



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 07:50 pm BST

PDB ID : 4EBA  
Title : Crystal structure of the Rna14-Rna15 complex  
Authors : Paulson, A.R.; Tong, L.  
Deposited on : 2012-03-23  
Resolution : 3.30 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

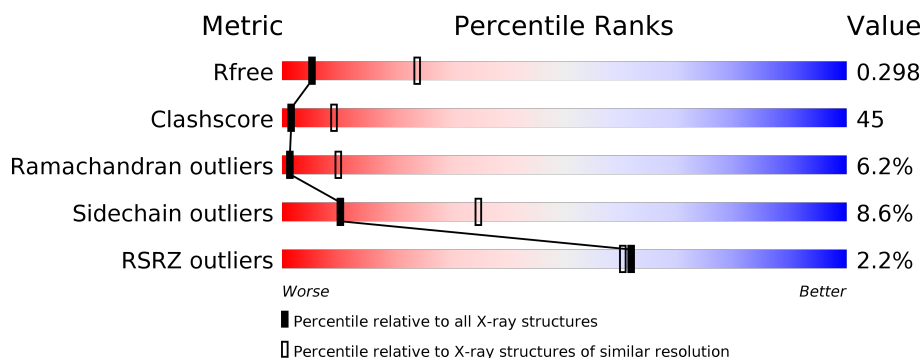
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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

Mol	Chain	Length	Quality of chain
1	A	645	<div> <div>27%</div> <div>53%</div> <div>9%</div> <div>•</div> <div>9%</div> </div>
1	B	645	<div> <div>29%</div> <div>49%</div> <div>8%</div> <div>•</div> <div>13%</div> </div>
1	C	645	<div> <div>2%</div> <div>35%</div> <div>49%</div> <div>6%</div> <div>•</div> <div>9%</div> </div>
1	D	645	<div> <div>%</div> <div>32%</div> <div>47%</div> <div>7%</div> <div>15%</div> </div>
1	E	645	<div> <div>7%</div> <div>27%</div> <div>52%</div> <div>10%</div> <div>10%</div> </div>
1	F	645	<div> <div>%</div> <div>30%</div> <div>48%</div> <div>7%</div> <div>•</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	174	<div><div></div><div>16%24%7%53%</div></div>
2	H	174	<div><div>2%</div><div></div><div>11%28%6%53%</div></div>
2	I	174	<div><div>%</div><div></div><div>13%27%6%53%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 30268 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 mRNA 3'-end-processing protein Rna14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4874	3149	803	897	25			
1	B	558	Total	C	N	O	S	0	0	0
			4646	2990	772	859	25			
1	C	585	Total	C	N	O	S	0	0	0
			4874	3149	803	897	25			
1	D	551	Total	C	N	O	S	0	0	0
			4589	2957	759	848	25			
1	E	578	Total	C	N	O	S	0	0	0
			4823	3118	795	885	25			
1	F	553	Total	C	N	O	S	0	0	0
			4608	2967	764	852	25			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MET	-	EXPRESSION TAG	UNP Q6CII8
B	17	MET	-	EXPRESSION TAG	UNP Q6CII8
C	17	MET	-	EXPRESSION TAG	UNP Q6CII8
D	17	MET	-	EXPRESSION TAG	UNP Q6CII8
E	17	MET	-	EXPRESSION TAG	UNP Q6CII8
F	17	MET	-	EXPRESSION TAG	UNP Q6CII8

- Molecule 2 is a protein called Rna15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	81	Total	C	N	O	S	0	0	0
			618	395	98	119	6			
2	I	81	Total	C	N	O	S	0	0	0
			618	395	98	119	6			
2	H	81	Total	C	N	O	S	0	0	0
			618	395	98	119	6			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	85	MET	-	EXPRESSION TAG	UNP Q6CKN2
G	86	GLY	-	EXPRESSION TAG	UNP Q6CKN2
G	87	SER	-	EXPRESSION TAG	UNP Q6CKN2
G	88	SER	-	EXPRESSION TAG	UNP Q6CKN2
G	89	HIS	-	EXPRESSION TAG	UNP Q6CKN2
G	90	HIS	-	EXPRESSION TAG	UNP Q6CKN2
G	91	HIS	-	EXPRESSION TAG	UNP Q6CKN2
G	92	HIS	-	EXPRESSION TAG	UNP Q6CKN2
G	93	HIS	-	EXPRESSION TAG	UNP Q6CKN2
G	94	HIS	-	EXPRESSION TAG	UNP Q6CKN2
G	95	SER	-	EXPRESSION TAG	UNP Q6CKN2
G	96	SER	-	EXPRESSION TAG	UNP Q6CKN2
G	97	GLY	-	EXPRESSION TAG	UNP Q6CKN2
G	98	LEU	-	EXPRESSION TAG	UNP Q6CKN2
G	99	VAL	-	EXPRESSION TAG	UNP Q6CKN2
G	100	PRO	-	EXPRESSION TAG	UNP Q6CKN2
G	101	ARG	-	EXPRESSION TAG	UNP Q6CKN2
G	102	GLY	-	EXPRESSION TAG	UNP Q6CKN2
G	103	SER	-	EXPRESSION TAG	UNP Q6CKN2
G	104	HIS	-	EXPRESSION TAG	UNP Q6CKN2
I	85	MET	-	EXPRESSION TAG	UNP Q6CKN2
I	86	GLY	-	EXPRESSION TAG	UNP Q6CKN2
I	87	SER	-	EXPRESSION TAG	UNP Q6CKN2
I	88	SER	-	EXPRESSION TAG	UNP Q6CKN2
I	89	HIS	-	EXPRESSION TAG	UNP Q6CKN2
I	90	HIS	-	EXPRESSION TAG	UNP Q6CKN2
I	91	HIS	-	EXPRESSION TAG	UNP Q6CKN2
I	92	HIS	-	EXPRESSION TAG	UNP Q6CKN2
I	93	HIS	-	EXPRESSION TAG	UNP Q6CKN2
I	94	HIS	-	EXPRESSION TAG	UNP Q6CKN2
I	95	SER	-	EXPRESSION TAG	UNP Q6CKN2
I	96	SER	-	EXPRESSION TAG	UNP Q6CKN2
I	97	GLY	-	EXPRESSION TAG	UNP Q6CKN2
I	98	LEU	-	EXPRESSION TAG	UNP Q6CKN2
I	99	VAL	-	EXPRESSION TAG	UNP Q6CKN2
I	100	PRO	-	EXPRESSION TAG	UNP Q6CKN2
I	101	ARG	-	EXPRESSION TAG	UNP Q6CKN2
I	102	GLY	-	EXPRESSION TAG	UNP Q6CKN2
I	103	SER	-	EXPRESSION TAG	UNP Q6CKN2
I	104	HIS	-	EXPRESSION TAG	UNP Q6CKN2
H	85	MET	-	EXPRESSION TAG	UNP Q6CKN2
H	86	GLY	-	EXPRESSION TAG	UNP Q6CKN2

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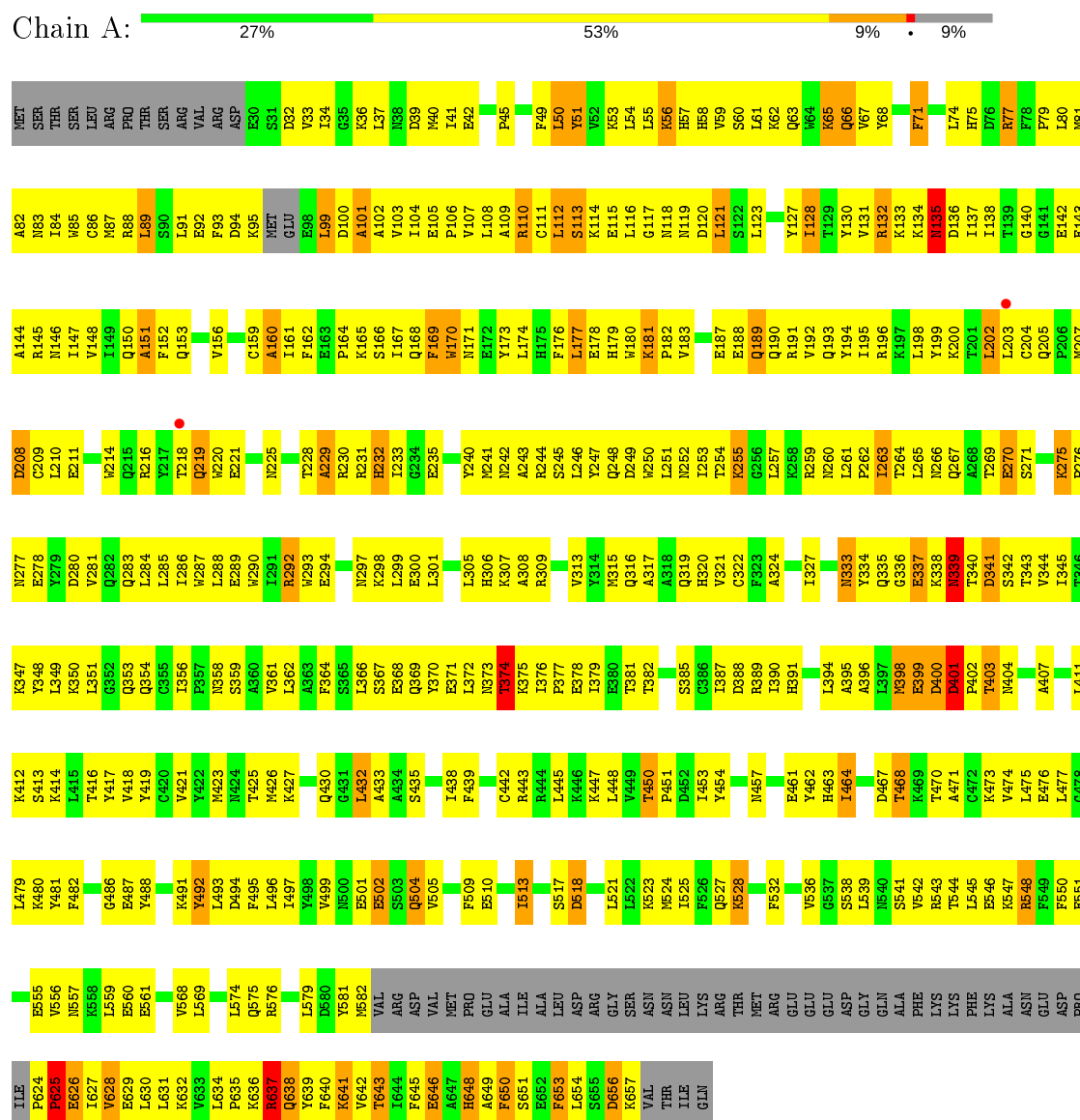
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Chain	Residue	Modelled	Actual	Comment	Reference
H	87	SER	-	EXPRESSION TAG	UNP Q6CKN2
H	88	SER	-	EXPRESSION TAG	UNP Q6CKN2
H	89	HIS	-	EXPRESSION TAG	UNP Q6CKN2
H	90	HIS	-	EXPRESSION TAG	UNP Q6CKN2
H	91	HIS	-	EXPRESSION TAG	UNP Q6CKN2
H	92	HIS	-	EXPRESSION TAG	UNP Q6CKN2
H	93	HIS	-	EXPRESSION TAG	UNP Q6CKN2
H	94	HIS	-	EXPRESSION TAG	UNP Q6CKN2
H	95	SER	-	EXPRESSION TAG	UNP Q6CKN2
H	96	SER	-	EXPRESSION TAG	UNP Q6CKN2
H	97	GLY	-	EXPRESSION TAG	UNP Q6CKN2
H	98	LEU	-	EXPRESSION TAG	UNP Q6CKN2
H	99	VAL	-	EXPRESSION TAG	UNP Q6CKN2
H	100	PRO	-	EXPRESSION TAG	UNP Q6CKN2
H	101	ARG	-	EXPRESSION TAG	UNP Q6CKN2
H	102	GLY	-	EXPRESSION TAG	UNP Q6CKN2
H	103	SER	-	EXPRESSION TAG	UNP Q6CKN2
H	104	HIS	-	EXPRESSION TAG	UNP Q6CKN2

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

#### • Molecule 1: mRNA 3'-end-processing protein RNA14



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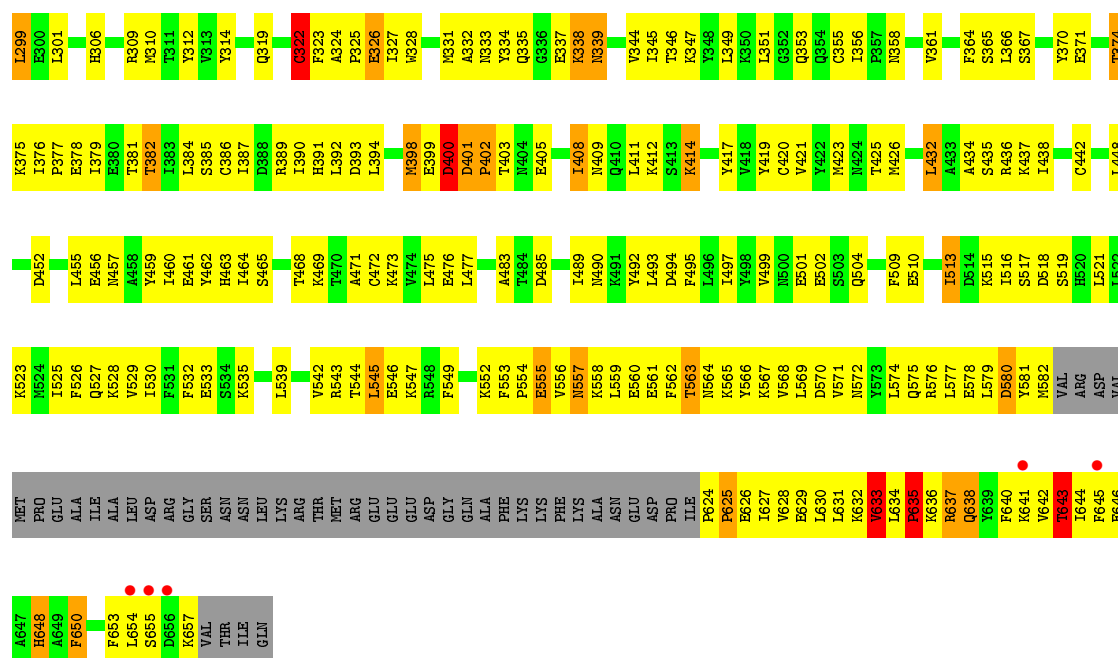


PRO	F562	D494	T425	L349	V281	M146	M81	MET
GLU	T563	F495	M426	K350	Q283	I147	A82	THR
ILE	N564	L496	K427	L351	Q282	V148	N83	SER
VAL	K565	I497	R428	G352	Q215	I149	I84	THR
GLU		V498	I429	Q353	L285	Q150	W85	LEU
LEU	V568	V499		Q354	I286	A151	C86	ARG
L569		M500	A434	C355	W287	F152	M87	
LYS	M572	E501	S435	L356	L288	R88	L89	P23
VAL		E502	K505	P357	E289	V155	S25	R26
LEU		S503	I438	N358	W290		S90	G26
PRO	Q575	Q504	F439	S359	I291	C159	I91	V27
LYS	R576	V505	G440		R292	A160	E92	R28
ARG	L577	K506	K441	F364		I161	F93	D29
GLN	E578	S507	C442	S365	D296	F162	D94	E30
TYR	L579	L508	R443	L366	I297		K95	S31
PHE	D580	F509	R444	E367	K298	R230	MET	
LYS	Y581		L445	S368	L299	R231	GLU	
VAL	M582	I513	K446	Q369		H232	E98	V33
THR	VAL	I516	K447	Y370	S302	I167	L99	I34
ILE	ILE	ARG	T448	E371	D303	Q168	G35	
GLU	ASP	ASP	V449	L443	R304	F169	D100	K36
PHE	GLU	GLU	T450	G376	L305	W170	A101	L37
ALA	VAL	L521	N450	I376	D305	M171	A102	N38
MET	MET	L522	P451	P377	K306	E172	V103	D59
HIS	PRO	K523	D452	E378	K307	Y173	I104	M40
ALA	GLU	M524	I463	I379	A308	F176	E105	I41
PHE	ALA	I525			R309	L177	P106	E42
ILE	ILE	F526	E456	T382	N310	H178	V107	E43
SER	GLU	Q527	N457		T311	H179	L108	Q44
GLU	LEU	K528		R389		W180		
PHE	ASP	V529	Y462	I390	Y314	E187	C111	I48
LEU	ASP	ILE	H463	H391	Q315	K181	L112	F49
SER	ARG	I530	I464	L392	R316	P182	S113	
GLY	ASP	F531	K465	L392	D249	V183	K114	
LYS	VAL	F532	S465	D393	A317	M184	V51	
ASN	ASN	ASN	K466	L394	A318	K185	E115	V52
ASN	ASN	K535	D467	L395	Q319	F186	L116	K53
LEU	LEU	V536	T468	A396	H320	E187	G117	L54
ASN	LEU	G537	K469	L397	R520	M118	L118	L55
LYS	LYS	S538	T470	M398	C322	Q189	D120	K56
ARG	ARG	L539	A471	E399	F323	R190	N119	H57
THR	THR		C472	D400	A324	Q190	L121	H58
MET	MET		K473	D401	P325	R191	S122	V59
ARG	ARG	V542	V474	F402		V192	L123	S60
GLU	GLU	R543				Q193		
GLU	GLU	T544	L475	T403	R331	L61	Y127	K62
GLU	GLU	L545	E476	E432	A332	Y194	I128	Q63
ASP	E546	K547	L477		R333	I195	T129	W64
GLY	GLY	K547	G478	I408	Y334	R196	K197	K65
GLN	GLN	R548	L479		Q335	K197	V131	
ALA	ALA	F549	K480	L411	G336	L198	R132	Q66
PHE	PHE	F550	Y481	K412	G337	Y199	K133	Y68
LYS	LYS	K551	F482	S413	R338	K200	K134	E69
LYS	LYS	F552		K414	R339	T201		
PHE	PHE	F553	D485	L415	T340	L202	N135	T70
LYS	LYS	P554	G486	D341	Q342	L203	D136	F71
ALA	ALA	E555	E487	T416	S342	C204	I137	
GLU	GLU	V556	Y488	Y419	P274	Q205	I138	L74
ASN	ASN	N557	I489	C420	V344	P206	T139	
GLU	GLU	K558	N490	Y421	T345	M207	G140	
ASP	ASP	L559	K491	Y422	R278	D208		F77
PRO	PRO		E560	Y492	E278			F78
ILE	ILE	P561	I493	M423	K347	Y279	C269	P79
PRO	PRO		N493	N424	Y280	L310	A144	A144
							R145	

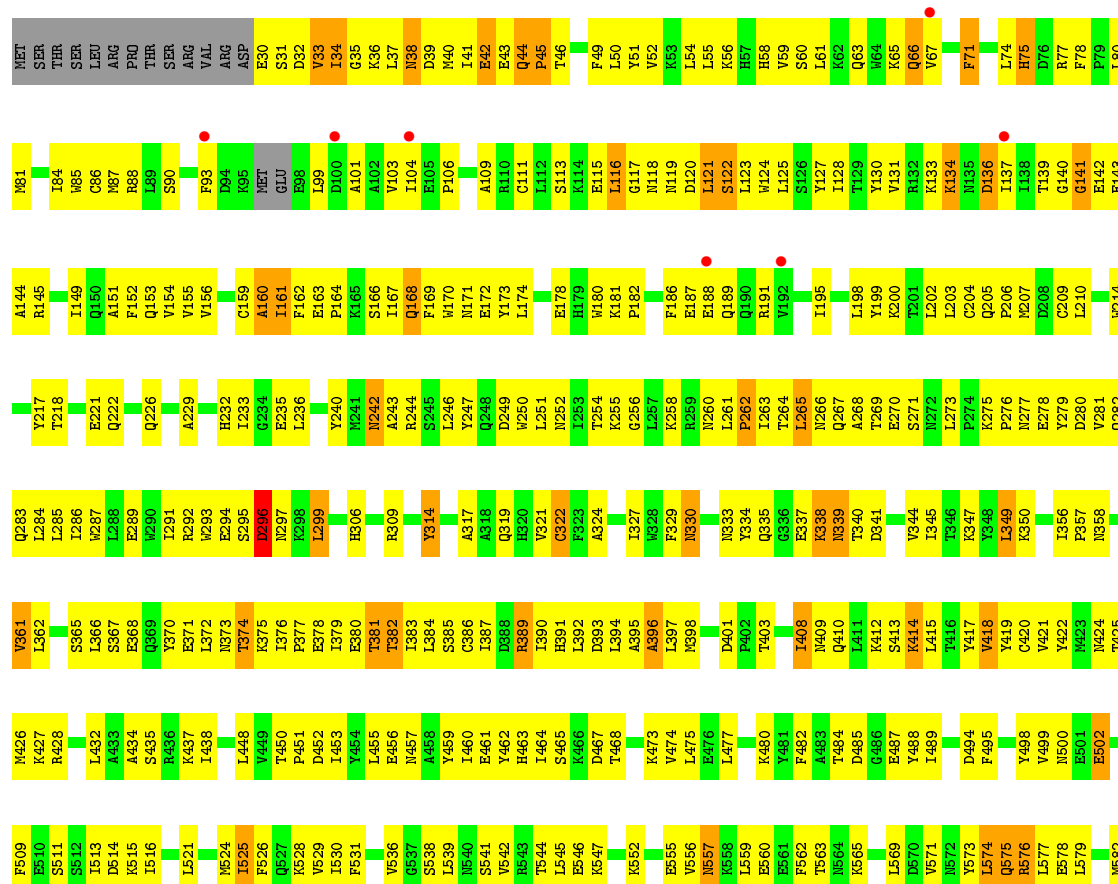
• Molecule 1: mRNA 3'-end-processing protein RNA14



MET	SER	THR	SER	THR	LEU	ARG	PRO	THR	SER	GLU	VAL	ARG	ASP	E30	S31	D32	V33	I34	G35	K36	L37	N38	D39	I40	E41	E42	E43	Q44	P45	T46	F47	T48	F49	L50	K53	L54	L55	H58	V59	S60	K62	Q63	D66	T70	F71	L74	H75	F78	P79	L80	P81	I84	
M85	M88	E92	K95	MET	GLU	E98	A101	A102	V103	I104	E105	P106	V107	L108	A109	R110	C111	L112	S113	K114	E115	L116	G117	N118	L121	S122	L123	M124	L125	S126	Y127	I128	Y131	K134	N135	D136	I137	I138	T139	G140	G141	E142	E143	A144	R145	M146	I147	Q150	A151	F152	Q153		
V154	V155	V156	D157	K158	C159	A160	I161	E163	K165	S166	I167	Q168	F169	W170	Y173	L174	H175	F176	L177	E178	H179	W180	K181	P182	F186	E187	E188	R191	A192	Q193	R196	K197	L198	Y199	T201	L202	L203	C204	Q205	P206	M207	D208	C209	L210	E211	Y217	T218	Q226	L227	T228			
R231	H232	I233	G234	E235	L236	S237	Y240	M241	M242	A243	R244	S245	L246	Y247	Q248	D249	W250	L251	N252	I253	G256	L257	P262	L263	T264	L265	N266	Q267	R268	A268	T269	E270	S271	N272	L273	K274	K275	P276	M277	E278	Y279	D280	Q281	Q282	L284	L285	L286	W287	W290	S295	D296	N297	E298

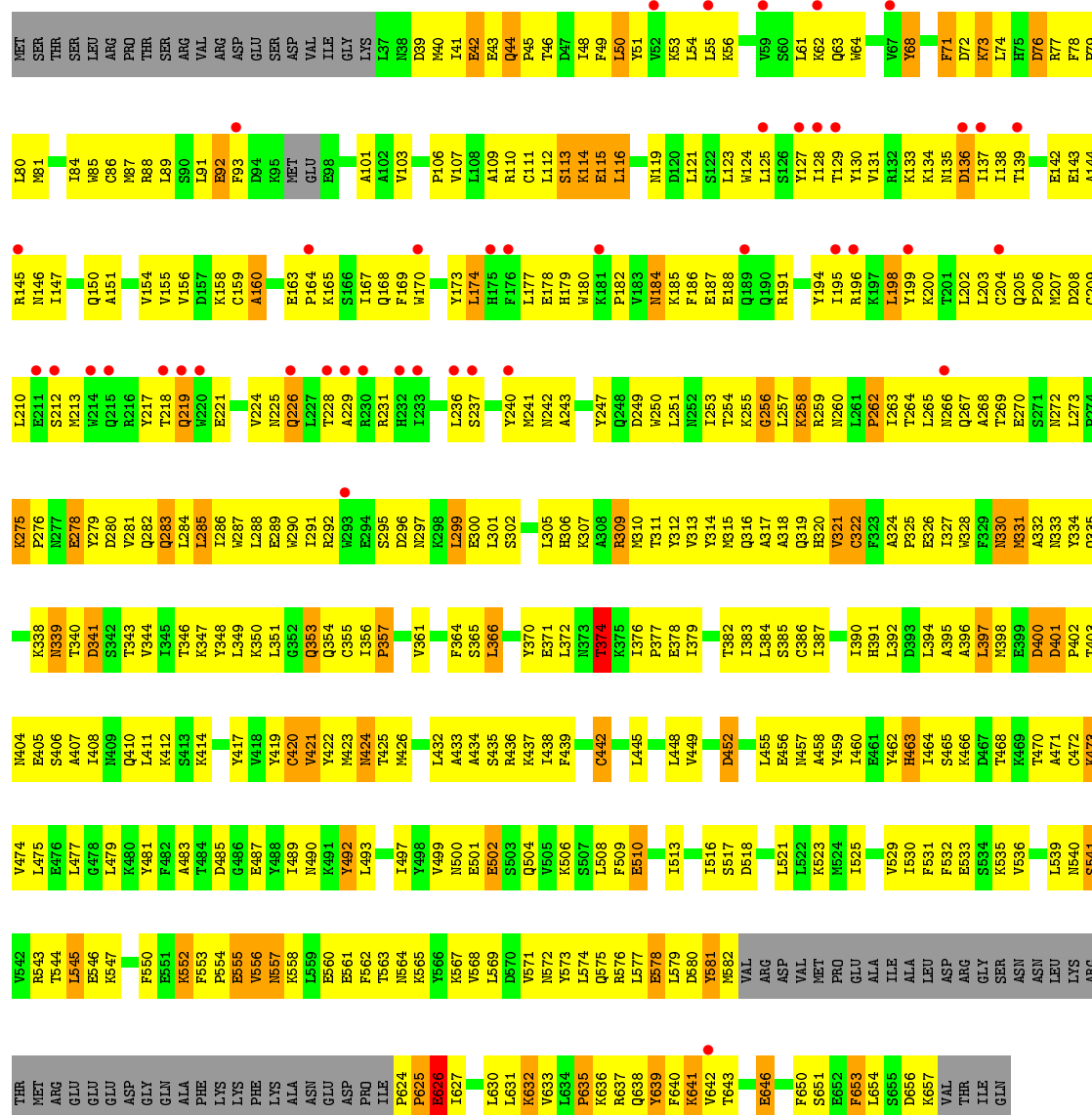


• Molecule 1: mRNA 3'-end-processing protein RNA14

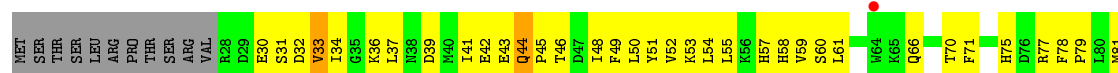


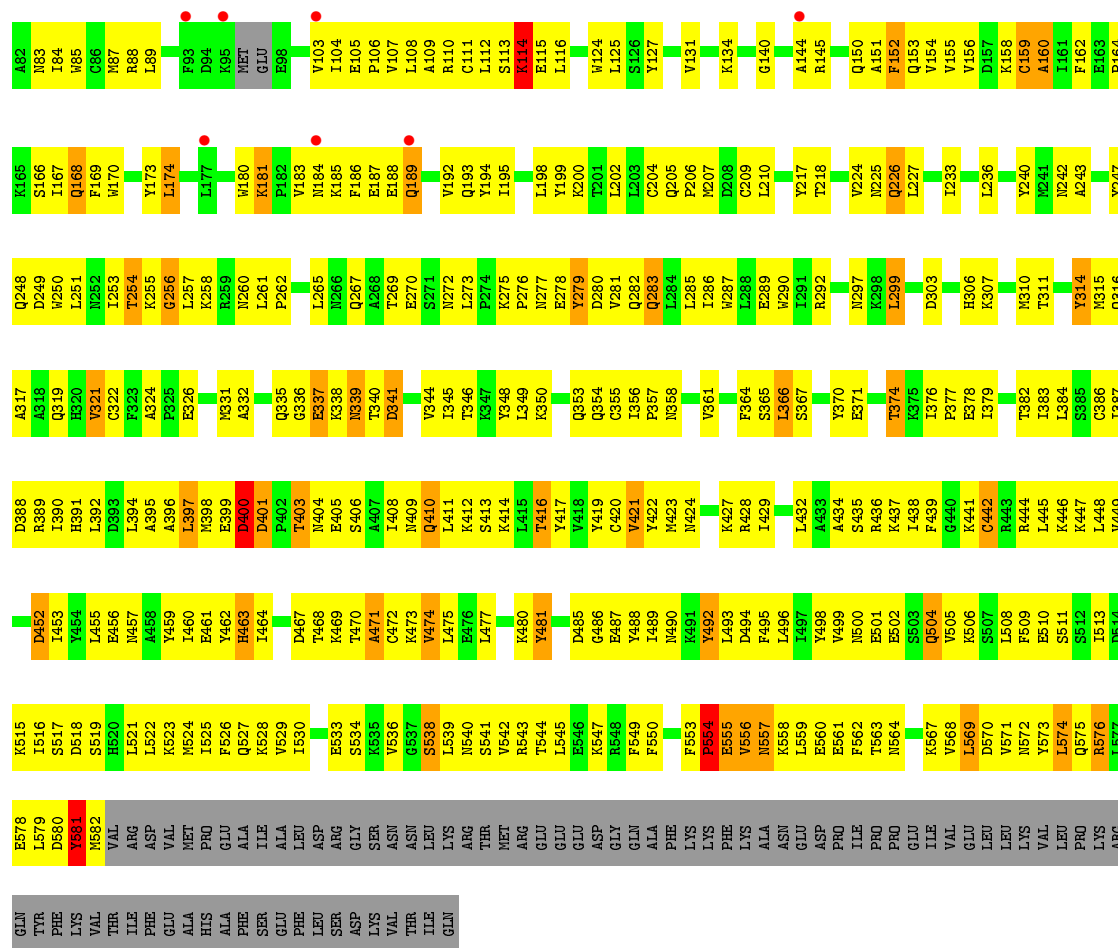
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- Molecule 1: mRNA 3'-end-processing protein RNA14

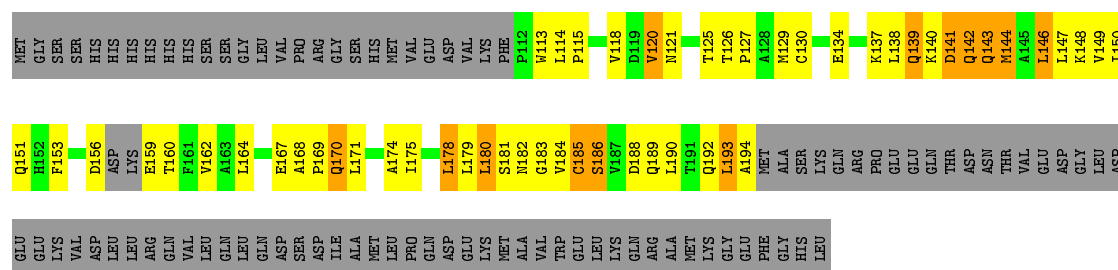
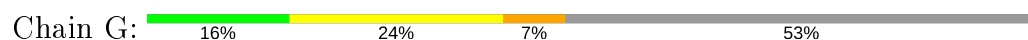


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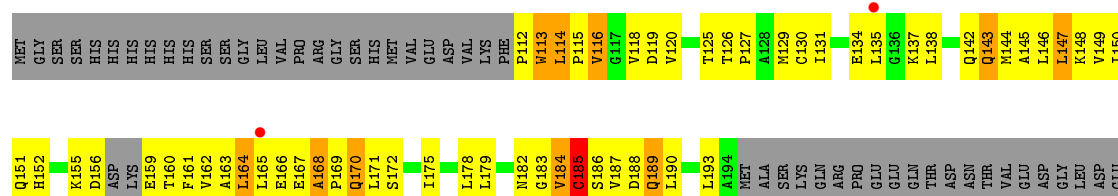
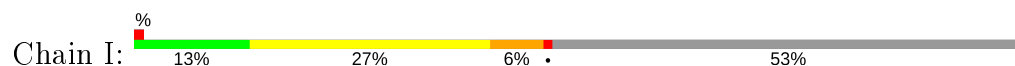




- Molecule 2: Rna15

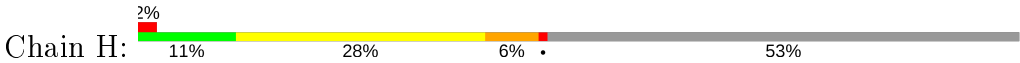


- Molecule 2: Rna15



GLU  
LYS  
VAL  
ASP  
LEU  
LEU  
ARG  
GLN  
GLN  
GLN  
GLN  
GLN  
ASP  
SER  
ASP  
ASP  
ILE  
ALA  
GLY  
MET  
LEU  
PRO  
GLN  
ASP  
GLU  
LYS  
LYS  
MET  
ALA  
VAL  
TRP  
GLU  
LEU  
LEU  
LYS  
GLN  
ARG  
ALA  
MET  
LYS  
GLY  
GLU  
PHE  
GLY  
HIS  
LEU

● Molecule 2: Rna15



MET  
GLY  
SER  
SER  
Q151  
HIS  
HIS  
HIS  
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HIS  
HIS  
HIS  
SER  
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W113  
L114  
P115  
V116  
G117  
V118  
D119  
V120  
H121  
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C130  
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E134  
L135  
G136  
K137  
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D141  
Q142  
Q143  
F144  
A145  
L146  
L147

K148  
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E167  
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ALA  
MET  
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GLU  
PHE  
GLY  
HIS  
LEU

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.04Å 162.04Å 177.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.79 – 3.30 47.79 – 3.30	Depositor EDS
% Data completeness (in resolution range)	86.4 (47.79-3.30) 86.3 (47.79-3.30)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 3.33Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.226 , 0.298 0.226 , 0.298	Depositor DCC
$R_{free}$ test set	3646 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	84.8	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 76.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l 0.038 for h,-h-k,-l 0.025 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	30268	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.09% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.46	0/4982	0.64	0/6732
1	B	0.44	0/4747	0.67	1/6416 (0.0%)
1	C	0.40	0/4982	0.60	0/6732
1	D	0.40	0/4689	0.59	0/6338
1	E	0.46	0/4931	0.66	1/6664 (0.0%)
1	F	0.42	0/4708	0.61	0/6363
2	G	0.39	0/626	0.71	0/849
2	H	0.37	0/626	0.67	0/849
2	I	0.38	0/626	0.63	0/849
All	All	0.43	0/30917	0.63	2/41792 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	SER	N-CA-C	-5.59	95.91	111.00
1	E	112	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	4874	0	4885	509	0
1	B	4646	0	4650	399	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4874	0	4885	391	0
1	D	4589	0	4591	385	0
1	E	4823	0	4834	511	0
1	F	4608	0	4608	398	0
2	G	618	0	632	81	0
2	H	618	0	632	93	0
2	I	618	0	632	92	0
All	All	30268	0	30349	2735	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 45.

All (2735) 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:D:563:THR:HG22	1:D:574:LEU:HD12	1.23	1.17
1:C:557:ASN:HD22	1:C:560:GLU:HB2	1.11	1.16
1:D:468:THR:HG21	1:D:499:VAL:HG11	1.31	1.07
1:A:345:ILE:HD12	1:A:345:ILE:H	1.19	1.03
1:A:225:ASN:HB2	1:A:229:ALA:HB2	1.37	1.02
2:H:170:GLN:HE21	2:H:170:GLN:N	1.56	1.02
1:A:548:ARG:HG2	1:A:548:ARG:HH11	1.23	1.01
1:F:299:LEU:H	1:F:299:LEU:HD12	1.21	1.01
1:D:468:THR:CG2	1:D:499:VAL:HG11	1.91	1.00
2:G:125:THR:HG22	2:G:126:THR:H	1.23	1.00
1:E:311:THR:HG22	1:E:315:MET:HE2	1.40	1.00
1:E:74:LEU:HD13	1:E:84:ILE:HG23	1.42	1.00
1:C:638:GLN:HA	1:C:641:LYS:HB3	1.44	0.99
1:C:202:LEU:HB2	1:C:207:MET:HE1	1.44	0.99
1:F:398:MET:HG2	1:F:408:ILE:HD11	1.44	0.99
1:E:178:GLU:HA	1:E:191:ARG:NH2	1.79	0.98
1:B:258:LYS:HE2	2:H:152:HIS:HB2	1.46	0.97
1:A:364:PHE:CZ	1:A:421:VAL:HG11	1.99	0.97
1:E:335:GLN:HE21	1:E:348:TYR:HE1	1.10	0.97
1:E:125:LEU:HD23	1:E:128:ILE:HD12	1.43	0.97
1:D:489:ILE:HG13	1:D:516:ILE:HD11	1.46	0.95
1:A:638:GLN:HA	1:A:641:LYS:HG3	1.49	0.95
2:H:193:LEU:HD12	2:H:194:ALA:H	1.30	0.95
1:E:564:ASN:O	1:E:567:LYS:HG3	1.67	0.94
2:H:170:GLN:HE21	2:H:170:GLN:H	0.95	0.94
1:D:434:ALA:HA	1:D:437:LYS:HE3	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:ASN:HB3	2:I:152:HIS:NE2	1.84	0.93
1:A:99:LEU:HB2	1:A:134:LYS:NZ	1.84	0.92
1:E:563:THR:HG22	1:E:574:LEU:HD12	1.50	0.92
1:F:557:ASN:HD22	1:F:560:GLU:HB2	1.34	0.92
1:E:115:GLU:HG2	1:E:116:LEU:H	1.32	0.92
2:H:170:GLN:NE2	2:H:170:GLN:H	1.67	0.92
1:B:200:LYS:HG2	1:B:236:LEU:HD11	1.49	0.92
1:C:262:PRO:HG3	1:C:273:LEU:HD21	1.50	0.92
1:B:524:MET:HA	1:B:527:GLN:HE21	1.35	0.91
1:C:398:MET:HA	1:C:408:ILE:HD11	1.50	0.91
1:B:396:ALA:O	1:B:400:ASP:HB2	1.69	0.91
2:G:170:GLN:NE2	2:G:170:GLN:H	1.66	0.91
2:G:170:GLN:HE21	2:G:170:GLN:H	0.91	0.91
1:A:137:ILE:HG23	1:A:145:ARG:HB2	1.54	0.90
1:F:390:ILE:HD13	1:F:414:LYS:HD3	1.51	0.90
1:F:489:ILE:HG13	1:F:516:ILE:HD11	1.53	0.90
1:B:548:ARG:HG2	1:B:548:ARG:HH11	1.36	0.89
2:G:170:GLN:N	2:G:170:GLN:HE21	1.71	0.89
1:F:576:ARG:HB3	1:F:576:ARG:HH11	1.36	0.89
1:F:48:ILE:HG22	1:F:273:LEU:HD13	1.53	0.89
1:A:568:VAL:HG12	1:A:569:LEU:HD22	1.55	0.89
2:G:185:CYS:SG	2:G:188:ASP:HB2	2.13	0.89
1:E:637:ARG:O	1:E:641:LYS:HB3	1.72	0.88
1:E:74:LEU:HD13	1:E:84:ILE:CG2	2.04	0.88
1:A:111:CYS:SG	1:A:112:LEU:HD23	2.11	0.88
1:A:259:ARG:HG2	1:A:320:HIS:NE2	1.88	0.88
1:E:325:PRO:HD3	1:E:356:ILE:HD13	1.56	0.88
1:F:314:TYR:HB3	1:F:331:MET:HE3	1.55	0.88
1:A:264:THR:HB	1:A:267:GLN:HG2	1.54	0.88
1:E:390:ILE:HD13	1:E:414:LYS:HD3	1.56	0.87
1:A:180:TRP:HB3	1:A:191:ARG:HH12	1.40	0.87
2:I:170:GLN:HE21	2:I:170:GLN:H	1.21	0.87
1:A:579:LEU:HD13	1:A:582:MET:HE1	1.57	0.87
1:E:475:LEU:H	1:E:475:LEU:HD12	1.40	0.87
1:C:364:PHE:CZ	1:C:421:VAL:HG11	2.10	0.87
1:A:180:TRP:CZ3	1:A:191:ARG:HA	2.10	0.87
1:E:364:PHE:CZ	1:E:421:VAL:HG11	2.10	0.87
1:A:631:LEU:HD21	2:G:171:LEU:HD22	1.56	0.87
1:C:572:ASN:ND2	1:C:575:GLN:HE21	1.73	0.86
1:A:180:TRP:HB3	1:A:191:ARG:NH1	1.91	0.86
1:A:283:GLN:HA	1:A:286:ILE:HD12	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:193:LEU:HG	2:G:194:ALA:H	1.41	0.86
2:H:185:CYS:HB3	2:H:188:ASP:HB3	1.58	0.86
2:H:179:LEU:HG	2:H:184:VAL:HG21	1.58	0.86
1:B:521:LEU:O	1:B:525:ILE:HG12	1.76	0.86
1:C:361:VAL:HG22	1:D:574:LEU:HD11	1.57	0.85
1:C:200:LYS:HG2	1:C:236:LEU:HD11	1.56	0.85
1:A:364:PHE:HZ	1:A:421:VAL:HG11	1.34	0.84
1:A:99:LEU:HB2	1:A:134:LYS:HZ3	1.42	0.84
1:E:206:PRO:HA	1:E:210:LEU:HD11	1.57	0.84
1:A:65:LYS:O	1:A:65:LYS:HD3	1.76	0.84
1:C:61:LEU:HB2	1:C:63:GLN:HE21	1.42	0.84
2:G:143:GLN:HG2	2:G:182:ASN:HD21	1.43	0.84
1:C:468:THR:CG2	1:C:499:VAL:HG11	2.07	0.83
1:A:281:VAL:O	1:A:285:LEU:HD12	1.78	0.83
1:C:574:LEU:HD11	1:D:361:VAL:HG22	1.60	0.83
1:E:341:ASP:HB3	1:E:344:VAL:HG23	1.59	0.83
1:F:140:GLY:HA3	1:F:144:ALA:HB3	1.60	0.83
2:I:170:GLN:NE2	2:I:170:GLN:H	1.74	0.83
1:A:33:VAL:HA	1:A:36:LYS:HD2	1.61	0.83
1:A:632:LYS:HG2	2:G:115:PRO:HG2	1.61	0.83
1:F:202:LEU:HB2	1:F:207:MET:HE1	1.60	0.82
2:H:193:LEU:HD12	2:H:194:ALA:N	1.94	0.82
1:A:86:CYS:HB3	1:A:263:ILE:HG13	1.60	0.82
1:B:61:LEU:HB2	1:B:63:GLN:HE21	1.43	0.82
1:C:557:ASN:ND2	1:C:560:GLU:HB2	1.92	0.82
1:E:546:GLU:OE2	1:E:565:LYS:HE2	1.80	0.82
2:H:155:LYS:HD3	2:H:155:LYS:H	1.44	0.82
1:E:81:MET:HE1	1:E:318:ALA:O	1.80	0.81
1:F:43:GLU:O	1:F:44:GLN:HG2	1.80	0.81
1:C:299:LEU:HD12	1:C:299:LEU:H	1.45	0.81
1:D:124:TRP:O	1:D:127:TYR:HB3	1.78	0.81
2:G:147:LEU:HD11	2:G:178:LEU:HD22	1.60	0.81
1:D:90:SER:HB3	1:D:264:THR:HG23	1.60	0.81
1:E:557:ASN:HD22	1:E:560:GLU:HB2	1.44	0.81
1:C:152:PHE:O	1:C:156:VAL:HG23	1.80	0.81
1:D:80:LEU:HA	1:D:118:ASN:HD21	1.43	0.81
1:A:81:MET:HB3	1:A:84:ILE:HD13	1.60	0.81
1:D:71:PHE:CE2	1:D:88:ARG:HB2	2.15	0.81
1:E:165:LYS:HD3	1:E:208:ASP:HB3	1.63	0.81
1:D:218:THR:HA	1:D:233:ILE:HD11	1.62	0.80
1:E:455:LEU:HB2	1:F:569:LEU:HD11	1.60	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:LEU:HD21	1:C:169:PHE:HD1	1.47	0.80
1:D:210:LEU:HD13	1:D:244:ARG:HA	1.62	0.80
1:D:299:LEU:H	1:D:299:LEU:HD12	1.46	0.80
1:D:557:ASN:HD22	1:D:560:GLU:H	1.26	0.80
1:A:108:LEU:O	1:A:112:LEU:HB2	1.81	0.80
1:E:502:GLU:OE2	1:E:536:VAL:HG11	1.81	0.80
1:C:378:GLU:O	1:C:382:THR:HG22	1.82	0.80
1:E:165:LYS:HE2	1:E:250:TRP:CZ3	2.17	0.80
1:A:140:GLY:HA3	1:A:144:ALA:HB2	1.64	0.79
2:H:135:LEU:HD22	2:H:178:LEU:HD21	1.63	0.79
1:B:89:LEU:HD21	1:B:107:VAL:HG11	1.65	0.79
1:E:521:LEU:O	1:E:525:ILE:HD13	1.83	0.79
1:F:557:ASN:ND2	1:F:560:GLU:H	1.79	0.79
1:F:51:TYR:O	1:F:55:LEU:HG	1.82	0.79
1:A:137:ILE:H	1:A:137:ILE:HD12	1.46	0.79
1:F:48:ILE:CG2	1:F:273:LEU:HD13	2.12	0.79
1:A:180:TRP:HZ3	1:A:191:ARG:HA	1.45	0.78
1:B:394:LEU:HA	1:B:411:LEU:HD23	1.64	0.78
1:C:115:GLU:H	1:C:115:GLU:CD	1.86	0.78
1:E:479:LEU:HD23	1:E:483:ALA:HA	1.65	0.78
1:E:557:ASN:ND2	1:E:560:GLU:H	1.80	0.78
1:A:447:LYS:HG2	1:A:481:TYR:HB3	1.63	0.78
1:E:124:TRP:CE3	1:E:155:VAL:HG22	2.18	0.78
1:B:145:ARG:NH2	1:B:180:TRP:HE1	1.82	0.78
1:B:496:LEU:HB3	1:B:505:VAL:HG22	1.65	0.78
1:E:327:ILE:HG23	1:E:328:TRP:N	1.99	0.78
1:F:79:PRO:HB2	1:F:116:LEU:HD13	1.66	0.78
2:I:190:LEU:O	2:I:193:LEU:HG	1.83	0.78
1:A:204:CYS:HB2	1:A:205:GLN:HE21	1.49	0.78
1:E:632:LYS:HG2	2:I:115:PRO:HB3	1.66	0.78
2:H:189:GLN:O	2:H:192:GLN:HB2	1.84	0.78
1:D:51:TYR:O	1:D:55:LEU:HG	1.85	0.77
1:E:312:TYR:O	1:E:316:GLN:HG2	1.83	0.77
1:B:178:GLU:CD	1:B:216:ARG:HH22	1.88	0.77
1:E:417:TYR:HB2	1:F:573:TYR:HD1	1.48	0.77
1:B:99:LEU:HB2	1:B:134:LYS:HZ3	1.48	0.77
1:E:327:ILE:CG2	1:E:328:TRP:H	1.98	0.77
1:E:423:MET:HA	1:E:438:ILE:HD12	1.66	0.77
1:B:145:ARG:CZ	1:B:180:TRP:HE1	1.98	0.77
1:C:529:VAL:HG12	1:C:545:LEU:HD11	1.67	0.77
1:E:631:LEU:HD23	2:I:171:LEU:HD13	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:LYS:HG2	2:G:115:PRO:CG	2.14	0.77
1:B:206:PRO:HB3	1:B:247:TYR:HB2	1.65	0.77
1:E:156:VAL:HA	1:E:160:ALA:CB	2.15	0.77
1:E:539:LEU:HD13	1:F:371:GLU:OE1	1.85	0.77
1:F:299:LEU:N	1:F:299:LEU:HD12	1.98	0.77
1:F:115:GLU:H	1:F:115:GLU:CD	1.88	0.76
1:F:124:TRP:O	1:F:127:TYR:HB3	1.85	0.76
2:H:150:ILE:HD13	2:H:175:ILE:HG12	1.66	0.76
2:I:143:GLN:HG2	2:I:182:ASN:ND2	2.00	0.76
1:B:101:ALA:HB1	1:B:105:GLU:HG3	1.66	0.76
1:D:459:TYR:O	1:D:463:HIS:HB2	1.86	0.76
1:F:400:ASP:O	1:F:401:ASP:HB3	1.84	0.76
1:A:548:ARG:HG2	1:A:548:ARG:NH1	1.98	0.76
1:F:563:THR:HG22	1:F:572:ASN:HD21	1.51	0.76
1:C:629:GLU:HA	1:C:632:LYS:HE3	1.68	0.76
1:A:394:LEU:HA	1:A:411:LEU:HD23	1.67	0.76
1:C:624:PRO:N	1:C:625:PRO:HD3	2.00	0.76
1:A:462:TYR:CZ	1:A:499:VAL:HG11	2.19	0.76
1:E:93:PHE:HZ	1:E:130:TYR:HB2	1.51	0.76
1:D:330:ASN:HD22	1:D:330:ASN:N	1.84	0.76
1:E:364:PHE:HZ	1:E:421:VAL:HG11	1.47	0.76
1:D:573:TYR:O	1:D:577:LEU:HB2	1.85	0.75
2:G:193:LEU:HD23	2:G:193:LEU:H	1.52	0.75
2:I:185:CYS:SG	2:I:188:ASP:HB3	2.25	0.75
1:C:648:HIS:NE2	2:H:162:VAL:HB	2.01	0.75
1:D:557:ASN:ND2	1:D:560:GLU:H	1.85	0.75
1:E:109:ALA:O	1:E:113:SER:HB3	1.87	0.75
1:F:71:PHE:CE2	1:F:88:ARG:HB2	2.21	0.75
2:G:190:LEU:HA	2:G:193:LEU:HD21	1.67	0.75
1:C:181:LYS:HD2	1:C:181:LYS:O	1.85	0.75
1:F:579:LEU:O	1:F:582:MET:HB2	1.86	0.75
1:B:218:THR:HG22	1:B:233:ILE:HD13	1.68	0.75
1:C:282:GLN:O	1:C:286:ILE:HG13	1.86	0.75
1:A:364:PHE:CE2	1:A:421:VAL:HG21	2.22	0.75
1:D:140:GLY:HA3	1:D:144:ALA:HB3	1.66	0.75
1:C:71:PHE:CE2	1:C:88:ARG:HB2	2.21	0.74
1:D:204:CYS:HB2	1:D:205:GLN:HE21	1.50	0.74
1:A:182:PRO:HG3	1:A:191:ARG:HD2	1.67	0.74
1:B:509:PHE:CD1	1:B:529:VAL:HG21	2.22	0.74
1:A:356:ILE:HG22	1:A:359:SER:HB2	1.69	0.74
1:A:396:ALA:O	1:A:400:ASP:HB2	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:LEU:O	1:B:63:GLN:HG3	1.87	0.74
1:E:398:MET:HA	1:E:408:ILE:HD11	1.69	0.74
1:B:218:THR:HA	1:B:233:ILE:HD11	1.68	0.74
1:B:524:MET:HA	1:B:527:GLN:NE2	2.03	0.74
1:C:111:CYS:O	1:C:118:ASN:HB2	1.88	0.74
1:C:574:LEU:O	1:C:574:LEU:HD13	1.86	0.74
1:E:269:THR:HG23	1:E:272:ASN:HD21	1.51	0.74
1:C:635:PRO:HG3	2:H:120:VAL:HG21	1.70	0.74
1:D:115:GLU:H	1:D:115:GLU:CD	1.92	0.74
1:F:405:GLU:HA	1:F:408:ILE:HG22	1.69	0.74
2:G:168:ALA:HA	2:G:170:GLN:HE22	1.53	0.74
1:A:378:GLU:O	1:A:382:THR:HG22	1.88	0.73
1:B:376:ILE:HB	1:B:377:PRO:HD3	1.70	0.73
1:B:66:GLN:HE21	1:B:66:GLN:N	1.84	0.73
1:E:465:SER:O	1:E:466:LYS:HB2	1.87	0.73
1:E:509:PHE:CZ	1:E:513:ILE:HD11	2.23	0.73
1:F:200:LYS:HG2	1:F:236:LEU:HD11	1.69	0.73
1:F:83:ASN:O	1:F:87:MET:HG3	1.88	0.73
1:A:205:GLN:O	1:A:207:MET:HG3	1.87	0.73
1:A:462:TYR:CE2	1:A:499:VAL:HG11	2.23	0.73
1:C:280:ASP:HB3	1:C:283:GLN:HB2	1.70	0.73
1:E:473:LYS:O	1:E:477:LEU:HD13	1.88	0.73
1:D:136:ASP:HB3	1:D:139:THR:HB	1.68	0.73
1:C:107:VAL:HA	1:C:110:ARG:HD3	1.70	0.73
1:E:200:LYS:HG2	1:E:236:LEU:HD11	1.69	0.73
1:F:181:LYS:O	1:F:181:LYS:HD2	1.89	0.73
1:E:287:TRP:O	1:E:290:TRP:HB3	1.89	0.73
1:E:468:THR:CG2	1:E:499:VAL:HG11	2.19	0.73
1:A:568:VAL:HG12	1:A:569:LEU:CD2	2.18	0.73
1:F:218:THR:HG23	1:F:233:ILE:HD13	1.69	0.73
2:I:179:LEU:O	2:I:184:VAL:HB	1.89	0.73
1:D:42:GLU:OE1	1:D:43:GLU:HG3	1.89	0.72
1:D:202:LEU:HD12	1:D:203:LEU:N	2.05	0.72
1:E:71:PHE:CE2	1:E:88:ARG:HB2	2.23	0.72
1:B:463:HIS:O	1:B:464:ILE:HG13	1.89	0.72
1:A:638:GLN:HA	1:A:641:LYS:CG	2.19	0.72
1:E:471:ALA:O	1:E:474:VAL:HB	1.90	0.72
1:F:371:GLU:HB2	1:F:379:ILE:HD11	1.71	0.72
1:A:654:LEU:HD21	2:G:150:ILE:HG22	1.72	0.72
1:B:137:ILE:HD12	1:B:137:ILE:H	1.53	0.72
1:B:351:LEU:HA	1:B:354:GLN:HG3	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:ASP:O	1:B:401:ASP:HB3	1.89	0.72
1:C:572:ASN:OD1	1:C:575:GLN:HG2	1.88	0.72
1:C:654:LEU:O	1:C:654:LEU:HD23	1.89	0.72
1:D:394:LEU:HD21	1:D:448:LEU:HD11	1.71	0.72
1:C:101:ALA:HB2	1:C:134:LYS:NZ	2.05	0.72
1:F:127:TYR:O	1:F:131:VAL:HG23	1.90	0.71
1:E:200:LYS:HG2	1:E:236:LEU:HD21	1.71	0.71
1:E:254:THR:HG23	1:E:257:LEU:HD22	1.71	0.71
1:A:75:HIS:HB3	1:A:110:ARG:HH21	1.54	0.71
1:E:313:VAL:O	1:E:316:GLN:HB2	1.90	0.71
1:E:578:GLU:O	1:E:579:LEU:HD23	1.90	0.71
1:F:289:GLU:HG3	1:F:292:ARG:HH21	1.55	0.71
1:F:493:LEU:HD23	1:F:508:LEU:HD23	1.71	0.71
2:G:193:LEU:HG	2:G:194:ALA:N	2.05	0.71
1:C:226:GLN:H	1:C:226:GLN:NE2	1.89	0.71
1:A:61:LEU:HD12	1:A:63:GLN:NE2	2.05	0.71
1:B:43:GLU:HG2	2:G:113:TRP:HZ3	1.55	0.71
1:C:306:HIS:O	1:C:309:ARG:HB3	1.91	0.71
1:C:489:ILE:HG13	1:C:516:ILE:HD11	1.72	0.71
1:E:101:ALA:HB2	1:E:134:LYS:HE2	1.71	0.71
1:E:327:ILE:CG2	1:E:328:TRP:N	2.54	0.71
1:F:152:PHE:O	1:F:156:VAL:HG23	1.90	0.71
1:C:165:LYS:HD3	1:C:208:ASP:HB3	1.73	0.71
1:D:37:LEU:HD12	1:D:40:MET:CE	2.20	0.71
1:E:156:VAL:HA	1:E:160:ALA:HB3	1.73	0.71
1:E:425:THR:HG22	1:E:426:MET:HE3	1.71	0.71
1:F:563:THR:HG22	1:F:572:ASN:ND2	2.04	0.71
1:E:299:LEU:HD22	1:E:301:LEU:HD11	1.72	0.71
1:F:473:LYS:O	1:F:477:LEU:HD13	1.90	0.70
1:A:285:LEU:HA	1:A:288:LEU:HD12	1.72	0.70
1:B:202:LEU:HD21	1:B:213:MET:HG2	1.72	0.70
1:F:299:LEU:CD1	1:F:299:LEU:H	2.01	0.70
1:B:307:LYS:CE	1:B:338:LYS:HG3	2.22	0.70
1:B:51:TYR:O	1:B:55:LEU:HG	1.91	0.70
1:E:264:THR:HG22	1:E:266:ASN:H	1.55	0.70
1:E:631:LEU:CD2	2:I:171:LEU:HD13	2.20	0.70
1:D:43:GLU:O	1:D:44:GLN:HG2	1.91	0.70
1:C:115:GLU:O	1:C:117:GLY:N	2.24	0.70
1:F:432:LEU:HD11	1:F:461:GLU:OE2	1.90	0.70
1:E:174:LEU:O	1:E:178:GLU:HG3	1.91	0.70
1:F:78:PHE:HB3	1:F:81:MET:CG	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:VAL:O	1:C:161:ILE:HG12	1.91	0.70
1:F:152:PHE:HB3	1:F:173:TYR:CE1	2.26	0.70
1:A:463:HIS:O	1:A:464:ILE:HG13	1.92	0.70
1:F:46:THR:HG23	1:F:276:PRO:HG3	1.72	0.70
2:I:145:ALA:O	2:I:149:VAL:HG23	1.92	0.70
1:B:128:ILE:O	1:B:132:ARG:HB2	1.92	0.70
1:A:336:GLY:O	1:A:338:LYS:N	2.25	0.70
1:C:627:ILE:HD11	2:H:171:LEU:HD11	1.72	0.70
1:D:218:THR:HA	1:D:233:ILE:CD1	2.20	0.69
1:D:41:ILE:HG12	1:D:50:LEU:HB3	1.73	0.69
1:E:284:LEU:O	1:E:288:LEU:HG	1.91	0.69
1:A:462:TYR:OH	1:A:499:VAL:HG11	1.90	0.69
1:A:641:LYS:HD2	1:A:642:VAL:N	2.06	0.69
1:C:115:GLU:C	1:C:117:GLY:H	1.95	0.69
1:D:222:GLN:HB3	1:D:226:GLN:HG2	1.73	0.69
1:F:572:ASN:OD1	1:F:575:GLN:HG2	1.91	0.69
1:D:152:PHE:O	1:D:156:VAL:HG23	1.91	0.69
1:E:638:GLN:HA	1:E:641:LYS:HG2	1.74	0.69
1:C:49:PHE:CE2	1:C:53:LYS:HD2	2.26	0.69
1:D:182:PRO:HD3	1:D:191:ARG:NH1	2.06	0.69
1:D:297:ASN:HB2	1:D:306:HIS:CE1	2.27	0.69
1:C:654:LEU:HD12	2:H:179:LEU:HD22	1.74	0.69
1:E:341:ASP:OD2	1:E:343:THR:HG22	1.92	0.69
1:D:434:ALA:HA	1:D:437:LYS:CE	2.22	0.69
1:E:205:GLN:O	1:E:210:LEU:HD21	1.92	0.69
1:F:576:ARG:HH11	1:F:576:ARG:CB	2.05	0.69
1:B:24:THR:HB	1:B:43:GLU:OE1	1.93	0.69
1:D:394:LEU:CD2	1:D:448:LEU:HD11	2.23	0.69
1:E:327:ILE:HG23	1:E:328:TRP:H	1.58	0.69
1:E:553:PHE:O	1:E:556:VAL:HG23	1.92	0.69
1:E:569:LEU:HD12	1:F:452:ASP:OD1	1.92	0.69
1:F:553:PHE:O	1:F:556:VAL:HG23	1.92	0.69
1:C:434:ALA:HA	1:C:437:LYS:HE2	1.75	0.69
1:A:247:TYR:HE1	1:A:251:LEU:HD22	1.56	0.69
1:D:349:LEU:HD11	1:D:365:SER:HB3	1.74	0.69
1:F:376:ILE:HB	1:F:377:PRO:HD3	1.75	0.69
1:F:557:ASN:HD22	1:F:560:GLU:CB	2.04	0.69
1:E:76:ASP:O	1:E:79:PRO:HD3	1.93	0.68
1:F:445:LEU:HD22	1:F:448:LEU:HD23	1.74	0.68
1:A:81:MET:CB	1:A:84:ILE:HD13	2.23	0.68
1:D:37:LEU:HD23	1:D:54:LEU:CD1	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:CYS:O	1:C:390:ILE:HG13	1.92	0.68
1:D:37:LEU:HD23	1:D:54:LEU:HD12	1.75	0.68
1:C:48:ILE:HG22	1:C:273:LEU:HD13	1.74	0.68
1:B:80:LEU:HA	1:B:118:ASN:HD21	1.58	0.68
1:F:501:GLU:HB3	1:F:504:GLN:HG3	1.75	0.68
2:I:126:THR:HB	2:I:129:MET:HB2	1.75	0.68
1:A:376:ILE:HB	1:A:377:PRO:HD3	1.74	0.68
1:A:394:LEU:HA	1:A:411:LEU:CD2	2.22	0.68
1:A:624:PRO:HB2	1:A:627:ILE:HG22	1.75	0.68
1:B:204:CYS:HB2	1:B:205:GLN:HE21	1.59	0.68
1:B:262:PRO:HB3	1:B:272:ASN:HD21	1.56	0.68
1:B:77:ARG:HD3	1:B:78:PHE:HE1	1.58	0.68
2:G:143:GLN:HG2	2:G:182:ASN:ND2	2.07	0.68
1:A:476:GLU:O	1:A:479:LEU:HB2	1.93	0.68
1:D:578:GLU:O	1:D:579:LEU:HD23	1.94	0.68
1:F:297:ASN:HD22	1:F:306:HIS:CG	2.12	0.68
1:F:366:LEU:HD22	1:F:370:TYR:CE1	2.29	0.68
1:A:81:MET:HE1	1:A:319:GLN:HA	1.75	0.68
1:B:145:ARG:CZ	1:B:180:TRP:NE1	2.57	0.68
1:B:64:TRP:HE3	1:B:68:TYR:HE2	1.42	0.68
1:F:506:LYS:HE2	1:F:533:GLU:OE2	1.93	0.68
2:G:125:THR:HG22	2:G:126:THR:N	2.04	0.68
1:B:404:ASN:O	1:B:408:ILE:HB	1.94	0.67
1:B:487:GLU:HG3	1:B:491:LYS:HE3	1.73	0.67
1:D:463:HIS:HE1	1:D:498:TYR:HE2	1.41	0.67
1:D:557:ASN:HD22	1:D:560:GLU:N	1.92	0.67
1:E:432:LEU:HD13	1:E:464:ILE:CD1	2.24	0.67
1:A:576:ARG:HG3	1:A:576:ARG:HH11	1.58	0.67
1:B:26:ARG:HG3	1:B:26:ARG:O	1.94	0.67
1:E:361:VAL:HG23	1:F:578:GLU:OE2	1.94	0.67
1:E:405:GLU:HG3	1:E:406:SER:N	2.09	0.67
1:A:177:LEU:HB3	1:A:195:ILE:HG12	1.75	0.67
1:B:296:ASP:HB3	1:B:298:LYS:CD	2.24	0.67
1:C:567:LYS:HG2	1:C:572:ASN:HA	1.74	0.67
1:D:459:TYR:CE1	1:D:495:PHE:HD1	2.12	0.67
1:A:177:LEU:O	1:A:195:ILE:HD11	1.94	0.67
1:A:66:GLN:HE21	1:A:66:GLN:N	1.92	0.67
1:C:265:LEU:O	1:C:265:LEU:HD23	1.95	0.67
1:D:44:GLN:H	1:D:45:PRO:CD	2.08	0.67
1:A:42:GLU:O	1:A:45:PRO:HD3	1.94	0.67
1:C:364:PHE:HZ	1:C:421:VAL:HG11	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:147:LEU:HD22	2:H:179:LEU:HD13	1.76	0.67
2:I:183:GLY:O	2:I:184:VAL:HG23	1.95	0.67
1:D:282:GLN:O	1:D:286:ILE:HG13	1.94	0.67
1:E:170:TRP:CE3	1:E:202:LEU:HD23	2.30	0.67
1:A:634:LEU:HD11	2:G:174:ALA:HB2	1.77	0.67
1:B:427:LYS:HB2	1:B:435:SER:CB	2.24	0.67
1:C:389:ARG:HH21	1:C:392:LEU:HB2	1.59	0.67
1:E:228:THR:HG22	1:E:231:ARG:NE	2.10	0.67
1:B:24:THR:HG21	1:B:43:GLU:HG3	1.77	0.67
1:B:513:ILE:HA	1:B:522:LEU:HD11	1.75	0.67
1:C:196:ARG:HG2	1:C:200:LYS:HE2	1.76	0.67
1:C:497:ILE:HG23	1:C:532:PHE:CD1	2.30	0.67
1:E:217:TYR:CE2	1:E:236:LEU:HD12	2.30	0.67
1:E:254:THR:HG23	1:E:257:LEU:CD2	2.25	0.67
1:A:317:ALA:O	1:A:321:VAL:HG22	1.94	0.67
1:C:115:GLU:HG2	1:C:116:LEU:H	1.59	0.67
1:D:99:LEU:HD11	1:D:133:LYS:HD3	1.75	0.67
1:F:378:GLU:O	1:F:382:THR:HG22	1.94	0.67
1:A:71:PHE:CE1	1:A:88:ARG:HA	2.30	0.66
1:B:65:LYS:HD3	1:B:65:LYS:O	1.95	0.66
1:E:180:TRP:O	1:E:182:PRO:HD3	1.95	0.66
1:E:56:LYS:HE3	1:E:265:LEU:O	1.95	0.66
1:E:283:GLN:HA	1:E:283:GLN:OE1	1.94	0.66
1:A:100:ASP:OD1	1:A:103:VAL:HG23	1.95	0.66
1:A:625:PRO:O	1:A:626:GLU:HB2	1.95	0.66
1:B:434:ALA:O	1:B:438:ILE:HG13	1.94	0.66
1:B:444:ARG:HH21	2:G:167:GLU:CD	1.97	0.66
1:D:127:TYR:O	1:D:131:VAL:HG23	1.95	0.66
1:C:626:GLU:HB3	2:H:149:VAL:HG11	1.75	0.66
1:B:43:GLU:HG2	2:G:113:TRP:CZ3	2.30	0.66
1:F:254:THR:HG23	1:F:257:LEU:HB3	1.76	0.66
2:I:143:GLN:HG2	2:I:182:ASN:HD21	1.58	0.66
2:I:164:LEU:HD23	2:I:165:LEU:N	2.10	0.66
1:E:452:ASP:HA	1:E:455:LEU:HD23	1.75	0.66
1:F:103:VAL:O	1:F:106:PRO:HD2	1.95	0.66
1:C:654:LEU:HD22	2:H:154:CYS:SG	2.35	0.66
1:E:287:TRP:HZ2	1:E:320:HIS:CG	2.14	0.66
1:A:495:PHE:O	1:A:499:VAL:HG23	1.95	0.66
1:B:122:SER:HB3	1:B:263:ILE:HD12	1.78	0.66
1:E:554:PRO:O	1:E:555:GLU:HB3	1.96	0.66
1:E:115:GLU:HG2	1:E:116:LEU:N	2.07	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:335:GLN:NE2	1:E:348:TYR:HE1	1.88	0.66
1:A:225:ASN:HB2	1:A:229:ALA:CB	2.18	0.66
1:B:137:ILE:HG23	1:B:145:ARG:HB2	1.76	0.66
1:B:86:CYS:HB3	1:B:263:ILE:HG13	1.78	0.66
1:B:447:LYS:HG2	1:B:481:TYR:HB3	1.77	0.66
1:F:563:THR:HG23	1:F:574:LEU:HB3	1.78	0.66
1:B:390:ILE:HD13	1:B:414:LYS:HG2	1.78	0.66
1:D:262:PRO:HG3	1:D:273:LEU:HD21	1.77	0.66
1:E:501:GLU:HB3	1:E:504:GLN:HG3	1.78	0.66
1:A:140:GLY:HA3	1:A:144:ALA:CB	2.26	0.66
1:A:356:ILE:CG2	1:A:359:SER:HB2	2.25	0.66
1:B:23:PRO:HB3	1:B:26:ARG:NH1	2.11	0.66
1:C:275:LYS:H	1:C:275:LYS:HE2	1.61	0.66
2:I:159:GLU:C	2:I:161:PHE:H	1.99	0.66
1:D:396:ALA:O	1:D:398:MET:N	2.28	0.65
1:D:455:LEU:HA	1:D:475:LEU:HD21	1.77	0.65
1:F:41:ILE:CG1	1:F:50:LEU:HB3	2.26	0.65
1:D:299:LEU:N	1:D:299:LEU:HD12	2.12	0.65
1:F:392:LEU:HD13	2:I:113:TRP:CZ3	2.32	0.65
1:F:432:LEU:HA	1:F:435:SER:HB3	1.78	0.65
1:A:142:GLU:O	1:A:146:ASN:HB2	1.96	0.65
1:B:137:ILE:HD12	1:B:137:ILE:N	2.10	0.65
1:B:165:LYS:HD3	1:B:208:ASP:OD2	1.97	0.65
1:B:366:LEU:C	1:B:368:GLU:H	1.98	0.65
1:C:145:ARG:O	1:C:145:ARG:HD2	1.94	0.65
1:F:282:GLN:O	1:F:286:ILE:HG13	1.96	0.65
2:H:185:CYS:CB	2:H:188:ASP:HB3	2.24	0.65
1:B:204:CYS:HB2	1:B:205:GLN:NE2	2.11	0.65
1:B:206:PRO:HA	1:B:210:LEU:HD11	1.78	0.65
1:B:364:PHE:CZ	1:B:421:VAL:HG11	2.32	0.65
1:E:131:VAL:HG11	1:E:151:ALA:CB	2.26	0.65
1:F:280:ASP:O	1:F:283:GLN:HB2	1.97	0.65
2:G:174:ALA:O	2:G:178:LEU:HB2	1.95	0.65
1:E:489:ILE:HD12	1:E:508:LEU:HD11	1.78	0.65
1:A:173:TYR:CE2	1:A:198:LEU:HD22	2.32	0.65
1:A:462:TYR:HD2	1:A:463:HIS:NE2	1.94	0.65
1:E:434:ALA:HA	1:E:437:LYS:NZ	2.11	0.65
1:F:398:MET:CG	1:F:408:ILE:HD11	2.22	0.65
1:D:513:ILE:HG22	1:D:552:LYS:HE2	1.78	0.65
1:E:42:GLU:O	1:E:45:PRO:HD3	1.96	0.65
1:F:492:TYR:CE1	1:F:496:LEU:HD11	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:160:THR:O	2:I:163:ALA:HB3	1.96	0.65
1:A:111:CYS:HG	1:A:112:LEU:HD23	1.60	0.65
1:A:646:GLU:HB2	1:A:650:PHE:HD2	1.61	0.65
1:E:468:THR:HG21	1:E:499:VAL:HG11	1.78	0.65
1:F:468:THR:CG2	1:F:499:VAL:HG11	2.26	0.65
1:C:237:SER:O	1:C:241:MET:HG2	1.96	0.65
1:C:455:LEU:HD22	1:C:455:LEU:N	2.12	0.65
1:C:468:THR:HG21	1:C:499:VAL:HG11	1.78	0.65
1:C:523:LYS:HB2	1:C:553:PHE:CE2	2.32	0.65
1:D:575:GLN:C	1:D:577:LEU:H	1.99	0.65
1:E:61:LEU:HB2	1:E:63:GLN:HE21	1.60	0.65
2:H:134:GLU:C	2:H:136:GLY:H	2.01	0.65
1:D:460:ILE:O	1:D:464:ILE:HG13	1.97	0.65
1:E:432:LEU:HD13	1:E:464:ILE:HD11	1.77	0.65
1:E:638:GLN:NE2	1:F:384:LEU:HD12	2.12	0.65
2:H:134:GLU:O	2:H:137:LYS:HG2	1.96	0.64
1:E:299:LEU:H	1:E:299:LEU:HD12	1.62	0.64
1:F:523:LYS:HB2	1:F:553:PHE:CE2	2.31	0.64
2:I:114:LEU:H	2:I:114:LEU:HD12	1.61	0.64
1:E:335:GLN:HG3	1:E:348:TYR:CE1	2.32	0.64
1:F:85:TRP:CE3	1:F:111:CYS:HB3	2.32	0.64
1:E:568:VAL:HG23	1:F:417:TYR:HE1	1.62	0.64
1:A:119:ASN:OD1	1:A:159:CYS:HB2	1.97	0.64
1:B:556:VAL:HG22	1:B:557:ASN:H	1.62	0.64
1:C:493:LEU:O	1:C:497:ILE:HG13	1.98	0.64
1:D:156:VAL:HG13	1:D:170:TRP:HH2	1.63	0.64
1:D:52:VAL:HG11	1:D:268:ALA:HB3	1.79	0.64
2:G:147:LEU:HD22	2:G:179:LEU:HD23	1.79	0.64
1:A:167:ILE:HG23	1:A:168:GLN:H	1.62	0.64
1:C:552:LYS:C	1:C:554:PRO:HD3	2.17	0.64
1:D:81:MET:HE1	1:D:319:GLN:O	1.98	0.64
1:E:255:LYS:O	1:E:257:LEU:N	2.29	0.64
1:E:335:GLN:HG3	1:E:348:TYR:CD1	2.33	0.64
1:E:574:LEU:HD11	1:F:361:VAL:HG22	1.79	0.64
1:B:426:MET:HG3	1:B:438:ILE:HD11	1.79	0.64
1:E:198:LEU:O	1:E:198:LEU:HD12	1.98	0.64
2:G:143:GLN:HG3	2:G:178:LEU:HD21	1.80	0.64
2:H:146:LEU:O	2:H:150:ILE:HG13	1.97	0.64
1:A:218:THR:HG22	1:A:233:ILE:HG21	1.80	0.64
1:C:140:GLY:HA3	1:C:144:ALA:HB3	1.79	0.64
1:C:400:ASP:O	1:C:401:ASP:HB3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:563:THR:HG22	1:C:572:ASN:OD1	1.97	0.64
1:D:468:THR:HG21	1:D:499:VAL:CG1	2.20	0.64
1:E:384:LEU:HD23	1:E:387:ILE:HD12	1.80	0.64
1:A:99:LEU:HD12	1:A:99:LEU:H	1.61	0.64
1:C:631:LEU:HD12	2:H:115:PRO:HD2	1.79	0.64
2:H:143:GLN:CG	2:H:178:LEU:HD22	2.28	0.64
1:B:202:LEU:HD12	1:B:203:LEU:N	2.13	0.64
1:E:125:LEU:HD21	1:E:169:PHE:HD1	1.63	0.64
1:F:485:ASP:HB3	1:F:488:TYR:HB3	1.80	0.64
1:F:54:LEU:O	1:F:54:LEU:HG	1.97	0.64
2:I:189:GLN:NE2	2:I:189:GLN:H	1.96	0.64
1:A:345:ILE:CD1	1:A:345:ILE:H	1.97	0.64
1:D:287:TRP:O	1:D:291:ILE:HG13	1.97	0.64
2:G:125:THR:HG23	2:G:129:MET:HE3	1.80	0.64
1:E:631:LEU:HD21	2:I:171:LEU:HD22	1.79	0.64
1:A:32:ASP:O	1:A:36:LYS:HG3	1.99	0.63
1:A:462:TYR:HD2	1:A:463:HIS:CE1	2.16	0.63
1:C:174:LEU:O	1:C:178:GLU:HG3	1.98	0.63
1:C:283:GLN:HA	1:C:286:ILE:HD12	1.80	0.63
1:C:473:LYS:O	1:C:477:LEU:HD13	1.98	0.63
1:D:456:GLU:O	1:D:460:ILE:HG13	1.97	0.63
1:E:434:ALA:HA	1:E:437:LYS:HZ3	1.63	0.63
1:E:626:GLU:OE1	2:I:146:LEU:HG	1.98	0.63
1:A:108:LEU:HD13	1:A:127:TYR:HD1	1.61	0.63
1:D:152:PHE:HB3	1:D:173:TYR:CE1	2.34	0.63
1:E:412:LYS:HE2	1:E:448:LEU:HA	1.79	0.63
2:G:125:THR:HG23	2:G:129:MET:CE	2.28	0.63
2:H:186:SER:HA	2:H:189:GLN:HE21	1.62	0.63
1:C:30:GLU:HG3	1:C:31:SER:H	1.64	0.63
1:D:55:LEU:HD13	1:D:265:LEU:HD11	1.80	0.63
1:D:59:VAL:C	1:D:61:LEU:H	2.02	0.63
1:E:207:MET:H	1:E:210:LEU:HG	1.63	0.63
1:C:644:ILE:HG23	2:H:173:TYR:HE1	1.64	0.63
1:E:650:PHE:HD2	2:I:165:LEU:HD21	1.63	0.63
1:A:280:ASP:OD2	1:A:283:GLN:HG2	1.98	0.63
1:B:130:TYR:C	1:B:132:ARG:H	2.02	0.63
1:B:59:VAL:HG13	1:B:60:SER:N	2.13	0.63
1:C:635:PRO:HG3	2:H:120:VAL:CG2	2.28	0.63
1:E:200:LYS:CD	1:E:236:LEU:HD21	2.29	0.63
1:E:479:LEU:HD11	1:E:492:TYR:HE2	1.63	0.63
1:A:83:ASN:HB2	1:A:262:PRO:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:ILE:O	1:B:529:VAL:HG23	1.98	0.63
1:E:173:TYR:CD2	1:E:198:LEU:HD22	2.34	0.63
2:H:186:SER:O	2:H:190:LEU:HG	1.98	0.63
1:A:51:TYR:HD1	1:A:74:LEU:HB2	1.64	0.63
1:A:61:LEU:HB2	1:A:63:GLN:HE21	1.64	0.63
1:C:423:MET:HB2	1:C:438:ILE:HG21	1.79	0.63
1:D:542:VAL:O	1:D:546:GLU:HG3	1.97	0.63
1:E:136:ASP:HB3	1:E:139:THR:HB	1.81	0.63
1:E:186:PHE:C	1:E:188:GLU:H	2.02	0.63
1:E:43:GLU:O	1:E:44:GLN:HG2	1.98	0.63
1:A:265:LEU:HD23	1:A:265:LEU:O	1.98	0.63
1:D:378:GLU:O	1:D:382:THR:HG22	1.99	0.63
1:F:36:LYS:C	1:F:37:LEU:HD12	2.19	0.63
1:F:89:LEU:HD11	1:F:108:LEU:HD21	1.80	0.63
1:D:159:CYS:O	1:D:161:ILE:HG12	1.98	0.63
1:D:376:ILE:HB	1:D:377:PRO:HD3	1.80	0.63
1:A:202:LEU:HD12	1:A:203:LEU:N	2.13	0.63
1:A:579:LEU:CD1	1:A:582:MET:HE1	2.29	0.63
1:B:77:ARG:HB3	1:B:78:PHE:HD1	1.63	0.63
1:C:78:PHE:HB3	1:C:81:MET:HG2	1.78	0.63
1:D:180:TRP:CZ3	1:D:191:ARG:HB2	2.34	0.63
1:D:280:ASP:HB3	1:D:283:GLN:HB2	1.81	0.63
1:E:371:GLU:HA	1:E:379:ILE:HD11	1.81	0.63
1:A:341:ASP:O	1:A:344:VAL:HG23	1.99	0.62
1:A:395:ALA:O	1:A:399:GLU:HG3	1.99	0.62
1:A:470:THR:O	1:A:474:VAL:HG23	1.99	0.62
1:B:442:CYS:O	1:B:445:LEU:HB2	1.99	0.62
1:E:552:LYS:C	1:E:554:PRO:HD3	2.19	0.62
1:E:576:ARG:HB2	1:E:576:ARG:HH11	1.64	0.62
1:A:115:GLU:O	1:A:116:LEU:HD23	1.98	0.62
1:A:443:ARG:HD2	1:A:477:LEU:HG	1.81	0.62
1:A:49:PHE:HE2	1:A:53:LYS:HZ2	1.46	0.62
1:E:237:SER:O	1:E:241:MET:HG2	1.99	0.62
1:E:635:PRO:HB2	1:E:640:PHE:HE1	1.63	0.62
1:F:297:ASN:HB2	1:F:306:HIS:CE1	2.35	0.62
1:A:626:GLU:OE1	2:G:149:VAL:HG21	1.98	0.62
1:A:231:ARG:O	1:A:235:GLU:HG3	1.99	0.62
1:B:422:TYR:CE2	1:B:438:ILE:HD13	2.34	0.62
1:C:509:PHE:CD1	1:C:529:VAL:HG21	2.34	0.62
1:D:371:GLU:HA	1:D:379:ILE:HD11	1.81	0.62
1:E:253:ILE:HG23	1:E:289:GLU:HG2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:ILE:HG22	1:E:273:LEU:HD13	1.80	0.62
1:F:574:LEU:O	1:F:578:GLU:HB3	1.99	0.62
1:A:639:TYR:CE2	2:G:120:VAL:HG23	2.35	0.62
1:B:572:ASN:HD22	1:B:572:ASN:C	2.02	0.62
1:C:509:PHE:CZ	1:C:513:ILE:HD11	2.34	0.62
1:D:103:VAL:O	1:D:106:PRO:HD2	1.98	0.62
1:E:125:LEU:CD2	1:E:128:ILE:HD12	2.23	0.62
1:F:456:GLU:O	1:F:460:ILE:HG13	1.99	0.62
1:B:346:THR:OG1	1:B:369:GLN:HB3	1.98	0.62
1:B:85:TRP:CE3	1:B:111:CYS:HB3	2.33	0.62
1:D:426:MET:HG3	1:D:438:ILE:HD11	1.82	0.62
1:B:184:ASN:OD1	1:B:185:LYS:N	2.31	0.62
1:D:37:LEU:HA	1:D:40:MET:HE2	1.81	0.62
1:E:191:ARG:HE	1:E:195:ILE:HD11	1.64	0.62
2:H:186:SER:CA	2:H:189:GLN:HE21	2.11	0.62
1:C:178:GLU:HA	1:C:191:ARG:NH2	2.13	0.62
1:D:494:ASP:OD1	1:D:528:LYS:HD3	1.99	0.62
1:E:326:GLU:O	1:E:330:ASN:HB2	1.99	0.62
1:B:530:ILE:HG13	1:B:545:LEU:HD22	1.82	0.62
1:C:412:LYS:NZ	1:C:448:LEU:HA	2.14	0.62
1:F:371:GLU:OE2	1:F:429:ILE:HD11	2.00	0.62
2:G:186:SER:HA	2:G:189:GLN:OE1	1.99	0.62
1:A:99:LEU:HB2	1:A:134:LYS:HZ1	1.63	0.62
1:A:174:LEU:HD11	1:A:199:TYR:CZ	2.35	0.62
1:C:180:TRP:O	1:C:191:ARG:NH1	2.33	0.62
1:E:302:SER:OG	1:E:305:LEU:HG	1.99	0.62
1:E:573:TYR:HD1	1:F:417:TYR:HB2	1.64	0.62
1:A:513:ILE:N	1:A:513:ILE:HD12	2.15	0.62
1:D:41:ILE:O	1:D:41:ILE:HG22	1.99	0.62
1:E:200:LYS:CG	1:E:236:LEU:HD21	2.29	0.62
1:E:401:ASP:C	1:E:403:THR:H	2.03	0.62
1:E:557:ASN:ND2	1:E:560:GLU:N	2.48	0.62
1:B:378:GLU:N	1:B:378:GLU:OE2	2.32	0.61
1:B:427:LYS:HB2	1:B:435:SER:HB2	1.82	0.61
1:C:559:LEU:HA	1:D:329:PHE:HE1	1.63	0.61
1:E:209:CYS:HB2	1:E:212:SER:HB3	1.82	0.61
1:E:426:MET:HG3	1:E:438:ILE:HD11	1.80	0.61
1:A:65:LYS:C	1:A:65:LYS:HD3	2.20	0.61
1:B:218:THR:HA	1:B:233:ILE:CD1	2.30	0.61
1:B:281:VAL:HG12	1:B:285:LEU:HD11	1.81	0.61
1:C:640:PHE:HA	1:C:642:VAL:HG22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:400:ASP:O	1:E:401:ASP:HB3	2.00	0.61
1:E:560:GLU:O	1:E:563:THR:OG1	2.16	0.61
1:F:371:GLU:CB	1:F:379:ILE:HD11	2.30	0.61
1:A:92:GLU:OE2	1:A:103:VAL:HG11	2.00	0.61
1:A:165:LYS:HD3	1:A:208:ASP:HB3	1.81	0.61
1:C:226:GLN:CD	1:C:226:GLN:H	2.02	0.61
1:D:77:ARG:HB3	1:D:78:PHE:CD1	2.36	0.61
1:C:460:ILE:O	1:C:464:ILE:HG13	2.00	0.61
1:A:59:VAL:HG13	1:A:60:SER:N	2.16	0.61
1:B:140:GLY:HA3	1:B:144:ALA:HB2	1.83	0.61
1:C:569:LEU:O	1:C:571:VAL:HG23	2.01	0.61
1:C:74:LEU:HD13	1:C:84:ILE:CG2	2.31	0.61
1:E:159:CYS:SG	1:E:160:ALA:N	2.73	0.61
1:E:137:ILE:HD12	1:E:179:HIS:NE2	2.15	0.61
1:E:41:ILE:HG22	1:E:41:ILE:O	2.00	0.61
1:A:128:ILE:HG12	1:A:152:PHE:CE1	2.36	0.61
1:A:638:GLN:O	1:A:641:LYS:HE3	2.00	0.61
1:C:106:PRO:O	1:C:109:ALA:HB3	2.01	0.61
1:D:85:TRP:CE3	1:D:111:CYS:HB3	2.35	0.61
1:E:41:ILE:CG1	1:E:50:LEU:HD22	2.30	0.61
1:F:534:SER:HA	1:F:542:VAL:HG21	1.82	0.61
1:A:249:ASP:O	1:A:253:ILE:HG13	2.00	0.61
1:A:81:MET:CE	1:A:319:GLN:HA	2.31	0.61
1:A:510:GLU:OE1	1:A:548:ARG:NH2	2.34	0.61
1:C:103:VAL:O	1:C:106:PRO:HD2	2.00	0.61
1:C:432:LEU:HD22	1:C:464:ILE:HD13	1.81	0.61
1:E:311:THR:O	1:E:315:MET:HG3	2.00	0.61
1:E:265:LEU:HD23	1:E:265:LEU:O	2.01	0.61
1:E:280:ASP:HB3	1:E:283:GLN:HB2	1.82	0.61
1:E:638:GLN:O	1:E:641:LYS:HG3	2.01	0.61
1:A:387:ILE:CD1	1:A:418:VAL:HG12	2.31	0.61
1:C:247:TYR:CZ	1:C:251:LEU:HD13	2.36	0.61
1:C:501:GLU:O	1:C:504:GLN:N	2.31	0.61
1:D:546:GLU:OE2	1:D:565:LYS:HE2	2.01	0.61
1:A:283:GLN:CA	1:A:286:ILE:HD12	2.30	0.60
1:B:267:GLN:O	1:B:269:THR:HG23	2.00	0.60
1:B:390:ILE:HG22	1:B:415:LEU:HD13	1.81	0.60
1:B:506:LYS:NZ	1:B:545:LEU:HD12	2.16	0.60
1:E:135:ASN:ND2	1:E:147:ILE:HG21	2.15	0.60
1:A:634:LEU:HD11	2:G:174:ALA:CB	2.31	0.60
1:A:106:PRO:O	1:A:109:ALA:HB3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:GLU:HG2	1:A:270:GLU:O	2.01	0.60
1:B:202:LEU:HD12	1:B:202:LEU:C	2.20	0.60
1:C:205:GLN:O	1:C:207:MET:HG3	2.01	0.60
1:C:275:LYS:HE2	1:C:278:GLU:OE1	2.01	0.60
1:D:275:LYS:N	1:D:275:LYS:HD3	2.15	0.60
1:F:557:ASN:ND2	1:F:560:GLU:N	2.49	0.60
1:F:77:ARG:HB3	1:F:78:PHE:CD1	2.36	0.60
1:A:510:GLU:O	1:A:513:ILE:HD11	2.01	0.60
1:D:221:GLU:HB3	1:D:229:ALA:HB1	1.83	0.60
1:A:345:ILE:N	1:A:345:ILE:HD12	2.04	0.60
1:B:317:ALA:O	1:B:321:VAL:HG22	2.02	0.60
1:C:44:GLN:H	1:C:45:PRO:HD3	1.65	0.60
1:D:200:LYS:HG2	1:D:236:LEU:HD11	1.83	0.60
1:A:400:ASP:O	1:A:401:ASP:HB3	2.01	0.60
1:A:427:LYS:HB2	1:A:435:SER:OG	2.01	0.60
1:A:624:PRO:HB2	1:A:627:ILE:CG2	2.31	0.60
1:B:78:PHE:N	1:B:78:PHE:CD1	2.69	0.60
1:F:254:THR:HG23	1:F:257:LEU:CB	2.30	0.60
1:F:509:PHE:O	1:F:513:ILE:HG13	2.01	0.60
2:I:125:THR:HG22	2:I:129:MET:CE	2.31	0.60
1:A:58:HIS:HB3	1:A:67:VAL:HG23	1.84	0.60
1:C:574:LEU:HD11	1:D:361:VAL:CG2	2.30	0.60
2:H:114:LEU:H	2:H:114:LEU:HD12	1.66	0.60
2:H:134:GLU:HA	2:H:137:LYS:HE2	1.83	0.60
1:B:86:CYS:CB	1:B:263:ILE:HG13	2.31	0.60
1:E:263:ILE:HG22	1:E:267:GLN:NE2	2.17	0.60
1:E:325:PRO:HD3	1:E:356:ILE:CD1	2.30	0.60
1:E:41:ILE:HG13	1:E:50:LEU:HD22	1.82	0.60
1:F:156:VAL:HA	1:F:160:ALA:HB3	1.82	0.60
1:F:71:PHE:CD2	1:F:88:ARG:HB2	2.36	0.60
1:B:192:VAL:HG12	1:B:220:TRP:CH2	2.36	0.60
1:D:128:ILE:HA	1:D:131:VAL:HG23	1.84	0.60
1:E:631:LEU:HD12	2:I:115:PRO:HD2	1.84	0.60
2:I:118:VAL:HG12	2:I:119:ASP:N	2.17	0.60
2:I:138:LEU:O	2:I:142:GLN:HB3	2.02	0.60
2:I:188:ASP:C	2:I:190:LEU:H	2.04	0.60
1:A:339:ASN:HD22	1:A:339:ASN:C	2.05	0.60
1:B:307:LYS:HE3	1:B:338:LYS:HG3	1.83	0.60
1:B:356:ILE:O	1:B:358:ASN:N	2.35	0.60
1:C:81:MET:CE	1:C:319:GLN:HA	2.32	0.60
1:D:455:LEU:HD13	1:D:475:LEU:CD2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:332:ALA:O	1:E:335:GLN:HB2	2.02	0.60
2:G:159:GLU:O	2:G:162:VAL:HG22	2.02	0.60
1:A:179:HIS:CG	1:A:179:HIS:O	2.55	0.60
1:A:58:HIS:ND1	1:A:66:GLN:HB3	2.16	0.60
1:B:227:LEU:O	1:B:227:LEU:HD23	2.02	0.60
1:B:364:PHE:HZ	1:B:421:VAL:HG11	1.65	0.60
1:B:559:LEU:HD21	1:B:579:LEU:HD11	1.84	0.60
1:C:186:PHE:C	1:C:188:GLU:H	2.05	0.60
1:C:553:PHE:O	1:C:556:VAL:HG23	2.00	0.60
1:D:560:GLU:HA	1:D:582:MET:HE3	1.84	0.60
1:A:99:LEU:N	1:A:99:LEU:HD12	2.16	0.59
1:B:252:ASN:O	1:B:255:LYS:HG2	2.02	0.59
1:C:44:GLN:H	1:C:45:PRO:CD	2.15	0.59
1:F:354:GLN:O	1:F:357:PRO:HD3	2.02	0.59
1:F:533:GLU:HB3	1:F:542:VAL:HG22	1.82	0.59
1:F:576:ARG:NH1	1:F:576:ARG:HB3	2.14	0.59
1:C:131:VAL:HG11	1:C:151:ALA:HB2	1.83	0.59
1:E:309:ARG:O	1:E:312:TYR:N	2.29	0.59
1:E:449:VAL:O	1:E:449:VAL:HG23	2.00	0.59
1:C:542:VAL:O	1:C:546:GLU:HG3	2.02	0.59
1:E:394:LEU:O	1:E:398:MET:HG3	2.02	0.59
1:E:74:LEU:HD22	1:E:84:ILE:HD13	1.84	0.59
1:A:245:SER:O	1:A:248:GLN:HB2	2.02	0.59
1:B:548:ARG:NH1	1:B:548:ARG:HG2	2.10	0.59
1:C:30:GLU:HG3	1:C:31:SER:N	2.17	0.59
1:C:371:GLU:HA	1:C:379:ILE:HD11	1.84	0.59
1:C:74:LEU:HD22	1:C:84:ILE:HD13	1.83	0.59
1:C:79:PRO:O	1:C:80:LEU:HD23	2.02	0.59
1:D:222:GLN:HA	1:D:226:GLN:HA	1.84	0.59
2:H:150:ILE:HG23	2:H:161:PHE:HE1	1.66	0.59
1:B:99:LEU:HB2	1:B:134:LYS:NZ	2.16	0.59
1:C:218:THR:HA	1:C:233:ILE:HD11	1.83	0.59
1:D:428:ARG:O	1:D:428:ARG:HG2	2.00	0.59
1:E:259:ARG:HH12	1:E:290:TRP:HH2	1.48	0.59
1:E:523:LYS:HB2	1:E:553:PHE:CE2	2.37	0.59
1:E:563:THR:HG22	1:E:574:LEU:CD1	2.26	0.59
1:A:264:THR:HB	1:A:267:GLN:CG	2.31	0.59
1:A:89:LEU:N	1:A:89:LEU:HD23	2.17	0.59
1:B:259:ARG:HD3	1:B:287:TRP:CH2	2.38	0.59
1:B:524:MET:O	1:B:528:LYS:HG3	2.03	0.59
1:D:451:PRO:HG3	1:D:482:PHE:CD2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:LYS:HD2	1:A:334:TYR:OH	2.03	0.59
1:B:89:LEU:HD21	1:B:107:VAL:CG1	2.31	0.59
1:C:153:GLN:O	1:C:156:VAL:HB	2.02	0.59
1:C:425:THR:HG22	1:C:426:MET:CE	2.33	0.59
1:D:330:ASN:ND2	1:D:330:ASN:N	2.51	0.59
1:F:350:LYS:NZ	1:F:354:GLN:HE21	2.00	0.59
2:G:150:ILE:HG21	2:G:175:ILE:HD13	1.85	0.59
2:G:164:LEU:HD12	2:G:164:LEU:O	2.03	0.59
1:B:119:ASN:OD1	1:B:159:CYS:HB2	2.03	0.59
1:B:71:PHE:CE2	1:B:88:ARG:HB2	2.37	0.59
1:C:631:LEU:HD21	2:H:171:LEU:HD12	1.83	0.59
1:A:85:TRP:CD2	1:A:111:CYS:HB3	2.36	0.59
1:F:275:LYS:HE2	1:F:275:LYS:H	1.67	0.59
2:G:189:GLN:HG3	2:G:190:LEU:N	2.17	0.59
1:A:196:ARG:NH1	1:A:232:HIS:HE1	2.01	0.59
1:A:575:GLN:HE21	1:A:582:MET:CE	2.16	0.59
1:B:296:ASP:HB3	1:B:298:LYS:HD2	1.83	0.59
1:C:394:LEU:HA	1:C:411:LEU:HD23	1.84	0.59
1:D:455:LEU:N	1:D:455:LEU:HD22	2.18	0.59
1:E:284:LEU:HB2	1:E:321:VAL:HG11	1.85	0.59
1:E:44:GLN:H	1:E:45:PRO:HD3	1.68	0.59
1:C:563:THR:HG23	1:C:574:LEU:HD12	1.83	0.58
1:C:85:TRP:CD2	1:C:111:CYS:HB3	2.38	0.58
1:C:361:VAL:HG22	1:D:574:LEU:CD1	2.30	0.58
1:E:285:LEU:HD23	1:E:285:LEU:O	2.03	0.58
1:E:557:ASN:HD22	1:E:560:GLU:CB	2.13	0.58
1:A:451:PRO:HB3	1:A:488:TYR:CD1	2.38	0.58
1:D:284:LEU:O	1:D:287:TRP:N	2.35	0.58
1:D:412:LYS:O	1:D:415:LEU:HB3	2.04	0.58
1:E:165:LYS:HE2	1:E:250:TRP:HZ3	1.66	0.58
1:E:282:GLN:O	1:E:286:ILE:HG13	2.02	0.58
2:H:116:VAL:HG23	2:H:117:GLY:N	2.17	0.58
2:I:168:ALA:HB1	2:I:170:GLN:OE1	2.04	0.58
1:A:173:TYR:CE2	1:A:198:LEU:HD13	2.38	0.58
1:A:280:ASP:HB3	1:A:283:GLN:HB2	1.84	0.58
1:A:492:TYR:CE1	1:A:496:LEU:HD11	2.37	0.58
1:A:54:LEU:HG	1:A:58:HIS:HD2	1.68	0.58
1:B:305:LEU:O	1:B:308:ALA:HB3	2.03	0.58
1:E:470:THR:O	1:E:474:VAL:HG23	2.03	0.58
1:E:509:PHE:CD1	1:E:529:VAL:HG21	2.38	0.58
1:F:79:PRO:CB	1:F:116:LEU:HD13	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:167:ILE:HG13	1:F:209:CYS:HB3	1.84	0.58
1:A:521:LEU:O	1:A:525:ILE:HG12	2.03	0.58
1:B:180:TRP:CZ3	1:B:191:ARG:HA	2.37	0.58
1:B:219:GLN:NE2	1:B:220:TRP:N	2.51	0.58
1:C:34:ILE:HD13	1:C:58:HIS:CE1	2.38	0.58
1:D:262:PRO:CG	1:D:273:LEU:HD21	2.33	0.58
1:D:317:ALA:HB1	1:D:327:ILE:HD11	1.83	0.58
2:I:179:LEU:HG	2:I:184:VAL:HG21	1.84	0.58
1:B:77:ARG:HB3	1:B:78:PHE:CD1	2.37	0.58
1:D:32:ASP:O	1:D:34:ILE:N	2.36	0.58
1:C:543:ARG:CZ	1:D:372:LEU:HD11	2.34	0.58
1:F:490:ASN:HB3	1:F:528:LYS:HZ1	1.67	0.58
2:I:147:LEU:HD23	2:I:148:LYS:N	2.19	0.58
1:A:432:LEU:O	1:A:432:LEU:HD12	2.03	0.58
1:C:332:ALA:O	1:C:345:ILE:HG12	2.04	0.58
1:E:40:MET:HB3	1:E:50:LEU:HD21	1.85	0.58
1:A:103:VAL:O	1:A:106:PRO:HD2	2.03	0.58
1:B:180:TRP:HB3	1:B:191:ARG:NH1	2.18	0.58
1:B:341:ASP:C	1:B:343:THR:H	2.07	0.58
1:F:78:PHE:HB3	1:F:81:MET:HG2	1.85	0.58
1:A:79:PRO:C	1:A:80:LEU:HD23	2.24	0.58
1:C:636:LYS:C	1:C:638:GLN:H	2.06	0.58
1:D:502:GLU:OE2	1:D:536:VAL:HG11	2.03	0.58
1:E:156:VAL:O	1:E:160:ALA:HB3	2.04	0.58
1:E:442:CYS:O	1:E:445:LEU:HB2	2.04	0.58
1:E:48:ILE:HA	1:E:51:TYR:HD2	1.69	0.58
1:F:168:GLN:HG3	1:F:169:PHE:N	2.18	0.58
1:F:516:ILE:HG22	1:F:517:SER:O	2.04	0.58
1:A:412:LYS:NZ	1:A:448:LEU:HA	2.19	0.58
1:B:28:ARG:HH21	1:F:33:VAL:HG11	1.69	0.58
1:C:121:LEU:HG	1:C:159:CYS:SG	2.44	0.58
1:C:452:ASP:HA	1:C:455:LEU:HD23	1.86	0.58
1:D:136:ASP:HB3	1:D:139:THR:CB	2.32	0.58
1:D:186:PHE:C	1:D:188:GLU:H	2.07	0.58
1:D:358:ASN:HB3	1:D:389:ARG:HG3	1.85	0.58
1:F:81:MET:HE2	1:F:319:GLN:HA	1.86	0.58
1:A:210:LEU:HD11	1:A:243:ALA:HB1	1.85	0.58
1:A:351:LEU:HA	1:A:354:GLN:OE1	2.04	0.58
1:B:545:LEU:HA	1:B:548:ARG:HD3	1.86	0.58
1:C:370:TYR:CD1	1:C:378:GLU:HB3	2.39	0.58
1:C:371:GLU:OE2	1:D:539:LEU:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:336:GLY:HA3	1:F:345:ILE:HG13	1.86	0.58
1:F:580:ASP:C	1:F:582:MET:H	2.05	0.58
1:A:66:GLN:HE21	1:A:66:GLN:CA	2.17	0.57
1:B:314:TYR:HB3	1:B:331:MET:CE	2.34	0.57
1:D:33:VAL:H	1:D:36:LYS:NZ	2.01	0.57
1:D:457:ASN:O	1:D:461:GLU:HG2	2.04	0.57
1:A:178:GLU:O	1:A:191:ARG:NH2	2.33	0.57
1:A:182:PRO:HB3	1:A:188:GLU:HB2	1.86	0.57
1:B:462:TYR:CE1	1:B:468:THR:HG23	2.39	0.57
1:C:483:ALA:HB1	1:C:515:LYS:NZ	2.19	0.57
1:C:78:PHE:HB3	1:C:81:MET:CG	2.33	0.57
1:E:320:HIS:O	1:E:322:CYS:N	2.37	0.57
1:F:167:ILE:HG23	1:F:168:GLN:N	2.18	0.57
1:F:371:GLU:CA	1:F:379:ILE:HD11	2.34	0.57
1:A:180:TRP:O	1:A:182:PRO:HD3	2.05	0.57
1:A:324:ALA:O	1:A:327:ILE:HG22	2.03	0.57
1:A:398:MET:C	1:A:400:ASP:H	2.08	0.57
1:B:78:PHE:N	1:B:78:PHE:HD1	2.03	0.57
1:C:257:LEU:HD12	1:C:283:GLN:HE22	1.67	0.57
1:C:636:LYS:O	1:C:638:GLN:N	2.36	0.57
1:D:221:GLU:HB3	1:D:229:ALA:CB	2.34	0.57
1:D:434:ALA:O	1:D:438:ILE:HG13	2.03	0.57
1:E:115:GLU:CG	1:E:116:LEU:H	2.12	0.57
1:E:258:LYS:HG3	1:E:260:ASN:OD1	2.04	0.57
1:E:299:LEU:HD21	1:E:309:ARG:NH1	2.19	0.57
1:F:81:MET:HE1	1:F:322:CYS:HB3	1.86	0.57
1:B:419:TYR:OH	1:B:441:LYS:HE3	2.03	0.57
1:A:173:TYR:HE2	1:A:198:LEU:HD13	1.68	0.57
1:A:524:MET:HE2	1:A:528:LYS:HE2	1.86	0.57
1:B:191:ARG:HG3	1:B:191:ARG:HH11	1.70	0.57
1:C:325:PRO:HD3	1:C:356:ILE:HD13	1.87	0.57
1:C:394:LEU:HA	1:C:411:LEU:CD2	2.35	0.57
1:D:432:LEU:HD13	1:D:464:ILE:HD11	1.87	0.57
1:E:200:LYS:O	1:E:204:CYS:SG	2.57	0.57
1:E:394:LEU:HD12	1:E:411:LEU:HD23	1.87	0.57
1:F:240:TYR:O	1:F:243:ALA:HB3	2.05	0.57
1:A:85:TRP:CE3	1:A:111:CYS:HB3	2.39	0.57
1:A:202:LEU:HD13	1:A:207:MET:HE1	1.87	0.57
1:A:79:PRO:HG3	1:A:351:LEU:HD22	1.86	0.57
1:A:84:ILE:HA	1:A:87:MET:HE3	1.86	0.57
1:E:173:TYR:HE2	1:E:198:LEU:HB2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:275:LYS:H	1:E:275:LYS:HE2	1.70	0.57
1:A:191:ARG:HG3	1:A:191:ARG:HH11	1.68	0.57
1:A:284:LEU:HG	1:A:288:LEU:HD11	1.87	0.57
1:B:457:ASN:HB3	1:B:474:VAL:HG11	1.87	0.57
1:C:43:GLU:O	1:C:44:GLN:HG2	2.04	0.57
1:A:261:LEU:HD12	1:A:319:GLN:HE21	1.70	0.57
1:A:259:ARG:HG2	1:A:320:HIS:CD2	2.39	0.57
1:C:41:ILE:HG12	1:C:50:LEU:HB3	1.87	0.57
1:D:371:GLU:CA	1:D:379:ILE:HD11	2.35	0.57
1:F:278:GLU:O	1:F:279:TYR:HB3	2.03	0.57
1:F:341:ASP:HB3	1:F:344:VAL:HG23	1.87	0.57
1:F:386:CYS:O	1:F:390:ILE:HG13	2.05	0.57
1:D:128:ILE:HA	1:D:131:VAL:CG2	2.34	0.57
1:E:154:VAL:O	1:E:158:LYS:HG2	2.04	0.57
1:F:509:PHE:CE2	1:F:513:ILE:HD11	2.40	0.57
1:B:476:GLU:HA	1:B:479:LEU:HD12	1.87	0.57
1:F:394:LEU:HD12	1:F:411:LEU:HD23	1.85	0.57
1:F:364:PHE:HZ	1:F:421:VAL:HG11	1.69	0.57
1:B:258:LYS:CE	2:H:152:HIS:HB2	2.29	0.57
2:I:187:VAL:O	2:I:190:LEU:HG	2.05	0.57
2:I:186:SER:N	2:I:189:GLN:HE22	2.03	0.57
1:A:167:ILE:HG23	1:A:168:GLN:N	2.18	0.56
1:A:425:THR:HG22	1:A:426:MET:CE	2.34	0.56
1:C:208:ASP:HA	1:C:247:TYR:CZ	2.40	0.56
1:C:626:GLU:OE1	2:H:149:VAL:HG21	2.04	0.56
1:B:427:LYS:HB2	1:B:435:SER:HB3	1.86	0.56
1:C:37:LEU:HD23	1:C:54:LEU:HD13	1.87	0.56
1:D:115:GLU:C	1:D:117:GLY:H	2.07	0.56
1:D:167:ILE:HD12	1:D:209:CYS:HB3	1.86	0.56
1:E:145:ARG:NH2	1:E:180:TRP:CZ2	2.73	0.56
1:E:533:GLU:HG3	1:E:545:LEU:HD12	1.87	0.56
2:H:145:ALA:O	2:H:149:VAL:HG23	2.05	0.56
1:A:228:THR:HG22	1:A:231:ARG:HH22	1.69	0.56
1:A:93:PHE:HE2	1:A:104:ILE:HD13	1.70	0.56
1:B:552:LYS:C	1:B:554:PRO:HD3	2.25	0.56
1:C:168:GLN:HG3	1:C:169:PHE:N	2.20	0.56
1:C:459:TYR:CE1	1:C:495:PHE:HD1	2.22	0.56
1:C:472:CYS:SG	1:C:504:GLN:NE2	2.78	0.56
1:D:530:ILE:HA	1:D:545:LEU:HD13	1.87	0.56
1:E:114:LYS:N	1:E:114:LYS:HD3	2.20	0.56
1:E:309:ARG:O	1:E:312:TYR:HB3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:460:ILE:O	1:E:464:ILE:HG13	2.05	0.56
1:A:115:GLU:OE2	1:A:115:GLU:N	2.36	0.56
1:A:130:TYR:C	1:A:132:ARG:H	2.08	0.56
1:A:630:LEU:HD23	2:G:171:LEU:CD1	2.35	0.56
1:B:497:ILE:HG23	1:B:532:PHE:HD1	1.71	0.56
1:E:287:TRP:CZ2	1:E:320:HIS:CG	2.94	0.56
1:F:115:GLU:N	1:F:115:GLU:CD	2.59	0.56
1:B:167:ILE:HG23	1:B:168:GLN:N	2.21	0.56
1:C:553:PHE:HB3	1:C:556:VAL:HG21	1.88	0.56
1:C:54:LEU:HD23	1:C:70:THR:HG23	1.88	0.56
1:E:107:VAL:HA	1:E:110:ARG:CD	2.36	0.56
1:E:119:ASN:O	1:E:316:GLN:NE2	2.38	0.56
1:E:137:ILE:HG13	1:E:138:ILE:HG13	1.87	0.56
1:E:173:TYR:CE2	1:E:198:LEU:HD22	2.40	0.56
1:F:85:TRP:CD2	1:F:111:CYS:HB3	2.39	0.56
1:A:170:TRP:CZ3	1:A:202:LEU:HB3	2.41	0.56
1:A:49:PHE:CE2	1:A:53:LYS:HD3	2.40	0.56
1:C:217:TYR:CE2	1:C:236:LEU:HD12	2.41	0.56
1:C:456:GLU:O	1:C:460:ILE:HG13	2.06	0.56
1:E:344:VAL:O	1:E:347:LYS:HB3	2.05	0.56
1:F:78:PHE:HB3	1:F:81:MET:HG3	1.86	0.56
2:I:184:VAL:O	2:I:185:CYS:HB2	2.05	0.56
1:A:387:ILE:HG22	1:A:388:ASP:N	2.20	0.56
1:B:180:TRP:HB3	1:B:191:ARG:HH12	1.69	0.56
1:C:92:GLU:OE1	1:C:95:LYS:HE2	2.05	0.56
1:E:115:GLU:HG2	1:E:116:LEU:HG	1.87	0.56
1:E:206:PRO:HB3	1:E:247:TYR:CA	2.35	0.56
1:E:557:ASN:HD22	1:E:560:GLU:H	1.49	0.56
1:A:439:PHE:CZ	1:A:474:VAL:HG13	2.40	0.56
1:C:218:THR:HA	1:C:233:ILE:CD1	2.35	0.56
1:C:523:LYS:O	1:C:527:GLN:HG3	2.05	0.56
1:A:105:GLU:HB2	1:A:106:PRO:HD3	1.87	0.56
1:A:307:LYS:HE3	1:A:338:LYS:HG3	1.86	0.56
1:B:439:PHE:CZ	1:B:474:VAL:HG13	2.41	0.56
1:C:37:LEU:O	1:C:41:ILE:HG13	2.06	0.56
1:C:425:THR:HG22	1:C:426:MET:HE2	1.87	0.56
1:C:642:VAL:O	1:C:643:THR:HG23	2.06	0.56
1:D:181:LYS:O	1:D:181:LYS:HG3	2.06	0.56
1:A:116:LEU:O	1:A:118:ASN:N	2.38	0.56
1:A:33:VAL:HG12	1:A:37:LEU:HG	1.86	0.56
1:A:649:ALA:C	1:A:651:SER:H	2.10	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:LEU:HB2	1:D:569:LEU:HD11	1.88	0.56
1:D:289:GLU:OE2	1:D:292:ARG:NH2	2.39	0.56
1:D:297:ASN:HD22	1:D:306:HIS:CG	2.23	0.56
1:D:30:GLU:HG3	1:D:31:SER:N	2.21	0.56
1:D:324:ALA:O	1:D:327:ILE:HG22	2.06	0.56
1:D:414:LYS:O	1:D:418:VAL:HG23	2.05	0.56
1:E:178:GLU:HA	1:E:191:ARG:HH22	1.66	0.56
1:F:270:GLU:O	1:F:270:GLU:HG2	2.06	0.56
1:E:568:VAL:CG2	1:F:417:TYR:HE1	2.19	0.56
1:F:493:LEU:CD2	1:F:508:LEU:HD23	2.35	0.56
1:B:183:VAL:HG23	1:B:187:GLU:OE1	2.06	0.56
1:B:391:HIS:CD2	1:B:415:LEU:HD21	2.41	0.56
1:B:398:MET:HA	1:B:408:ILE:HD11	1.87	0.56
1:D:463:HIS:HE1	1:D:498:TYR:CE2	2.23	0.56
1:E:101:ALA:CB	1:E:134:LYS:HE2	2.36	0.56
1:F:83:ASN:ND2	1:F:261:LEU:HB3	2.21	0.56
1:F:432:LEU:HD22	1:F:464:ILE:CD1	2.35	0.56
1:F:563:THR:CG2	1:F:572:ASN:HD21	2.18	0.56
2:G:139:GLN:O	2:G:142:GLN:HG2	2.06	0.56
1:A:128:ILE:HG12	1:A:152:PHE:CD1	2.41	0.55
1:B:115:GLU:CD	1:B:115:GLU:H	2.10	0.55
1:B:427:LYS:HA	1:B:435:SER:HB3	1.88	0.55
1:E:177:LEU:O	1:E:195:ILE:HD11	2.07	0.55
1:F:578:GLU:O	1:F:579:LEU:HD23	2.06	0.55
1:A:247:TYR:CE1	1:A:251:LEU:HD22	2.39	0.55
1:D:295:SER:C	1:D:297:ASN:H	2.10	0.55
1:D:37:LEU:HA	1:D:40:MET:CE	2.35	0.55
1:E:174:LEU:HD11	1:E:199:TYR:CZ	2.41	0.55
1:E:306:HIS:O	1:E:309:ARG:HB3	2.06	0.55
1:E:468:THR:HG23	1:E:499:VAL:HG11	1.87	0.55
1:E:41:ILE:HD12	1:E:54:LEU:HD22	1.88	0.55
1:E:574:LEU:HD13	1:E:574:LEU:O	2.07	0.55
1:F:571:VAL:HB	1:F:573:TYR:CE2	2.42	0.55
1:A:361:VAL:HG23	1:B:578:GLU:OE1	2.06	0.55
1:B:416:THR:OG1	1:B:450:THR:HG23	2.06	0.55
1:B:473:LYS:O	1:B:477:LEU:HB2	2.07	0.55
1:B:580:ASP:C	1:B:582:MET:H	2.10	0.55
1:F:416:THR:OG1	1:F:449:VAL:HB	2.06	0.55
1:B:192:VAL:HG12	1:B:220:TRP:CZ2	2.40	0.55
1:E:489:ILE:HG13	1:E:516:ILE:HD11	1.88	0.55
1:F:521:LEU:O	1:F:525:ILE:HD13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:557:ASN:ND2	1:F:560:GLU:HB2	2.15	0.55
1:D:511:SER:O	1:D:515:LYS:HE2	2.07	0.55
1:F:364:PHE:CZ	1:F:421:VAL:HG11	2.42	0.55
1:A:480:LYS:HD3	1:A:480:LYS:N	2.22	0.55
1:B:559:LEU:O	1:B:562:PHE:HB3	2.07	0.55
1:D:345:ILE:O	1:D:349:LEU:HB2	2.06	0.55
1:C:566:TYR:OH	1:D:368:GLU:OE2	2.14	0.55
1:F:160:ALA:HB1	1:F:170:TRP:CZ2	2.42	0.55
1:A:54:LEU:HG	1:A:58:HIS:CD2	2.41	0.55
1:A:646:GLU:HG3	1:A:650:PHE:HE2	1.72	0.55
1:A:71:PHE:CD1	1:A:88:ARG:HD2	2.42	0.55
1:B:41:ILE:HD11	1:B:50:LEU:O	2.06	0.55
1:C:47:ASP:HB2	1:C:276:PRO:CG	2.37	0.55
1:D:269:THR:OG1	1:D:271:SER:HB3	2.07	0.55
1:D:279:TYR:CE2	1:D:324:ALA:HA	2.41	0.55
1:E:107:VAL:HA	1:E:110:ARG:HG3	1.89	0.55
1:E:49:PHE:CE2	1:E:270:GLU:HB2	2.42	0.55
2:G:125:THR:HA	2:G:129:MET:HE2	1.89	0.55
1:A:137:ILE:N	1:A:137:ILE:HD12	2.18	0.55
1:B:100:ASP:O	1:B:102:ALA:N	2.40	0.55
1:B:132:ARG:HH11	1:B:132:ARG:HG2	1.71	0.55
1:B:341:ASP:O	1:B:344:VAL:HG23	2.06	0.55
1:D:162:PHE:CD2	1:D:309:ARG:HG3	2.41	0.55
1:E:164:PRO:HG3	1:E:250:TRP:CZ2	2.41	0.55
1:E:471:ALA:O	1:E:475:LEU:HD12	2.06	0.55
2:I:175:ILE:O	2:I:179:LEU:HD13	2.07	0.55
1:B:58:HIS:CE1	1:B:66:GLN:HG2	2.41	0.55
1:B:59:VAL:CG1	1:B:60:SER:N	2.70	0.55
1:D:214:TRP:CH2	1:D:233:ILE:HG23	2.42	0.55
1:E:457:ASN:O	1:E:460:ILE:HB	2.07	0.55
1:E:580:ASP:C	1:E:582:MET:H	2.08	0.55
1:B:246:LEU:CD1	1:B:299:LEU:HD23	2.37	0.55
1:D:44:GLN:N	1:D:45:PRO:CD	2.68	0.55
1:E:125:LEU:C	1:E:127:TYR:H	2.08	0.55
1:F:258:LYS:HG3	1:F:260:ASN:OD1	2.07	0.55
1:A:147:ILE:O	1:A:150:GLN:HB2	2.07	0.54
1:A:366:LEU:HD22	1:A:370:TYR:CE1	2.41	0.54
1:A:371:GLU:HA	1:A:379:ILE:HD11	1.88	0.54
1:A:40:MET:HG2	1:A:50:LEU:CD1	2.36	0.54
1:D:103:VAL:C	1:D:106:PRO:HD2	2.27	0.54
1:D:258:LYS:HG3	1:D:260:ASN:OD1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:560:GLU:HA	1:D:582:MET:CE	2.37	0.54
1:F:536:VAL:HG12	1:F:536:VAL:O	2.06	0.54
1:B:325:PRO:HD3	1:B:356:ILE:HD13	1.89	0.54
1:F:60:SER:O	1:F:61:LEU:HD23	2.06	0.54
2:H:179:LEU:O	2:H:184:VAL:HB	2.08	0.54
2:I:167:GLU:O	2:I:168:ALA:HB2	2.08	0.54
1:B:103:VAL:O	1:B:106:PRO:HD2	2.07	0.54
1:C:455:LEU:H	1:C:455:LEU:HD22	1.71	0.54
1:E:568:VAL:CG2	1:F:417:TYR:CE1	2.91	0.54
1:F:145:ARG:NH2	1:F:180:TRP:CZ2	2.75	0.54
1:F:265:LEU:O	1:F:265:LEU:HD23	2.07	0.54
1:A:131:VAL:HG11	1:A:151:ALA:HB2	1.88	0.54
1:A:156:VAL:O	1:A:161:ILE:HG23	2.07	0.54
1:A:230:ARG:O	1:A:230:ARG:HG2	2.07	0.54
1:A:451:PRO:HG3	1:A:482:PHE:CD2	2.42	0.54
1:B:36:LYS:O	1:B:40:MET:HG3	2.06	0.54
1:B:451:PRO:HB3	1:B:488:TYR:CD1	2.43	0.54
1:C:399:GLU:HG3	1:C:400:ASP:N	2.22	0.54
1:D:167:ILE:HG12	1:D:171:ASN:ND2	2.22	0.54
1:E:459:TYR:O	1:E:463:HIS:HB2	2.07	0.54
1:A:517:SER:O	1:A:518:ASP:C	2.46	0.54
1:B:121:LEU:HG	1:B:159:CYS:SG	2.47	0.54
1:B:314:TYR:HB3	1:B:331:MET:HE3	1.89	0.54
1:B:61:LEU:HD12	1:B:63:GLN:NE2	2.22	0.54
1:C:529:VAL:HG12	1:C:545:LEU:CD1	2.37	0.54
1:D:557:ASN:HD22	1:D:560:GLU:HB2	1.73	0.54
1:D:59:VAL:HG22	1:D:67:VAL:HG21	1.88	0.54
1:D:71:PHE:HE2	1:D:88:ARG:HB2	1.68	0.54
1:F:460:ILE:O	1:F:464:ILE:HG13	2.07	0.54
2:H:134:GLU:C	2:H:136:GLY:N	2.61	0.54
2:I:170:GLN:N	2:I:170:GLN:HE21	1.98	0.54
1:A:115:GLU:CD	1:A:115:GLU:H	2.11	0.54
1:D:167:ILE:HG23	1:D:168:GLN:N	2.22	0.54
1:D:557:ASN:ND2	1:D:560:GLU:N	2.55	0.54
1:E:335:GLN:HA	1:E:335:GLN:OE1	2.07	0.54
1:F:463:HIS:HE1	1:F:498:TYR:HE2	1.55	0.54
1:B:38:ASN:N	1:B:38:ASN:HD22	2.04	0.54
1:C:122:SER:OG	1:C:263:ILE:HD11	2.08	0.54
1:D:159:CYS:O	1:D:161:ILE:N	2.41	0.54
1:E:165:LYS:HE2	1:E:250:TRP:CH2	2.42	0.54
1:F:200:LYS:HG2	1:F:236:LEU:CD1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:400:ASP:O	1:F:401:ASP:CB	2.55	0.54
1:F:55:LEU:HD13	1:F:71:PHE:CE1	2.42	0.54
1:B:523:LYS:HB2	1:B:553:PHE:CE2	2.43	0.54
1:A:417:TYR:HE1	1:B:568:VAL:HG23	1.72	0.54
1:D:217:TYR:CE2	1:D:236:LEU:HD12	2.43	0.54
2:G:185:CYS:O	2:G:186:SER:HB2	2.07	0.54
1:E:637:ARG:CZ	2:I:116:VAL:HG12	2.38	0.54
1:A:81:MET:HE2	1:A:319:GLN:HG3	1.90	0.54
1:B:100:ASP:C	1:B:102:ALA:H	2.12	0.54
1:D:384:LEU:O	1:D:387:ILE:N	2.41	0.54
1:E:93:PHE:CZ	1:E:130:TYR:HB2	2.39	0.54
1:E:81:MET:CE	1:E:319:GLN:HA	2.38	0.54
1:F:404:ASN:O	1:F:408:ILE:HB	2.08	0.54
2:H:155:LYS:O	2:H:159:GLU:N	2.41	0.54
1:A:254:THR:O	1:A:257:LEU:HB2	2.07	0.54
1:A:373:ASN:O	1:A:375:LYS:N	2.41	0.54
1:A:557:ASN:HB3	1:A:560:GLU:HB3	1.88	0.54
1:C:101:ALA:HB2	1:C:134:LYS:CE	2.38	0.54
1:D:145:ARG:HH11	1:D:149:ILE:HD11	1.73	0.54
1:F:81:MET:CE	1:F:319:GLN:HA	2.37	0.54
2:G:138:LEU:HB3	2:G:142:GLN:HG3	1.90	0.54
1:C:633:VAL:HA	2:H:118:VAL:CG2	2.38	0.54
2:I:187:VAL:N	2:I:189:GLN:HE22	2.06	0.54
1:A:629:GLU:OE1	1:A:632:LYS:HE2	2.09	0.53
1:C:115:GLU:C	1:C:117:GLY:N	2.60	0.53
1:C:501:GLU:O	1:C:502:GLU:C	2.47	0.53
1:D:37:LEU:HD12	1:D:40:MET:HE2	1.88	0.53
1:E:167:ILE:HD12	1:E:209:CYS:HB3	1.90	0.53
1:E:225:ASN:O	1:E:229:ALA:HB2	2.08	0.53
1:F:413:SER:O	1:F:416:THR:N	2.42	0.53
1:A:336:GLY:C	1:A:338:LYS:N	2.62	0.53
1:B:496:LEU:HD22	1:B:501:GLU:CB	2.37	0.53
1:F:151:ALA:O	1:F:154:VAL:HG12	2.08	0.53
1:F:353:GLN:O	1:F:357:PRO:HA	2.08	0.53
2:I:134:GLU:O	2:I:137:LYS:HE3	2.08	0.53
1:B:34:ILE:HG12	1:B:57:HIS:HD2	1.74	0.53
1:C:218:THR:HG23	1:C:233:ILE:CD1	2.38	0.53
1:E:314:TYR:HB3	1:E:331:MET:HG3	1.90	0.53
1:C:127:TYR:O	1:C:131:VAL:HG23	2.08	0.53
1:C:521:LEU:O	1:C:525:ILE:HD13	2.07	0.53
1:E:195:ILE:O	1:E:199:TYR:CD2	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:171:LEU:O	2:H:171:LEU:HD23	2.09	0.53
1:A:202:LEU:HD12	1:A:202:LEU:C	2.29	0.53
1:A:264:THR:HG22	1:A:266:ASN:H	1.73	0.53
1:A:343:THR:O	1:A:343:THR:HG22	2.08	0.53
1:B:206:PRO:CB	1:B:247:TYR:HB2	2.36	0.53
1:D:473:LYS:O	1:D:477:LEU:HD13	2.07	0.53
1:E:434:ALA:HB2	1:E:437:LYS:HZ1	1.74	0.53
1:E:571:VAL:HB	1:E:573:TYR:CE2	2.43	0.53
1:F:75:HIS:HB3	1:F:110:ARG:HH21	1.73	0.53
2:H:147:LEU:HD22	2:H:179:LEU:CD1	2.38	0.53
1:A:170:TRP:CE3	1:A:202:LEU:HD23	2.44	0.53
1:A:390:ILE:HD13	1:A:414:LYS:HG2	1.91	0.53
1:A:569:LEU:CD2	1:B:456:GLU:HG2	2.38	0.53
1:C:140:GLY:O	1:C:142:GLU:N	2.41	0.53
1:C:157:ASP:HA	1:C:161:ILE:HD11	1.90	0.53
1:C:490:ASN:ND2	1:C:525:ILE:CD1	2.72	0.53
1:D:206:PRO:HB3	1:D:247:TYR:HB2	1.91	0.53
1:D:81:MET:HE1	1:D:322:CYS:HB3	1.91	0.53
1:D:74:LEU:HD13	1:D:84:ILE:HD13	1.91	0.53
1:F:468:THR:HG21	1:F:499:VAL:HG11	1.90	0.53
1:F:486:GLY:C	1:F:521:LEU:HD22	2.29	0.53
1:A:162:PHE:HA	1:A:309:ARG:NH1	2.24	0.53
1:A:218:THR:HG22	1:A:233:ILE:CG2	2.38	0.53
1:A:542:VAL:HG12	1:A:546:GLU:HG3	1.90	0.53
1:B:132:ARG:NH1	1:B:132:ARG:HG2	2.24	0.53
1:B:130:TYR:C	1:B:132:ARG:N	2.62	0.53
1:B:530:ILE:CG1	1:B:545:LEU:HD22	2.38	0.53
1:C:471:ALA:HB1	1:C:495:PHE:CZ	2.44	0.53
1:D:121:LEU:HD12	1:D:163:GLU:HG2	1.90	0.53
1:E:103:VAL:C	1:E:106:PRO:HD2	2.29	0.53
1:F:275:LYS:HE2	1:F:278:GLU:HG2	1.90	0.53
1:A:89:LEU:HD21	1:A:107:VAL:HG11	1.91	0.53
1:C:218:THR:HG23	1:C:233:ILE:HD13	1.91	0.53
1:C:398:MET:HA	1:C:408:ILE:CD1	2.33	0.53
1:D:341:ASP:HB3	1:D:344:VAL:HG23	1.91	0.53
1:F:145:ARG:NH2	1:F:180:TRP:HZ2	2.07	0.53
2:H:155:LYS:HE2	2:H:156:ASP:OD1	2.09	0.53
2:H:168:ALA:HA	2:H:170:GLN:HE22	1.74	0.53
1:A:189:GLN:O	1:A:192:VAL:HG22	2.09	0.53
1:B:467:ASP:OD1	1:B:470:THR:HG23	2.09	0.53
1:B:479:LEU:O	1:B:480:LYS:C	2.47	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:572:ASN:OD1	1:B:575:GLN:HG3	2.09	0.53
1:B:61:LEU:HB2	1:B:63:GLN:NE2	2.20	0.53
1:C:228:THR:O	1:C:231:ARG:HB3	2.09	0.53
1:C:262:PRO:CG	1:C:273:LEU:HD21	2.31	0.53
1:C:392:LEU:O	1:C:393:ASP:C	2.46	0.53
1:C:468:THR:O	1:C:469:LYS:C	2.47	0.53
1:C:655:SER:O	2:H:151:GLN:NE2	2.42	0.53
1:D:269:THR:C	1:D:271:SER:H	2.12	0.53
1:F:226:GLN:C	1:F:227:LEU:HD12	2.29	0.53
1:F:281:VAL:HG12	1:F:285:LEU:HD12	1.91	0.53
1:E:627:ILE:HD11	2:I:171:LEU:HD21	1.91	0.53
1:A:135:ASN:ND2	1:A:147:ILE:HG21	2.23	0.53
1:A:374:THR:O	1:A:376:ILE:N	2.42	0.53
1:A:68:TYR:OH	1:A:92:GLU:OE2	2.27	0.53
1:B:179:HIS:CG	1:B:179:HIS:O	2.59	0.53
1:B:401:ASP:O	1:B:401:ASP:CG	2.48	0.53
1:B:24:THR:CG2	1:B:43:GLU:HG3	2.39	0.53
1:C:192:VAL:HG23	1:C:193:GLN:H	1.74	0.53
1:C:206:PRO:HG3	1:C:246:LEU:HB2	1.90	0.53
1:D:115:GLU:N	1:D:115:GLU:CD	2.60	0.53
1:E:281:VAL:O	1:E:285:LEU:HB2	2.10	0.53
1:F:553:PHE:O	1:F:554:PRO:O	2.27	0.53
2:I:146:LEU:HD23	2:I:146:LEU:O	2.08	0.53
1:B:55:LEU:HD21	1:B:70:THR:CG2	2.38	0.52
1:C:44:GLN:N	1:C:45:PRO:CD	2.73	0.52
1:C:554:PRO:O	1:C:555:GLU:HB3	2.08	0.52
1:D:38:ASN:HD22	1:D:38:ASN:N	2.06	0.52
1:D:52:VAL:HA	1:D:55:LEU:HD12	1.91	0.52
1:E:398:MET:HA	1:E:408:ILE:CD1	2.37	0.52
1:F:202:LEU:HD12	1:F:202:LEU:C	2.30	0.52
2:G:114:LEU:CD2	2:G:164:LEU:HD13	2.39	0.52
2:H:135:LEU:HD13	2:H:177:GLU:HG2	1.91	0.52
1:A:132:ARG:HH11	1:A:132:ARG:HG2	1.74	0.52
1:A:432:LEU:O	1:A:435:SER:HB3	2.08	0.52
1:A:41:ILE:HG23	1:A:51:TYR:CE2	2.45	0.52
1:A:576:ARG:HG3	1:A:576:ARG:NH1	2.24	0.52
1:B:277:ASN:HD22	1:B:277:ASN:N	2.06	0.52
1:B:289:GLU:OE2	1:B:292:ARG:HD2	2.09	0.52
1:C:48:ILE:N	1:C:48:ILE:HD12	2.24	0.52
1:C:516:ILE:HG22	1:C:517:SER:O	2.10	0.52
1:D:210:LEU:CD1	1:D:244:ARG:HA	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:321:VAL:HG23	1:E:321:VAL:O	2.09	0.52
1:E:568:VAL:O	1:E:569:LEU:C	2.47	0.52
1:E:639:TYR:HB3	2:I:127:PRO:CG	2.38	0.52
1:F:49:PHE:O	1:F:52:VAL:HB	2.10	0.52
2:H:126:THR:HB	2:H:129:MET:HB2	1.90	0.52
1:A:462:TYR:CD2	1:A:463:HIS:CE1	2.97	0.52
1:A:77:ARG:HB2	1:A:77:ARG:HH11	1.74	0.52
1:B:423:MET:HA	1:B:438:ILE:HD12	1.91	0.52
1:D:392:LEU:HD13	2:H:113:TRP:CZ3	2.44	0.52
1:E:200:LYS:HD2	1:E:236:LEU:HD21	1.91	0.52
1:E:347:LYS:O	1:E:351:LEU:HG	2.09	0.52
1:E:485:ASP:OD1	1:E:487:GLU:HB3	2.08	0.52
1:E:580:ASP:O	1:E:582:MET:N	2.41	0.52
1:F:424:ASN:O	1:F:427:LYS:HB3	2.09	0.52
1:F:490:ASN:HB3	1:F:528:LYS:NZ	2.24	0.52
1:F:556:VAL:O	1:F:557:ASN:C	2.48	0.52
2:G:147:LEU:HD22	2:G:179:LEU:CD2	2.39	0.52
1:C:627:ILE:CD1	2:H:171:LEU:HD11	2.38	0.52
1:A:61:LEU:HB2	1:A:63:GLN:HG3	1.90	0.52
1:B:376:ILE:O	1:B:379:ILE:HB	2.10	0.52
1:E:206:PRO:HB3	1:E:247:TYR:HB2	1.90	0.52
1:E:456:GLU:O	1:E:460:ILE:HG13	2.08	0.52
1:E:44:GLN:H	1:E:45:PRO:CD	2.22	0.52
1:E:88:ARG:CZ	1:E:107:VAL:HG21	2.38	0.52
1:F:45:PRO:O	1:F:51:TYR:HE2	1.93	0.52
1:F:37:LEU:HD21	1:F:53:LYS:HE3	1.90	0.52
1:F:55:LEU:HD22	1:F:71:PHE:CD1	2.44	0.52
1:A:341:ASP:HB3	1:A:344:VAL:HG23	1.90	0.52
1:A:387:ILE:HD11	1:A:418:VAL:HG12	1.91	0.52
1:A:37:LEU:HB2	1:A:54:LEU:HD13	1.91	0.52
1:B:262:PRO:HD3	1:B:272:ASN:ND2	2.24	0.52
1:B:364:PHE:HA	1:B:367:SER:OG	2.09	0.52
1:B:99:LEU:HD12	1:B:99:LEU:N	2.25	0.52
1:C:472:CYS:O	1:C:476:GLU:HG3	2.10	0.52
1:C:61:LEU:HB2	1:C:63:GLN:NE2	2.20	0.52
1:D:275:LYS:N	1:D:275:LYS:CD	2.72	0.52
1:E:191:ARG:HE	1:E:195:ILE:CD1	2.22	0.52
1:E:299:LEU:HB2	1:E:301:LEU:HG	1.91	0.52
1:E:351:LEU:HA	1:E:354:GLN:OE1	2.09	0.52
1:E:557:ASN:HD22	1:E:560:GLU:N	2.07	0.52
1:F:167:ILE:CG2	1:F:168:GLN:N	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:189:GLN:O	1:F:193:GLN:HG3	2.10	0.52
1:F:341:ASP:HB3	1:F:344:VAL:CG2	2.40	0.52
1:C:633:VAL:HA	2:H:118:VAL:HG23	1.92	0.52
1:A:401:ASP:C	1:A:403:THR:H	2.13	0.52
1:A:89:LEU:HD11	1:A:108:LEU:HD21	1.92	0.52
1:C:180:TRP:O	1:C:182:PRO:HD3	2.10	0.52
1:C:495:PHE:O	1:C:499:VAL:HG23	2.09	0.52
1:D:575:GLN:C	1:D:577:LEU:N	2.63	0.52
1:E:196:ARG:NH2	1:E:221:GLU:OE1	2.43	0.52
1:E:207:MET:H	1:E:210:LEU:CD1	2.22	0.52
1:F:509:PHE:CD1	1:F:529:VAL:HG21	2.45	0.52
2:G:150:ILE:HG22	2:G:150:ILE:O	2.08	0.52
1:A:247:TYR:CD1	1:A:247:TYR:O	2.63	0.52
1:C:326:GLU:O	1:C:326:GLU:HG3	2.08	0.52
1:C:344:VAL:O	1:C:347:LYS:HB3	2.10	0.52
1:D:115:GLU:HG2	1:D:116:LEU:H	1.75	0.52
1:D:521:LEU:O	1:D:525:ILE:HD13	2.10	0.52
1:F:164:PRO:HG3	1:F:250:TRP:CE2	2.45	0.52
1:F:417:TYR:O	1:F:421:VAL:HG12	2.09	0.52
1:A:33:VAL:HA	1:A:36:LYS:CD	2.35	0.52
1:C:412:LYS:HZ1	1:C:448:LEU:HA	1.75	0.52
1:D:93:PHE:HZ	1:D:130:TYR:HB2	1.75	0.52
1:E:198:LEU:O	1:E:202:LEU:HG	2.10	0.52
1:E:284:LEU:HD22	1:E:324:ALA:HB1	1.91	0.52
1:F:262:PRO:CG	1:F:273:LEU:HD21	2.40	0.52
1:F:55:LEU:O	1:F:59:VAL:HG23	2.10	0.52
1:A:121:LEU:HG	1:A:159:CYS:SG	2.50	0.52
1:A:32:ASP:CG	1:A:32:ASP:O	2.48	0.52
1:B:206:PRO:HB3	1:B:247:TYR:CB	2.36	0.52
1:B:34:ILE:HG12	1:B:57:HIS:CD2	2.45	0.52
1:B:371:GLU:OE1	1:B:428:ARG:NH2	2.43	0.52
1:C:81:MET:HE2	1:C:319:GLN:HA	1.91	0.52
1:D:49:PHE:O	1:D:52:VAL:N	2.41	0.52
1:D:556:VAL:O	1:D:557:ASN:C	2.47	0.52
1:E:151:ALA:O	1:E:155:VAL:HG23	2.09	0.52
1:E:259:ARG:NH1	1:E:290:TRP:CH2	2.78	0.52
1:F:311:THR:O	1:F:315:MET:HG2	2.09	0.52
1:F:526:PHE:CD2	1:F:549:PHE:HB2	2.45	0.52
1:F:557:ASN:HD22	1:F:560:GLU:H	1.56	0.52
2:I:159:GLU:OE2	2:I:160:THR:N	2.43	0.52
1:A:509:PHE:CD1	1:A:525:ILE:HG22	2.46	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:GLU:CD	1:B:216:ARG:NH2	2.61	0.52
1:F:564:ASN:HA	1:F:567:LYS:HD2	1.92	0.52
1:A:518:ASP:CG	1:A:521:LEU:HD13	2.30	0.51
1:A:628:VAL:HG12	1:A:629:GLU:OE2	2.09	0.51
1:D:292:ARG:O	1:D:295:SER:N	2.40	0.51
1:D:338:LYS:O	1:D:339:ASN:HB3	2.10	0.51
1:E:340:THR:O	1:E:341:ASP:C	2.48	0.51
1:F:486:GLY:HA3	1:F:521:LEU:HD13	1.92	0.51
1:B:366:LEU:O	1:B:368:GLU:N	2.42	0.51
1:D:58:HIS:CE1	1:D:66:GLN:HG2	2.44	0.51
1:A:80:LEU:HD21	1:A:116:LEU:HD22	1.90	0.51
1:A:49:PHE:CZ	1:A:270:GLU:HB2	2.44	0.51
1:A:298:LYS:O	1:A:300:GLU:OE2	2.29	0.51
1:A:398:MET:O	1:A:402:PRO:HD3	2.10	0.51
1:B:95:LYS:HB2	1:B:95:LYS:NZ	2.25	0.51
1:C:103:VAL:C	1:C:106:PRO:HD2	2.31	0.51
1:D:202:LEU:HD12	1:D:203:LEU:HG	1.92	0.51
1:D:413:SER:OG	1:D:450:THR:HG21	2.10	0.51
1:D:85:TRP:CD2	1:D:111:CYS:HB3	2.45	0.51
1:E:405:GLU:C	1:E:407:ALA:N	2.63	0.51
1:E:516:ILE:HG22	1:E:517:SER:O	2.09	0.51
1:F:41:ILE:HD11	1:F:50:LEU:C	2.30	0.51
2:G:189:GLN:HG3	2:G:190:LEU:H	1.75	0.51
1:C:645:PHE:O	2:H:193:LEU:HA	2.11	0.51
2:I:159:GLU:C	2:I:161:PHE:N	2.64	0.51
1:A:369:GLN:O	1:A:372:LEU:HB3	2.11	0.51
1:A:635:PRO:HB3	2:G:120:VAL:HG21	1.92	0.51
1:B:259:ARG:HD3	1:B:287:TRP:CZ2	2.46	0.51
1:C:417:TYR:HE2	1:D:574:LEU:HD23	1.76	0.51
1:D:178:GLU:HA	1:D:191:ARG:HH21	1.76	0.51
1:D:86:CYS:HB3	1:D:263:ILE:HG13	1.91	0.51
1:D:90:SER:CB	1:D:264:THR:HG23	2.36	0.51
1:E:156:VAL:CA	1:E:160:ALA:HB3	2.40	0.51
1:E:165:LYS:HD3	1:E:208:ASP:CB	2.38	0.51
1:E:180:TRP:CZ3	1:E:191:ARG:HB2	2.44	0.51
1:F:336:GLY:HA3	1:F:345:ILE:CG1	2.41	0.51
1:A:457:ASN:O	1:A:461:GLU:HG2	2.10	0.51
1:C:338:LYS:O	1:C:339:ASN:HB3	2.10	0.51
1:C:409:ASN:O	1:C:412:LYS:HB2	2.11	0.51
1:E:550:PHE:CD1	1:E:558:LYS:HE2	2.46	0.51
1:F:358:ASN:HB3	1:F:389:ARG:CG	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:185:CYS:HB3	2:I:189:GLN:HE21	1.74	0.51
1:A:49:PHE:CE2	1:A:270:GLU:HB2	2.45	0.51
1:B:84:ILE:HG22	1:B:85:TRP:N	2.25	0.51
1:C:642:VAL:HG23	1:C:643:THR:N	2.26	0.51
1:D:221:GLU:HG3	1:D:233:ILE:HG13	1.93	0.51
1:D:262:PRO:HG3	1:D:273:LEU:CD2	2.41	0.51
1:D:455:LEU:H	1:D:455:LEU:CD2	2.24	0.51
1:D:531:PHE:C	1:D:531:PHE:CD1	2.84	0.51
1:E:544:THR:O	1:E:547:LYS:HB3	2.11	0.51
2:G:150:ILE:N	2:G:150:ILE:HD12	2.25	0.51
2:G:185:CYS:SG	2:G:188:ASP:CB	2.94	0.51
2:I:125:THR:HG22	2:I:129:MET:SD	2.51	0.51
1:A:99:LEU:HD11	1:A:133:LYS:HD3	1.93	0.51
1:B:190:GLN:HA	1:B:193:GLN:HG3	1.91	0.51
1:B:66:GLN:NE2	1:B:66:GLN:N	2.58	0.51
1:D:408:ILE:HG22	1:D:409:ASN:N	2.25	0.51
1:D:86:CYS:SG	1:D:123:LEU:HA	2.51	0.51
1:E:51:TYR:O	1:E:54:LEU:N	2.43	0.51
1:E:88:ARG:O	1:E:88:ARG:HG2	2.11	0.51
1:F:125:LEU:C	1:F:127:TYR:H	2.14	0.51
1:F:310:MET:O	1:F:314:TYR:HB2	2.11	0.51
1:F:432:LEU:HD22	1:F:464:ILE:HD13	1.93	0.51
1:F:49:PHE:O	1:F:52:VAL:N	2.43	0.51
1:F:89:LEU:HD11	1:F:108:LEU:CD2	2.39	0.51
1:A:173:TYR:CD2	1:A:198:LEU:HD22	2.46	0.51
1:B:51:TYR:CB	1:B:74:LEU:HD13	2.41	0.51
1:C:405:GLU:HA	1:C:408:ILE:HB	1.92	0.51
1:C:653:PHE:O	1:C:657:LYS:CG	2.59	0.51
1:E:275:LYS:N	1:E:275:LYS:HE2	2.26	0.51
1:E:299:LEU:HD21	1:E:309:ARG:CZ	2.41	0.51
1:A:55:LEU:C	1:A:57:HIS:H	2.15	0.51
1:B:296:ASP:HB3	1:B:298:LYS:HD3	1.91	0.51
1:B:353:GLN:HG3	1:B:353:GLN:O	2.10	0.51
1:B:425:THR:O	1:B:429:ILE:HG12	2.11	0.51
1:E:553:PHE:O	1:E:554:PRO:C	2.49	0.51
1:F:152:PHE:HB3	1:F:173:TYR:CD1	2.46	0.51
1:F:279:TYR:CE2	1:F:324:ALA:HA	2.46	0.51
1:F:468:THR:HG23	1:F:499:VAL:HG11	1.93	0.51
2:I:179:LEU:HB3	2:I:184:VAL:HB	1.92	0.51
1:A:92:GLU:C	1:A:94:ASP:H	2.14	0.51
1:B:122:SER:HB3	1:B:263:ILE:CD1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:GLU:C	1:B:94:ASP:H	2.14	0.51
1:C:575:GLN:C	1:C:577:LEU:H	2.14	0.51
1:D:121:LEU:HD21	1:D:169:PHE:HB2	1.93	0.51
1:D:191:ARG:O	1:D:195:ILE:HG13	2.10	0.51
1:D:420:CYS:SG	1:D:453:ILE:HA	2.51	0.51
1:E:46:THR:HG23	1:E:276:PRO:HG3	1.93	0.51
1:F:455:LEU:H	1:F:455:LEU:CD2	2.24	0.51
1:F:444:ARG:HD2	2:I:166:GLU:OE2	2.11	0.51
1:A:417:TYR:O	1:A:421:VAL:HG12	2.11	0.50
1:B:336:GLY:C	1:B:338:LYS:H	2.14	0.50
1:B:65:LYS:HD2	1:B:66:GLN:HE22	1.76	0.50
1:E:249:ASP:O	1:E:253:ILE:HG13	2.11	0.50
1:E:81:MET:SD	1:E:319:GLN:O	2.69	0.50
1:E:432:LEU:O	1:E:435:SER:HB3	2.11	0.50
1:F:409:ASN:HA	1:F:412:LYS:HB2	1.93	0.50
1:E:420:CYS:HB3	1:F:568:VAL:HG11	1.93	0.50
2:G:192:GLN:HA	2:G:192:GLN:OE1	2.11	0.50
2:I:168:ALA:HA	2:I:170:GLN:HE22	1.75	0.50
2:I:188:ASP:C	2:I:190:LEU:N	2.64	0.50
1:C:37:LEU:HD23	1:C:54:LEU:CD1	2.41	0.50
1:D:280:ASP:O	1:D:283:GLN:HB2	2.12	0.50
1:E:129:THR:HG23	1:E:133:LYS:HE3	1.94	0.50
1:E:509:PHE:CG	1:E:529:VAL:HG21	2.46	0.50
1:E:624:PRO:N	1:E:625:PRO:HD3	2.26	0.50
1:F:173:TYR:CD2	1:F:198:LEU:HD22	2.47	0.50
1:F:315:MET:HE1	1:F:348:TYR:HE2	1.76	0.50
1:F:455:LEU:CD2	1:F:455:LEU:N	2.74	0.50
1:F:55:LEU:HD22	1:F:71:PHE:CE1	2.46	0.50
1:A:166:SER:O	1:A:170:TRP:HD1	1.94	0.50
1:B:281:VAL:O	1:B:284:LEU:HB3	2.12	0.50
1:B:447:LYS:CG	1:B:481:TYR:HB3	2.41	0.50
1:B:481:TYR:N	1:B:481:TYR:CD1	2.80	0.50
1:C:529:VAL:CG1	1:C:545:LEU:HD11	2.39	0.50
1:D:455:LEU:HD13	1:D:475:LEU:HD22	1.93	0.50
1:E:115:GLU:H	1:E:115:GLU:CD	2.15	0.50
1:E:351:LEU:O	1:E:354:GLN:HB2	2.11	0.50
1:F:502:GLU:OE2	1:F:536:VAL:HG11	2.11	0.50
1:A:635:PRO:HB3	2:G:120:VAL:CG2	2.42	0.50
2:G:180:LEU:HD12	2:G:185:CYS:O	2.11	0.50
1:B:390:ILE:HD11	1:B:414:LYS:HE2	1.94	0.50
1:B:472:CYS:HB3	1:B:504:GLN:HE22	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:THR:HG23	1:D:233:ILE:CD1	2.41	0.50
1:D:464:ILE:HG22	1:D:465:SER:N	2.26	0.50
1:D:93:PHE:CZ	1:D:130:TYR:HB2	2.46	0.50
1:E:125:LEU:HD23	1:E:128:ILE:CD1	2.29	0.50
1:E:378:GLU:OE2	1:E:378:GLU:N	2.42	0.50
1:E:555:GLU:OE1	1:E:555:GLU:C	2.49	0.50
1:E:641:LYS:O	1:E:643:THR:N	2.44	0.50
1:F:337:GLU:HG2	1:F:337:GLU:O	2.11	0.50
1:F:401:ASP:CG	1:F:401:ASP:O	2.48	0.50
2:H:184:VAL:O	2:H:185:CYS:SG	2.67	0.50
1:B:366:LEU:C	1:B:368:GLU:N	2.65	0.50
1:D:222:GLN:O	1:D:226:GLN:HG3	2.10	0.50
1:D:65:LYS:HB3	1:D:66:GLN:OE1	2.12	0.50
1:E:424:ASN:ND2	1:E:456:GLU:OE1	2.45	0.50
1:E:85:TRP:CD2	1:E:111:CYS:HB3	2.47	0.50
1:F:522:LEU:O	1:F:525:ILE:N	2.44	0.50
1:F:561:GLU:O	1:F:562:PHE:C	2.48	0.50
2:G:184:VAL:O	2:G:185:CYS:SG	2.69	0.50
2:I:137:LYS:HG3	2:I:138:LEU:HG	1.92	0.50
1:B:335:GLN:HB3	1:B:344:VAL:HG11	1.94	0.50
1:D:275:LYS:HE2	1:D:275:LYS:H	1.76	0.50
1:D:314:TYR:O	1:D:317:ALA:HB3	2.12	0.50
1:D:44:GLN:H	1:D:45:PRO:HD3	1.76	0.50
1:E:306:HIS:O	1:E:310:MET:HG2	2.12	0.50
1:F:480:LYS:HB2	1:F:481:TYR:CD1	2.47	0.50
1:F:523:LYS:O	1:F:527:GLN:HG3	2.11	0.50
2:I:179:LEU:CG	2:I:184:VAL:HG21	2.41	0.50
1:A:447:LYS:CG	1:A:481:TYR:HB3	2.37	0.50
1:B:89:LEU:CD2	1:B:107:VAL:HG11	2.39	0.50
1:C:543:ARG:NE	1:D:372:LEU:HD11	2.26	0.50
1:D:525:ILE:HG22	1:D:526:PHE:N	2.26	0.50
1:E:366:LEU:HD22	1:E:370:TYR:CE1	2.47	0.50
1:E:370:TYR:CE1	1:E:378:GLU:HB3	2.47	0.50
1:E:509:PHE:CE2	1:E:513:ILE:HD11	2.46	0.50
1:E:638:GLN:HA	1:E:641:LYS:CG	2.41	0.50
1:F:374:THR:O	1:F:374:THR:HG22	2.12	0.50
1:A:259:ARG:HG2	1:A:320:HIS:CE1	2.46	0.50
1:C:475:LEU:HD13	1:C:492:TYR:CE1	2.47	0.50
1:E:207:MET:H	1:E:210:LEU:CG	2.24	0.50
1:E:68:TYR:N	1:E:68:TYR:HD2	2.10	0.50
1:F:481:TYR:CD1	1:F:481:TYR:N	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:494:ASP:O	1:F:498:TYR:HB2	2.12	0.50
1:F:78:PHE:CD1	1:F:78:PHE:N	2.80	0.50
2:I:147:LEU:HD23	2:I:147:LEU:C	2.31	0.50
1:A:173:TYR:O	1:A:176:PHE:HB3	2.12	0.50
1:A:462:TYR:CD2	1:A:463:HIS:NE2	2.78	0.50
1:A:463:HIS:O	1:A:464:ILE:CG1	2.60	0.50
1:B:160:ALA:C	1:B:162:PHE:H	2.15	0.50
1:B:202:LEU:HB2	1:B:207:MET:HE1	1.93	0.50
1:B:501:GLU:O	1:B:505:VAL:HG23	2.12	0.50
1:C:358:ASN:HB3	1:C:389:ARG:HG3	1.93	0.50
1:D:200:LYS:HG2	1:D:236:LEU:CD1	2.41	0.50
1:D:370:TYR:HB2	1:D:379:ILE:HG12	1.94	0.50
1:D:530:ILE:HG12	1:D:545:LEU:HB3	1.93	0.50
1:E:56:LYS:HG3	1:E:265:LEU:HD21	1.93	0.50
1:F:474:VAL:HG12	1:F:475:LEU:N	2.25	0.50
2:G:144:MET:O	2:G:148:LYS:HG2	2.12	0.50
2:I:146:LEU:HD23	2:I:150:ILE:HD13	1.93	0.50
1:A:289:GLU:O	1:A:292:ARG:HG3	2.12	0.49
1:A:631:LEU:CD1	2:G:114:LEU:HD23	2.42	0.49
1:B:356:ILE:CG2	1:B:359:SER:HB2	2.41	0.49
1:B:568:VAL:HG12	1:B:569:LEU:HG	1.92	0.49
1:B:81:MET:HE2	1:B:319:GLN:HG3	1.93	0.49
1:C:125:LEU:CD2	1:C:169:PHE:HD1	2.23	0.49
1:C:561:GLU:O	1:C:562:PHE:C	2.50	0.49
1:C:563:THR:HG23	1:C:574:LEU:HB3	1.94	0.49
1:D:390:ILE:HD13	1:D:414:LYS:CD	2.42	0.49
1:E:386:CYS:O	1:E:390:ILE:HG13	2.12	0.49
2:H:134:GLU:O	2:H:136:GLY:N	2.44	0.49
1:A:110:ARG:HG2	1:A:110:ARG:HH11	1.76	0.49
1:A:89:LEU:N	1:A:89:LEU:CD2	2.75	0.49
1:C:173:TYR:CD2	1:C:198:LEU:HD22	2.47	0.49
1:C:247:TYR:O	1:C:251:LEU:HB2	2.12	0.49
1:C:501:GLU:HB3	1:C:504:GLN:HG3	1.93	0.49
1:C:55:LEU:O	1:C:59:VAL:HG23	2.12	0.49
1:E:574:LEU:CD1	1:F:361:VAL:HG22	2.42	0.49
1:F:529:VAL:HG12	1:F:545:LEU:HD11	1.94	0.49
2:H:178:LEU:C	2:H:180:LEU:H	2.15	0.49
1:F:388:ASP:OD2	2:I:116:VAL:HG11	2.11	0.49
1:B:496:LEU:HD22	1:B:501:GLU:HB2	1.93	0.49
1:C:563:THR:CG2	1:C:574:LEU:HB3	2.42	0.49
1:C:74:LEU:HD13	1:C:84:ILE:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:ILE:HG21	1:D:130:TYR:CE1	2.46	0.49
1:D:291:ILE:HD13	1:D:314:TYR:CE1	2.47	0.49
1:D:41:ILE:CG1	1:D:50:LEU:HB3	2.41	0.49
1:E:124:TRP:CZ3	1:E:155:VAL:HG22	2.48	0.49
1:F:394:LEU:CD1	1:F:411:LEU:HD23	2.42	0.49
1:F:41:ILE:HG13	1:F:50:LEU:HB3	1.94	0.49
1:A:305:LEU:O	1:A:308:ALA:HB3	2.12	0.49
1:A:544:THR:O	1:A:547:LYS:HB3	2.12	0.49
1:A:640:PHE:C	1:A:642:VAL:N	2.66	0.49
1:B:364:PHE:CZ	1:B:421:VAL:CG1	2.95	0.49
1:B:572:ASN:ND2	1:B:575:GLN:H	2.10	0.49
1:C:322:CYS:SG	1:C:323:PHE:N	2.86	0.49
1:C:563:THR:HB	1:C:572:ASN:HD21	1.78	0.49
1:C:578:GLU:HG2	1:C:578:GLU:O	2.12	0.49
1:D:434:ALA:CA	1:D:437:LYS:HE3	2.33	0.49
1:E:121:LEU:CD1	1:E:163:GLU:HG2	2.42	0.49
1:E:156:VAL:HG13	1:E:170:TRP:CH2	2.48	0.49
1:E:44:GLN:N	1:E:45:PRO:CD	2.75	0.49
1:F:563:THR:HG22	1:F:572:ASN:CG	2.32	0.49
2:H:116:VAL:CG2	2:H:117:GLY:N	2.76	0.49
2:H:143:GLN:HG3	2:H:178:LEU:HD22	1.93	0.49
1:B:185:LYS:HG2	1:B:186:PHE:N	2.26	0.49
1:C:347:LYS:O	1:C:351:LEU:HG	2.13	0.49
1:C:375:LYS:HB3	1:C:378:GLU:OE2	2.13	0.49
1:C:546:GLU:OE2	1:C:565:LYS:HE2	2.12	0.49
1:D:557:ASN:HD22	1:D:560:GLU:CB	2.24	0.49
1:D:74:LEU:O	1:D:75:HIS:C	2.48	0.49
1:D:84:ILE:O	1:D:84:ILE:HG22	2.12	0.49
1:E:68:TYR:N	1:E:68:TYR:CD2	2.80	0.49
1:F:39:ASP:O	1:F:42:GLU:N	2.43	0.49
1:F:580:ASP:O	1:F:582:MET:N	2.32	0.49
1:A:362:LEU:O	1:A:366:LEU:HB2	2.12	0.49
1:A:416:THR:OG1	1:A:450:THR:HG23	2.12	0.49
1:B:81:MET:HE1	1:B:319:GLN:HA	1.94	0.49
1:C:101:ALA:CB	1:C:134:LYS:HE2	2.43	0.49
1:C:376:ILE:HB	1:C:377:PRO:HD3	1.94	0.49
1:C:399:GLU:CG	1:C:400:ASP:N	2.75	0.49
1:D:169:PHE:CD2	1:D:170:TRP:N	2.81	0.49
1:D:247:TYR:CZ	1:D:251:LEU:HD13	2.47	0.49
1:C:559:LEU:HB2	1:D:329:PHE:HD1	1.78	0.49
1:D:541:SER:O	1:D:544:THR:HB	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:559:LEU:O	1:D:562:PHE:HB3	2.12	0.49
1:E:135:ASN:ND2	1:E:147:ILE:CG2	2.75	0.49
1:F:563:THR:HG22	1:F:572:ASN:OD1	2.12	0.49
1:F:77:ARG:HB3	1:F:78:PHE:CE1	2.46	0.49
1:A:334:TYR:O	1:A:335:GLN:C	2.51	0.49
1:A:418:VAL:HA	1:A:421:VAL:CG1	2.43	0.49
1:A:425:THR:HG22	1:A:426:MET:HE1	1.94	0.49
1:A:646:GLU:HG3	1:A:650:PHE:CE2	2.46	0.49
1:B:137:ILE:CD1	1:B:137:ILE:H	2.24	0.49
1:B:81:MET:CE	1:B:319:GLN:HA	2.43	0.49
1:B:74:LEU:HD21	1:B:84:ILE:HG12	1.94	0.49
1:D:482:PHE:C	1:D:484:THR:H	2.15	0.49
1:E:417:TYR:O	1:E:420:CYS:HB2	2.13	0.49
2:H:186:SER:HA	2:H:189:GLN:NE2	2.25	0.49
1:A:170:TRP:HE3	1:A:198:LEU:HD11	1.78	0.49
1:A:152:PHE:CD2	1:A:173:TYR:HD1	2.31	0.49
1:A:287:TRP:CH2	1:A:316:GLN:HB3	2.48	0.49
1:A:398:MET:O	1:A:400:ASP:N	2.43	0.49
1:B:162:PHE:CD2	1:B:309:ARG:HG3	2.48	0.49
1:B:166:SER:O	1:B:170:TRP:HD1	1.95	0.49
1:B:487:GLU:N	1:B:521:LEU:HD23	2.28	0.49
1:B:496:LEU:CB	1:B:505:VAL:HG22	2.41	0.49
1:C:371:GLU:CA	1:C:379:ILE:HD11	2.43	0.49
1:C:539:LEU:CD2	1:D:371:GLU:HB3	2.43	0.49
1:D:142:GLU:HA	1:D:142:GLU:OE1	2.12	0.49
1:D:427:LYS:HB2	1:D:435:SER:HB2	1.93	0.49
1:E:289:GLU:OE2	1:E:292:ARG:NH2	2.46	0.49
1:F:455:LEU:HD22	1:F:455:LEU:N	2.28	0.49
2:H:125:THR:HA	2:H:129:MET:HE2	1.94	0.49
2:I:164:LEU:HD23	2:I:165:LEU:H	1.76	0.49
1:B:302:SER:OG	1:B:303:ASP:N	2.44	0.49
1:B:351:LEU:CA	1:B:354:GLN:HG3	2.39	0.49
1:B:85:TRP:CZ3	1:B:111:CYS:HB3	2.48	0.49
1:E:313:VAL:O	1:E:316:GLN:CB	2.59	0.49
1:F:114:LYS:HG2	1:F:115:GLU:OE2	2.13	0.49
1:A:634:LEU:CD1	2:G:174:ALA:HB2	2.43	0.49
1:B:108:LEU:HD22	1:B:127:TYR:HD1	1.78	0.49
1:C:309:ARG:O	1:C:312:TYR:HB3	2.12	0.49
1:C:624:PRO:O	1:C:627:ILE:HG22	2.11	0.49
1:D:299:LEU:H	1:D:299:LEU:CD1	2.23	0.49
1:E:103:VAL:O	1:E:106:PRO:HD2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:ARG:HG3	1:E:292:ARG:HH11	1.78	0.49
1:E:316:GLN:O	1:E:319:GLN:HB3	2.12	0.49
1:E:324:ALA:O	1:E:325:PRO:C	2.51	0.49
1:E:419:TYR:O	1:E:422:TYR:HB3	2.12	0.49
1:A:196:ARG:HD3	1:A:232:HIS:CE1	2.48	0.48
1:A:247:TYR:CD1	1:A:247:TYR:C	2.86	0.48
1:A:387:ILE:HD12	1:A:418:VAL:HG12	1.95	0.48
1:C:526:PHE:O	1:C:530:ILE:HG13	2.12	0.48
1:C:34:ILE:HD13	1:C:58:HIS:HE1	1.77	0.48
1:C:653:PHE:CG	2:H:192:GLN:NE2	2.81	0.48
1:D:84:ILE:HG12	1:D:87:MET:CE	2.43	0.48
1:E:370:TYR:CD1	1:E:378:GLU:HB3	2.48	0.48
1:F:262:PRO:HD3	1:F:272:ASN:OD1	2.13	0.48
1:F:540:ASN:HD22	1:F:543:ARG:NH2	2.11	0.48
1:A:569:LEU:HD22	1:B:456:GLU:HG2	1.95	0.48
1:D:392:LEU:O	1:D:395:ALA:N	2.46	0.48
1:D:77:ARG:HB3	1:D:78:PHE:HD1	1.77	0.48
1:E:167:ILE:HG23	1:E:168:GLN:N	2.28	0.48
1:E:262:PRO:HB3	1:E:268:ALA:HA	1.94	0.48
1:E:479:LEU:HD11	1:E:492:TYR:CE2	2.46	0.48
1:E:55:LEU:HB3	1:E:265:LEU:HD11	1.94	0.48
1:F:289:GLU:HG3	1:F:292:ARG:NH2	2.27	0.48
1:F:438:ILE:O	1:F:442:CYS:HB2	2.13	0.48
1:F:540:ASN:HD22	1:F:543:ARG:HH21	1.59	0.48
1:A:335:GLN:HG3	1:A:348:TYR:CE1	2.48	0.48
1:A:366:LEU:C	1:A:368:GLU:H	2.16	0.48
1:A:79:PRO:CG	1:A:351:LEU:HD22	2.43	0.48
1:C:192:VAL:HG23	1:C:193:GLN:N	2.28	0.48
1:D:297:ASN:ND2	1:D:306:HIS:CG	2.81	0.48
1:D:390:ILE:HD13	1:D:414:LYS:HD3	1.94	0.48
1:D:81:MET:CE	1:D:319:GLN:HA	2.43	0.48
1:E:125:LEU:HD11	1:E:169:PHE:HB2	1.94	0.48
1:E:177:LEU:HD11	1:E:194:TYR:HB3	1.96	0.48
1:F:580:ASP:C	1:F:582:MET:N	2.66	0.48
2:I:159:GLU:O	2:I:162:VAL:HG22	2.14	0.48
1:A:275:LYS:O	1:A:278:GLU:HB3	2.13	0.48
1:B:145:ARG:HG2	1:B:145:ARG:O	2.12	0.48
1:B:155:VAL:HG11	1:B:169:PHE:CE1	2.49	0.48
1:C:180:TRP:HZ3	1:C:191:ARG:HA	1.77	0.48
1:C:432:LEU:HD13	1:C:464:ILE:HD11	1.94	0.48
1:E:423:MET:HB2	1:E:438:ILE:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:194:TYR:N	1:F:194:TYR:HD1	2.12	0.48
1:F:553:PHE:N	1:F:554:PRO:HD3	2.29	0.48
1:F:52:VAL:HA	1:F:55:LEU:HD12	1.96	0.48
1:A:214:TRP:CH2	1:A:233:ILE:HG23	2.48	0.48
1:A:341:ASP:OD2	1:A:343:THR:HB	2.12	0.48
1:A:358:ASN:HB3	1:A:389:ARG:CG	2.43	0.48
1:C:554:PRO:O	1:C:555:GLU:CB	2.60	0.48
1:D:455:LEU:H	1:D:455:LEU:HD22	1.77	0.48
1:D:56:LYS:O	1:D:60:SER:HB2	2.13	0.48
1:E:86:CYS:SG	1:E:123:LEU:HA	2.54	0.48
1:E:434:ALA:CB	1:E:437:LYS:HZ1	2.26	0.48
1:E:71:PHE:CD2	1:E:88:ARG:HB2	2.49	0.48
1:F:166:SER:O	1:F:167:ILE:C	2.51	0.48
1:F:152:PHE:CG	1:F:173:TYR:CD1	3.02	0.48
1:F:46:THR:HG21	1:F:276:PRO:HB3	1.95	0.48
2:G:139:GLN:O	2:G:141:ASP:N	2.46	0.48
2:I:165:LEU:HD11	2:I:172:SER:HB2	1.96	0.48
1:A:509:PHE:CE1	1:A:525:ILE:HG22	2.49	0.48
1:A:497:ILE:HG23	1:A:532:PHE:CD1	2.49	0.48
1:A:94:ASP:O	1:A:95:LYS:HB3	2.14	0.48
1:B:449:VAL:HG23	1:B:450:THR:O	2.12	0.48
1:B:560:GLU:O	1:B:562:PHE:N	2.47	0.48
1:D:264:THR:HG22	1:D:266:ASN:H	1.79	0.48
1:D:292:ARG:O	1:D:294:GLU:N	2.47	0.48
1:E:144:ALA:HA	1:E:147:ILE:CD1	2.42	0.48
1:F:563:THR:HG23	1:F:574:LEU:CB	2.43	0.48
2:G:179:LEU:O	2:G:180:LEU:C	2.52	0.48
2:H:131:ILE:CG2	2:H:135:LEU:HD12	2.44	0.48
1:A:180:TRP:CZ3	1:A:191:ARG:CA	2.90	0.48
1:A:59:VAL:CG1	1:A:60:SER:N	2.77	0.48
1:D:168:GLN:HG3	1:D:169:PHE:N	2.29	0.48
1:D:297:ASN:ND2	1:D:306:HIS:HB2	2.27	0.48
1:E:61:LEU:O	1:E:63:GLN:HG3	2.13	0.48
1:F:421:VAL:HA	1:F:424:ASN:HD22	1.78	0.48
2:H:150:ILE:O	2:H:154:CYS:SG	2.67	0.48
1:A:80:LEU:HA	1:A:118:ASN:HD21	1.78	0.48
1:B:195:ILE:HG22	1:B:199:TYR:HD2	1.78	0.48
1:B:364:PHE:HZ	1:B:421:VAL:CG1	2.26	0.48
1:C:269:THR:HG23	1:C:272:ASN:HD21	1.79	0.48
1:D:125:LEU:C	1:D:127:TYR:H	2.15	0.48
1:D:156:VAL:HG22	1:D:170:TRP:CZ3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:569:LEU:HD12	1:D:452:ASP:OD1	2.13	0.48
1:E:423:MET:HA	1:E:438:ILE:CD1	2.40	0.48
1:F:254:THR:CG2	1:F:257:LEU:HB3	2.44	0.48
1:E:569:LEU:HD11	1:F:455:LEU:HB2	1.95	0.48
1:A:51:TYR:CD1	1:A:74:LEU:HB2	2.47	0.48
1:A:559:LEU:HD21	1:A:579:LEU:HD11	1.95	0.48
1:B:333:ASN:O	1:B:337:GLU:HB2	2.14	0.48
1:B:516:ILE:CD1	1:B:525:ILE:HG13	2.43	0.48
1:C:135:ASN:ND2	1:C:147:ILE:HG21	2.28	0.48
1:C:401:ASP:C	1:C:403:THR:H	2.15	0.48
1:C:533:GLU:HG3	1:C:545:LEU:HD12	1.95	0.48
1:C:653:PHE:O	1:C:657:LYS:HG3	2.14	0.48
1:E:87:MET:HG2	1:E:264:THR:C	2.33	0.48
1:E:501:GLU:O	1:E:504:GLN:N	2.47	0.48
1:F:553:PHE:O	1:F:554:PRO:C	2.51	0.48
2:G:134:GLU:O	2:G:137:LYS:HG2	2.14	0.48
1:A:101:ALA:HA	1:A:130:TYR:OH	2.14	0.48
1:A:130:TYR:C	1:A:132:ARG:N	2.66	0.48
1:A:169:PHE:CD2	1:A:170:TRP:N	2.82	0.48
1:A:231:ARG:HB3	1:A:231:ARG:NH1	2.28	0.48
1:A:536:VAL:O	1:A:536:VAL:HG22	2.13	0.48
1:B:74:LEU:HD21	1:B:84:ILE:CG1	2.44	0.48
1:C:275:LYS:N	1:C:275:LYS:HE2	2.28	0.48
1:D:247:TYR:CE1	1:D:251:LEU:HD13	2.49	0.48
1:D:499:VAL:O	1:D:499:VAL:HG12	2.14	0.48
1:E:398:MET:HG2	1:E:408:ILE:HD13	1.95	0.48
1:F:186:PHE:C	1:F:188:GLU:H	2.17	0.48
1:F:405:GLU:HA	1:F:408:ILE:CG2	2.42	0.48
1:F:442:CYS:SG	1:F:453:ILE:HG12	2.53	0.48
1:F:525:ILE:HG22	1:F:526:PHE:N	2.28	0.48
1:A:182:PRO:HG2	1:A:188:GLU:HG3	1.95	0.47
1:A:283:GLN:OE1	1:A:283:GLN:HA	2.13	0.47
1:A:66:GLN:NE2	1:A:66:GLN:CA	2.76	0.47
1:B:341:ASP:O	1:B:343:THR:N	2.45	0.47
1:C:283:GLN:HA	1:C:286:ILE:CD1	2.44	0.47
1:D:153:GLN:O	1:D:156:VAL:N	2.47	0.47
1:E:154:VAL:HG13	1:E:155:VAL:HG23	1.95	0.47
1:E:170:TRP:CE3	1:E:198:LEU:CD1	2.97	0.47
1:E:364:PHE:CZ	1:E:421:VAL:CG1	2.92	0.47
1:E:396:ALA:O	1:E:397:LEU:C	2.51	0.47
1:F:109:ALA:O	1:F:113:SER:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:249:ASP:O	1:F:253:ILE:HG13	2.14	0.47
1:F:441:LYS:HA	1:F:444:ARG:HE	1.78	0.47
1:F:538:SER:O	1:F:541:SER:HB2	2.14	0.47
1:A:135:ASN:CG	1:A:147:ILE:HG21	2.34	0.47
1:A:628:VAL:O	1:A:632:LYS:HG3	2.13	0.47
1:B:264:THR:O	1:B:266:ASN:N	2.47	0.47
1:B:408:ILE:O	1:B:412:LYS:HG3	2.14	0.47
1:C:640:PHE:CA	1:C:642:VAL:HG22	2.44	0.47
1:D:204:CYS:HB2	1:D:205:GLN:NE2	2.25	0.47
1:D:255:LYS:HB3	1:D:256:GLY:H	1.46	0.47
1:D:392:LEU:HA	1:D:395:ALA:HB3	1.95	0.47
1:D:509:PHE:CD1	1:D:529:VAL:HG21	2.49	0.47
1:D:502:GLU:CD	1:D:536:VAL:HG11	2.34	0.47
1:E:472:CYS:HB3	1:E:504:GLN:HE22	1.79	0.47
1:E:576:ARG:O	1:E:577:LEU:HD23	2.14	0.47
1:F:472:CYS:O	1:F:473:LYS:C	2.51	0.47
1:F:499:VAL:O	1:F:499:VAL:HG12	2.13	0.47
2:I:112:PRO:N	2:I:114:LEU:CD1	2.77	0.47
1:A:510:GLU:C	1:A:513:ILE:HD11	2.34	0.47
1:C:628:VAL:C	1:C:630:LEU:H	2.17	0.47
1:D:474:VAL:HG12	1:D:475:LEU:N	2.29	0.47
1:E:156:VAL:HA	1:E:160:ALA:HB2	1.93	0.47
1:E:462:TYR:HD2	1:E:463:HIS:HD1	1.61	0.47
1:F:32:ASP:O	1:F:34:ILE:N	2.38	0.47
2:H:120:VAL:HG22	2:H:130:CYS:SG	2.54	0.47
1:A:646:GLU:HB2	1:A:650:PHE:CD2	2.47	0.47
1:A:67:VAL:HG12	1:A:68:TYR:CD2	2.49	0.47
1:B:356:ILE:HG21	1:B:359:SER:HB2	1.96	0.47
1:B:44:GLN:HE22	1:B:389:ARG:NH2	2.12	0.47
1:C:202:LEU:HD12	1:C:202:LEU:C	2.35	0.47
1:C:210:LEU:HD13	1:C:244:ARG:HA	1.96	0.47
1:C:452:ASP:OD1	1:D:569:LEU:HD12	2.14	0.47
1:D:455:LEU:HD13	1:D:475:LEU:HD21	1.95	0.47
1:E:131:VAL:HG11	1:E:151:ALA:HB3	1.95	0.47
1:F:459:TYR:CE1	1:F:495:PHE:HD1	2.32	0.47
1:F:522:LEU:O	1:F:525:ILE:HB	2.14	0.47
1:E:640:PHE:CZ	2:I:131:ILE:HD11	2.49	0.47
1:A:204:CYS:HB2	1:A:205:GLN:NE2	2.24	0.47
1:A:545:LEU:O	1:A:545:LEU:HD23	2.13	0.47
1:E:396:ALA:O	1:E:398:MET:N	2.48	0.47
1:E:465:SER:O	1:E:466:LYS:CB	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:124:TRP:CE3	1:F:155:VAL:HG22	2.49	0.47
1:A:67:VAL:O	1:A:71:PHE:HB2	2.14	0.47
1:B:83:ASN:HB2	1:B:262:PRO:O	2.15	0.47
1:B:425:THR:HG22	1:B:426:MET:HE3	1.96	0.47
1:D:160:ALA:HB1	1:D:170:TRP:CZ2	2.50	0.47
1:C:417:TYR:HB2	1:D:573:TYR:CD1	2.49	0.47
1:E:553:PHE:N	1:E:554:PRO:HD3	2.30	0.47
1:F:277:ASN:N	1:F:277:ASN:HD22	2.13	0.47
2:G:147:LEU:CD1	2:G:178:LEU:HD22	2.38	0.47
1:A:400:ASP:O	1:A:401:ASP:CB	2.61	0.47
1:B:196:ARG:O	1:B:197:LYS:C	2.53	0.47
1:B:462:TYR:CD2	1:B:463:HIS:CE1	3.03	0.47
1:B:503:SER:OG	1:B:504:GLN:N	2.46	0.47
1:C:264:THR:HG22	1:C:266:ASN:H	1.79	0.47
1:C:314:TYR:HB3	1:C:331:MET:CE	2.45	0.47
1:C:417:TYR:HB2	1:D:573:TYR:HD1	1.79	0.47
1:C:644:ILE:HG23	2:H:173:TYR:CE1	2.47	0.47
1:E:571:VAL:HB	1:E:573:TYR:CD2	2.50	0.47
1:F:167:ILE:CG1	1:F:209:CYS:HB3	2.44	0.47
1:F:194:TYR:CD1	1:F:194:TYR:N	2.80	0.47
1:F:455:LEU:HD21	1:F:488:TYR:CD1	2.50	0.47
1:F:553:PHE:N	1:F:554:PRO:CD	2.78	0.47
1:E:455:LEU:CB	1:F:569:LEU:HD11	2.38	0.47
2:I:137:LYS:O	2:I:138:LEU:HB2	2.13	0.47
1:A:631:LEU:HD11	2:G:164:LEU:HD11	1.97	0.47
1:B:462:TYR:O	1:B:466:LYS:HA	2.14	0.47
1:B:65:LYS:HD3	1:B:65:LYS:C	2.35	0.47
1:C:206:PRO:HB3	1:C:247:TYR:CA	2.44	0.47
1:C:264:THR:CG2	1:C:266:ASN:HD22	2.28	0.47
1:C:327:ILE:CG2	1:C:328:TRP:N	2.78	0.47
1:C:627:ILE:CG1	2:H:171:LEU:HD11	2.44	0.47
1:D:169:PHE:O	1:D:172:GLU:N	2.47	0.47
1:D:267:GLN:O	1:D:269:THR:HG23	2.14	0.47
1:E:269:THR:HG23	1:E:272:ASN:ND2	2.24	0.47
1:E:284:LEU:HD11	1:E:288:LEU:HD21	1.97	0.47
1:E:417:TYR:HB2	1:F:573:TYR:CD1	2.39	0.47
1:F:159:CYS:O	1:F:162:PHE:N	2.44	0.47
1:F:55:LEU:HD21	1:F:70:THR:CG2	2.44	0.47
2:I:169:PRO:O	2:I:172:SER:HB3	2.15	0.47
1:B:358:ASN:HB3	1:B:389:ARG:CG	2.45	0.47
1:B:77:ARG:HD3	1:B:78:PHE:CE1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:CYS:O	1:C:423:MET:N	2.48	0.47
1:C:475:LEU:HB3	1:C:492:TYR:CZ	2.50	0.47
1:C:572:ASN:OD1	1:C:572:ASN:O	2.33	0.47
1:C:572:ASN:HD21	1:C:575:GLN:HE21	1.55	0.47
1:D:202:LEU:HD12	1:D:202:LEU:C	2.35	0.47
1:D:33:VAL:HA	1:D:36:LYS:NZ	2.30	0.47
1:D:41:ILE:HD11	1:D:50:LEU:O	2.15	0.47
1:E:353:GLN:O	1:E:353:GLN:HG3	2.14	0.47
1:E:374:THR:O	1:E:376:ILE:HG12	2.15	0.47
1:E:378:GLU:O	1:E:382:THR:HG22	2.15	0.47
1:E:405:GLU:C	1:E:407:ALA:H	2.17	0.47
1:F:554:PRO:O	1:F:555:GLU:HB3	2.15	0.47
2:I:171:LEU:O	2:I:175:ILE:HG13	2.14	0.47
1:A:180:TRP:O	1:A:191:ARG:NH1	2.48	0.47
1:C:400:ASP:O	1:C:401:ASP:CB	2.61	0.47
1:C:628:VAL:C	1:C:630:LEU:N	2.68	0.47
1:D:202:LEU:CD1	1:D:203:LEU:HG	2.45	0.47
1:D:366:LEU:O	1:D:367:SER:C	2.53	0.47
1:E:417:TYR:O	1:E:421:VAL:HG12	2.15	0.47
1:F:370:TYR:CG	1:F:378:GLU:HB3	2.49	0.47
1:F:524:MET:HE2	1:F:528:LYS:HE3	1.97	0.47
1:A:132:ARG:NH1	1:A:132:ARG:HG2	2.30	0.47
1:A:202:LEU:O	1:A:207:MET:HE2	2.15	0.47
1:A:221:GLU:HB3	1:A:229:ALA:HB1	1.96	0.47
1:A:245:SER:O	1:A:248:GLN:N	2.46	0.47
1:B:23:PRO:HD3	1:B:26:ARG:NH2	2.30	0.47
1:C:563:THR:HG21	1:C:575:GLN:HB3	1.97	0.47
1:D:119:ASN:HA	1:D:124:TRP:HE1	1.80	0.47
1:D:59:VAL:C	1:D:61:LEU:N	2.63	0.47
1:E:145:ARG:NH2	1:E:180:TRP:HZ2	2.12	0.47
1:E:279:TYR:CE2	1:E:324:ALA:HA	2.51	0.47
1:E:556:VAL:O	1:E:557:ASN:C	2.51	0.47
1:E:638:GLN:O	1:E:640:PHE:N	2.48	0.47
1:F:225:ASN:C	1:F:227:LEU:H	2.17	0.47
2:H:131:ILE:HG23	2:H:135:LEU:HD12	1.96	0.47
1:A:128:ILE:HD11	1:A:152:PHE:N	2.30	0.46
1:A:137:ILE:H	1:A:137:ILE:CD1	2.22	0.46
1:A:164:PRO:HG3	1:A:250:TRP:CE2	2.50	0.46
1:A:250:TRP:CH2	1:A:254:THR:HG21	2.51	0.46
1:C:167:ILE:HG23	1:C:168:GLN:N	2.30	0.46
1:C:299:LEU:HB2	1:C:301:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:SER:OG	1:C:379:ILE:HG23	2.15	0.46
1:C:384:LEU:O	1:C:387:ILE:N	2.48	0.46
1:D:153:GLN:O	1:D:156:VAL:HB	2.15	0.46
1:D:366:LEU:HD23	1:D:366:LEU:HA	1.71	0.46
1:F:350:LYS:HZ1	1:F:354:GLN:HE21	1.61	0.46
1:F:559:LEU:O	1:F:562:PHE:HB3	2.15	0.46
1:A:156:VAL:HA	1:A:160:ALA:HB3	1.96	0.46
1:A:167:ILE:HG12	1:A:171:ASN:ND2	2.30	0.46
1:A:294:GLU:HG3	1:A:313:VAL:HG21	1.97	0.46
1:A:542:VAL:CG1	1:A:546:GLU:HG3	2.44	0.46
1:B:398:MET:C	1:B:400:ASP:H	2.18	0.46
1:B:557:ASN:OD1	1:B:557:ASN:C	2.53	0.46
1:C:624:PRO:N	1:C:625:PRO:CD	2.76	0.46
1:D:198:LEU:O	1:D:202:LEU:HG	2.15	0.46
1:D:275:LYS:CE	1:D:275:LYS:H	2.29	0.46
1:E:144:ALA:HA	1:E:147:ILE:HD12	1.97	0.46
1:E:163:GLU:OE2	1:E:165:LYS:N	2.46	0.46
1:E:226:GLN:HA	1:E:229:ALA:HB2	1.96	0.46
1:E:41:ILE:HG12	1:E:50:LEU:HD22	1.96	0.46
1:E:555:GLU:CD	1:E:555:GLU:C	2.74	0.46
1:F:183:VAL:HG12	1:F:183:VAL:O	2.16	0.46
1:A:289:GLU:OE2	1:A:292:ARG:HD2	2.15	0.46
1:A:401:ASP:C	1:A:403:THR:N	2.68	0.46
1:A:417:TYR:HE1	1:B:568:VAL:CG2	2.28	0.46
1:C:641:LYS:O	1:C:642:VAL:C	2.53	0.46
1:E:200:LYS:HG2	1:E:236:LEU:CD2	2.43	0.46
2:G:114:LEU:HD21	2:G:164:LEU:HD13	1.96	0.46
2:H:118:VAL:HG12	2:H:119:ASP:N	2.29	0.46
2:H:150:ILE:HG23	2:H:161:PHE:CE1	2.48	0.46
2:I:112:PRO:O	2:I:113:TRP:CD1	2.68	0.46
2:I:184:VAL:O	2:I:185:CYS:CB	2.63	0.46
1:A:196:ARG:NH1	1:A:232:HIS:CE1	2.82	0.46
1:A:629:GLU:HA	1:A:632:LYS:HG3	1.97	0.46
1:B:202:LEU:CD1	1:B:202:LEU:C	2.84	0.46
1:B:230:ARG:HD3	1:B:230:ARG:O	2.15	0.46
1:B:480:LYS:HB2	1:B:481:TYR:CD1	2.51	0.46
1:B:529:VAL:O	1:B:532:PHE:HB3	2.16	0.46
1:D:121:LEU:O	1:D:124:TRP:HB2	2.15	0.46
1:D:373:ASN:O	1:D:375:LYS:HG2	2.16	0.46
1:D:417:TYR:O	1:D:420:CYS:N	2.48	0.46
1:D:425:THR:HG22	1:D:426:MET:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:VAL:HG21	1:E:151:ALA:HB1	1.97	0.46
1:E:355:CYS:O	1:E:357:PRO:HD2	2.16	0.46
1:E:390:ILE:CD1	1:E:414:LYS:HD3	2.39	0.46
1:E:438:ILE:O	1:E:442:CYS:HB2	2.15	0.46
2:I:126:THR:HG23	2:I:127:PRO:HD2	1.97	0.46
1:A:641:LYS:C	1:A:641:LYS:HD2	2.35	0.46
1:B:336:GLY:C	1:B:338:LYS:N	2.67	0.46
1:D:37:LEU:O	1:D:40:MET:HE3	2.16	0.46
1:D:571:VAL:HG11	1:D:573:TYR:CE2	2.50	0.46
1:F:156:VAL:HG13	1:F:170:TRP:CH2	2.50	0.46
2:H:135:LEU:HD22	2:H:178:LEU:HD11	1.98	0.46
1:A:137:ILE:HG23	1:A:145:ARG:CB	2.36	0.46
1:A:169:PHE:O	1:A:171:ASN:N	2.48	0.46
1:B:206:PRO:HB3	1:B:247:TYR:CA	2.46	0.46
1:E:107:VAL:HG13	1:E:110:ARG:HD3	1.98	0.46
1:E:81:MET:HE2	1:E:319:GLN:HA	1.97	0.46
1:E:41:ILE:CG2	1:E:41:ILE:O	2.63	0.46
1:E:576:ARG:HB2	1:E:576:ARG:NH1	2.28	0.46
1:F:111:CYS:SG	1:F:112:LEU:HG	2.55	0.46
1:F:153:GLN:O	1:F:156:VAL:N	2.42	0.46
2:I:146:LEU:HA	2:I:149:VAL:HG23	1.97	0.46
1:A:351:LEU:O	1:A:354:GLN:HB2	2.16	0.46
1:A:427:LYS:HB2	1:A:435:SER:CB	2.46	0.46
1:B:485:ASP:O	1:B:489:ILE:HG12	2.15	0.46
1:C:36:LYS:O	1:C:39:ASP:HB2	2.14	0.46
1:C:436:ARG:NH2	1:C:461:GLU:OE1	2.46	0.46
1:D:247:TYR:O	1:D:250:TRP:HB3	2.15	0.46
1:D:295:SER:C	1:D:297:ASN:N	2.68	0.46
2:I:186:SER:CA	2:I:189:GLN:HE22	2.29	0.46
1:A:401:ASP:O	1:A:403:THR:N	2.49	0.46
1:A:473:LYS:O	1:A:477:LEU:HB2	2.16	0.46
1:A:568:VAL:CG1	1:A:569:LEU:HD22	2.37	0.46
1:B:279:TYR:CE2	1:B:324:ALA:HA	2.51	0.46
1:D:199:TYR:O	1:D:203:LEU:HG	2.16	0.46
1:D:455:LEU:N	1:D:455:LEU:CD2	2.79	0.46
1:F:55:LEU:HD21	1:F:70:THR:HG22	1.98	0.46
1:F:81:MET:HG3	1:F:84:ILE:HD12	1.97	0.46
2:H:180:LEU:HD22	2:H:189:GLN:OE1	2.16	0.46
2:I:138:LEU:HB3	2:I:142:GLN:CG	2.46	0.46
2:I:175:ILE:HG22	2:I:175:ILE:O	2.15	0.46
1:B:113:SER:OG	1:B:115:GLU:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:TRP:O	1:C:127:TYR:HB3	2.16	0.46
1:C:242:ASN:O	1:C:246:LEU:HG	2.16	0.46
1:E:191:ARG:NE	1:E:195:ILE:HD11	2.31	0.46
1:E:200:LYS:HG2	1:E:236:LEU:CD1	2.43	0.46
1:F:370:TYR:CD1	1:F:378:GLU:HB3	2.51	0.46
2:H:180:LEU:HD13	2:H:189:GLN:HE22	1.80	0.46
2:I:162:VAL:O	2:I:166:GLU:HB2	2.16	0.46
1:A:336:GLY:C	1:A:338:LYS:H	2.18	0.46
1:A:345:ILE:HB	1:A:369:GLN:OE1	2.16	0.46
1:A:358:ASN:HB3	1:A:389:ARG:HG3	1.98	0.46
1:B:116:LEU:O	1:B:118:ASN:N	2.44	0.46
1:B:181:LYS:HD2	1:B:181:LYS:N	2.31	0.46
1:B:52:VAL:HG11	1:B:268:ALA:CB	2.45	0.46
1:B:71:PHE:HB3	1:B:88:ARG:NH1	2.30	0.46
1:C:544:THR:O	1:C:547:LYS:HB3	2.16	0.46
1:C:580:ASP:C	1:C:582:MET:H	2.18	0.46
1:D:125:LEU:C	1:D:127:TYR:N	2.69	0.46
1:D:166:SER:O	1:D:167:ILE:C	2.55	0.46
1:E:135:ASN:HB3	1:E:144:ALA:O	2.16	0.46
1:E:170:TRP:CD2	1:E:202:LEU:HD23	2.51	0.46
1:E:579:LEU:HD22	1:E:581:TYR:OH	2.16	0.46
2:I:160:THR:O	2:I:160:THR:HG22	2.16	0.46
1:A:177:LEU:HD11	1:A:194:TYR:HB3	1.97	0.45
1:A:442:CYS:HA	1:A:445:LEU:HD12	1.98	0.45
1:B:168:GLN:O	1:B:169:PHE:C	2.54	0.45
1:B:199:TYR:O	1:B:203:LEU:HG	2.16	0.45
1:C:169:PHE:O	1:C:170:TRP:C	2.54	0.45
1:C:55:LEU:HD13	1:C:71:PHE:CE1	2.50	0.45
1:C:61:LEU:HD12	1:C:63:GLN:NE2	2.31	0.45
1:D:207:MET:O	1:D:247:TYR:CD2	2.69	0.45
1:E:170:TRP:CE2	1:E:202:LEU:HB3	2.51	0.45
1:E:191:ARG:O	1:E:195:ILE:HG13	2.16	0.45
1:E:119:ASN:HD22	1:E:312:TYR:HD1	1.64	0.45
1:E:394:LEU:HD12	1:E:411:LEU:CD2	2.46	0.45
1:F:255:LYS:C	1:F:257:LEU:H	2.19	0.45
1:F:326:GLU:HG3	1:F:326:GLU:O	2.15	0.45
1:E:333:ASN:HD22	1:F:558:LYS:HD3	1.81	0.45
1:A:39:ASP:O	1:A:42:GLU:HB3	2.17	0.45
1:A:640:PHE:C	1:A:642:VAL:H	2.18	0.45
1:B:145:ARG:NE	1:B:180:TRP:NE1	2.64	0.45
1:B:242:ASN:O	1:B:246:LEU:HG	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:GLU:HA	1:C:240:TYR:OH	2.16	0.45
1:C:567:LYS:HG2	1:C:572:ASN:CA	2.45	0.45
1:D:249:ASP:O	1:D:252:ASN:HB2	2.15	0.45
1:D:356:ILE:O	1:D:358:ASN:N	2.50	0.45
1:F:255:LYS:HB3	1:F:256:GLY:H	1.44	0.45
1:B:444:ARG:NH2	2:G:167:GLU:OE2	2.49	0.45
1:A:241:MET:O	1:A:244:ARG:N	2.50	0.45
1:A:252:ASN:O	1:A:255:LYS:HG2	2.16	0.45
1:A:486:GLY:C	1:A:521:LEU:HD23	2.36	0.45
1:B:335:GLN:OE1	1:B:335:GLN:HA	2.17	0.45
1:B:478:GLY:O	1:B:482:PHE:HB2	2.16	0.45
1:B:57:HIS:C	1:B:59:VAL:N	2.70	0.45
1:B:71:PHE:HB3	1:B:88:ARG:HH11	1.81	0.45
1:C:203:LEU:HD12	1:C:236:LEU:HD13	1.99	0.45
1:C:249:ASP:O	1:C:253:ILE:HG13	2.16	0.45
1:C:346:THR:HG21	1:C:370:TYR:HE2	1.82	0.45
1:C:642:VAL:HG23	1:C:643:THR:H	1.81	0.45
1:D:207:MET:H	1:D:210:LEU:HG	1.81	0.45
1:D:462:TYR:HA	1:D:467:ASP:O	2.16	0.45
1:E:41:ILE:HD11	1:E:51:TYR:HA	1.98	0.45
1:E:577:LEU:O	1:E:578:GLU:HB2	2.15	0.45
1:A:113:SER:HB2	1:A:115:GLU:OE1	2.16	0.45
1:A:127:TYR:O	1:A:131:VAL:HG23	2.17	0.45
1:A:297:ASN:HB2	1:A:306:HIS:CE1	2.52	0.45
1:A:423:MET:HA	1:A:438:ILE:HD12	1.99	0.45
1:E:392:LEU:HA	1:E:395:ALA:HB3	1.98	0.45
1:E:78:PHE:N	1:E:78:PHE:CD1	2.83	0.45
1:F:420:CYS:O	1:F:423:MET:N	2.49	0.45
1:A:153:GLN:O	1:A:156:VAL:HB	2.16	0.45
1:A:179:HIS:O	1:A:179:HIS:ND1	2.49	0.45
1:A:182:PRO:CG	1:A:191:ARG:HD2	2.43	0.45
1:A:305:LEU:O	1:A:306:HIS:C	2.54	0.45
1:A:49:PHE:HE2	1:A:53:LYS:NZ	2.14	0.45
1:A:61:LEU:HB2	1:A:63:GLN:NE2	2.28	0.45
1:B:191:ARG:HG3	1:B:191:ARG:NH1	2.31	0.45
1:C:455:LEU:CD2	1:C:455:LEU:H	2.29	0.45
1:C:494:ASP:OD1	1:C:528:LYS:HD3	2.16	0.45
1:D:306:HIS:CD2	1:D:306:HIS:O	2.70	0.45
1:D:546:GLU:O	1:D:547:LYS:C	2.54	0.45
1:E:314:TYR:CD1	1:E:331:MET:HB2	2.51	0.45
1:B:30:GLU:HG2	1:F:61:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:PHE:O	1:B:499:VAL:HG22	2.17	0.45
1:C:178:GLU:HA	1:C:191:ARG:HH21	1.78	0.45
1:C:240:TYR:O	1:C:243:ALA:HB3	2.16	0.45
1:C:392:LEU:O	1:C:394:LEU:N	2.50	0.45
1:C:54:LEU:HD23	1:C:70:THR:CG2	2.46	0.45
1:E:282:GLN:NE2	1:E:282:GLN:HA	2.32	0.45
1:E:432:LEU:O	1:E:433:ALA:C	2.54	0.45
1:E:568:VAL:HG21	1:F:417:TYR:CE1	2.51	0.45
1:B:182:PRO:HB3	1:B:188:GLU:HB2	1.99	0.45
1:B:162:PHE:HD2	1:B:309:ARG:HG3	1.81	0.45
1:B:506:LYS:HZ1	1:B:545:LEU:HD12	1.82	0.45
1:C:79:PRO:HB2	1:C:116:LEU:HD22	1.98	0.45
1:C:564:ASN:HA	1:C:567:LYS:HE2	1.99	0.45
1:E:178:GLU:HA	1:E:191:ARG:CZ	2.43	0.45
1:F:199:TYR:CD1	1:F:217:TYR:HB2	2.51	0.45
2:G:126:THR:HB	2:G:129:MET:H	1.82	0.45
1:E:630:LEU:CD1	2:I:135:LEU:HD21	2.46	0.45
1:A:101:ALA:O	1:A:105:GLU:HG3	2.17	0.45
1:A:542:VAL:O	1:A:543:ARG:C	2.55	0.45
1:B:240:TYR:O	1:B:243:ALA:HB3	2.17	0.45
1:B:486:GLY:C	1:B:521:LEU:HD23	2.37	0.45
1:B:539:LEU:C	1:B:539:LEU:HD23	2.37	0.45
1:C:455:LEU:CD2	1:C:455:LEU:N	2.80	0.45
1:E:372:LEU:CD1	1:F:543:ARG:NE	2.80	0.45
1:E:40:MET:C	1:E:42:GLU:H	2.19	0.45
1:E:533:GLU:OE1	1:E:541:SER:HB3	2.16	0.45
1:E:71:PHE:CE1	1:E:265:LEU:HD12	2.52	0.45
1:F:124:TRP:O	1:F:127:TYR:N	2.43	0.45
1:F:307:LYS:HD3	1:F:338:LYS:HG3	1.99	0.45
2:H:163:ALA:O	2:H:167:GLU:HG2	2.17	0.45
1:B:180:TRP:HZ3	1:B:191:ARG:HA	1.82	0.45
1:B:281:VAL:O	1:B:285:LEU:HD12	2.17	0.45
1:C:112:LEU:HD23	1:C:112:LEU:HA	1.82	0.45
1:C:128:ILE:HD11	1:C:155:VAL:HG21	1.98	0.45
1:E:131:VAL:HG11	1:E:151:ALA:HB2	1.99	0.45
1:E:164:PRO:CG	1:E:250:TRP:CZ2	2.99	0.45
1:E:210:LEU:HD21	1:E:243:ALA:HB1	1.98	0.45
1:E:540:ASN:ND2	1:E:543:ARG:NH2	2.65	0.45
1:F:180:TRP:CZ2	1:F:187:GLU:HG2	2.51	0.45
1:F:563:THR:CG2	1:F:572:ASN:OD1	2.65	0.45
2:I:144:MET:HA	2:I:147:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:GLU:OE1	1:A:105:GLU:HA	2.17	0.45
1:B:95:LYS:O	1:B:98:GLU:N	2.49	0.45
1:C:181:LYS:CD	1:C:181:LYS:O	2.61	0.45
1:D:137:ILE:O	1:D:141:GLY:HA2	2.17	0.45
1:D:84:ILE:O	1:D:84:ILE:CG2	2.64	0.45
1:E:317:ALA:O	1:E:321:VAL:HG22	2.16	0.45
1:F:204:CYS:HB2	1:F:205:GLN:HE21	1.82	0.45
1:F:568:VAL:O	1:F:569:LEU:C	2.56	0.45
1:A:93:PHE:HE2	1:A:104:ILE:CD1	2.29	0.44
1:B:105:GLU:HB2	1:B:106:PRO:HD3	1.99	0.44
1:B:135:ASN:ND2	1:B:147:ILE:HG21	2.32	0.44
1:B:240:TYR:CZ	1:B:244:ARG:HD2	2.52	0.44
1:B:542:VAL:O	1:B:543:ARG:C	2.53	0.44
1:B:556:VAL:HG22	1:B:557:ASN:N	2.30	0.44
1:C:125:LEU:HD21	1:C:169:PHE:CD1	2.38	0.44
1:C:509:PHE:CG	1:C:529:VAL:HG21	2.51	0.44
1:D:221:GLU:O	1:D:229:ALA:HB2	2.17	0.44
1:D:242:ASN:O	1:D:246:LEU:HG	2.16	0.44
1:E:173:TYR:O	1:E:173:TYR:CG	2.70	0.44
1:E:262:PRO:CB	1:E:268:ALA:HA	2.47	0.44
1:E:401:ASP:O	1:E:403:THR:N	2.49	0.44
1:F:145:ARG:CZ	1:F:180:TRP:CZ2	3.00	0.44
1:F:226:GLN:O	1:F:226:GLN:HG2	2.17	0.44
1:F:332:ALA:O	1:F:345:ILE:HG12	2.16	0.44
1:F:358:ASN:HB3	1:F:389:ARG:HG3	1.99	0.44
1:F:392:LEU:C	1:F:394:LEU:N	2.70	0.44
2:I:137:LYS:O	2:I:138:LEU:CB	2.65	0.44
1:A:220:TRP:HZ3	1:A:221:GLU:OE2	1.99	0.44
1:A:492:TYR:HE1	1:A:496:LEU:HD11	1.81	0.44
1:B:378:GLU:O	1:B:382:THR:OG1	2.28	0.44
1:B:83:ASN:ND2	1:B:84:ILE:HD12	2.32	0.44
1:C:125:LEU:C	1:C:127:TYR:H	2.19	0.44
1:D:330:ASN:H	1:D:330:ASN:ND2	2.15	0.44
1:D:33:VAL:H	1:D:36:LYS:HZ3	1.65	0.44
1:C:417:TYR:CE2	1:D:574:LEU:HD23	2.52	0.44
1:E:124:TRP:O	1:E:127:TYR:HB3	2.17	0.44
1:E:426:MET:CE	1:E:426:MET:HA	2.48	0.44
1:C:633:VAL:O	2:H:134:GLU:HG3	2.17	0.44
1:A:315:MET:O	1:A:316:GLN:C	2.55	0.44
1:A:334:TYR:O	1:A:336:GLY:N	2.51	0.44
1:A:88:ARG:HG3	1:A:88:ARG:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:GLY:O	1:B:119:ASN:N	2.50	0.44
1:B:572:ASN:C	1:B:572:ASN:ND2	2.70	0.44
1:C:265:LEU:O	1:C:268:ALA:HB3	2.17	0.44
1:C:306:HIS:CD2	1:C:310:MET:HG2	2.52	0.44
1:D:136:ASP:CB	1:D:139:THR:HB	2.44	0.44
1:E:247:TYR:CZ	1:E:251:LEU:HD13	2.53	0.44
1:E:287:TRP:CZ2	1:E:320:HIS:ND1	2.86	0.44
1:E:384:LEU:O	1:E:385:SER:C	2.55	0.44
1:E:529:VAL:O	1:E:532:PHE:HB3	2.17	0.44
1:A:351:LEU:HD23	1:A:354:GLN:OE1	2.18	0.44
1:A:418:VAL:O	1:A:418:VAL:HG12	2.16	0.44
1:B:203:LEU:HD13	1:B:214:TRP:CE3	2.52	0.44
1:B:401:ASP:C	1:B:403:THR:H	2.21	0.44
1:B:527:GLN:HB2	1:B:527:GLN:HE21	1.61	0.44
1:B:559:LEU:O	1:B:563:THR:HG23	2.17	0.44
1:C:137:ILE:HG21	1:C:176:PHE:HE1	1.81	0.44
1:C:262:PRO:HG3	1:C:273:LEU:CD2	2.36	0.44
1:C:576:ARG:O	1:C:577:LEU:HD23	2.17	0.44
1:C:55:LEU:HD22	1:C:71:PHE:CD1	2.53	0.44
1:D:432:LEU:O	1:D:435:SER:HB3	2.17	0.44
1:F:504:GLN:O	1:F:505:VAL:C	2.55	0.44
2:H:142:GLN:O	2:H:145:ALA:HB3	2.17	0.44
2:H:135:LEU:CD1	2:H:177:GLU:HG2	2.47	0.44
1:A:152:PHE:HB3	1:A:173:TYR:CD1	2.53	0.44
1:A:225:ASN:O	1:A:229:ALA:HB3	2.17	0.44
1:A:364:PHE:CD1	1:A:364:PHE:N	2.85	0.44
1:A:493:LEU:O	1:A:494:ASP:C	2.56	0.44
1:A:630:LEU:HD23	2:G:171:LEU:HD13	1.99	0.44
1:B:225:ASN:CB	1:B:228:THR:HB	2.48	0.44
1:B:51:TYR:CG	1:B:74:LEU:HD13	2.53	0.44
1:B:77:ARG:CD	1:B:78:PHE:HE1	2.27	0.44
1:C:199:TYR:O	1:C:203:LEU:HG	2.18	0.44
1:C:335:GLN:OE1	1:C:335:GLN:HA	2.18	0.44
1:C:517:SER:O	1:C:518:ASP:HB3	2.18	0.44
1:D:261:LEU:HD23	1:D:261:LEU:HA	1.76	0.44
1:E:477:LEU:N	1:E:477:LEU:HD12	2.33	0.44
1:E:77:ARG:HH11	1:E:77:ARG:HG3	1.81	0.44
1:F:383:ILE:HG21	1:F:422:TYR:CG	2.53	0.44
1:F:533:GLU:OE1	1:F:541:SER:HB3	2.17	0.44
2:G:179:LEU:O	2:G:181:SER:N	2.50	0.44
1:A:147:ILE:HG22	1:A:148:VAL:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:PHE:HA	1:A:309:ARG:HH12	1.82	0.44
1:A:183:VAL:HG23	1:A:187:GLU:OE1	2.18	0.44
1:A:404:ASN:OD1	1:A:407:ALA:N	2.45	0.44
1:A:574:LEU:HA	1:A:574:LEU:HD12	1.61	0.44
1:B:205:GLN:NE2	1:B:205:GLN:H	2.15	0.44
1:B:580:ASP:O	1:B:582:MET:N	2.50	0.44
1:C:167:ILE:HD12	1:C:209:CYS:HB3	1.99	0.44
1:C:475:LEU:HB3	1:C:492:TYR:CE1	2.53	0.44
1:C:572:ASN:ND2	1:C:575:GLN:NE2	2.53	0.44
1:D:295:SER:O	1:D:297:ASN:N	2.51	0.44
1:D:477:LEU:O	1:D:480:LYS:HG2	2.18	0.44
1:E:297:ASN:HB2	1:E:306:HIS:CE1	2.53	0.44
1:F:405:GLU:HG3	1:F:406:SER:N	2.32	0.44
1:A:624:PRO:HG3	2:G:153:PHE:CE1	2.52	0.44
2:G:168:ALA:CA	2:G:170:GLN:HE22	2.27	0.44
1:A:100:ASP:O	1:A:100:ASP:OD1	2.35	0.44
1:A:538:SER:N	1:A:541:SER:OG	2.50	0.44
1:B:427:LYS:CA	1:B:435:SER:HB3	2.48	0.44
1:B:25:SER:HB2	1:B:43:GLU:CD	2.38	0.44
1:D:115:GLU:C	1:D:117:GLY:N	2.71	0.44
1:D:361:VAL:HG12	1:D:362:LEU:N	2.33	0.44
1:E:143:GLU:C	1:E:145:ARG:H	2.20	0.44
1:E:186:PHE:C	1:E:188:GLU:N	2.69	0.44
1:E:313:VAL:O	1:E:316:GLN:N	2.51	0.44
1:F:346:THR:O	1:F:350:LYS:HB2	2.17	0.44
1:F:470:THR:O	1:F:472:CYS:N	2.50	0.44
1:E:361:VAL:HG11	1:F:559:LEU:HD11	1.98	0.44
1:F:568:VAL:O	1:F:570:ASP:N	2.50	0.44
2:G:138:LEU:O	2:G:139:GLN:C	2.56	0.44
1:E:651:SER:HB2	2:I:162:VAL:CG1	2.48	0.44
1:A:300:GLU:N	1:A:300:GLU:OE2	2.51	0.44
1:B:274:PRO:HB2	1:B:323:PHE:CE1	2.53	0.44
1:B:86:CYS:HB3	1:B:263:ILE:CG1	2.46	0.44
1:C:279:TYR:CE2	1:C:324:ALA:HA	2.53	0.44
1:C:579:LEU:HD22	1:C:581:TYR:CZ	2.53	0.44
1:D:575:GLN:O	1:D:577:LEU:N	2.51	0.44
1:E:103:VAL:O	1:E:103:VAL:HG12	2.17	0.44
1:E:119:ASN:O	1:E:312:TYR:CE1	2.70	0.44
1:E:219:GLN:HE21	1:E:219:GLN:HB3	1.58	0.44
1:E:474:VAL:O	1:E:477:LEU:HB2	2.18	0.44
1:E:493:LEU:O	1:E:497:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:631:LEU:O	1:E:633:VAL:N	2.51	0.44
1:F:349:LEU:HD11	1:F:365:SER:HB3	1.99	0.44
1:F:529:VAL:CG1	1:F:545:LEU:HD11	2.48	0.44
1:F:54:LEU:HG	1:F:58:HIS:CD2	2.52	0.44
2:I:193:LEU:HD12	2:I:193:LEU:C	2.38	0.44
1:A:196:ARG:CG	1:A:200:LYS:HE2	2.48	0.44
1:A:207:MET:C	1:A:209:CYS:H	2.21	0.44
1:A:636:LYS:O	1:A:638:GLN:N	2.46	0.44
1:B:192:VAL:O	1:B:193:GLN:C	2.55	0.44
1:B:366:LEU:HB3	1:B:382:THR:HG21	1.99	0.44
1:C:110:ARG:HG2	1:C:110:ARG:HH11	1.82	0.44
1:C:327:ILE:HG23	1:C:328:TRP:N	2.33	0.44
1:D:101:ALA:HB2	1:D:134:LYS:HZ3	1.83	0.44
1:D:232:HIS:HA	1:D:235:GLU:OE1	2.17	0.44
1:D:296:ASP:O	1:D:297:ASN:C	2.56	0.44
1:D:424:ASN:O	1:D:427:LYS:HB3	2.18	0.44
1:E:371:GLU:OE2	1:F:539:LEU:HB2	2.17	0.44
1:E:497:ILE:HG23	1:E:532:PHE:CD1	2.53	0.44
1:F:394:LEU:O	1:F:395:ALA:C	2.57	0.44
1:F:410:GLN:HB3	1:F:410:GLN:HE21	1.52	0.44
1:A:269:THR:O	1:A:271:SER:N	2.42	0.43
1:A:51:TYR:N	1:A:51:TYR:CD2	2.86	0.43
1:B:181:LYS:HD3	1:B:181:LYS:O	2.18	0.43
1:B:376:ILE:HB	1:B:377:PRO:CD	2.45	0.43
1:C:297:ASN:HB2	1:C:306:HIS:CE1	2.53	0.43
1:C:314:TYR:CD1	1:C:331:MET:HB2	2.53	0.43
1:C:464:ILE:HG22	1:C:465:SER:N	2.33	0.43
1:D:269:THR:C	1:D:271:SER:N	2.71	0.43
1:D:386:CYS:O	1:D:390:ILE:HG13	2.18	0.43
1:E:423:MET:HB2	1:E:438:ILE:HG21	2.00	0.43
1:E:554:PRO:O	1:E:555:GLU:CB	2.64	0.43
1:F:281:VAL:O	1:F:282:GLN:C	2.54	0.43
1:F:287:TRP:CZ3	1:F:290:TRP:CZ3	3.06	0.43
2:H:118:VAL:CG1	2:H:119:ASP:N	2.81	0.43
1:E:631:LEU:CD1	2:I:115:PRO:HD2	2.47	0.43
1:A:254:THR:O	1:A:255:LYS:C	2.56	0.43
1:A:532:PHE:O	1:A:536:VAL:HG12	2.17	0.43
1:B:61:LEU:O	1:B:62:LYS:C	2.57	0.43
1:B:68:TYR:OH	1:B:103:VAL:HG11	2.18	0.43
1:C:174:LEU:HD11	1:C:199:TYR:CZ	2.52	0.43
1:D:162:PHE:HA	1:D:309:ARG:NH1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:LEU:HG	1:E:163:GLU:HG2	1.99	0.43
1:E:164:PRO:HG2	1:E:165:LYS:H	1.83	0.43
1:E:412:LYS:CE	1:E:448:LEU:HA	2.46	0.43
1:F:183:VAL:HG23	1:F:187:GLU:OE1	2.18	0.43
1:F:487:GLU:N	1:F:521:LEU:HD22	2.33	0.43
1:C:644:ILE:HA	2:H:173:TYR:OH	2.18	0.43
1:A:219:GLN:C	1:A:219:GLN:NE2	2.72	0.43
1:A:364:PHE:CZ	1:A:421:VAL:CG1	2.86	0.43
1:A:373:ASN:C	1:A:375:LYS:H	2.21	0.43
1:A:462:TYR:HD1	1:A:471:ALA:HB3	1.84	0.43
1:A:575:GLN:HE21	1:A:582:MET:HE3	1.83	0.43
1:B:225:ASN:HB2	1:B:228:THR:HB	2.00	0.43
1:B:281:VAL:O	1:B:284:LEU:N	2.51	0.43
1:C:296:ASP:O	1:C:297:ASN:C	2.57	0.43
1:D:164:PRO:HG3	1:D:250:TRP:CE2	2.54	0.43
1:D:275:LYS:CD	1:D:275:LYS:H	2.31	0.43
1:D:455:LEU:HD21	1:D:488:TYR:CD1	2.52	0.43
1:E:371:GLU:CA	1:E:379:ILE:HD11	2.45	0.43
1:F:105:GLU:HB2	1:F:106:PRO:HD3	2.00	0.43
2:G:169:PRO:HD2	2:G:170:GLN:NE2	2.32	0.43
1:A:128:ILE:CD1	1:A:151:ALA:HB1	2.49	0.43
1:A:334:TYR:HA	1:A:337:GLU:HB3	2.01	0.43
1:A:41:ILE:HD11	1:A:51:TYR:HA	1.99	0.43
1:A:418:VAL:HA	1:A:421:VAL:HG12	2.00	0.43
1:B:559:LEU:HD21	1:B:579:LEU:CD1	2.47	0.43
1:B:560:GLU:O	1:B:563:THR:N	2.51	0.43
1:B:61:LEU:O	1:B:63:GLN:CG	2.63	0.43
1:D:169:PHE:O	1:D:170:TRP:C	2.56	0.43
1:D:167:ILE:CD1	1:D:209:CYS:HB3	2.49	0.43
1:D:240:TYR:O	1:D:243:ALA:HB3	2.19	0.43
1:D:52:VAL:HG21	1:D:268:ALA:HB1	2.00	0.43
1:E:206:PRO:HB3	1:E:247:TYR:CB	2.48	0.43
1:E:394:LEU:HA	1:E:411:LEU:CD2	2.49	0.43
1:F:125:LEU:HD11	1:F:168:GLN:HG3	2.01	0.43
1:F:434:ALA:HA	1:F:437:LYS:HE3	2.01	0.43
1:F:540:ASN:ND2	1:F:543:ARG:NH2	2.67	0.43
2:I:185:CYS:HB3	2:I:189:GLN:NE2	2.33	0.43
1:A:169:PHE:O	1:A:170:TRP:C	2.56	0.43
1:A:132:ARG:HH21	1:A:176:PHE:HD1	1.67	0.43
1:A:513:ILE:H	1:A:513:ILE:HD12	1.84	0.43
1:A:51:TYR:CB	1:A:74:LEU:HD12	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:ILE:HD12	1:B:508:LEU:HD11	2.01	0.43
1:B:59:VAL:O	1:B:62:LYS:N	2.51	0.43
1:B:66:GLN:HE21	1:B:66:GLN:CA	2.31	0.43
1:C:125:LEU:C	1:C:127:TYR:N	2.70	0.43
1:F:349:LEU:HB3	1:F:366:LEU:HG	2.01	0.43
1:F:387:ILE:HG22	1:F:388:ASP:N	2.33	0.43
1:F:468:THR:O	1:F:469:LYS:C	2.56	0.43
1:A:350:LYS:HA	1:A:366:LEU:HD11	2.00	0.43
1:A:579:LEU:HA	1:A:579:LEU:HD23	1.82	0.43
1:A:87:MET:HG2	1:A:265:LEU:N	2.33	0.43
1:B:111:CYS:SG	1:B:112:LEU:HD23	2.58	0.43
1:B:127:TYR:O	1:B:131:VAL:HG23	2.19	0.43
1:D:120:ASP:O	1:D:121:LEU:C	2.57	0.43
1:D:33:VAL:HA	1:D:36:LYS:HZ1	1.83	0.43
1:D:80:LEU:HA	1:D:118:ASN:ND2	2.23	0.43
1:E:327:ILE:HG22	1:E:328:TRP:H	1.78	0.43
1:E:394:LEU:HD23	1:E:448:LEU:HD11	2.00	0.43
1:E:573:TYR:C	1:E:575:GLN:N	2.72	0.43
1:F:254:THR:HG22	1:F:255:LYS:N	2.32	0.43
1:F:428:ARG:HG2	1:F:428:ARG:O	2.17	0.43
1:A:247:TYR:O	1:A:251:LEU:HB2	2.18	0.43
1:A:387:ILE:HD12	1:A:418:VAL:CG1	2.49	0.43
1:A:414:LYS:HB2	1:B:577:LEU:HD13	2.00	0.43
1:A:509:PHE:O	1:A:513:ILE:HG13	2.19	0.43
1:A:57:HIS:C	1:A:59:VAL:N	2.72	0.43
1:B:121:LEU:O	1:B:123:LEU:N	2.52	0.43
1:B:350:LYS:NZ	1:B:354:GLN:HE21	2.15	0.43
1:B:501:GLU:HB3	1:B:504:GLN:HB2	2.00	0.43
1:C:265:LEU:C	1:C:265:LEU:HD23	2.38	0.43
1:C:414:LYS:HA	1:D:577:LEU:HD13	2.00	0.43
1:D:54:LEU:HG	1:D:58:HIS:CD2	2.53	0.43
1:E:203:LEU:HD22	1:E:240:TYR:CD1	2.54	0.43
1:F:511:SER:O	1:F:515:LYS:HG3	2.19	0.43
1:F:533:GLU:HG3	1:F:545:LEU:HD12	2.01	0.43
1:F:567:LYS:HG2	1:F:572:ASN:HA	2.01	0.43
2:H:162:VAL:O	2:H:166:GLU:HG3	2.19	0.43
1:A:240:TYR:O	1:A:243:ALA:HB3	2.18	0.43
1:A:401:ASP:O	1:A:401:ASP:CG	2.55	0.43
1:B:314:TYR:HB3	1:B:331:MET:HE2	2.01	0.43
1:B:93:PHE:O	1:B:94:ASP:OD1	2.37	0.43
1:B:94:ASP:O	1:B:95:LYS:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:LEU:HD11	1:C:412:LYS:HG3	2.01	0.43
1:C:546:GLU:O	1:C:549:PHE:N	2.52	0.43
1:D:339:ASN:ND2	1:D:340:THR:O	2.52	0.43
1:D:60:SER:O	1:D:61:LEU:HD23	2.18	0.43
1:E:376:ILE:HB	1:E:377:PRO:HD3	1.99	0.43
1:E:87:MET:SD	1:E:268:ALA:HB2	2.59	0.43
1:F:471:ALA:HB1	1:F:495:PHE:CZ	2.54	0.43
1:A:333:ASN:HA	1:A:333:ASN:HD22	1.68	0.43
1:A:394:LEU:HD12	1:A:411:LEU:HD23	2.01	0.43
1:A:496:LEU:HB3	1:A:505:VAL:HG22	2.01	0.43
1:B:550:PHE:HE2	1:B:558:LYS:HD2	1.84	0.43
1:C:131:VAL:HG11	1:C:151:ALA:CB	2.47	0.43
1:C:323:PHE:CE2	1:C:355:CYS:O	2.72	0.43
1:D:170:TRP:HA	1:D:170:TRP:CE3	2.53	0.43
1:D:513:ILE:CG2	1:D:552:LYS:HE2	2.49	0.43
1:E:107:VAL:HA	1:E:110:ARG:CG	2.47	0.43
1:E:324:ALA:O	1:E:327:ILE:HG22	2.18	0.43
1:E:394:LEU:HA	1:E:411:LEU:HD21	2.01	0.43
1:E:532:PHE:O	1:E:535:LYS:N	2.49	0.43
1:E:653:PHE:O	1:E:657:LYS:HB3	2.18	0.43
1:F:248:GLN:O	1:F:251:LEU:N	2.51	0.43
1:F:54:LEU:HG	1:F:58:HIS:HD2	1.84	0.43
2:I:135:LEU:HD22	2:I:178:LEU:HD21	2.01	0.43
2:I:189:GLN:CD	2:I:189:GLN:H	2.23	0.43
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.78	0.43
1:A:398:MET:C	1:A:400:ASP:N	2.72	0.43
1:A:49:PHE:CZ	1:A:53:LYS:HD3	2.54	0.43
1:A:501:GLU:O	1:A:502:GLU:C	2.57	0.43
1:A:542:VAL:HG12	1:A:543:ARG:N	2.34	0.43
1:A:83:ASN:O	1:A:84:ILE:C	2.57	0.43
1:B:128:ILE:HD13	1:B:152:PHE:CE1	2.54	0.43
1:B:490:ASN:OD1	1:B:525:ILE:HD13	2.18	0.43
1:C:398:MET:O	1:C:402:PRO:HD3	2.18	0.43
1:D:294:GLU:OE1	1:D:309:ARG:NE	2.45	0.43
1:D:36:LYS:HA	1:D:39:ASP:OD2	2.18	0.43
1:D:574:LEU:HA	1:D:574:LEU:HD22	1.78	0.43
1:D:560:GLU:CA	1:D:582:MET:HE3	2.48	0.43
1:E:170:TRP:CZ3	1:E:198:LEU:HD13	2.54	0.43
1:F:125:LEU:HD11	1:F:168:GLN:CG	2.49	0.43
1:F:156:VAL:HG13	1:F:170:TRP:HH2	1.83	0.43
1:E:281:VAL:HG21	1:F:581:TYR:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:84:ILE:HG22	1:F:84:ILE:O	2.18	0.43
2:I:118:VAL:CG1	2:I:119:ASP:N	2.82	0.43
1:A:209:CYS:O	1:A:210:LEU:C	2.57	0.42
1:A:462:TYR:HD1	1:A:471:ALA:CB	2.32	0.42
1:B:195:ILE:HG22	1:B:199:TYR:CD2	2.54	0.42
1:B:553:PHE:N	1:B:554:PRO:HD3	2.34	0.42
1:D:33:VAL:C	1:D:35:GLY:N	2.71	0.42
1:E:439:PHE:CD2	1:E:457:ASN:OD1	2.72	0.42
1:E:539:LEU:HD22	1:F:371:GLU:HB3	2.01	0.42
1:E:575:GLN:C	1:E:577:LEU:H	2.23	0.42
2:I:155:LYS:O	2:I:156:ASP:HB3	2.18	0.42
2:I:170:GLN:N	2:I:170:GLN:NE2	2.55	0.42
1:A:101:ALA:HB1	1:A:105:GLU:CG	2.49	0.42
1:A:244:ARG:O	1:A:247:TYR:N	2.51	0.42
1:A:290:TRP:O	1:A:293:TRP:HB3	2.19	0.42
1:A:493:LEU:O	1:A:497:ILE:HG13	2.19	0.42
1:B:149:ILE:O	1:B:150:GLN:C	2.58	0.42
1:B:149:ILE:O	1:B:152:PHE:N	2.51	0.42
1:B:553:PHE:O	1:B:556:VAL:HB	2.19	0.42
1:B:66:GLN:NE2	1:B:66:GLN:CA	2.82	0.42
1:C:121:LEU:HD12	1:C:163:GLU:HG2	2.02	0.42
1:C:270:GLU:HG2	1:C:270:GLU:O	2.19	0.42
1:C:628:VAL:O	1:C:630:LEU:N	2.52	0.42
1:D:182:PRO:HD3	1:D:191:ARG:HH11	1.81	0.42
1:D:63:GLN:O	1:D:67:VAL:HG23	2.19	0.42
1:E:88:ARG:NH2	1:E:107:VAL:HG21	2.34	0.42
1:E:349:LEU:CD1	1:E:365:SER:HB3	2.49	0.42
1:F:152:PHE:CG	1:F:173:TYR:HD1	2.37	0.42
1:F:49:PHE:O	1:F:50:LEU:C	2.55	0.42
2:G:148:LYS:O	2:G:151:GLN:HB3	2.19	0.42
1:A:182:PRO:HB3	1:A:188:GLU:CB	2.48	0.42
1:A:191:ARG:HG3	1:A:191:ARG:NH1	2.32	0.42
1:A:636:LYS:HG3	2:G:118:VAL:O	2.20	0.42
1:B:347:LYS:HG2	1:B:348:TYR:N	2.33	0.42
1:D:122:SER:O	1:D:125:LEU:N	2.51	0.42
1:D:81:MET:HE2	1:D:319:GLN:HA	2.00	0.42
1:E:255:LYS:HB3	1:E:256:GLY:H	1.67	0.42
1:E:349:LEU:HD11	1:E:365:SER:HB3	2.01	0.42
1:E:432:LEU:HD21	1:E:436:ARG:HH21	1.84	0.42
1:F:462:TYR:HA	1:F:467:ASP:O	2.19	0.42
1:F:432:LEU:HD13	1:F:464:ILE:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:125:THR:HG22	2:H:126:THR:N	2.33	0.42
2:H:135:LEU:HD13	2:H:177:GLU:HB3	2.01	0.42
2:H:174:ALA:O	2:H:177:GLU:HB3	2.19	0.42
2:H:187:VAL:HG12	2:H:187:VAL:O	2.19	0.42
1:A:167:ILE:CG1	1:A:171:ASN:HD21	2.32	0.42
1:A:174:LEU:HD11	1:A:199:TYR:CE1	2.54	0.42
1:A:340:THR:HB	1:A:341:ASP:H	1.63	0.42
1:A:624:PRO:O	1:A:625:PRO:C	2.56	0.42
1:A:71:PHE:CZ	1:A:88:ARG:HA	2.53	0.42
1:B:99:LEU:CD2	1:B:133:LYS:HD2	2.49	0.42
1:B:203:LEU:HD13	1:B:214:TRP:HE3	1.83	0.42
1:B:544:THR:O	1:B:547:LYS:HB3	2.19	0.42
1:C:101:ALA:HB2	1:C:134:LYS:HZ1	1.83	0.42
1:C:349:LEU:CD1	1:C:365:SER:HB3	2.49	0.42
1:C:562:PHE:CZ	1:C:566:TYR:CE2	3.08	0.42
1:D:106:PRO:O	1:D:109:ALA:HB3	2.20	0.42
1:D:468:THR:HG23	1:D:499:VAL:HG11	1.90	0.42
1:E:72:ASP:C	1:E:74:LEU:N	2.72	0.42
1:E:88:ARG:O	1:E:92:GLU:OE1	2.38	0.42
1:F:247:TYR:O	1:F:250:TRP:HB3	2.19	0.42
1:F:398:MET:HG2	1:F:408:ILE:CD1	2.33	0.42
1:F:436:ARG:O	1:F:439:PHE:N	2.50	0.42
2:H:138:LEU:O	2:H:139:GLN:C	2.58	0.42
1:A:156:VAL:O	1:A:161:ILE:HG12	2.19	0.42
1:B:543:ARG:HD3	1:B:543:ARG:HA	1.82	0.42
1:B:38:ASN:HD21	1:B:54:LEU:CD2	2.33	0.42
1:C:392:LEU:C	1:C:394:LEU:N	2.69	0.42
1:C:518:ASP:O	1:C:519:SER:C	2.57	0.42
1:D:140:GLY:O	1:D:142:GLU:N	2.53	0.42
1:D:140:GLY:C	1:D:142:GLU:H	2.23	0.42
1:D:78:PHE:N	1:D:78:PHE:CD1	2.87	0.42
1:E:295:SER:HB3	1:E:310:MET:CE	2.49	0.42
1:E:479:LEU:CD1	1:E:492:TYR:HE2	2.28	0.42
1:E:41:ILE:HD11	1:E:50:LEU:O	2.19	0.42
1:F:107:VAL:HG12	1:F:108:LEU:N	2.33	0.42
1:F:272:ASN:OD1	1:F:273:LEU:HG	2.20	0.42
1:F:321:VAL:HG23	1:F:321:VAL:O	2.19	0.42
1:F:489:ILE:HG13	1:F:516:ILE:CD1	2.37	0.42
1:A:638:GLN:HE21	1:A:638:GLN:HB2	1.66	0.42
1:A:648:HIS:O	1:A:651:SER:HB2	2.20	0.42
1:A:89:LEU:HD11	1:A:108:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:THR:HG22	1:B:426:MET:CE	2.50	0.42
1:C:121:LEU:HD11	1:C:166:SER:HB3	2.01	0.42
1:C:135:ASN:ND2	1:C:147:ILE:CG2	2.83	0.42
1:C:232:HIS:C	1:C:234:GLY:N	2.72	0.42
1:D:154:VAL:HG13	1:D:155:VAL:N	2.34	0.42
1:D:333:ASN:O	1:D:334:TYR:C	2.57	0.42
1:D:380:GLU:O	1:D:381:THR:C	2.56	0.42
1:D:59:VAL:HG22	1:D:67:VAL:CG2	2.49	0.42
1:E:405:GLU:HG3	1:E:406:SER:H	1.84	0.42
1:E:499:VAL:HG12	1:E:499:VAL:O	2.18	0.42
1:E:572:ASN:ND2	1:E:575:GLN:NE2	2.67	0.42
1:F:206:PRO:HA	1:F:210:LEU:HD11	2.01	0.42
1:F:267:GLN:O	1:F:269:THR:HG23	2.19	0.42
1:A:181:LYS:CD	1:A:181:LYS:H	2.32	0.42
1:A:219:GLN:NE2	1:A:220:TRP:N	2.68	0.42
1:A:349:LEU:HD23	1:A:349:LEU:HA	1.71	0.42
1:A:467:ASP:OD1	1:A:467:ASP:O	2.38	0.42
1:A:51:TYR:N	1:A:51:TYR:HD2	2.17	0.42
1:C:167:ILE:CD1	1:C:209:CYS:HB3	2.50	0.42
1:C:256:GLY:O	1:C:283:GLN:OE1	2.37	0.42
1:C:30:GLU:CG	1:C:31:SER:H	2.27	0.42
1:C:546:GLU:HA	1:C:549:PHE:HB3	2.01	0.42
1:C:568:VAL:O	1:C:569:LEU:C	2.57	0.42
1:D:392:LEU:O	1:D:393:ASP:C	2.58	0.42
1:D:582:MET:HE2	1:D:582:MET:HB3	1.96	0.42
1:E:136:ASP:HB3	1:E:139:THR:CB	2.49	0.42
1:E:142:GLU:O	1:E:146:ASN:ND2	2.53	0.42
1:E:506:LYS:O	1:E:510:GLU:HB2	2.19	0.42
1:E:523:LYS:HB2	1:E:553:PHE:HE2	1.85	0.42
1:E:653:PHE:CD1	1:E:657:LYS:HD3	2.55	0.42
1:A:202:LEU:HD12	1:A:203:LEU:HG	2.02	0.42
1:A:248:GLN:O	1:A:251:LEU:N	2.53	0.42
1:A:327:ILE:HD12	1:A:327:ILE:HA	1.81	0.42
1:A:656:ASP:OD2	1:A:657:LYS:HG3	2.19	0.42
1:B:167:ILE:O	1:B:171:ASN:ND2	2.53	0.42
1:B:194:TYR:CD1	1:B:194:TYR:N	2.88	0.42
1:B:99:LEU:CD1	1:B:133:LYS:HD3	2.49	0.42
1:C:55:LEU:HB3	1:C:265:LEU:HD11	2.02	0.42
1:D:420:CYS:SG	1:D:453:ILE:HD12	2.60	0.42
1:C:641:LYS:HE3	1:D:437:LYS:NZ	2.35	0.42
1:D:524:MET:O	1:D:525:ILE:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:ILE:HG22	1:E:267:GLN:HE22	1.84	0.42
1:E:405:GLU:O	1:E:407:ALA:N	2.52	0.42
1:E:425:THR:HG22	1:E:426:MET:CE	2.44	0.42
1:E:56:LYS:HG3	1:E:265:LEU:CD2	2.49	0.42
1:E:654:LEU:HG	2:I:151:GLN:OE1	2.20	0.42
1:F:262:PRO:HG3	1:F:273:LEU:HD21	2.01	0.42
1:F:335:GLN:O	1:F:339:ASN:OD1	2.38	0.42
1:F:383:ILE:HG21	1:F:422:TYR:HB2	2.01	0.42
1:F:462:TYR:CZ	1:F:499:VAL:HG22	2.54	0.42
1:F:57:HIS:HD2	1:F:57:HIS:O	2.03	0.42
2:I:130:CYS:O	2:I:134:GLU:HB2	2.19	0.42
1:A:276:PRO:C	1:A:278:GLU:H	2.24	0.42
1:B:290:TRP:C	1:B:290:TRP:CD1	2.93	0.42
1:C:101:ALA:HB2	1:C:134:LYS:HE2	2.01	0.42
1:C:295:SER:C	1:C:297:ASN:H	2.23	0.42
1:C:334:TYR:O	1:C:335:GLN:C	2.56	0.42
1:C:432:LEU:O	1:C:435:SER:HB3	2.20	0.42
1:D:104:ILE:HG21	1:D:130:TYR:CD1	2.54	0.42
1:D:101:ALA:HB2	1:D:134:LYS:NZ	2.35	0.42
1:D:337:GLU:O	1:D:339:ASN:N	2.52	0.42
1:D:42:GLU:C	1:D:45:PRO:HD3	2.40	0.42
1:E:341:ASP:CG	1:E:343:THR:HG22	2.40	0.42
1:E:350:LYS:O	1:E:354:GLN:HG3	2.20	0.42
1:E:401:ASP:C	1:E:403:THR:N	2.72	0.42
1:E:401:ASP:OD2	1:E:404:ASN:HB2	2.20	0.42
1:E:439:PHE:CG	1:E:457:ASN:OD1	2.73	0.42
1:F:104:ILE:O	1:F:107:VAL:HB	2.20	0.42
2:G:150:ILE:HG21	2:G:175:ILE:CD1	2.48	0.42
2:I:179:LEU:HB3	2:I:184:VAL:CB	2.49	0.42
1:A:253:ILE:HG23	1:A:289:GLU:HG3	2.02	0.42
1:A:412:LYS:HZ1	1:A:448:LEU:HA	1.83	0.42
1:B:219:GLN:HE21	1:B:220:TRP:N	2.18	0.42
1:B:59:VAL:CG1	1:B:60:SER:H	2.32	0.42
1:C:462:TYR:C	1:C:464:ILE:H	2.24	0.42
1:C:552:LYS:HB2	1:C:552:LYS:NZ	2.35	0.42
1:C:556:VAL:O	1:C:558:LYS:N	2.52	0.42
1:C:569:LEU:O	1:C:571:VAL:N	2.53	0.42
1:D:261:LEU:HD22	1:D:262:PRO:HD2	2.02	0.42
1:D:347:LYS:O	1:D:350:LYS:HB3	2.19	0.42
1:D:383:ILE:HG21	1:D:422:TYR:CD1	2.54	0.42
1:E:135:ASN:HD21	1:E:147:ILE:HG21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:561:GLU:O	1:E:562:PHE:C	2.57	0.42
1:F:401:ASP:O	1:F:403:THR:N	2.53	0.42
1:F:383:ILE:HG21	1:F:422:TYR:CD1	2.55	0.42
2:H:112:PRO:O	2:H:114:LEU:N	2.53	0.42
1:A:128:ILE:HD12	1:A:151:ALA:HB1	2.02	0.41
1:A:174:LEU:O	1:A:178:GLU:N	2.51	0.41
1:A:442:CYS:O	1:A:445:LEU:N	2.51	0.41
1:B:56:LYS:HE3	1:B:265:LEU:O	2.19	0.41
1:B:257:LEU:HB2	1:B:286:ILE:HG21	2.02	0.41
1:B:311:THR:O	1:B:315:MET:HG2	2.20	0.41
1:B:335:GLN:HB3	1:B:344:VAL:CG1	2.50	0.41
1:B:439:PHE:O	1:B:442:CYS:HB2	2.20	0.41
1:B:64:TRP:CH2	1:B:95:LYS:HD2	2.55	0.41
1:C:559:LEU:HA	1:D:329:PHE:CE1	2.50	0.41
1:C:634:LEU:O	1:C:635:PRO:C	2.58	0.41
1:D:122:SER:O	1:D:123:LEU:C	2.59	0.41
1:D:124:TRP:CE3	1:D:155:VAL:HG22	2.54	0.41
1:D:401:ASP:C	1:D:403:THR:N	2.73	0.41
1:D:44:GLN:N	1:D:45:PRO:HD2	2.34	0.41
1:D:485:ASP:OD1	1:D:487:GLU:HB3	2.19	0.41
1:D:509:PHE:CE2	1:D:513:ILE:HD11	2.55	0.41
1:E:577:LEU:HD13	1:F:414:LYS:HB2	2.02	0.41
1:E:641:LYS:C	1:E:643:THR:N	2.71	0.41
1:F:462:TYR:C	1:F:464:ILE:H	2.23	0.41
1:E:372:LEU:HD11	1:F:543:ARG:CZ	2.49	0.41
2:G:169:PRO:HD2	2:G:170:GLN:HE22	1.85	0.41
1:A:202:LEU:HD13	1:A:207:MET:CE	2.50	0.41
1:A:501:GLU:HB3	1:A:504:GLN:HB2	2.01	0.41
1:B:149:ILE:HD13	1:B:194:TYR:CE2	2.55	0.41
1:C:287:TRP:CZ3	1:C:290:TRP:CZ3	3.08	0.41
1:C:423:MET:CB	1:C:438:ILE:HG21	2.48	0.41
1:E:159:CYS:O	1:E:160:ALA:C	2.57	0.41
1:E:228:THR:HG22	1:E:231:ARG:HE	1.80	0.41
1:E:275:LYS:O	1:E:278:GLU:HB2	2.19	0.41
1:E:64:TRP:HE3	1:E:68:TYR:HE2	1.68	0.41
1:F:509:PHE:CG	1:F:529:VAL:HG21	2.54	0.41
1:A:632:LYS:CG	2:G:115:PRO:HG2	2.42	0.41
2:G:125:THR:HG23	2:G:129:MET:HE2	2.01	0.41
2:G:127:PRO:O	2:G:130:CYS:HB3	2.21	0.41
1:A:100:ASP:C	1:A:102:ALA:H	2.23	0.41
1:A:335:GLN:HA	1:A:335:GLN:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:TYR:C	1:A:336:GLY:N	2.71	0.41
1:A:475:LEU:HD13	1:A:492:TYR:CD1	2.56	0.41
1:A:548:ARG:CG	1:A:548:ARG:NH1	2.73	0.41
1:A:556:VAL:HG22	1:A:561:GLU:HG2	2.01	0.41
1:B:101:ALA:HB2	1:B:130:TYR:OH	2.20	0.41
1:B:264:THR:C	1:B:266:ASN:N	2.74	0.41
1:B:340:THR:OG1	1:B:341:ASP:N	2.53	0.41
1:B:427:LYS:CB	1:B:435:SER:HB3	2.50	0.41
1:C:366:LEU:HD23	1:C:366:LEU:HA	1.82	0.41
1:C:370:TYR:HB2	1:C:379:ILE:HG12	2.02	0.41
1:D:80:LEU:CA	1:D:118:ASN:HD21	2.22	0.41
1:D:560:GLU:CB	1:D:582:MET:HE3	2.50	0.41
1:E:442:CYS:HA	1:E:445:LEU:HD12	2.01	0.41
1:E:458:ALA:C	1:E:460:ILE:N	2.74	0.41
1:E:479:LEU:HD23	1:E:483:ALA:CA	2.42	0.41
1:F:154:VAL:O	1:F:158:LYS:HB2	2.20	0.41
1:F:195:ILE:HG22	1:F:199:TYR:HD2	1.84	0.41
1:F:316:GLN:O	1:F:319:GLN:HB3	2.20	0.41
1:F:408:ILE:O	1:F:412:LYS:HB2	2.20	0.41
1:F:494:ASP:O	1:F:498:TYR:N	2.52	0.41
1:F:71:PHE:HE2	1:F:88:ARG:HB2	1.79	0.41
2:H:190:LEU:O	2:H:193:LEU:HG	2.20	0.41
1:A:367:SER:HB2	1:A:379:ILE:HG23	2.01	0.41
1:B:100:ASP:C	1:B:102:ALA:N	2.74	0.41
1:C:324:ALA:O	1:C:325:PRO:C	2.59	0.41
1:D:167:ILE:CG2	1:D:168:GLN:N	2.84	0.41
1:D:167:ILE:CG1	1:D:171:ASN:ND2	2.84	0.41
1:D:33:VAL:O	1:D:35:GLY:N	2.53	0.41
1:D:54:LEU:HG	1:D:58:HIS:HD2	1.85	0.41
1:E:339:ASN:ND2	1:E:340:THR:H	2.18	0.41
1:E:412:LYS:HE2	1:E:448:LEU:CA	2.47	0.41
1:E:638:GLN:OE1	1:E:638:GLN:N	2.53	0.41
1:F:446:LYS:C	1:F:448:LEU:H	2.24	0.41
1:F:471:ALA:O	1:F:475:LEU:HD12	2.20	0.41
1:F:550:PHE:O	1:F:554:PRO:HG3	2.19	0.41
2:H:155:LYS:HE2	2:H:155:LYS:HB2	1.91	0.41
2:H:185:CYS:HB3	2:H:186:SER:H	1.56	0.41
1:A:181:LYS:O	1:A:182:PRO:C	2.58	0.41
1:A:344:VAL:O	1:A:347:LYS:HB3	2.20	0.41
1:B:202:LEU:HD13	1:B:207:MET:CE	2.50	0.41
1:B:89:LEU:C	1:B:91:LEU:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:GLN:O	1:C:154:VAL:HG12	2.21	0.41
1:C:48:ILE:H	1:C:48:ILE:HD12	1.84	0.41
1:C:80:LEU:HD23	1:C:80:LEU:HA	1.75	0.41
1:E:346:THR:O	1:E:350:LYS:HB2	2.20	0.41
1:E:382:THR:HG23	1:E:383:ILE:N	2.35	0.41
1:E:530:ILE:O	1:E:531:PHE:C	2.59	0.41
1:A:167:ILE:HG12	1:A:171:ASN:HD21	1.85	0.41
1:A:34:ILE:HD11	1:A:57:HIS:NE2	2.36	0.41
1:A:523:LYS:O	1:A:527:GLN:HG3	2.20	0.41
1:A:550:PHE:CD2	1:A:550:PHE:N	2.89	0.41
1:A:637:ARG:H	1:A:637:ARG:HG3	1.46	0.41
1:A:81:MET:O	1:A:84:ILE:HB	2.21	0.41
1:B:123:LEU:HA	1:B:123:LEU:HD12	1.82	0.41
1:C:173:TYR:CE2	1:C:198:LEU:HD22	2.56	0.41
1:C:579:LEU:O	1:C:581:TYR:N	2.54	0.41
1:C:74:LEU:O	1:C:75:HIS:C	2.59	0.41
1:D:218:THR:HG23	1:D:233:ILE:HD13	2.02	0.41
1:D:74:LEU:O	1:D:77:ARG:N	2.43	0.41
1:E:150:GLN:O	1:E:154:VAL:HG12	2.21	0.41
1:E:284:LEU:CD1	1:E:288:LEU:HD21	2.50	0.41
1:E:539:LEU:HD22	1:F:371:GLU:CG	2.51	0.41
1:F:492:TYR:HD1	1:F:492:TYR:O	2.04	0.41
1:F:518:ASP:O	1:F:519:SER:C	2.59	0.41
1:F:578:GLU:C	1:F:579:LEU:HD23	2.40	0.41
2:G:138:LEU:O	2:G:139:GLN:O	2.38	0.41
1:A:113:SER:HB2	1:A:115:GLU:CD	2.40	0.41
1:A:121:LEU:C	1:A:123:LEU:H	2.23	0.41
1:B:152:PHE:HB3	1:B:173:TYR:CE1	2.55	0.41
1:B:190:GLN:O	1:B:193:GLN:HB2	2.21	0.41
1:B:228:THR:O	1:B:230:ARG:N	2.54	0.41
1:B:281:VAL:HG12	1:B:285:LEU:CD1	2.48	0.41
1:C:180:TRP:CZ3	1:C:191:ARG:HB2	2.55	0.41
1:C:210:LEU:CD1	1:C:244:ARG:HA	2.49	0.41
1:D:125:LEU:HD23	1:D:125:LEU:HA	1.87	0.41
1:D:160:ALA:O	1:D:162:PHE:N	2.53	0.41
1:D:242:ASN:O	1:D:242:ASN:ND2	2.54	0.41
1:D:251:LEU:HD12	1:D:251:LEU:HA	1.81	0.41
1:D:270:GLU:O	1:D:270:GLU:HG2	2.21	0.41
1:D:292:ARG:C	1:D:294:GLU:N	2.74	0.41
1:D:394:LEU:HD23	1:D:448:LEU:HD11	2.01	0.41
1:D:71:PHE:CD2	1:D:88:ARG:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:LEU:HD11	1:E:199:TYR:OH	2.21	0.41
1:E:228:THR:HA	1:E:231:ARG:HG2	2.01	0.41
1:E:254:THR:HG23	1:E:257:LEU:HB2	2.02	0.41
1:E:299:LEU:O	1:E:300:GLU:HB2	2.20	0.41
1:F:501:GLU:O	1:F:504:GLN:N	2.40	0.41
1:F:574:LEU:HA	1:F:574:LEU:HD23	1.81	0.41
1:A:178:GLU:CD	1:A:216:ARG:NH2	2.74	0.41
1:A:248:GLN:O	1:A:249:ASP:C	2.59	0.41
1:A:261:LEU:CD1	1:A:319:GLN:HE21	2.33	0.41
1:B:493:LEU:O	1:B:494:ASP:C	2.59	0.41
1:B:502:GLU:HA	1:B:502:GLU:OE1	2.21	0.41
1:C:61:LEU:O	1:C:62:LYS:C	2.59	0.41
2:G:190:LEU:HA	2:G:193:LEU:CD2	2.45	0.41
1:A:181:LYS:H	1:A:181:LYS:HD2	1.85	0.41
1:A:82:ALA:HB1	1:A:120:ASP:OD2	2.21	0.41
1:B:259:ARG:HD3	1:B:287:TRP:HH2	1.83	0.41
1:B:468:THR:O	1:B:471:ALA:HB3	2.21	0.41
1:B:493:LEU:O	1:B:497:ILE:HG13	2.20	0.41
1:B:495:PHE:HB3	1:B:496:LEU:H	1.76	0.41
1:C:384:LEU:O	1:C:385:SER:C	2.57	0.41
1:C:457:ASN:HA	1:C:460:ILE:HD12	2.03	0.41
1:C:483:ALA:HB1	1:C:515:LYS:HZ2	1.83	0.41
1:D:169:PHE:HD2	1:D:170:TRP:N	2.18	0.41
1:D:401:ASP:C	1:D:403:THR:H	2.23	0.41
1:E:42:GLU:OE1	1:E:43:GLU:HG3	2.21	0.41
1:E:43:GLU:O	1:E:44:GLN:CG	2.69	0.41
1:E:48:ILE:O	1:E:51:TYR:HB2	2.20	0.41
1:E:49:PHE:CZ	1:E:270:GLU:HB2	2.56	0.41
1:E:54:LEU:HA	1:E:54:LEU:HD12	1.78	0.41
1:F:315:MET:O	1:F:316:GLN:C	2.58	0.41
1:F:317:ALA:O	1:F:321:VAL:HG22	2.21	0.41
1:F:339:ASN:HD22	1:F:340:THR:H	1.69	0.41
1:F:358:ASN:HB3	1:F:389:ARG:HG2	2.02	0.41
1:F:399:GLU:CG	1:F:400:ASP:N	2.84	0.41
1:F:463:HIS:HE1	1:F:498:TYR:CE2	2.36	0.41
1:F:572:ASN:OD1	1:F:572:ASN:O	2.38	0.41
1:F:563:THR:HG21	1:F:575:GLN:HE21	1.86	0.41
1:E:636:LYS:HG2	2:I:116:VAL:O	2.20	0.41
1:A:85:TRP:CE2	1:A:111:CYS:HB3	2.56	0.41
1:A:40:MET:HG2	1:A:50:LEU:HD11	2.03	0.41
1:B:262:PRO:CB	1:B:272:ASN:HD21	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ILE:O	1:B:49:PHE:C	2.59	0.41
1:B:536:VAL:HG13	1:B:537:GLY:N	2.35	0.41
1:B:64:TRP:CE3	1:B:68:TYR:HE2	2.29	0.41
1:C:186:PHE:C	1:C:188:GLU:N	2.72	0.41
1:F:227:LEU:N	1:F:227:LEU:HD12	2.36	0.41
1:F:355:CYS:C	1:F:356:ILE:HG13	2.41	0.41
1:F:37:LEU:N	1:F:37:LEU:HD12	2.35	0.41
1:F:544:THR:O	1:F:547:LYS:HB3	2.21	0.41
2:G:139:GLN:HB2	2:G:142:GLN:OE1	2.21	0.41
2:H:185:CYS:SG	2:H:188:ASP:CB	3.09	0.41
1:A:89:LEU:C	1:A:91:LEU:H	2.23	0.41
1:B:189:GLN:HE21	1:B:189:GLN:HB3	1.54	0.41
1:B:23:PRO:HA	1:B:26:ARG:HG2	2.03	0.41
1:B:462:TYR:CZ	1:B:468:THR:HG23	2.54	0.41
1:B:503:SER:O	1:B:506:LYS:N	2.54	0.41
1:C:217:TYR:CZ	1:C:236:LEU:HD12	2.56	0.41
1:C:457:ASN:O	1:C:461:GLU:HG2	2.21	0.41
1:D:143:GLU:C	1:D:145:ARG:H	2.24	0.41
1:D:37:LEU:CD2	1:D:54:LEU:HA	2.50	0.41
1:E:262:PRO:HG3	1:E:273:LEU:CD2	2.50	0.41
1:E:291:ILE:HG21	1:E:314:TYR:CZ	2.56	0.41
1:E:525:ILE:O	1:E:529:VAL:HG23	2.21	0.41
1:E:656:ASP:O	1:E:657:LYS:HB2	2.20	0.41
1:F:115:GLU:HG2	1:F:116:LEU:H	1.86	0.41
1:F:170:TRP:NE1	1:F:207:MET:SD	2.94	0.41
1:F:339:ASN:ND2	1:F:340:THR:H	2.18	0.41
1:F:367:SER:O	1:F:379:ILE:HG12	2.21	0.41
2:G:146:LEU:O	2:G:149:VAL:N	2.54	0.41
2:G:168:ALA:HA	2:G:170:GLN:NE2	2.30	0.41
1:A:231:ARG:HH11	1:A:231:ARG:HB3	1.86	0.40
1:A:284:LEU:HG	1:A:288:LEU:CD1	2.50	0.40
1:A:307:LYS:CE	1:A:338:LYS:HG3	2.51	0.40
1:B:173:TYR:O	1:B:176:PHE:HB3	2.21	0.40
1:B:305:LEU:HD23	1:B:305:LEU:HA	1.86	0.40
1:B:307:LYS:CD	1:B:338:LYS:HG3	2.51	0.40
1:B:580:ASP:C	1:B:582:MET:N	2.74	0.40
1:C:134:LYS:HA	1:C:134:LYS:HD3	1.80	0.40
1:D:186:PHE:HE1	1:D:189:GLN:NE2	2.18	0.40
1:D:206:PRO:HA	1:D:210:LEU:HD11	2.04	0.40
1:D:276:PRO:O	1:D:277:ASN:HB2	2.21	0.40
1:C:539:LEU:HD22	1:D:371:GLU:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:LEU:O	1:D:385:SER:C	2.59	0.40
1:D:451:PRO:HG3	1:D:482:PHE:CG	2.56	0.40
1:E:184:ASN:HB2	1:E:185:LYS:H	1.58	0.40
1:E:40:MET:C	1:E:42:GLU:N	2.74	0.40
1:E:477:LEU:N	1:E:477:LEU:CD1	2.84	0.40
1:E:639:TYR:CE1	2:I:120:VAL:HB	2.56	0.40
1:F:174:LEU:HD11	1:F:199:TYR:CZ	2.55	0.40
1:F:225:ASN:O	1:F:227:LEU:N	2.54	0.40
1:F:376:ILE:O	1:F:379:ILE:HB	2.21	0.40
1:F:530:ILE:CG1	1:F:545:LEU:HD22	2.51	0.40
2:G:156:ASP:O	2:G:159:GLU:N	2.54	0.40
1:A:190:GLN:O	1:A:193:GLN:HB2	2.21	0.40
1:A:211:GLU:HA	1:A:240:TYR:OH	2.20	0.40
1:A:56:LYS:HE3	1:A:265:LEU:O	2.22	0.40
1:A:299:LEU:HB2	1:A:301:LEU:HG	2.04	0.40
1:A:394:LEU:HD21	1:A:448:LEU:HD11	2.03	0.40
1:B:246:LEU:HD12	1:B:299:LEU:HD23	2.04	0.40
1:B:453:ILE:HD12	1:B:453:ILE:HA	1.81	0.40
1:C:124:TRP:NE1	1:C:159:CYS:HB2	2.36	0.40
1:C:509:PHE:CE2	1:C:513:ILE:HD11	2.56	0.40
1:D:131:VAL:HG11	1:D:151:ALA:CB	2.51	0.40
1:D:81:MET:CE	1:D:322:CYS:HB3	2.51	0.40
1:E:134:LYS:HA	1:E:134:LYS:HD3	1.87	0.40
1:E:307:LYS:HD2	1:E:334:TYR:OH	2.21	0.40
1:F:59:VAL:C	1:F:61:LEU:H	2.23	0.40
2:H:112:PRO:N	2:H:114:LEU:CD1	2.84	0.40
2:I:179:LEU:HD23	2:I:184:VAL:HG11	2.02	0.40
1:A:135:ASN:O	1:A:136:ASP:C	2.60	0.40
1:A:376:ILE:HB	1:A:377:PRO:CD	2.49	0.40
1:A:487:GLU:HG3	1:A:491:LYS:HE3	2.02	0.40
1:A:538:SER:O	1:A:539:LEU:C	2.60	0.40
1:A:68:TYR:CD2	1:A:68:TYR:N	2.89	0.40
1:B:121:LEU:C	1:B:123:LEU:H	2.24	0.40
1:B:29:ASP:OD1	1:B:32:ASP:OD2	2.39	0.40
1:B:99:LEU:HD11	1:B:133:LYS:HD3	2.03	0.40
1:C:182:PRO:HD3	1:C:191:ARG:HH11	1.86	0.40
1:C:196:ARG:CG	1:C:200:LYS:HE2	2.48	0.40
1:C:275:LYS:CE	1:C:278:GLU:OE1	2.68	0.40
1:C:543:ARG:NH2	1:D:372:LEU:HD11	2.37	0.40
1:E:91:LEU:HB3	1:E:92:GLU:OE1	2.21	0.40
1:F:353:GLN:O	1:F:357:PRO:CA	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:439:PHE:HB2	1:F:457:ASN:ND2	2.35	0.40
1:F:502:GLU:H	1:F:502:GLU:HG2	1.69	0.40
1:F:561:GLU:O	1:F:564:ASN:N	2.55	0.40
2:H:150:ILE:O	2:H:154:CYS:N	2.53	0.40
2:H:155:LYS:HB2	2:H:156:ASP:H	1.77	0.40
2:I:155:LYS:O	2:I:156:ASP:CB	2.70	0.40
1:A:181:LYS:N	1:A:181:LYS:HD2	2.36	0.40
1:A:202:LEU:CD1	1:A:202:LEU:C	2.90	0.40
1:A:221:GLU:O	1:A:229:ALA:CB	2.69	0.40
1:A:196:ARG:HH11	1:A:232:HIS:HE1	1.70	0.40
1:A:299:LEU:O	1:A:301:LEU:HD23	2.21	0.40
1:A:453:ILE:HG23	1:A:454:TYR:N	2.36	0.40
1:A:56:LYS:CE	1:A:265:LEU:O	2.70	0.40
1:A:636:LYS:C	1:A:638:GLN:H	2.25	0.40
1:A:653:PHE:CD1	1:A:657:LYS:HD3	2.56	0.40
1:B:206:PRO:HA	1:B:210:LEU:CD1	2.49	0.40
1:B:28:ARG:HD2	1:B:28:ARG:HA	1.92	0.40
1:B:564:ASN:O	1:B:565:LYS:C	2.59	0.40
1:C:105:GLU:N	1:C:106:PRO:CD	2.84	0.40
1:C:115:GLU:CD	1:C:115:GLU:N	2.66	0.40
1:C:81:MET:HE1	1:C:319:GLN:HA	2.02	0.40
1:C:337:GLU:C	1:C:339:ASN:H	2.24	0.40
1:C:394:LEU:HD21	1:C:448:LEU:HD11	2.03	0.40
1:D:125:LEU:HD21	1:D:169:PHE:CD1	2.56	0.40
1:D:482:PHE:C	1:D:484:THR:N	2.74	0.40
1:E:198:LEU:HD12	1:E:202:LEU:HD23	2.03	0.40
1:E:71:PHE:HE1	1:E:265:LEU:HD12	1.87	0.40
1:E:327:ILE:HD12	1:E:327:ILE:HA	1.80	0.40
1:E:49:PHE:CE2	1:E:53:LYS:HD2	2.56	0.40
1:E:73:LYS:HE2	1:E:73:LYS:HB2	1.99	0.40
1:F:350:LYS:NZ	1:F:354:GLN:NE2	2.68	0.40
1:F:517:SER:O	1:F:518:ASP:HB3	2.21	0.40
1:A:250:TRP:CE2	1:A:254:THR:OG1	2.73	0.40
1:A:336:GLY:O	1:A:337:GLU:C	2.60	0.40
1:A:344:VAL:O	1:A:347:LYS:N	2.54	0.40
1:B:228:THR:O	1:B:229:ALA:C	2.60	0.40
1:C:636:LYS:C	1:C:638:GLN:N	2.73	0.40
1:C:650:PHE:HD1	1:C:650:PHE:O	2.04	0.40
1:C:650:PHE:CD1	1:C:650:PHE:O	2.74	0.40
1:E:209:CYS:SG	1:E:213:MET:HE2	2.62	0.40
1:F:125:LEU:C	1:F:127:TYR:N	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:192:VAL:HG23	1:F:193:GLN:N	2.36	0.40
1:F:397:LEU:O	1:F:397:LEU:HG	2.22	0.40
2:H:139:GLN:O	2:H:141:ASP:N	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	579/645 (90%)	433 (75%)	110 (19%)	36 (6%)	1	10
1	B	554/645 (86%)	414 (75%)	108 (20%)	32 (6%)	1	11
1	C	579/645 (90%)	435 (75%)	110 (19%)	34 (6%)	1	10
1	D	547/645 (85%)	398 (73%)	117 (21%)	32 (6%)	1	10
1	E	572/645 (89%)	429 (75%)	106 (18%)	37 (6%)	1	9
1	F	549/645 (85%)	422 (77%)	95 (17%)	32 (6%)	1	11
2	G	77/174 (44%)	57 (74%)	12 (16%)	8 (10%)	0	3
2	H	77/174 (44%)	56 (73%)	12 (16%)	9 (12%)	0	2
2	I	77/174 (44%)	58 (75%)	14 (18%)	5 (6%)	1	9
All	All	3611/4392 (82%)	2702 (75%)	684 (19%)	225 (6%)	1	10

All (225) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	LYS
1	A	110	ARG
1	A	135	ASN
1	A	255	LYS
1	A	337	GLU

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Mol	Chain	Res	Type
1	A	374	THR
1	A	401	ASP
1	A	464	ILE
1	A	625	PRO
1	A	626	GLU
1	B	30	GLU
1	B	101	ALA
1	B	118	ASN
1	B	229	ALA
1	B	255	LYS
1	B	401	ASP
1	B	464	ILE
1	B	502	GLU
1	C	44	GLN
1	C	169	PHE
1	C	339	ASN
1	C	401	ASP
1	C	570	ASP
1	C	637	ARG
1	D	33	VAL
1	D	44	GLN
1	D	113	SER
1	D	160	ALA
1	D	338	LYS
1	D	374	THR
1	D	396	ALA
1	D	397	LEU
1	E	44	GLN
1	E	160	ALA
1	E	625	PRO
1	E	639	TYR
1	F	30	GLU
1	F	339	ASN
1	F	341	ASP
1	F	401	ASP
1	F	569	LEU
2	G	139	GLN
2	G	186	SER
2	I	168	ALA
2	H	137	LYS
1	A	113	SER
1	A	138	ILE

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Mol	Chain	Res	Type
1	A	160	ALA
1	A	339	ASN
1	A	433	ALA
1	A	502	GLU
1	A	581	TYR
1	A	637	ARG
1	A	653	PHE
1	B	62	LYS
1	B	135	ASN
1	B	168	GLN
1	B	265	LEU
1	B	340	THR
1	B	342	SER
1	B	556	VAL
1	B	581	TYR
1	C	116	LEU
1	C	141	GLY
1	C	170	TRP
1	C	400	ASP
1	C	463	HIS
1	C	485	ASP
1	C	513	ILE
1	C	557	ASN
1	C	635	PRO
1	C	643	THR
1	D	168	GLN
1	D	293	TRP
1	D	339	ASN
1	D	382	THR
1	E	113	SER
1	E	256	GLY
1	E	258	LYS
1	E	321	VAL
1	E	339	ASN
1	E	374	THR
1	E	401	ASP
1	E	452	ASP
1	E	578	GLU
1	E	581	TYR
1	E	626	GLU
1	E	632	LYS
1	F	160	ALA

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Mol	Chain	Res	Type
1	F	184	ASN
1	F	224	VAL
1	F	226	GLN
1	F	400	ASP
1	F	452	ASP
1	F	463	HIS
2	G	140	LYS
2	G	183	GLY
2	I	184	VAL
2	H	113	TRP
2	H	140	LYS
2	H	141	ASP
1	A	56	LYS
1	A	117	GLY
1	A	151	ALA
1	A	169	PHE
1	A	170	TRP
1	A	208	ASP
1	A	277	ASN
1	B	122	SER
1	B	169	PHE
1	B	322	CYS
1	B	367	SER
1	B	561	GLU
1	C	110	ARG
1	C	117	GLY
1	C	187	GLU
1	C	322	CYS
1	C	326	GLU
1	C	580	ASP
1	D	122	SER
1	D	254	THR
1	D	322	CYS
1	D	389	ARG
1	D	557	ASN
1	E	62	LYS
1	E	76	ASP
1	E	116	LEU
1	E	224	VAL
1	E	309	ARG
1	E	341	ASP
1	E	397	LEU

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Mol	Chain	Res	Type
1	E	642	VAL
1	E	646	GLU
1	E	653	PHE
1	F	114	LYS
1	F	254	THR
1	F	396	ALA
1	F	471	ALA
1	F	554	PRO
1	F	557	ASN
1	F	581	TYR
2	G	121	ASN
2	G	180	LEU
2	I	185	CYS
2	H	135	LEU
1	A	229	ALA
1	A	322	CYS
1	A	398	MET
1	A	399	GLU
1	A	468	THR
1	A	518	ASP
1	A	643	THR
1	B	24	THR
1	B	184	ASN
1	B	357	PRO
1	B	495	PHE
1	C	111	CYS
1	C	142	GLU
1	C	338	LYS
1	C	374	THR
1	C	432	LEU
1	D	45	PRO
1	D	75	HIS
1	D	141	GLY
1	D	296	ASP
1	E	187	GLU
1	E	262	PRO
1	E	518	ASP
1	F	44	GLN
1	F	168	GLN
1	F	279	TYR
1	F	397	LEU
1	F	447	LYS

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Mol	Chain	Res	Type
1	F	556	VAL
2	H	186	SER
1	A	101	ALA
1	A	270	GLU
1	A	341	ASP
1	B	117	GLY
1	B	161	ILE
1	B	268	ALA
1	B	302	SER
1	C	625	PRO
1	D	187	GLU
1	D	357	PRO
1	E	184	ASN
1	E	338	LYS
1	E	420	CYS
1	E	556	VAL
1	E	557	ASN
1	F	321	VAL
1	F	374	THR
2	G	141	ASP
2	G	185	CYS
2	I	113	TRP
2	I	114	LEU
2	H	180	LEU
1	B	49	PHE
1	C	161	ILE
1	C	256	GLY
1	C	398	MET
1	D	116	LEU
1	D	161	ILE
1	D	262	PRO
1	D	381	THR
1	D	525	ILE
1	D	576	ARG
1	F	159	CYS
1	F	474	VAL
1	C	33	VAL
1	C	402	PRO
1	C	633	VAL
1	E	357	PRO
1	E	402	PRO
1	F	33	VAL

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Mol	Chain	Res	Type
1	F	421	VAL
2	H	114	LEU
2	H	184	VAL
1	D	361	VAL
1	D	418	VAL
1	F	256	GLY
1	B	138	ILE
1	D	34	ILE
1	B	48	ILE
1	E	635	PRO

### 5.3.2 Protein sidechains [i](#)

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	544/598 (91%)	483 (89%)	61 (11%)	6	23
1	B	519/598 (87%)	472 (91%)	47 (9%)	9	31
1	C	544/598 (91%)	506 (93%)	38 (7%)	15	43
1	D	512/598 (86%)	476 (93%)	36 (7%)	15	43
1	E	538/598 (90%)	487 (90%)	51 (10%)	8	29
1	F	514/598 (86%)	479 (93%)	35 (7%)	16	44
2	G	71/154 (46%)	62 (87%)	9 (13%)	4	19
2	H	71/154 (46%)	65 (92%)	6 (8%)	10	35
2	I	71/154 (46%)	64 (90%)	7 (10%)	8	28
All	All	3384/4050 (84%)	3094 (91%)	290 (9%)	10	35

All (290) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LEU
1	A	51	TYR
1	A	65	LYS
1	A	66	GLN

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Mol	Chain	Res	Type
1	A	71	PHE
1	A	77	ARG
1	A	89	LEU
1	A	99	LEU
1	A	112	LEU
1	A	114	LYS
1	A	121	LEU
1	A	128	ILE
1	A	132	ARG
1	A	135	ASN
1	A	143	GLU
1	A	177	LEU
1	A	181	LYS
1	A	189	GLN
1	A	202	LEU
1	A	219	GLN
1	A	232	HIS
1	A	242	ASN
1	A	260	ASN
1	A	263	ILE
1	A	275	LYS
1	A	292	ARG
1	A	333	ASN
1	A	339	ASN
1	A	342	SER
1	A	353	GLN
1	A	374	THR
1	A	381	THR
1	A	385	SER
1	A	391	HIS
1	A	400	ASP
1	A	401	ASP
1	A	403	THR
1	A	413	SER
1	A	419	TYR
1	A	430	GLN
1	A	432	LEU
1	A	450	THR
1	A	468	THR
1	A	492	TYR
1	A	504	GLN
1	A	513	ILE

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Mol	Chain	Res	Type
1	A	528	LYS
1	A	548	ARG
1	A	551	GLU
1	A	555	GLU
1	A	625	PRO
1	A	628	VAL
1	A	637	ARG
1	A	638	GLN
1	A	641	LYS
1	A	643	THR
1	A	645	PHE
1	A	646	GLU
1	A	648	HIS
1	A	650	PHE
1	A	656	ASP
1	B	25	SER
1	B	28	ARG
1	B	29	ASP
1	B	30	GLU
1	B	66	GLN
1	B	71	PHE
1	B	78	PHE
1	B	84	ILE
1	B	95	LYS
1	B	114	LYS
1	B	115	GLU
1	B	128	ILE
1	B	135	ASN
1	B	150	GLN
1	B	152	PHE
1	B	181	LYS
1	B	189	GLN
1	B	202	LEU
1	B	219	GLN
1	B	231	ARG
1	B	249	ASP
1	B	260	ASN
1	B	265	LEU
1	B	276	PRO
1	B	277	ASN
1	B	283	GLN
1	B	292	ARG

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Mol	Chain	Res	Type
1	B	296	ASP
1	B	298	LYS
1	B	353	GLN
1	B	391	HIS
1	B	392	LEU
1	B	399	GLU
1	B	400	ASP
1	B	401	ASP
1	B	413	SER
1	B	449	VAL
1	B	450	THR
1	B	481	TYR
1	B	492	TYR
1	B	527	GLN
1	B	535	LYS
1	B	548	ARG
1	B	551	GLU
1	B	555	GLU
1	B	556	VAL
1	B	572	ASN
1	C	42	GLU
1	C	66	GLN
1	C	71	PHE
1	C	114	LYS
1	C	124	TRP
1	C	136	ASP
1	C	174	LEU
1	C	181	LYS
1	C	204	CYS
1	C	242	ASN
1	C	275	LYS
1	C	285	LEU
1	C	299	LEU
1	C	322	CYS
1	C	333	ASN
1	C	353	GLN
1	C	374	THR
1	C	381	THR
1	C	382	THR
1	C	391	HIS
1	C	400	ASP
1	C	408	ILE

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Mol	Chain	Res	Type
1	C	414	LYS
1	C	419	TYR
1	C	442	CYS
1	C	510	GLU
1	C	535	LYS
1	C	545	LEU
1	C	555	GLU
1	C	563	THR
1	C	633	VAL
1	C	635	PRO
1	C	637	ARG
1	C	638	GLN
1	C	643	THR
1	C	646	GLU
1	C	648	HIS
1	C	650	PHE
1	D	38	ASN
1	D	42	GLU
1	D	46	THR
1	D	66	GLN
1	D	71	PHE
1	D	121	LEU
1	D	134	LYS
1	D	136	ASP
1	D	174	LEU
1	D	242	ASN
1	D	265	LEU
1	D	278	GLU
1	D	281	VAL
1	D	285	LEU
1	D	296	ASP
1	D	299	LEU
1	D	314	TYR
1	D	321	VAL
1	D	330	ASN
1	D	335	GLN
1	D	349	LEU
1	D	374	THR
1	D	391	HIS
1	D	408	ILE
1	D	410	GLN
1	D	414	LYS

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Mol	Chain	Res	Type
1	D	419	TYR
1	D	421	VAL
1	D	500	ASN
1	D	502	GLU
1	D	514	ASP
1	D	538	SER
1	D	555	GLU
1	D	574	LEU
1	D	575	GLN
1	D	576	ARG
1	E	39	ASP
1	E	42	GLU
1	E	50	LEU
1	E	68	TYR
1	E	71	PHE
1	E	73	LYS
1	E	80	LEU
1	E	89	LEU
1	E	92	GLU
1	E	114	LYS
1	E	115	GLU
1	E	136	ASP
1	E	174	LEU
1	E	198	LEU
1	E	218	THR
1	E	219	GLN
1	E	226	GLN
1	E	242	ASN
1	E	275	LYS
1	E	278	GLU
1	E	283	GLN
1	E	285	LEU
1	E	296	ASP
1	E	299	LEU
1	E	322	CYS
1	E	330	ASN
1	E	331	MET
1	E	353	GLN
1	E	366	LEU
1	E	374	THR
1	E	391	HIS
1	E	400	ASP

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Mol	Chain	Res	Type
1	E	410	GLN
1	E	421	VAL
1	E	424	ASN
1	E	442	CYS
1	E	463	HIS
1	E	473	LYS
1	E	481	TYR
1	E	490	ASN
1	E	492	TYR
1	E	500	ASN
1	E	502	GLU
1	E	510	GLU
1	E	541	SER
1	E	545	LEU
1	E	552	LYS
1	E	555	GLU
1	E	626	GLU
1	E	641	LYS
1	E	646	GLU
1	F	31	SER
1	F	66	GLN
1	F	114	LYS
1	F	134	LYS
1	F	150	GLN
1	F	152	PHE
1	F	174	LEU
1	F	181	LYS
1	F	185	LYS
1	F	189	GLN
1	F	242	ASN
1	F	283	GLN
1	F	299	LEU
1	F	303	ASP
1	F	314	TYR
1	F	337	GLU
1	F	366	LEU
1	F	391	HIS
1	F	400	ASP
1	F	403	THR
1	F	410	GLN
1	F	416	THR
1	F	419	TYR

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Mol	Chain	Res	Type
1	F	442	CYS
1	F	481	TYR
1	F	492	TYR
1	F	500	ASN
1	F	504	GLN
1	F	510	GLU
1	F	538	SER
1	F	554	PRO
1	F	555	GLU
1	F	574	LEU
1	F	576	ARG
1	F	581	TYR
2	G	120	VAL
2	G	142	GLN
2	G	143	GLN
2	G	144	MET
2	G	146	LEU
2	G	160	THR
2	G	170	GLN
2	G	178	LEU
2	G	193	LEU
2	I	116	VAL
2	I	143	GLN
2	I	147	LEU
2	I	164	LEU
2	I	170	GLN
2	I	185	CYS
2	I	189	GLN
2	H	122	ILE
2	H	141	ASP
2	H	155	LYS
2	H	162	VAL
2	H	170	GLN
2	H	188	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (144) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	58	HIS
1	A	63	GLN
1	A	66	GLN

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Mol	Chain	Res	Type
1	A	118	ASN
1	A	171	ASN
1	A	189	GLN
1	A	205	GLN
1	A	219	GLN
1	A	232	HIS
1	A	242	ASN
1	A	252	ASN
1	A	266	ASN
1	A	267	GLN
1	A	277	ASN
1	A	282	GLN
1	A	306	HIS
1	A	316	GLN
1	A	333	ASN
1	A	339	ASN
1	A	504	GLN
1	A	527	GLN
1	A	540	ASN
1	A	564	ASN
1	A	575	GLN
1	B	38	ASN
1	B	44	GLN
1	B	57	HIS
1	B	58	HIS
1	B	63	GLN
1	B	66	GLN
1	B	118	ASN
1	B	135	ASN
1	B	189	GLN
1	B	205	GLN
1	B	215	GLN
1	B	219	GLN
1	B	232	HIS
1	B	266	ASN
1	B	277	ASN
1	B	354	GLN
1	B	391	HIS
1	B	463	HIS
1	B	500	ASN
1	B	504	GLN
1	B	527	GLN

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Mol	Chain	Res	Type
1	B	572	ASN
1	C	38	ASN
1	C	57	HIS
1	C	58	HIS
1	C	63	GLN
1	C	135	ASN
1	C	189	GLN
1	C	219	GLN
1	C	226	GLN
1	C	232	HIS
1	C	242	ASN
1	C	266	ASN
1	C	267	GLN
1	C	409	ASN
1	C	463	HIS
1	C	504	GLN
1	C	540	ASN
1	C	557	ASN
1	C	564	ASN
1	C	575	GLN
1	D	38	ASN
1	D	58	HIS
1	D	118	ASN
1	D	146	ASN
1	D	171	ASN
1	D	189	GLN
1	D	205	GLN
1	D	219	GLN
1	D	226	GLN
1	D	242	ASN
1	D	267	GLN
1	D	277	ASN
1	D	330	ASN
1	D	339	ASN
1	D	354	GLN
1	D	391	HIS
1	D	410	GLN
1	D	463	HIS
1	D	504	GLN
1	D	540	ASN
1	D	557	ASN
1	D	575	GLN

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Mol	Chain	Res	Type
1	E	63	GLN
1	E	75	HIS
1	E	118	ASN
1	E	135	ASN
1	E	146	ASN
1	E	171	ASN
1	E	189	GLN
1	E	215	GLN
1	E	219	GLN
1	E	225	ASN
1	E	242	ASN
1	E	267	GLN
1	E	282	GLN
1	E	316	GLN
1	E	330	ASN
1	E	333	ASN
1	E	410	GLN
1	E	504	GLN
1	E	540	ASN
1	E	557	ASN
1	E	564	ASN
1	E	575	GLN
1	F	38	ASN
1	F	57	HIS
1	F	58	HIS
1	F	83	ASN
1	F	118	ASN
1	F	189	GLN
1	F	205	GLN
1	F	219	GLN
1	F	226	GLN
1	F	242	ASN
1	F	282	GLN
1	F	330	ASN
1	F	354	GLN
1	F	373	ASN
1	F	410	GLN
1	F	424	ASN
1	F	463	HIS
1	F	504	GLN
1	F	540	ASN
1	F	557	ASN

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Mol	Chain	Res	Type
1	F	575	GLN
2	G	170	GLN
2	G	182	ASN
2	I	170	GLN
2	I	182	ASN
2	I	189	GLN
2	H	139	GLN
2	H	142	GLN
2	H	143	GLN
2	H	151	GLN
2	H	170	GLN
2	H	182	ASN
2	H	189	GLN
2	H	192	GLN

### 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](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	585/645 (90%)	-0.29	2 (0%) 94 94	39, 76, 136, 149	0
1	B	558/645 (86%)	-0.29	0 100 100	36, 73, 136, 148	0
1	C	585/645 (90%)	-0.10	13 (2%) 62 60	60, 106, 149, 151	0
1	D	551/645 (85%)	-0.13	7 (1%) 77 77	58, 104, 149, 151	0
1	E	578/645 (89%)	0.20	43 (7%) 14 14	57, 106, 150, 151	0
1	F	553/645 (85%)	-0.08	8 (1%) 75 75	55, 104, 148, 151	0
2	G	81/174 (46%)	-0.30	0 100 100	63, 102, 138, 151	0
2	H	81/174 (46%)	0.06	4 (4%) 29 27	90, 128, 148, 151	0
2	I	81/174 (46%)	-0.03	2 (2%) 57 54	96, 125, 147, 151	0
All	All	3653/4392 (83%)	-0.11	79 (2%) 62 60	36, 99, 148, 151	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	125	LEU	4.9
1	E	214	TRP	4.3
1	E	215	GLN	4.3
1	E	218	THR	4.1
1	C	655	SER	4.0
1	E	195	ILE	3.9
1	E	164	PRO	3.8
1	E	189	GLN	3.8
1	E	199	TYR	3.6
1	E	233	ILE	3.5
1	E	181	LYS	3.5
1	F	189	GLN	3.4
1	F	144	ALA	3.4
1	E	236	LEU	3.4
1	C	641	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	230	ARG	3.2
1	E	226	GLN	3.2
1	E	229	ALA	3.2
1	D	104	ILE	3.2
1	E	237	SER	3.0
1	C	645	PHE	3.0
1	E	204	CYS	3.0
1	E	128	ILE	3.0
1	E	67	VAL	2.9
1	C	34	ILE	2.8
1	C	33	VAL	2.8
1	E	228	THR	2.8
1	E	93	PHE	2.8
1	E	170	TRP	2.7
1	E	220	TRP	2.6
1	E	219	GLN	2.6
1	C	236	LEU	2.6
1	C	186	PHE	2.6
1	E	52	VAL	2.6
1	D	67	VAL	2.5
1	C	233	ILE	2.5
1	A	203	LEU	2.5
1	E	266	ASN	2.5
1	E	55	LEU	2.5
1	E	139	THR	2.5
1	D	137	ILE	2.5
1	F	177	LEU	2.4
1	C	199	TYR	2.4
1	F	95	LYS	2.4
1	C	137	ILE	2.4
1	C	656	ASP	2.4
1	A	218	THR	2.4
2	H	192	GLN	2.4
1	E	59	VAL	2.3
2	I	165	LEU	2.3
1	E	240	TYR	2.3
1	E	62	LYS	2.3
1	D	93	PHE	2.3
1	E	129	THR	2.3
1	C	138	ILE	2.3
2	I	135	LEU	2.3
1	E	127	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	211	GLU	2.2
1	F	184	ASN	2.2
2	H	171	LEU	2.2
1	E	293	TRP	2.2
1	E	137	ILE	2.2
2	H	175	ILE	2.2
1	E	175	HIS	2.2
1	C	654	LEU	2.2
1	E	145	ARG	2.2
1	F	64	TRP	2.2
1	D	100	ASP	2.2
1	F	93	PHE	2.2
1	E	196	ARG	2.2
1	D	188	GLU	2.1
1	E	212	SER	2.1
1	E	232	HIS	2.1
1	D	192	VAL	2.1
1	E	642	VAL	2.1
2	H	193	LEU	2.1
1	F	103	VAL	2.0
1	E	176	PHE	2.0
1	E	136	ASP	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.