



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:55 PM GMT

PDB ID : 1HT2  
Title : Nucleotide-Dependent Conformational Changes in a Protease-Associated ATPase HslU  
Authors : Wang, J.; Song, J.J.; Seong, I.S.; Franklin, M.C.; Kamtekar, S.; Eom, S.H.; Chung, C.H.  
Deposited on : 2000-12-27  
Resolution : 2.80 Å(reported)

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

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

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

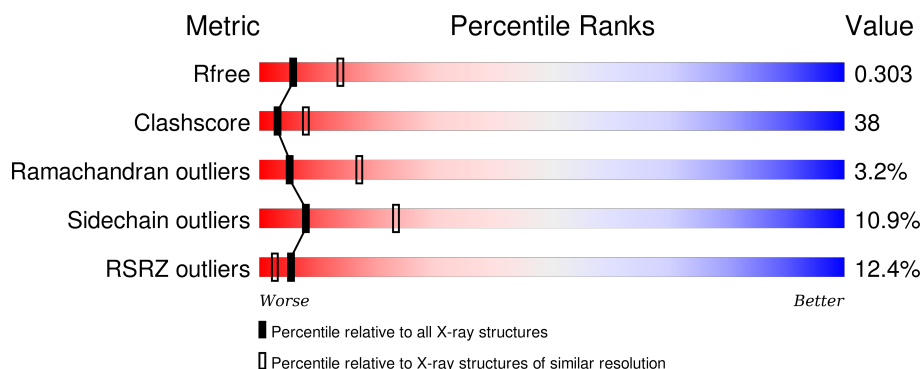
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	175	<div> <div>2%</div> <div>57%</div> <div>37%</div> <div>5%</div> <div>..</div> </div>
1	B	175	<div> <div>8%</div> <div>43%</div> <div>47%</div> <div>9%</div> <div>.</div> </div>
1	C	175	<div> <div>5%</div> <div>50%</div> <div>42%</div> <div>7%</div> <div>.</div> </div>
1	D	175	<div> <div>7%</div> <div>43%</div> <div>49%</div> <div>7%</div> <div>.</div> </div>
1	I	175	<div> <div>2%</div> <div>57%</div> <div>37%</div> <div>6%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	J	175	<div><div></div><div>3%</div><div>49%</div><div>43%</div><div>7%</div><div></div></div>
1	K	175	<div><div></div><div>11%</div><div>56%</div><div>38%</div><div>5%</div><div></div></div>
1	L	175	<div><div></div><div>5%</div><div>53%</div><div>38%</div><div>8%</div><div></div></div>
2	E	449	<div><div></div><div>13%</div><div>42%</div><div>41%</div><div>6%</div><div></div><div>9%</div></div>
2	F	449	<div><div></div><div>20%</div><div>41%</div><div>39%</div><div>10%</div><div></div><div>9%</div></div>
2	G	449	<div><div></div><div>14%</div><div>46%</div><div>36%</div><div>7%</div><div></div><div>9%</div></div>
2	H	449	<div><div></div><div>19%</div><div>37%</div><div>42%</div><div>11%</div><div></div><div>9%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23636 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 HEAT SHOCK LOCUS HSLV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			
1	B	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			
1	C	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			
1	D	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			
1	I	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			
1	J	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			
1	K	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			
1	L	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			

- Molecule 2 is a protein called HEAT SHOCK LOCUS HSLU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	408	Total	C	N	O	S	0	0	0
			3226	2014	577	625	10			
2	F	408	Total	C	N	O	S	0	0	0
			3226	2014	577	625	10			
2	G	408	Total	C	N	O	S	0	0	0
			3226	2014	577	625	10			
2	H	408	Total	C	N	O	S	0	0	0
			3226	2014	577	625	10			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	HIS	-	EXPRESSION TAG	UNP P0A6H5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	EXPRESSION TAG	UNP P0A6H5
E	-3	HIS	-	EXPRESSION TAG	UNP P0A6H5
E	-2	HIS	-	EXPRESSION TAG	UNP P0A6H5
E	-1	HIS	-	EXPRESSION TAG	UNP P0A6H5
E	0	HIS	-	EXPRESSION TAG	UNP P0A6H5
E	1	HIS	-	EXPRESSION TAG	UNP P0A6H5
F	-5	HIS	-	EXPRESSION TAG	UNP P0A6H5
F	-4	HIS	-	EXPRESSION TAG	UNP P0A6H5
F	-3	HIS	-	EXPRESSION TAG	UNP P0A6H5
F	-2	HIS	-	EXPRESSION TAG	UNP P0A6H5
F	-1	HIS	-	EXPRESSION TAG	UNP P0A6H5
F	0	HIS	-	EXPRESSION TAG	UNP P0A6H5
F	1	HIS	-	EXPRESSION TAG	UNP P0A6H5
G	-5	HIS	-	EXPRESSION TAG	UNP P0A6H5
G	-4	HIS	-	EXPRESSION TAG	UNP P0A6H5
G	-3	HIS	-	EXPRESSION TAG	UNP P0A6H5
G	-2	HIS	-	EXPRESSION TAG	UNP P0A6H5
G	-1	HIS	-	EXPRESSION TAG	UNP P0A6H5
G	0	HIS	-	EXPRESSION TAG	UNP P0A6H5
G	1	HIS	-	EXPRESSION TAG	UNP P0A6H5
H	-5	HIS	-	EXPRESSION TAG	UNP P0A6H5
H	-4	HIS	-	EXPRESSION TAG	UNP P0A6H5
H	-3	HIS	-	EXPRESSION TAG	UNP P0A6H5
H	-2	HIS	-	EXPRESSION TAG	UNP P0A6H5
H	-1	HIS	-	EXPRESSION TAG	UNP P0A6H5
H	0	HIS	-	EXPRESSION TAG	UNP P0A6H5
H	1	HIS	-	EXPRESSION TAG	UNP P0A6H5

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

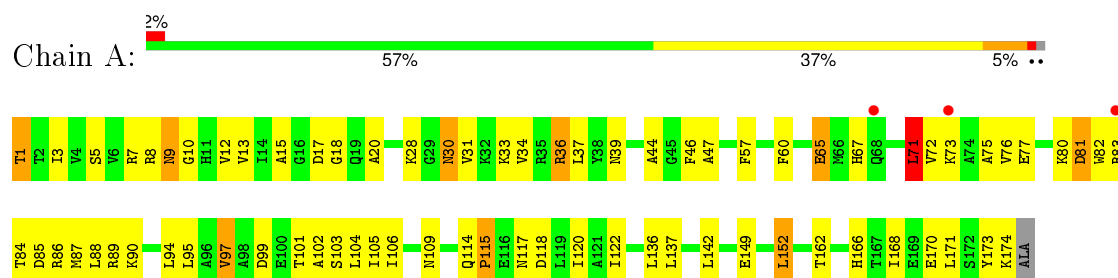


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

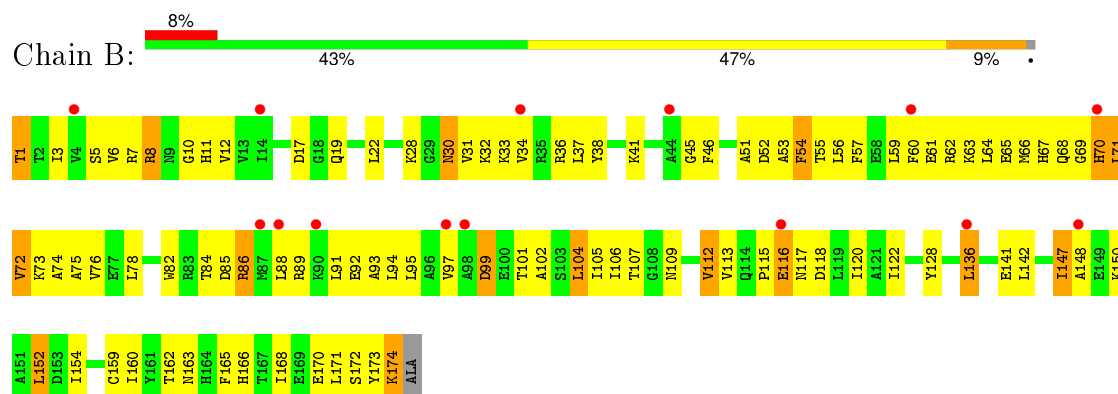
### 3 Residue-property plots

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

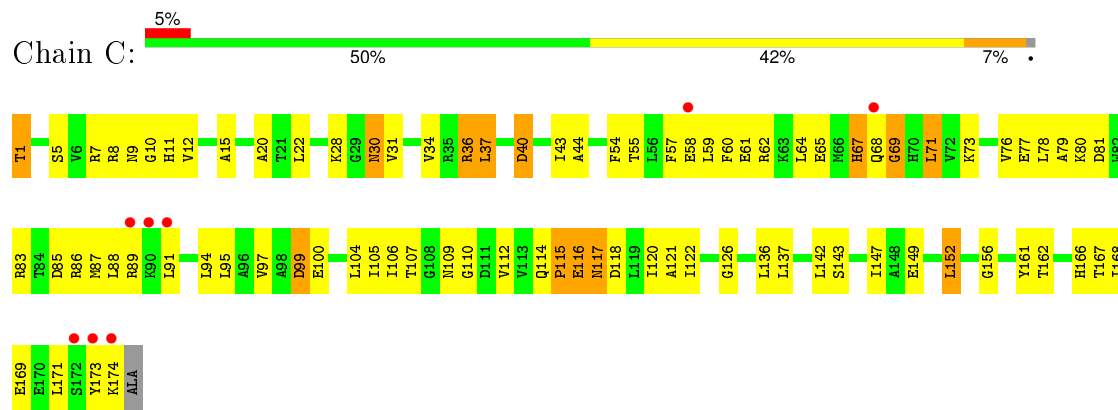
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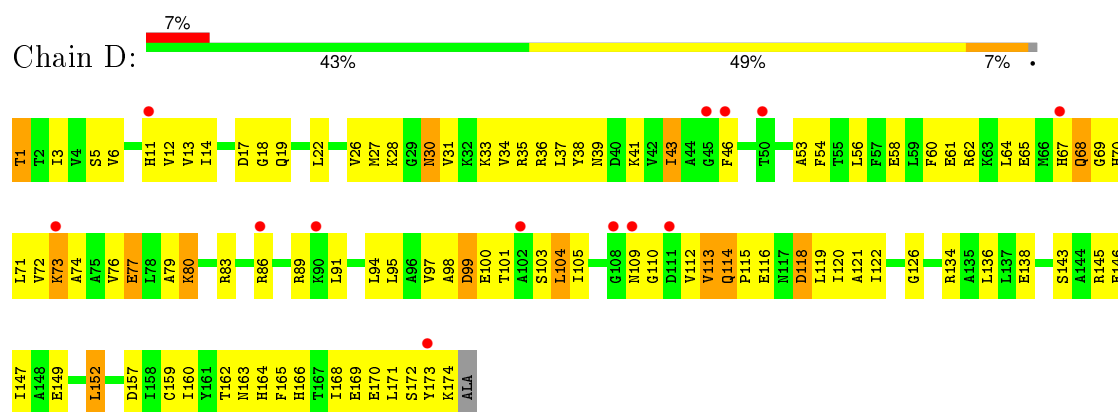
#### • Molecule 1: HEAT SHOCK LOCUS HSLV



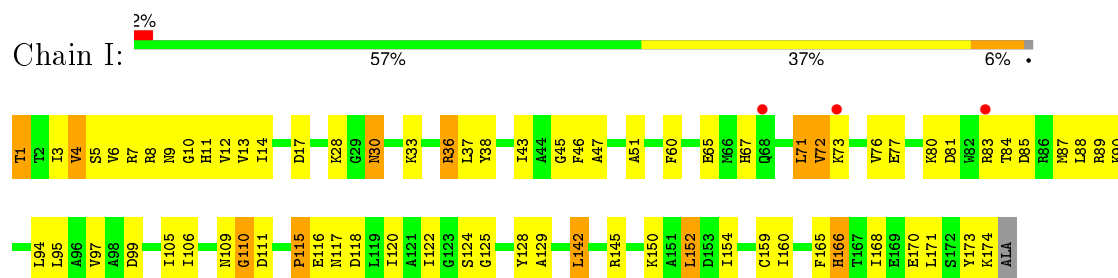
#### • Molecule 1: HEAT SHOCK LOCUS HSLV



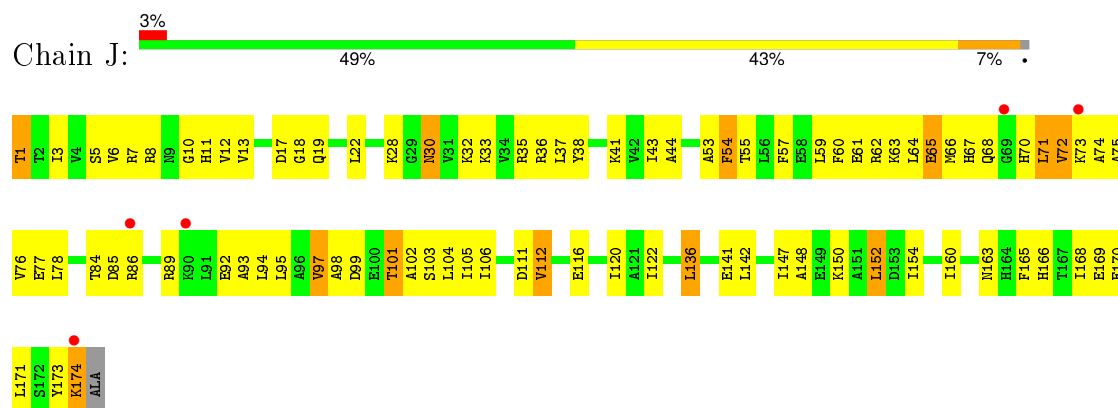
#### • Molecule 1: HEAT SHOCK LOCUS HSLV



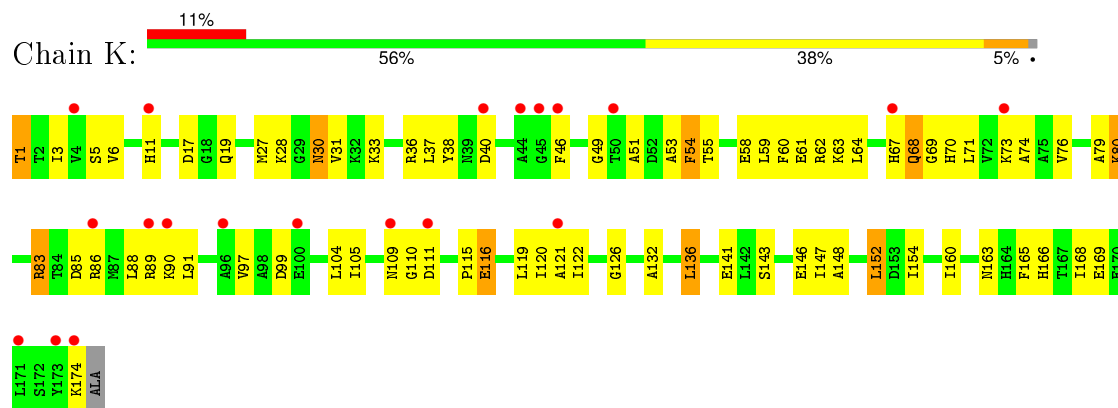
• Molecule 1: HEAT SHOCK LOCUS HSLV



• Molecule 1: HEAT SHOCK LOCUS HSLV

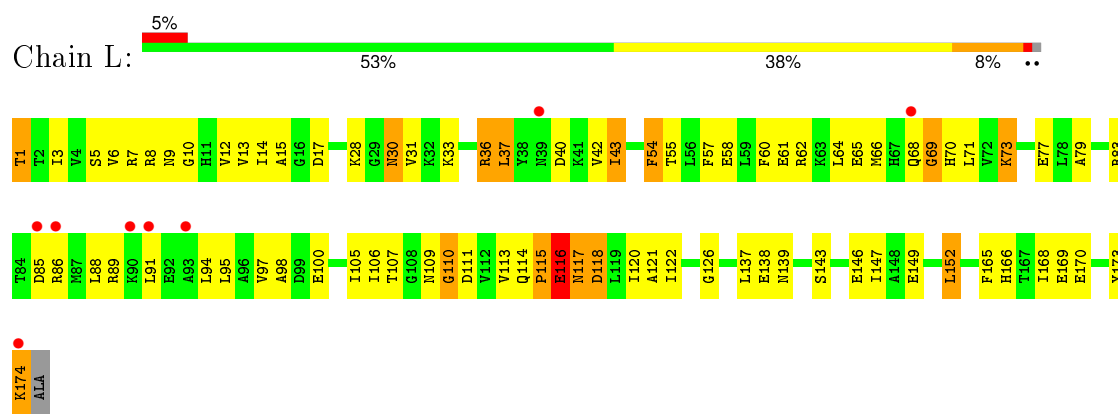


• Molecule 1: HEAT SHOCK LOCUS HSLV

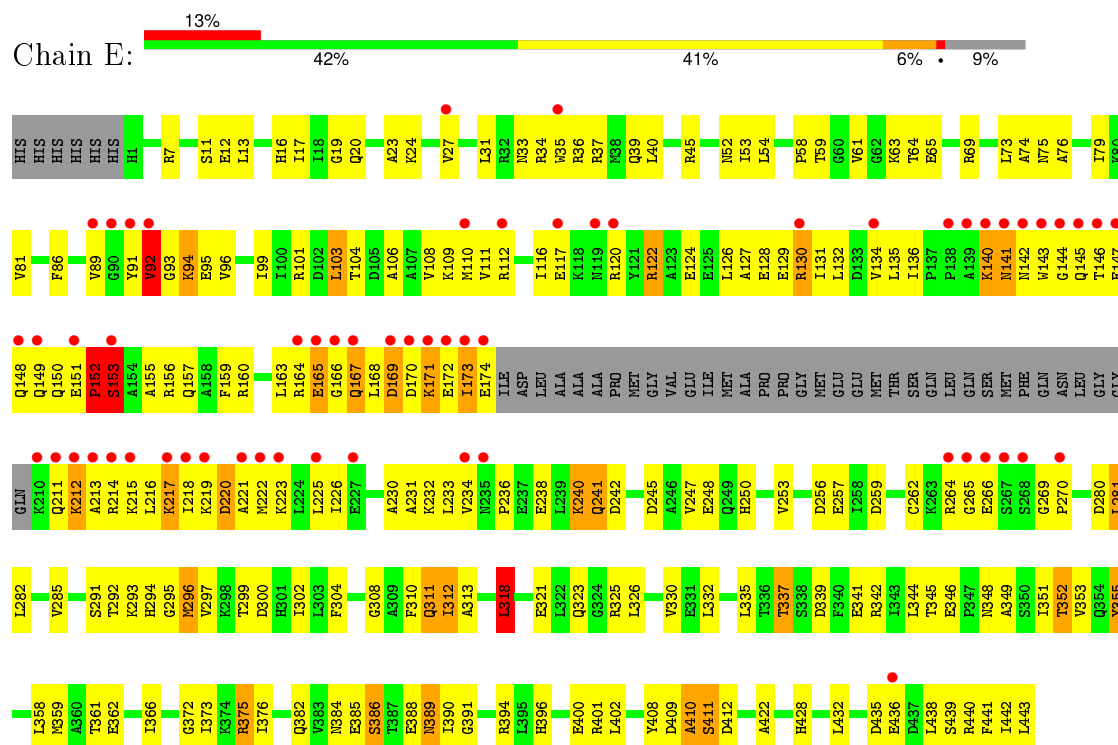


• Molecule 1: HEAT SHOCK LOCUS HSLV

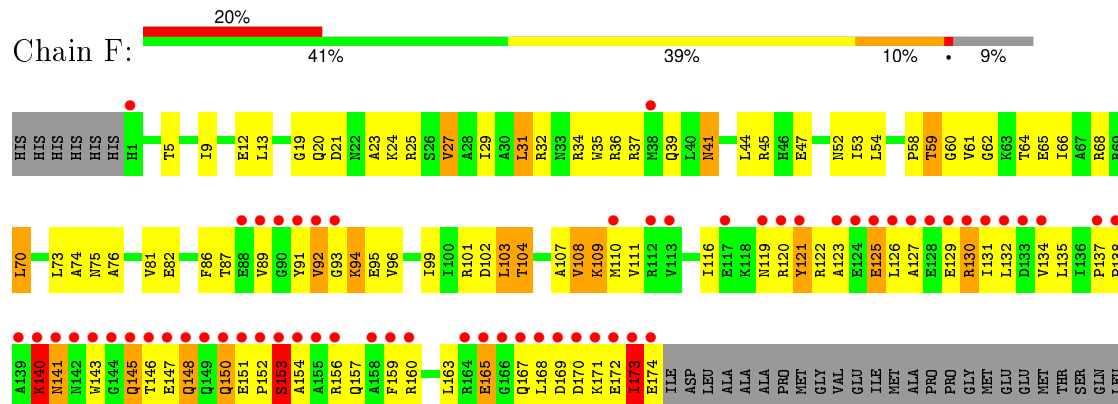


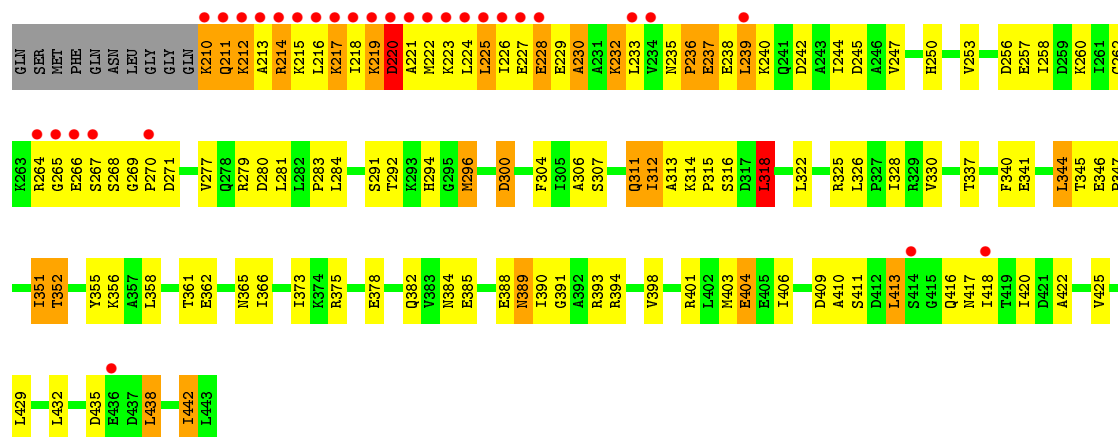


- Molecule 2: HEAT SHOCK LOCUS HSLU

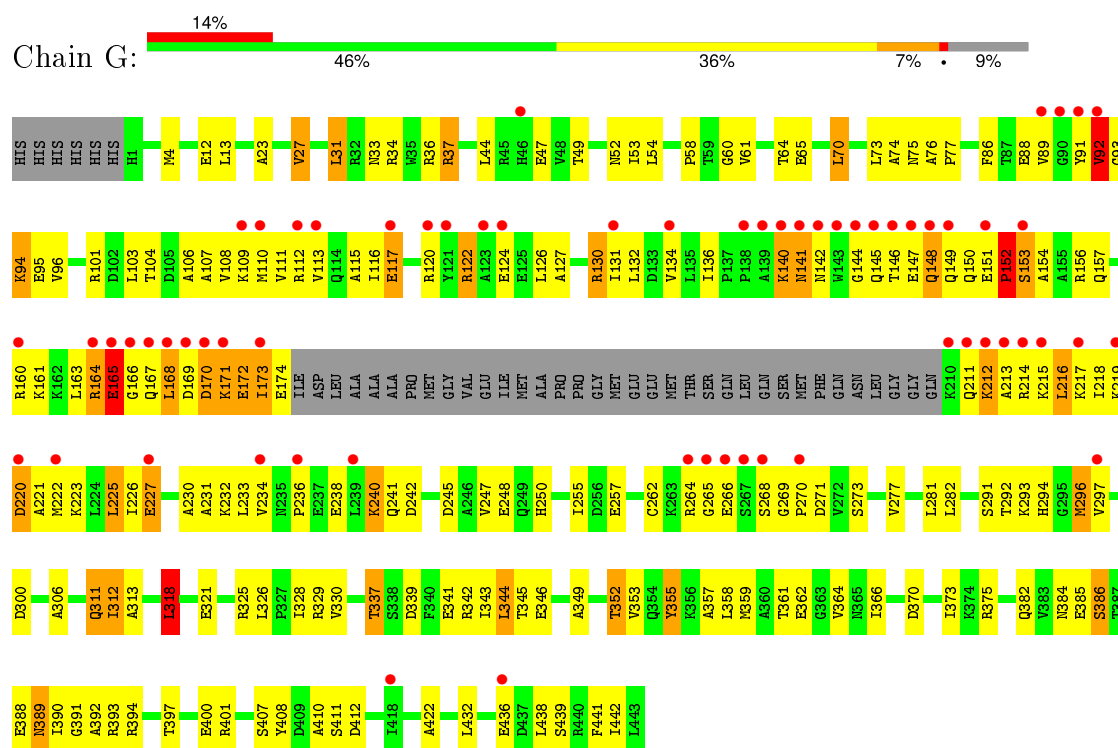


- Molecule 2: HEAT SHOCK LOCUS HSLU

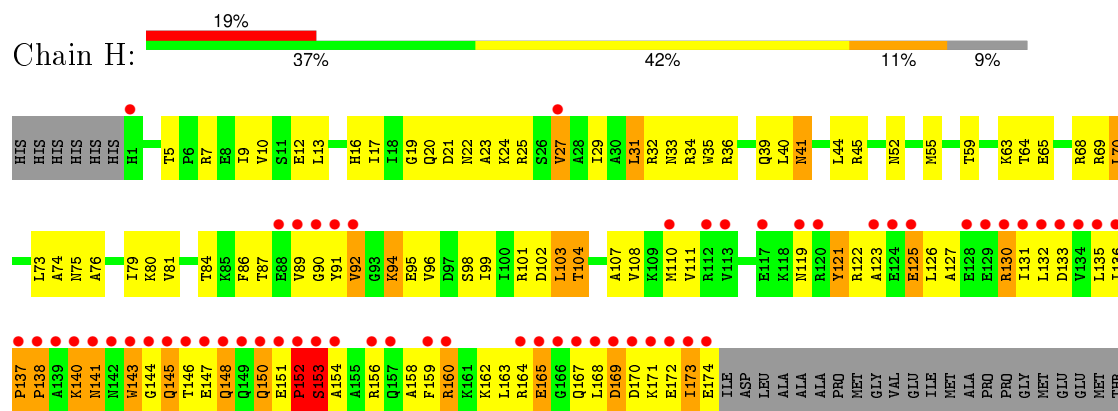


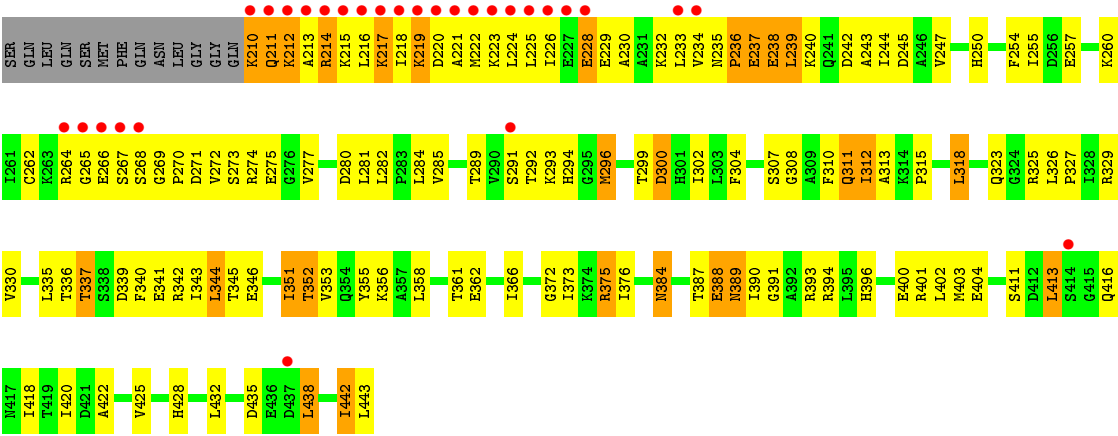


- Molecule 2: HEAT SHOCK LOCUS HSLU



- Molecule 2: HEAT SHOCK LOCUS HSLU





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 1 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.02Å 172.02Å 276.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.62 – 2.80 29.62 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.5 (29.62-2.80) 92.5 (29.62-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.49 (at 2.80Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.262 , 0.310 0.254 , 0.303	Depositor DCC
$R_{free}$ test set	10803 reflections (11.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.1	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.8	EDS
Estimated twinning fraction	0.499 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	16 of 119676 reflections (0.013%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	23636	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 61.11 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.3765e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.45	0/1345	0.72	0/1817
1	B	0.41	0/1345	0.67	0/1817
1	C	0.39	0/1345	0.67	0/1817
1	D	0.34	0/1345	0.62	0/1817
1	I	0.45	0/1345	0.73	0/1817
1	J	0.41	0/1345	0.67	0/1817
1	K	0.32	0/1345	0.60	0/1817
1	L	0.34	0/1345	0.63	0/1817
2	E	0.44	0/3266	0.71	5/4400 (0.1%)
2	F	0.44	0/3266	0.71	4/4400 (0.1%)
2	G	0.43	1/3266 (0.0%)	0.69	3/4400 (0.1%)
2	H	0.45	1/3266 (0.0%)	0.70	2/4400 (0.0%)
All	All	0.42	2/23824 (0.0%)	0.68	14/32136 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	152	PRO	CA-C	-6.59	1.39	1.52
2	G	152	PRO	CA-C	-5.91	1.41	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	152	PRO	CA-N-CD	-6.83	101.94	111.50
2	E	152	PRO	CA-N-CD	-6.78	102.02	111.50
2	F	220	ASP	CB-CA-C	-6.51	97.38	110.40
2	G	318	LEU	CA-CB-CG	6.31	129.80	115.30
2	E	153	SER	C-N-CA	6.07	136.87	121.70
2	F	153	SER	CB-CA-C	5.86	121.24	110.10
2	H	153	SER	CB-CA-C	5.75	121.02	110.10
2	E	318	LEU	CA-CB-CG	5.73	128.47	115.30
2	E	153	SER	CB-CA-C	5.52	120.59	110.10
2	F	318	LEU	CA-CB-CG	5.46	127.86	115.30
2	F	153	SER	C-N-CA	5.45	135.32	121.70
2	H	152	PRO	CA-N-CD	-5.30	104.07	111.50
2	E	152	PRO	C-N-CA	-5.24	108.60	121.70
2	G	152	PRO	C-N-CA	-5.04	109.10	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	128	TYR	Sidechain

## 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	1328	0	1348	94	0
1	B	1328	0	1348	105	0
1	C	1328	0	1348	82	0
1	D	1328	0	1348	108	1
1	I	1328	0	1348	75	0
1	J	1328	0	1348	102	0
1	K	1328	0	1348	74	1
1	L	1328	0	1348	92	0
2	E	3226	0	3293	267	1
2	F	3226	0	3293	290	1
2	G	3226	0	3293	309	0
2	H	3226	0	3293	348	0
3	E	27	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	27	0	12	3	0
3	G	27	0	12	2	0
3	H	27	0	12	3	0
All	All	23636	0	24004	1831	3

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 38.

All (1831) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:152:PRO:O	2:G:154:ALA:CA	1.76	1.33
2:G:152:PRO:O	2:G:153:SER:C	1.74	1.22
2:G:152:PRO:C	2:G:154:ALA:N	1.72	1.22
2:G:109:LYS:HB2	2:H:296:MET:HG2	1.32	1.10
2:E:174:GLU:HB3	2:E:211:GLN:HG3	1.30	1.10
2:H:216:LEU:HG	2:H:221:ALA:HB2	1.32	1.09
1:I:80:LYS:HA	1:I:83:ARG:HH12	1.12	1.09
2:G:174:GLU:HB3	2:G:211:GLN:HG3	1.34	1.08
2:G:109:LYS:HD3	2:H:296:MET:HB3	1.31	1.08
1:L:83:ARG:HB3	1:L:83:ARG:NH1	1.66	1.08
2:G:168:LEU:HG	2:G:219:LYS:HD3	1.30	1.07
2:G:152:PRO:HB2	2:G:156:ARG:HB2	1.37	1.06
1:C:83:ARG:NH1	1:C:83:ARG:HB3	1.72	1.05
1:L:83:ARG:HB3	1:L:83:ARG:HH11	1.12	1.03
2:E:212:LYS:HD3	2:E:216:LEU:HD21	1.41	1.03
2:G:130:ARG:HD2	2:G:225:LEU:HD11	1.38	1.03
1:A:13:VAL:HG12	1:A:170:GLU:HG3	1.41	1.01
2:H:150:GLN:O	2:H:153:SER:HB2	1.61	1.00
1:K:105:ILE:HD11	1:K:120:ILE:HG23	1.41	1.00
2:E:312:ILE:H	2:E:312:ILE:HD13	1.27	1.00
2:F:122:ARG:HH11	2:F:126:LEU:HD23	1.27	1.00
2:E:152:PRO:HB2	2:E:156:ARG:HB2	1.43	0.99
2:H:351:ILE:HD13	2:H:351:ILE:H	1.27	0.98
2:G:220:ASP:HA	2:G:223:LYS:HD2	1.43	0.98
1:B:65:GLU:HG2	2:F:143:TRP:CD1	1.97	0.97
2:G:92:VAL:HG21	2:H:92:VAL:HG13	1.42	0.97
2:H:123:ALA:HA	2:H:127:ALA:HB3	1.46	0.96
2:G:88:GLU:HB3	2:H:90:GLY:HA2	1.44	0.96
2:G:170:ASP:HA	2:G:217:LYS:HA	1.44	0.96
2:F:132:LEU:HD11	2:F:160:ARG:HG3	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:92:VAL:HG21	2:H:92:VAL:CG1	1.94	0.96
1:I:80:LYS:HA	1:I:83:ARG:NH1	1.81	0.95
1:A:80:LYS:HA	1:A:83:ARG:NH1	1.81	0.95
2:H:312:ILE:HD13	2:H:312:ILE:H	1.31	0.95
2:G:94:LYS:HA	2:G:94:LYS:HE2	1.49	0.95
2:H:135:LEU:HD23	2:H:171:LYS:HE2	1.46	0.95
1:B:65:GLU:HB3	2:F:143:TRP:HA	1.47	0.95
2:G:103:LEU:HD22	2:G:247:VAL:HG22	1.48	0.94
1:A:80:LYS:HA	1:A:83:ARG:HH12	1.29	0.94
2:F:94:LYS:HE2	2:F:94:LYS:HA	1.48	0.93
2:H:172:GLU:HB3	2:H:215:LYS:HD2	1.51	0.93
2:H:132:LEU:HD11	2:H:160:ARG:HG3	1.50	0.91
1:J:71:LEU:HB2	1:J:99:ASP:OD2	1.71	0.91
1:D:83:ARG:NH1	1:D:83:ARG:HB3	1.86	0.91
2:G:130:ARG:HB2	2:G:130:ARG:NH2	1.85	0.91
2:F:351:ILE:HD13	2:F:351:ILE:H	1.35	0.91
2:F:59:THR:HG22	2:F:393:ARG:NH2	1.84	0.90
1:B:65:GLU:OE1	2:F:143:TRP:CD1	2.25	0.90
2:H:122:ARG:HH11	2:H:126:LEU:HD23	1.34	0.90
1:I:85:ASP:O	1:I:89:ARG:HB2	1.70	0.90
1:D:83:ARG:HH11	1:D:83:ARG:HB3	1.37	0.89
2:E:94:LYS:HE2	2:E:94:LYS:HA	1.52	0.89
2:H:94:LYS:HA	2:H:94:LYS:HE2	1.53	0.88
1:D:105:ILE:HD11	1:D:120:ILE:HG21	1.54	0.88
2:G:344:LEU:O	2:G:352:THR:HB	1.73	0.87
2:E:299:THR:HA	2:E:302:ILE:HD13	1.55	0.87
1:I:10:GLY:HA3	1:I:174:LYS:HA	1.55	0.87
2:G:64:THR:HB	3:G:2450:ADP:O2A	1.74	0.87
2:H:216:LEU:CG	2:H:221:ALA:HB2	2.05	0.87
1:B:104:LEU:HD12	1:B:112:VAL:HG12	1.57	0.86
2:E:344:LEU:O	2:E:352:THR:HB	1.75	0.86
1:K:105:ILE:HD11	1:K:120:ILE:CG2	2.05	0.86
1:L:174:LYS:NZ	1:L:174:LYS:HA	1.90	0.86
2:H:312:ILE:CD1	2:H:312:ILE:H	1.89	0.86
1:I:1:THR:HB	1:I:33:LYS:HZ3	1.39	0.86
2:G:397:THR:HG22	2:H:327:PRO:HA	1.58	0.85
1:B:65:GLU:OE1	2:F:143:TRP:CG	2.29	0.85
2:E:132:LEU:HD11	2:E:160:ARG:HG3	1.58	0.85
1:D:152:LEU:HD13	1:D:166:HIS:ND1	1.91	0.84
1:I:47:ALA:HB3	1:I:94:LEU:HB2	1.58	0.84
2:G:312:ILE:H	2:G:312:ILE:HD13	1.40	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ARG:HH11	1:C:83:ARG:HB3	1.34	0.84
1:A:85:ASP:O	1:A:89:ARG:HB2	1.76	0.84
2:F:91:TYR:O	2:F:92:VAL:HG13	1.78	0.84
1:B:17:ASP:HA	1:B:165:PHE:O	1.78	0.84
2:H:132:LEU:HA	2:H:135:LEU:HD12	1.58	0.84
1:B:65:GLU:CG	2:F:143:TRP:CD1	2.60	0.84
2:F:59:THR:HG22	2:F:393:ARG:HH21	1.42	0.84
2:E:130:ARG:NH2	2:E:130:ARG:HB2	1.92	0.84
2:E:214:ARG:HD3	2:E:216:LEU:HD22	1.59	0.83
2:H:174:GLU:HA	2:H:213:ALA:H	1.43	0.83
1:B:72:VAL:O	1:B:76:VAL:HG23	1.78	0.83
2:G:362:GLU:OE2	2:H:32:ARG:NH2	2.08	0.83
2:E:64:THR:HB	3:E:450:ADP:O2A	1.78	0.83
2:F:123:ALA:HA	2:F:127:ALA:HB3	1.59	0.83
2:E:131:ILE:HD11	2:E:218:ILE:HG12	1.61	0.83
2:G:91:TYR:HB2	2:H:90:GLY:O	1.78	0.82
1:J:72:VAL:O	1:J:76:VAL:HG23	1.79	0.82
2:F:103:LEU:HD13	2:F:247:VAL:HG22	1.61	0.82
2:G:220:ASP:O	2:G:223:LYS:N	2.10	0.82
2:E:145:GLN:HB2	2:E:148:GLN:HB2	1.62	0.82
2:G:361:THR:HG22	2:H:35:TRP:CZ3	2.15	0.82
1:A:10:GLY:HA2	1:A:173:TYR:CE1	2.15	0.82
2:F:173:ILE:HG12	2:F:212:LYS:HD2	1.59	0.82
2:F:171:LYS:NZ	2:F:218:ILE:HD11	1.94	0.81
2:E:312:ILE:H	2:E:312:ILE:CD1	1.93	0.81
2:H:173:ILE:HG12	2:H:212:LYS:HD2	1.63	0.81
2:F:312:ILE:H	2:F:312:ILE:HD13	1.46	0.81
1:D:71:LEU:HD21	1:D:97:VAL:HG11	1.62	0.80
1:K:152:LEU:HD13	1:K:166:HIS:ND1	1.96	0.80
2:H:171:LYS:NZ	2:H:218:ILE:HD11	1.96	0.80
1:D:43:ILE:H	1:D:43:ILE:HD13	1.46	0.80
2:H:131:ILE:HD11	2:H:218:ILE:HD13	1.64	0.80
2:F:64:THR:HB	3:F:1450:ADP:O2A	1.82	0.80
2:E:150:GLN:O	2:E:153:SER:HB2	1.82	0.79
1:L:1:THR:HB	1:L:33:LYS:HZ3	1.47	0.79
2:F:27:VAL:HG13	2:F:70:LEU:HG	1.62	0.79
2:E:173:ILE:HG12	2:E:212:LYS:HD2	1.64	0.79
2:G:211:GLN:HG2	2:G:212:LYS:H	1.47	0.79
2:G:92:VAL:HG11	2:H:92:VAL:CG1	2.12	0.79
1:I:10:GLY:HA2	1:I:173:TYR:CE1	2.18	0.79
2:E:389:ASN:ND2	2:E:391:GLY:H	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:62:ARG:O	1:L:66:MET:HB2	1.82	0.79
2:H:345:THR:CG2	2:H:373:ILE:HD13	2.13	0.79
2:E:152:PRO:HB3	2:E:156:ARG:H	1.48	0.79
1:D:105:ILE:HD11	1:D:120:ILE:CG2	2.13	0.79
2:H:389:ASN:ND2	2:H:391:GLY:H	1.81	0.79
2:H:384:ASN:ND2	2:H:394:ARG:HE	1.80	0.79
2:E:389:ASN:C	2:E:389:ASN:HD22	1.83	0.78
2:F:224:LEU:O	2:F:228:GLU:HB2	1.83	0.78
1:L:13:VAL:HG12	1:L:170:GLU:HG3	1.64	0.78
1:J:57:PHE:O	1:J:61:GLU:HG3	1.83	0.78
2:G:147:GLU:HA	2:G:150:GLN:HG3	1.66	0.78
2:F:172:GLU:HB3	2:F:215:LYS:HD2	1.64	0.78
2:H:91:TYR:O	2:H:92:VAL:HG13	1.83	0.78
1:B:65:GLU:HG2	2:F:143:TRP:HD1	1.46	0.77
2:F:223:LYS:HA	2:F:226:ILE:HG12	1.64	0.77
2:H:132:LEU:HD23	2:H:135:LEU:HD12	1.66	0.77
2:E:211:GLN:HG2	2:E:212:LYS:H	1.49	0.76
1:A:10:GLY:HA3	1:A:174:LYS:HA	1.65	0.76
2:G:109:LYS:CD	2:H:296:MET:HB3	2.13	0.76
1:B:105:ILE:HD11	1:B:120:ILE:HG23	1.68	0.76
2:F:257:GLU:HB2	2:F:260:LYS:HG3	1.68	0.76
2:F:148:GLN:OE1	2:F:151:GLU:HG3	1.85	0.76
2:H:103:LEU:HD13	2:H:247:VAL:HG22	1.68	0.76
2:H:217:LYS:NZ	2:H:217:LYS:HB2	2.01	0.75
1:B:170:GLU:HG2	1:B:171:LEU:H	1.51	0.75
2:G:142:ASN:HB2	2:G:149:GLN:HE22	1.51	0.75
1:L:30:ASN:H	1:L:30:ASN:HD22	1.31	0.75
1:D:54:PHE:O	1:D:58:GLU:HB2	1.86	0.75
1:L:105:ILE:HD11	1:L:120:ILE:HG23	1.68	0.75
2:H:64:THR:HB	3:H:3450:ADP:O2A	1.85	0.75
1:J:104:LEU:HD12	1:J:112:VAL:HG12	1.68	0.75
2:E:130:ARG:HD2	2:E:225:LEU:HD11	1.67	0.75
1:B:1:THR:HB	1:B:33:LYS:NZ	2.01	0.75
2:G:152:PRO:CB	2:G:156:ARG:HB2	2.16	0.74
2:E:384:ASN:ND2	2:E:394:ARG:HE	1.85	0.74
2:G:291:SER:HA	2:G:296:MET:HE2	1.69	0.74
1:J:1:THR:HB	1:J:33:LYS:NZ	2.03	0.74
2:E:174:GLU:HA	2:E:213:ALA:H	1.51	0.74
2:G:136:ILE:O	2:G:136:ILE:HG22	1.88	0.74
2:G:152:PRO:O	2:G:154:ALA:N	0.59	0.74
2:H:130:ARG:HH21	2:H:229:GLU:HG3	1.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:83:ARG:HG2	1:I:83:ARG:HH11	1.52	0.74
1:B:60:PHE:CD1	1:B:78:LEU:HD22	2.23	0.74
2:E:104:THR:HG21	2:E:292:THR:HG21	1.69	0.74
1:L:64:LEU:HB3	1:L:69:GLY:HA2	1.69	0.74
2:F:384:ASN:ND2	2:F:394:ARG:HE	1.85	0.74
2:G:168:LEU:HA	2:G:219:LYS:HB3	1.68	0.73
1:B:57:PHE:O	1:B:61:GLU:HG3	1.88	0.73
1:L:138:GLU:C	1:L:139:ASN:HD22	1.90	0.73
2:H:108:VAL:HA	2:H:111:VAL:HG22	1.68	0.73
2:G:145:GLN:HB2	2:G:148:GLN:HB2	1.70	0.73
2:H:130:ARG:HG2	2:H:225:LEU:HD11	1.70	0.73
1:B:28:LYS:HZ2	1:B:30:ASN:HD21	1.36	0.73
2:F:122:ARG:NH1	2:F:126:LEU:HD23	2.02	0.73
1:C:85:ASP:HB3	1:C:88:LEU:HB2	1.69	0.73
2:H:356:LYS:HG3	2:H:366:ILE:HG22	1.71	0.73
2:G:389:ASN:ND2	2:G:391:GLY:H	1.86	0.73
2:E:167:GLN:NE2	2:E:168:LEU:HG	2.04	0.73
2:H:147:GLU:O	2:H:151:GLU:HG2	1.89	0.73
1:J:19:GLN:HB2	1:J:163:ASN:ND2	2.03	0.73
1:D:3:ILE:HB	1:D:122:ILE:HG12	1.71	0.72
1:L:30:ASN:ND2	1:L:30:ASN:H	1.87	0.72
1:L:115:PRO:HG3	1:L:120:ILE:HG12	1.68	0.72
2:H:219:LYS:HA	2:H:219:LYS:HE3	1.71	0.72
1:C:136:LEU:HB3	1:C:147:ILE:HD12	1.72	0.72
1:B:36:ARG:O	1:B:37:LEU:HD23	1.88	0.72
2:H:232:LYS:H	2:H:232:LYS:HD2	1.54	0.72
2:G:312:ILE:H	2:G:312:ILE:CD1	2.02	0.72
1:B:86:ARG:HA	1:B:89:ARG:NE	2.03	0.72
2:F:356:LYS:HG3	2:F:366:ILE:HG22	1.70	0.72
2:H:220:ASP:O	2:H:224:LEU:HD23	1.88	0.72
2:G:91:TYR:HD1	2:H:91:TYR:CD2	2.06	0.72
1:K:71:LEU:HG	1:K:99:ASP:OD1	1.88	0.72
1:L:152:LEU:HD13	1:L:166:HIS:CE1	2.24	0.72
2:E:167:GLN:HE22	2:E:168:LEU:HG	1.54	0.72
1:D:71:LEU:HD21	1:D:97:VAL:CG1	2.19	0.72
2:E:124:GLU:HA	2:E:127:ALA:HB3	1.72	0.72
1:D:79:ALA:HB1	1:D:110:GLY:HA2	1.69	0.72
1:J:152:LEU:HD13	1:J:166:HIS:ND1	2.05	0.72
2:E:91:TYR:O	2:E:92:VAL:HG13	1.89	0.72
2:G:362:GLU:HG2	2:G:410:ALA:HB1	1.72	0.72
2:F:81:VAL:HG11	2:F:99:ILE:HG12	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:171:LYS:HG3	2:E:218:ILE:HD11	1.72	0.71
2:H:242:ASP:HA	2:H:245:ASP:OD1	1.90	0.71
2:G:389:ASN:C	2:G:389:ASN:HD22	1.92	0.71
2:E:140:LYS:O	2:E:141:ASN:HB2	1.90	0.71
1:D:115:PRO:HG3	1:D:120:ILE:HG12	1.71	0.71
2:G:361:THR:CG2	2:H:35:TRP:CZ3	2.74	0.71
1:J:5:SER:HB3	1:J:120:ILE:HD13	1.72	0.71
2:G:153:SER:O	2:G:157:GLN:NE2	2.23	0.71
2:G:124:GLU:HA	2:G:127:ALA:HB3	1.73	0.71
1:L:174:LYS:HZ3	1:L:174:LYS:HA	1.53	0.71
2:G:92:VAL:CG2	2:H:91:TYR:C	2.59	0.71
1:B:28:LYS:NZ	1:B:30:ASN:HD21	1.88	0.70
1:J:105:ILE:HD11	1:J:120:ILE:HG23	1.73	0.70
1:K:64:LEU:HD23	1:K:74:ALA:CB	2.20	0.70
2:F:108:VAL:HG21	2:F:294:HIS:HD2	1.56	0.70
2:G:130:ARG:HH21	2:G:130:ARG:HB2	1.54	0.70
2:H:344:LEU:O	2:H:352:THR:HB	1.90	0.70
2:F:242:ASP:HA	2:F:245:ASP:OD1	1.90	0.70
2:F:312:ILE:H	2:F:312:ILE:CD1	2.04	0.70
1:D:14:ILE:HD13	1:D:43:ILE:CG1	2.22	0.70
1:B:63:LYS:HA	1:B:66:MET:HE3	1.72	0.70
2:F:174:GLU:HA	2:F:213:ALA:H	1.56	0.70
1:I:1:THR:HB	1:I:33:LYS:NZ	2.05	0.70
1:L:43:ILE:HD13	1:L:43:ILE:H	1.57	0.70
2:G:91:TYR:HD1	2:H:91:TYR:CE2	2.09	0.70
1:B:1:THR:HB	1:B:33:LYS:HZ3	1.56	0.70
2:H:217:LYS:O	2:H:221:ALA:N	2.13	0.69
2:G:91:TYR:O	2:G:92:VAL:HG13	1.91	0.69
1:D:6:VAL:HG21	1:D:147:ILE:HG22	1.74	0.69
2:F:344:LEU:O	2:F:352:THR:HB	1.92	0.69
2:E:165:GLU:HG2	2:E:166:GLY:H	1.55	0.69
2:G:174:GLU:HA	2:G:212:LYS:HB3	1.73	0.69
2:F:217:LYS:HB2	2:F:217:LYS:NZ	2.07	0.69
2:H:174:GLU:HB3	2:H:211:GLN:HB2	1.74	0.69
1:J:104:LEU:CD1	1:J:112:VAL:HG12	2.22	0.69
2:E:293:LYS:HG3	2:E:294:HIS:CD2	2.28	0.69
2:H:148:GLN:HA	2:H:151:GLU:HG3	1.72	0.69
2:H:27:VAL:HG13	2:H:70:LEU:HG	1.75	0.69
1:A:71:LEU:HD23	1:A:99:ASP:OD2	1.92	0.69
1:B:86:ARG:HA	1:B:89:ARG:CZ	2.23	0.69
1:J:86:ARG:HA	1:J:89:ARG:CZ	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:86:ARG:HA	1:K:89:ARG:NH1	2.06	0.69
1:I:8:ARG:HG2	1:I:9:ASN:ND2	2.08	0.69
2:E:170:ASP:HA	2:E:217:LYS:HA	1.73	0.69
1:J:141:GLU:OE2	1:J:141:GLU:HA	1.93	0.69
2:E:312:ILE:HG12	2:E:313:ALA:H	1.58	0.69
2:G:91:TYR:CD1	2:H:91:TYR:CE2	2.81	0.69
1:B:104:LEU:CD1	1:B:112:VAL:HG12	2.22	0.69
2:G:359:MET:HG3	2:G:366:ILE:HG13	1.74	0.69
2:E:359:MET:HG3	2:E:366:ILE:HG13	1.75	0.69
1:B:65:GLU:CD	2:F:143:TRP:CD1	2.65	0.68
2:G:345:THR:HG21	2:G:373:ILE:HD13	1.74	0.68
2:H:389:ASN:HD22	2:H:391:GLY:H	1.41	0.68
2:H:236:PRO:HG2	2:H:237:GLU:H	1.58	0.68
2:E:337:THR:O	2:E:341:GLU:HG3	1.92	0.68
2:E:214:ARG:HG2	2:E:215:LYS:N	2.08	0.68
2:H:223:LYS:HA	2:H:226:ILE:HG12	1.76	0.68
1:I:77:GLU:O	1:I:80:LYS:HB2	1.93	0.68
2:H:235:ASN:HB2	2:H:236:PRO:HD2	1.73	0.68
2:F:264:ARG:NE	2:F:265:GLY:H	1.91	0.68
2:F:375:ARG:CZ	2:F:422:ALA:HB1	2.23	0.68
2:F:108:VAL:C	2:F:110:MET:H	1.96	0.68
1:I:10:GLY:HA2	1:I:173:TYR:CZ	2.29	0.68
2:E:122:ARG:CZ	2:E:126:LEU:HD21	2.24	0.68
2:H:375:ARG:CZ	2:H:422:ALA:HB1	2.23	0.68
2:G:152:PRO:HB2	2:G:156:ARG:CB	2.21	0.68
2:E:291:SER:HA	2:E:296:MET:HE2	1.76	0.68
2:H:135:LEU:HB3	2:H:159:PHE:CD2	2.28	0.68
1:D:28:LYS:HD3	1:D:31:VAL:HG22	1.74	0.68
1:K:73:LYS:HA	1:K:76:VAL:HG12	1.76	0.68
2:G:359:MET:CE	2:H:36:ARG:NH1	2.57	0.67
2:E:174:GLU:CB	2:E:211:GLN:HG3	2.18	0.67
2:G:173:ILE:N	2:G:173:ILE:HD13	2.09	0.67
2:H:96:VAL:HG11	2:H:281:LEU:HD12	1.75	0.67
1:A:1:THR:HB	1:A:33:LYS:HZ3	1.59	0.67
2:G:147:GLU:HG3	2:G:150:GLN:NE2	2.10	0.67
1:J:86:ARG:HA	1:J:89:ARG:NE	2.09	0.67
1:C:11:HIS:NE2	1:C:174:LYS:HE2	2.08	0.67
2:E:216:LEU:HD23	2:E:216:LEU:H	1.60	0.67
2:F:163:LEU:HD11	2:F:222:MET:CE	2.24	0.67
1:B:152:LEU:HD13	1:B:166:HIS:ND1	2.10	0.67
2:G:153:SER:HA	2:G:157:GLN:HG3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:82:GLU:HB3	2:F:257:GLU:OE2	1.93	0.67
2:G:130:ARG:CD	2:G:225:LEU:HD11	2.20	0.67
2:F:216:LEU:HD11	2:F:221:ALA:HA	1.76	0.67
2:G:384:ASN:ND2	2:G:394:ARG:HE	1.92	0.67
2:G:140:LYS:O	2:G:141:ASN:HB2	1.95	0.67
2:F:152:PRO:HB2	2:F:156:ARG:HB2	1.77	0.67
1:D:73:LYS:NZ	1:D:77:GLU:HG2	2.09	0.67
1:C:152:LEU:HD13	1:C:166:HIS:CE1	2.29	0.67
2:G:89:VAL:HG12	2:G:93:GLY:HA3	1.77	0.66
1:J:85:ASP:O	1:J:89:ARG:HG3	1.95	0.66
1:A:65:GLU:CD	2:E:141:ASN:HB3	2.15	0.66
1:C:10:GLY:HA2	1:C:173:TYR:CE1	2.30	0.66
2:F:223:LYS:HD2	2:F:223:LYS:N	2.09	0.66
1:B:19:GLN:HB2	1:B:163:ASN:ND2	2.11	0.66
1:C:79:ALA:HB1	1:C:110:GLY:HA2	1.78	0.66
2:E:136:ILE:O	2:E:136:ILE:HG22	1.95	0.66
2:F:135:LEU:CD2	2:F:171:LYS:HE2	2.25	0.66
2:F:389:ASN:ND2	2:F:391:GLY:H	1.93	0.66
1:A:28:LYS:NZ	1:A:30:ASN:ND2	2.43	0.66
2:F:130:ARG:HD2	2:F:225:LEU:HD11	1.77	0.66
1:J:8:ARG:NH1	1:J:142:LEU:O	2.26	0.66
1:K:27:MET:SD	1:L:113:VAL:HG21	2.35	0.66
2:E:211:GLN:HG2	2:E:212:LYS:N	2.11	0.66
2:H:130:ARG:HG2	2:H:225:LEU:CD1	2.26	0.66
2:H:130:ARG:NH2	2:H:229:GLU:HG3	2.10	0.66
2:G:173:ILE:HG12	2:G:212:LYS:HD2	1.76	0.66
2:F:174:GLU:HA	2:F:212:LYS:HB3	1.76	0.66
2:F:291:SER:HA	2:F:296:MET:HE2	1.77	0.66
2:F:211:GLN:HE21	2:F:212:LYS:H	1.43	0.66
2:E:122:ARG:O	2:E:126:LEU:HD23	1.96	0.66
1:A:65:GLU:OE1	2:E:141:ASN:CB	2.44	0.66
2:F:362:GLU:HG2	2:F:410:ALA:CB	2.25	0.66
2:E:103:LEU:HD22	2:E:247:VAL:HG22	1.78	0.66
1:J:36:ARG:O	1:J:37:LEU:HD23	1.95	0.66
2:F:151:GLU:HB2	2:F:152:PRO:CD	2.26	0.66
2:G:174:GLU:HB3	2:G:211:GLN:CG	2.20	0.65
1:B:62:ARG:HA	1:B:65:GLU:HG3	1.77	0.65
2:G:92:VAL:HG21	2:H:91:TYR:C	2.15	0.65
1:C:73:LYS:HA	1:C:76:VAL:HG12	1.78	0.65
2:G:293:LYS:HG3	2:G:294:HIS:CD2	2.31	0.65
2:E:52:ASN:HB2	2:E:325:ARG:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:223:LYS:HA	2:H:226:ILE:CG1	2.27	0.65
2:E:345:THR:CG2	2:E:373:ILE:HD13	2.27	0.65
1:J:28:LYS:NZ	1:J:30:ASN:HD21	1.94	0.65
1:J:1:THR:HB	1:J:33:LYS:HZ3	1.60	0.65
1:J:28:LYS:HZ2	1:J:30:ASN:HD21	1.44	0.65
2:H:108:VAL:C	2:H:110:MET:H	1.98	0.65
2:G:92:VAL:HG11	2:H:92:VAL:HG12	1.76	0.65
1:B:28:LYS:NZ	1:B:30:ASN:ND2	2.44	0.65
2:H:168:LEU:O	2:H:217:LYS:HD2	1.97	0.65
2:F:89:VAL:HG11	2:F:94:LYS:O	1.97	0.65
2:F:130:ARG:CD	2:F:225:LEU:HD11	2.27	0.65
2:H:219:LYS:O	2:H:223:LYS:HD3	1.96	0.65
2:H:229:GLU:HA	2:H:232:LYS:HD3	1.78	0.65
2:H:148:GLN:OE1	2:H:151:GLU:HG3	1.97	0.65
1:K:168:ILE:HD12	1:K:168:ILE:N	2.12	0.65
2:F:145:GLN:HB2	2:F:148:GLN:HG2	1.78	0.64
1:D:30:ASN:H	1:D:30:ASN:HD22	1.45	0.64
2:F:210:LYS:HD3	2:F:210:LYS:N	2.12	0.64
2:G:92:VAL:CG2	2:H:92:VAL:HG13	2.23	0.64
2:H:389:ASN:HD22	2:H:389:ASN:C	2.01	0.64
1:J:168:ILE:HD12	1:J:168:ILE:H	1.63	0.64
1:K:115:PRO:HG3	1:K:120:ILE:HG12	1.80	0.64
2:G:361:THR:HG21	2:H:36:ARG:HA	1.79	0.64
2:G:152:PRO:HB3	2:G:156:ARG:H	1.63	0.64
1:A:1:THR:HB	1:A:33:LYS:NZ	2.11	0.64
1:L:91:LEU:HD12	1:L:91:LEU:O	1.98	0.64
1:J:17:ASP:HA	1:J:165:PHE:O	1.98	0.64
2:G:142:ASN:CB	2:G:149:GLN:HE22	2.10	0.64
1:I:152:LEU:HD13	1:I:166:HIS:CE1	2.32	0.64
2:E:173:ILE:N	2:E:173:ILE:HD13	2.12	0.64
2:E:174:GLU:HB3	2:E:211:GLN:CG	2.19	0.64
2:E:147:GLU:HA	2:E:150:GLN:HG3	1.80	0.64
1:D:30:ASN:HD22	1:D:30:ASN:N	1.95	0.64
1:D:17:ASP:HA	1:D:165:PHE:O	1.97	0.64
2:G:112:ARG:HH11	2:G:112:ARG:HG3	1.62	0.64
2:H:214:ARG:HE	2:H:216:LEU:HB3	1.61	0.64
2:H:145:GLN:HB2	2:H:148:GLN:HG2	1.80	0.64
1:I:168:ILE:HD12	1:I:168:ILE:N	2.13	0.64
2:H:232:LYS:N	2:H:232:LYS:HD2	2.11	0.64
2:F:132:LEU:HA	2:F:135:LEU:HD12	1.80	0.64
2:F:127:ALA:HA	2:F:130:ARG:NH2	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:168:ILE:HD12	1:K:168:ILE:H	1.63	0.64
1:L:79:ALA:HB1	1:L:110:GLY:HA2	1.80	0.64
1:D:19:GLN:HB2	1:D:163:ASN:ND2	2.12	0.64
1:C:30:ASN:H	1:C:30:ASN:HD22	1.43	0.64
2:F:123:ALA:HA	2:F:127:ALA:CB	2.27	0.64
2:H:167:GLN:O	2:H:168:LEU:HB3	1.98	0.64
1:D:34:VAL:HG12	1:D:169:GLU:HG3	1.80	0.64
2:G:122:ARG:CZ	2:G:126:LEU:HD21	2.28	0.64
2:E:116:ILE:O	2:E:120:ARG:HB2	1.98	0.64
1:A:84:THR:HG23	1:A:85:ASP:H	1.63	0.63
1:C:28:LYS:HD2	1:D:113:VAL:HG13	1.79	0.63
1:A:7:ARG:HB2	1:A:12:VAL:HG23	1.80	0.63
2:G:408:TYR:HB2	2:H:29:ILE:HD11	1.80	0.63
1:A:88:LEU:H	1:A:88:LEU:HD12	1.63	0.63
1:I:67:HIS:CD2	1:I:73:LYS:HD2	2.33	0.63
2:E:152:PRO:HB2	2:E:156:ARG:CB	2.25	0.63
2:E:375:ARG:CZ	2:E:422:ALA:HB1	2.27	0.63
2:E:311:GLN:HE21	2:E:311:GLN:CA	2.11	0.63
2:F:147:GLU:O	2:F:151:GLU:HG2	1.99	0.63
2:F:236:PRO:HG2	2:F:237:GLU:H	1.64	0.63
1:C:83:ARG:CZ	1:C:83:ARG:HB3	2.29	0.63
2:F:132:LEU:HD11	2:F:160:ARG:CG	2.27	0.63
2:H:174:GLU:HA	2:H:212:LYS:HB3	1.81	0.63
2:F:235:ASN:HB2	2:F:236:PRO:HD2	1.81	0.63
1:K:83:ARG:HH11	1:K:83:ARG:HG3	1.63	0.63
1:J:28:LYS:NZ	1:J:30:ASN:ND2	2.47	0.63
1:K:36:ARG:O	1:K:37:LEU:HD23	1.98	0.63
2:H:312:ILE:N	2:H:312:ILE:HD13	2.08	0.63
1:I:8:ARG:O	1:I:11:HIS:HB2	1.99	0.63
2:F:41:ASN:C	2:F:41:ASN:HD22	2.02	0.63
1:A:67:HIS:HD2	1:A:73:LYS:HD2	1.62	0.63
2:F:96:VAL:HG11	2:F:281:LEU:HD12	1.80	0.63
2:F:132:LEU:HD23	2:F:135:LEU:HD12	1.80	0.63
2:H:315:PRO:O	2:H:318:LEU:HB2	1.99	0.63
1:L:6:VAL:HG21	1:L:147:ILE:HG22	1.79	0.63
2:G:88:GLU:CB	2:H:90:GLY:HA2	2.25	0.63
2:G:375:ARG:CZ	2:G:422:ALA:HB1	2.29	0.63
2:F:27:VAL:CG1	2:F:70:LEU:HG	2.30	0.62
1:I:36:ARG:HH11	1:I:36:ARG:HB3	1.63	0.62
2:F:131:ILE:HD13	2:F:222:MET:HE1	1.80	0.62
2:F:147:GLU:CG	2:F:150:GLN:NE2	2.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:211:GLN:NE2	2:F:212:LYS:H	1.97	0.62
1:D:37:LEU:HD11	1:D:60:PHE:HD2	1.63	0.62
1:A:65:GLU:CD	2:E:141:ASN:CB	2.68	0.62
2:F:101:ARG:O	2:F:104:THR:HB	1.99	0.62
2:F:31:LEU:HD11	2:F:74:ALA:HB2	1.81	0.62
1:L:95:LEU:HB2	1:L:106:ILE:HB	1.81	0.62
2:H:123:ALA:HA	2:H:127:ALA:CB	2.24	0.62
2:G:359:MET:HE2	2:H:36:ARG:NH1	2.14	0.62
2:F:401:ARG:NH2	2:F:442:ILE:HG13	2.15	0.62
2:G:170:ASP:HB3	2:G:217:LYS:HD3	1.81	0.62
1:B:28:LYS:HD3	1:B:31:VAL:HG22	1.82	0.62
1:L:152:LEU:HD13	1:L:166:HIS:ND1	2.13	0.62
2:F:108:VAL:HG21	2:F:294:HIS:CD2	2.34	0.62
1:J:86:ARG:HA	1:J:89:ARG:NH1	2.14	0.62
1:K:28:LYS:HE2	1:K:30:ASN:ND2	2.15	0.62
2:E:130:ARG:CZ	2:E:130:ARG:HB2	2.30	0.62
2:E:389:ASN:HD22	2:E:391:GLY:H	1.46	0.62
1:A:65:GLU:OE1	2:E:141:ASN:HB3	2.00	0.62
2:G:231:ALA:C	2:G:233:LEU:H	2.03	0.62
2:E:312:ILE:N	2:E:312:ILE:HD13	2.09	0.62
2:E:312:ILE:HG12	2:E:313:ALA:N	2.14	0.62
2:G:362:GLU:HG2	2:G:410:ALA:CB	2.30	0.62
2:F:219:LYS:O	2:F:223:LYS:HD3	2.00	0.62
2:H:239:LEU:HD23	2:H:240:LYS:N	2.14	0.62
1:B:46:PHE:CE2	1:B:53:ALA:HB2	2.35	0.61
2:F:129:GLU:HB2	2:F:130:ARG:NH1	2.15	0.61
2:H:221:ALA:O	2:H:225:LEU:HD23	2.00	0.61
2:E:140:LYS:HD3	2:E:140:LYS:H	1.66	0.61
1:L:55:THR:O	1:L:58:GLU:HB3	2.00	0.61
1:I:87:MET:CE	1:J:84:THR:HA	2.30	0.61
2:H:81:VAL:HG11	2:H:99:ILE:HG12	1.82	0.61
2:G:140:LYS:H	2:G:140:LYS:HD3	1.65	0.61
2:F:362:GLU:HG2	2:F:410:ALA:HB1	1.80	0.61
2:H:20:GLN:O	2:H:24:LYS:HG3	2.00	0.61
2:H:19:GLY:O	2:H:24:LYS:HE3	2.00	0.61
1:D:38:TYR:HE1	1:D:65:GLU:HB3	1.64	0.61
1:D:86:ARG:HA	1:D:89:ARG:CZ	2.30	0.61
2:G:148:GLN:HA	2:G:151:GLU:HG2	1.82	0.61
2:H:393:ARG:HH11	2:H:393:ARG:HG2	1.65	0.61
2:E:293:LYS:HG3	2:E:294:HIS:HD2	1.65	0.61
2:G:108:VAL:HG21	2:G:294:HIS:ND1	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:ILE:HD12	1:B:168:ILE:N	2.15	0.61
1:L:1:THR:HB	1:L:33:LYS:NZ	2.16	0.61
1:A:8:ARG:NH1	1:A:142:LEU:O	2.23	0.61
2:E:152:PRO:CB	2:E:156:ARG:H	2.13	0.61
2:F:170:ASP:HA	2:F:217:LYS:HA	1.81	0.61
2:G:345:THR:HG22	2:G:352:THR:HG21	1.82	0.61
1:A:88:LEU:H	1:A:88:LEU:CD1	2.13	0.61
2:F:116:ILE:O	2:F:120:ARG:HB2	2.01	0.61
2:H:123:ALA:CA	2:H:127:ALA:HB3	2.25	0.61
1:C:95:LEU:HB2	1:C:106:ILE:HB	1.83	0.60
1:B:65:GLU:OE1	2:F:143:TRP:CD2	2.55	0.60
1:D:13:VAL:HG12	1:D:170:GLU:HA	1.82	0.60
2:H:262:CYS:SG	2:H:318:LEU:HD13	2.41	0.60
1:D:86:ARG:HA	1:D:89:ARG:NH1	2.15	0.60
1:A:105:ILE:CD1	1:A:120:ILE:HG23	2.30	0.60
2:G:109:LYS:HB2	2:H:296:MET:CG	2.21	0.60
2:H:127:ALA:HA	2:H:130:ARG:NH2	2.15	0.60
2:G:214:ARG:NH2	2:H:233:LEU:HD13	2.16	0.60
2:G:359:MET:HE1	2:H:36:ARG:HH12	1.66	0.60
1:J:168:ILE:HD12	1:J:168:ILE:N	2.16	0.60
2:G:242:ASP:HA	2:G:245:ASP:OD1	2.02	0.60
1:J:19:GLN:HB2	1:J:163:ASN:HD22	1.65	0.60
2:H:63:LYS:HE2	2:H:307:SER:OG	2.01	0.60
2:F:312:ILE:HG12	2:F:313:ALA:N	2.15	0.60
2:H:108:VAL:HG21	2:H:294:HIS:HD2	1.67	0.60
2:H:375:ARG:HB3	2:H:425:VAL:HG11	1.83	0.60
2:H:132:LEU:HD23	2:H:135:LEU:CD1	2.31	0.60
2:H:211:GLN:NE2	2:H:212:LYS:H	2.00	0.60
1:B:70:HIS:HE1	1:B:72:VAL:HB	1.67	0.60
1:D:14:ILE:HD13	1:D:43:ILE:HG13	1.83	0.60
2:H:25:ARG:O	2:H:29:ILE:HG12	2.02	0.60
1:C:55:THR:O	1:C:58:GLU:HB3	2.02	0.60
2:F:212:LYS:NZ	2:F:212:LYS:HB2	2.17	0.60
2:G:389:ASN:HD22	2:G:391:GLY:H	1.49	0.60
2:H:291:SER:HA	2:H:296:MET:HE2	1.83	0.60
2:G:219:LYS:O	2:G:223:LYS:HE3	2.01	0.60
2:E:168:LEU:HA	2:E:219:LYS:HB3	1.84	0.60
2:F:130:ARG:CG	2:F:225:LEU:HD11	2.32	0.60
1:D:14:ILE:HD13	1:D:43:ILE:HG12	1.83	0.60
2:F:19:GLY:O	2:F:24:LYS:HE3	2.02	0.60
1:C:94:LEU:CD2	1:C:107:THR:HG22	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:136:LEU:HB3	1:K:147:ILE:HD12	1.82	0.60
2:F:86:PHE:O	2:F:89:VAL:HG22	2.02	0.60
1:L:174:LYS:HZ2	1:L:174:LYS:HA	1.65	0.60
2:E:168:LEU:HD23	2:E:219:LYS:HB3	1.82	0.60
2:E:33:ASN:ND2	2:E:36:ARG:HD2	2.17	0.60
1:I:14:ILE:HD12	1:I:43:ILE:HG13	1.84	0.60
2:H:311:GLN:HA	2:H:311:GLN:NE2	2.17	0.60
2:G:88:GLU:HB3	2:H:90:GLY:CA	2.25	0.60
1:A:77:GLU:O	1:A:80:LYS:HB2	2.01	0.60
2:F:229:GLU:OE2	2:F:232:LYS:HD2	2.02	0.60
2:F:147:GLU:HG2	2:F:150:GLN:NE2	2.16	0.60
2:G:131:ILE:HD11	2:G:218:ILE:HG12	1.83	0.60
2:H:337:THR:O	2:H:341:GLU:HG3	2.02	0.60
2:E:131:ILE:HD11	2:E:218:ILE:CG1	2.30	0.59
2:H:218:ILE:O	2:H:222:MET:HB3	2.02	0.59
2:G:174:GLU:HA	2:G:213:ALA:H	1.67	0.59
2:G:142:ASN:HB2	2:G:149:GLN:NE2	2.15	0.59
1:I:105:ILE:CD1	1:I:120:ILE:HG23	2.31	0.59
2:F:12:GLU:HG2	2:F:73:LEU:CD1	2.32	0.59
2:E:432:LEU:H	2:E:432:LEU:HD12	1.67	0.59
2:G:153:SER:CA	2:G:157:GLN:HG3	2.32	0.59
1:I:83:ARG:HG2	1:I:83:ARG:NH1	2.17	0.59
2:H:212:LYS:HB2	2:H:212:LYS:NZ	2.18	0.59
2:F:59:THR:CG2	2:F:393:ARG:HH21	2.13	0.59
2:E:130:ARG:CD	2:E:225:LEU:HD11	2.33	0.59
1:L:30:ASN:HD22	1:L:30:ASN:N	1.96	0.59
2:E:33:ASN:HD22	2:E:36:ARG:HD2	1.66	0.59
2:H:311:GLN:CA	2:H:311:GLN:HE21	2.15	0.59
2:G:174:GLU:C	2:G:211:GLN:HB2	2.22	0.59
2:H:108:VAL:HG21	2:H:294:HIS:CD2	2.36	0.59
2:H:264:ARG:NE	2:H:265:GLY:H	1.99	0.59
2:H:169:ASP:O	2:H:218:ILE:HG13	2.02	0.59
2:F:389:ASN:HD22	2:F:391:GLY:H	1.51	0.59
2:G:312:ILE:HG12	2:G:313:ALA:N	2.18	0.59
2:F:340:PHE:O	2:F:344:LEU:HD22	2.03	0.59
1:A:39:ASN:OD1	2:E:143:TRP:CZ2	2.55	0.59
2:G:311:GLN:CA	2:G:311:GLN:HE21	2.15	0.59
1:J:38:TYR:HB2	1:J:64:LEU:CD1	2.33	0.59
2:G:152:PRO:O	2:G:154:ALA:C	2.41	0.59
2:F:351:ILE:N	2:F:351:ILE:HD13	2.13	0.59
1:J:6:VAL:HG12	1:J:7:ARG:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:10:GLY:HA2	1:L:173:TYR:CZ	2.38	0.59
2:H:335:LEU:HD22	2:H:339:ASP:HB3	1.84	0.59
2:E:174:GLU:HA	2:E:212:LYS:HB3	1.83	0.59
1:I:17:ASP:HA	1:I:165:PHE:O	2.03	0.59
1:J:62:ARG:HA	1:J:65:GLU:HG3	1.83	0.59
2:F:65:GLU:HG3	3:F:1450:ADP:H2'	1.84	0.59
2:H:12:GLU:HG2	2:H:73:LEU:HD11	1.84	0.59
2:F:218:ILE:C	2:F:220:ASP:H	2.06	0.59
1:J:98:ALA:CB	1:J:103:SER:HB3	2.33	0.59
1:K:54:PHE:O	1:K:58:GLU:HB2	2.02	0.59
1:L:83:ARG:HH11	1:L:83:ARG:CB	2.01	0.58
2:F:130:ARG:HH21	2:F:229:GLU:HG3	1.67	0.58
1:L:8:ARG:NH2	1:L:137:LEU:HD12	2.18	0.58
2:E:89:VAL:HG12	2:E:93:GLY:HA3	1.84	0.58
2:E:96:VAL:HG11	2:E:281:LEU:HD12	1.85	0.58
2:G:145:GLN:C	2:G:147:GLU:H	2.05	0.58
1:D:14:ILE:HD11	1:D:98:ALA:HB3	1.84	0.58
2:F:366:ILE:HD12	2:F:418:ILE:HB	1.84	0.58
1:C:100:GLU:OE2	1:C:173:TYR:HB2	2.04	0.58
1:L:57:PHE:O	1:L:61:GLU:HG2	2.02	0.58
2:E:142:ASN:HB2	2:E:149:GLN:HE22	1.67	0.58
2:F:131:ILE:HD11	2:F:218:ILE:HD13	1.83	0.58
1:B:86:ARG:HA	1:B:89:ARG:NH1	2.18	0.58
2:E:124:GLU:HA	2:E:127:ALA:CB	2.33	0.58
2:E:362:GLU:HG2	2:E:410:ALA:HB1	1.84	0.58
2:H:401:ARG:NH2	2:H:442:ILE:HG13	2.18	0.58
1:A:90:LYS:NZ	1:B:89:ARG:NH2	2.51	0.58
2:G:58:PRO:HG2	2:G:61:VAL:HG11	1.84	0.58
2:G:116:ILE:O	2:G:120:ARG:HB2	2.03	0.58
2:E:89:VAL:HA	2:E:93:GLY:N	2.17	0.58
1:L:143:SER:OG	1:L:146:GLU:HG3	2.03	0.58
2:E:382:GLN:O	2:E:386:SER:HB3	2.03	0.58
1:B:115:PRO:HG3	1:B:120:ILE:HG12	1.85	0.58
1:L:14:ILE:HD12	1:L:43:ILE:HG12	1.85	0.58
1:D:159:CYS:HB3	1:D:162:THR:HB	1.84	0.58
2:F:389:ASN:C	2:F:389:ASN:HD22	2.06	0.58
2:G:389:ASN:HD22	2:G:390:ILE:N	2.02	0.58
1:L:15:ALA:HB1	1:L:152:LEU:HD12	1.86	0.58
2:G:217:LYS:HG3	2:G:219:LYS:HZ1	1.69	0.58
2:E:132:LEU:HD11	2:E:160:ARG:CG	2.32	0.58
2:H:345:THR:HG21	2:H:373:ILE:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:LYS:HA	1:D:76:VAL:HG12	1.85	0.58
1:C:30:ASN:H	1:C:30:ASN:ND2	2.01	0.58
1:A:149:GLU:HG2	1:A:168:ILE:HD11	1.85	0.58
1:K:59:LEU:HD11	1:K:63:LYS:HE2	1.86	0.58
1:D:67:HIS:CD2	1:D:73:LYS:HE2	2.38	0.58
1:I:117:ASN:O	1:I:118:ASP:HB2	2.03	0.58
1:B:141:GLU:HA	1:B:141:GLU:OE2	2.04	0.58
2:H:351:ILE:H	2:H:351:ILE:CD1	2.07	0.57
2:F:123:ALA:CA	2:F:127:ALA:HB3	2.33	0.57
1:L:64:LEU:O	1:L:69:GLY:N	2.36	0.57
2:F:76:ALA:HB1	2:F:250:HIS:O	2.03	0.57
2:E:222:MET:O	2:E:226:ILE:HG12	2.04	0.57
2:H:52:ASN:HB2	2:H:325:ARG:O	2.04	0.57
2:G:92:VAL:HG21	2:H:92:VAL:CA	2.34	0.57
1:D:170:GLU:HG2	1:D:171:LEU:H	1.69	0.57
1:A:67:HIS:CD2	1:A:73:LYS:HD2	2.38	0.57
2:F:413:LEU:O	2:F:416:GLN:HG3	2.03	0.57
2:G:31:LEU:HD12	2:G:70:LEU:CD2	2.34	0.57
2:F:311:GLN:CA	2:F:311:GLN:HE21	2.17	0.57
2:E:172:GLU:HG3	2:E:214:ARG:O	2.05	0.57
2:E:389:ASN:ND2	2:E:389:ASN:C	2.56	0.57
2:G:131:ILE:O	2:G:134:VAL:HG12	2.04	0.57
2:G:170:ASP:CB	2:G:217:LYS:HD3	2.34	0.57
2:F:218:ILE:C	2:F:220:ASP:N	2.57	0.57
1:J:60:PHE:CD1	1:J:78:LEU:HD22	2.39	0.57
1:A:10:GLY:HA3	1:A:174:LYS:CA	2.33	0.57
1:A:12:VAL:HG12	1:A:171:LEU:HB3	1.86	0.57
1:J:38:TYR:CD2	1:J:41:LYS:HD2	2.39	0.57
1:B:159:CYS:HB3	1:B:162:THR:HB	1.87	0.57
2:E:131:ILE:CD1	2:E:218:ILE:HG12	2.31	0.57
2:F:151:GLU:CB	2:F:152:PRO:CD	2.82	0.57
2:G:122:ARG:NH1	2:G:126:LEU:HD21	2.20	0.57
2:F:140:LYS:O	2:F:141:ASN:HB3	2.05	0.57
1:A:37:LEU:HD21	1:A:57:PHE:HB3	1.86	0.57
1:B:60:PHE:HD1	1:B:78:LEU:HD22	1.69	0.57
1:C:71:LEU:HD12	1:C:104:LEU:HD21	1.86	0.57
2:H:211:GLN:HE21	2:H:212:LYS:H	1.52	0.57
2:F:223:LYS:HA	2:F:226:ILE:CG1	2.31	0.57
2:F:108:VAL:C	2:F:110:MET:N	2.58	0.57
2:F:258:ILE:HG22	2:F:307:SER:O	2.05	0.57
2:G:257:GLU:O	2:G:257:GLU:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:145:GLN:HG3	2:G:148:GLN:HG3	1.87	0.57
2:G:130:ARG:HB2	2:G:130:ARG:CZ	2.35	0.57
2:H:145:GLN:HE21	2:H:145:GLN:CA	2.17	0.57
2:G:240:LYS:HE3	2:G:294:HIS:O	2.04	0.57
2:H:432:LEU:HD12	2:H:432:LEU:N	2.18	0.57
1:A:86:ARG:HA	1:A:89:ARG:NH2	2.20	0.57
2:H:103:LEU:O	2:H:107:ALA:HB2	2.04	0.57
1:D:28:LYS:NZ	1:D:30:ASN:ND2	2.52	0.57
1:C:10:GLY:HA2	1:C:173:TYR:CZ	2.39	0.57
2:G:293:LYS:HG3	2:G:294:HIS:HD2	1.68	0.57
2:H:168:LEU:HD12	2:H:217:LYS:HD2	1.87	0.57
2:E:145:GLN:HG3	2:E:148:GLN:HG3	1.86	0.57
1:D:46:PHE:CE2	1:D:53:ALA:HB2	2.39	0.57
2:G:312:ILE:HG12	2:G:313:ALA:H	1.69	0.57
2:F:145:GLN:HB2	2:F:148:GLN:CG	2.35	0.57
1:C:7:ARG:HB2	1:C:12:VAL:HG23	1.87	0.57
2:G:441:PHE:HA	2:H:315:PRO:HG2	1.87	0.57
1:I:4:VAL:HG11	1:I:129:ALA:HB1	1.86	0.57
2:H:171:LYS:HZ2	2:H:218:ILE:HD11	1.67	0.56
1:A:65:GLU:OE1	2:E:141:ASN:HB2	2.05	0.56
1:C:105:ILE:HD11	1:C:120:ILE:HG23	1.87	0.56
2:F:52:ASN:HB2	2:F:325:ARG:O	2.05	0.56
2:F:89:VAL:HA	2:F:92:VAL:O	2.05	0.56
2:E:170:ASP:HB3	2:E:217:LYS:HD3	1.87	0.56
1:B:8:ARG:NH1	1:B:142:LEU:O	2.39	0.56
1:I:88:LEU:CD1	1:I:88:LEU:H	2.18	0.56
2:G:174:GLU:CB	2:G:211:GLN:HG3	2.21	0.56
1:L:28:LYS:HD3	1:L:31:VAL:HG22	1.88	0.56
2:G:27:VAL:HG13	2:G:70:LEU:HG	1.88	0.56
2:G:269:GLY:N	2:G:270:PRO:HD2	2.21	0.56
1:B:152:LEU:HD13	1:B:166:HIS:CE1	2.40	0.56
2:G:122:ARG:NE	2:G:126:LEU:HD21	2.21	0.56
1:A:88:LEU:N	1:A:88:LEU:HD12	2.21	0.56
2:G:147:GLU:HA	2:G:150:GLN:CG	2.34	0.56
2:F:168:LEU:O	2:F:217:LYS:HD2	2.04	0.56
2:G:4:MET:HE1	2:G:73:LEU:HD11	1.88	0.56
1:D:68:GLN:O	1:D:70:HIS:N	2.38	0.56
2:H:228:GLU:O	2:H:232:LYS:HE2	2.05	0.56
2:G:211:GLN:HG2	2:G:212:LYS:N	2.18	0.56
2:E:148:GLN:HA	2:E:151:GLU:HG2	1.87	0.56
2:H:351:ILE:N	2:H:351:ILE:HD13	2.10	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:86:PHE:O	2:G:89:VAL:HG22	2.06	0.56
2:G:89:VAL:HG12	2:G:93:GLY:CA	2.35	0.56
2:G:88:GLU:CD	2:H:90:GLY:HA3	2.26	0.56
2:F:211:GLN:HE21	2:F:212:LYS:N	2.03	0.56
1:J:63:LYS:HA	1:J:66:MET:HE3	1.86	0.56
1:J:59:LEU:HG	1:J:78:LEU:HD13	1.88	0.56
1:K:86:ARG:HA	1:K:89:ARG:HH12	1.69	0.56
1:I:150:LYS:O	1:I:154:ILE:HG12	2.04	0.56
2:E:257:GLU:HG3	2:E:257:GLU:O	2.06	0.56
2:E:131:ILE:HD11	2:E:218:ILE:CD1	2.35	0.56
1:C:136:LEU:HB3	1:C:147:ILE:CD1	2.35	0.56
1:J:120:ILE:HD12	1:J:120:ILE:N	2.21	0.56
2:E:86:PHE:O	2:E:89:VAL:HG22	2.05	0.56
2:G:312:ILE:N	2:G:312:ILE:HD13	2.18	0.56
2:H:108:VAL:C	2:H:110:MET:N	2.58	0.56
2:H:244:ILE:HD11	2:H:294:HIS:O	2.06	0.56
1:J:98:ALA:HB2	1:J:103:SER:HB3	1.87	0.56
2:H:389:ASN:HD22	2:H:390:ILE:N	2.03	0.55
2:E:311:GLN:NE2	2:E:311:GLN:HA	2.21	0.55
2:E:109:LYS:HG3	2:E:109:LYS:O	2.05	0.55
2:F:32:ARG:O	2:F:36:ARG:HG3	2.06	0.55
2:G:60:GLY:N	2:G:393:ARG:NH2	2.54	0.55
2:G:92:VAL:HG21	2:H:92:VAL:N	2.20	0.55
2:G:89:VAL:HA	2:G:93:GLY:N	2.22	0.55
2:H:312:ILE:HG12	2:H:313:ALA:N	2.21	0.55
2:F:130:ARG:HG2	2:F:225:LEU:HD11	1.88	0.55
2:E:108:VAL:HG21	2:E:294:HIS:ND1	2.22	0.55
2:E:108:VAL:C	2:E:110:MET:H	2.09	0.55
2:G:37:ARG:HB3	2:G:37:ARG:HH11	1.72	0.55
1:I:33:LYS:HA	1:I:46:PHE:CE1	2.41	0.55
2:F:151:GLU:HB2	2:F:152:PRO:HD2	1.88	0.55
1:L:109:ASN:O	1:L:110:GLY:C	2.45	0.55
2:G:52:ASN:HB2	2:G:325:ARG:O	2.06	0.55
2:E:160:ARG:HH12	2:E:164:ARG:HH22	1.52	0.55
2:E:130:ARG:CG	2:E:225:LEU:HD11	2.36	0.55
2:E:211:GLN:O	2:E:212:LYS:HB2	2.06	0.55
2:H:64:THR:HG21	2:H:68:ARG:NH1	2.21	0.55
1:A:149:GLU:OE1	1:A:168:ILE:HD11	2.06	0.55
1:B:150:LYS:O	1:B:154:ILE:HG12	2.07	0.55
2:E:242:ASP:HA	2:E:245:ASP:OD1	2.06	0.55
2:E:212:LYS:CD	2:E:216:LEU:HD21	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:171:LYS:HZ2	2:F:218:ILE:HD11	1.72	0.55
1:I:105:ILE:HD11	1:I:120:ILE:HG23	1.89	0.55
1:L:8:ARG:HG2	1:L:9:ASN:ND2	2.22	0.55
1:L:83:ARG:HB3	1:L:83:ARG:CZ	2.36	0.55
1:A:87:MET:HE3	1:B:84:THR:O	2.06	0.55
2:E:441:PHE:CZ	2:F:314:LYS:HG2	2.42	0.55
2:E:151:GLU:CB	2:E:152:PRO:CD	2.84	0.55
2:F:219:LYS:C	2:F:223:LYS:HD3	2.27	0.55
1:A:33:LYS:HA	1:A:46:PHE:CE1	2.42	0.55
1:K:51:ALA:HB3	1:L:110:GLY:O	2.07	0.55
2:H:151:GLU:HB2	2:H:152:PRO:CD	2.37	0.54
1:B:72:VAL:O	1:B:75:ALA:HB3	2.07	0.54
1:K:86:ARG:HG3	1:K:89:ARG:HH22	1.71	0.54
2:F:174:GLU:C	2:F:211:GLN:HB2	2.28	0.54
2:H:211:GLN:HE21	2:H:212:LYS:N	2.05	0.54
1:J:59:LEU:O	1:J:59:LEU:HD12	2.06	0.54
2:H:41:ASN:C	2:H:41:ASN:HD22	2.10	0.54
2:E:134:VAL:HG13	2:E:171:LYS:HD3	1.88	0.54
2:E:152:PRO:CB	2:E:156:ARG:HB2	2.29	0.54
2:F:390:ILE:O	2:F:393:ARG:HB2	2.07	0.54
2:E:165:GLU:HG2	2:E:166:GLY:N	2.23	0.54
2:G:131:ILE:CD1	2:G:218:ILE:HG12	2.37	0.54
1:D:86:ARG:HA	1:D:89:ARG:NH2	2.22	0.54
2:H:217:LYS:HB2	2:H:217:LYS:HZ3	1.72	0.54
2:F:389:ASN:HD22	2:F:390:ILE:N	2.05	0.54
2:E:103:LEU:HD13	2:E:247:VAL:HG13	1.90	0.54
1:L:37:LEU:HB2	1:L:61:GLU:OE1	2.07	0.54
2:H:362:GLU:HG3	2:H:411:SER:HA	1.88	0.54
2:G:442:ILE:HG22	2:G:442:ILE:O	2.07	0.54
2:H:174:GLU:CA	2:H:212:LYS:HB3	2.38	0.54
1:J:71:LEU:HD11	1:J:104:LEU:HD21	1.90	0.54
1:D:143:SER:OG	1:D:146:GLU:HG3	2.06	0.54
2:G:147:GLU:CA	2:G:150:GLN:HG3	2.37	0.54
2:E:212:LYS:NZ	2:E:212:LYS:HB2	2.21	0.54
2:E:147:GLU:HA	2:E:150:GLN:CG	2.36	0.54
2:H:122:ARG:NH1	2:H:126:LEU:HD23	2.12	0.54
2:G:264:ARG:CZ	2:G:265:GLY:H	2.20	0.54
2:G:145:GLN:O	2:G:147:GLU:N	2.41	0.54
2:G:132:LEU:HB3	2:G:156:ARG:NH1	2.23	0.54
2:H:135:LEU:CD2	2:H:171:LYS:HE2	2.29	0.54
1:K:5:SER:HB3	1:K:120:ILE:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:89:VAL:HG11	2:H:94:LYS:O	2.07	0.54
2:H:167:GLN:NE2	2:H:219:LYS:NZ	2.56	0.54
2:G:127:ALA:HA	2:G:130:ARG:HH22	1.73	0.54
2:G:168:LEU:HD12	2:G:219:LYS:HB3	1.89	0.54
2:F:135:LEU:HD23	2:F:171:LYS:HE2	1.89	0.54
1:C:149:GLU:CD	1:C:168:ILE:HD11	2.27	0.54
2:H:12:GLU:HG2	2:H:73:LEU:CD1	2.38	0.54
2:H:413:LEU:O	2:H:416:GLN:HG3	2.08	0.54
1:J:13:VAL:HG12	1:J:170:GLU:HG3	1.90	0.54
1:C:43:ILE:O	1:C:43:ILE:HG13	2.08	0.54
2:F:345:THR:HG22	2:F:352:THR:HG21	1.89	0.54
2:H:96:VAL:HG21	2:H:280:ASP:HB3	1.90	0.54
1:D:70:HIS:CE1	1:D:72:VAL:HB	2.43	0.54
1:B:3:ILE:HB	1:B:122:ILE:HG12	1.90	0.54
2:H:210:LYS:HD3	2:H:210:LYS:N	2.23	0.54
2:F:432:LEU:N	2:F:432:LEU:HD12	2.22	0.54
1:C:91:LEU:O	1:C:91:LEU:HD12	2.07	0.54
1:K:64:LEU:HD23	1:K:74:ALA:HB3	1.89	0.54
2:F:167:GLN:O	2:F:168:LEU:HB3	2.07	0.53
1:A:28:LYS:HZ3	1:A:30:ASN:ND2	2.05	0.53
2:G:359:MET:HE1	2:H:36:ARG:NH1	2.21	0.53
1:L:30:ASN:ND2	1:L:30:ASN:N	2.50	0.53
2:H:340:PHE:O	2:H:344:LEU:HD22	2.07	0.53
1:D:30:ASN:ND2	1:D:30:ASN:N	2.55	0.53
2:G:134:VAL:CG1	2:G:171:LYS:HD3	2.38	0.53
1:L:73:LYS:HZ2	1:L:77:GLU:HG2	1.73	0.53
2:E:335:LEU:HD22	2:E:339:ASP:HB3	1.90	0.53
2:E:134:VAL:CG1	2:E:171:LYS:HD3	2.39	0.53
1:I:10:GLY:HA3	1:I:174:LYS:CA	2.34	0.53
1:J:70:HIS:HE1	1:J:72:VAL:HB	1.73	0.53
1:D:99:ASP:OD1	1:D:101:THR:N	2.40	0.53
1:D:43:ILE:HD12	1:D:171:LEU:HD22	1.91	0.53
1:D:73:LYS:HZ2	1:D:77:GLU:HG2	1.71	0.53
1:I:109:ASN:O	1:I:110:GLY:C	2.46	0.53
1:J:3:ILE:HB	1:J:122:ILE:HG12	1.91	0.53
1:B:10:GLY:HA2	1:B:173:TYR:CZ	2.43	0.53
2:F:239:LEU:HD23	2:F:240:LYS:N	2.23	0.53
2:H:119:ASN:ND2	2:H:233:LEU:HD23	2.24	0.53
2:E:217:LYS:HG3	2:E:219:LYS:NZ	2.23	0.53
2:H:33:ASN:ND2	2:H:36:ARG:HD2	2.24	0.53
2:H:420:ILE:N	2:H:420:ILE:HD12	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:ARG:HA	1:B:89:ARG:HE	1.72	0.53
2:E:441:PHE:CE2	2:F:314:LYS:HG2	2.44	0.53
2:G:268:SER:HA	2:G:271:ASP:OD2	2.09	0.53
1:L:68:GLN:O	1:L:70:HIS:N	2.41	0.53
1:K:115:PRO:HB2	1:K:119:LEU:O	2.08	0.53
2:F:173:ILE:HD13	2:F:173:ILE:N	2.23	0.53
1:C:64:LEU:HB3	1:C:69:GLY:HA2	1.90	0.53
1:I:125:GLY:HA2	1:I:128:TYR:CD2	2.43	0.53
2:E:34:ARG:CZ	2:E:250:HIS:HA	2.38	0.53
2:H:223:LYS:N	2:H:223:LYS:HD2	2.23	0.53
1:A:13:VAL:CG1	1:A:170:GLU:HG3	2.29	0.53
1:K:148:ALA:O	1:K:152:LEU:HB2	2.09	0.53
2:F:269:GLY:N	2:F:270:PRO:HD2	2.22	0.53
2:E:58:PRO:HG2	2:E:61:VAL:HG11	1.91	0.53
2:F:315:PRO:O	2:F:318:LEU:HB2	2.08	0.53
1:I:80:LYS:O	1:I:84:THR:HG22	2.09	0.53
1:K:91:LEU:O	1:K:91:LEU:HD12	2.09	0.53
2:H:145:GLN:C	2:H:147:GLU:H	2.12	0.53
2:H:91:TYR:O	2:H:92:VAL:HG22	2.08	0.53
1:J:71:LEU:CD1	1:J:104:LEU:HD21	2.37	0.53
1:I:87:MET:HE3	1:J:84:THR:O	2.09	0.53
2:G:349:ALA:CB	2:H:44:LEU:HD23	2.39	0.53
1:K:17:ASP:HA	1:K:165:PHE:O	2.09	0.53
2:H:255:ILE:HD11	2:H:304:PHE:HD2	1.74	0.53
1:B:104:LEU:N	1:B:104:LEU:HD23	2.23	0.53
2:F:103:LEU:CD1	2:F:247:VAL:HG13	2.38	0.53
1:A:10:GLY:HA2	1:A:173:TYR:CD1	2.42	0.53
1:K:83:ARG:HG3	1:K:109:ASN:O	2.09	0.53
1:L:6:VAL:HG21	1:L:147:ILE:CG2	2.38	0.53
1:L:10:GLY:HA2	1:L:173:TYR:CE1	2.43	0.53
2:G:432:LEU:HD12	2:G:432:LEU:N	2.23	0.53
2:G:94:LYS:HA	2:G:94:LYS:CE	2.30	0.53
2:F:41:ASN:HD21	2:F:44:LEU:H	1.57	0.53
1:L:58:GLU:O	1:L:61:GLU:HB2	2.09	0.53
2:E:432:LEU:N	2:E:432:LEU:HD12	2.22	0.53
2:E:361:THR:HG21	2:F:36:ARG:HA	1.90	0.53
2:H:358:LEU:O	2:H:361:THR:HB	2.08	0.53
2:E:81:VAL:HG11	2:E:99:ILE:HG12	1.90	0.53
2:H:5:THR:O	2:H:9:ILE:HG12	2.09	0.53
1:J:95:LEU:HD12	1:J:95:LEU:H	1.74	0.53
1:D:83:ARG:HD3	1:D:109:ASN:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:PRO:HG3	1:D:120:ILE:CG1	2.39	0.53
1:C:152:LEU:HD13	1:C:166:HIS:ND1	2.24	0.53
2:G:104:THR:HG21	2:G:292:THR:HG21	1.91	0.53
1:K:30:ASN:H	1:K:30:ASN:HD22	1.57	0.53
1:D:56:LEU:HD13	1:D:95:LEU:HD11	1.91	0.53
1:D:115:PRO:HB2	1:D:119:LEU:O	2.09	0.53
2:F:103:LEU:O	2:F:107:ALA:HB2	2.09	0.53
2:F:375:ARG:HB3	2:F:425:VAL:HG11	1.91	0.53
1:J:53:ALA:C	1:J:55:THR:H	2.11	0.53
1:L:36:ARG:HH11	1:L:36:ARG:HB3	1.74	0.53
2:F:54:LEU:HD12	2:F:306:ALA:HB3	1.90	0.53
1:B:136:LEU:HB3	1:B:147:ILE:CD1	2.39	0.53
2:G:132:LEU:HD11	2:G:160:ARG:CG	2.39	0.52
1:I:88:LEU:HD12	1:I:88:LEU:H	1.74	0.52
2:F:89:VAL:HA	2:F:92:VAL:C	2.30	0.52
2:H:122:ARG:HA	2:H:122:ARG:NE	2.25	0.52
1:L:54:PHE:O	1:L:58:GLU:HB2	2.09	0.52
2:H:21:ASP:O	2:H:24:LYS:HB2	2.08	0.52
2:G:150:GLN:O	2:G:153:SER:HB2	2.09	0.52
2:H:160:ARG:HG2	2:H:160:ARG:HH11	1.74	0.52
2:G:168:LEU:HA	2:G:219:LYS:CB	2.39	0.52
2:F:147:GLU:HG3	2:F:150:GLN:NE2	2.24	0.52
1:I:67:HIS:HD2	1:I:73:LYS:HD2	1.71	0.52
2:E:372:GLY:O	2:E:376:ILE:HG13	2.09	0.52
2:F:5:THR:O	2:F:9:ILE:HG12	2.08	0.52
1:J:10:GLY:HA2	1:J:173:TYR:CZ	2.43	0.52
2:G:127:ALA:HA	2:G:130:ARG:NH2	2.24	0.52
2:G:92:VAL:HG21	2:H:91:TYR:O	2.09	0.52
1:L:28:LYS:NZ	1:L:30:ASN:ND2	2.57	0.52
2:F:73:LEU:HG	2:F:73:LEU:O	2.10	0.52
1:I:28:LYS:NZ	1:I:30:ASN:ND2	2.58	0.52
1:D:36:ARG:C	1:D:37:LEU:HD23	2.30	0.52
1:I:90:LYS:NZ	1:J:89:ARG:NH2	2.58	0.52
2:F:12:GLU:HG2	2:F:73:LEU:HD13	1.92	0.52
2:G:147:GLU:CG	2:G:150:GLN:NE2	2.73	0.52
2:G:89:VAL:HG12	2:G:93:GLY:C	2.29	0.52
2:F:256:ASP:O	2:F:257:GLU:HG2	2.10	0.52
1:I:5:SER:HB2	1:I:14:ILE:HG12	1.92	0.52
1:D:64:LEU:HD23	1:D:74:ALA:CB	2.40	0.52
2:H:152:PRO:HB2	2:H:156:ARG:HB2	1.90	0.52
1:A:152:LEU:HD13	1:A:166:HIS:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:3:ILE:HD11	1:K:46:PHE:O	2.10	0.52
1:K:28:LYS:HD3	1:K:31:VAL:HG22	1.92	0.52
1:K:83:ARG:CZ	1:K:83:ARG:HB3	2.40	0.52
2:H:396:HIS:O	2:H:400:GLU:HB2	2.10	0.52
2:E:269:GLY:N	2:E:270:PRO:HD2	2.25	0.52
2:F:119:ASN:ND2	2:F:233:LEU:HD23	2.24	0.52
1:B:38:TYR:HB2	1:B:64:LEU:HD12	1.92	0.52
1:K:91:LEU:HB3	1:L:83:ARG:HE	1.74	0.52
2:H:173:ILE:N	2:H:173:ILE:HD13	2.25	0.52
2:F:153:SER:HA	2:F:157:GLN:H	1.74	0.52
2:H:366:ILE:HD11	2:H:420:ILE:HD11	1.92	0.52
2:E:311:GLN:NE2	2:E:311:GLN:CA	2.73	0.52
2:E:401:ARG:HG2	2:E:443:LEU:HD21	1.91	0.52
2:H:269:GLY:N	2:H:270:PRO:HD2	2.23	0.52
1:K:19:GLN:HB2	1:K:163:ASN:ND2	2.24	0.52
2:F:108:VAL:HA	2:F:111:VAL:HG22	1.91	0.52
1:C:8:ARG:HG2	1:C:9:ASN:ND2	2.25	0.52
2:G:34:ARG:CZ	2:G:250:HIS:HA	2.39	0.52
2:E:214:ARG:HG2	2:E:215:LYS:H	1.76	0.51
2:G:212:LYS:NZ	2:G:212:LYS:HB2	2.25	0.51
1:A:37:LEU:CD2	1:A:57:PHE:HB3	2.40	0.51
2:F:262:CYS:SG	2:F:318:LEU:HD13	2.50	0.51
2:F:312:ILE:HG12	2:F:313:ALA:H	1.75	0.51
1:K:71:LEU:C	1:K:71:LEU:HD13	2.31	0.51
1:I:115:PRO:HG3	1:I:120:ILE:HG12	1.92	0.51
2:E:94:LYS:CE	2:E:94:LYS:HA	2.32	0.51
1:D:94:LEU:HD13	1:D:122:ILE:HB	1.93	0.51
1:J:72:VAL:O	1:J:75:ALA:HB3	2.10	0.51
1:L:73:LYS:NZ	1:L:77:GLU:HG2	2.24	0.51
2:E:153:SER:O	2:E:157:GLN:NE2	2.43	0.51
2:H:35:TRP:O	2:H:39:GLN:HG2	2.10	0.51
1:D:170:GLU:HG2	1:D:171:LEU:N	2.25	0.51
1:D:43:ILE:HD13	1:D:98:ALA:O	2.10	0.51
1:L:62:ARG:HA	1:L:65:GLU:CG	2.41	0.51
2:H:255:ILE:HD12	2:H:255:ILE:N	2.26	0.51
1:D:100:GLU:OE2	1:D:173:TYR:HB2	2.11	0.51
2:G:401:ARG:NH2	2:H:329:ARG:O	2.42	0.51
2:G:86:PHE:HA	2:G:89:VAL:HG13	1.93	0.51
2:E:217:LYS:HB3	2:E:219:LYS:HZ3	1.75	0.51
2:G:389:ASN:C	2:G:389:ASN:ND2	2.64	0.51
1:D:18:GLY:C	1:D:163:ASN:HD21	2.12	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:311:GLN:CA	2:H:311:GLN:NE2	2.74	0.51
2:G:117:GLU:OE2	2:G:120:ARG:NH2	2.41	0.51
2:H:95:GLU:H	2:H:95:GLU:CD	2.14	0.51
2:F:174:GLU:HB3	2:F:211:GLN:HB2	1.90	0.51
1:A:28:LYS:HD2	1:B:113:VAL:CG1	2.40	0.51
2:G:358:LEU:HD22	2:H:36:ARG:HB2	1.93	0.51
1:I:87:MET:CE	1:J:84:THR:HG23	2.40	0.51
2:E:362:GLU:HG2	2:E:410:ALA:CB	2.40	0.51
2:G:349:ALA:HB1	2:H:44:LEU:HD23	1.91	0.51
2:E:76:ALA:HB1	2:E:250:HIS:O	2.11	0.51
1:J:95:LEU:HD12	1:J:95:LEU:N	2.25	0.51
2:F:54:LEU:CD1	2:F:306:ALA:HB3	2.41	0.51
2:G:124:GLU:HA	2:G:127:ALA:CB	2.41	0.51
2:H:150:GLN:O	2:H:153:SER:CB	2.48	0.51
2:F:174:GLU:CA	2:F:212:LYS:HB3	2.40	0.51
2:G:122:ARG:O	2:G:126:LEU:HD23	2.11	0.51
2:H:339:ASP:O	2:H:343:ILE:HG13	2.10	0.51
2:G:412:ASP:CG	2:H:7:ARG:HE	2.14	0.51
2:E:130:ARG:HH21	2:E:130:ARG:HB2	1.71	0.51
2:G:358:LEU:HD23	2:H:36:ARG:HB3	1.92	0.51
1:J:18:GLY:HA2	1:J:33:LYS:HE3	1.91	0.51
1:B:59:LEU:HD12	1:B:59:LEU:O	2.11	0.51
1:K:85:ASP:O	1:K:89:ARG:HB2	2.11	0.51
1:I:36:ARG:O	1:I:37:LEU:HD23	2.11	0.51
2:H:217:LYS:O	2:H:220:ASP:HB2	2.11	0.51
2:G:91:TYR:C	2:G:92:VAL:HG22	2.31	0.51
2:F:292:THR:C	2:F:294:HIS:H	2.14	0.51
2:G:112:ARG:HG3	2:G:112:ARG:NH1	2.26	0.51
2:F:280:ASP:O	2:F:283:PRO:HD2	2.09	0.51
1:L:36:ARG:HH12	1:L:40:ASP:C	2.14	0.51
2:H:31:LEU:HD11	2:H:74:ALA:HB2	1.93	0.51
2:E:171:LYS:HB2	2:E:218:ILE:HG13	1.93	0.51
1:I:81:ASP:HA	1:I:84:THR:CG2	2.41	0.51
1:A:86:ARG:HA	1:A:89:ARG:CZ	2.41	0.51
2:F:20:GLN:O	2:F:24:LYS:HG3	2.10	0.51
2:E:401:ARG:HD2	2:E:432:LEU:CD2	2.41	0.51
1:J:170:GLU:HG2	1:J:171:LEU:H	1.76	0.51
1:C:36:ARG:HD3	1:C:40:ASP:OD1	2.10	0.51
2:E:23:ALA:HA	2:E:330:VAL:HG21	1.92	0.51
2:G:355:TYR:CE2	2:G:400:GLU:OE2	2.64	0.50
2:F:312:ILE:HD13	2:F:312:ILE:N	2.21	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:PHE:CE2	1:B:97:VAL:HG21	2.46	0.50
1:A:36:ARG:HH11	1:A:36:ARG:HB3	1.76	0.50
2:E:128:GLU:O	2:E:131:ILE:HG22	2.11	0.50
2:H:217:LYS:HB2	2:H:217:LYS:HZ2	1.76	0.50
2:H:345:THR:HG21	2:H:373:ILE:CD1	2.41	0.50
1:A:65:GLU:CG	2:E:141:ASN:HB3	2.41	0.50
1:D:28:LYS:HG2	1:D:30:ASN:ND2	2.26	0.50
1:K:83:ARG:CG	1:K:83:ARG:HH11	2.21	0.50
1:A:39:ASN:OD1	2:E:143:TRP:CH2	2.65	0.50
2:E:408:TYR:HA	2:F:29:ILE:CD1	2.40	0.50
2:G:357:ALA:HB1	2:H:40:LEU:HD22	1.93	0.50
2:F:351:ILE:CD1	2:F:351:ILE:H	2.14	0.50
2:E:122:ARG:NE	2:E:126:LEU:HD21	2.27	0.50
1:D:13:VAL:C	1:D:14:ILE:HD12	2.32	0.50
2:E:89:VAL:HG12	2:E:93:GLY:CA	2.41	0.50
2:F:34:ARG:CZ	2:F:250:HIS:HA	2.41	0.50
2:G:442:ILE:CG2	2:G:442:ILE:O	2.59	0.50
2:E:230:ALA:O	2:E:233:LEU:HB3	2.10	0.50
2:G:151:GLU:CB	2:G:152:PRO:CD	2.89	0.50
2:H:216:LEU:CD2	2:H:221:ALA:HB2	2.41	0.50
2:H:211:GLN:O	2:H:212:LYS:HB2	2.11	0.50
1:B:92:GLU:O	1:B:93:ALA:HB2	2.11	0.50
2:H:145:GLN:HE21	2:H:145:GLN:HA	1.77	0.50
2:G:92:VAL:CG2	2:H:92:VAL:N	2.74	0.50
2:G:355:TYR:HH	2:G:400:GLU:CD	2.15	0.50
2:F:346:GLU:HB2	2:F:347:PRO:HD3	1.94	0.50
2:F:148:GLN:HA	2:F:151:GLU:CG	2.42	0.50
1:D:28:LYS:HZ3	1:D:30:ASN:HD21	1.59	0.50
1:K:58:GLU:HG3	1:K:62:ARG:NH2	2.27	0.50
1:C:105:ILE:CD1	1:C:120:ILE:HG23	2.42	0.50
1:C:77:GLU:O	1:C:80:LYS:HB3	2.11	0.50
2:H:76:ALA:HB1	2:H:250:HIS:O	2.11	0.50
2:H:101:ARG:O	2:H:104:THR:HB	2.11	0.50
2:F:135:LEU:HD22	2:F:159:PHE:CD2	2.47	0.50
1:A:84:THR:HG23	1:A:85:ASP:N	2.26	0.50
1:J:1:THR:HB	1:J:33:LYS:HZ2	1.76	0.50
1:C:143:SER:O	1:C:147:ILE:HG12	2.11	0.50
2:H:235:ASN:HB2	2:H:236:PRO:CD	2.42	0.50
1:A:5:SER:HB3	1:A:120:ILE:HB	1.92	0.50
1:L:117:ASN:O	1:L:118:ASP:HB2	2.10	0.50
1:L:86:ARG:HA	1:L:89:ARG:HH12	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:23:ALA:HA	2:H:330:VAL:HG21	1.93	0.50
2:H:167:GLN:CD	2:H:219:LYS:HZ1	2.14	0.50
1:A:28:LYS:HE3	1:B:113:VAL:HG13	1.93	0.50
2:H:41:ASN:ND2	2:H:44:LEU:HB2	2.27	0.50
1:B:38:TYR:HB2	1:B:64:LEU:CD1	2.40	0.50
2:F:95:GLU:H	2:F:95:GLU:CD	2.15	0.50
2:G:147:GLU:HG3	2:G:150:GLN:CD	2.32	0.50
2:G:109:LYS:HD3	2:H:296:MET:O	2.12	0.50
2:F:221:ALA:O	2:F:225:LEU:HD23	2.12	0.50
1:D:145:ARG:NH1	1:D:168:ILE:HD12	2.27	0.50
2:E:91:TYR:C	2:E:92:VAL:HG22	2.32	0.50
1:C:10:GLY:HA3	1:C:174:LYS:HA	1.93	0.50
1:C:8:ARG:NH1	1:C:142:LEU:O	2.45	0.50
1:D:91:LEU:O	1:D:91:LEU:HD12	2.12	0.50
2:H:94:LYS:NZ	2:H:101:ARG:HH12	2.10	0.49
1:D:73:LYS:HZ1	1:D:77:GLU:HG2	1.76	0.49
1:L:85:ASP:HB3	1:L:88:LEU:HB2	1.93	0.49
2:F:235:ASN:OD1	2:F:238:GLU:HB2	2.12	0.49
1:A:103:SER:OG	1:A:118:ASP:HB3	2.12	0.49
2:H:131:ILE:HG21	2:H:222:MET:HE1	1.93	0.49
1:I:88:LEU:HD12	1:I:88:LEU:N	2.26	0.49
2:H:151:GLU:CB	2:H:152:PRO:CD	2.91	0.49
1:K:105:ILE:HD12	1:K:122:ILE:HG21	1.94	0.49
2:E:152:PRO:HB3	2:E:155:ALA:HB3	1.94	0.49
2:G:77:PRO:HB2	2:G:103:LEU:HD21	1.94	0.49
2:E:108:VAL:C	2:E:110:MET:N	2.63	0.49
1:J:6:VAL:HG12	1:J:7:ARG:H	1.75	0.49
1:J:10:GLY:HA2	1:J:173:TYR:CE1	2.46	0.49
1:I:84:THR:HG23	1:I:85:ASP:H	1.76	0.49
2:E:167:GLN:OE1	2:E:168:LEU:N	2.46	0.49
2:F:108:VAL:O	2:F:110:MET:N	2.45	0.49
1:B:53:ALA:O	1:B:55:THR:N	2.45	0.49
1:L:37:LEU:HD13	1:L:57:PHE:HB3	1.93	0.49
1:I:4:VAL:CG1	1:I:129:ALA:HB1	2.42	0.49
1:I:30:ASN:ND2	1:I:30:ASN:H	2.11	0.49
2:H:270:PRO:O	2:H:274:ARG:HD2	2.11	0.49
2:G:382:GLN:O	2:G:386:SER:HB3	2.12	0.49
2:E:318:LEU:O	2:E:323:GLN:NE2	2.44	0.49
2:H:352:THR:HG22	2:H:353:VAL:N	2.27	0.49
1:A:18:GLY:HA2	1:A:33:LYS:HE3	1.94	0.49
1:C:12:VAL:HG12	1:C:171:LEU:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:108:VAL:C	2:G:110:MET:H	2.16	0.49
1:J:28:LYS:HZ1	1:J:30:ASN:ND2	2.10	0.49
1:C:28:LYS:HG2	1:C:30:ASN:ND2	2.27	0.49
2:E:382:GLN:HA	2:E:382:GLN:NE2	2.27	0.49
2:F:25:ARG:O	2:F:29:ILE:HG12	2.13	0.49
2:E:95:GLU:OE1	2:E:101:ARG:NH1	2.43	0.49
2:H:135:LEU:HD13	2:H:159:PHE:HB3	1.94	0.49
2:G:103:LEU:HD13	2:G:247:VAL:HG13	1.93	0.49
2:F:384:ASN:HD21	2:F:390:ILE:HG12	1.77	0.49
1:B:71:LEU:HB2	1:B:99:ASP:OD1	2.12	0.49
2:G:362:GLU:HG3	2:G:411:SER:HA	1.95	0.49
2:H:345:THR:CG2	2:H:373:ILE:CD1	2.88	0.49
2:H:393:ARG:NH1	2:H:393:ARG:HG2	2.27	0.49
2:F:74:ALA:O	2:F:75:ASN:C	2.51	0.49
2:E:89:VAL:HG12	2:E:93:GLY:C	2.32	0.49
1:J:136:LEU:HB3	1:J:147:ILE:CD1	2.42	0.49
1:B:65:GLU:OE1	2:F:143:TRP:CE2	2.65	0.49
2:E:163:LEU:HG	2:E:163:LEU:O	2.12	0.49
2:H:147:GLU:CG	2:H:150:GLN:NE2	2.75	0.49
2:E:151:GLU:HB2	2:E:152:PRO:HD2	1.95	0.49
1:D:36:ARG:O	1:D:37:LEU:HB3	2.13	0.49
2:F:345:THR:CG2	2:F:373:ILE:HD13	2.43	0.49
2:F:140:LYS:H	2:F:140:LYS:HD3	1.78	0.49
2:H:432:LEU:HD12	2:H:432:LEU:H	1.77	0.49
1:L:86:ARG:HA	1:L:89:ARG:NH1	2.28	0.49
2:H:435:ASP:CG	2:H:438:LEU:HB2	2.32	0.49
2:G:145:GLN:C	2:G:147:GLU:N	2.66	0.49
2:G:136:ILE:O	2:G:136:ILE:CG2	2.60	0.49
2:H:292:THR:C	2:H:294:HIS:H	2.16	0.49
1:A:65:GLU:HG3	2:E:141:ASN:HB3	1.94	0.49
1:I:90:LYS:HZ1	1:J:89:ARG:NH2	2.11	0.49
2:G:131:ILE:HD11	2:G:218:ILE:CD1	2.43	0.49
2:G:31:LEU:HD12	2:G:70:LEU:HD22	1.95	0.49
1:A:103:SER:O	1:A:104:LEU:HB3	2.13	0.49
2:H:257:GLU:HB2	2:H:260:LYS:HG3	1.95	0.49
2:G:248:GLU:HG2	2:G:297:VAL:HG13	1.95	0.49
2:E:282:LEU:HD11	2:E:321:GLU:HB3	1.94	0.49
1:D:12:VAL:HG13	1:D:12:VAL:O	2.13	0.49
2:F:132:LEU:HD23	2:F:135:LEU:CD1	2.41	0.49
1:D:3:ILE:HB	1:D:122:ILE:CG1	2.41	0.49
2:F:232:LYS:HZ2	2:F:232:LYS:HB2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:384:ASN:HD21	2:H:390:ILE:HG12	1.77	0.49
1:I:5:SER:HB3	1:I:120:ILE:HB	1.94	0.49
1:J:53:ALA:O	1:J:55:THR:N	2.46	0.49
2:E:355:TYR:HE2	2:E:400:GLU:OE2	1.94	0.49
2:E:217:LYS:CB	2:E:219:LYS:HZ3	2.26	0.49
2:H:108:VAL:HA	2:H:111:VAL:CG2	2.41	0.49
1:B:64:LEU:HD23	1:B:74:ALA:CB	2.43	0.49
2:H:164:ARG:O	2:H:165:GLU:HB3	2.13	0.49
1:J:35:ARG:O	1:J:169:GLU:HG3	2.13	0.49
2:E:145:GLN:C	2:E:147:GLU:H	2.16	0.48
2:H:64:THR:CG2	2:H:68:ARG:NH1	2.76	0.48
1:L:43:ILE:HG12	1:L:43:ILE:O	2.13	0.48
1:I:109:ASN:N	1:I:109:ASN:HD22	2.09	0.48
1:A:104:LEU:HD12	1:A:104:LEU:O	2.13	0.48
2:G:132:LEU:HD11	2:G:160:ARG:HG2	1.96	0.48
2:E:171:LYS:HE3	2:E:172:GLU:N	2.27	0.48
2:H:170:ASP:HB3	2:H:217:LYS:HD3	1.95	0.48
2:G:168:LEU:HG	2:G:219:LYS:CD	2.21	0.48
1:C:83:ARG:CB	1:C:83:ARG:HH11	2.17	0.48
2:E:147:GLU:O	2:E:150:GLN:HG3	2.13	0.48
2:E:362:GLU:OE1	2:F:36:ARG:NE	2.46	0.48
1:C:5:SER:HB3	1:C:120:ILE:HB	1.95	0.48
1:A:47:ALA:HB3	1:A:94:LEU:HB2	1.95	0.48
2:F:132:LEU:CD1	2:F:160:ARG:HG3	2.31	0.48
1:L:5:SER:HB3	1:L:120:ILE:HB	1.94	0.48
1:C:60:PHE:CZ	1:C:97:VAL:HG11	2.48	0.48
2:E:256:ASP:O	2:E:257:GLU:HG2	2.12	0.48
2:G:95:GLU:CD	2:G:95:GLU:H	2.15	0.48
2:G:355:TYR:HE2	2:G:400:GLU:OE2	1.96	0.48
2:E:311:GLN:HA	2:E:311:GLN:HE21	1.77	0.48
2:G:231:ALA:C	2:G:233:LEU:N	2.67	0.48
2:E:362:GLU:HG3	2:E:411:SER:HA	1.95	0.48
2:G:211:GLN:O	2:G:212:LYS:HB2	2.13	0.48
2:G:212:LYS:C	2:G:214:ARG:H	2.15	0.48
2:F:153:SER:HB3	2:F:157:GLN:HG3	1.95	0.48
1:A:105:ILE:HD11	1:A:120:ILE:HG23	1.95	0.48
1:C:71:LEU:HD11	1:C:97:VAL:HG12	1.94	0.48
1:J:12:VAL:HG12	1:J:171:LEU:HB3	1.95	0.48
1:C:64:LEU:O	1:C:69:GLY:N	2.39	0.48
2:F:86:PHE:HB2	2:F:277:VAL:HG13	1.94	0.48
1:B:70:HIS:CE1	1:B:72:VAL:HB	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:44:ALA:HB2	1:J:97:VAL:HG23	1.96	0.48
2:G:408:TYR:CB	2:H:29:ILE:HD11	2.43	0.48
2:F:279:ARG:O	2:F:283:PRO:HD3	2.14	0.48
2:H:318:LEU:O	2:H:323:GLN:NE2	2.45	0.48
2:F:240:LYS:O	2:F:244:ILE:HD13	2.14	0.48
2:H:34:ARG:CZ	2:H:250:HIS:HA	2.44	0.48
1:A:117:ASN:O	1:A:118:ASP:HB2	2.13	0.48
1:K:49:GLY:HA2	1:L:111:ASP:OD1	2.14	0.48
2:H:140:LYS:O	2:H:141:ASN:HB3	2.14	0.48
2:E:299:THR:HA	2:E:302:ILE:CD1	2.38	0.48
2:G:361:THR:HG22	2:H:35:TRP:HZ3	1.74	0.48
2:G:361:THR:HG23	2:H:39:GLN:HG3	1.96	0.48
2:H:103:LEU:HD13	2:H:247:VAL:CG2	2.42	0.48
1:K:85:ASP:HB3	1:K:88:LEU:HB2	1.94	0.48
2:F:311:GLN:HA	2:F:311:GLN:NE2	2.29	0.48
1:A:20:ALA:HB2	1:A:31:VAL:HG21	1.94	0.48
1:L:71:LEU:HD21	1:L:97:VAL:CG1	2.44	0.48
1:L:94:LEU:CD2	1:L:107:THR:HG22	2.44	0.48
1:C:83:ARG:O	1:C:83:ARG:HG2	2.13	0.48
1:D:71:LEU:C	1:D:71:LEU:HD13	2.34	0.48
2:F:366:ILE:HD11	2:F:406:ILE:HD13	1.95	0.48
1:D:17:ASP:O	1:D:33:LYS:HD2	2.14	0.48
1:C:30:ASN:N	1:C:30:ASN:HD22	2.04	0.48
2:E:442:ILE:CG2	2:E:442:ILE:O	2.62	0.48
1:I:109:ASN:N	1:I:109:ASN:ND2	2.62	0.48
1:I:95:LEU:HB2	1:I:106:ILE:HB	1.95	0.48
2:E:240:LYS:HE3	2:E:294:HIS:O	2.13	0.48
2:G:31:LEU:HD12	2:G:70:LEU:HD21	1.96	0.48
1:J:3:ILE:HB	1:J:122:ILE:CG1	2.43	0.48
2:H:267:SER:O	2:H:271:ASP:OD2	2.32	0.48
2:H:89:VAL:HA	2:H:92:VAL:C	2.34	0.48
2:F:152:PRO:CB	2:F:156:ARG:HB2	2.43	0.48
1:B:59:LEU:HG	1:B:78:LEU:CD1	2.44	0.48
1:A:99:ASP:OD1	1:A:99:ASP:C	2.52	0.48
2:E:345:THR:HG21	2:E:373:ILE:HD13	1.95	0.48
2:E:112:ARG:HH11	2:E:112:ARG:HG3	1.78	0.48
1:B:174:LYS:HD2	1:B:174:LYS:N	2.29	0.48
2:G:221:ALA:O	2:G:225:LEU:HD23	2.14	0.47
2:H:122:ARG:CZ	2:H:122:ARG:HA	2.43	0.47
2:E:130:ARG:HG2	2:E:225:LEU:HD11	1.95	0.47
1:B:5:SER:HB3	1:B:120:ILE:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:THR:HB	1:B:33:LYS:HZ2	1.77	0.47
1:D:28:LYS:HZ2	1:D:30:ASN:ND2	2.12	0.47
2:G:222:MET:O	2:G:226:ILE:HG12	2.14	0.47
1:K:17:ASP:O	1:K:33:LYS:HD2	2.14	0.47
2:H:23:ALA:HB1	2:H:55:MET:HE2	1.96	0.47
1:I:60:PHE:CE2	1:I:97:VAL:HG21	2.49	0.47
1:I:77:GLU:HA	1:I:80:LYS:HD2	1.97	0.47
1:B:65:GLU:OE1	2:F:143:TRP:NE1	2.47	0.47
2:F:163:LEU:HD11	2:F:222:MET:HE1	1.94	0.47
2:E:170:ASP:CB	2:E:217:LYS:HD3	2.45	0.47
2:G:407:SER:OG	2:H:29:ILE:HG23	2.13	0.47
1:K:136:LEU:HB3	1:K:147:ILE:CD1	2.43	0.47
2:H:272:VAL:HA	2:H:275:GLU:HB2	1.96	0.47
2:F:23:ALA:HA	2:F:330:VAL:HG21	1.97	0.47
2:E:142:ASN:CB	2:E:149:GLN:HE22	2.27	0.47
1:D:94:LEU:HB3	1:D:122:ILE:HD12	1.96	0.47
1:B:105:ILE:HG22	1:B:106:ILE:N	2.29	0.47
2:H:103:LEU:CD1	2:H:247:VAL:HG13	2.44	0.47
1:B:170:GLU:CG	1:B:171:LEU:H	2.22	0.47
1:L:105:ILE:CD1	1:L:120:ILE:HG23	2.41	0.47
1:A:115:PRO:HG3	1:A:120:ILE:HG12	1.96	0.47
2:G:116:ILE:O	2:G:116:ILE:HG22	2.14	0.47
1:B:38:TYR:CD2	1:B:41:LYS:HD2	2.49	0.47
2:F:134:VAL:HG21	2:F:172:GLU:O	2.15	0.47
1:D:36:ARG:NH1	1:D:43:ILE:HG22	2.29	0.47
1:D:99:ASP:HA	1:D:171:LEU:CD2	2.45	0.47
2:E:401:ARG:HD2	2:E:432:LEU:HD21	1.96	0.47
1:J:98:ALA:HB2	1:J:103:SER:CB	2.45	0.47
1:K:11:HIS:HE1	1:K:174:LYS:NZ	2.11	0.47
2:H:86:PHE:HB2	2:H:277:VAL:HG13	1.95	0.47
1:A:80:LYS:O	1:A:81:ASP:C	2.52	0.47
2:H:27:VAL:CG1	2:H:70:LEU:HG	2.43	0.47
2:G:408:TYR:CA	2:H:29:ILE:HD11	2.45	0.47
2:F:235:ASN:ND2	2:F:238:GLU:OE1	2.47	0.47
2:H:167:GLN:NE2	2:H:219:LYS:HZ2	2.12	0.47
2:F:216:LEU:HG	2:F:221:ALA:HB2	1.96	0.47
2:F:219:LYS:HE3	2:F:219:LYS:HA	1.95	0.47
1:C:149:GLU:OE1	1:C:166:HIS:CD2	2.67	0.47
2:G:108:VAL:C	2:G:110:MET:N	2.67	0.47
2:H:133:ASP:O	2:H:137:PRO:HA	2.13	0.47
2:F:365:ASN:ND2	2:F:417:ASN:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:LYS:HA	1:D:174:LYS:HZ2	1.80	0.47
2:E:131:ILE:O	2:E:134:VAL:HG12	2.14	0.47
2:G:217:LYS:HB3	2:G:219:LYS:HZ3	1.80	0.47
2:G:214:ARG:HG2	2:G:215:LYS:N	2.28	0.47
2:H:147:GLU:HG3	2:H:150:GLN:NE2	2.30	0.47
2:H:94:LYS:NZ	2:H:98:SER:HB3	2.29	0.47
1:A:83:ARG:HH11	1:A:83:ARG:HG2	1.80	0.47
2:G:358:LEU:CD2	2:H:36:ARG:HB3	2.44	0.47
2:H:393:ARG:NH2	3:H:3450:ADP:O1B	2.47	0.47
2:H:356:LYS:CG	2:H:366:ILE:HG22	2.42	0.47
1:I:8:ARG:NH1	1:I:142:LEU:O	2.48	0.47
2:F:41:ASN:ND2	2:F:44:LEU:HB2	2.30	0.47
1:L:8:ARG:HH21	1:L:137:LEU:HD12	1.80	0.47
2:G:76:ALA:HB1	2:G:250:HIS:O	2.15	0.47
1:C:1:THR:N	1:C:161:TYR:O	2.47	0.47
1:C:67:HIS:ND1	1:C:67:HIS:N	2.62	0.47
1:K:68:GLN:O	1:K:70:HIS:N	2.48	0.47
2:F:62:GLY:O	2:F:66:ILE:HG13	2.15	0.47
1:K:132:ALA:HB2	1:K:154:ILE:HG21	1.97	0.47
2:E:348:ASN:O	2:E:349:ALA:HB3	2.15	0.47
2:F:435:ASP:CG	2:F:438:LEU:HB2	2.35	0.47
1:I:33:LYS:O	1:I:45:GLY:HA2	2.15	0.47
2:H:65:GLU:HG3	3:H:3450:ADP:H2'	1.97	0.47
1:J:30:ASN:HD22	1:J:30:ASN:C	2.17	0.47
1:K:36:ARG:NE	1:K:169:GLU:OE1	2.47	0.47
1:K:6:VAL:HG21	1:K:147:ILE:HG22	1.96	0.47
2:E:432:LEU:H	2:E:432:LEU:CD1	2.27	0.47
1:L:36:ARG:NH1	1:L:36:ARG:HB3	2.30	0.47
2:G:382:GLN:HA	2:G:382:GLN:NE2	2.30	0.47
1:B:51:ALA:O	1:B:52:ASP:C	2.52	0.47
2:G:74:ALA:O	2:G:75:ASN:C	2.53	0.47
2:E:171:LYS:HB3	2:E:172:GLU:H	1.53	0.47
2:E:173:ILE:HG12	2:E:212:LYS:CD	2.42	0.47
2:H:219:LYS:HA	2:H:223:LYS:HZ3	1.80	0.47
2:G:165:GLU:HG2	2:G:166:GLY:N	2.29	0.47
2:E:132:LEU:HB3	2:E:156:ARG:NH1	2.29	0.47
2:G:345:THR:CG2	2:G:373:ILE:HD13	2.43	0.47
1:B:12:VAL:HG12	1:B:171:LEU:HB3	1.97	0.47
1:D:28:LYS:CD	1:D:31:VAL:HG22	2.45	0.47
2:F:96:VAL:CG1	2:F:281:LEU:HD12	2.45	0.47
1:K:121:ALA:HB1	1:K:126:GLY:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:259:ASP:HB3	2:E:310:PHE:CZ	2.50	0.47
2:G:217:LYS:HG3	2:G:219:LYS:NZ	2.30	0.47
2:H:145:GLN:NE2	2:H:145:GLN:HA	2.30	0.47
2:E:153:SER:HA	2:E:157:GLN:HG3	1.97	0.47
2:F:60:GLY:H	2:F:393:ARG:NH2	2.12	0.47
1:A:90:LYS:HZ2	1:B:89:ARG:NH2	2.12	0.47
1:K:55:THR:O	1:K:58:GLU:HB3	2.15	0.47
2:F:358:LEU:O	2:F:361:THR:HB	2.14	0.47
1:I:3:ILE:HB	1:I:122:ILE:HG12	1.97	0.47
1:L:37:LEU:N	1:L:37:LEU:HD23	2.30	0.46
2:H:131:ILE:HG23	2:H:132:LEU:N	2.31	0.46
2:H:135:LEU:HD13	2:H:159:PHE:HD2	1.80	0.46
2:F:135:LEU:HD13	2:F:159:PHE:HD2	1.79	0.46
1:D:5:SER:HB3	1:D:120:ILE:HB	1.96	0.46
1:J:60:PHE:CE2	1:J:97:VAL:HG21	2.50	0.46
2:H:236:PRO:O	2:H:238:GLU:N	2.47	0.46
1:L:12:VAL:HG13	1:L:12:VAL:O	2.15	0.46
2:H:167:GLN:CD	2:H:219:LYS:NZ	2.68	0.46
2:G:220:ASP:O	2:G:221:ALA:C	2.53	0.46
2:H:172:GLU:O	2:H:173:ILE:HG23	2.15	0.46
1:D:3:ILE:O	1:D:121:ALA:HA	2.15	0.46
2:F:148:GLN:HA	2:F:151:GLU:HG3	1.96	0.46
2:F:102:ASP:C	2:F:104:THR:H	2.18	0.46
2:G:311:GLN:HA	2:G:311:GLN:HE21	1.80	0.46
1:A:149:GLU:CG	1:A:168:ILE:HD11	2.46	0.46
1:L:168:ILE:HG22	1:L:169:GLU:N	2.29	0.46
2:G:109:LYS:O	2:G:113:VAL:HG23	2.15	0.46
2:H:366:ILE:HG13	2:H:420:ILE:HD13	1.97	0.46
1:K:71:LEU:HD21	1:K:97:VAL:CG1	2.45	0.46
2:G:171:LYS:NZ	2:G:171:LYS:HA	2.30	0.46
2:E:409:ASP:O	2:E:410:ALA:C	2.54	0.46
2:G:60:GLY:H	2:G:393:ARG:HH22	1.62	0.46
1:A:80:LYS:O	1:A:82:TRP:N	2.49	0.46
1:J:99:ASP:OD1	1:J:101:THR:HB	2.16	0.46
2:F:130:ARG:NH2	2:F:229:GLU:HG3	2.31	0.46
2:E:240:LYS:HD3	2:E:241:GLN:N	2.29	0.46
1:K:73:LYS:HA	1:K:76:VAL:CG1	2.44	0.46
1:A:149:GLU:HG2	1:A:168:ILE:CD1	2.46	0.46
2:H:163:LEU:HD11	2:H:222:MET:CE	2.45	0.46
2:G:91:TYR:O	2:G:92:VAL:HG22	2.14	0.46
1:D:46:PHE:HA	1:D:94:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:358:LEU:CD2	2:H:36:ARG:CB	2.93	0.46
1:C:117:ASN:O	1:C:118:ASP:HB2	2.15	0.46
2:E:221:ALA:O	2:E:225:LEU:HD23	2.15	0.46
2:E:389:ASN:HD22	2:E:390:ILE:N	2.12	0.46
1:B:3:ILE:HB	1:B:122:ILE:CG1	2.45	0.46
1:K:80:LYS:HD2	1:K:80:LYS:C	2.36	0.46
2:H:86:PHE:O	2:H:89:VAL:HG22	2.16	0.46
2:F:163:LEU:HD11	2:F:222:MET:HE3	1.98	0.46
2:F:217:LYS:HG3	2:F:218:ILE:H	1.81	0.46
1:A:80:LYS:O	1:A:84:THR:HG22	2.15	0.46
1:D:83:ARG:CB	1:D:83:ARG:HH11	2.17	0.46
2:F:147:GLU:HG2	2:F:150:GLN:HE21	1.79	0.46
1:A:90:LYS:HZ1	1:B:89:ARG:NH2	2.13	0.46
1:C:28:LYS:HE2	1:D:114:GLN:O	2.16	0.46
2:E:442:ILE:O	2:E:442:ILE:HG22	2.15	0.46
2:E:234:VAL:O	2:E:236:PRO:HD3	2.15	0.46
2:G:92:VAL:CG2	2:H:92:VAL:CG1	2.80	0.46
2:H:312:ILE:HG12	2:H:313:ALA:H	1.81	0.46
2:F:223:LYS:CD	2:F:223:LYS:N	2.79	0.46
2:F:145:GLN:CA	2:F:145:GLN:HE21	2.28	0.46
2:F:362:GLU:HG2	2:F:410:ALA:C	2.36	0.46
2:F:53:ILE:HG12	2:F:328:ILE:HB	1.97	0.46
2:H:372:GLY:O	2:H:376:ILE:HG13	2.16	0.46
2:E:352:THR:HG22	2:E:353:VAL:N	2.31	0.46
1:A:17:ASP:CB	1:A:162:THR:HG23	2.46	0.46
1:C:36:ARG:HH12	1:C:40:ASP:C	2.19	0.46
2:G:95:GLU:OE1	2:G:101:ARG:NH1	2.47	0.46
2:F:169:ASP:O	2:F:218:ILE:HG13	2.15	0.45
1:D:105:ILE:HD12	1:D:122:ILE:HG21	1.98	0.45
1:K:86:ARG:HA	1:K:89:ARG:CZ	2.47	0.45
1:A:17:ASP:HB3	1:A:162:THR:HG23	1.98	0.45
1:D:62:ARG:O	1:D:65:GLU:HG2	2.16	0.45
2:H:17:ILE:HD12	2:H:17:ILE:N	2.31	0.45
2:E:436:GLU:O	2:E:439:SER:HB2	2.16	0.45
2:E:147:GLU:CA	2:E:150:GLN:HG3	2.46	0.45
2:F:236:PRO:O	2:F:238:GLU:N	2.49	0.45
2:E:308:GLY:HA3	2:E:310:PHE:CE2	2.51	0.45
1:B:95:LEU:N	1:B:95:LEU:HD12	2.31	0.45
2:G:262:CYS:SG	2:G:318:LEU:HD13	2.55	0.45
2:F:122:ARG:CZ	2:F:122:ARG:HA	2.46	0.45
2:F:212:LYS:HZ2	2:F:212:LYS:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:100:GLU:OE2	1:L:173:TYR:HB2	2.16	0.45
1:K:90:LYS:NZ	1:L:89:ARG:CZ	2.80	0.45
1:L:89:ARG:NH1	1:L:89:ARG:HB3	2.31	0.45
2:H:135:LEU:O	2:H:136:ILE:HD13	2.17	0.45
2:F:171:LYS:O	2:F:172:GLU:HB3	2.17	0.45
1:J:148:ALA:O	1:J:152:LEU:HB2	2.15	0.45
2:E:95:GLU:H	2:E:95:GLU:CD	2.20	0.45
2:F:398:VAL:HG13	2:F:429:LEU:HD13	1.97	0.45
1:C:22:LEU:C	1:C:22:LEU:HD23	2.36	0.45
1:J:71:LEU:HD13	1:J:71:LEU:C	2.37	0.45
1:J:86:ARG:HA	1:J:89:ARG:HE	1.82	0.45
1:K:73:LYS:O	1:K:76:VAL:HG12	2.16	0.45
2:G:311:GLN:HA	2:G:311:GLN:NE2	2.31	0.45
2:F:233:LEU:HD12	2:F:233:LEU:O	2.17	0.45
1:I:51:ALA:CB	1:J:111:ASP:OD2	2.65	0.45
2:E:169:ASP:O	2:E:218:ILE:CG1	2.65	0.45
2:G:173:ILE:HD11	2:G:221:ALA:HB1	1.98	0.45
2:E:312:ILE:CG1	2:E:313:ALA:H	2.27	0.45
2:G:88:GLU:CD	2:H:90:GLY:CA	2.85	0.45
2:F:160:ARG:HG2	2:F:160:ARG:HH11	1.82	0.45
1:A:95:LEU:HB2	1:A:106:ILE:HB	1.99	0.45
2:G:358:LEU:HD22	2:H:36:ARG:CB	2.46	0.45
2:F:121:TYR:O	2:F:125:GLU:HB2	2.17	0.45
1:A:10:GLY:HA2	1:A:173:TYR:CZ	2.51	0.45
1:L:62:ARG:HA	1:L:65:GLU:HG2	1.98	0.45
2:F:41:ASN:ND2	2:F:44:LEU:H	2.14	0.45
2:F:96:VAL:HG12	2:F:284:LEU:HD11	1.97	0.45
1:K:58:GLU:O	1:K:61:GLU:HB2	2.16	0.45
2:E:86:PHE:HA	2:E:89:VAL:HG13	1.98	0.45
2:F:119:ASN:HD21	2:F:233:LEU:HD23	1.81	0.45
1:J:136:LEU:HB3	1:J:147:ILE:HD12	1.97	0.45
2:G:54:LEU:HD12	2:G:306:ALA:HB3	1.98	0.45
2:G:153:SER:N	2:G:156:ARG:HB3	2.32	0.45
2:E:214:ARG:CG	2:E:215:LYS:N	2.79	0.45
1:L:64:LEU:CB	1:L:69:GLY:HA2	2.43	0.45
2:G:227:GLU:O	2:G:230:ALA:N	2.49	0.45
2:G:230:ALA:O	2:G:233:LEU:HB3	2.17	0.45
1:I:87:MET:HE1	1:J:84:THR:HA	1.98	0.45
1:J:94:LEU:HB3	1:J:122:ILE:HD12	1.98	0.45
1:B:38:TYR:CE2	1:B:41:LYS:HD2	2.52	0.45
2:E:402:LEU:HD12	2:E:428:HIS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:264:ARG:NE	2:E:265:GLY:H	2.15	0.45
1:I:85:ASP:OD1	1:I:88:LEU:HD13	2.17	0.45
2:G:216:LEU:CD1	2:G:221:ALA:HB2	2.47	0.45
1:J:60:PHE:HB2	1:J:78:LEU:HD22	1.97	0.45
1:J:70:HIS:CE1	1:J:72:VAL:HB	2.51	0.45
2:F:312:ILE:CG1	2:F:313:ALA:N	2.78	0.45
1:C:11:HIS:CE1	1:C:174:LYS:HE2	2.52	0.45
1:C:7:ARG:O	1:C:8:ARG:HB2	2.17	0.45
1:K:58:GLU:HG3	1:K:62:ARG:HH21	1.82	0.45
2:F:311:GLN:CA	2:F:311:GLN:NE2	2.80	0.45
2:H:308:GLY:HA3	2:H:310:PHE:CE2	2.52	0.45
2:E:134:VAL:HG22	2:E:134:VAL:O	2.17	0.45
1:J:104:LEU:HD23	1:J:104:LEU:N	2.31	0.45
2:E:126:LEU:O	2:E:130:ARG:NH2	2.45	0.45
1:D:73:LYS:O	1:D:76:VAL:HG12	2.17	0.45
2:G:171:LYS:HG3	2:G:218:ILE:HD11	1.98	0.45
1:I:17:ASP:O	1:I:33:LYS:HD2	2.17	0.45
2:E:65:GLU:O	2:E:69:ARG:HG2	2.17	0.45
2:E:384:ASN:HD21	2:E:390:ILE:HG12	1.82	0.45
1:C:8:ARG:O	1:C:11:HIS:HB2	2.16	0.45
2:G:140:LYS:O	2:G:141:ASN:CB	2.63	0.45
2:E:96:VAL:HG21	2:E:280:ASP:HB3	1.99	0.45
1:L:89:ARG:CB	1:L:89:ARG:NH1	2.80	0.45
2:E:53:ILE:HG22	2:E:54:LEU:N	2.32	0.45
2:G:109:LYS:HG3	2:G:109:LYS:O	2.17	0.44
2:G:130:ARG:HD2	2:G:225:LEU:CD1	2.27	0.44
2:F:211:GLN:O	2:F:212:LYS:HB2	2.17	0.44
1:A:71:LEU:O	1:A:75:ALA:N	2.49	0.44
2:E:89:VAL:HA	2:E:93:GLY:HA3	1.99	0.44
1:I:72:VAL:O	1:I:76:VAL:HG23	2.18	0.44
2:G:23:ALA:HA	2:G:330:VAL:HG21	1.99	0.44
1:A:34:VAL:HG13	1:A:44:ALA:O	2.17	0.44
2:G:152:PRO:O	2:G:154:ALA:CB	2.58	0.44
2:F:135:LEU:HB3	2:F:159:PHE:CD2	2.52	0.44
1:A:30:ASN:HD22	1:A:30:ASN:C	2.20	0.44
2:F:345:THR:CG2	2:F:373:ILE:CD1	2.95	0.44
1:I:8:ARG:HG2	1:I:9:ASN:CG	2.38	0.44
2:E:262:CYS:SG	2:E:318:LEU:HD13	2.57	0.44
1:C:156:GLY:HA2	1:C:162:THR:HG22	1.99	0.44
1:J:66:MET:C	1:J:67:HIS:ND1	2.70	0.44
1:D:98:ALA:HA	1:D:103:SER:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:ASP:HA	1:D:171:LEU:HD23	1.99	0.44
1:D:28:LYS:HZ3	1:D:30:ASN:ND2	2.15	0.44
1:K:73:LYS:CA	1:K:76:VAL:HG12	2.47	0.44
2:H:255:ILE:HD12	2:H:255:ILE:H	1.80	0.44
1:C:116:GLU:C	1:C:118:ASP:H	2.21	0.44
1:C:20:ALA:HB2	1:C:31:VAL:HG21	1.98	0.44
2:E:19:GLY:O	2:E:24:LYS:HE3	2.17	0.44
2:G:153:SER:C	2:G:157:GLN:HG3	2.37	0.44
2:E:216:LEU:HD23	2:E:216:LEU:N	2.31	0.44
2:H:167:GLN:CG	2:H:219:LYS:HZ1	2.31	0.44
2:G:165:GLU:HG2	2:G:166:GLY:H	1.82	0.44
2:F:217:LYS:HZ2	2:F:217:LYS:HB2	1.80	0.44
1:A:28:LYS:NZ	1:A:30:ASN:HD21	2.12	0.44
1:D:41:LYS:O	1:D:171:LEU:HD21	2.16	0.44
1:D:73:LYS:HD2	1:D:76:VAL:CG1	2.47	0.44
2:F:362:GLU:HG3	2:F:411:SER:HA	2.00	0.44
2:E:89:VAL:HA	2:E:93:GLY:CA	2.48	0.44
2:E:408:TYR:HD1	2:F:29:ILE:HD11	1.82	0.44
2:E:264:ARG:CZ	2:E:265:GLY:H	2.30	0.44
2:E:248:GLU:HG2	2:E:297:VAL:HG13	1.99	0.44
2:H:158:ALA:HB1	2:H:162:LYS:NZ	2.33	0.44
1:I:85:ASP:CG	1:I:88:LEU:HD13	2.37	0.44
2:H:119:ASN:OD1	2:H:234:VAL:HG23	2.16	0.44
2:G:362:GLU:HB3	2:G:364:VAL:HG23	2.00	0.44
1:D:168:ILE:HG22	1:D:169:GLU:N	2.32	0.44
2:F:150:GLN:O	2:F:153:SER:HB2	2.18	0.44
2:G:408:TYR:CE1	2:H:10:VAL:HG21	2.52	0.44
2:F:21:ASP:O	2:F:24:LYS:HB2	2.17	0.44
1:D:70:HIS:HE1	1:D:72:VAL:HB	1.83	0.44
2:E:35:TRP:O	2:E:39:GLN:HG2	2.17	0.44
1:C:121:ALA:HB1	1:C:126:GLY:O	2.18	0.44
2:H:121:TYR:O	2:H:125:GLU:HB2	2.18	0.44
2:H:214:ARG:NE	2:H:216:LEU:HB3	2.32	0.44
2:H:145:GLN:HB2	2:H:148:GLN:CG	2.46	0.44
2:E:145:GLN:HB2	2:E:148:GLN:CB	2.39	0.44
1:B:65:GLU:CD	2:F:143:TRP:NE1	2.71	0.44
1:B:65:GLU:O	2:F:143:TRP:O	2.35	0.44
2:F:172:GLU:O	2:F:173:ILE:HG23	2.18	0.44
2:E:220:ASP:HA	2:E:223:LYS:HD2	1.98	0.44
1:J:62:ARG:O	1:J:66:MET:HG3	2.18	0.44
1:D:11:HIS:HA	1:D:171:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:299:THR:O	2:H:302:ILE:HG12	2.18	0.44
1:B:59:LEU:HG	1:B:78:LEU:HD13	1.99	0.44
2:H:356:LYS:HG3	2:H:366:ILE:CG2	2.46	0.44
2:E:342:ARG:NH2	2:E:346:GLU:OE2	2.40	0.44
2:H:282:LEU:HD12	2:H:282:LEU:HA	1.76	0.44
2:H:151:GLU:HB2	2:H:152:PRO:HD2	1.99	0.44
2:F:345:THR:HG21	2:F:373:ILE:CD1	2.47	0.44
2:F:41:ASN:O	2:F:45:ARG:HG3	2.17	0.44
2:G:34:ARG:NH2	2:G:250:HIS:HA	2.32	0.44
2:H:16:HIS:HB2	2:H:17:ILE:HD12	1.99	0.44
2:F:268:SER:HA	2:F:271:ASP:OD2	2.16	0.44
2:H:167:GLN:OE1	2:H:168:LEU:N	2.51	0.44
1:I:84:THR:HG23	1:I:85:ASP:N	2.32	0.44
1:K:115:PRO:HG3	1:K:120:ILE:CG1	2.47	0.44
2:F:174:GLU:HB3	2:F:211:GLN:NE2	2.33	0.44
2:E:219:LYS:O	2:E:223:LYS:HG3	2.18	0.44
1:A:60:PHE:CE2	1:A:97:VAL:HG21	2.53	0.44
2:H:96:VAL:HG12	2:H:284:LEU:HD11	2.00	0.44
1:L:60:PHE:CZ	1:L:97:VAL:HG11	2.53	0.44
1:K:79:ALA:HB1	1:K:110:GLY:HA2	2.00	0.44
1:J:92:GLU:O	1:J:93:ALA:HB2	2.17	0.44
1:C:34:VAL:HB	1:C:167:THR:HG22	1.99	0.44
2:H:127:ALA:HB1	2:H:229:GLU:HB3	1.99	0.44
1:K:91:LEU:HB3	1:L:83:ARG:NE	2.32	0.44
2:H:102:ASP:C	2:H:104:THR:H	2.21	0.44
1:J:37:LEU:HD11	1:J:57:PHE:CD1	2.53	0.44
1:L:149:GLU:OE1	1:L:166:HIS:CD2	2.71	0.44
1:A:1:THR:HA	1:A:17:ASP:OD1	2.18	0.44
2:G:171:LYS:HB3	2:G:172:GLU:H	1.48	0.44
1:J:38:TYR:HB2	1:J:64:LEU:HD12	1.99	0.44
1:A:15:ALA:HB1	1:A:152:LEU:HD12	2.00	0.44
2:G:436:GLU:O	2:G:439:SER:HB2	2.17	0.44
2:G:255:ILE:HD13	2:G:281:LEU:HD21	2.00	0.44
1:K:143:SER:OG	1:K:146:GLU:HG3	2.18	0.44
1:A:72:VAL:O	1:A:76:VAL:HG23	2.18	0.44
2:G:126:LEU:N	2:G:126:LEU:HD22	2.33	0.43
2:G:311:GLN:CA	2:G:311:GLN:NE2	2.81	0.43
2:H:432:LEU:H	2:H:432:LEU:CD1	2.30	0.43
1:L:89:ARG:HH11	1:L:89:ARG:CB	2.31	0.43
1:D:157:ASP:OD2	1:D:164:HIS:NE2	2.37	0.43
2:F:47:GLU:OE1	2:F:47:GLU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:47:GLU:OE1	2:G:47:GLU:HA	2.18	0.43
2:G:53:ILE:HA	2:G:328:ILE:HB	2.00	0.43
2:E:169:ASP:O	2:E:218:ILE:HG13	2.18	0.43
2:E:122:ARG:NH1	2:E:126:LEU:HD21	2.33	0.43
2:H:103:LEU:HD22	2:H:103:LEU:O	2.18	0.43
1:K:60:PHE:CZ	1:K:97:VAL:HG11	2.53	0.43
2:E:91:TYR:O	2:E:92:VAL:HG22	2.18	0.43
1:A:88:LEU:N	1:A:88:LEU:CD1	2.80	0.43
1:L:37:LEU:H	1:L:37:LEU:HD23	1.83	0.43
2:E:401:ARG:CZ	2:E:442:ILE:HG23	2.48	0.43
2:H:220:ASP:O	2:H:224:LEU:N	2.44	0.43
2:F:170:ASP:HB3	2:F:217:LYS:HD3	2.00	0.43
1:D:115:PRO:HG2	1:D:118:ASP:HA	2.00	0.43
2:F:58:PRO:HG2	2:F:61:VAL:HG11	2.00	0.43
1:B:7:ARG:NE	1:B:118:ASP:OD2	2.48	0.43
2:E:12:GLU:HG2	2:E:73:LEU:HD11	2.00	0.43
2:E:74:ALA:O	2:E:75:ASN:C	2.56	0.43
1:L:17:ASP:HA	1:L:165:PHE:O	2.18	0.43
2:F:60:GLY:N	2:F:393:ARG:NH2	2.66	0.43
2:F:214:ARG:HD3	2:F:214:ARG:O	2.19	0.43
1:D:11:HIS:HE1	1:D:172:SER:OG	2.01	0.43
2:H:65:GLU:O	2:H:69:ARG:HG2	2.18	0.43
1:B:148:ALA:O	1:B:152:LEU:HB2	2.19	0.43
1:C:15:ALA:HB1	1:C:152:LEU:HD12	2.00	0.43
2:G:106:ALA:O	2:G:110:MET:HB2	2.18	0.43
1:J:64:LEU:HD23	1:J:74:ALA:CB	2.48	0.43
2:E:358:LEU:O	2:E:361:THR:HB	2.17	0.43
2:G:257:GLU:CG	2:G:257:GLU:O	2.65	0.43
1:D:104:LEU:HD22	1:D:112:VAL:HG12	2.00	0.43
2:G:273:SER:O	2:G:277:VAL:HG23	2.18	0.43
2:H:296:MET:CE	2:H:296:MET:HA	2.48	0.43
2:E:174:GLU:C	2:E:211:GLN:HB2	2.39	0.43
1:A:28:LYS:HZ1	1:A:30:ASN:ND2	2.12	0.43
2:F:129:GLU:HB2	2:F:130:ARG:HH11	1.83	0.43
2:H:96:VAL:CG1	2:H:281:LEU:HD12	2.45	0.43
2:E:79:ILE:CG2	2:E:103:LEU:HG	2.48	0.43
2:F:236:PRO:C	2:F:238:GLU:H	2.22	0.43
1:K:83:ARG:CG	1:K:83:ARG:NH1	2.80	0.43
1:K:28:LYS:CE	1:K:30:ASN:ND2	2.81	0.43
2:H:140:LYS:HD3	2:H:140:LYS:H	1.83	0.43
1:I:12:VAL:HG12	1:I:171:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:63:LYS:HG2	2:E:332:LEU:HD13	2.00	0.43
1:C:112:VAL:O	1:C:112:VAL:HG12	2.18	0.43
2:G:173:ILE:HG12	2:G:212:LYS:CD	2.45	0.43
2:H:94:LYS:HA	2:H:94:LYS:CE	2.35	0.43
2:F:91:TYR:O	2:F:92:VAL:HG22	2.19	0.43
1:J:65:GLU:HB3	2:H:143:TRP:HA	2.00	0.43
1:D:13:VAL:HG11	1:D:145:ARG:HB2	1.99	0.43
2:E:292:THR:HB	2:E:295:GLY:O	2.18	0.43
2:G:384:ASN:HD21	2:G:390:ILE:HG12	1.84	0.43
2:F:341:GLU:O	2:F:344:LEU:HB2	2.19	0.43
2:G:134:VAL:HG13	2:G:171:LYS:HD3	1.99	0.43
1:I:109:ASN:O	1:I:111:ASP:N	2.51	0.43
2:E:20:GLN:O	2:E:24:LYS:HG3	2.18	0.43
2:F:322:LEU:HA	2:F:322:LEU:HD12	1.77	0.43
2:G:282:LEU:HD11	2:G:321:GLU:HB3	2.00	0.43
2:G:212:LYS:HZ2	2:G:212:LYS:HB2	1.84	0.43
1:K:3:ILE:HB	1:K:122:ILE:CG1	2.49	0.43
1:K:46:PHE:CD2	1:K:53:ALA:HB2	2.54	0.43
2:F:159:PHE:O	2:F:163:LEU:HB2	2.18	0.43
2:H:122:ARG:HH21	2:H:122:ARG:HG2	1.84	0.43
1:B:99:ASP:OD1	1:B:101:THR:HB	2.18	0.43
1:B:99:ASP:OD2	1:B:101:THR:N	2.29	0.43
2:F:312:ILE:CG1	2:F:313:ALA:H	2.31	0.43
2:F:227:GLU:O	2:F:228:GLU:C	2.56	0.43
2:G:384:ASN:HA	2:G:384:ASN:HD22	1.61	0.43
2:G:292:THR:HG22	2:G:293:LYS:N	2.34	0.43
1:C:28:LYS:NZ	1:C:30:ASN:ND2	2.67	0.43
2:G:231:ALA:O	2:G:233:LEU:N	2.51	0.43
2:F:267:SER:O	2:F:271:ASP:OD2	2.35	0.43
2:G:96:VAL:HG11	2:G:281:LEU:HD12	2.00	0.43
2:G:342:ARG:NH2	2:G:346:GLU:OE2	2.37	0.43
2:F:388:GLU:OE2	2:F:388:GLU:N	2.52	0.43
2:H:224:LEU:O	2:H:228:GLU:HB2	2.19	0.43
2:G:165:GLU:O	2:G:167:GLN:HG3	2.18	0.43
2:E:140:LYS:O	2:E:141:ASN:CB	2.65	0.43
1:A:101:THR:O	1:A:102:ALA:HB2	2.18	0.43
2:H:236:PRO:C	2:H:238:GLU:H	2.22	0.43
2:G:108:VAL:O	2:G:110:MET:N	2.52	0.43
2:F:102:ASP:C	2:F:104:THR:N	2.71	0.43
1:C:86:ARG:HA	1:C:89:ARG:NH2	2.34	0.43
2:H:136:ILE:HD11	2:H:159:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:223:LYS:C	2:H:225:LEU:H	2.21	0.43
2:G:174:GLU:HG3	2:G:213:ALA:HA	2.01	0.43
2:F:214:ARG:HE	2:F:216:LEU:HB3	1.84	0.43
2:F:123:ALA:HB2	2:F:229:GLU:O	2.19	0.43
1:J:60:PHE:HD1	1:J:78:LEU:HD22	1.81	0.43
2:H:111:VAL:HG21	2:H:243:ALA:HB2	2.01	0.43
2:H:366:ILE:HD12	2:H:418:ILE:HB	2.00	0.43
2:F:35:TRP:O	2:F:39:GLN:HG2	2.19	0.43
1:I:145:ARG:NE	1:I:170:GLU:OE1	2.44	0.43
2:G:89:VAL:HA	2:G:92:VAL:C	2.40	0.43
1:D:37:LEU:HB2	1:D:61:GLU:OE1	2.19	0.43
2:H:108:VAL:O	2:H:110:MET:N	2.51	0.43
1:A:102:ALA:HB1	1:A:114:GLN:OE1	2.19	0.43
1:K:86:ARG:HG3	1:K:89:ARG:NH2	2.34	0.43
1:D:28:LYS:HG2	1:D:30:ASN:HD22	1.82	0.43
1:C:36:ARG:NH1	1:C:40:ASP:CA	2.82	0.43
2:G:54:LEU:HB3	2:G:329:ARG:HD3	2.01	0.43
2:G:337:THR:O	2:G:341:GLU:HG3	2.19	0.43
2:F:403:MET:SD	2:F:420:ILE:HD13	2.59	0.43
2:E:16:HIS:HB2	2:E:17:ILE:HD12	2.00	0.43
2:G:65:GLU:OE2	2:G:65:GLU:HA	2.19	0.43
1:J:67:HIS:CD2	1:J:73:LYS:HD2	2.54	0.42
2:H:79:ILE:HG21	2:H:103:LEU:HB2	2.00	0.42
1:C:85:ASP:CB	1:C:88:LEU:HD12	2.49	0.42
1:C:36:ARG:NH1	1:C:40:ASP:HB3	2.34	0.42
2:G:164:ARG:HH11	2:G:164:ARG:HA	1.83	0.42
2:G:145:GLN:HB2	2:G:148:GLN:CB	2.44	0.42
2:G:151:GLU:HB2	2:G:152:PRO:HD2	2.01	0.42
1:D:152:LEU:HB3	1:D:166:HIS:CE1	2.54	0.42
2:F:264:ARG:HE	2:F:265:GLY:H	1.64	0.42
1:C:168:ILE:HG22	1:C:169:GLU:N	2.34	0.42
2:G:170:ASP:HB3	2:G:217:LYS:CD	2.47	0.42
2:F:135:LEU:HD22	2:F:159:PHE:CE2	2.54	0.42
1:D:121:ALA:HB1	1:D:126:GLY:O	2.18	0.42
2:G:392:ALA:HB3	3:G:2450:ADP:C8	2.55	0.42
2:G:358:LEU:O	2:G:361:THR:HB	2.18	0.42
2:F:125:GLU:C	2:F:127:ALA:H	2.22	0.42
1:L:14:ILE:HD12	1:L:43:ILE:O	2.19	0.42
2:E:296:MET:HE2	2:E:296:MET:HA	2.00	0.42
2:E:116:ILE:HG22	2:E:116:ILE:O	2.18	0.42
1:K:30:ASN:H	1:K:30:ASN:ND2	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:116:GLU:C	1:L:118:ASP:H	2.22	0.42
2:E:435:ASP:OD1	2:E:438:LEU:HB2	2.19	0.42
1:C:37:LEU:HB3	1:C:61:GLU:OE1	2.19	0.42
1:A:109:ASN:N	1:A:109:ASN:HD22	2.16	0.42
2:H:174:GLU:C	2:H:212:LYS:HB3	2.40	0.42
2:E:217:LYS:O	2:E:221:ALA:N	2.36	0.42
1:D:43:ILE:H	1:D:43:ILE:CD1	2.24	0.42
2:G:140:LYS:HD3	2:G:140:LYS:N	2.33	0.42
2:E:351:ILE:HD13	2:E:396:HIS:ND1	2.34	0.42
2:H:84:THR:C	2:H:86:PHE:H	2.22	0.42
2:H:312:ILE:CG1	2:H:313:ALA:N	2.82	0.42
1:J:70:HIS:ND1	1:J:73:LYS:HB2	2.34	0.42
2:E:108:VAL:HA	2:E:111:VAL:HG22	2.01	0.42
1:K:38:TYR:HB2	1:K:64:LEU:CD1	2.50	0.42
1:C:67:HIS:O	1:C:68:GLN:C	2.57	0.42
1:K:67:HIS:O	1:K:68:GLN:C	2.57	0.42
1:D:22:LEU:HD12	1:D:27:MET:CE	2.49	0.42
2:G:163:LEU:O	2:G:163:LEU:HG	2.19	0.42
1:J:59:LEU:HD11	1:J:63:LYS:HE2	2.02	0.42
2:G:33:ASN:ND2	2:G:36:ARG:HD2	2.35	0.42
1:J:150:LYS:O	1:J:154:ILE:HG12	2.18	0.42
1:J:32:LYS:HE3	1:J:32:LYS:HB2	1.78	0.42
2:E:232:LYS:HB3	2:E:232:LYS:NZ	2.33	0.42
2:G:216:LEU:HD12	2:G:216:LEU:O	2.19	0.42
2:H:147:GLU:HG2	2:H:150:GLN:NE2	2.35	0.42
2:F:264:ARG:CZ	2:F:265:GLY:H	2.31	0.42
2:H:96:VAL:CG1	2:H:99:ILE:HD12	2.49	0.42
2:G:293:LYS:C	2:G:294:HIS:HD2	2.23	0.42
2:H:432:LEU:N	2:H:432:LEU:CD1	2.83	0.42
2:G:349:ALA:HB1	2:H:44:LEU:CD2	2.50	0.42
2:E:231:ALA:C	2:E:233:LEU:N	2.73	0.42
1:D:134:ARG:HD2	1:D:138:GLU:OE1	2.19	0.42
1:B:11:HIS:CE1	1:B:172:SER:OG	2.73	0.42
1:B:32:LYS:HE3	1:B:32:LYS:HB2	1.78	0.42
1:K:141:GLU:HA	1:K:141:GLU:OE2	2.20	0.42
1:A:86:ARG:HG2	1:A:89:ARG:HH22	1.85	0.42
1:A:28:LYS:HD2	1:B:113:VAL:HG13	2.01	0.42
1:B:104:LEU:HB2	1:B:113:VAL:O	2.19	0.42
2:E:217:LYS:HG3	2:E:219:LYS:HZ1	1.82	0.42
1:J:8:ARG:O	1:J:11:HIS:HB2	2.20	0.42
1:B:117:ASN:O	1:B:118:ASP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:40:LEU:O	2:E:45:ARG:NH1	2.53	0.42
2:E:151:GLU:C	2:E:153:SER:N	2.71	0.42
2:G:366:ILE:HA	2:G:366:ILE:HD13	1.92	0.42
1:B:53:ALA:O	1:B:56:LEU:N	2.53	0.42
1:L:89:ARG:HH11	1:L:89:ARG:HB2	1.84	0.42
1:I:6:VAL:HG12	1:I:7:ARG:N	2.35	0.42
2:G:214:ARG:HD3	2:G:216:LEU:HD23	2.02	0.42
2:H:94:LYS:HZ1	2:H:101:ARG:HH12	1.68	0.42
2:E:299:THR:CA	2:E:302:ILE:HD13	2.38	0.42
2:H:32:ARG:O	2:H:36:ARG:HG3	2.20	0.42
1:J:63:LYS:HD2	1:J:77:GLU:HB3	2.01	0.42
2:F:151:GLU:CB	2:F:152:PRO:HD3	2.50	0.42
1:D:1:THR:HB	1:D:33:LYS:NZ	2.35	0.42
1:B:6:VAL:HG12	1:B:7:ARG:N	2.34	0.42
2:H:40:LEU:O	2:H:45:ARG:NH1	2.52	0.42
2:H:342:ARG:O	2:H:346:GLU:HB2	2.20	0.42
2:E:173:ILE:N	2:E:173:ILE:CD1	2.82	0.41
2:H:218:ILE:C	2:H:220:ASP:N	2.73	0.41
2:G:174:GLU:OE2	2:G:213:ALA:HA	2.19	0.41
2:G:92:VAL:CG1	2:H:92:VAL:CG1	2.93	0.41
1:A:99:ASP:OD1	1:A:101:THR:N	2.36	0.41
1:C:95:LEU:HD12	1:C:95:LEU:N	2.35	0.41
2:G:349:ALA:CB	2:H:44:LEU:CD2	2.98	0.41
2:H:257:GLU:HB2	2:H:260:LYS:CG	2.50	0.41
2:G:161:LYS:O	2:G:164:ARG:HB2	2.19	0.41
1:C:114:GLN:O	1:C:115:PRO:O	2.38	0.41
2:H:289:THR:CG2	2:H:296:MET:HG3	2.50	0.41
2:H:135:LEU:HB3	2:H:159:PHE:HD2	1.80	0.41
1:D:43:ILE:HD13	1:D:43:ILE:N	2.25	0.41
2:G:131:ILE:HD11	2:G:218:ILE:CG1	2.49	0.41
2:E:257:GLU:O	2:E:257:GLU:CG	2.63	0.41
2:H:285:VAL:HG12	2:H:304:PHE:CD1	2.55	0.41
2:H:74:ALA:O	2:H:75:ASN:C	2.58	0.41
2:E:408:TYR:CB	2:F:29:ILE:HD11	2.50	0.41
2:H:80:LYS:HG3	2:H:254:PHE:HD1	1.85	0.41
1:C:44:ALA:HB1	1:C:57:PHE:CE1	2.55	0.41
1:D:160:ILE:HA	1:D:160:ILE:HD13	1.86	0.41
2:E:214:ARG:CD	2:E:216:LEU:HD22	2.41	0.41
2:H:148:GLN:HA	2:H:151:GLU:CG	2.44	0.41
2:G:89:VAL:HA	2:G:93:GLY:HA3	2.02	0.41
2:G:400:GLU:HG3	2:H:327:PRO:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:389:ASN:ND2	2:H:389:ASN:C	2.72	0.41
2:E:106:ALA:O	2:E:110:MET:HB2	2.20	0.41
1:C:73:LYS:HD2	1:C:76:VAL:HG11	2.02	0.41
2:E:231:ALA:C	2:E:233:LEU:H	2.22	0.41
2:G:91:TYR:CE1	2:H:91:TYR:CE2	3.09	0.41
2:H:89:VAL:HA	2:H:92:VAL:O	2.20	0.41
2:F:212:LYS:O	2:F:213:ALA:HB3	2.20	0.41
2:F:168:LEU:HD12	2:F:217:LYS:HG2	2.02	0.41
1:C:8:ARG:NH2	1:C:137:LEU:HD12	2.35	0.41
1:C:73:LYS:HA	1:C:73:LYS:HD2	1.92	0.41
2:F:311:GLN:HA	2:F:311:GLN:HE21	1.83	0.41
2:H:41:ASN:HD21	2:H:44:LEU:HB2	1.84	0.41
2:H:269:GLY:N	2:H:270:PRO:CD	2.84	0.41
2:H:355:TYR:CE1	2:H:403:MET:HE3	2.56	0.41
1:L:42:VAL:HG13	1:L:98:ALA:O	2.21	0.41
1:I:38:TYR:HE1	1:I:65:GLU:HG2	1.85	0.41
2:F:167:GLN:OE1	2:F:168:LEU:N	2.53	0.41
1:J:101:THR:HG22	1:J:102:ALA:N	2.34	0.41
2:F:223:LYS:HD2	2:F:223:LYS:H	1.84	0.41
2:F:109:LYS:O	2:F:109:LYS:HG3	2.19	0.41
2:G:408:TYR:HE1	2:H:10:VAL:HG21	1.85	0.41
1:L:3:ILE:HB	1:L:122:ILE:HG12	2.02	0.41
1:L:121:ALA:HB1	1:L:126:GLY:O	2.20	0.41
2:H:387:THR:OG1	2:H:388:GLU:N	2.53	0.41
2:G:147:GLU:O	2:G:150:GLN:HG3	2.21	0.41
2:G:113:VAL:C	2:G:115:ALA:H	2.23	0.41
2:E:312:ILE:CG1	2:E:313:ALA:N	2.81	0.41
2:F:89:VAL:HG12	2:F:93:GLY:HA3	2.02	0.41
1:B:73:LYS:HA	1:B:76:VAL:HG23	2.03	0.41
2:F:103:LEU:HD13	2:F:247:VAL:CG2	2.43	0.41
1:A:173:TYR:O	1:A:174:LYS:C	2.58	0.41
1:B:28:LYS:HZ1	1:B:30:ASN:ND2	2.17	0.41
1:B:85:ASP:O	1:B:86:ARG:C	2.59	0.41
1:K:71:LEU:HD21	1:K:97:VAL:HG12	2.02	0.41
1:J:105:ILE:HG22	1:J:106:ILE:N	2.35	0.41
2:E:296:MET:CE	2:E:296:MET:HA	2.50	0.41
1:C:152:LEU:HD22	1:C:166:HIS:CE1	2.56	0.41
2:G:12:GLU:HG2	2:G:73:LEU:CD1	2.51	0.41
2:F:94:LYS:HA	2:F:94:LYS:CE	2.29	0.41
2:F:384:ASN:HD21	2:F:394:ARG:HE	1.62	0.41
1:B:17:ASP:HB2	1:B:163:ASN:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:247:VAL:O	2:H:302:ILE:HD13	2.21	0.41
1:B:170:GLU:HG2	1:B:171:LEU:N	2.27	0.41
2:H:236:PRO:CG	2:H:237:GLU:H	2.32	0.41
2:F:375:ARG:HA	2:F:378:GLU:HB2	2.02	0.41
1:C:99:ASP:HA	1:C:171:LEU:HD22	2.01	0.41
1:L:6:VAL:HG12	1:L:7:ARG:N	2.36	0.41
2:H:268:SER:HA	2:H:271:ASP:OD2	2.20	0.41
2:F:403:MET:O	2:F:404:GLU:C	2.59	0.41
1:B:88:LEU:HD12	1:B:91:LEU:HD11	2.03	0.41
2:G:148:GLN:OE1	2:G:151:GLU:HG3	2.21	0.41
2:G:173:ILE:N	2:G:173:ILE:CD1	2.79	0.41
2:G:212:LYS:HD3	2:G:216:LEU:HD11	2.02	0.41
2:F:217:LYS:CG	2:F:218:ILE:H	2.31	0.41
1:J:99:ASP:OD1	1:J:101:THR:N	2.53	0.41
2:E:352:THR:CG2	2:E:353:VAL:N	2.84	0.41
1:B:101:THR:HG22	1:B:102:ALA:N	2.35	0.41
2:F:96:VAL:HG21	2:F:280:ASP:HB3	2.03	0.41
2:F:432:LEU:N	2:F:432:LEU:CD1	2.83	0.41
1:K:1:THR:HB	1:K:33:LYS:HZ3	1.86	0.41
2:G:107:ALA:O	2:G:111:VAL:HG22	2.20	0.41
2:H:443:LEU:HD23	2:H:443:LEU:HA	1.94	0.41
1:J:174:LYS:HD2	1:J:174:LYS:N	2.36	0.41
2:E:174:GLU:CA	2:E:212:LYS:HB3	2.51	0.41
2:H:145:GLN:H	2:H:148:GLN:HB2	1.86	0.41
2:G:92:VAL:CG2	2:H:91:TYR:O	2.69	0.41
2:E:168:LEU:HD22	2:E:219:LYS:HD3	2.02	0.41
1:D:149:GLU:CD	1:D:168:ILE:HD11	2.41	0.41
2:F:145:GLN:C	2:F:147:GLU:H	2.23	0.41
1:A:71:LEU:HD11	1:A:97:VAL:HG13	2.02	0.41
1:C:152:LEU:HD22	1:C:166:HIS:HE1	1.86	0.41
2:F:41:ASN:C	2:F:41:ASN:ND2	2.72	0.41
2:G:226:ILE:O	2:G:230:ALA:HB2	2.20	0.41
1:J:38:TYR:HB2	1:J:64:LEU:HD13	2.03	0.41
2:G:27:VAL:CG1	2:G:70:LEU:HG	2.51	0.41
1:B:6:VAL:HG21	1:B:147:ILE:HG22	2.02	0.41
1:D:64:LEU:HA	1:D:74:ALA:HB2	2.03	0.41
2:E:408:TYR:CD1	2:F:29:ILE:HD11	2.55	0.41
2:E:285:VAL:HG12	2:E:304:PHE:CD1	2.56	0.41
2:H:402:LEU:HD12	2:H:428:HIS:HB2	2.03	0.41
2:E:135:LEU:HB3	2:E:159:PHE:CD2	2.55	0.41
1:A:3:ILE:HB	1:A:122:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:223:LYS:C	2:H:225:LEU:N	2.74	0.41
2:H:220:ASP:C	2:H:224:LEU:HD23	2.42	0.41
1:I:88:LEU:N	1:I:88:LEU:CD1	2.82	0.41
2:H:145:GLN:NE2	2:H:145:GLN:CA	2.84	0.41
1:A:82:TRP:CH2	1:A:95:LEU:HD13	2.56	0.41
2:H:174:GLU:HB3	2:H:211:GLN:NE2	2.36	0.41
1:J:59:LEU:C	1:J:59:LEU:HD12	2.40	0.41
1:L:28:LYS:HG2	1:L:30:ASN:ND2	2.36	0.41
2:E:292:THR:C	2:E:294:HIS:H	2.24	0.41
2:H:293:LYS:HG3	2:H:294:HIS:CE1	2.56	0.41
1:J:12:VAL:CG1	1:J:171:LEU:HB3	2.50	0.41
1:J:53:ALA:C	1:J:55:THR:N	2.75	0.41
1:I:28:LYS:HZ1	1:I:30:ASN:ND2	2.18	0.41
1:D:80:LYS:O	1:D:80:LYS:HD2	2.21	0.41
1:C:59:LEU:HD23	1:C:78:LEU:HD12	2.03	0.41
2:G:167:GLN:OE1	2:G:168:LEU:N	2.53	0.40
2:F:384:ASN:ND2	2:F:390:ILE:H	2.19	0.40
2:G:312:ILE:CG1	2:G:313:ALA:N	2.84	0.40
1:B:71:LEU:O	1:B:72:VAL:C	2.60	0.40
2:E:65:GLU:HG3	3:E:450:ADP:H2'	2.02	0.40
2:F:61:VAL:C	3:F:1450:ADP:N7	2.74	0.40
2:H:235:ASN:OD1	2:H:238:GLU:HB2	2.20	0.40
1:C:28:LYS:HG2	1:C:30:ASN:HD22	1.86	0.40
2:H:336:THR:H	2:H:339:ASP:HB2	1.86	0.40
2:H:270:PRO:O	2:H:273:SER:HB3	2.21	0.40
1:A:109:ASN:N	1:A:109:ASN:ND2	2.69	0.40
2:E:440:ARG:HB3	2:F:316:SER:OG	2.20	0.40
2:E:215:LYS:HG3	2:E:215:LYS:O	2.21	0.40
2:F:122:ARG:NE	2:F:122:ARG:HA	2.36	0.40
2:E:149:GLN:C	2:E:151:GLU:H	2.25	0.40
2:E:151:GLU:HB2	2:E:152:PRO:CD	2.51	0.40
1:A:83:ARG:NH1	1:A:83:ARG:HG2	2.36	0.40
1:D:60:PHE:CZ	1:D:97:VAL:HG11	2.56	0.40
2:H:384:ASN:HA	2:H:384:ASN:HD22	1.60	0.40
1:L:114:GLN:O	1:L:115:PRO:O	2.39	0.40
2:E:240:LYS:HD3	2:E:240:LYS:C	2.41	0.40
2:F:108:VAL:HG12	2:F:109:LYS:N	2.35	0.40
1:C:109:ASN:O	1:C:110:GLY:C	2.60	0.40
1:L:85:ASP:CB	1:L:88:LEU:HD12	2.52	0.40
1:I:30:ASN:HD22	1:I:30:ASN:C	2.25	0.40
1:I:171:LEU:HD12	1:I:171:LEU:HA	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:253:VAL:HB	2:E:304:PHE:CD2	2.56	0.40
1:B:34:VAL:HA	1:B:45:GLY:HA2	2.03	0.40
2:E:128:GLU:O	2:E:129:GLU:C	2.60	0.40
2:H:160:ARG:HG2	2:H:160:ARG:NH1	2.36	0.40
2:H:168:LEU:HD12	2:H:217:LYS:CD	2.49	0.40
2:E:220:ASP:O	2:E:221:ALA:C	2.59	0.40
2:H:366:ILE:HG13	2:H:420:ILE:CD1	2.51	0.40
1:B:66:MET:O	1:B:67:HIS:ND1	2.54	0.40
2:G:408:TYR:CE1	2:H:25:ARG:HG2	2.55	0.40
2:G:131:ILE:HG21	2:G:222:MET:HE3	2.03	0.40
1:C:105:ILE:HD12	1:C:122:ILE:CG2	2.52	0.40
2:G:339:ASP:O	2:G:343:ILE:HG13	2.22	0.40
2:F:253:VAL:HB	2:F:304:PHE:CD2	2.57	0.40
2:H:22:ASN:HA	2:H:22:ASN:HD22	1.66	0.40
1:C:62:ARG:HA	1:C:65:GLU:OE2	2.21	0.40
2:G:145:GLN:HG3	2:G:148:GLN:CG	2.50	0.40
2:F:168:LEU:O	2:F:168:LEU:HG	2.21	0.40
2:E:108:VAL:O	2:E:110:MET:N	2.55	0.40
1:D:26:VAL:HG12	1:D:28:LYS:O	2.22	0.40
1:B:168:ILE:CD1	1:B:168:ILE:N	2.84	0.40
1:J:6:VAL:CG1	1:J:7:ARG:N	2.83	0.40
1:J:43:ILE:HG12	1:J:98:ALA:O	2.21	0.40
1:B:94:LEU:HB3	1:B:122:ILE:HD12	2.03	0.40
2:E:355:TYR:CE2	2:E:400:GLU:OE2	2.73	0.40
1:I:13:VAL:HG12	1:I:170:GLU:HG3	2.03	0.40
1:I:124:SER:HB3	1:I:159:CYS:SG	2.62	0.40
1:B:107:THR:C	1:B:109:ASN:N	2.75	0.40
2:G:234:VAL:O	2:G:236:PRO:HD3	2.22	0.40
2:E:145:GLN:C	2:E:147:GLU:N	2.75	0.40
2:F:229:GLU:O	2:F:230:ALA:HB2	2.22	0.40
2:F:219:LYS:HA	2:F:223:LYS:HZ3	1.86	0.40
1:B:66:MET:C	1:B:67:HIS:ND1	2.75	0.40
1:L:88:LEU:O	1:L:91:LEU:HG	2.22	0.40
1:L:95:LEU:N	1:L:95:LEU:HD12	2.36	0.40
2:F:12:GLU:HG2	2:F:73:LEU:HD11	2.02	0.40
2:G:432:LEU:HD12	2:G:432:LEU:H	1.87	0.40
1:B:107:THR:O	1:B:109:ASN:N	2.54	0.40
1:A:137:LEU:O	1:A:137:LEU:HD23	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:7:ARG:NH2	2:F:409:ASP:OD2[2_665]	2.01	0.19
1:K:160:ILE:CG2	1:K:160:ILE:CG2[4_666]	2.04	0.16
1:D:160:ILE:CG2	1:D:160:ILE:CG2[6_577]	2.19	0.01

## 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	172/175 (98%)	152 (88%)	16 (9%)	4 (2%)	8	26
1	B	172/175 (98%)	137 (80%)	25 (14%)	10 (6%)	2	5
1	C	172/175 (98%)	150 (87%)	17 (10%)	5 (3%)	6	19
1	D	172/175 (98%)	145 (84%)	23 (13%)	4 (2%)	8	26
1	I	172/175 (98%)	147 (86%)	20 (12%)	5 (3%)	6	19
1	J	172/175 (98%)	140 (81%)	26 (15%)	6 (4%)	4	15
1	K	172/175 (98%)	146 (85%)	23 (13%)	3 (2%)	11	36
1	L	172/175 (98%)	149 (87%)	18 (10%)	5 (3%)	6	19
2	E	404/449 (90%)	348 (86%)	47 (12%)	9 (2%)	8	28
2	F	404/449 (90%)	344 (85%)	43 (11%)	17 (4%)	3	11
2	G	404/449 (90%)	344 (85%)	48 (12%)	12 (3%)	5	18
2	H	404/449 (90%)	343 (85%)	45 (11%)	16 (4%)	4	12
All	All	2992/3196 (94%)	2545 (85%)	351 (12%)	96 (3%)	5	17

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	71	LEU
1	B	72	VAL
1	B	116	GLU
2	E	92	VAL
2	E	144	GLY

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Mol	Chain	Res	Type
2	E	153	SER
2	E	212	LYS
2	F	92	VAL
2	F	153	SER
2	F	165	GLU
2	F	212	LYS
2	F	237	GLU
1	C	116	GLU
1	D	69	GLY
1	J	116	GLU
2	G	92	VAL
2	G	144	GLY
2	G	146	THR
2	G	153	SER
2	G	212	LYS
2	H	92	VAL
2	H	153	SER
2	H	165	GLU
2	H	212	LYS
2	H	236	PRO
2	H	237	GLU
1	L	116	GLU
1	A	9	ASN
1	B	54	PHE
2	E	165	GLU
2	E	410	ALA
2	F	230	ALA
2	F	236	PRO
2	F	300	ASP
1	D	68	GLN
1	D	113	VAL
1	J	54	PHE
2	G	165	GLU
2	G	170	ASP
2	H	138	PRO
2	H	154	ALA
2	H	228	GLU
2	H	230	ALA
2	H	300	ASP
1	K	68	GLN
1	K	69	GLY
1	K	116	GLU

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Mol	Chain	Res	Type
1	L	69	GLY
1	A	115	PRO
1	B	68	GLN
2	E	141	ASN
2	E	146	THR
2	F	138	PRO
1	C	115	PRO
1	C	117	ASN
1	I	71	LEU
1	I	115	PRO
1	J	71	LEU
1	J	101	THR
2	G	141	ASN
2	G	227	GLU
2	G	232	LYS
2	H	143	TRP
2	H	146	THR
1	L	115	PRO
1	A	71	LEU
1	A	81	ASP
1	B	70	HIS
2	E	217	LYS
2	F	109	LYS
2	F	125	GLU
2	F	137	PRO
1	I	110	GLY
1	I	142	LEU
1	J	68	GLN
2	G	44	LEU
2	G	172	GLU
2	H	125	GLU
1	L	117	ASN
2	F	140	LYS
2	F	228	GLU
1	D	99	ASP
2	H	137	PRO
1	B	69	GLY
1	B	82	TRP
1	B	86	ARG
2	F	146	THR
2	F	154	ALA
1	C	40	ASP

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Mol	Chain	Res	Type
1	L	110	GLY
1	C	69	GLY
2	H	144	GLY
2	F	173	ILE
1	J	72	VAL
1	B	147	ILE
1	I	72	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	136/136 (100%)	127 (93%)	9 (7%)	21	51
1	B	136/136 (100%)	123 (90%)	13 (10%)	10	29
1	C	136/136 (100%)	125 (92%)	11 (8%)	15	39
1	D	136/136 (100%)	122 (90%)	14 (10%)	9	26
1	I	136/136 (100%)	126 (93%)	10 (7%)	17	43
1	J	136/136 (100%)	125 (92%)	11 (8%)	15	39
1	K	136/136 (100%)	125 (92%)	11 (8%)	15	39
1	L	136/136 (100%)	125 (92%)	11 (8%)	15	39
2	E	350/383 (91%)	310 (89%)	40 (11%)	7	21
2	F	350/383 (91%)	300 (86%)	50 (14%)	4	12
2	G	350/383 (91%)	306 (87%)	44 (13%)	5	17
2	H	350/383 (91%)	302 (86%)	48 (14%)	4	13
All	All	2488/2620 (95%)	2216 (89%)	272 (11%)	8	23

All (272) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	9	ASN
1	A	30	ASN

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Mol	Chain	Res	Type
1	A	36	ARG
1	A	65	GLU
1	A	71	LEU
1	A	97	VAL
1	A	136	LEU
1	A	152	LEU
1	B	1	THR
1	B	8	ARG
1	B	22	LEU
1	B	30	ASN
1	B	54	PHE
1	B	99	ASP
1	B	104	LEU
1	B	112	VAL
1	B	116	GLU
1	B	136	LEU
1	B	152	LEU
1	B	160	ILE
1	B	174	LYS
2	E	11	SER
2	E	13	LEU
2	E	27	VAL
2	E	31	LEU
2	E	37	ARG
2	E	59	THR
2	E	92	VAL
2	E	94	LYS
2	E	103	LEU
2	E	117	GLU
2	E	122	ARG
2	E	130	ARG
2	E	140	LYS
2	E	152	PRO
2	E	167	GLN
2	E	169	ASP
2	E	171	LYS
2	E	173	ILE
2	E	220	ASP
2	E	238	GLU
2	E	240	LYS
2	E	241	GLN
2	E	266	GLU

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Mol	Chain	Res	Type
2	E	281	LEU
2	E	296	MET
2	E	300	ASP
2	E	311	GLN
2	E	312	ILE
2	E	318	LEU
2	E	326	LEU
2	E	337	THR
2	E	352	THR
2	E	355	TYR
2	E	375	ARG
2	E	385	GLU
2	E	386	SER
2	E	388	GLU
2	E	389	ASN
2	E	411	SER
2	E	412	ASP
2	F	13	LEU
2	F	27	VAL
2	F	31	LEU
2	F	37	ARG
2	F	41	ASN
2	F	59	THR
2	F	68	ARG
2	F	70	LEU
2	F	87	THR
2	F	94	LYS
2	F	103	LEU
2	F	104	THR
2	F	108	VAL
2	F	121	TYR
2	F	130	ARG
2	F	140	LYS
2	F	141	ASN
2	F	145	GLN
2	F	148	GLN
2	F	150	GLN
2	F	165	GLU
2	F	173	ILE
2	F	210	LYS
2	F	211	GLN
2	F	214	ARG

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Mol	Chain	Res	Type
2	F	217	LYS
2	F	219	LYS
2	F	220	ASP
2	F	225	LEU
2	F	232	LYS
2	F	239	LEU
2	F	266	GLU
2	F	296	MET
2	F	300	ASP
2	F	311	GLN
2	F	312	ILE
2	F	318	LEU
2	F	326	LEU
2	F	337	THR
2	F	344	LEU
2	F	351	ILE
2	F	352	THR
2	F	355	TYR
2	F	382	GLN
2	F	385	GLU
2	F	389	ASN
2	F	404	GLU
2	F	413	LEU
2	F	438	LEU
2	F	442	ILE
1	C	1	THR
1	C	30	ASN
1	C	36	ARG
1	C	37	LEU
1	C	54	PHE
1	C	67	HIS
1	C	71	LEU
1	C	81	ASP
1	C	87	MET
1	C	99	ASP
1	C	152	LEU
1	D	1	THR
1	D	30	ASN
1	D	35	ARG
1	D	39	ASN
1	D	43	ILE
1	D	73	LYS

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Mol	Chain	Res	Type
1	D	77	GLU
1	D	80	LYS
1	D	104	LEU
1	D	114	GLN
1	D	116	GLU
1	D	118	ASP
1	D	136	LEU
1	D	152	LEU
1	I	1	THR
1	I	4	VAL
1	I	30	ASN
1	I	36	ARG
1	I	71	LEU
1	I	99	ASP
1	I	116	GLU
1	I	152	LEU
1	I	160	ILE
1	I	166	HIS
1	J	1	THR
1	J	22	LEU
1	J	30	ASN
1	J	54	PHE
1	J	65	GLU
1	J	97	VAL
1	J	112	VAL
1	J	136	LEU
1	J	152	LEU
1	J	160	ILE
1	J	174	LYS
2	G	13	LEU
2	G	27	VAL
2	G	31	LEU
2	G	37	ARG
2	G	49	THR
2	G	70	LEU
2	G	92	VAL
2	G	94	LYS
2	G	117	GLU
2	G	122	ARG
2	G	130	ARG
2	G	140	LYS
2	G	148	GLN

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Mol	Chain	Res	Type
2	G	152	PRO
2	G	164	ARG
2	G	165	GLU
2	G	168	LEU
2	G	169	ASP
2	G	171	LYS
2	G	173	ILE
2	G	216	LEU
2	G	220	ASP
2	G	225	LEU
2	G	238	GLU
2	G	240	LYS
2	G	241	GLN
2	G	266	GLU
2	G	296	MET
2	G	300	ASP
2	G	311	GLN
2	G	312	ILE
2	G	318	LEU
2	G	326	LEU
2	G	337	THR
2	G	344	LEU
2	G	352	THR
2	G	353	VAL
2	G	355	TYR
2	G	370	ASP
2	G	385	GLU
2	G	386	SER
2	G	388	GLU
2	G	389	ASN
2	G	438	LEU
2	H	13	LEU
2	H	27	VAL
2	H	31	LEU
2	H	41	ASN
2	H	59	THR
2	H	70	LEU
2	H	87	THR
2	H	94	LYS
2	H	103	LEU
2	H	104	THR
2	H	121	TYR

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Mol	Chain	Res	Type
2	H	130	ARG
2	H	138	PRO
2	H	140	LYS
2	H	141	ASN
2	H	145	GLN
2	H	148	GLN
2	H	150	GLN
2	H	152	PRO
2	H	160	ARG
2	H	169	ASP
2	H	173	ILE
2	H	210	LYS
2	H	211	GLN
2	H	214	ARG
2	H	217	LYS
2	H	219	LYS
2	H	238	GLU
2	H	239	LEU
2	H	266	GLU
2	H	296	MET
2	H	300	ASP
2	H	311	GLN
2	H	312	ILE
2	H	318	LEU
2	H	326	LEU
2	H	337	THR
2	H	344	LEU
2	H	351	ILE
2	H	352	THR
2	H	375	ARG
2	H	384	ASN
2	H	388	GLU
2	H	389	ASN
2	H	404	GLU
2	H	413	LEU
2	H	438	LEU
2	H	442	ILE
1	K	1	THR
1	K	30	ASN
1	K	40	ASP
1	K	54	PHE
1	K	80	LYS

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Mol	Chain	Res	Type
1	K	83	ARG
1	K	104	LEU
1	K	111	ASP
1	K	116	GLU
1	K	136	LEU
1	K	152	LEU
1	L	1	THR
1	L	30	ASN
1	L	36	ARG
1	L	37	LEU
1	L	43	ILE
1	L	54	PHE
1	L	73	LYS
1	L	116	GLU
1	L	118	ASP
1	L	152	LEU
1	L	174	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	39	ASN
1	A	109	ASN
1	A	166	HIS
1	B	11	HIS
1	B	30	ASN
1	B	109	ASN
1	B	130	GLN
2	E	22	ASN
2	E	33	ASN
2	E	75	ASN
2	E	114	GLN
2	E	141	ASN
2	E	149	GLN
2	E	150	GLN
2	E	241	GLN
2	E	294	HIS
2	E	311	GLN
2	E	348	ASN
2	E	382	GLN
2	E	384	ASN

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Mol	Chain	Res	Type
2	E	389	ASN
2	E	416	GLN
2	E	428	HIS
2	F	22	ASN
2	F	41	ASN
2	F	75	ASN
2	F	114	GLN
2	F	119	ASN
2	F	141	ASN
2	F	142	ASN
2	F	145	GLN
2	F	149	GLN
2	F	150	GLN
2	F	211	GLN
2	F	311	GLN
2	F	348	ASN
2	F	384	ASN
2	F	389	ASN
2	F	416	GLN
1	C	9	ASN
1	C	30	ASN
1	D	11	HIS
1	D	30	ASN
1	D	114	GLN
1	I	9	ASN
1	I	30	ASN
1	I	39	ASN
1	I	109	ASN
1	J	30	ASN
1	J	109	ASN
1	J	130	GLN
2	G	22	ASN
2	G	33	ASN
2	G	75	ASN
2	G	114	GLN
2	G	149	GLN
2	G	150	GLN
2	G	241	GLN
2	G	294	HIS
2	G	311	GLN
2	G	348	ASN
2	G	382	GLN

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Mol	Chain	Res	Type
2	G	384	ASN
2	G	389	ASN
2	G	416	GLN
2	G	428	HIS
2	H	22	ASN
2	H	33	ASN
2	H	41	ASN
2	H	75	ASN
2	H	114	GLN
2	H	119	ASN
2	H	142	ASN
2	H	145	GLN
2	H	149	GLN
2	H	150	GLN
2	H	167	GLN
2	H	211	GLN
2	H	311	GLN
2	H	348	ASN
2	H	384	ASN
2	H	389	ASN
2	H	416	GLN
2	H	428	HIS
1	K	30	ASN
1	K	39	ASN
1	K	114	GLN
1	L	9	ASN
1	L	11	HIS
1	L	30	ASN
1	L	114	GLN
1	L	139	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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



## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	ADP	E	450	-	22,29,29	1.60	6 (27%)	27,45,45	2.21	5 (18%)
3	ADP	F	1450	-	22,29,29	1.46	4 (18%)	27,45,45	2.07	5 (18%)
3	ADP	G	2450	-	22,29,29	1.54	6 (27%)	27,45,45	2.15	5 (18%)
3	ADP	H	3450	-	22,29,29	1.54	5 (22%)	27,45,45	2.13	5 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	E	450	-	-	0/12/32/32	0/3/3/3
3	ADP	F	1450	-	-	0/12/32/32	0/3/3/3
3	ADP	G	2450	-	-	0/12/32/32	0/3/3/3
3	ADP	H	3450	-	-	0/12/32/32	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	450	ADP	C8-N7	-3.95	1.27	1.34
3	H	3450	ADP	C8-N7	-3.91	1.27	1.34
3	G	2450	ADP	C8-N7	-3.78	1.27	1.34
3	F	1450	ADP	C8-N7	-3.69	1.27	1.34
3	E	450	ADP	PA-O1A	-2.35	1.42	1.51
3	E	450	ADP	PA-O2A	-2.17	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2450	ADP	PA-O2A	-2.13	1.45	1.54
3	H	3450	ADP	PA-O1A	-2.08	1.43	1.51
3	F	1450	ADP	PB-O3B	-2.07	1.47	1.54
3	G	2450	ADP	PB-O3B	-2.04	1.47	1.54
3	F	1450	ADP	C2-N3	2.22	1.36	1.32
3	G	2450	ADP	C2-N3	2.25	1.36	1.32
3	G	2450	ADP	O4'-C1'	2.32	1.44	1.41
3	F	1450	ADP	C4-N3	2.34	1.39	1.35
3	H	3450	ADP	O4'-C1'	2.35	1.44	1.41
3	E	450	ADP	C2-N3	2.35	1.36	1.32
3	E	450	ADP	C4-N3	2.37	1.39	1.35
3	G	2450	ADP	C4-N3	2.42	1.39	1.35
3	H	3450	ADP	C2-N3	2.44	1.36	1.32
3	E	450	ADP	O4'-C1'	2.47	1.44	1.41
3	H	3450	ADP	C4-N3	2.62	1.39	1.35

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	450	ADP	C2'-C1'-N9	-5.41	106.03	114.29
3	H	3450	ADP	N3-C2-N1	-5.27	124.86	128.89
3	F	1450	ADP	N3-C2-N1	-5.09	125.00	128.89
3	G	2450	ADP	N3-C2-N1	-4.98	125.08	128.89
3	E	450	ADP	N3-C2-N1	-4.82	125.20	128.89
3	G	2450	ADP	C2'-C1'-N9	-4.25	107.79	114.29
3	H	3450	ADP	C2'-C1'-N9	-3.85	108.41	114.29
3	F	1450	ADP	C2'-C1'-N9	-3.65	108.71	114.29
3	F	1450	ADP	O3A-PA-O5'	2.61	109.85	102.94
3	G	2450	ADP	O3A-PA-O5'	2.82	110.41	102.94
3	H	3450	ADP	O3A-PA-O5'	2.88	110.58	102.94
3	F	1450	ADP	C2'-C3'-C4'	2.92	108.61	102.61
3	E	450	ADP	C2'-C3'-C4'	2.96	108.70	102.61
3	E	450	ADP	O3A-PA-O5'	3.00	110.91	102.94
3	H	3450	ADP	C2'-C3'-C4'	3.04	108.86	102.61
3	G	2450	ADP	C2'-C3'-C4'	3.05	108.88	102.61
3	E	450	ADP	C4'-O4'-C1'	6.68	117.05	109.72
3	F	1450	ADP	C4'-O4'-C1'	6.75	117.13	109.72
3	H	3450	ADP	C4'-O4'-C1'	6.76	117.15	109.72
3	G	2450	ADP	C4'-O4'-C1'	6.88	117.28	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	450	ADP	2	0
3	F	1450	ADP	3	0
3	G	2450	ADP	2	0
3	H	3450	ADP	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	174/175 (99%)	0.19	3 (1%) 73 63	33, 58, 91, 99	0
1	B	174/175 (99%)	0.78	14 (8%) 15 7	38, 70, 101, 102	0
1	C	174/175 (99%)	0.39	8 (4%) 36 25	51, 68, 98, 101	0
1	D	174/175 (99%)	0.67	13 (7%) 17 9	54, 87, 101, 102	0
1	I	174/175 (99%)	0.15	3 (1%) 73 63	29, 56, 89, 97	0
1	J	174/175 (99%)	0.50	5 (2%) 55 43	36, 70, 100, 102	0
1	K	174/175 (99%)	0.78	20 (11%) 6 3	62, 95, 102, 102	0
1	L	174/175 (99%)	0.56	8 (4%) 36 25	57, 80, 102, 102	0
2	E	408/449 (90%)	0.72	60 (14%) 3 2	32, 59, 102, 102	0
2	F	408/449 (90%)	1.28	91 (22%) 1 1	35, 61, 102, 102	0
2	G	408/449 (90%)	0.82	63 (15%) 3 1	35, 62, 102, 102	0
2	H	408/449 (90%)	1.16	87 (21%) 1 1	35, 63, 102, 102	0
All	All	3024/3196 (94%)	0.77	375 (12%) 5 2	29, 66, 102, 102	0

All (375) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	144	GLY	13.1
2	G	144	GLY	12.4
2	H	141	ASN	11.8
2	F	141	ASN	11.0
2	F	145	GLN	10.9
2	F	146	THR	10.8
2	E	144	GLY	10.5
2	H	144	GLY	10.3
2	H	146	THR	9.0
2	G	90	GLY	8.8
2	F	222	MET	8.7

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Mol	Chain	Res	Type	RSRZ
2	G	145	GLN	8.3
2	F	264	ARG	8.1
2	F	143	TRP	8.1
2	F	90	GLY	7.9
2	F	153	SER	7.9
2	G	153	SER	7.9
2	H	145	GLN	7.8
2	H	154	ALA	7.8
2	F	169	ASP	7.6
2	H	91	TYR	7.5
2	H	168	LEU	7.4
2	E	143	TRP	7.3
2	F	219	LYS	7.2
2	H	139	ALA	7.2
2	G	140	LYS	7.2
2	H	169	ASP	7.1
2	H	153	SER	7.0
2	F	139	ALA	6.9
2	H	170	ASP	6.9
2	F	151	GLU	6.8
2	E	140	LYS	6.8
2	F	89	VAL	6.8
2	E	90	GLY	6.8
2	F	91	TYR	6.7
2	F	165	GLU	6.7
2	G	143	TRP	6.6
2	H	89	VAL	6.6
2	H	134	VAL	6.6
2	F	140	LYS	6.5
2	H	90	GLY	6.5
2	F	134	VAL	6.4
2	E	267	SER	6.4
2	E	89	VAL	6.3
2	H	143	TRP	6.2
2	E	145	GLN	6.2
2	E	91	TYR	6.1
2	G	91	TYR	6.1
2	G	267	SER	6.1
2	G	265	GLY	6.0
2	F	133	ASP	6.0
2	F	211	GLN	5.9
2	H	221	ALA	5.9

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Mol	Chain	Res	Type	RSRZ
2	F	266	GLU	5.9
2	F	128	GLU	5.8
2	H	152	PRO	5.8
2	H	210	LYS	5.8
2	F	226	ILE	5.8
2	H	123	ALA	5.8
2	E	264	ARG	5.8
2	F	173	ILE	5.7
2	F	170	ASP	5.7
2	H	267	SER	5.6
2	H	227	GLU	5.6
2	F	265	GLY	5.6
2	H	138	PRO	5.6
2	E	153	SER	5.5
2	F	154	ALA	5.5
2	F	92	VAL	5.5
2	H	117	GLU	5.5
2	F	125	GLU	5.5
2	E	148	GLN	5.4
2	F	147	GLU	5.4
2	E	142	ASN	5.4
2	G	264	ARG	5.3
1	D	173	TYR	5.3
2	H	165	GLU	5.2
2	H	140	LYS	5.2
2	E	141	ASN	5.2
2	H	211	GLN	5.2
2	F	267	SER	5.2
2	G	147	GLU	5.1
2	G	146	THR	5.1
2	E	139	ALA	5.1
2	F	138	PRO	5.0
2	H	226	ILE	5.0
2	F	124	GLU	4.9
2	F	152	PRO	4.9
2	F	130	ARG	4.9
2	H	166	GLY	4.9
2	G	141	ASN	4.9
2	H	130	ARG	4.9
2	H	132	LEU	4.9
2	G	215	LYS	4.9
2	G	148	GLN	4.9

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Mol	Chain	Res	Type	RSRZ
2	H	142	ASN	4.9
2	E	146	THR	4.9
2	H	264	ARG	4.8
2	F	132	LEU	4.8
1	K	174	LYS	4.8
2	G	266	GLU	4.8
2	F	168	LEU	4.7
2	E	265	GLY	4.7
2	G	139	ALA	4.6
2	F	1	HIS	4.6
2	F	228	GLU	4.6
2	F	221	ALA	4.5
2	H	167	GLN	4.5
2	G	123	ALA	4.5
2	H	222	MET	4.5
2	H	223	LYS	4.4
2	E	266	GLU	4.4
2	G	170	ASP	4.4
2	G	219	LYS	4.4
2	E	218	ILE	4.4
2	F	88	GLU	4.4
2	G	214	ARG	4.4
2	H	151	GLU	4.3
2	H	266	GLU	4.3
2	F	214	ARG	4.3
2	E	147	GLU	4.3
2	F	155	ALA	4.3
2	H	124	GLU	4.3
2	G	210	LYS	4.2
2	F	119	ASN	4.2
2	F	129	GLU	4.2
1	K	173	TYR	4.2
2	G	89	VAL	4.2
2	H	150	GLN	4.2
2	F	210	LYS	4.2
2	H	219	LYS	4.2
2	F	167	GLN	4.1
2	F	123	ALA	4.1
2	F	215	LYS	4.1
2	H	128	GLU	4.1
2	E	210	LYS	4.1
2	H	173	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
2	G	112	ARG	4.1
2	F	223	LYS	4.0
2	H	217	LYS	4.0
2	G	117	GLU	3.9
2	E	215	LYS	3.9
2	F	112	ARG	3.9
2	F	137	PRO	3.9
1	C	90	LYS	3.9
2	H	92	VAL	3.9
2	E	112	ARG	3.9
2	H	265	GLY	3.8
2	F	227	GLU	3.8
1	L	68	GLN	3.8
2	G	212	LYS	3.8
1	L	91	LEU	3.8
2	F	220	ASP	3.8
2	H	136	ILE	3.8
2	H	214	ARG	3.7
2	E	170	ASP	3.7
2	H	88	GLU	3.7
2	F	117	GLU	3.6
2	E	151	GLU	3.6
2	F	126	LEU	3.6
2	G	171	LYS	3.6
2	H	215	LYS	3.6
2	E	219	LYS	3.6
2	F	113	VAL	3.6
2	E	134	VAL	3.6
2	E	117	GLU	3.6
2	H	1	HIS	3.6
2	F	131	ILE	3.6
2	G	165	GLU	3.6
2	H	218	ILE	3.6
1	D	90	LYS	3.5
2	E	211	GLN	3.5
1	K	111	ASP	3.5
2	H	147	GLU	3.5
2	F	172	GLU	3.5
2	F	216	LEU	3.5
2	G	134	VAL	3.5
1	L	90	LYS	3.5
2	G	270	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
2	H	133	ASP	3.4
2	H	224	LEU	3.3
1	D	11	HIS	3.3
2	G	211	GLN	3.3
2	E	171	LYS	3.3
2	F	166	GLY	3.3
1	J	86	ARG	3.3
1	A	68	GLN	3.2
2	G	167	GLN	3.2
2	F	93	GLY	3.2
2	G	227	GLU	3.2
2	F	174	GLU	3.2
2	E	217	LYS	3.2
2	E	92	VAL	3.2
2	F	270	PRO	3.2
2	H	129	GLU	3.2
1	B	88	LEU	3.2
2	F	142	ASN	3.2
2	H	225	LEU	3.2
1	J	69	GLY	3.1
1	K	11	HIS	3.1
2	G	92	VAL	3.1
2	F	213	ALA	3.1
2	F	225	LEU	3.1
2	G	234	VAL	3.1
2	E	169	ASP	3.1
1	K	89	ARG	3.1
1	B	60	PHE	3.1
2	H	174	GLU	3.1
2	F	234	VAL	3.1
1	K	96	ALA	3.0
2	H	113	VAL	3.0
2	F	218	ILE	3.0
2	H	157	GLN	3.0
1	C	91	LEU	3.0
2	E	120	ARG	3.0
2	E	235	ASN	3.0
2	F	217	LYS	3.0
2	H	131	ILE	3.0
2	F	121	TYR	3.0
2	E	225	LEU	3.0
2	H	172	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	173	TYR	3.0
2	F	150	GLN	3.0
2	E	149	GLN	3.0
1	C	172	SER	2.9
2	F	120	ARG	2.9
2	G	220	ASP	2.9
2	H	112	ARG	2.9
2	F	159	PHE	2.9
2	E	212	LYS	2.9
2	G	151	GLU	2.9
2	F	418	ILE	2.9
2	H	216	LEU	2.9
2	H	137	PRO	2.8
1	J	90	LYS	2.8
2	F	171	LYS	2.8
2	G	268	SER	2.8
2	E	173	ILE	2.8
2	H	148	GLN	2.8
2	E	436	GLU	2.8
2	G	109	LYS	2.8
1	D	45	GLY	2.8
2	H	110	MET	2.8
1	K	73	LYS	2.8
2	H	233	LEU	2.7
1	L	39	ASN	2.7
1	L	86	ARG	2.7
2	H	149	GLN	2.7
1	L	93	ALA	2.7
1	K	50	THR	2.7
2	G	168	LEU	2.7
1	K	67	HIS	2.7
2	E	167	GLN	2.7
2	E	234	VAL	2.7
2	H	125	GLU	2.7
2	E	119	ASN	2.6
2	G	149	GLN	2.6
2	H	220	ASP	2.6
2	G	124	GLU	2.6
1	B	87	MET	2.6
1	J	73	LYS	2.6
2	F	110	MET	2.6
1	I	68	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	160	ARG	2.6
1	K	171	LEU	2.6
2	F	149	GLN	2.6
2	G	160	ARG	2.6
2	E	268	SER	2.6
2	G	222	MET	2.6
1	D	67	HIS	2.6
2	F	224	LEU	2.6
1	K	86	ARG	2.5
2	F	164	ARG	2.5
2	H	213	ALA	2.5
1	B	70	HIS	2.5
1	K	100	GLU	2.5
2	E	214	ARG	2.5
1	D	73	LYS	2.5
2	G	120	ARG	2.5
2	G	239	LEU	2.5
1	D	111	ASP	2.5
2	H	159	PHE	2.5
2	E	166	GLY	2.5
2	E	227	GLU	2.5
2	H	164	ARG	2.5
2	H	234	VAL	2.5
2	H	171	LYS	2.5
1	C	68	GLN	2.5
1	K	44	ALA	2.5
2	G	138	PRO	2.5
1	L	174	LYS	2.5
2	E	270	PRO	2.4
1	B	116	GLU	2.4
1	D	86	ARG	2.4
2	F	414	SER	2.4
2	E	110	MET	2.4
2	H	156	ARG	2.4
2	G	213	ALA	2.4
1	K	90	LYS	2.4
2	H	120	ARG	2.4
1	D	50	THR	2.4
2	E	27	VAL	2.4
1	D	102	ALA	2.4
2	G	164	ARG	2.4
2	G	217	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	G	46	HIS	2.4
2	E	222	MET	2.3
1	D	46	PHE	2.3
1	A	83	ARG	2.3
2	E	172	GLU	2.3
2	G	110	MET	2.3
2	F	212	LYS	2.3
2	G	418	ILE	2.3
2	F	148	GLN	2.3
2	F	160	ARG	2.3
2	E	138	PRO	2.3
2	G	121	TYR	2.3
2	G	142	ASN	2.3
1	D	108	GLY	2.3
1	I	73	LYS	2.3
2	G	236	PRO	2.3
1	I	83	ARG	2.3
2	H	268	SER	2.3
2	G	436	GLU	2.3
1	C	174	LYS	2.3
1	J	174	LYS	2.3
2	F	127	ALA	2.3
2	G	113	VAL	2.3
1	K	45	GLY	2.3
2	F	233	LEU	2.3
1	K	46	PHE	2.2
1	K	109	ASN	2.2
2	E	130	ARG	2.2
2	E	223	LYS	2.2
2	H	119	ASN	2.2
1	B	136	LEU	2.2
2	F	156	ARG	2.2
2	F	239	LEU	2.2
1	D	109	ASN	2.2
1	B	97	VAL	2.2
1	K	40	ASP	2.2
2	F	158	ALA	2.2
2	G	169	ASP	2.2
2	E	35	TRP	2.2
1	K	121	ALA	2.2
2	F	436	GLU	2.2
2	G	131	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	4	VAL	2.2
1	B	148	ALA	2.1
2	H	414	SER	2.1
2	G	166	GLY	2.1
2	E	164	ARG	2.1
2	H	437	ASP	2.1
1	A	73	LYS	2.1
2	E	213	ALA	2.1
2	H	291	SER	2.1
1	C	58	GLU	2.1
2	E	165	GLU	2.1
1	B	98	ALA	2.1
2	E	221	ALA	2.1
2	E	174	GLU	2.1
1	B	34	VAL	2.1
2	H	27	VAL	2.1
2	F	38	MET	2.0
1	B	90	LYS	2.0
2	G	297	VAL	2.0
1	B	44	ALA	2.0
2	H	135	LEU	2.0
2	H	212	LYS	2.0
1	L	85	ASP	2.0
1	C	89	ARG	2.0
1	B	14	ILE	2.0
2	G	173	ILE	2.0
1	B	4	VAL	2.0
2	H	228	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ADP	E	450	27/27	0.93	0.25	1.10	46,50,60,62	0
3	ADP	G	2450	27/27	0.90	0.26	0.93	43,51,61,61	0
3	ADP	H	3450	27/27	0.92	0.25	0.71	53,55,58,61	0
3	ADP	F	1450	27/27	0.93	0.23	0.62	45,50,57,59	0

## 6.5 Other polymers

There are no such residues in this entry.