

### 3 Residue-property plots

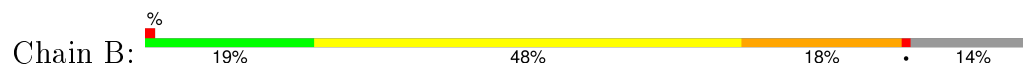
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 (cytosine-5)-methyltransferase 1



R828	ALA	GLN
L829	ALA	
Q830	ARG	
	ALA	
D834	SER	
Y835	PRO	
Y836	VAL	
Y837	GLY	
Y838	THR	
Y839	PRO	
	ALA	
L842	GLY	
L843	GLU	
E844	VAL	
K845	VAL	
L846	GLU	
L847	GLN	
Y848		
Y849		
G850		
G851		
A852		
Y853		
P856		
Y857		
L861		
Y862		
Y863		
Y864		
L865		
G866		
Y867		
A868		
Y869		
L870		
E874		
G875		
S876		
D877		
P878		
L879		
Y880		
Q881		
L882		
P883		
P884		
S885		
P886		
THR		
SER		
VAL		
GLY		
ANG		
THR		
ALA		
GLY		

• Molecule 1: DNA (cytosine-5)-methyltransferase 1



SER	Y192	L253	SER	A380	F441	P503	D563	A633	L693	L772	P833	ALA
ALA	Y193	S254	ASP	C381	V442	L504	I564	P634	S694	V773	D834	GLY
GLY	Y194	S255	THR	Q382	V443	P505	L565	M635	R695	P774	Y835	GLU
ASP	K195	E256	ALA	S383	E444	G506	G506	A636	R696	D775	VAL	VAL
	A196		GLY	L384	K445	V507	G570	F637	D697	Y776	R837	VAL
E134	G197	L262	SER	L385	L446	V508	Y571	S638	M698	A777	L838	GLU
P135	A198	D263	ILE	Y386	V447	D509	L572	Q639	L699	M778	F839	GLN
E136	E199	C264	SER	N387	G448	V510	G573	Q640	D700	S779	G840	
F137	E200	C265	SER	H388	L449	I511	A574	M641	W701	F780	P841	
Y138	A201	L266	ASP	P389	C450	G512	Y575	V642	S702	K781	L842	
G139	G202	K268	ASP	Q390	Y451	G513	A576	A643	F703	K782	K843	
S140	D203	K269	VAL	T391	G452	G514	L577	Y644		G783	E844	
P141	G204	L270	ASP	E392	G453	P515	C578	D645	D710	K784	K845	
V142	Y203	K271	LEU	E393	S454	P516	C579	E846		S785	Y846	
A143		L272	GLU	R394	D455	C517	L580	T647	K713	P788	L847	
A144	R206	I271	THR	N395	R456	Q518	V581	Q648	L714	F789	Q848	
L145	T208	V272	SER	P395	E457	G519	A582	K649	L715	G790		
E146	E209	K273	SER	K396	L460	G520	M583	P650	D716	R791		
A147	F210	V274	SER	F401	L461	G521	K584	S651	H717	L792		
A148	E211	D275	THR	E402	F462	G522	Y585	L652	Q718	L793		
S149	E212	F276	THR	F403	K463	A587	Q586	K653	P719	W794		
G150	G213	K277	THR	L402	L403	A588	Y589	A655	L720	Y795		
Y151	D214	K278	THR	L404	L405	A589	G590	L656	L721	E796		
P152	D215	P280	THR	L406	L407	A590	G591	L657	L722	T797		
K153	Q216	K281	THR	L408	L409	A591	G592	L658	L723	Y798		
R154	C217	A282	THR	K464	L410	A592	G593	L659	L724	P799		
Y155	H218	K283	THR	K465	L411	A593	G594	L660	L725	T800		
F156	Y219	K284	THR	K466	L412	A594	G595	L661	L726	Y801		
G157	F220	K285	THR	K467	L413	A595	G596	L662	L727	V802		
A157	Y221	K286	THR	K468	L414	A596	G597	L663	L728	T803		
SER	C222	K287	THR	K469	L415	A597	G598	L664	L729	R804		
THR	R223	K288	THR	K470	L416	A598	G599	L665	L730	A805		
ALA	W224	K289	THR	K471	L417	A599	G600	L666	L731	E806		
ALA	F225	K290	THR	K472	L418	A600	G601	L667	L732	P807		
LYS	F226	K291	THR	K473	L419	A601	G602	L668	L733	R808		
LYS	R227	K292	THR	K474	L420	A602	G603	L669	L734	H809		
PRO	A228	K293	THR	K475	L421	A603	G604	L670	L735	N809		
ASP	E229	K294	THR	K476	L422	A604	G605	L671	L736	Q810		
GLU	D230	K295	THR	K477	L423	A605	G606	L672	L737	V811		
GLU	T231	K296	THR	K478	L424	A606	G607	L673	L738	L812		
GLU	V232	K297	THR	K479	L425	A607	G608	L674	L739	I813		
GLU	N234	K298	THR	K480	L426	A608	G609	L675	L740	H814		
L170	L170	K299	THR	K481	L427	A609	G610	L676	L741	P815		
K171	S235	K300	THR	K482	L428	A610	G611	L677	L742	T816		
	L236	K301	THR	K483	L429	A611	G612	L678	L743	Q817		
C174	V237	K302	THR	K484	L430	A612	G613	L679	L744	A818		
H175	S238	K303	THR	K485	L431	A613	G614	L680	L745	M819		
Y176	I239	K304	THR	K486	L432	A614	G615	L681	L746	R819		
R177	S240	K305	THR	K487	L433	A615	G616	L682	L747	G820		
S178	V241	K306	THR	K488	L434	A616	G617	L683	L748	L821		
A179	D242	K307	THR	K489	L435	A617	G618	L684	L749	T822		
K180	G243	K308	THR	K490	L436	A618	G619	L685	L750	I823		
V181	H244	K309	THR	K491	L437	A619	G620	L686	L751	R824		
D182	K245	K310	THR	K492	L438	A620	G621	L687	L752	E825		
N183	H246	K311	THR	K493	L439	A621	G622	L688	L753	N826		
V184	D247	K312	THR	K494	L440	A622	G623	L689	L754	A827		
GLY	P248	K313	THR	K495	L441	A623	G624	L690	L755	R828		
ASN	D249	K314	THR	K496	L442	A624	G625	L691	L756	L829		
GLY	P249	K315	THR	K497	L443	A625	G626	L692	L757	S767		
GLY	R249	K316	THR	K498	L444	A626	G627	L693	L758	Q830		
GLY	R250	K317	THR	K499	L445	A627	G628	L694	L759	S768		
GLY	R251	K318	THR	K500	L446	A628	G629	L695	L760	G831		
GLY	F252	K319	THR	K501	L447	A629	G630	L696	L761	T832		
D191		K320	THR	K502	L448	A630	G631	L697	L762	F832		

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.86Å 88.95Å 113.49Å 93.47° 95.53° 110.41°	Depositor
Resolution (Å)	40.25 – 3.20 48.87 – 3.19	Depositor EDS
% Data completeness (in resolution range)	97.6 (40.25-3.20) 95.6 (48.87-3.19)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 3.19Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.1_743)	Depositor
R, $R_{free}$	0.240 , 0.263 0.233 , 0.254	Depositor DCC
$R_{free}$ test set	1937 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.9	Xtriage
Anisotropy	0.609	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 68.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 38702 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	10631	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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: SAH

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.64	0/5445	0.79	5/7358 (0.1%)
1	B	0.63	1/5362 (0.0%)	0.82	12/7252 (0.2%)
All	All	0.63	1/10807 (0.0%)	0.80	17/14610 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	579	CYS	CB-SG	-5.50	1.72	1.81

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	535	ASP	CB-CG-OD1	-9.04	110.17	118.30
1	A	632	GLY	N-CA-C	-8.60	91.61	113.10
1	B	535	ASP	N-CA-C	8.56	134.12	111.00
1	B	146	GLU	N-CA-C	-6.83	92.56	111.00
1	B	746	GLY	N-CA-C	-6.81	96.08	113.10
1	A	809	ASN	N-CA-C	6.74	129.18	111.00
1	B	680	GLY	N-CA-C	-6.54	96.76	113.10
1	B	699	LEU	CA-CB-CG	-6.52	100.31	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	810	GLN	N-CA-C	6.51	128.59	111.00
1	A	649	LYS	N-CA-C	-6.46	93.57	111.00
1	B	657	LEU	CA-CB-CG	-6.36	100.67	115.30
1	A	418	ASP	N-CA-C	-6.25	94.13	111.00
1	B	279	ASP	N-CA-CB	-6.17	99.50	110.60
1	B	139	GLY	N-CA-C	-5.96	98.19	113.10
1	B	279	ASP	C-N-CD	-5.96	107.49	120.60
1	B	589	LEU	CA-CB-CG	5.08	126.98	115.30
1	A	879	LEU	CB-CG-CD2	-5.05	102.41	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	ASP	Peptide
1	A	455	ASP	Peptide
1	A	507	ASP	Peptide
1	B	504	LEU	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	5331	0	5166	987	0
1	B	5248	0	5023	1014	0
2	A	26	0	19	6	0
2	B	26	0	19	6	0
All	All	10631	0	10227	1998	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 96.

All (1998) 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)
1:B:695:ARG:HG2	1:B:835:TYR:CD1	1.50	1.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:LEU:C	1:B:657:LEU:HD12	1.33	1.45
1:A:134:GLU:HB3	1:A:135:PRO:CD	1.43	1.38
1:B:883:PRO:CG	1:B:884:PRO:HD2	1.53	1.37
1:B:695:ARG:HG2	1:B:835:TYR:CE1	1.64	1.32
1:B:699:LEU:HD12	1:B:701:TRP:NE1	1.44	1.31
1:B:142:VAL:HG11	1:B:174:CYS:SG	1.75	1.26
1:B:883:PRO:HG2	1:B:884:PRO:CD	1.66	1.25
1:B:457:GLU:HB2	1:B:461:TYR:OH	1.35	1.24
1:A:134:GLU:CB	1:A:135:PRO:HD2	1.64	1.23
1:A:784:LYS:C	1:A:786:LEU:HD12	1.58	1.23
1:B:656:LEU:O	1:B:657:LEU:HD12	1.39	1.22
1:A:404:LEU:O	1:A:404:LEU:HD12	1.34	1.22
1:B:142:VAL:CG1	1:B:174:CYS:SG	2.29	1.20
1:A:784:LYS:CA	1:A:786:LEU:HD12	1.72	1.20
1:B:279:ASP:O	1:B:283:LYS:HG3	1.38	1.18
1:B:279:ASP:CB	1:B:280:PRO:HD3	1.74	1.17
1:A:822:THR:HG22	1:A:825:GLU:OE2	1.44	1.17
1:A:781:ILE:N	1:A:781:ILE:HD13	1.57	1.16
1:A:209:GLU:HB2	1:A:221:THR:CG2	1.75	1.16
1:A:273:HIS:HB2	1:A:294:TYR:CE2	1.81	1.15
1:B:699:LEU:HD12	1:B:701:TRP:CD1	1.82	1.15
1:B:279:ASP:HB3	1:B:280:PRO:HD3	1.23	1.14
1:A:456:ARG:HH21	1:A:456:ARG:HG2	1.04	1.14
1:B:604:MSE:SE	1:B:641:MSE:HE1	1.97	1.14
1:B:695:ARG:CG	1:B:695:ARG:HH11	1.59	1.14
1:B:134:GLU:OE1	1:B:135:PRO:HD3	1.44	1.14
1:A:664:ASP:O	1:A:664:ASP:OD1	1.66	1.13
1:A:780:PHE:HE2	1:A:809:ASN:ND2	1.45	1.13
1:A:273:HIS:HB2	1:A:294:TYR:HE2	1.00	1.12
1:B:691:ILE:CD1	1:B:833:PRO:HA	1.78	1.12
1:B:699:LEU:HD11	1:B:701:TRP:CD2	1.83	1.12
1:A:209:GLU:CB	1:A:221:THR:HG22	1.79	1.12
1:B:691:ILE:HD11	1:B:833:PRO:HA	1.13	1.12
1:A:412:CYS:O	1:A:416:VAL:HG23	1.46	1.11
1:B:148:ARG:HH11	1:B:148:ARG:HG2	1.07	1.11
1:B:772:LEU:O	1:B:773:VAL:HG22	1.47	1.11
1:B:227:ARG:HB2	1:B:230:ASP:OD2	1.48	1.11
1:B:837:ARG:HH11	1:B:837:ARG:HG3	1.14	1.11
1:A:250:ARG:NH1	1:A:252:PHE:HE2	1.48	1.10
1:B:883:PRO:HB2	1:B:884:PRO:HD3	1.25	1.10
1:A:879:LEU:HD22	1:A:879:LEU:N	1.67	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:ALA:HA	2:A:1000:SAH:OXT	1.49	1.09
1:A:195:LYS:NZ	1:A:264:CYS:HA	1.67	1.09
1:A:784:LYS:CB	1:A:786:LEU:CD1	2.30	1.09
1:B:206:ARG:HH11	1:B:206:ARG:HG3	0.98	1.09
1:B:645:ASP:O	1:B:646:GLU:HB3	1.45	1.09
1:A:440:GLU:HG2	1:A:441:PHE:H	1.09	1.09
1:B:667:LYS:HA	1:B:817:GLN:OE1	1.52	1.08
1:A:540:GLN:HA	1:A:540:GLN:NE2	1.47	1.08
1:B:226:PHE:CE2	1:B:254:SER:HB2	1.89	1.08
1:B:796:GLU:HG3	1:B:797:THR:H	1.19	1.08
1:A:781:ILE:HG12	1:A:786:LEU:HD21	1.34	1.08
1:B:143:ALA:O	1:B:144:ALA:HB3	1.54	1.07
1:A:279:ASP:HB2	1:A:280:PRO:HD2	1.31	1.07
1:B:649:LYS:HD2	1:B:652:LEU:HD12	1.36	1.07
1:A:154:ARG:HH22	1:A:209:GLU:CD	1.55	1.07
1:A:417:GLN:NE2	1:A:417:GLN:HA	1.66	1.07
1:B:685:THR:HG22	1:B:688:GLN:H	1.18	1.06
1:B:883:PRO:CB	1:B:884:PRO:CD	2.34	1.06
1:B:699:LEU:CD1	1:B:701:TRP:CD1	2.38	1.06
1:A:784:LYS:O	1:A:786:LEU:HD12	1.53	1.06
1:A:592:MSE:HE1	1:A:861:LEU:HD21	1.11	1.06
1:B:852:ALA:HA	2:B:1000:SAH:OXT	1.55	1.06
1:B:667:LYS:HG3	1:B:817:GLN:OE1	1.55	1.06
1:B:820:VAL:HG13	1:B:821:LEU:H	1.01	1.06
1:B:695:ARG:HG3	1:B:695:ARG:HH11	0.91	1.05
1:A:214:THR:O	1:A:215:ASP:HB2	1.55	1.05
1:A:209:GLU:HB3	1:A:221:THR:HG22	1.38	1.05
1:A:173:ARG:HH11	1:A:212:GLU:CD	1.56	1.05
1:A:733:ILE:CG2	1:A:791:ARG:HH21	1.68	1.05
1:B:134:GLU:OE1	1:B:134:GLU:HA	1.47	1.05
1:A:733:ILE:HG22	1:A:791:ARG:HH21	1.22	1.05
1:B:231:THR:OG1	1:B:233:ILE:HG23	1.55	1.05
1:B:278:MSE:HB3	1:B:282:ALA:HB3	1.39	1.05
1:A:478:PRO:HG2	1:A:481:ASN:HB2	1.06	1.05
1:B:791:ARG:HD2	1:B:792:LEU:H	1.16	1.05
1:A:154:ARG:HB3	1:A:170:LEU:HD23	1.34	1.04
1:A:250:ARG:NH1	1:A:252:PHE:CE2	2.24	1.04
1:B:699:LEU:CD1	1:B:701:TRP:CE2	2.41	1.04
1:B:748:ARG:CB	1:B:756:GLU:H	1.71	1.04
1:A:281:LYS:HA	1:A:284:ALA:HB3	1.37	1.04
1:B:685:THR:CG2	1:B:688:GLN:H	1.70	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:676:VAL:CG1	1:B:713:LYS:CE	2.36	1.03
1:A:652:LEU:O	1:A:653:LYS:C	1.96	1.03
1:B:656:LEU:C	1:B:657:LEU:CD1	2.27	1.03
1:B:676:VAL:HG13	1:B:713:LYS:CE	1.89	1.03
1:B:723:ASN:OD1	1:B:726:ASP:HB2	1.58	1.03
1:A:229:GLU:HG3	1:A:237:VAL:HG11	1.39	1.02
1:B:695:ARG:CG	1:B:835:TYR:CD1	2.43	1.02
1:B:676:VAL:HG13	1:B:713:LYS:HE2	1.41	1.02
1:A:596:CYS:HB3	1:A:623:PRO:HB3	1.39	1.02
1:A:273:HIS:CB	1:A:294:TYR:HE2	1.72	1.02
1:B:793:TRP:HB3	1:B:815:PRO:HB3	1.42	1.02
1:A:367:LYS:HE3	1:A:701:TRP:CH2	1.93	1.02
1:A:759:PRO:O	1:A:760:GLU:HB2	1.60	1.01
1:B:379:PHE:CD2	1:B:844:GLU:HG2	1.95	1.01
1:B:646:GLU:HG2	1:B:646:GLU:O	1.60	1.01
1:A:715:LEU:HD22	1:A:837:ARG:HG2	1.42	1.01
1:A:772:LEU:HD13	1:A:773:VAL:HG22	1.38	1.00
1:A:725:ASP:HA	1:A:766:LEU:CD1	1.90	1.00
1:B:339:ARG:HG2	1:B:339:ARG:HH11	1.23	1.00
1:B:772:LEU:C	1:B:774:PRO:CD	2.30	1.00
1:B:729:ARG:HH21	1:B:772:LEU:HA	1.25	1.00
1:A:879:LEU:HD22	1:A:879:LEU:H	1.17	0.99
1:B:695:ARG:HG2	1:B:835:TYR:HD1	1.16	0.99
1:A:541:MSE:SE	1:A:558:MSE:HE1	2.12	0.99
1:B:699:LEU:HD12	1:B:701:TRP:CE2	1.96	0.99
1:A:515:PRO:HG2	1:A:558:MSE:HE3	1.43	0.99
1:A:646:GLU:HA	1:A:646:GLU:OE2	1.58	0.99
1:B:883:PRO:HB2	1:B:884:PRO:CD	1.90	0.98
1:B:549:ALA:HA	1:B:583:MSE:HE2	1.43	0.98
1:A:803:THR:HA	1:A:850:GLY:HA3	1.39	0.98
1:A:300:VAL:O	1:A:300:VAL:HG23	1.63	0.98
1:B:691:ILE:HD11	1:B:833:PRO:CA	1.93	0.98
1:A:784:LYS:CB	1:A:786:LEU:HD11	1.93	0.98
1:B:206:ARG:CG	1:B:206:ARG:HH11	1.76	0.98
1:B:820:VAL:HG13	1:B:821:LEU:N	1.78	0.97
1:B:676:VAL:CG1	1:B:713:LYS:HE2	1.94	0.97
1:A:134:GLU:HB3	1:A:135:PRO:HD2	0.99	0.97
1:A:784:LYS:H	1:A:786:LEU:CD1	1.76	0.97
1:B:206:ARG:HG3	1:B:206:ARG:NH1	1.68	0.97
1:B:143:ALA:O	1:B:144:ALA:CB	2.12	0.97
1:B:134:GLU:CD	1:B:135:PRO:HD3	1.85	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:LEU:HD21	1:A:814:HIS:HE1	1.29	0.96
1:A:353:MSE:HB2	1:A:853:VAL:HG11	1.47	0.96
1:A:540:GLN:HA	1:A:540:GLN:HE21	1.25	0.96
1:B:445:LYS:O	1:B:446:LEU:HD23	1.65	0.96
1:B:773:VAL:N	1:B:774:PRO:HD2	1.79	0.95
1:A:784:LYS:CA	1:A:786:LEU:CD1	2.44	0.95
1:A:502:LEU:HD23	1:A:503:PRO:HD2	1.45	0.95
1:B:773:VAL:N	1:B:774:PRO:CD	2.29	0.95
1:B:518:GLN:HB2	1:B:537:LYS:HB3	1.48	0.95
1:A:787:LYS:N	1:A:788:PRO:HD3	1.81	0.95
1:A:727:TYR:HE2	1:A:731:GLN:OE1	1.48	0.95
1:B:685:THR:HG22	1:B:688:GLN:N	1.80	0.95
1:B:772:LEU:C	1:B:774:PRO:HD3	1.86	0.95
1:A:209:GLU:CB	1:A:221:THR:CG2	2.41	0.95
1:A:784:LYS:N	1:A:786:LEU:CD1	2.30	0.94
1:B:645:ASP:O	1:B:645:ASP:OD1	1.85	0.94
1:A:879:LEU:N	1:A:879:LEU:CD2	2.30	0.94
1:B:699:LEU:CD1	1:B:701:TRP:NE1	2.30	0.94
1:A:663:SER:HB3	1:A:688:GLN:HE22	1.31	0.94
1:B:379:PHE:HD2	1:B:844:GLU:HG2	1.30	0.94
1:B:814:HIS:CD2	1:B:816:THR:H	1.85	0.94
1:B:142:VAL:HG13	1:B:174:CYS:SG	2.06	0.94
1:B:279:ASP:CB	1:B:280:PRO:CD	2.43	0.94
1:A:589:LEU:HA	1:A:620:TYR:OH	1.68	0.94
1:A:220:PHE:H	1:A:220:PHE:HD2	1.14	0.94
1:B:226:PHE:HE2	1:B:254:SER:HB2	1.26	0.94
1:B:814:HIS:HD2	1:B:816:THR:H	1.10	0.93
1:B:699:LEU:HD23	1:B:699:LEU:O	1.68	0.93
1:A:714:LEU:HD21	1:A:717:HIS:HB2	1.48	0.93
1:A:404:LEU:C	1:A:404:LEU:HD12	1.72	0.93
1:A:772:LEU:O	1:A:774:PRO:HD3	1.68	0.93
1:A:220:PHE:CE2	1:A:260:ASN:HB2	2.03	0.93
1:A:772:LEU:HD13	1:A:773:VAL:H	1.33	0.93
1:A:764:VAL:HG21	1:A:772:LEU:HG	1.48	0.93
1:B:307:ASN:ND2	1:B:586:GLN:CD	2.22	0.93
1:B:355:THR:HG22	1:B:388:HIS:NE2	1.83	0.92
1:A:786:LEU:HB3	1:A:788:PRO:HD3	1.48	0.92
1:A:780:PHE:CE2	1:A:809:ASN:ND2	2.37	0.92
1:B:796:GLU:HG3	1:B:797:THR:N	1.79	0.92
1:A:605:ARG:HG2	1:A:605:ARG:HH11	1.31	0.92
1:A:154:ARG:CZ	1:A:170:LEU:HD21	1.98	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:695:ARG:CG	1:B:835:TYR:CE1	2.53	0.92
1:A:171:LYS:O	1:A:213:GLY:HA2	1.69	0.92
1:B:814:HIS:HD2	1:B:816:THR:N	1.66	0.92
1:A:668:VAL:H	1:A:817:GLN:HE22	1.01	0.92
1:A:572:LEU:HD22	1:A:572:LEU:H	1.35	0.92
1:B:685:THR:HG23	1:B:687:PHE:N	1.85	0.92
1:A:279:ASP:HB2	1:A:280:PRO:CD	1.99	0.92
1:B:833:PRO:HB2	1:B:835:TYR:CE2	2.04	0.92
1:B:562:VAL:HG21	1:B:604:MSE:HE3	1.51	0.92
1:A:605:ARG:HH11	1:A:605:ARG:CG	1.83	0.91
1:A:648:GLN:OE1	1:A:648:GLN:HA	1.67	0.91
1:A:781:ILE:N	1:A:781:ILE:CD1	2.30	0.91
1:A:668:VAL:H	1:A:817:GLN:NE2	1.67	0.91
1:A:151:TRP:HE1	1:A:175:HIS:CE1	1.87	0.91
1:A:478:PRO:CG	1:A:481:ASN:HB2	1.99	0.91
1:B:236:LEU:HD13	1:B:574:LYS:HB2	1.51	0.91
1:B:676:VAL:O	1:B:676:VAL:HG12	1.68	0.91
1:B:599:LEU:HD11	1:B:856:PRO:HG2	1.50	0.91
1:A:727:TYR:CE2	1:A:731:GLN:OE1	2.24	0.90
1:A:740:ASN:ND2	1:A:742:ARG:HG3	1.87	0.90
1:B:820:VAL:CG1	1:B:821:LEU:H	1.85	0.90
1:B:881:GLN:OE1	1:B:882:LEU:N	2.05	0.90
1:A:781:ILE:CG1	1:A:786:LEU:HD21	2.02	0.89
1:A:555:TYR:HE2	1:A:618:PRO:HD3	1.37	0.89
1:A:171:LYS:HB2	1:A:214:THR:HG23	1.54	0.89
1:A:415:TYR:CD2	1:A:490:ARG:HG2	2.08	0.89
1:A:154:ARG:NH2	1:A:209:GLU:CD	2.26	0.89
1:B:699:LEU:CD1	1:B:701:TRP:CG	2.56	0.89
1:A:784:LYS:CB	1:A:786:LEU:HD12	1.99	0.89
1:B:844:GLU:O	1:B:847:ILE:HG13	1.72	0.89
1:A:173:ARG:HH11	1:A:212:GLU:CG	1.86	0.89
1:A:644:TYR:CE2	1:A:649:LYS:HG3	2.07	0.89
1:B:279:ASP:CG	1:B:280:PRO:HD3	1.93	0.88
1:B:279:ASP:O	1:B:283:LYS:CG	2.20	0.88
1:A:879:LEU:H	1:A:879:LEU:CD2	1.84	0.88
1:A:444:GLU:O	1:A:488:LYS:HE3	1.73	0.88
1:B:695:ARG:HG3	1:B:695:ARG:NH1	1.63	0.88
1:B:279:ASP:HB3	1:B:280:PRO:CD	2.01	0.88
1:B:748:ARG:CB	1:B:756:GLU:N	2.36	0.88
1:A:379:PHE:CD2	1:A:844:GLU:HG2	2.09	0.88
1:A:195:LYS:HZ3	1:A:264:CYS:HA	1.35	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:PHE:CE2	1:B:254:SER:CB	2.55	0.88
1:A:236:LEU:HD13	1:A:574:LYS:HB2	1.54	0.88
1:B:883:PRO:CB	1:B:884:PRO:HD3	2.01	0.88
1:A:727:TYR:O	1:A:727:TYR:HD2	1.56	0.88
1:A:220:PHE:CD2	1:A:260:ASN:O	2.26	0.88
1:B:554:LYS:HD3	1:B:615:MSE:HE3	1.55	0.88
1:A:748:ARG:CB	1:A:755:VAL:HA	2.03	0.88
1:B:408:TRP:O	1:B:412:CYS:HB2	1.74	0.88
1:A:633:ALA:O	1:A:634:PRO:O	1.90	0.88
1:B:644:TYR:O	1:B:645:ASP:HB3	1.73	0.87
1:B:443:VAL:HG12	1:B:466:TRP:CE3	2.09	0.87
1:A:554:LYS:HB3	1:A:615:MSE:HE3	1.55	0.87
1:B:692:ARG:O	1:B:693:LEU:HD12	1.74	0.87
1:B:814:HIS:ND1	1:B:819:ARG:NH2	2.23	0.87
1:A:215:ASP:O	1:A:216:GLN:HG3	1.73	0.87
1:B:671:HIS:HD2	1:B:721:ARG:NH1	1.72	0.87
1:B:391:THR:CG2	1:B:392:GLU:N	2.37	0.87
1:A:599:LEU:HD11	1:A:856:PRO:HG2	1.55	0.87
1:B:695:ARG:HD3	1:B:700:ASP:CG	1.94	0.87
1:B:729:ARG:HH21	1:B:772:LEU:CA	1.85	0.87
1:A:577:LEU:HD22	1:A:589:LEU:HD21	1.54	0.87
1:A:725:ASP:HA	1:A:766:LEU:HD13	1.56	0.87
1:A:728:GLU:OE1	1:A:766:LEU:HD21	1.74	0.87
1:B:445:LYS:C	1:B:446:LEU:HD23	1.95	0.87
1:A:279:ASP:CB	1:A:280:PRO:CD	2.51	0.87
1:B:699:LEU:HD11	1:B:701:TRP:CG	2.08	0.87
1:B:657:LEU:HD12	1:B:657:LEU:N	1.70	0.86
1:B:619:LYS:HG3	1:B:880:TYR:HB2	1.57	0.86
1:B:791:ARG:CD	1:B:792:LEU:H	1.88	0.86
1:A:714:LEU:HD21	1:A:717:HIS:CB	2.04	0.86
1:B:714:LEU:HD21	1:B:717:HIS:HB2	1.55	0.86
1:A:672:GLN:NE2	1:A:674:ASN:HB2	1.90	0.86
1:B:699:LEU:CD1	1:B:701:TRP:CD2	2.56	0.86
1:A:822:THR:CG2	1:A:825:GLU:OE2	2.23	0.86
1:A:351:GLY:O	1:A:355:THR:HG23	1.74	0.86
1:A:174:CYS:SG	1:A:212:GLU:OE1	2.33	0.86
1:B:339:ARG:CG	1:B:339:ARG:HH11	1.87	0.86
1:B:690:TYR:O	1:B:693:LEU:HD13	1.75	0.86
1:A:209:GLU:HB2	1:A:221:THR:HG23	1.57	0.86
1:B:729:ARG:HE	1:B:773:VAL:HG22	1.41	0.86
1:B:456:ARG:HG2	1:B:456:ARG:HH21	1.40	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:596:CYS:HB3	1:B:623:PRO:HB3	1.56	0.86
1:B:212:GLU:OE1	1:B:216:GLN:HG2	1.75	0.85
1:B:837:ARG:NH1	1:B:837:ARG:HG3	1.88	0.85
1:A:136:GLU:OE2	1:A:137:PHE:HB2	1.75	0.85
1:B:140:SER:OG	1:B:141:PRO:HD3	1.77	0.85
1:B:791:ARG:HD2	1:B:792:LEU:N	1.91	0.85
1:A:154:ARG:HB3	1:A:170:LEU:CD2	2.06	0.85
1:A:772:LEU:CD1	1:A:773:VAL:HG22	2.06	0.85
1:A:725:ASP:HA	1:A:766:LEU:HD11	1.56	0.85
1:A:780:PHE:HE2	1:A:809:ASN:CG	1.80	0.85
1:A:478:PRO:HG2	1:A:481:ASN:CB	2.01	0.85
1:A:588:ARG:NH2	1:A:878:PRO:HA	1.91	0.85
1:B:656:LEU:O	1:B:657:LEU:CD1	2.23	0.85
1:B:695:ARG:HA	1:B:835:TYR:CE1	2.11	0.85
1:A:772:LEU:CD1	1:A:773:VAL:H	1.89	0.85
1:B:605:ARG:HG2	1:B:605:ARG:HH11	1.42	0.85
1:A:236:LEU:HD23	1:A:239:ILE:HD11	1.58	0.84
1:B:658:LEU:HB3	1:B:794:TRP:HA	1.58	0.84
1:B:814:HIS:CD2	1:B:817:GLN:H	1.95	0.84
1:A:134:GLU:HB3	1:A:135:PRO:HD3	1.55	0.84
1:A:787:LYS:HB3	1:A:811:VAL:HG12	1.59	0.84
1:A:665:LEU:HD13	1:A:665:LEU:O	1.74	0.84
1:B:534:LYS:NZ	1:B:535:ASP:HB2	1.91	0.84
1:A:440:GLU:HG2	1:A:441:PHE:N	1.92	0.84
1:B:676:VAL:HG22	1:B:713:LYS:HE2	1.60	0.84
1:A:353:MSE:HB2	1:A:853:VAL:CG1	2.06	0.84
1:A:659:GLY:O	1:A:663:SER:HB2	1.78	0.84
1:A:220:PHE:CD2	1:A:220:PHE:O	2.30	0.84
1:B:235:SER:OG	1:B:236:LEU:N	2.09	0.84
1:A:764:VAL:HG21	1:A:772:LEU:CD1	2.08	0.84
1:A:171:LYS:CB	1:A:214:THR:HG23	2.08	0.84
1:A:173:ARG:NH1	1:A:212:GLU:CG	2.40	0.84
1:A:764:VAL:HG21	1:A:772:LEU:CG	2.08	0.84
1:A:247:ASP:OD1	1:A:248:PRO:HD2	1.76	0.83
1:A:540:GLN:CA	1:A:540:GLN:NE2	2.30	0.83
1:B:466:TRP:HZ2	1:B:475:THR:HG22	1.42	0.83
1:A:186:TYR:CE2	1:A:265:ILE:HG21	2.13	0.83
1:B:695:ARG:HD3	1:B:700:ASP:CB	2.09	0.83
1:A:134:GLU:N	1:A:180:LYS:HZ2	1.76	0.83
1:A:668:VAL:HG21	1:A:677:MSE:HE1	1.61	0.83
1:B:774:PRO:HB3	1:B:778:MSE:CE	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:728:GLU:OE1	1:A:766:LEU:CD2	2.26	0.83
1:B:307:ASN:HD22	1:B:586:GLN:CD	1.79	0.83
1:A:173:ARG:NH1	1:A:212:GLU:HG2	1.91	0.83
1:B:193:TYR:CE1	1:B:269:VAL:HG13	2.14	0.83
1:A:154:ARG:NH1	1:A:211:PHE:CD2	2.47	0.83
1:B:676:VAL:CG1	1:B:713:LYS:HE3	2.08	0.83
1:B:879:LEU:HD22	1:B:879:LEU:H	1.42	0.83
1:B:379:PHE:HA	1:B:382:GLN:HG3	1.59	0.82
1:B:774:PRO:HB3	1:B:778:MSE:HE2	1.58	0.82
1:A:440:GLU:CG	1:A:441:PHE:H	1.92	0.82
1:A:624:THR:O	1:A:653:LYS:HG3	1.79	0.82
1:B:140:SER:CB	1:B:141:PRO:HD3	2.09	0.82
1:B:695:ARG:CG	1:B:835:TYR:HD1	1.85	0.82
1:A:449:ILE:HD13	1:A:462:PHE:CE1	2.15	0.82
1:B:880:TYR:CE2	1:B:881:GLN:O	2.33	0.82
1:B:236:LEU:O	1:B:239:ILE:HD11	1.79	0.82
1:B:667:LYS:CA	1:B:817:GLN:OE1	2.27	0.82
1:B:553:PRO:HD2	1:B:585:TYR:OH	1.80	0.82
1:B:222:CYS:SG	1:B:224:TRP:CH2	2.73	0.81
1:A:648:GLN:O	1:A:650:PRO:HD3	1.79	0.81
1:B:391:THR:HG23	1:B:392:GLU:N	1.92	0.81
1:B:685:THR:O	1:B:689:ARG:HG3	1.79	0.81
1:A:151:TRP:NE1	1:A:175:HIS:CE1	2.46	0.81
1:B:274:VAL:HG23	1:B:278:MSE:HG3	1.61	0.81
1:B:671:HIS:CD2	1:B:721:ARG:NH1	2.48	0.81
1:B:883:PRO:CG	1:B:884:PRO:CD	2.30	0.81
1:A:281:LYS:O	1:A:285:GLN:HG2	1.81	0.81
1:A:412:CYS:O	1:A:416:VAL:CG2	2.29	0.81
1:B:676:VAL:CG2	1:B:713:LYS:HE2	2.10	0.81
1:A:415:TYR:CD2	1:A:490:ARG:HA	2.16	0.81
1:A:484:ASP:N	1:A:484:ASP:OD1	2.11	0.81
1:A:456:ARG:NH2	1:A:456:ARG:HG2	1.79	0.81
1:B:134:GLU:CD	1:B:135:PRO:CD	2.48	0.81
1:A:784:LYS:O	1:A:786:LEU:CD1	2.29	0.81
1:A:220:PHE:HE2	1:A:260:ASN:C	1.84	0.81
1:A:564:ILE:HG22	1:A:565:LEU:HD23	1.62	0.81
1:B:817:GLN:HB3	1:B:819:ARG:HG2	1.63	0.80
1:A:291:ASP:O	1:A:292:LEU:HD23	1.81	0.80
1:A:733:ILE:HG22	1:A:791:ARG:NH2	1.96	0.80
1:B:484:ASP:O	1:B:486:PRO:HD3	1.81	0.80
1:B:279:ASP:OD1	1:B:280:PRO:N	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:646:GLU:OE2	1:B:647:THR:CG2	2.30	0.80
1:B:254:SER:OG	1:B:256:GLU:HB2	1.82	0.80
1:B:487:GLN:N	1:B:487:GLN:OE1	2.15	0.80
1:B:148:ARG:NH1	1:B:148:ARG:HG2	1.86	0.80
1:B:696:LYS:CD	1:B:696:LYS:O	2.30	0.80
1:A:792:LEU:HD23	1:A:792:LEU:N	1.96	0.80
1:B:410:VAL:HG13	1:B:411:LEU:H	1.47	0.80
1:B:828:ARG:HH21	1:B:828:ARG:HG3	1.46	0.80
1:B:577:LEU:O	1:B:581:VAL:HG12	1.81	0.80
1:A:415:TYR:HD2	1:A:490:ARG:HG2	1.45	0.80
1:B:447:VAL:O	1:B:447:VAL:CG2	2.30	0.80
1:B:440:GLU:OE1	1:B:440:GLU:CA	2.30	0.80
1:A:273:HIS:NE2	1:A:274:VAL:O	2.15	0.80
1:A:456:ARG:HD2	1:A:458:ASN:OD1	1.81	0.80
1:B:656:LEU:N	1:B:656:LEU:HD23	1.95	0.79
1:B:227:ARG:O	1:B:230:ASP:HB2	1.82	0.79
1:A:787:LYS:N	1:A:788:PRO:CD	2.45	0.79
1:B:362:ALA:CB	1:B:699:LEU:HD22	2.13	0.79
1:B:646:GLU:O	1:B:646:GLU:CG	2.30	0.79
1:B:696:LYS:CE	1:B:696:LYS:O	2.30	0.79
1:B:699:LEU:CD2	1:B:699:LEU:O	2.30	0.79
1:B:278:MSE:O	1:B:279:ASP:HB3	1.80	0.79
1:A:294:TYR:HD2	1:A:294:TYR:O	1.66	0.79
1:A:355:THR:HG22	1:A:388:HIS:NE2	1.97	0.79
1:B:699:LEU:HD11	1:B:701:TRP:CE2	2.13	0.79
1:A:417:GLN:HE21	1:A:417:GLN:HA	1.46	0.79
1:B:772:LEU:O	1:B:773:VAL:CG2	2.30	0.79
1:A:648:GLN:CA	1:A:648:GLN:OE1	2.30	0.79
1:A:204:ILE:O	1:A:224:TRP:HE3	1.65	0.79
1:A:375:ASP:OD2	1:A:376:PHE:N	2.16	0.79
1:A:154:ARG:HD3	1:A:172:ALA:HB2	1.63	0.79
1:A:671:HIS:HD2	1:A:721:ARG:NH1	1.80	0.78
1:B:833:PRO:CB	1:B:835:TYR:HE2	1.96	0.78
1:B:278:MSE:HB3	1:B:282:ALA:CB	2.12	0.78
1:B:134:GLU:HG3	1:B:135:PRO:HD2	1.63	0.78
1:B:667:LYS:CG	1:B:817:GLN:OE1	2.31	0.78
1:A:730:VAL:HG21	1:A:818:ALA:O	1.82	0.78
1:B:134:GLU:OE1	1:B:134:GLU:CA	2.30	0.78
1:B:772:LEU:CB	1:B:774:PRO:CD	2.61	0.78
1:B:657:LEU:CD1	1:B:657:LEU:N	2.41	0.78
1:B:239:ILE:HD13	1:B:578:SER:HB3	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:GLN:O	1:A:498:LYS:HD3	1.82	0.78
1:B:715:LEU:HD22	1:B:837:ARG:HG2	1.65	0.78
1:B:676:VAL:HG11	1:B:713:LYS:CE	2.14	0.78
1:B:554:LYS:HD3	1:B:615:MSE:CE	2.14	0.78
1:A:852:ALA:CA	2:A:1000:SAH:OXT	2.32	0.78
1:A:646:GLU:CA	1:A:646:GLU:OE2	2.30	0.78
1:B:457:GLU:HB2	1:B:461:TYR:HH	1.49	0.77
1:A:740:ASN:HD22	1:A:742:ARG:HG3	1.46	0.77
1:B:828:ARG:HH22	1:B:834:ASP:CG	1.87	0.77
1:B:278:MSE:SE	1:B:282:ALA:HB1	2.34	0.77
1:A:300:VAL:O	1:A:300:VAL:CG2	2.30	0.77
1:B:675:ASP:HA	1:B:718:GLN:NE2	1.99	0.77
1:A:569:ASP:N	1:A:569:ASP:OD2	2.17	0.77
1:B:723:ASN:OD1	1:B:726:ASP:CB	2.33	0.77
1:A:250:ARG:HH21	1:A:584:LYS:HE2	1.47	0.77
1:B:772:LEU:C	1:B:774:PRO:HD2	2.00	0.77
1:B:549:ALA:HA	1:B:583:MSE:CE	2.13	0.77
1:B:880:TYR:CG	1:B:881:GLN:N	2.52	0.77
1:B:279:ASP:CG	1:B:280:PRO:CD	2.52	0.77
1:A:671:HIS:CD2	1:A:721:ARG:NH1	2.53	0.77
1:A:784:LYS:N	1:A:786:LEU:HD12	1.96	0.77
1:A:685:THR:O	1:A:689:ARG:HG3	1.85	0.77
1:B:220:PHE:CD2	1:B:262:LEU:HA	2.20	0.77
1:A:220:PHE:HD2	1:A:260:ASN:O	1.67	0.77
1:A:154:ARG:HD2	1:A:175:HIS:NE2	2.00	0.77
1:B:142:VAL:CG1	1:B:175:HIS:H	1.98	0.77
1:A:866:GLY:O	1:A:870:LEU:HD12	1.85	0.77
1:A:309:SER:O	1:A:310:SER:CB	2.33	0.76
1:B:837:ARG:O	1:B:838:LEU:HD12	1.85	0.76
1:B:135:PRO:CG	1:B:135:PRO:O	2.30	0.76
1:A:690:TYR:O	1:A:693:LEU:HD13	1.86	0.76
1:A:338:THR:HG21	1:A:367:LYS:NZ	1.99	0.76
1:A:134:GLU:CB	1:A:135:PRO:CD	2.30	0.76
1:A:449:ILE:HD13	1:A:462:PHE:CZ	2.21	0.76
1:B:659:GLY:CA	1:B:794:TRP:HB3	2.15	0.76
1:A:294:TYR:O	1:A:294:TYR:CD2	2.37	0.76
1:B:729:ARG:NH2	1:B:772:LEU:HA	2.00	0.76
1:B:699:LEU:CG	1:B:699:LEU:O	2.30	0.76
1:A:728:GLU:CD	1:A:766:LEU:HG	2.06	0.76
1:A:883:PRO:HB2	1:A:884:PRO:HD3	1.67	0.76
1:B:821:LEU:HG	1:B:825:GLU:OE1	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:TRP:HZ2	1:A:475:THR:HG1	1.33	0.76
1:B:457:GLU:CB	1:B:461:TYR:OH	2.27	0.76
1:B:138:ILE:HG12	1:B:139:GLY:H	1.51	0.76
1:A:469:TYR:CE1	1:B:806:GLU:OE1	2.40	0.75
1:B:227:ARG:CB	1:B:230:ASP:OD2	2.29	0.75
1:B:676:VAL:HG13	1:B:713:LYS:HE3	1.65	0.75
1:A:487:GLN:HA	1:A:487:GLN:NE2	2.01	0.75
1:A:206:ARG:O	1:A:222:CYS:HB2	1.87	0.75
1:A:828:ARG:NH2	1:A:834:ASP:OD1	2.20	0.75
1:A:748:ARG:CB	1:A:756:GLU:H	1.99	0.75
1:B:671:HIS:ND1	1:B:673:PRO:HD3	2.00	0.75
1:B:413:LYS:HZ2	1:B:414:LYS:HG2	1.51	0.75
1:B:535:ASP:O	1:B:535:ASP:OD1	2.04	0.75
1:A:823:ILE:HD13	1:A:845:LYS:HG3	1.68	0.75
1:A:289:SER:O	1:A:289:SER:OG	2.00	0.75
1:B:833:PRO:CG	1:B:835:TYR:HE2	2.00	0.75
1:A:717:HIS:CE1	1:A:822:THR:HG21	2.22	0.75
1:A:277:ASN:N	1:A:277:ASN:OD1	2.15	0.75
1:A:728:GLU:OE1	1:A:766:LEU:HG	1.86	0.75
1:A:134:GLU:HB2	1:A:135:PRO:HD2	1.68	0.75
1:A:781:ILE:H	1:A:781:ILE:HD13	1.52	0.75
1:A:564:ILE:O	1:A:570:GLY:HA2	1.86	0.75
1:B:685:THR:HG23	1:B:687:PHE:H	1.51	0.74
1:A:195:LYS:CE	1:A:264:CYS:HA	2.15	0.74
1:A:766:LEU:HD23	1:A:768:SER:H	1.50	0.74
1:A:763:ARG:O	1:A:764:VAL:HG13	1.87	0.74
1:B:599:LEU:HD23	1:B:829:LEU:O	1.86	0.74
1:A:141:PRO:O	1:A:142:VAL:HG22	1.85	0.74
1:B:605:ARG:HG2	1:B:605:ARG:NH1	2.02	0.74
1:B:774:PRO:O	1:B:777:ALA:N	2.21	0.74
1:B:626:ASP:OD2	1:B:655:ALA:N	2.21	0.74
1:B:729:ARG:HD3	1:B:773:VAL:HG21	1.69	0.74
1:A:811:VAL:O	1:A:811:VAL:HG22	1.86	0.74
1:A:225:PHE:CE1	1:A:294:TYR:CD1	2.76	0.74
1:B:134:GLU:OE1	1:B:135:PRO:CD	2.29	0.74
1:B:811:VAL:O	1:B:811:VAL:HG22	1.87	0.74
1:A:780:PHE:HB3	1:A:786:LEU:HD22	1.69	0.74
1:B:134:GLU:CG	1:B:135:PRO:HD2	2.17	0.74
1:B:696:LYS:O	1:B:696:LYS:HD2	1.86	0.74
1:A:666:PRO:HG3	1:A:679:TYR:O	1.87	0.74
1:B:502:LEU:HD23	1:B:503:PRO:HD2	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:PHE:CE2	1:A:809:ASN:CG	2.61	0.74
1:A:663:SER:CB	1:A:688:GLN:HE22	2.00	0.74
1:A:249:ARG:O	1:A:249:ARG:HG3	1.87	0.74
1:A:662:ILE:O	1:A:665:LEU:HG	1.88	0.74
1:B:462:PHE:O	1:B:464:VAL:HG12	1.88	0.73
1:B:143:ALA:CB	1:B:147:ALA:HB2	2.18	0.73
1:A:214:THR:O	1:A:215:ASP:CB	2.35	0.73
1:A:635:ASN:OD1	1:A:636:ALA:N	2.20	0.73
1:B:695:ARG:HG2	1:B:835:TYR:HE1	1.46	0.73
1:B:820:VAL:CG1	1:B:821:LEU:N	2.44	0.73
1:B:273:HIS:HD2	1:B:274:VAL:N	1.85	0.73
1:A:692:ARG:O	1:A:693:LEU:HD12	1.89	0.73
1:A:668:VAL:N	1:A:817:GLN:HE22	1.83	0.73
1:B:879:LEU:HD22	1:B:879:LEU:N	2.03	0.73
1:A:883:PRO:HB2	1:A:884:PRO:CD	2.19	0.73
1:B:197:GLY:HA3	1:B:200:GLU:OE2	1.89	0.73
1:B:741:PHE:N	1:B:789:PHE:O	2.21	0.73
1:A:276:PRO:HG2	1:A:277:ASN:OD1	1.88	0.73
1:A:221:THR:HB	1:A:259:ASP:OD1	1.88	0.73
1:A:557:LEU:HD21	1:A:861:LEU:HD13	1.69	0.73
1:B:135:PRO:O	1:B:135:PRO:HG2	1.89	0.73
1:A:220:PHE:CE2	1:A:260:ASN:O	2.42	0.73
1:A:677:MSE:HG3	1:A:714:LEU:HD22	1.71	0.72
1:A:733:ILE:CG2	1:A:791:ARG:NH2	2.50	0.72
1:A:151:TRP:NE1	1:A:175:HIS:ND1	2.37	0.72
1:B:454:SER:O	1:B:456:ARG:HG3	1.88	0.72
1:B:484:ASP:OD1	1:B:485:CYS:N	2.22	0.72
1:A:154:ARG:NE	1:A:170:LEU:HD21	2.03	0.72
1:B:218:HIS:CB	1:B:262:LEU:HD11	2.19	0.72
1:A:838:LEU:C	1:A:839:PHE:HD1	1.93	0.72
1:A:557:LEU:HD12	1:A:558:MSE:N	2.05	0.72
1:A:812:ILE:HG23	1:A:820:VAL:HG22	1.71	0.72
1:B:791:ARG:CD	1:B:813:ILE:O	2.37	0.72
1:A:728:GLU:OE1	1:A:766:LEU:CG	2.37	0.72
1:B:443:VAL:O	1:B:488:LYS:HE2	1.89	0.72
1:B:249:ARG:NH2	1:B:287:ILE:O	2.21	0.72
1:B:231:THR:HG1	1:B:233:ILE:HG23	1.55	0.72
1:B:148:ARG:HB3	1:B:155:TYR:CD2	2.25	0.72
1:A:588:ARG:HH21	1:A:878:PRO:HA	1.52	0.72
1:A:837:ARG:HB3	1:A:839:PHE:HE1	1.54	0.72
1:A:515:PRO:HG2	1:A:558:MSE:CE	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:ARG:HD3	1:A:772:LEU:O	1.90	0.72
1:A:220:PHE:CE2	1:A:260:ASN:C	2.63	0.72
1:B:138:ILE:CG1	1:B:139:GLY:H	2.02	0.72
1:A:486:PRO:HB2	1:A:490:ARG:HD2	1.71	0.72
1:A:772:LEU:HD13	1:A:773:VAL:N	2.04	0.71
1:B:449:ILE:O	1:B:449:ILE:HG23	1.89	0.71
1:B:549:ALA:HB2	1:B:583:MSE:HE1	1.71	0.71
1:B:793:TRP:CB	1:B:815:PRO:HB3	2.19	0.71
1:B:819:ARG:O	1:B:820:VAL:HG12	1.90	0.71
1:B:181:VAL:HG12	1:B:186:TYR:OH	1.90	0.71
1:B:460:ILE:CD1	1:B:460:ILE:N	2.53	0.71
1:A:232:VAL:HG12	1:A:233:ILE:HG22	1.73	0.71
1:A:737:LYS:NZ	1:A:795:ASP:OD2	2.23	0.71
1:B:273:HIS:HB2	1:B:294:TYR:CE1	2.26	0.71
1:A:250:ARG:NH2	1:A:295:ASP:OD2	2.24	0.71
1:B:644:TYR:O	1:B:645:ASP:CB	2.36	0.71
1:B:143:ALA:HB3	1:B:147:ALA:HB2	1.72	0.71
1:A:724:ASN:O	1:A:728:GLU:HG3	1.89	0.71
1:A:605:ARG:NH1	1:A:605:ARG:HG2	1.99	0.71
1:B:814:HIS:N	1:B:820:VAL:O	2.22	0.71
1:A:442:VAL:HG13	1:A:467:GLU:HG3	1.71	0.71
1:A:138:ILE:HG23	1:A:139:GLY:N	2.05	0.71
1:A:215:ASP:C	1:A:216:GLN:CG	2.57	0.71
1:A:250:ARG:HH21	1:A:584:LYS:CE	2.04	0.71
1:B:226:PHE:HE2	1:B:254:SER:CB	1.96	0.71
1:A:670:ASN:ND2	1:A:722:LEU:HD22	2.06	0.71
1:B:518:GLN:NE2	1:B:518:GLN:HA	2.05	0.70
1:B:413:LYS:NZ	1:B:414:LYS:HG2	2.04	0.70
1:B:819:ARG:NH2	1:B:825:GLU:OE2	2.24	0.70
1:A:375:ASP:CG	2:A:1000:SAH:O2'	2.28	0.70
1:B:191:ASP:OD1	1:B:206:ARG:NH1	2.24	0.70
1:A:136:GLU:HG3	1:A:218:HIS:CE1	2.25	0.70
1:A:536:GLU:O	1:A:537:LYS:C	2.30	0.70
1:B:603:ARG:CZ	1:B:830:GLN:HE22	2.05	0.70
1:A:277:ASN:O	1:A:278:MSE:HG3	1.91	0.70
1:A:648:GLN:O	1:A:650:PRO:CD	2.40	0.70
1:B:440:GLU:C	1:B:440:GLU:OE1	2.30	0.70
1:A:695:ARG:HB3	1:A:700:ASP:HB3	1.73	0.70
1:B:646:GLU:OE2	1:B:647:THR:HG22	1.90	0.70
1:A:644:TYR:CD2	1:A:649:LYS:HG3	2.25	0.70
1:A:236:LEU:HD13	1:A:574:LYS:CB	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:GLU:OE1	1:A:221:THR:HG21	1.92	0.70
1:B:239:ILE:HD13	1:B:578:SER:CB	2.22	0.70
1:B:637:PHE:N	1:B:637:PHE:CD2	2.59	0.70
1:B:774:PRO:O	1:B:775:ASP:C	2.30	0.70
1:A:733:ILE:HG21	1:A:791:ARG:HH21	1.54	0.70
1:A:220:PHE:HE2	1:A:260:ASN:CB	2.04	0.70
1:B:467:GLU:O	1:B:469:TYR:CE2	2.45	0.70
1:A:215:ASP:O	1:A:216:GLN:CG	2.40	0.70
1:B:459:GLY:O	1:B:461:TYR:CD2	2.45	0.70
1:A:780:PHE:C	1:A:781:ILE:HD13	2.13	0.70
1:B:771:PRO:C	1:B:773:VAL:H	1.95	0.70
1:B:583:MSE:O	1:B:584:LYS:HB2	1.91	0.70
1:A:464:VAL:HG11	1:A:466:TRP:CH2	2.27	0.70
1:A:631:GLY:HA3	1:A:641:MSE:HE1	1.73	0.70
1:A:279:ASP:CB	1:A:280:PRO:HD2	2.12	0.69
1:A:220:PHE:CE2	1:A:260:ASN:CB	2.75	0.69
1:B:376:PHE:O	1:B:395:ASN:ND2	2.24	0.69
1:A:173:ARG:N	1:A:212:GLU:O	2.25	0.69
1:A:535:ASP:C	1:A:535:ASP:OD2	2.30	0.69
1:A:739:ALA:HB3	1:A:791:ARG:HG2	1.74	0.69
1:B:592:MSE:SE	1:B:861:LEU:HD21	2.42	0.69
1:B:339:ARG:HG2	1:B:339:ARG:NH1	1.96	0.69
1:A:727:TYR:O	1:A:727:TYR:CD2	2.45	0.69
1:A:649:LYS:O	1:A:649:LYS:HD3	1.93	0.69
1:A:140:SER:HB3	1:A:141:PRO:HD2	1.75	0.69
1:A:793:TRP:HB3	1:A:795:ASP:OD1	1.92	0.69
1:B:220:PHE:CE2	1:B:262:LEU:HA	2.27	0.69
1:A:793:TRP:CE3	1:A:793:TRP:HA	2.27	0.69
1:B:833:PRO:HB2	1:B:835:TYR:HE2	1.47	0.69
1:B:144:ALA:C	1:B:145:ASP:OD2	2.30	0.69
1:A:787:LYS:HB2	1:A:809:ASN:O	1.92	0.69
1:A:814:HIS:HD2	1:A:816:THR:H	1.41	0.69
1:B:440:GLU:OE1	1:B:440:GLU:HA	1.91	0.69
1:A:145:ASP:OD1	1:A:148:ARG:NH1	2.26	0.69
1:A:540:GLN:CA	1:A:540:GLN:HE21	1.89	0.69
1:A:274:VAL:HG23	1:A:295:ASP:HA	1.74	0.68
1:A:460:ILE:CG2	1:A:462:PHE:CE2	2.76	0.68
1:A:211:PHE:CD1	1:A:211:PHE:C	2.67	0.68
1:B:273:HIS:CD2	1:B:274:VAL:N	2.60	0.68
1:A:515:PRO:CG	1:A:558:MSE:HE3	2.21	0.68
1:B:700:ASP:OD1	1:B:702:SER:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ASP:O	1:A:395:ASN:HA	1.94	0.68
1:B:575:TYR:O	1:B:579:CYS:SG	2.50	0.68
1:B:404:LEU:HB2	1:B:451:TYR:HB3	1.75	0.68
1:A:154:ARG:HB2	1:A:171:LYS:HA	1.75	0.68
1:A:176:TYR:HE1	1:A:212:GLU:HG3	1.57	0.68
1:A:225:PHE:HE1	1:A:294:TYR:CD1	2.10	0.68
1:B:729:ARG:NE	1:B:773:VAL:HG22	2.08	0.68
1:A:464:VAL:CG1	1:A:466:TRP:CZ2	2.77	0.68
1:A:231:THR:OG1	1:A:233:ILE:HG23	1.93	0.68
1:A:668:VAL:CG2	1:A:677:MSE:HE1	2.24	0.68
1:B:215:ASP:O	1:B:216:GLN:HB2	1.94	0.68
1:B:802:VAL:HG12	1:B:804:ARG:H	1.59	0.68
1:B:805:ALA:HA	1:B:810:GLN:NE2	2.09	0.68
1:A:784:LYS:O	1:A:785:SER:C	2.30	0.68
1:A:253:LEU:HD12	1:A:294:TYR:CE1	2.29	0.68
1:B:467:GLU:O	1:B:469:TYR:CD2	2.47	0.68
1:B:222:CYS:SG	1:B:224:TRP:CZ3	2.87	0.68
1:A:227:ARG:HB2	1:A:230:ASP:OD2	1.94	0.68
1:B:658:LEU:O	1:B:659:GLY:C	2.30	0.67
1:B:685:THR:HG23	1:B:686:GLU:N	2.06	0.67
1:A:781:ILE:HG12	1:A:786:LEU:CD2	2.19	0.67
1:B:635:ASN:OD1	1:B:636:ALA:N	2.27	0.67
1:B:646:GLU:OE2	1:B:647:THR:CA	2.42	0.67
1:A:648:GLN:O	1:A:649:LYS:C	2.30	0.67
1:B:699:LEU:HG	1:B:701:TRP:CD1	2.29	0.67
1:A:641:MSE:HG3	1:A:642:VAL:N	2.08	0.67
1:A:142:VAL:HA	1:A:175:HIS:O	1.95	0.67
1:A:786:LEU:CB	1:A:788:PRO:HD3	2.22	0.67
1:B:443:VAL:HG12	1:B:466:TRP:HE3	1.56	0.67
1:A:714:LEU:C	1:A:714:LEU:HD23	2.15	0.67
1:A:204:ILE:O	1:A:224:TRP:CE3	2.47	0.67
1:B:771:PRO:C	1:B:773:VAL:N	2.46	0.67
1:B:667:LYS:HG3	1:B:817:GLN:CD	2.14	0.67
1:B:791:ARG:HG2	1:B:814:HIS:O	1.95	0.67
1:B:218:HIS:HB3	1:B:262:LEU:HD11	1.76	0.67
1:A:466:TRP:N	1:A:466:TRP:CD1	2.62	0.67
1:A:691:ILE:HG23	1:A:834:ASP:OD1	1.95	0.67
1:A:879:LEU:O	1:A:879:LEU:HD23	1.95	0.67
1:A:377:ASN:OD1	1:A:379:PHE:N	2.28	0.67
1:A:220:PHE:HE2	1:A:260:ASN:HB2	1.60	0.67
1:A:154:ARG:NH1	1:A:175:HIS:CE1	2.63	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:TYR:HB3	1:B:473:GLU:HB2	1.76	0.67
1:A:599:LEU:HD23	1:A:829:LEU:O	1.95	0.67
1:A:672:GLN:HE21	1:A:674:ASN:HB2	1.60	0.67
1:B:696:LYS:HE3	1:B:696:LYS:O	1.95	0.67
1:B:657:LEU:O	1:B:660:ASP:HB2	1.94	0.67
1:B:273:HIS:HB2	1:B:294:TYR:CZ	2.30	0.67
1:A:255:GLU:HG3	1:A:255:GLU:O	1.95	0.67
1:B:345:ASP:CG	1:B:348:SER:HB3	2.15	0.66
1:B:279:ASP:CG	1:B:280:PRO:N	2.47	0.66
1:B:646:GLU:OE2	1:B:647:THR:HA	1.96	0.66
1:A:651:SER:O	1:A:652:LEU:C	2.30	0.66
1:A:788:PRO:O	1:A:789:PHE:C	2.30	0.66
1:B:239:ILE:HD12	1:B:239:ILE:H	1.61	0.66
1:B:662:ILE:HG21	1:B:825:GLU:HB3	1.77	0.66
1:B:884:PRO:O	1:B:885:SER:C	2.34	0.66
1:B:599:LEU:HD23	1:B:601:GLN:HE21	1.59	0.66
1:A:729:ARG:HG3	1:A:729:ARG:HH11	1.60	0.66
1:A:289:SER:O	1:A:290:CYS:HB3	1.95	0.66
1:A:171:LYS:HB3	1:A:214:THR:CG2	2.25	0.66
1:A:690:TYR:CE1	1:A:698:MSE:SE	2.99	0.66
1:A:671:HIS:HD2	1:A:721:ARG:HH12	1.42	0.66
1:B:699:LEU:HG	1:B:699:LEU:O	1.94	0.66
1:A:220:PHE:CZ	1:A:260:ASN:HB2	2.31	0.66
1:A:449:ILE:HD11	1:A:460:ILE:HG23	1.77	0.66
1:A:874:GLU:HG3	1:A:875:GLY:H	1.61	0.66
1:B:344:LEU:HD12	1:B:372:TRP:HB2	1.78	0.66
1:B:235:SER:O	1:B:237:VAL:HG23	1.96	0.66
1:A:803:THR:CA	1:A:850:GLY:HA3	2.21	0.66
1:B:599:LEU:HD11	1:B:856:PRO:CG	2.22	0.66
1:B:447:VAL:O	1:B:447:VAL:HG22	1.96	0.66
1:B:648:GLN:O	1:B:650:PRO:HD3	1.96	0.66
1:A:171:LYS:O	1:A:213:GLY:CA	2.44	0.66
1:B:449:ILE:CG2	1:B:449:ILE:O	2.44	0.66
1:B:290:CYS:HB2	1:B:292:LEU:O	1.96	0.66
1:B:278:MSE:O	1:B:280:PRO:HD2	1.94	0.66
1:A:456:ARG:HH21	1:A:456:ARG:CG	1.93	0.66
1:A:498:LYS:HD3	1:A:498:LYS:H	1.61	0.66
1:B:677:MSE:O	1:B:714:LEU:HB3	1.96	0.65
1:B:226:PHE:CD2	1:B:254:SER:HB2	2.31	0.65
1:B:589:LEU:HA	1:B:620:TYR:OH	1.95	0.65
1:A:495:GLU:HA	1:A:495:GLU:OE1	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ARG:CD	1:A:172:ALA:HB2	2.26	0.65
1:B:806:GLU:H	1:B:810:GLN:HE21	1.44	0.65
1:B:286:LEU:O	1:B:289:SER:N	2.28	0.65
1:A:478:PRO:O	1:A:482:LEU:HD23	1.97	0.65
1:B:518:GLN:HB2	1:B:537:LYS:CB	2.24	0.65
1:A:465:GLN:HG3	1:A:474:ASP:OD1	1.96	0.65
1:B:275:ASP:HB2	1:B:276:PRO:HD2	1.78	0.65
1:A:154:ARG:CD	1:A:172:ALA:CB	2.74	0.65
1:B:235:SER:O	1:B:237:VAL:N	2.29	0.65
1:B:410:VAL:O	1:B:413:LYS:N	2.29	0.65
1:B:671:HIS:HE1	1:B:673:PRO:HB3	1.62	0.65
1:B:534:LYS:HZ2	1:B:535:ASP:HB2	1.60	0.65
1:A:464:VAL:HG11	1:A:466:TRP:CZ2	2.30	0.65
1:B:353:MSE:HE2	1:B:512:CYS:HB3	1.79	0.65
1:B:676:VAL:HG21	1:B:713:LYS:NZ	2.12	0.65
1:B:272:VAL:CG1	1:B:273:HIS:N	2.60	0.65
1:B:660:ASP:O	1:B:688:GLN:NE2	2.30	0.65
1:B:685:THR:CG2	1:B:688:GLN:N	2.45	0.65
1:B:549:ALA:CA	1:B:583:MSE:CE	2.75	0.65
1:A:309:SER:O	1:A:310:SER:HB3	1.96	0.65
1:A:752:ASN:C	1:A:754:ILE:H	2.00	0.65
1:B:686:GLU:HA	1:B:689:ARG:NH2	2.11	0.65
1:A:723:ASN:HD22	1:A:723:ASN:C	2.01	0.65
1:B:564:ILE:HG23	1:B:572:LEU:HB2	1.77	0.65
1:A:557:LEU:HD12	1:A:558:MSE:H	1.60	0.64
1:B:646:GLU:OE2	1:B:647:THR:N	2.30	0.64
1:A:145:ASP:CG	1:A:148:ARG:NH1	2.49	0.64
1:B:699:LEU:CG	1:B:701:TRP:CD1	2.79	0.64
1:A:541:MSE:HG3	1:A:541:MSE:O	1.95	0.64
1:B:347:TYR:CD2	1:B:516:PRO:HD3	2.32	0.64
1:B:648:GLN:N	1:B:648:GLN:OE1	2.30	0.64
1:B:413:LYS:HZ1	1:B:414:LYS:HE2	1.62	0.64
1:B:254:SER:HG	1:B:256:GLU:HB2	1.61	0.64
1:B:649:LYS:C	1:B:651:SER:H	2.00	0.64
1:B:388:HIS:HA	1:B:702:SER:HG	1.62	0.64
1:B:657:LEU:HB3	1:B:794:TRP:O	1.98	0.64
1:A:195:LYS:HG2	1:A:266:ILE:HD11	1.80	0.64
1:A:781:ILE:O	1:A:782:LYS:CB	2.44	0.64
1:A:585:TYR:CD1	1:A:610:GLY:O	2.50	0.64
1:B:626:ASP:OD2	1:B:655:ALA:HB2	1.98	0.64
1:B:883:PRO:HG2	1:B:884:PRO:HD2	0.71	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:LEU:C	1:A:839:PHE:CD1	2.71	0.64
1:A:279:ASP:OD1	1:A:279:ASP:N	2.29	0.64
1:A:729:ARG:CD	1:A:772:LEU:O	2.45	0.64
1:A:555:TYR:HE2	1:A:618:PRO:CD	2.10	0.64
1:B:508:VAL:CG1	1:B:511:ILE:HG22	2.28	0.64
1:A:592:MSE:HE2	1:A:620:TYR:CD1	2.33	0.64
1:A:631:GLY:CA	1:A:641:MSE:HE1	2.28	0.64
1:A:417:GLN:HE21	1:A:417:GLN:CA	2.09	0.64
1:A:376:PHE:CD2	1:A:376:PHE:C	2.70	0.64
1:B:229:GLU:HG3	1:B:237:VAL:HG21	1.79	0.64
1:A:490:ARG:O	1:A:494:GLN:HG3	1.98	0.64
1:B:804:ARG:O	1:B:810:GLN:NE2	2.30	0.63
1:A:287:ILE:HD12	1:A:288:GLU:N	2.13	0.63
1:A:603:ARG:CZ	1:A:830:GLN:HE22	2.10	0.63
1:B:466:TRP:NE1	1:B:473:GLU:O	2.31	0.63
1:B:695:ARG:CG	1:B:835:TYR:HE1	2.07	0.63
1:A:809:ASN:CG	1:A:809:ASN:O	2.35	0.63
1:A:664:ASP:OD1	1:A:828:ARG:NH1	2.29	0.63
1:A:247:ASP:OD1	1:A:248:PRO:CD	2.46	0.63
1:B:791:ARG:HG3	1:B:792:LEU:O	1.97	0.63
1:B:383:SER:HB3	1:B:838:LEU:HA	1.80	0.63
1:A:822:THR:HG22	1:A:825:GLU:CD	2.19	0.63
1:A:665:LEU:O	1:A:666:PRO:C	2.37	0.63
1:B:676:VAL:HG11	1:B:713:LYS:HE3	1.78	0.63
1:B:464:VAL:HG13	1:B:475:THR:O	1.99	0.63
1:A:884:PRO:O	1:A:885:SER:C	2.36	0.63
1:B:250:ARG:HH21	1:B:295:ASP:CG	2.01	0.63
1:B:349:GLY:HA2	1:B:380:ALA:HB1	1.80	0.63
1:A:727:TYR:C	1:A:727:TYR:CD2	2.67	0.63
1:B:687:PHE:O	1:B:690:TYR:N	2.31	0.63
1:B:469:TYR:HB3	1:B:473:GLU:CB	2.28	0.63
1:A:757:TRP:HZ3	1:A:773:VAL:CG2	2.11	0.63
1:A:469:TYR:HB3	1:A:473:GLU:HB2	1.80	0.63
1:B:540:GLN:OE1	1:B:540:GLN:HA	1.99	0.63
1:B:735:VAL:HG22	1:B:735:VAL:O	1.99	0.63
1:B:828:ARG:CG	1:B:828:ARG:HH21	2.12	0.63
1:B:348:SER:HA	2:B:1000:SAH:N	2.13	0.63
1:B:659:GLY:N	1:B:794:TRP:HB3	2.13	0.63
1:B:802:VAL:CG1	1:B:803:THR:N	2.62	0.62
1:A:664:ASP:OD2	1:A:692:ARG:NH1	2.32	0.62
1:B:609:TRP:CD1	1:B:620:TYR:CE1	2.86	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:691:ILE:O	1:B:691:ILE:HD12	1.99	0.62
1:A:726:ASP:OD1	1:A:729:ARG:NH1	2.32	0.62
1:B:448:GLY:O	1:B:462:PHE:HA	1.99	0.62
1:A:555:TYR:CE2	1:A:618:PRO:HD3	2.26	0.62
1:B:847:ILE:HD12	1:B:848:GLN:N	2.13	0.62
1:A:138:ILE:HG21	1:A:178:SER:HB2	1.79	0.62
1:A:137:PHE:CE2	1:A:218:HIS:HB3	2.34	0.62
1:A:668:VAL:O	1:A:817:GLN:NE2	2.33	0.62
1:B:578:SER:HA	1:B:581:VAL:CG1	2.29	0.62
1:B:648:GLN:N	1:B:648:GLN:CD	2.49	0.62
1:B:572:LEU:HD12	1:B:572:LEU:H	1.64	0.62
1:A:587:ALA:HA	1:A:609:TRP:O	1.99	0.62
1:B:549:ALA:HB2	1:B:583:MSE:CE	2.28	0.62
1:B:364:SER:CB	1:B:866:GLY:HA3	2.29	0.62
1:B:714:LEU:HD23	1:B:715:LEU:N	2.15	0.62
1:B:792:LEU:CD2	1:B:796:GLU:HB3	2.29	0.62
1:A:171:LYS:CB	1:A:214:THR:CG2	2.77	0.62
1:B:135:PRO:CD	1:B:135:PRO:O	2.48	0.62
1:B:440:GLU:CG	1:B:440:GLU:O	2.44	0.62
1:A:242:ASP:OD1	1:A:243:GLY:N	2.32	0.62
1:A:788:PRO:HA	1:A:808:HIS:O	1.98	0.62
1:B:445:LYS:O	1:B:446:LEU:CD2	2.43	0.62
1:B:464:VAL:HG21	1:B:466:TRP:CH2	2.35	0.62
1:B:411:LEU:C	1:B:411:LEU:HD23	2.20	0.62
1:B:733:ILE:HG13	1:B:734:PRO:HD2	1.82	0.62
1:A:727:TYR:C	1:A:727:TYR:HD2	2.02	0.62
1:A:541:MSE:SE	1:A:558:MSE:CE	2.94	0.62
1:A:776:TYR:CD2	1:A:777:ALA:N	2.68	0.62
1:B:833:PRO:HB2	1:B:835:TYR:CD2	2.34	0.62
1:B:272:VAL:HG12	1:B:273:HIS:N	2.14	0.62
1:A:710:ASP:HB3	1:A:715:LEU:HD21	1.82	0.62
1:B:772:LEU:O	1:B:774:PRO:HD3	1.98	0.62
1:B:813:ILE:HA	1:B:820:VAL:HA	1.82	0.62
1:A:784:LYS:H	1:A:786:LEU:HD13	1.62	0.62
1:A:225:PHE:CE1	1:A:294:TYR:HD1	2.18	0.62
1:A:449:ILE:HD12	1:A:461:TYR:O	2.00	0.62
1:B:648:GLN:OE1	1:B:648:GLN:CA	2.48	0.62
1:B:343:LEU:HD12	1:B:344:LEU:H	1.65	0.61
1:A:154:ARG:HD3	1:A:172:ALA:CB	2.29	0.61
1:A:195:LYS:HG2	1:A:266:ILE:CD1	2.31	0.61
1:A:254:SER:OG	1:A:256:GLU:HB2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:LEU:C	1:A:879:LEU:HD23	2.19	0.61
1:A:579:CYS:O	1:A:583:MSE:HG3	2.00	0.61
1:A:787:LYS:H	1:A:788:PRO:HD3	1.65	0.61
1:B:791:ARG:HD3	1:B:813:ILE:O	2.00	0.61
1:B:805:ALA:HA	1:B:810:GLN:HE22	1.65	0.61
1:B:821:LEU:CG	1:B:825:GLU:OE1	2.48	0.61
1:A:249:ARG:O	1:A:293:TYR:HE2	1.82	0.61
1:B:601:GLN:OE1	1:B:801:VAL:HG12	2.00	0.61
1:A:280:PRO:O	1:A:281:LYS:HB2	2.01	0.61
1:A:377:ASN:C	1:A:377:ASN:OD1	2.38	0.61
1:B:570:GLY:O	1:B:574:LYS:HG2	2.01	0.61
1:A:664:ASP:CG	1:A:692:ARG:HH11	2.03	0.61
1:A:250:ARG:NH1	1:A:252:PHE:CZ	2.67	0.61
1:A:453:GLY:O	1:A:456:ARG:HB2	1.99	0.61
1:B:236:LEU:O	1:B:239:ILE:CD1	2.48	0.61
1:B:589:LEU:HD23	1:B:608:LEU:HD12	1.83	0.61
1:B:153:LYS:O	1:B:171:LYS:NZ	2.28	0.61
1:A:272:VAL:O	1:A:293:TYR:HA	2.00	0.61
1:B:549:ALA:CB	1:B:583:MSE:CE	2.79	0.61
1:B:443:VAL:HG12	1:B:466:TRP:CZ3	2.35	0.61
1:B:671:HIS:HD2	1:B:721:ARG:CZ	2.13	0.61
1:A:726:ASP:HA	1:A:729:ARG:HH11	1.65	0.61
1:A:415:TYR:HD2	1:A:490:ARG:HA	1.65	0.61
1:B:695:ARG:CG	1:B:695:ARG:NH1	2.30	0.61
1:A:584:LYS:HB3	1:A:584:LYS:HZ3	1.65	0.61
1:B:714:LEU:CD2	1:B:717:HIS:HB2	2.28	0.60
1:A:663:SER:OG	1:A:684:LYS:HE2	2.01	0.60
1:B:250:ARG:NH2	1:B:295:ASP:OD2	2.29	0.60
1:A:407:GLU:O	1:A:411:LEU:HD13	2.01	0.60
1:B:675:ASP:OD1	1:B:675:ASP:N	2.34	0.60
1:B:710:ASP:OD2	1:B:837:ARG:NH1	2.34	0.60
1:B:273:HIS:CD2	1:B:273:HIS:C	2.74	0.60
1:A:791:ARG:NH1	1:A:815:PRO:O	2.34	0.60
1:A:338:THR:HB	1:A:367:LYS:HD3	1.82	0.60
1:B:880:TYR:CZ	1:B:881:GLN:O	2.53	0.60
1:B:181:VAL:CG1	1:B:186:TYR:OH	2.49	0.60
1:A:154:ARG:CZ	1:A:175:HIS:CE1	2.83	0.60
1:A:700:ASP:O	1:A:702:SER:N	2.34	0.60
1:A:601:GLN:NE2	1:A:830:GLN:OE1	2.34	0.60
1:A:580:LEU:HD22	1:A:608:LEU:CD2	2.31	0.60
1:A:726:ASP:HA	1:A:729:ARG:NH1	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:VAL:O	1:B:488:LYS:CE	2.49	0.60
1:B:772:LEU:CB	1:B:774:PRO:HD3	2.31	0.60
1:A:652:LEU:O	1:A:654:LYS:N	2.34	0.60
1:B:445:LYS:HB3	1:B:465:GLN:HB2	1.82	0.60
1:B:138:ILE:CG1	1:B:139:GLY:N	2.65	0.60
1:A:410:VAL:O	1:A:413:LYS:HB3	2.01	0.60
1:B:740:ASN:HA	1:B:789:PHE:O	2.01	0.60
1:A:154:ARG:HH12	1:A:211:PHE:HD2	1.45	0.60
1:B:649:LYS:O	1:B:651:SER:N	2.30	0.60
1:A:792:LEU:H	1:A:792:LEU:HD23	1.67	0.60
1:A:772:LEU:H	1:A:772:LEU:HD12	1.66	0.60
1:A:344:LEU:HD12	1:A:372:TRP:HB2	1.84	0.60
1:A:338:THR:HG21	1:A:367:LYS:HZ3	1.66	0.60
1:B:405:LEU:HD21	1:B:503:PRO:HG2	1.84	0.60
1:A:379:PHE:HD2	1:A:844:GLU:HG2	1.63	0.60
1:A:394:ARG:NE	1:A:396:GLU:OE1	2.34	0.60
1:B:649:LYS:HD2	1:B:652:LEU:CD1	2.21	0.60
1:B:785:SER:O	1:B:788:PRO:CD	2.50	0.59
1:B:833:PRO:CB	1:B:835:TYR:CE2	2.76	0.59
1:A:226:PHE:O	1:A:251:VAL:HG12	2.02	0.59
1:B:604:MSE:O	1:B:605:ARG:NH1	2.35	0.59
1:A:763:ARG:NH1	1:A:771:PRO:CB	2.64	0.59
1:A:384:LEU:HD13	1:A:388:HIS:HD2	1.67	0.59
1:B:459:GLY:O	1:B:461:TYR:CE2	2.55	0.59
1:A:780:PHE:O	1:A:783:GLY:N	2.29	0.59
1:A:698:MSE:C	1:A:699:LEU:HD12	2.22	0.59
1:B:646:GLU:C	1:B:646:GLU:OE2	2.41	0.59
1:A:657:LEU:HD23	1:A:795:ASP:HA	1.84	0.59
1:B:790:GLY:O	1:B:811:VAL:HA	2.01	0.59
1:B:830:GLN:HA	1:B:830:GLN:OE1	2.01	0.59
1:B:676:VAL:CG2	1:B:713:LYS:CE	2.80	0.59
1:B:410:VAL:HG13	1:B:411:LEU:N	2.16	0.59
1:B:561:VAL:HG23	1:B:563:ASP:H	1.65	0.59
1:B:734:PRO:O	1:B:735:VAL:CG1	2.51	0.59
1:A:469:TYR:HE1	1:B:806:GLU:OE1	1.85	0.59
1:B:586:GLN:NE2	1:B:615:MSE:O	2.35	0.59
1:A:498:LYS:HD3	1:A:498:LYS:N	2.17	0.59
1:B:170:LEU:HD21	1:B:211:PHE:CE1	2.37	0.59
1:B:343:LEU:HD13	1:B:510:VAL:HB	1.85	0.59
1:B:788:PRO:CB	1:B:808:HIS:O	2.50	0.59
1:B:362:ALA:HB1	1:B:699:LEU:HD22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ARG:HB3	1:B:155:TYR:CE2	2.37	0.59
1:A:664:ASP:OD2	1:A:683:PRO:HA	2.02	0.59
1:A:279:ASP:CB	1:A:280:PRO:HD3	2.32	0.59
1:B:414:LYS:O	1:B:415:TYR:HB2	2.03	0.59
1:A:737:LYS:HE3	1:A:796:GLU:OE1	2.02	0.59
1:B:649:LYS:CD	1:B:652:LEU:HD12	2.24	0.59
1:B:196:ALA:HB1	1:B:203:TYR:CZ	2.37	0.59
1:A:544:PHE:CD1	1:A:558:MSE:SE	3.06	0.59
1:A:752:ASN:C	1:A:754:ILE:N	2.53	0.59
1:B:246:HIS:CE1	1:B:582:ALA:HB2	2.36	0.59
1:B:475:THR:HG23	1:B:477:GLU:HG2	1.84	0.59
1:B:484:ASP:C	1:B:486:PRO:HD3	2.21	0.59
1:B:212:GLU:HG3	1:B:216:GLN:HA	1.85	0.59
1:B:553:PRO:HD2	1:B:585:TYR:HH	1.67	0.59
1:B:686:GLU:HA	1:B:689:ARG:HH21	1.67	0.59
1:A:211:PHE:CD1	1:A:211:PHE:O	2.56	0.59
1:B:454:SER:OG	1:B:455:ASP:N	2.36	0.59
1:B:453:GLY:O	1:B:456:ARG:HG2	2.03	0.59
1:A:362:ALA:HB1	1:A:699:LEU:HD22	1.84	0.59
1:A:823:ILE:HD11	1:A:842:ILE:HG23	1.84	0.59
1:B:227:ARG:N	1:B:230:ASP:OD2	2.29	0.59
1:A:580:LEU:HD22	1:A:608:LEU:HD21	1.84	0.59
1:A:586:GLN:NE2	1:A:615:MSE:O	2.35	0.59
1:B:830:GLN:HB3	1:B:832:PHE:HD2	1.68	0.58
1:B:772:LEU:CA	1:B:774:PRO:HD2	2.33	0.58
1:B:233:ILE:CG1	1:B:233:ILE:O	2.50	0.58
1:B:881:GLN:HA	1:B:881:GLN:OE1	2.03	0.58
1:B:285:GLN:O	1:B:288:GLU:HB2	2.02	0.58
1:B:791:ARG:HG2	1:B:814:HIS:C	2.23	0.58
1:B:209:GLU:HB2	1:B:221:THR:CG2	2.34	0.58
1:B:278:MSE:CB	1:B:282:ALA:HB3	2.26	0.58
1:A:280:PRO:O	1:A:280:PRO:CG	2.51	0.58
1:B:542:VAL:O	1:B:546:ASP:OD1	2.21	0.58
1:A:772:LEU:CD1	1:A:773:VAL:N	2.64	0.58
1:A:347:TYR:CD1	1:A:515:PRO:HA	2.38	0.58
1:B:233:ILE:HG13	1:B:233:ILE:O	2.03	0.58
1:B:648:GLN:CD	1:B:648:GLN:H	2.05	0.58
1:A:562:VAL:HG21	1:A:604:MSE:SE	2.53	0.58
1:B:375:ASP:OD1	2:B:1000:SAH:O2'	2.21	0.58
1:B:343:LEU:HD21	1:B:512:CYS:SG	2.43	0.58
1:B:207:ILE:HD11	1:B:209:GLU:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:MSE:CG	1:A:714:LEU:HD22	2.33	0.58
1:A:220:PHE:CD2	1:A:220:PHE:N	2.59	0.58
1:B:387:ASN:H	1:B:387:ASN:HD22	1.51	0.58
1:A:413:LYS:CG	1:A:420:ASP:HB3	2.34	0.58
1:B:728:GLU:HA	1:B:731:GLN:NE2	2.17	0.58
1:A:281:LYS:HA	1:A:284:ALA:CB	2.24	0.58
1:A:367:LYS:HE3	1:A:701:TRP:HH2	1.64	0.58
1:A:364:SER:CB	1:A:866:GLY:HA3	2.34	0.58
1:A:341:ALA:O	1:A:368:LEU:HD23	2.04	0.58
1:A:146:GLU:O	1:A:150:ASN:N	2.24	0.58
1:A:416:VAL:O	1:A:417:GLN:NE2	2.30	0.58
1:A:195:LYS:CG	1:A:266:ILE:HD11	2.33	0.58
1:B:664:ASP:HB2	1:B:688:GLN:OE1	2.04	0.58
1:B:342:THR:HB	1:B:371:ARG:HG3	1.85	0.58
1:A:567:PHE:HD2	1:A:572:LEU:HD21	1.68	0.58
1:B:649:LYS:C	1:B:651:SER:N	2.57	0.58
1:B:508:VAL:HG21	1:B:551:LEU:HD13	1.86	0.58
1:A:572:LEU:CD2	1:A:572:LEU:H	2.11	0.58
1:A:729:ARG:HG3	1:A:729:ARG:NH1	2.17	0.58
1:B:590:GLY:HA2	1:B:640:CYS:HB3	1.86	0.58
1:A:600:PRO:HG2	1:A:661:ALA:HB2	1.85	0.58
1:B:504:LEU:O	1:B:507:ASP:N	2.29	0.58
1:B:142:VAL:HG12	1:B:175:HIS:H	1.68	0.58
1:B:485:CYS:HB3	1:B:488:LYS:HD2	1.84	0.58
1:B:534:LYS:C	1:B:534:LYS:HZ3	2.07	0.58
1:B:621:PRO:HG3	1:B:860:ALA:HB1	1.86	0.58
1:A:814:HIS:CD2	1:A:816:THR:H	2.22	0.57
1:B:732:GLN:HG3	1:B:732:GLN:O	2.02	0.57
1:A:154:ARG:HH22	1:A:209:GLU:CG	2.15	0.57
1:A:215:ASP:C	1:A:216:GLN:HG3	2.20	0.57
1:B:599:LEU:CD1	1:B:856:PRO:HG2	2.27	0.57
1:A:186:TYR:HE2	1:A:265:ILE:HG21	1.66	0.57
1:A:464:VAL:O	1:A:474:ASP:CG	2.42	0.57
1:B:685:THR:HG21	1:B:687:PHE:HB3	1.85	0.57
1:A:226:PHE:HB2	1:A:252:PHE:O	2.04	0.57
1:A:250:ARG:HG3	1:A:293:TYR:CZ	2.38	0.57
1:B:440:GLU:O	1:B:440:GLU:CD	2.42	0.57
1:A:781:ILE:HG12	1:A:786:LEU:HD11	1.85	0.57
1:A:670:ASN:HD21	1:A:722:LEU:HD22	1.68	0.57
1:B:741:PHE:HB3	1:B:789:PHE:HB2	1.87	0.57
1:A:786:LEU:HB3	1:A:788:PRO:CD	2.27	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:LEU:HB2	1:B:451:TYR:CB	2.33	0.57
1:B:456:ARG:HH21	1:B:456:ARG:CG	2.16	0.57
1:A:220:PHE:HE2	1:A:260:ASN:CA	2.18	0.57
1:B:879:LEU:H	1:B:879:LEU:CD2	2.14	0.57
1:A:192:VAL:HA	1:A:268:LYS:HA	1.86	0.57
1:B:439:ASP:OD1	1:B:440:GLU:N	2.38	0.57
1:B:170:LEU:HD21	1:B:211:PHE:HE1	1.69	0.57
1:A:170:LEU:HD12	1:A:259:ASP:OD2	2.05	0.57
1:A:273:HIS:CD2	1:A:274:VAL:O	2.57	0.57
1:A:541:MSE:CE	1:A:572:LEU:O	2.52	0.57
1:A:338:THR:HG21	1:A:367:LYS:HZ2	1.70	0.57
1:B:302:TYR:HB3	1:B:588:ARG:HG3	1.85	0.57
1:B:192:VAL:N	1:B:269:VAL:HG23	2.20	0.57
1:A:809:ASN:O	1:A:809:ASN:OD1	2.22	0.57
1:A:764:VAL:CG2	1:A:772:LEU:CD1	2.83	0.57
1:B:672:GLN:NE2	1:B:673:PRO:HD2	2.19	0.57
1:B:535:ASP:O	1:B:535:ASP:CG	2.43	0.57
1:B:513:GLY:HA3	1:B:558:MSE:HA	1.87	0.57
1:B:788:PRO:O	1:B:807:PRO:O	2.23	0.57
1:B:134:GLU:CG	1:B:135:PRO:CD	2.80	0.57
1:A:792:LEU:CD2	1:A:792:LEU:N	2.64	0.57
1:A:236:LEU:CD1	1:A:574:LYS:HB2	2.32	0.57
1:B:142:VAL:HG12	1:B:143:ALA:H	1.70	0.57
1:B:622:LEU:HD12	1:B:880:TYR:O	2.05	0.57
1:B:715:LEU:HD12	1:B:715:LEU:H	1.69	0.56
1:B:225:PHE:HE1	1:B:294:TYR:CD2	2.23	0.56
1:B:472:GLU:O	1:B:473:GLU:HB2	2.05	0.56
1:B:617:LEU:HD12	1:B:618:PRO:HD2	1.86	0.56
1:A:236:LEU:HD23	1:A:239:ILE:CD1	2.32	0.56
1:A:455:ASP:CB	1:A:461:TYR:HE2	2.18	0.56
1:B:637:PHE:HB3	1:B:640:CYS:SG	2.44	0.56
1:A:671:HIS:C	1:A:671:HIS:ND1	2.58	0.56
1:B:785:SER:O	1:B:788:PRO:HD3	2.06	0.56
1:A:247:ASP:HB3	1:A:250:ARG:HB2	1.86	0.56
1:A:517:CYS:SG	1:A:517:CYS:O	2.63	0.56
1:A:670:ASN:ND2	1:A:722:LEU:CD2	2.68	0.56
1:A:460:ILE:HG21	1:A:462:PHE:CE2	2.39	0.56
1:B:460:ILE:HD13	1:B:460:ILE:N	2.20	0.56
1:B:351:GLY:O	1:B:355:THR:HG23	2.06	0.56
1:A:757:TRP:HZ3	1:A:773:VAL:HG21	1.70	0.56
1:B:443:VAL:O	1:B:488:LYS:NZ	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:GLU:O	1:B:495:GLU:OE1	2.24	0.56
1:A:141:PRO:HB2	1:A:143:ALA:H	1.69	0.56
1:A:154:ARG:O	1:A:155:TYR:HB2	2.05	0.56
1:A:714:LEU:HD11	1:A:717:HIS:HD2	1.70	0.56
1:A:592:MSE:CE	1:A:861:LEU:HD21	2.07	0.56
1:A:722:LEU:N	1:A:722:LEU:HD13	2.20	0.56
1:A:803:THR:OG1	1:A:847:ILE:HA	2.05	0.56
1:A:555:TYR:CE1	1:A:615:MSE:HG2	2.41	0.56
1:A:136:GLU:CG	1:A:218:HIS:CE1	2.88	0.56
1:A:136:GLU:HG2	1:A:137:PHE:H	1.71	0.56
1:A:137:PHE:CD2	1:A:218:HIS:HB3	2.40	0.56
1:A:839:PHE:HD1	1:A:839:PHE:N	2.03	0.56
1:A:635:ASN:O	1:A:638:SER:N	2.36	0.56
1:B:194:VAL:HB	1:B:203:TYR:HB2	1.87	0.56
1:B:351:GLY:N	1:B:384:LEU:HD12	2.20	0.56
1:B:695:ARG:HH11	1:B:835:TYR:HD1	1.53	0.56
1:B:220:PHE:HD2	1:B:262:LEU:HA	1.69	0.56
1:A:780:PHE:HB3	1:A:786:LEU:CD2	2.35	0.56
1:A:609:TRP:CD1	1:A:620:TYR:CE1	2.93	0.56
1:B:236:LEU:HD23	1:B:239:ILE:CG1	2.36	0.56
1:B:388:HIS:HA	1:B:702:SER:OG	2.06	0.56
1:B:508:VAL:HG11	1:B:511:ILE:HG22	1.88	0.56
1:B:218:HIS:HB2	1:B:262:LEU:HD11	1.87	0.56
1:A:541:MSE:HE2	1:A:572:LEU:HB3	1.88	0.56
1:A:302:TYR:CD2	1:A:878:PRO:HB3	2.41	0.56
1:A:236:LEU:O	1:A:239:ILE:HD13	2.05	0.56
1:B:675:ASP:HA	1:B:718:GLN:HE21	1.70	0.56
1:B:281:LYS:O	1:B:284:ALA:HB3	2.05	0.56
1:A:714:LEU:HD21	1:A:717:HIS:HB3	1.84	0.56
1:A:495:GLU:CG	1:A:499:ARG:HH21	2.19	0.56
1:A:784:LYS:N	1:A:786:LEU:HD11	2.18	0.56
1:A:347:TYR:OH	1:A:540:GLN:NE2	2.39	0.56
1:A:355:THR:HG22	1:A:388:HIS:CE1	2.41	0.56
1:B:658:LEU:HD21	1:B:791:ARG:NH2	2.21	0.55
1:B:485:CYS:SG	1:B:488:LYS:NZ	2.77	0.55
1:B:483:SER:O	1:B:486:PRO:HG3	2.06	0.55
1:B:374:VAL:HG22	1:B:394:ARG:HB2	1.88	0.55
1:B:741:PHE:O	1:B:744:LEU:N	2.29	0.55
1:A:817:GLN:O	1:A:818:ALA:HB3	2.05	0.55
1:B:645:ASP:O	1:B:645:ASP:CG	2.45	0.55
1:A:338:THR:HG22	1:A:339:ARG:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:GLU:O	1:A:410:VAL:HB	2.06	0.55
1:B:664:ASP:HB2	1:B:688:GLN:CD	2.26	0.55
1:B:791:ARG:CG	1:B:792:LEU:N	2.69	0.55
1:A:664:ASP:CG	1:A:664:ASP:O	2.44	0.55
1:A:723:ASN:ND2	1:A:723:ASN:C	2.58	0.55
1:B:599:LEU:CD2	1:B:601:GLN:HE21	2.19	0.55
1:B:823:ILE:CD1	1:B:845:LYS:HD2	2.36	0.55
1:B:278:MSE:O	1:B:280:PRO:CD	2.54	0.55
1:A:665:LEU:HD21	1:A:814:HIS:CE1	2.22	0.55
1:A:652:LEU:O	1:A:653:LYS:O	2.23	0.55
1:B:879:LEU:N	1:B:879:LEU:CD2	2.70	0.55
1:A:511:ILE:CG2	1:A:553:PRO:HB3	2.36	0.55
1:A:444:GLU:HG3	1:A:445:LYS:N	2.20	0.55
1:B:391:THR:HG23	1:B:392:GLU:H	1.68	0.55
1:A:735:VAL:O	1:A:735:VAL:CG1	2.55	0.55
1:B:796:GLU:CG	1:B:797:THR:N	2.58	0.55
1:B:802:VAL:CG1	1:B:803:THR:H	2.20	0.55
1:A:558:MSE:O	1:A:607:PHE:HA	2.06	0.55
1:A:631:GLY:HA3	1:A:641:MSE:CE	2.35	0.55
1:B:176:TYR:O	1:B:210:PHE:HB2	2.07	0.55
1:A:704:GLY:O	1:A:705:GLU:HB3	2.07	0.55
1:B:814:HIS:ND1	1:B:819:ARG:CZ	2.69	0.55
1:B:543:THR:O	1:B:547:ILE:HG12	2.07	0.55
1:B:147:ALA:O	1:B:151:TRP:N	2.39	0.55
1:A:535:ASP:OD2	1:A:536:GLU:N	2.39	0.55
1:B:772:LEU:CB	1:B:774:PRO:HD2	2.35	0.55
1:A:652:LEU:N	1:A:652:LEU:HD23	2.21	0.55
1:B:672:GLN:OE1	1:B:674:ASN:O	2.25	0.55
1:A:704:GLY:O	1:A:705:GLU:CB	2.55	0.55
1:A:142:VAL:HG12	1:A:176:TYR:CE2	2.42	0.55
1:A:780:PHE:C	1:A:782:LYS:N	2.60	0.55
1:A:786:LEU:C	1:A:788:PRO:HD3	2.27	0.55
1:A:273:HIS:CB	1:A:294:TYR:CE2	2.62	0.55
1:A:280:PRO:HG2	1:A:280:PRO:O	2.07	0.55
1:A:596:CYS:O	1:A:625:TYR:N	2.40	0.55
1:A:605:ARG:NH1	1:A:605:ARG:CG	2.53	0.55
1:A:568:ALA:O	1:A:569:ASP:C	2.44	0.55
1:B:349:GLY:O	1:B:350:CYS:SG	2.65	0.54
1:B:281:LYS:HG3	1:B:282:ALA:N	2.22	0.54
1:B:645:ASP:O	1:B:646:GLU:CB	2.30	0.54
1:B:667:LYS:CB	1:B:817:GLN:OE1	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:LEU:C	1:A:845:LYS:HE2	2.27	0.54
1:B:206:ARG:CG	1:B:206:ARG:NH1	2.45	0.54
1:B:239:ILE:HG21	1:B:575:TYR:CE1	2.43	0.54
1:A:555:TYR:OH	1:A:868:ALA:HB1	2.08	0.54
1:A:839:PHE:N	1:A:839:PHE:CD1	2.74	0.54
1:A:234:ASN:O	1:A:235:SER:HB3	2.07	0.54
1:A:394:ARG:NH2	1:A:396:GLU:OE1	2.38	0.54
1:A:154:ARG:CZ	1:A:175:HIS:HE1	2.21	0.54
1:A:249:ARG:CG	1:A:249:ARG:O	2.56	0.54
1:A:195:LYS:CG	1:A:266:ILE:CD1	2.85	0.54
1:A:585:TYR:HD1	1:A:610:GLY:O	1.89	0.54
1:B:387:ASN:CB	1:B:836:TYR:CE2	2.90	0.54
1:A:269:VAL:HG22	1:A:271:ILE:HG13	1.90	0.54
1:A:772:LEU:N	1:A:772:LEU:HD12	2.22	0.54
1:A:415:TYR:CD2	1:A:490:ARG:CG	2.88	0.54
1:B:139:GLY:HA3	1:B:178:SER:HB3	1.88	0.54
1:A:186:TYR:CE2	1:A:265:ILE:CG2	2.89	0.54
1:A:413:LYS:HG2	1:A:420:ASP:HB3	1.90	0.54
1:A:505:PRO:HD3	1:A:550:TYR:CE1	2.42	0.54
1:B:690:TYR:C	1:B:693:LEU:HD13	2.27	0.54
1:B:459:GLY:O	1:B:461:TYR:HD2	1.88	0.54
1:A:727:TYR:CE2	1:A:731:GLN:CD	2.80	0.54
1:A:280:PRO:O	1:A:281:LYS:CB	2.56	0.54
1:A:644:TYR:CE1	1:A:649:LYS:HB3	2.42	0.54
1:A:599:LEU:HD11	1:A:856:PRO:CG	2.33	0.54
1:B:266:ILE:HG22	1:B:267:SER:HB3	1.89	0.54
1:B:685:THR:CG2	1:B:687:PHE:N	2.66	0.54
1:B:691:ILE:HG23	1:B:692:ARG:HG3	1.89	0.54
1:B:151:TRP:CE3	1:B:175:HIS:CE1	2.96	0.54
1:A:716:ASP:OD2	1:A:838:LEU:HB2	2.08	0.54
1:A:253:LEU:HD12	1:A:294:TYR:HE1	1.70	0.54
1:A:538:ASN:C	1:A:540:GLN:N	2.55	0.54
1:B:223:ARG:HA	1:B:256:GLU:O	2.08	0.54
1:B:387:ASN:ND2	1:B:387:ASN:N	2.56	0.54
1:B:404:LEU:HD22	1:B:404:LEU:O	2.07	0.54
1:A:793:TRP:HA	1:A:793:TRP:HE3	1.68	0.54
1:B:156:GLY:O	1:B:157:ARG:C	2.46	0.54
1:A:173:ARG:NH1	1:A:212:GLU:CD	2.41	0.54
1:A:785:SER:O	1:A:786:LEU:HB2	2.06	0.54
1:A:405:LEU:HD21	1:A:503:PRO:HG2	1.89	0.54
1:B:139:GLY:CA	1:B:178:SER:HB3	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:PHE:HE1	1:A:210:PHE:HB3	1.73	0.53
1:B:676:VAL:CB	1:B:713:LYS:HE2	2.38	0.53
1:A:766:LEU:HD23	1:A:767:SER:N	2.23	0.53
1:A:502:LEU:CD2	1:A:503:PRO:HD2	2.30	0.53
1:A:449:ILE:CD1	1:A:460:ILE:HG23	2.36	0.53
1:B:714:LEU:HD23	1:B:714:LEU:C	2.29	0.53
1:A:134:GLU:O	1:A:136:GLU:N	2.41	0.53
1:A:285:GLN:HA	1:A:285:GLN:OE1	2.08	0.53
1:B:456:ARG:NH2	1:B:456:ARG:HG2	2.17	0.53
1:A:757:TRP:CH2	1:A:763:ARG:NH2	2.76	0.53
1:A:220:PHE:HD2	1:A:220:PHE:N	1.87	0.53
1:B:834:ASP:C	1:B:836:TYR:H	2.10	0.53
1:A:227:ARG:N	1:A:230:ASP:OD2	2.38	0.53
1:B:389:PRO:HD2	1:B:702:SER:OG	2.08	0.53
1:A:715:LEU:HD22	1:A:837:ARG:CG	2.29	0.53
1:A:250:ARG:CZ	1:A:295:ASP:OD2	2.56	0.53
1:A:273:HIS:CE1	1:A:274:VAL:O	2.62	0.53
1:B:447:VAL:O	1:B:447:VAL:HG23	2.06	0.53
1:A:198:GLU:O	1:A:199:ASN:HB2	2.07	0.53
1:B:802:VAL:HG13	1:B:803:THR:H	1.72	0.53
1:A:730:VAL:CG2	1:A:818:ALA:O	2.53	0.53
1:B:578:SER:O	1:B:579:CYS:C	2.44	0.53
1:A:619:LYS:HB3	1:A:878:PRO:O	2.08	0.53
1:B:247:ASP:C	1:B:247:ASP:OD1	2.47	0.53
1:A:195:LYS:HE2	1:A:264:CYS:HA	1.89	0.53
1:A:367:LYS:HE3	1:A:701:TRP:CZ3	2.40	0.53
1:A:633:ALA:C	1:A:634:PRO:O	2.42	0.53
1:A:148:ARG:CG	1:A:155:TYR:CD1	2.91	0.53
1:A:375:ASP:OD2	2:A:1000:SAH:O2'	2.27	0.53
1:A:814:HIS:CD2	1:A:815:PRO:HD2	2.42	0.53
1:B:443:VAL:CG1	1:B:466:TRP:CE3	2.89	0.53
1:B:622:LEU:HB3	1:B:623:PRO:HD2	1.90	0.53
1:B:672:GLN:CD	1:B:674:ASN:H	2.11	0.53
1:B:404:LEU:HD11	1:B:502:LEU:HD21	1.91	0.53
1:B:352:GLY:N	2:B:1000:SAH:O	2.41	0.53
1:B:833:PRO:CG	1:B:835:TYR:CE2	2.88	0.53
1:A:136:GLU:CD	1:A:137:PHE:N	2.62	0.53
1:B:209:GLU:HB2	1:B:221:THR:HB	1.90	0.53
1:A:417:GLN:O	1:A:418:ASP:C	2.45	0.53
1:A:729:ARG:NE	1:A:772:LEU:O	2.41	0.53
1:A:617:LEU:HD12	1:A:618:PRO:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:602:PHE:O	1:B:799:PRO:O	2.27	0.53
1:B:695:ARG:NH1	1:B:835:TYR:CD1	2.77	0.53
1:A:140:SER:HB3	1:A:141:PRO:CD	2.38	0.53
1:B:148:ARG:HH11	1:B:148:ARG:CG	1.97	0.53
1:A:375:ASP:C	1:A:375:ASP:OD2	2.46	0.53
1:A:822:THR:CG2	1:A:825:GLU:CD	2.78	0.52
1:A:672:GLN:HE22	1:A:674:ASN:HB2	1.71	0.52
1:B:828:ARG:NH2	1:B:834:ASP:OD1	2.42	0.52
1:A:232:VAL:CG1	1:A:233:ILE:HG22	2.38	0.52
1:A:622:LEU:HD12	1:A:880:TYR:O	2.09	0.52
1:A:763:ARG:NH1	1:A:771:PRO:HB2	2.24	0.52
1:A:223:ARG:HD2	1:A:255:GLU:HA	1.92	0.52
1:A:399:ASP:N	1:A:399:ASP:OD1	2.35	0.52
1:B:347:TYR:HD2	1:B:516:PRO:HD3	1.72	0.52
1:A:176:TYR:OH	1:A:212:GLU:OE2	2.28	0.52
1:A:740:ASN:N	1:A:740:ASN:OD1	2.42	0.52
1:A:716:ASP:OD1	1:A:716:ASP:N	2.40	0.52
1:B:772:LEU:CA	1:B:774:PRO:CD	2.87	0.52
1:B:605:ARG:CG	1:B:605:ARG:HH11	2.16	0.52
1:B:729:ARG:NH2	1:B:771:PRO:O	2.43	0.52
1:B:443:VAL:CG1	1:B:466:TRP:CZ3	2.92	0.52
1:A:714:LEU:HD23	1:A:715:LEU:N	2.24	0.52
1:A:837:ARG:HB3	1:A:839:PHE:CE1	2.39	0.52
1:A:284:ALA:HA	1:A:287:ILE:CG1	2.40	0.52
1:B:729:ARG:CZ	1:B:729:ARG:HB3	2.38	0.52
1:B:549:ALA:CB	1:B:583:MSE:HE1	2.38	0.52
1:A:340:THR:HA	1:A:367:LYS:O	2.09	0.52
1:B:411:LEU:HD21	1:B:493:VAL:CG2	2.39	0.52
1:B:534:LYS:HZ1	1:B:535:ASP:HB2	1.73	0.52
1:A:671:HIS:HE1	1:A:673:PRO:CG	2.23	0.52
1:A:464:VAL:HG13	1:A:466:TRP:CZ2	2.43	0.52
1:B:544:PHE:CE1	1:B:558:MSE:HE3	2.45	0.52
1:A:495:GLU:CG	1:A:499:ARG:NH2	2.73	0.52
1:B:252:PHE:HD2	1:B:296:MSE:HB3	1.74	0.52
1:A:148:ARG:HH11	1:A:148:ARG:HG3	1.75	0.52
1:A:180:LYS:HB2	1:A:185:VAL:HG13	1.92	0.52
1:A:624:THR:O	1:A:624:THR:HG22	2.09	0.52
1:A:763:ARG:HH11	1:A:771:PRO:CB	2.23	0.52
1:A:723:ASN:HD21	1:A:725:ASP:HB2	1.75	0.52
1:A:384:LEU:HD13	1:A:388:HIS:CD2	2.44	0.52
1:B:489:ILE:HG12	1:B:490:ARG:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:ASP:HB3	1:A:461:TYR:HE2	1.75	0.52
1:A:215:ASP:O	1:A:216:GLN:CB	2.57	0.52
1:A:391:THR:CG2	1:A:393:VAL:HG23	2.40	0.52
1:A:601:GLN:HB3	1:A:798:VAL:HG23	1.91	0.52
1:B:511:ILE:HD11	1:B:548:VAL:HG22	1.92	0.51
1:A:140:SER:O	1:A:141:PRO:C	2.48	0.51
1:A:154:ARG:HD2	1:A:172:ALA:HB3	1.93	0.51
1:B:766:LEU:C	1:B:768:SER:O	2.48	0.51
1:A:136:GLU:CG	1:A:137:PHE:N	2.73	0.51
1:B:209:GLU:HB2	1:B:221:THR:HG22	1.92	0.51
1:A:272:VAL:HG21	1:A:286:LEU:CD2	2.39	0.51
1:B:619:LYS:HB2	1:B:878:PRO:O	2.10	0.51
1:B:720:LEU:HD12	1:B:805:ALA:O	2.11	0.51
1:A:700:ASP:HB2	1:A:835:TYR:OH	2.10	0.51
1:A:763:ARG:C	1:A:764:VAL:HG22	2.31	0.51
1:A:605:ARG:HG3	1:A:605:ARG:HH11	1.74	0.51
1:B:555:TYR:HE2	1:B:618:PRO:HD3	1.74	0.51
1:B:538:ASN:N	1:B:538:ASN:ND2	2.57	0.51
1:A:211:PHE:C	1:A:211:PHE:HD1	2.14	0.51
1:A:691:ILE:CG2	1:A:834:ASP:OD1	2.58	0.51
1:A:727:TYR:CE2	1:A:731:GLN:NE2	2.78	0.51
1:A:273:HIS:CG	1:A:294:TYR:HE2	2.26	0.51
1:B:729:ARG:CD	1:B:773:VAL:HG21	2.38	0.51
1:A:580:LEU:HD23	1:A:587:ALA:CB	2.41	0.51
1:A:764:VAL:HG21	1:A:772:LEU:HD12	1.89	0.51
1:B:622:LEU:HD11	1:B:879:LEU:HB2	1.92	0.51
1:B:665:LEU:HB3	1:B:717:HIS:HE2	1.76	0.51
1:A:656:LEU:C	1:A:657:LEU:HD12	2.30	0.51
1:B:195:LYS:HE2	1:B:264:CYS:HA	1.92	0.51
1:B:229:GLU:OE1	1:B:229:GLU:N	2.29	0.51
1:A:596:CYS:HA	1:A:627:VAL:CG1	2.41	0.51
1:A:501:ILE:HG12	1:A:502:LEU:N	2.24	0.51
1:B:404:LEU:HD13	1:B:404:LEU:C	2.30	0.51
1:B:572:LEU:HD12	1:B:572:LEU:N	2.25	0.51
1:A:154:ARG:CD	1:A:172:ALA:HB3	2.39	0.51
1:A:154:ARG:HD2	1:A:172:ALA:CB	2.40	0.51
1:A:172:ALA:HA	1:A:213:GLY:HA2	1.92	0.51
1:B:217:CYS:HB2	1:B:219:TYR:CE2	2.46	0.51
1:B:192:VAL:CA	1:B:269:VAL:HG23	2.41	0.51
1:B:266:ILE:HG22	1:B:267:SER:N	2.25	0.51
1:B:814:HIS:CD2	1:B:815:PRO:N	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:TRP:CD1	1:A:175:HIS:CE1	2.98	0.51
1:B:362:ALA:HB2	1:B:699:LEU:HD22	1.90	0.51
1:A:415:TYR:CE2	1:A:490:ARG:HG2	2.46	0.51
1:B:186:TYR:HD1	1:B:268:LYS:HG3	1.76	0.51
1:A:234:ASN:ND2	1:A:234:ASN:O	2.43	0.51
1:B:274:VAL:HA	1:B:278:MSE:HE3	1.93	0.51
1:A:249:ARG:O	1:A:293:TYR:CE2	2.64	0.51
1:B:231:THR:OG1	1:B:233:ILE:CG2	2.44	0.51
1:B:241:VAL:HG21	1:B:579:CYS:HB3	1.93	0.51
1:B:676:VAL:HG21	1:B:713:LYS:HZ1	1.76	0.51
1:A:564:ILE:HG23	1:A:573:GLY:N	2.26	0.51
1:A:575:TYR:CE1	1:A:579:CYS:SG	3.04	0.51
1:A:648:GLN:C	1:A:649:LYS:O	2.43	0.51
1:B:304:THR:HG21	1:B:588:ARG:NH2	2.25	0.51
1:B:671:HIS:CE1	1:B:673:PRO:HD3	2.46	0.51
1:B:508:VAL:HG11	1:B:511:ILE:CG2	2.41	0.50
1:B:272:VAL:CG1	1:B:273:HIS:H	2.24	0.50
1:A:671:HIS:HE1	1:A:673:PRO:HG3	1.75	0.50
1:B:460:ILE:HD12	1:B:460:ILE:N	2.26	0.50
1:B:154:ARG:HH21	1:B:209:GLU:CD	2.15	0.50
1:A:609:TRP:HD1	1:A:620:TYR:CE1	2.29	0.50
1:B:464:VAL:HG23	1:B:465:GLN:N	2.24	0.50
1:B:695:ARG:NE	1:B:703:PHE:HE2	2.08	0.50
1:B:224:TRP:O	1:B:254:SER:HB3	2.11	0.50
1:B:642:VAL:O	1:B:642:VAL:CG2	2.59	0.50
1:A:675:ASP:N	1:A:675:ASP:OD1	2.43	0.50
1:A:715:LEU:HD12	1:A:834:ASP:O	2.11	0.50
1:A:253:LEU:HD22	1:A:254:SER:O	2.11	0.50
1:A:544:PHE:HD1	1:A:558:MSE:SE	2.43	0.50
1:B:411:LEU:HD23	1:B:412:CYS:N	2.26	0.50
1:B:413:LYS:HZ1	1:B:414:LYS:CE	2.23	0.50
1:B:140:SER:CB	1:B:141:PRO:CD	2.85	0.50
1:B:766:LEU:O	1:B:768:SER:O	2.29	0.50
1:B:685:THR:HG21	1:B:688:GLN:H	1.67	0.50
1:B:821:LEU:CB	1:B:825:GLU:OE1	2.60	0.50
1:A:557:LEU:HD22	1:A:609:TRP:CH2	2.47	0.50
1:A:733:ILE:CG2	1:A:791:ARG:HE	2.25	0.50
1:A:814:HIS:HD2	1:A:816:THR:N	2.06	0.50
1:A:757:TRP:CZ3	1:A:773:VAL:CG2	2.95	0.50
1:B:307:ASN:ND2	1:B:586:GLN:NE2	2.60	0.50
1:B:622:LEU:CD1	1:B:879:LEU:HB2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:LEU:O	1:B:405:LEU:HB2	2.11	0.50
1:B:250:ARG:NH2	1:B:295:ASP:OD1	2.44	0.50
1:A:505:PRO:HD3	1:A:550:TYR:HE1	1.76	0.50
1:A:196:ALA:HB2	1:A:203:TYR:CE1	2.47	0.50
1:A:690:TYR:HE1	1:A:698:MSE:SE	2.45	0.50
1:A:823:ILE:HG12	1:A:846:TYR:CE2	2.47	0.50
1:A:412:CYS:C	1:A:416:VAL:HG23	2.28	0.50
1:A:370:THR:O	1:A:391:THR:OG1	2.24	0.50
1:A:195:LYS:NZ	1:A:263:ASP:O	2.28	0.50
1:B:410:VAL:O	1:B:413:LYS:HB3	2.11	0.50
1:B:814:HIS:HA	1:B:821:LEU:HD13	1.93	0.50
1:A:136:GLU:CG	1:A:137:PHE:H	2.24	0.50
1:A:141:PRO:O	1:A:142:VAL:HG13	2.11	0.50
1:A:148:ARG:HG2	1:A:155:TYR:CD1	2.46	0.50
1:A:148:ARG:HG2	1:A:155:TYR:CG	2.45	0.50
1:A:154:ARG:NH1	1:A:211:PHE:CG	2.80	0.50
1:A:584:LYS:NZ	1:A:584:LYS:HB3	2.25	0.50
1:A:456:ARG:NH2	1:A:456:ARG:CG	2.59	0.50
1:B:646:GLU:OE2	1:B:647:THR:HG23	2.09	0.50
1:A:665:LEU:O	1:A:665:LEU:CD1	2.53	0.50
1:A:670:ASN:O	1:A:670:ASN:OD1	2.30	0.50
1:B:413:LYS:NZ	1:B:414:LYS:CE	2.75	0.50
1:B:186:TYR:CD1	1:B:268:LYS:HG3	2.47	0.50
1:B:186:TYR:CZ	1:B:265:ILE:HG21	2.47	0.50
1:A:495:GLU:HG3	1:A:499:ARG:NH2	2.26	0.50
1:B:728:GLU:O	1:B:731:GLN:HG2	2.12	0.50
1:A:397:LYS:HB2	1:A:400:GLU:OE1	2.11	0.50
1:A:287:ILE:CD1	1:A:288:GLU:HG2	2.42	0.50
1:B:774:PRO:O	1:B:776:TYR:N	2.45	0.50
1:A:591:MSE:HG3	1:A:640:CYS:O	2.12	0.50
1:A:455:ASP:HB3	1:A:461:TYR:CE2	2.47	0.50
1:B:591:MSE:CE	1:B:640:CYS:HB2	2.42	0.50
1:B:375:ASP:OD1	1:B:376:PHE:N	2.45	0.50
1:B:658:LEU:CD2	1:B:791:ARG:NH2	2.74	0.50
1:B:791:ARG:CG	1:B:813:ILE:O	2.59	0.50
1:B:192:VAL:HG13	1:B:193:TYR:N	2.27	0.50
1:A:474:ASP:C	1:A:475:THR:HG23	2.32	0.50
1:A:447:VAL:HG13	1:A:463:LYS:HG2	1.93	0.50
1:B:378:SER:O	1:B:382:GLN:CG	2.60	0.49
1:B:884:PRO:O	1:B:885:SER:O	2.30	0.49
1:B:208:THR:OG1	1:B:221:THR:CG2	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:PHE:C	1:A:782:LYS:H	2.12	0.49
1:A:250:ARG:NH2	1:A:584:LYS:HE2	2.23	0.49
1:A:865:LEU:O	1:A:868:ALA:N	2.45	0.49
1:A:657:LEU:HD23	1:A:795:ASP:CA	2.42	0.49
1:B:791:ARG:HG2	1:B:813:ILE:O	2.12	0.49
1:B:810:GLN:O	1:B:811:VAL:HG13	2.11	0.49
1:B:207:ILE:HD12	1:B:221:THR:O	2.12	0.49
1:B:281:LYS:HA	1:B:284:ALA:HB3	1.94	0.49
1:A:823:ILE:HG12	1:A:846:TYR:CD2	2.46	0.49
1:A:204:ILE:HB	1:A:225:PHE:HB2	1.94	0.49
1:B:774:PRO:CB	1:B:778:MSE:CE	2.86	0.49
1:A:364:SER:OG	1:A:863:TYR:O	2.30	0.49
1:B:535:ASP:OD2	1:B:539:LYS:HE3	2.12	0.49
1:A:242:ASP:CG	1:A:243:GLY:H	2.15	0.49
1:B:679:TYR:O	1:B:681:GLY:N	2.43	0.49
1:B:791:ARG:CG	1:B:792:LEU:H	2.25	0.49
1:A:140:SER:CB	1:A:141:PRO:CD	2.90	0.49
1:B:143:ALA:N	1:B:175:HIS:O	2.44	0.49
1:B:472:GLU:H	1:B:472:GLU:CD	2.16	0.49
1:B:413:LYS:NZ	1:B:414:LYS:NZ	2.60	0.49
1:A:389:PRO:CD	1:A:390:GLN:H	2.26	0.49
1:A:174:CYS:O	1:A:212:GLU:N	2.26	0.49
1:A:176:TYR:O	1:A:210:PHE:HB2	2.12	0.49
1:A:837:ARG:O	1:A:838:LEU:HD12	2.11	0.49
1:A:343:LEU:HD21	1:A:512:CYS:SG	2.52	0.49
1:A:536:GLU:O	1:A:538:ASN:OD1	2.30	0.49
1:A:195:LYS:HB2	1:A:264:CYS:HB3	1.94	0.49
1:B:696:LYS:C	1:B:698:MSE:N	2.64	0.49
1:B:387:ASN:HB2	1:B:836:TYR:CE2	2.46	0.49
1:B:387:ASN:HD22	1:B:387:ASN:N	2.10	0.49
1:A:206:ARG:O	1:A:222:CYS:CB	2.57	0.49
1:B:275:ASP:OD2	1:B:277:ASN:HB2	2.12	0.49
1:A:394:ARG:HH21	1:A:396:GLU:CD	2.16	0.49
1:B:394:ARG:NH2	1:B:396:GLU:OE2	2.42	0.49
1:B:272:VAL:HG11	1:B:286:LEU:HD23	1.95	0.49
1:A:250:ARG:NH2	1:A:584:LYS:HD2	2.28	0.49
1:B:375:ASP:O	1:B:395:ASN:HA	2.12	0.49
1:B:687:PHE:C	1:B:687:PHE:CD2	2.86	0.49
1:B:672:GLN:HE21	1:B:672:GLN:HA	1.78	0.49
1:B:140:SER:HB3	1:B:141:PRO:HD3	1.91	0.49
1:A:874:GLU:HG3	1:A:875:GLY:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:ILE:O	1:B:548:VAL:C	2.50	0.49
1:A:179:ALA:O	1:A:185:VAL:HA	2.13	0.49
1:B:723:ASN:OD1	1:B:726:ASP:OD2	2.30	0.49
1:A:645:ASP:O	1:A:646:GLU:OE2	2.30	0.49
1:A:843:LYS:O	1:A:847:ILE:HD12	2.13	0.49
1:B:535:ASP:OD1	1:B:539:LYS:HE3	2.13	0.49
1:B:679:TYR:C	1:B:681:GLY:N	2.65	0.49
1:B:378:SER:O	1:B:382:GLN:HG2	2.13	0.49
1:B:207:ILE:HD13	1:B:220:PHE:HB2	1.94	0.49
1:A:454:SER:C	1:A:456:ARG:N	2.66	0.49
1:A:376:PHE:C	1:A:395:ASN:OD1	2.51	0.49
1:A:339:ARG:O	1:A:367:LYS:HB2	2.13	0.49
1:B:622:LEU:CD1	1:B:880:TYR:O	2.60	0.49
1:B:626:ASP:OD2	1:B:655:ALA:CB	2.61	0.49
1:B:561:VAL:HG23	1:B:563:ASP:HB2	1.95	0.49
1:B:180:LYS:CE	1:B:183:ASN:HA	2.42	0.49
1:B:343:LEU:HB2	1:B:368:LEU:CD2	2.43	0.49
1:B:692:ARG:C	1:B:693:LEU:HD12	2.32	0.49
1:B:668:VAL:O	1:B:817:GLN:HG2	2.13	0.49
1:A:537:LYS:C	1:A:539:LYS:H	2.15	0.49
1:A:757:TRP:CZ3	1:A:773:VAL:HG21	2.48	0.49
1:B:624:THR:O	1:B:624:THR:HG22	2.13	0.49
1:B:671:HIS:CE1	1:B:673:PRO:HB3	2.44	0.49
1:B:349:GLY:C	1:B:351:GLY:H	2.16	0.49
1:B:361:ALA:CB	1:B:368:LEU:HB2	2.43	0.49
1:A:151:TRP:O	1:A:151:TRP:CD1	2.66	0.49
1:A:785:SER:OG	1:A:786:LEU:N	2.43	0.49
1:B:565:LEU:HD11	1:B:606:VAL:HG21	1.95	0.49
1:B:349:GLY:CA	1:B:380:ALA:HB1	2.42	0.48
1:A:555:TYR:CE2	1:A:618:PRO:CG	2.95	0.48
1:A:585:TYR:CE1	1:A:612:LEU:HG	2.48	0.48
1:A:442:VAL:HG11	1:A:467:GLU:OE2	2.13	0.48
1:A:413:LYS:HG3	1:A:420:ASP:HB3	1.95	0.48
1:B:346:LEU:O	1:B:347:TYR:HB2	2.12	0.48
1:B:812:ILE:HG12	1:B:812:ILE:O	2.13	0.48
1:B:457:GLU:O	1:B:461:TYR:OH	2.30	0.48
1:B:227:ARG:O	1:B:230:ASP:CB	2.58	0.48
1:B:802:VAL:HG12	1:B:803:THR:N	2.27	0.48
1:B:603:ARG:NH2	1:B:830:GLN:HE22	2.11	0.48
1:B:603:ARG:NH1	1:B:852:ALA:O	2.45	0.48
1:A:456:ARG:O	1:A:456:ARG:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:728:GLU:CD	1:A:766:LEU:CG	2.78	0.48
1:B:671:HIS:HE1	1:B:673:PRO:CB	2.27	0.48
1:B:553:PRO:O	1:B:553:PRO:CD	2.61	0.48
1:A:464:VAL:HG12	1:A:475:THR:O	2.13	0.48
1:B:689:ARG:O	1:B:693:LEU:CD1	2.62	0.48
1:B:717:HIS:C	1:B:718:GLN:HG3	2.32	0.48
1:B:144:ALA:O	1:B:145:ASP:CB	2.60	0.48
1:A:733:ILE:HG21	1:A:791:ARG:NH2	2.22	0.48
1:B:235:SER:O	1:B:236:LEU:C	2.50	0.48
1:B:676:VAL:CG2	1:B:713:LYS:NZ	2.76	0.48
1:A:496:GLY:O	1:A:501:ILE:HG23	2.13	0.48
1:A:465:GLN:CG	1:A:474:ASP:OD1	2.62	0.48
1:B:621:PRO:HD3	1:B:864:CYS:SG	2.53	0.48
1:B:785:SER:O	1:B:788:PRO:HD2	2.12	0.48
1:A:141:PRO:CB	1:A:143:ALA:H	2.26	0.48
1:B:562:VAL:HG21	1:B:604:MSE:CE	2.34	0.48
1:A:347:TYR:HD1	1:A:516:PRO:HD3	1.77	0.48
1:A:367:LYS:CE	1:A:701:TRP:CH2	2.82	0.48
1:B:170:LEU:CD2	1:B:211:PHE:CZ	2.97	0.48
1:B:621:PRO:CG	1:B:860:ALA:HB1	2.43	0.48
1:B:171:LYS:O	1:B:214:THR:HG23	2.13	0.48
1:B:239:ILE:HD12	1:B:239:ILE:N	2.28	0.48
1:A:309:SER:O	1:A:310:SER:OG	2.30	0.48
1:B:841:PRO:HB2	1:B:843:LYS:HE3	1.95	0.48
1:B:345:ASP:OD2	1:B:348:SER:HB3	2.13	0.48
1:B:814:HIS:CE1	1:B:819:ARG:NH2	2.80	0.48
1:B:362:ALA:HA	1:B:366:LEU:O	2.13	0.48
1:A:248:PRO:HD2	1:A:249:ARG:H	1.78	0.48
1:B:229:GLU:H	1:B:229:GLU:CD	2.13	0.48
1:B:195:LYS:HG3	1:B:266:ILE:HD12	1.95	0.48
1:B:345:ASP:HA	1:B:512:CYS:HB2	1.95	0.48
1:A:379:PHE:HA	1:A:382:GLN:HG2	1.96	0.48
1:A:757:TRP:HZ3	1:A:773:VAL:HG23	1.79	0.48
1:B:588:ARG:NH1	1:B:618:PRO:O	2.47	0.48
1:A:866:GLY:O	1:A:870:LEU:CD1	2.60	0.48
1:B:607:PHE:CD2	1:B:861:LEU:HD11	2.49	0.48
1:B:695:ARG:CD	1:B:700:ASP:CB	2.85	0.48
1:B:739:ALA:O	1:B:790:GLY:HA3	2.13	0.48
1:B:601:GLN:OE1	1:B:801:VAL:CG1	2.62	0.48
1:B:673:PRO:HG2	1:B:674:ASN:ND2	2.29	0.48
1:A:191:ASP:HB2	1:A:269:VAL:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:ASN:O	1:B:541:MSE:HB3	2.13	0.48
1:B:689:ARG:O	1:B:693:LEU:HD11	2.14	0.48
1:B:790:GLY:C	1:B:813:ILE:HG13	2.35	0.48
1:A:175:HIS:HA	1:A:211:PHE:HA	1.95	0.48
1:A:787:LYS:HB2	1:A:809:ASN:C	2.34	0.48
1:A:514:GLY:O	1:A:515:PRO:C	2.53	0.48
1:B:599:LEU:HD12	1:B:599:LEU:N	2.28	0.48
1:B:601:GLN:HB3	1:B:798:VAL:O	2.14	0.48
1:A:415:TYR:HD2	1:A:490:ARG:CG	2.21	0.48
1:A:498:LYS:CD	1:A:498:LYS:N	2.76	0.48
1:B:387:ASN:HB2	1:B:836:TYR:HE2	1.78	0.48
1:B:695:ARG:HG2	1:B:695:ARG:HH11	1.68	0.47
1:B:741:PHE:CD2	1:B:788:PRO:HG2	2.49	0.47
1:A:811:VAL:O	1:A:811:VAL:CG2	2.58	0.47
1:B:729:ARG:HD3	1:B:773:VAL:CG2	2.38	0.47
1:A:220:PHE:CD2	1:A:220:PHE:C	2.84	0.47
1:B:236:LEU:HD23	1:B:239:ILE:HG13	1.95	0.47
1:A:724:ASN:OD1	1:A:724:ASN:N	2.41	0.47
1:B:834:ASP:C	1:B:836:TYR:N	2.68	0.47
1:B:440:GLU:HG3	1:B:440:GLU:O	2.13	0.47
1:A:807:PRO:HA	1:A:812:ILE:HG22	1.96	0.47
1:B:830:GLN:HB3	1:B:832:PHE:CD2	2.49	0.47
1:A:137:PHE:CD1	1:A:176:TYR:CD1	3.02	0.47
1:B:729:ARG:HG2	1:B:729:ARG:H	1.51	0.47
1:A:763:ARG:HB3	1:A:764:VAL:H	1.37	0.47
1:B:464:VAL:HG21	1:B:466:TRP:CZ2	2.49	0.47
1:A:599:LEU:CD1	1:A:856:PRO:HG2	2.36	0.47
1:A:179:ALA:HB1	1:A:262:LEU:CD2	2.44	0.47
1:A:404:LEU:CD1	1:A:404:LEU:C	2.49	0.47
1:B:225:PHE:CE1	1:B:294:TYR:CD2	3.03	0.47
1:A:554:LYS:HA	1:A:612:LEU:HD12	1.96	0.47
1:B:414:LYS:O	1:B:415:TYR:CB	2.62	0.47
1:B:274:VAL:HG23	1:B:278:MSE:CG	2.38	0.47
1:A:305:PHE:N	1:A:305:PHE:CD2	2.83	0.47
1:A:544:PHE:CE1	1:A:558:MSE:SE	3.17	0.47
1:A:220:PHE:CE2	1:A:260:ASN:CA	2.98	0.47
1:A:619:LYS:CD	1:A:877:ASP:O	2.62	0.47
1:A:563:ASP:O	1:A:564:ILE:C	2.49	0.47
1:B:252:PHE:CD2	1:B:296:MSE:HB3	2.49	0.47
1:B:514:GLY:N	1:B:515:PRO:CD	2.78	0.47
1:A:154:ARG:NH2	1:A:209:GLU:OE1	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ILE:HD12	1:A:288:GLU:HG2	1.97	0.47
1:B:364:SER:OG	1:B:863:TYR:O	2.32	0.47
1:B:515:PRO:O	1:B:560:ASN:ND2	2.48	0.47
1:B:174:CYS:SG	1:B:175:HIS:N	2.87	0.47
1:B:774:PRO:HB3	1:B:778:MSE:HE3	1.96	0.47
1:B:774:PRO:CB	1:B:778:MSE:HE3	2.44	0.47
1:B:779:SER:O	1:B:780:PHE:C	2.52	0.47
1:B:246:HIS:HE1	1:B:581:VAL:HG13	1.80	0.47
1:A:220:PHE:O	1:A:220:PHE:CG	2.68	0.47
1:A:455:ASP:CB	1:A:461:TYR:CE2	2.97	0.47
1:B:591:MSE:CG	1:B:606:VAL:HG22	2.44	0.47
1:B:440:GLU:OE1	1:B:440:GLU:O	2.33	0.47
1:A:719:PRO:HB3	1:A:820:VAL:O	2.14	0.47
1:A:641:MSE:HG3	1:A:642:VAL:H	1.78	0.47
1:B:394:ARG:NE	1:B:396:GLU:OE2	2.42	0.47
1:B:669:GLN:OE1	1:B:669:GLN:N	2.42	0.47
1:B:375:ASP:OD1	1:B:377:ASN:N	2.48	0.47
1:B:659:GLY:HA2	1:B:794:TRP:HB3	1.95	0.47
1:B:456:ARG:O	1:B:457:GLU:C	2.51	0.47
1:B:565:LEU:HD11	1:B:606:VAL:CG2	2.45	0.47
1:A:394:ARG:HB3	1:A:394:ARG:HE	1.53	0.47
1:B:806:GLU:HA	1:B:807:PRO:HD3	1.72	0.47
1:B:771:PRO:HB2	1:B:773:VAL:H	1.80	0.47
1:B:235:SER:O	1:B:237:VAL:CG2	2.63	0.47
1:A:591:MSE:HE1	1:A:634:PRO:HD2	1.96	0.47
1:B:250:ARG:NH2	1:B:295:ASP:CG	2.68	0.47
1:A:508:VAL:HG11	1:A:551:LEU:HB3	1.97	0.47
1:A:664:ASP:HB3	1:A:688:GLN:OE1	2.15	0.47
1:A:717:HIS:ND1	1:A:822:THR:HG21	2.29	0.47
1:B:301:ALA:C	1:B:302:TYR:CD2	2.88	0.47
1:B:387:ASN:CB	1:B:836:TYR:HE2	2.28	0.47
1:A:464:VAL:HG13	1:A:466:TRP:CE2	2.50	0.47
1:A:550:TYR:HD1	1:A:551:LEU:HG	1.80	0.47
1:B:349:GLY:O	1:B:351:GLY:N	2.46	0.46
1:A:468:GLY:HA3	1:B:808:HIS:CE1	2.50	0.46
1:B:819:ARG:O	1:B:820:VAL:CG1	2.62	0.46
1:A:208:THR:OG1	1:A:221:THR:O	2.24	0.46
1:A:787:LYS:HG3	1:A:809:ASN:O	2.16	0.46
1:A:280:PRO:O	1:A:280:PRO:CD	2.62	0.46
1:A:589:LEU:HA	1:A:620:TYR:HH	1.78	0.46
1:A:483:SER:OG	1:A:484:ASP:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:558:MSE:HB2	1:B:558:MSE:HE3	1.49	0.46
1:B:346:LEU:HB3	1:B:347:TYR:HD1	1.80	0.46
1:B:695:ARG:HA	1:B:835:TYR:CD1	2.48	0.46
1:A:150:ASN:HB3	1:A:151:TRP:CE3	2.50	0.46
1:A:384:LEU:C	1:A:384:LEU:HD12	2.36	0.46
1:B:561:VAL:CG2	1:B:563:ASP:HB2	2.46	0.46
1:A:389:PRO:HD2	1:A:390:GLN:H	1.80	0.46
1:A:741:PHE:CD1	1:A:741:PHE:C	2.88	0.46
1:A:404:LEU:O	1:A:404:LEU:CD1	2.30	0.46
1:A:700:ASP:C	1:A:702:SER:H	2.18	0.46
1:A:542:VAL:HG12	1:A:543:THR:N	2.28	0.46
1:A:555:TYR:CZ	1:A:615:MSE:HG2	2.49	0.46
1:B:411:LEU:HD21	1:B:493:VAL:HG21	1.97	0.46
1:A:659:GLY:HA2	1:A:794:TRP:HE3	1.81	0.46
1:A:296:MSE:HE3	1:A:306:ALA:HA	1.97	0.46
1:A:725:ASP:OD2	1:A:766:LEU:HD22	2.15	0.46
1:A:487:GLN:O	1:A:491:GLU:HB3	2.16	0.46
1:A:829:LEU:HA	1:A:829:LEU:HD12	1.74	0.46
1:A:413:LYS:O	1:A:420:ASP:HB2	2.15	0.46
1:B:716:ASP:N	1:B:716:ASP:OD1	2.49	0.46
1:B:353:MSE:HE2	1:B:512:CYS:CB	2.45	0.46
1:A:727:TYR:O	1:A:730:VAL:HG13	2.15	0.46
1:A:347:TYR:CD1	1:A:516:PRO:HD3	2.50	0.46
1:B:676:VAL:HG22	1:B:713:LYS:CE	2.39	0.46
1:A:670:ASN:HD21	1:A:722:LEU:CD2	2.28	0.46
1:A:486:PRO:HB2	1:A:490:ARG:CD	2.45	0.46
1:A:233:ILE:O	1:A:234:ASN:C	2.54	0.46
1:B:715:LEU:N	1:B:715:LEU:HD12	2.31	0.46
1:B:788:PRO:HG2	1:B:789:PHE:H	1.79	0.46
1:B:817:GLN:O	1:B:818:ALA:HB3	2.15	0.46
1:A:284:ALA:HA	1:A:287:ILE:HD11	1.97	0.46
1:A:252:PHE:HA	1:A:296:MSE:O	2.15	0.46
1:B:202:ASP:O	1:B:227:ARG:NH2	2.49	0.46
1:B:241:VAL:O	1:B:242:ASP:C	2.53	0.46
1:B:477:GLU:HB2	1:B:482:LEU:HD21	1.98	0.46
1:A:303:SER:OG	1:A:640:CYS:SG	2.68	0.46
1:A:233:ILE:CG1	1:A:233:ILE:O	2.63	0.46
1:B:345:ASP:C	1:B:346:LEU:HD13	2.35	0.46
1:B:684:LYS:HB2	1:B:688:GLN:OE1	2.16	0.46
1:B:695:ARG:CD	1:B:700:ASP:HB3	2.46	0.46
1:B:729:ARG:CD	1:B:773:VAL:CG2	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:831:GLY:HA3	1:B:856:PRO:HD3	1.97	0.46
1:B:221:THR:O	1:B:221:THR:HG22	2.16	0.46
1:B:729:ARG:HH21	1:B:772:LEU:C	2.18	0.46
1:B:231:THR:HB	1:B:298:TYR:CE1	2.51	0.46
1:B:583:MSE:O	1:B:584:LYS:CB	2.61	0.46
1:A:339:ARG:O	1:A:367:LYS:N	2.32	0.46
1:A:644:TYR:CD1	1:A:649:LYS:HB3	2.50	0.46
1:B:215:ASP:HB2	1:B:217:CYS:SG	2.56	0.46
1:B:535:ASP:OD1	1:B:539:LYS:CE	2.64	0.46
1:B:547:ILE:H	1:B:547:ILE:HG12	1.49	0.46
1:A:687:PHE:O	1:A:690:TYR:N	2.47	0.46
1:A:344:LEU:HD21	1:A:346:LEU:HD21	1.96	0.46
1:A:725:ASP:CA	1:A:766:LEU:HD13	2.38	0.46
1:A:511:ILE:HG23	1:A:553:PRO:CB	2.46	0.46
1:B:589:LEU:CD1	1:B:589:LEU:C	2.84	0.46
1:B:828:ARG:NH2	1:B:834:ASP:OD2	2.29	0.46
1:A:509:ASP:OD1	1:A:509:ASP:N	2.46	0.46
1:A:593:VAL:HG11	1:A:602:PHE:CD1	2.50	0.46
1:B:209:GLU:HB2	1:B:221:THR:CB	2.45	0.46
1:A:653:LYS:HA	1:A:653:LYS:HE3	1.97	0.46
1:B:464:VAL:CG2	1:B:466:TRP:CZ2	2.98	0.46
1:A:505:PRO:HA	1:A:551:LEU:HD23	1.97	0.46
1:B:343:LEU:HB2	1:B:368:LEU:HD22	1.97	0.45
1:B:783:GLY:O	1:B:784:LYS:C	2.54	0.45
1:B:805:ALA:HB1	1:B:812:ILE:HD13	1.97	0.45
1:B:699:LEU:HG	1:B:701:TRP:CG	2.51	0.45
1:B:279:ASP:H	1:B:283:LYS:HD3	1.81	0.45
1:A:663:SER:CB	1:A:688:GLN:NE2	2.75	0.45
1:B:460:ILE:H	1:B:460:ILE:HD13	1.80	0.45
1:A:642:VAL:O	1:A:642:VAL:HG23	2.15	0.45
1:A:411:LEU:CD1	1:A:411:LEU:N	2.80	0.45
1:B:144:ALA:O	1:B:145:ASP:HB2	2.17	0.45
1:A:415:TYR:N	1:A:415:TYR:CD1	2.85	0.45
1:B:580:LEU:HD22	1:B:608:LEU:HD21	1.98	0.45
1:B:733:ILE:CG1	1:B:734:PRO:HD2	2.46	0.45
1:B:805:ALA:O	1:B:806:GLU:HG3	2.15	0.45
1:A:686:GLU:HA	1:A:689:ARG:CZ	2.46	0.45
1:B:729:ARG:NE	1:B:773:VAL:CG2	2.76	0.45
1:B:779:SER:O	1:B:782:LYS:N	2.48	0.45
1:B:670:ASN:HD21	1:B:722:LEU:H	1.64	0.45
1:A:186:TYR:CD1	1:A:268:LYS:HD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:ILE:HD13	1:A:462:PHE:CD1	2.51	0.45
1:A:233:ILE:O	1:A:233:ILE:HG13	2.16	0.45
1:B:180:LYS:HE3	1:B:183:ASN:HA	1.97	0.45
1:A:626:ASP:C	1:A:626:ASP:OD1	2.55	0.45
1:B:687:PHE:O	1:B:690:TYR:HB3	2.17	0.45
1:B:739:ALA:HB3	1:B:791:ARG:H	1.81	0.45
1:B:805:ALA:HB2	1:B:846:TYR:CE1	2.51	0.45
1:A:145:ASP:OD2	1:A:148:ARG:NH1	2.50	0.45
1:A:174:CYS:C	1:A:175:HIS:HD2	2.20	0.45
1:A:810:GLN:O	1:A:811:VAL:CG1	2.64	0.45
1:A:723:ASN:ND2	1:A:723:ASN:O	2.50	0.45
1:B:307:ASN:HD21	1:B:586:GLN:CD	2.12	0.45
1:B:535:ASP:CG	1:B:539:LYS:HE3	2.36	0.45
1:B:734:PRO:O	1:B:735:VAL:HG13	2.16	0.45
1:A:741:PHE:HD2	1:A:788:PRO:HB2	1.82	0.45
1:A:772:LEU:HD12	1:A:773:VAL:H	1.78	0.45
1:A:619:LYS:HD3	1:A:877:ASP:O	2.15	0.45
1:B:170:LEU:CD2	1:B:211:PHE:CE1	2.98	0.45
1:B:740:ASN:CA	1:B:789:PHE:O	2.64	0.45
1:B:811:VAL:CG2	1:B:811:VAL:O	2.58	0.45
1:A:787:LYS:CB	1:A:809:ASN:O	2.62	0.45
1:A:285:GLN:O	1:A:286:LEU:C	2.55	0.45
1:B:776:TYR:O	1:B:779:SER:N	2.49	0.45
1:A:347:TYR:CD2	1:A:347:TYR:N	2.83	0.45
1:B:223:ARG:HD2	1:B:253:LEU:HD22	1.98	0.45
1:B:469:TYR:HD1	1:B:473:GLU:HB3	1.82	0.45
1:A:801:VAL:HG21	1:A:829:LEU:HB3	1.99	0.45
1:B:730:VAL:O	1:B:733:ILE:HB	2.17	0.45
1:B:171:LYS:HA	1:B:171:LYS:HE2	1.99	0.45
1:B:218:HIS:O	1:B:262:LEU:HG	2.17	0.45
1:A:676:VAL:HA	1:A:714:LEU:O	2.17	0.45
1:A:683:PRO:HB2	1:A:689:ARG:HA	1.99	0.45
1:B:446:LEU:HD23	1:B:446:LEU:N	2.22	0.45
1:B:823:ILE:O	1:B:826:ASN:N	2.49	0.45
1:A:660:ASP:OD2	1:A:660:ASP:N	2.50	0.45
1:B:375:ASP:CG	2:B:1000:SAH:HO2'	2.21	0.45
1:B:343:LEU:HD12	1:B:344:LEU:N	2.30	0.45
1:B:349:GLY:C	1:B:350:CYS:SG	2.96	0.45
1:B:718:GLN:N	1:B:822:THR:HB	2.32	0.45
1:B:791:ARG:CD	1:B:792:LEU:N	2.64	0.45
1:B:691:ILE:HD11	1:B:832:PHE:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:787:LYS:HB3	1:A:811:VAL:CG1	2.41	0.45
1:A:553:PRO:HB2	1:A:555:TYR:O	2.16	0.45
1:A:555:TYR:CE2	1:A:618:PRO:CD	2.94	0.45
1:A:363:LEU:HB3	1:A:863:TYR:CD1	2.52	0.45
1:A:672:GLN:HG3	1:A:672:GLN:O	2.16	0.45
1:B:565:LEU:HB3	1:B:637:PHE:CE2	2.52	0.45
1:A:447:VAL:O	1:A:447:VAL:CG2	2.64	0.45
1:B:791:ARG:NE	1:B:813:ILE:O	2.50	0.45
1:B:793:TRP:HB2	1:B:794:TRP:CD1	2.52	0.45
1:A:281:LYS:O	1:A:285:GLN:CG	2.60	0.45
1:B:646:GLU:CD	1:B:646:GLU:C	2.74	0.45
1:A:596:CYS:HB3	1:A:623:PRO:CB	2.28	0.45
1:B:287:ILE:HD11	1:B:293:TYR:CE2	2.52	0.45
1:B:823:ILE:HD13	1:B:845:LYS:CB	2.47	0.45
1:B:395:ASN:C	1:B:395:ASN:HD22	2.20	0.44
1:B:793:TRP:N	1:B:793:TRP:CD1	2.84	0.44
1:B:820:VAL:O	1:B:821:LEU:HD13	2.17	0.44
1:A:173:ARG:NH2	1:A:216:GLN:HA	2.32	0.44
1:A:653:LYS:HD2	1:A:653:LYS:H	1.83	0.44
1:A:487:GLN:O	1:A:491:GLU:CB	2.65	0.44
1:A:451:TYR:HD1	1:A:460:ILE:HD12	1.81	0.44
1:A:484:ASP:O	1:A:485:CYS:C	2.55	0.44
1:A:483:SER:C	1:A:485:CYS:H	2.21	0.44
1:A:570:GLY:O	1:A:571:TYR:C	2.54	0.44
1:B:557:LEU:HD21	1:B:861:LEU:HD13	1.99	0.44
1:B:364:SER:HA	1:B:863:TYR:HE1	1.83	0.44
1:B:675:ASP:CA	1:B:718:GLN:NE2	2.75	0.44
1:A:516:PRO:O	1:A:517:CYS:C	2.56	0.44
1:A:596:CYS:N	1:A:627:VAL:HG11	2.32	0.44
1:B:670:ASN:C	1:B:670:ASN:OD1	2.55	0.44
1:B:186:TYR:HD1	1:B:268:LYS:CG	2.29	0.44
1:A:143:ALA:CB	1:A:177:ARG:HH21	2.30	0.44
1:B:142:VAL:HG12	1:B:175:HIS:O	2.17	0.44
1:A:780:PHE:HD2	1:A:786:LEU:CD2	2.30	0.44
1:A:278:MSE:C	1:A:279:ASP:OD1	2.55	0.44
1:A:376:PHE:CD2	1:A:377:ASN:N	2.86	0.44
1:B:577:LEU:HD12	1:B:577:LEU:HA	1.77	0.44
1:A:752:ASN:O	1:A:753:ASN:CB	2.66	0.44
1:A:602:PHE:O	1:A:799:PRO:O	2.35	0.44
1:B:718:GLN:C	1:B:822:THR:HB	2.38	0.44
1:A:792:LEU:O	1:A:815:PRO:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:THR:OG1	1:A:356:GLY:N	2.51	0.44
1:B:589:LEU:HD12	1:B:589:LEU:O	2.18	0.44
1:B:591:MSE:HE2	1:B:640:CYS:HB2	2.00	0.44
1:B:157:ARG:HB3	1:B:157:ARG:HE	1.42	0.44
1:A:173:ARG:CB	1:A:212:GLU:O	2.66	0.44
1:B:549:ALA:CA	1:B:583:MSE:HE1	2.48	0.44
1:A:479:ILE:O	1:A:482:LEU:HB2	2.18	0.44
1:A:653:LYS:HD2	1:A:653:LYS:N	2.32	0.44
1:A:812:ILE:CG2	1:A:820:VAL:HG22	2.45	0.44
1:B:338:THR:O	1:B:338:THR:CG2	2.66	0.44
1:B:616:VAL:O	1:B:868:ALA:HB1	2.17	0.44
1:A:279:ASP:HB3	1:A:280:PRO:HD3	1.98	0.44
1:B:772:LEU:N	1:B:774:PRO:HD2	2.32	0.44
1:A:542:VAL:HG22	1:A:575:TYR:OH	2.17	0.44
1:B:298:TYR:HD1	1:B:305:PHE:CE1	2.35	0.44
1:B:579:CYS:O	1:B:583:MSE:HB2	2.18	0.44
1:A:193:TYR:CE1	1:A:269:VAL:HB	2.53	0.44
1:B:496:GLY:CA	1:B:501:ILE:HD13	2.46	0.44
1:B:821:LEU:HD12	1:B:821:LEU:HA	1.80	0.44
1:B:837:ARG:NH1	1:B:837:ARG:CG	2.65	0.44
1:A:757:TRP:CD2	1:A:778:MSE:HE3	2.53	0.44
1:B:304:THR:HG23	1:B:588:ARG:HB2	2.00	0.44
1:A:302:TYR:O	1:A:303:SER:C	2.50	0.44
1:B:391:THR:HG22	1:B:393:VAL:HG23	2.00	0.44
1:B:589:LEU:CD1	1:B:640:CYS:SG	3.05	0.44
1:B:451:TYR:CD2	1:B:452:GLY:N	2.86	0.44
1:B:686:GLU:CA	1:B:689:ARG:NH2	2.79	0.44
1:B:791:ARG:HB2	1:B:813:ILE:HG13	2.00	0.44
1:B:657:LEU:HD23	1:B:795:ASP:O	2.18	0.44
1:B:812:ILE:HG23	1:B:820:VAL:HG22	1.99	0.44
1:B:457:GLU:CB	1:B:461:TYR:HH	2.17	0.44
1:A:456:ARG:HA	1:A:456:ARG:HD3	1.78	0.44
1:A:557:LEU:HD22	1:A:609:TRP:CZ2	2.52	0.44
1:A:179:ALA:O	1:A:185:VAL:HG12	2.18	0.44
1:B:143:ALA:HB1	1:B:147:ALA:HB2	1.96	0.44
1:B:207:ILE:HD12	1:B:209:GLU:H	1.83	0.44
1:A:787:LYS:CG	1:A:809:ASN:O	2.66	0.44
1:B:233:ILE:HD12	1:B:578:SER:OG	2.18	0.44
1:A:232:VAL:HG12	1:A:233:ILE:CG2	2.46	0.44
1:A:593:VAL:CG1	1:A:602:PHE:CD1	3.01	0.44
1:B:663:SER:HB2	1:B:688:GLN:HE22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:784:LYS:O	1:B:785:SER:C	2.55	0.43
1:B:828:ARG:CG	1:B:828:ARG:NH2	2.73	0.43
1:B:603:ARG:CZ	1:B:830:GLN:NE2	2.79	0.43
1:B:142:VAL:CG1	1:B:175:HIS:N	2.76	0.43
1:A:722:LEU:HB3	1:A:726:ASP:HB2	1.99	0.43
1:B:554:LYS:O	1:B:611:ALA:HA	2.17	0.43
1:A:444:GLU:CG	1:A:445:LYS:N	2.81	0.43
1:B:184:VAL:CG1	1:B:186:TYR:CE1	3.00	0.43
1:A:737:LYS:HZ1	1:A:795:ASP:CG	2.21	0.43
1:B:386:TYR:HB2	1:B:839:PHE:CE2	2.53	0.43
1:B:781:ILE:O	1:B:782:LYS:C	2.55	0.43
1:A:194:VAL:HG12	1:A:195:LYS:N	2.33	0.43
1:A:733:ILE:HD12	1:A:739:ALA:HB1	2.00	0.43
1:B:719:PRO:HB3	1:B:820:VAL:HG12	1.99	0.43
1:B:790:GLY:N	1:B:813:ILE:HD11	2.33	0.43
1:A:254:SER:OG	1:A:256:GLU:N	2.51	0.43
1:A:347:TYR:O	2:A:1000:SAH:HG1	2.18	0.43
1:A:645:ASP:N	1:A:645:ASP:OD1	2.29	0.43
1:A:384:LEU:C	1:A:384:LEU:CD1	2.87	0.43
1:B:139:GLY:O	1:B:140:SER:HB3	2.17	0.43
1:B:580:LEU:O	1:B:585:TYR:HB2	2.17	0.43
1:B:589:LEU:HD12	1:B:589:LEU:C	2.39	0.43
1:B:734:PRO:O	1:B:735:VAL:HG12	2.16	0.43
1:A:143:ALA:O	1:A:144:ALA:C	2.56	0.43
1:A:154:ARG:NH2	1:A:170:LEU:HD21	2.33	0.43
1:B:772:LEU:CB	1:B:774:PRO:CG	2.97	0.43
1:B:227:ARG:O	1:B:230:ASP:N	2.51	0.43
1:A:343:LEU:HB3	1:A:370:THR:HA	2.00	0.43
1:A:763:ARG:HH11	1:A:771:PRO:HB3	1.82	0.43
1:B:446:LEU:HA	1:B:446:LEU:HD22	1.71	0.43
1:A:586:GLN:N	1:A:611:ALA:O	2.51	0.43
1:B:391:THR:CG2	1:B:393:VAL:HG23	2.49	0.43
1:A:308:ILE:HG23	1:A:309:SER:N	2.32	0.43
1:B:703:PHE:N	1:B:703:PHE:CD2	2.87	0.43
1:B:175:HIS:HE1	1:B:209:GLU:HG2	1.83	0.43
1:A:274:VAL:HG23	1:A:295:ASP:CA	2.47	0.43
1:B:546:ASP:O	1:B:549:ALA:HB3	2.19	0.43
1:A:615:MSE:HE2	1:A:615:MSE:HB2	1.83	0.43
1:B:439:ASP:O	1:B:440:GLU:HB3	2.19	0.43
1:B:740:ASN:C	1:B:789:PHE:O	2.57	0.43
1:B:806:GLU:O	1:B:810:GLN:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:TRP:O	1:A:151:TRP:HD1	2.01	0.43
1:B:286:LEU:HA	1:B:289:SER:OG	2.17	0.43
1:B:229:GLU:O	1:B:234:ASN:OD1	2.37	0.43
1:B:237:VAL:HG13	1:B:246:HIS:CD2	2.53	0.43
1:A:564:ILE:CG2	1:A:573:GLY:CA	2.97	0.43
1:B:694:SER:OG	1:B:697:ASP:OD2	2.37	0.43
1:A:172:ALA:CB	1:A:175:HIS:NE2	2.82	0.43
1:A:155:TYR:CE2	1:A:172:ALA:HB3	2.54	0.43
1:A:806:GLU:O	1:A:810:GLN:HG2	2.19	0.43
1:A:247:ASP:HA	1:A:248:PRO:HD3	1.72	0.43
1:A:556:VAL:HB	1:A:610:GLY:HA3	2.00	0.43
1:B:413:LYS:NZ	1:B:414:LYS:CG	2.80	0.43
1:B:672:GLN:HE21	1:B:673:PRO:HD2	1.84	0.43
1:B:672:GLN:NE2	1:B:674:ASN:H	2.15	0.43
1:A:635:ASN:O	1:A:637:PHE:N	2.51	0.43
1:B:504:LEU:HB3	1:B:505:PRO:CD	2.49	0.43
1:B:498:LYS:HA	1:B:498:LYS:HD3	1.50	0.43
1:B:817:GLN:HB2	1:B:817:GLN:HE21	1.57	0.43
1:A:155:TYR:OH	1:A:175:HIS:CD2	2.72	0.43
1:A:580:LEU:HD23	1:A:587:ALA:HB1	2.01	0.43
1:B:621:PRO:HG3	1:B:860:ALA:CB	2.48	0.43
1:B:658:LEU:O	1:B:660:ASP:N	2.52	0.43
1:A:278:MSE:HB2	1:A:283:LYS:HE3	2.01	0.43
1:A:482:LEU:N	1:A:482:LEU:CD2	2.82	0.43
1:A:625:TYR:HA	1:A:653:LYS:HB2	2.01	0.43
1:A:452:GLY:HA3	1:A:455:ASP:HB2	2.01	0.43
1:B:249:ARG:O	1:B:293:TYR:CE2	2.71	0.43
1:A:389:PRO:CG	1:A:390:GLN:N	2.81	0.43
1:B:559:GLU:OE2	1:B:605:ARG:HD2	2.19	0.42
1:B:237:VAL:CG1	1:B:246:HIS:HD2	2.31	0.42
1:A:186:TYR:HE2	1:A:265:ILE:CG2	2.29	0.42
1:B:300:VAL:HG23	1:B:300:VAL:O	2.19	0.42
1:B:656:LEU:CD2	1:B:656:LEU:N	2.69	0.42
1:B:675:ASP:O	1:B:715:LEU:HA	2.19	0.42
1:B:221:THR:O	1:B:221:THR:CG2	2.63	0.42
1:A:658:LEU:HD11	1:A:662:ILE:HD13	2.00	0.42
1:B:237:VAL:CG1	1:B:246:HIS:CD2	3.02	0.42
1:B:814:HIS:CD2	1:B:815:PRO:HD2	2.54	0.42
1:B:699:LEU:CG	1:B:701:TRP:CG	3.00	0.42
1:A:376:PHE:HD2	1:A:377:ASN:N	2.16	0.42
1:B:574:LYS:HG2	1:B:574:LYS:H	1.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:TYR:CD2	1:B:878:PRO:HB3	2.55	0.42
1:A:474:ASP:C	1:A:475:THR:CG2	2.87	0.42
1:A:665:LEU:CD2	1:A:814:HIS:HE1	2.17	0.42
1:A:624:THR:O	1:A:653:LYS:CG	2.60	0.42
1:A:588:ARG:HH11	1:A:617:LEU:HG	1.85	0.42
1:A:493:VAL:O	1:A:494:GLN:C	2.55	0.42
1:B:410:VAL:CG1	1:B:411:LEU:H	2.26	0.42
1:B:186:TYR:CD2	1:B:186:TYR:N	2.87	0.42
1:B:750:GLY:O	1:B:751:ALA:C	2.58	0.42
1:B:790:GLY:H	1:B:813:ILE:HD11	1.84	0.42
1:A:249:ARG:HB2	1:A:292:LEU:CD2	2.49	0.42
1:A:537:LYS:C	1:A:539:LYS:N	2.72	0.42
1:A:603:ARG:NH1	1:A:852:ALA:O	2.52	0.42
1:B:138:ILE:CD1	1:B:139:GLY:H	2.32	0.42
1:B:170:LEU:HD22	1:B:211:PHE:HZ	1.85	0.42
1:A:786:LEU:C	1:A:788:PRO:CD	2.88	0.42
1:A:343:LEU:HD22	1:A:344:LEU:N	2.33	0.42
1:A:589:LEU:HD23	1:A:589:LEU:N	2.34	0.42
1:A:653:LYS:O	1:A:654:LYS:C	2.58	0.42
1:A:759:PRO:O	1:A:760:GLU:CB	2.43	0.42
1:B:624:THR:CG2	1:B:624:THR:O	2.68	0.42
1:B:589:LEU:HD12	1:B:640:CYS:SG	2.59	0.42
1:A:411:LEU:N	1:A:411:LEU:HD12	2.35	0.42
1:B:735:VAL:CG2	1:B:735:VAL:O	2.65	0.42
1:B:737:LYS:HA	1:B:793:TRP:CE2	2.55	0.42
1:A:137:PHE:C	1:A:138:ILE:O	2.55	0.42
1:A:211:PHE:HD1	1:A:213:GLY:N	2.17	0.42
1:A:375:ASP:OD1	2:A:1000:SAH:O2'	2.36	0.42
1:A:580:LEU:HD12	1:A:580:LEU:HA	1.76	0.42
1:A:757:TRP:CE3	1:A:778:MSE:HE3	2.55	0.42
1:A:763:ARG:NH1	1:A:773:VAL:O	2.44	0.42
1:B:586:GLN:O	1:B:610:GLY:HA2	2.19	0.42
1:B:250:ARG:HH22	1:B:296:MSE:HE2	1.84	0.42
1:A:628:VAL:O	1:A:628:VAL:CG1	2.67	0.42
1:B:347:TYR:OH	1:B:540:GLN:OE1	2.35	0.42
1:B:658:LEU:HD21	1:B:791:ARG:HH21	1.85	0.42
1:B:727:TYR:O	1:B:730:VAL:CG1	2.68	0.42
1:A:272:VAL:HG21	1:A:286:LEU:HD23	2.02	0.42
1:A:343:LEU:CD2	1:A:344:LEU:N	2.83	0.42
1:A:734:PRO:O	1:A:791:ARG:NE	2.52	0.42
1:A:764:VAL:CG2	1:A:772:LEU:HD12	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:VAL:CG2	1:A:186:TYR:CE2	3.02	0.42
1:A:880:TYR:HD1	1:A:881:GLN:H	1.68	0.42
1:B:832:PHE:CZ	1:B:852:ALA:CB	3.02	0.42
1:A:139:GLY:O	1:A:140:SER:HB2	2.19	0.42
1:A:141:PRO:O	1:A:142:VAL:CG2	2.62	0.42
1:A:575:TYR:C	1:A:575:TYR:CD1	2.93	0.42
1:A:812:ILE:HG13	1:A:812:ILE:O	2.20	0.42
1:B:198:GLU:O	1:B:199:ASN:C	2.57	0.42
1:B:822:THR:H	1:B:825:GLU:CD	2.23	0.42
1:B:838:LEU:C	1:B:839:PHE:CD2	2.94	0.42
1:A:272:VAL:CG1	1:A:286:LEU:HD22	2.50	0.42
1:A:273:HIS:ND1	1:A:294:TYR:CE2	2.88	0.42
1:B:229:GLU:O	1:B:234:ASN:CG	2.58	0.42
1:A:477:GLU:OE1	1:A:481:ASN:ND2	2.52	0.42
1:A:447:VAL:O	1:A:447:VAL:HG22	2.20	0.42
1:A:500:LYS:NZ	1:A:507:ASP:OD2	2.38	0.42
1:B:741:PHE:HB3	1:B:789:PHE:CB	2.49	0.41
1:A:225:PHE:CZ	1:A:294:TYR:CD1	3.08	0.41
1:B:596:CYS:O	1:B:624:THR:N	2.53	0.41
1:B:247:ASP:O	1:B:249:ARG:N	2.53	0.41
1:B:633:ALA:HA	1:B:634:PRO:HD3	1.86	0.41
1:A:148:ARG:HG3	1:A:155:TYR:CD1	2.55	0.41
1:A:440:GLU:CG	1:A:441:PHE:N	2.64	0.41
1:A:338:THR:CG2	1:A:367:LYS:HZ3	2.31	0.41
1:B:391:THR:HG22	1:B:392:GLU:N	2.20	0.41
1:A:635:ASN:O	1:A:636:ALA:C	2.58	0.41
1:A:793:TRP:N	1:A:796:GLU:OE2	2.36	0.41
1:B:180:LYS:HE2	1:B:182:ASP:O	2.20	0.41
1:A:419:VAL:HG12	1:A:419:VAL:O	2.20	0.41
1:B:659:GLY:H	1:B:794:TRP:HB3	1.85	0.41
1:B:278:MSE:SE	1:B:282:ALA:CB	3.13	0.41
1:A:737:LYS:NZ	1:A:795:ASP:CG	2.73	0.41
1:B:353:MSE:O	1:B:357:LEU:HB2	2.20	0.41
1:B:793:TRP:HA	1:B:815:PRO:HG3	2.02	0.41
1:B:386:TYR:CD2	1:B:837:ARG:HB2	2.56	0.41
1:A:180:LYS:HB2	1:A:185:VAL:CG1	2.51	0.41
1:B:154:ARG:NE	1:B:209:GLU:OE1	2.52	0.41
1:A:692:ARG:C	1:A:693:LEU:HD12	2.39	0.41
1:A:512:CYS:HA	1:A:557:LEU:O	2.20	0.41
1:A:757:TRP:CH2	1:A:763:ARG:CZ	3.04	0.41
1:A:803:THR:OG1	1:A:847:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:TYR:O	1:A:303:SER:HB2	2.20	0.41
1:B:814:HIS:CD2	1:B:816:THR:N	2.55	0.41
1:B:695:ARG:CA	1:B:835:TYR:CE1	2.96	0.41
1:B:280:PRO:CG	1:B:281:LYS:N	2.84	0.41
1:B:772:LEU:C	1:B:773:VAL:HG22	2.31	0.41
1:A:555:TYR:CE2	1:A:618:PRO:HG3	2.56	0.41
1:A:656:LEU:HA	1:A:656:LEU:HD22	1.90	0.41
1:B:513:GLY:N	1:B:557:LEU:O	2.53	0.41
1:A:735:VAL:O	1:A:735:VAL:HG12	2.19	0.41
1:A:447:VAL:HG13	1:A:463:LYS:HB3	2.01	0.41
1:B:841:PRO:HG2	1:B:843:LYS:HE3	2.02	0.41
1:A:402:LEU:HD22	1:A:547:ILE:HG12	2.02	0.41
1:B:545:MSE:HE3	1:B:576:ALA:HA	2.01	0.41
1:B:810:GLN:O	1:B:811:VAL:CG1	2.69	0.41
1:A:154:ARG:NE	1:A:170:LEU:CD2	2.80	0.41
1:B:154:ARG:O	1:B:171:LYS:HE2	2.21	0.41
1:A:781:ILE:CD1	1:A:786:LEU:HD21	2.49	0.41
1:A:838:LEU:O	1:A:845:LYS:HE2	2.19	0.41
1:B:617:LEU:HD12	1:B:618:PRO:CD	2.51	0.41
1:A:865:LEU:CD2	1:A:865:LEU:C	2.88	0.41
1:A:486:PRO:O	1:A:487:GLN:C	2.58	0.41
1:A:876:SER:OG	1:A:876:SER:O	2.30	0.41
1:B:659:GLY:O	1:B:663:SER:OG	2.37	0.41
1:B:806:GLU:N	1:B:810:GLN:HE21	2.13	0.41
1:B:819:ARG:CZ	1:B:825:GLU:OE2	2.69	0.41
1:B:134:GLU:CD	1:B:135:PRO:HD2	2.29	0.41
1:A:543:THR:O	1:A:544:PHE:C	2.57	0.41
1:A:557:LEU:HD11	1:A:607:PHE:HB3	2.03	0.41
1:A:266:ILE:H	1:A:266:ILE:HG12	1.31	0.41
1:A:739:ALA:HB3	1:A:791:ARG:CG	2.47	0.41
1:A:652:LEU:H	1:A:652:LEU:HD23	1.85	0.41
1:B:445:LYS:HB3	1:B:465:GLN:OE1	2.19	0.41
1:B:462:PHE:HE2	1:B:479:ILE:HD13	1.85	0.41
1:B:554:LYS:HD3	1:B:615:MSE:HE2	1.99	0.41
1:A:267:SER:OG	1:A:268:LYS:N	2.52	0.41
1:A:269:VAL:CG2	1:A:270:LYS:N	2.84	0.41
1:B:180:LYS:HE2	1:B:183:ASN:HA	2.03	0.41
1:A:593:VAL:HG21	1:A:602:PHE:HE1	1.85	0.41
1:B:571:TYR:CD2	1:B:571:TYR:C	2.94	0.41
1:B:510:VAL:HG12	1:B:511:ILE:N	2.35	0.41
1:B:144:ALA:O	1:B:145:ASP:OD2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:HIS:HB2	1:B:262:LEU:CD1	2.48	0.41
1:A:822:THR:HG23	1:A:825:GLU:CG	2.50	0.41
1:B:604:MSE:SE	1:B:641:MSE:CE	2.92	0.41
1:B:343:LEU:HD12	1:B:511:ILE:HA	2.03	0.41
1:B:455:ASP:O	1:B:456:ARG:HB2	2.21	0.41
1:B:457:GLU:O	1:B:461:TYR:CE2	2.74	0.41
1:A:686:GLU:HA	1:A:689:ARG:NH1	2.36	0.41
1:A:249:ARG:HB2	1:A:292:LEU:HD22	2.02	0.41
1:A:204:ILE:HD13	1:A:204:ILE:HG21	1.78	0.41
1:B:135:PRO:HD2	1:B:135:PRO:O	2.19	0.41
1:A:541:MSE:HE3	1:A:572:LEU:O	2.21	0.41
1:A:580:LEU:HD23	1:A:587:ALA:HB2	2.03	0.41
1:B:223:ARG:HD2	1:B:253:LEU:CD2	2.50	0.41
1:A:814:HIS:CD2	1:A:815:PRO:N	2.89	0.41
1:B:855:VAL:N	1:B:856:PRO:CD	2.84	0.41
1:B:138:ILE:HG12	1:B:139:GLY:N	2.24	0.41
1:A:657:LEU:HD23	1:A:795:ASP:C	2.42	0.41
1:B:400:GLU:H	1:B:400:GLU:HG3	1.70	0.41
1:B:353:MSE:N	2:B:1000:SAH:O	2.47	0.41
1:B:733:ILE:HA	1:B:734:PRO:HD3	1.92	0.41
1:A:307:ASN:ND2	1:A:586:GLN:NE2	2.69	0.41
1:A:776:TYR:C	1:A:776:TYR:CD2	2.95	0.41
1:B:491:GLU:O	1:B:494:GLN:HB2	2.21	0.41
1:B:842:ILE:N	1:B:842:ILE:HD12	2.36	0.41
1:A:153:LYS:HE3	1:A:153:LYS:HB2	1.40	0.41
1:A:629:VAL:HG23	1:A:629:VAL:O	2.21	0.41
1:B:362:ALA:HB2	1:B:699:LEU:CD2	2.51	0.40
1:B:145:ASP:O	1:B:148:ARG:HG3	2.21	0.40
1:B:272:VAL:HG13	1:B:273:HIS:H	1.84	0.40
1:A:714:LEU:C	1:A:714:LEU:CD2	2.87	0.40
1:A:284:ALA:O	1:A:288:GLU:HG2	2.21	0.40
1:A:454:SER:C	1:A:456:ARG:H	2.22	0.40
1:A:457:GLU:O	1:A:458:ASN:C	2.56	0.40
1:B:622:LEU:HB3	1:B:623:PRO:CD	2.51	0.40
1:B:637:PHE:N	1:B:637:PHE:HD2	2.13	0.40
1:B:404:LEU:HD13	1:B:405:LEU:N	2.36	0.40
1:B:865:LEU:O	1:B:865:LEU:HD12	2.20	0.40
1:B:347:TYR:CD1	1:B:347:TYR:N	2.89	0.40
1:B:733:ILE:HG13	1:B:739:ALA:HB1	2.03	0.40
1:B:819:ARG:O	1:B:820:VAL:CB	2.68	0.40
1:A:184:VAL:HG22	1:A:185:VAL:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:ARG:O	1:A:699:LEU:N	2.54	0.40
1:A:273:HIS:C	1:A:273:HIS:CD2	2.92	0.40
1:A:763:ARG:HD3	1:A:763:ARG:HA	1.93	0.40
1:B:798:VAL:HG21	1:B:829:LEU:HD21	2.02	0.40
1:A:568:ALA:C	1:A:569:ASP:OD2	2.60	0.40
1:B:244:HIS:CE1	1:B:552:LYS:NZ	2.89	0.40
1:A:534:LYS:HB3	1:A:534:LYS:HE2	1.64	0.40
1:B:794:TRP:N	1:B:794:TRP:CD1	2.83	0.40
1:B:803:THR:HG22	1:B:847:ILE:HA	2.03	0.40
1:A:176:TYR:OH	1:A:212:GLU:CD	2.60	0.40
1:A:814:HIS:CD2	1:A:815:PRO:CD	3.05	0.40
1:B:466:TRP:HZ2	1:B:475:THR:CG2	2.24	0.40
1:B:287:ILE:HD11	1:B:293:TYR:CZ	2.56	0.40
1:A:495:GLU:CA	1:A:495:GLU:OE1	2.66	0.40
1:A:594:ALA:HA	1:A:857:VAL:CG2	2.51	0.40
1:B:399:ASP:N	1:B:399:ASP:OD1	2.50	0.40
1:A:296:MSE:HE2	1:A:305:PHE:HB3	2.02	0.40
1:A:580:LEU:HD22	1:A:608:LEU:HD23	2.02	0.40
1:B:231:THR:C	1:B:233:ILE:N	2.75	0.40
1:B:723:ASN:OD1	1:B:726:ASP:CG	2.58	0.40
1:A:486:PRO:HG2	1:A:487:GLN:H	1.87	0.40
1:B:791:ARG:HG3	1:B:792:LEU:N	2.37	0.40
1:A:173:ARG:HH22	1:A:216:GLN:HA	1.87	0.40
1:A:741:PHE:O	1:A:742:ARG:C	2.59	0.40
1:A:659:GLY:HA3	1:A:794:TRP:HB3	2.03	0.40
1:B:722:LEU:O	1:B:723:ASN:C	2.60	0.40
1:A:865:LEU:O	1:A:866:GLY:C	2.60	0.40
1:B:534:LYS:C	1:B:534:LYS:NZ	2.73	0.40
1:B:728:GLU:OE2	1:B:767:SER:CB	2.69	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	670/784 (86%)	591 (88%)	62 (9%)	17 (2%)	7	41
1	B	665/784 (85%)	607 (91%)	43 (6%)	15 (2%)	8	44
All	All	1335/1568 (85%)	1198 (90%)	105 (8%)	32 (2%)	7	43

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	VAL
1	A	634	PRO
1	A	646	GLU
1	B	140	SER
1	B	279	ASP
1	B	773	VAL
1	B	775	ASP
1	B	883	PRO
1	A	764	VAL
1	B	646	GLU
1	B	820	VAL
1	A	135	PRO
1	A	417	GLN
1	A	567	PHE
1	A	650	PRO
1	A	760	GLU
1	A	883	PRO
1	A	653	LYS
1	A	781	ILE
1	B	144	ALA
1	B	350	CYS
1	A	140	SER
1	B	236	LEU
1	B	884	PRO
1	A	215	ASP
1	A	290	CYS
1	B	138	ILE
1	B	788	PRO
1	A	759	PRO
1	A	787	LYS
1	B	142	VAL
1	B	266	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	564/652 (86%)	413 (73%)	151 (27%)	0	2
1	B	544/652 (83%)	384 (71%)	160 (29%)	0	1
All	All	1108/1304 (85%)	797 (72%)	311 (28%)	0	1

All (311) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	ILE
1	A	140	SER
1	A	153	LYS
1	A	181	VAL
1	A	185	VAL
1	A	192	VAL
1	A	198	GLU
1	A	208	THR
1	A	211	PHE
1	A	214	THR
1	A	215	ASP
1	A	216	GLN
1	A	220	PHE
1	A	230	ASP
1	A	233	ILE
1	A	234	ASN
1	A	235	SER
1	A	238	SER
1	A	251	VAL
1	A	253	LEU
1	A	254	SER
1	A	257	LYS
1	A	266	ILE
1	A	267	SER
1	A	269	VAL
1	A	272	VAL
1	A	274	VAL

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Mol	Chain	Res	Type
1	A	275	ASP
1	A	277	ASN
1	A	279	ASP
1	A	286	LEU
1	A	293	TYR
1	A	294	TYR
1	A	299	SER
1	A	300	VAL
1	A	304	THR
1	A	305	PHE
1	A	308	ILE
1	A	309	SER
1	A	338	THR
1	A	343	LEU
1	A	350	CYS
1	A	357	LEU
1	A	363	LEU
1	A	368	LEU
1	A	376	PHE
1	A	377	ASN
1	A	378	SER
1	A	384	LEU
1	A	385	LYS
1	A	394	ARG
1	A	399	ASP
1	A	404	LEU
1	A	405	LEU
1	A	417	GLN
1	A	418	ASP
1	A	419	VAL
1	A	440	GLU
1	A	443	VAL
1	A	447	VAL
1	A	456	ARG
1	A	457	GLU
1	A	466	TRP
1	A	474	ASP
1	A	482	LEU
1	A	483	SER
1	A	484	ASP
1	A	485	CYS
1	A	487	GLN

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Mol	Chain	Res	Type
1	A	489	ILE
1	A	498	LYS
1	A	501	ILE
1	A	502	LEU
1	A	507	ASP
1	A	511	ILE
1	A	512	CYS
1	A	534	LYS
1	A	536	GLU
1	A	539	LYS
1	A	541	MSE
1	A	557	LEU
1	A	563	ASP
1	A	564	ILE
1	A	569	ASP
1	A	572	LEU
1	A	584	LYS
1	A	585	TYR
1	A	588	ARG
1	A	589	LEU
1	A	591	MSE
1	A	605	ARG
1	A	608	LEU
1	A	615	MSE
1	A	619	LYS
1	A	627	VAL
1	A	628	VAL
1	A	630	ARG
1	A	645	ASP
1	A	646	GLU
1	A	647	THR
1	A	648	GLN
1	A	649	LYS
1	A	651	SER
1	A	652	LEU
1	A	654	LYS
1	A	656	LEU
1	A	660	ASP
1	A	665	LEU
1	A	671	HIS
1	A	675	ASP
1	A	682	SER

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Mol	Chain	Res	Type
1	A	692	ARG
1	A	701	TRP
1	A	710	ASP
1	A	713	LYS
1	A	715	LEU
1	A	716	ASP
1	A	720	LEU
1	A	722	LEU
1	A	723	ASN
1	A	724	ASN
1	A	727	TYR
1	A	730	VAL
1	A	731	GLN
1	A	733	ILE
1	A	742	ARG
1	A	760	GLU
1	A	764	VAL
1	A	772	LEU
1	A	773	VAL
1	A	781	ILE
1	A	785	SER
1	A	786	LEU
1	A	787	LYS
1	A	791	ARG
1	A	792	LEU
1	A	793	TRP
1	A	796	GLU
1	A	797	THR
1	A	800	THR
1	A	813	ILE
1	A	821	LEU
1	A	822	THR
1	A	837	ARG
1	A	839	PHE
1	A	846	TYR
1	A	849	VAL
1	A	865	LEU
1	A	870	LEU
1	A	879	LEU
1	A	880	TYR
1	B	133	HIS
1	B	134	GLU

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Mol	Chain	Res	Type
1	B	136	GLU
1	B	138	ILE
1	B	145	ASP
1	B	148	ARG
1	B	149	SER
1	B	157	ARG
1	B	175	HIS
1	B	181	VAL
1	B	184	VAL
1	B	185	VAL
1	B	186	TYR
1	B	187	CYS
1	B	192	VAL
1	B	206	ARG
1	B	207	ILE
1	B	215	ASP
1	B	221	THR
1	B	223	ARG
1	B	227	ARG
1	B	231	THR
1	B	233	ILE
1	B	234	ASN
1	B	235	SER
1	B	236	LEU
1	B	238	SER
1	B	239	ILE
1	B	245	LYS
1	B	249	ARG
1	B	251	VAL
1	B	253	LEU
1	B	254	SER
1	B	255	GLU
1	B	256	GLU
1	B	262	LEU
1	B	269	VAL
1	B	270	LYS
1	B	273	HIS
1	B	274	VAL
1	B	281	LYS
1	B	283	LYS
1	B	299	SER
1	B	300	VAL

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Mol	Chain	Res	Type
1	B	303	SER
1	B	308	ILE
1	B	338	THR
1	B	339	ARG
1	B	342	THR
1	B	346	LEU
1	B	354	SER
1	B	367	LYS
1	B	368	LEU
1	B	370	THR
1	B	376	PHE
1	B	382	GLN
1	B	383	SER
1	B	387	ASN
1	B	390	GLN
1	B	391	THR
1	B	392	GLU
1	B	395	ASN
1	B	399	ASP
1	B	404	LEU
1	B	407	GLU
1	B	411	LEU
1	B	412	CYS
1	B	440	GLU
1	B	441	PHE
1	B	442	VAL
1	B	443	VAL
1	B	444	GLU
1	B	445	LYS
1	B	446	LEU
1	B	447	VAL
1	B	451	TYR
1	B	460	ILE
1	B	461	TYR
1	B	466	TRP
1	B	473	GLU
1	B	489	ILE
1	B	498	LYS
1	B	499	ARG
1	B	502	LEU
1	B	511	ILE
1	B	518	GLN

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Mol	Chain	Res	Type
1	B	534	LYS
1	B	538	ASN
1	B	546	ASP
1	B	547	ILE
1	B	552	LYS
1	B	558	MSE
1	B	563	ASP
1	B	574	LYS
1	B	577	LEU
1	B	580	LEU
1	B	583	MSE
1	B	589	LEU
1	B	601	GLN
1	B	605	ARG
1	B	608	LEU
1	B	614	SER
1	B	619	LYS
1	B	626	ASP
1	B	629	VAL
1	B	635	ASN
1	B	637	PHE
1	B	638	SER
1	B	639	GLN
1	B	642	VAL
1	B	646	GLU
1	B	648	GLN
1	B	651	SER
1	B	654	LYS
1	B	656	LEU
1	B	658	LEU
1	B	660	ASP
1	B	668	VAL
1	B	672	GLN
1	B	677	MSE
1	B	682	SER
1	B	685	THR
1	B	691	ILE
1	B	694	SER
1	B	695	ARG
1	B	696	LYS
1	B	697	ASP
1	B	698	MSE

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Mol	Chain	Res	Type
1	B	699	LEU
1	B	715	LEU
1	B	716	ASP
1	B	717	HIS
1	B	720	LEU
1	B	724	ASN
1	B	727	TYR
1	B	729	ARG
1	B	732	GLN
1	B	789	PHE
1	B	792	LEU
1	B	793	TRP
1	B	794	TRP
1	B	796	GLU
1	B	798	VAL
1	B	801	VAL
1	B	803	THR
1	B	809	ASN
1	B	811	VAL
1	B	813	ILE
1	B	817	GLN
1	B	819	ARG
1	B	820	VAL
1	B	821	LEU
1	B	825	GLU
1	B	828	ARG
1	B	835	TYR
1	B	836	TYR
1	B	837	ARG
1	B	843	LYS
1	B	844	GLU
1	B	879	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	GLN
1	A	234	ASN
1	A	540	GLN
1	A	586	GLN
1	A	670	ASN
1	A	671	HIS

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Mol	Chain	Res	Type
1	A	672	GLN
1	A	674	ASN
1	A	717	HIS
1	A	723	ASN
1	A	814	HIS
1	A	817	GLN
1	B	175	HIS
1	B	183	ASN
1	B	244	HIS
1	B	246	HIS
1	B	273	HIS
1	B	307	ASN
1	B	395	ASN
1	B	518	GLN
1	B	671	HIS
1	B	674	ASN
1	B	810	GLN
1	B	814	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SAH	A	1000	-	20,28,28	1.60	4 (20%)	19,40,40	3.59	4 (21%)
2	SAH	B	1000	-	20,28,28	1.60	4 (20%)	19,40,40	3.56	4 (21%)

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
2	SAH	A	1000	-	-	0/7/31/31	0/3/3/3
2	SAH	B	1000	-	-	0/7/31/31	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	SAH	C5-C4	-2.96	1.33	1.40
2	A	1000	SAH	C5-C4	-2.95	1.33	1.40
2	A	1000	SAH	O4'-C1'	2.15	1.43	1.41
2	B	1000	SAH	O4'-C1'	2.20	1.44	1.41
2	A	1000	SAH	C2-N1	3.19	1.40	1.33
2	B	1000	SAH	C2-N1	3.21	1.40	1.33
2	B	1000	SAH	C2-N3	4.48	1.40	1.32
2	A	1000	SAH	C2-N3	4.53	1.40	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	SAH	N3-C2-N1	-14.09	118.11	128.89
2	B	1000	SAH	N3-C2-N1	-14.00	118.18	128.89
2	A	1000	SAH	C4'-O4'-C1'	-5.32	103.87	109.72
2	B	1000	SAH	C4'-O4'-C1'	-5.27	103.93	109.72
2	A	1000	SAH	C2'-C1'-N9	-2.14	111.02	114.29
2	B	1000	SAH	C2'-C1'-N9	-2.13	111.04	114.29
2	B	1000	SAH	C5'-C4'-C3'	-2.12	109.50	114.98
2	A	1000	SAH	C5'-C4'-C3'	-2.11	109.52	114.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	SAH	6	0
2	B	1000	SAH	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	665/784 (84%)	-0.15	9 (1%) 78 65	21, 62, 129, 200	0
1	B	660/784 (84%)	-0.24	5 (0%) 87 80	17, 69, 134, 285	0
All	All	1325/1568 (84%)	-0.19	14 (1%) 82 72	17, 65, 132, 285	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	759	PRO	3.9
1	A	746	GLY	3.3
1	A	484	ASP	3.2
1	A	445	LYS	2.7
1	B	729	ARG	2.6
1	A	409	ALA	2.5
1	A	755	VAL	2.3
1	B	497	HIS	2.2
1	B	732	GLN	2.2
1	B	279	ASP	2.2
1	A	809	ASN	2.2
1	A	749	VAL	2.1
1	A	745	LYS	2.0
1	B	501	ILE	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( $\text{\AA}^2$ )	Q<0.9
2	SAH	A	1000	26/26	0.91	0.28	3.48	42,53,71,112	0
2	SAH	B	1000	26/26	0.95	0.19	-0.16	31,55,87,93	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.