



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 08:12 AM GMT

PDB ID : 1HT1  
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 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/ValidationPDFNotes.html>

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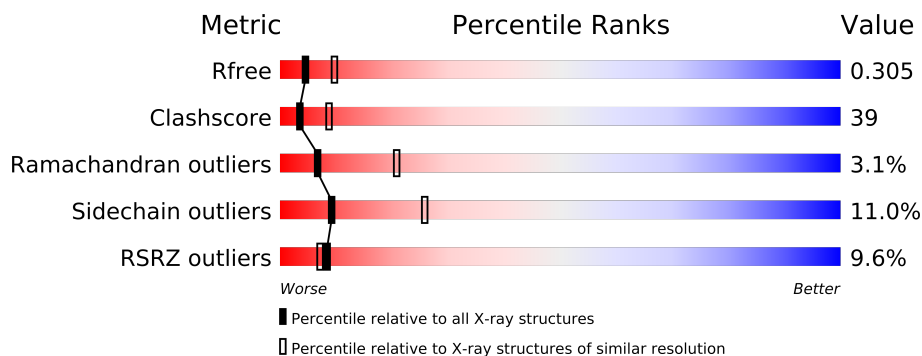
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance


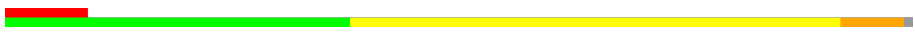
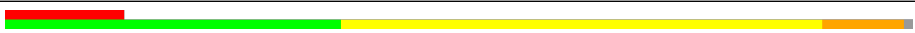
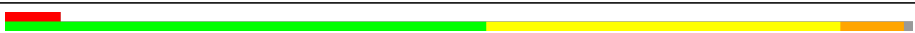
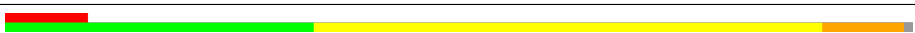

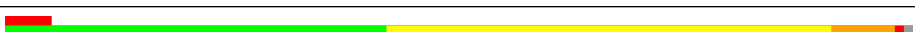

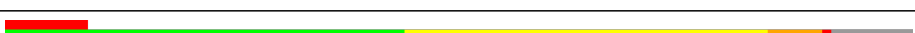
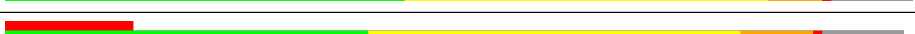


The reported resolution of this entry is 2.80 Å.

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))
$R_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	175	
1	B	175	
1	C	175	
1	D	175	
1	V	175	
1	X	175	
1	Y	175	
1	Z	175	
2	E	449	
2	F	449	
2	G	449	
2	I	449	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23636 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called HEAT SHOCK LOCUS HSLV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	V	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			
1	X	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			
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	Z	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			
1	Y	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	I	408	Total	C	N	O	S	0	0	0
			3226	2014	577	625	10			

There are 28 discrepancies between the modelled and reference sequences:

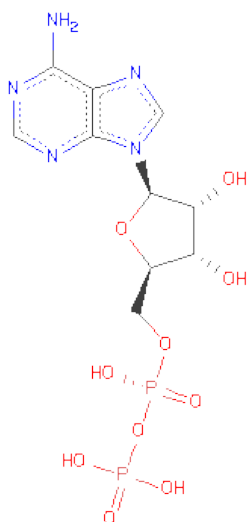
Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	HIS	-	EXPRESSION TAG	UNP P0A6H5

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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
I	-5	HIS	-	EXPRESSION TAG	UNP P0A6H5
I	-4	HIS	-	EXPRESSION TAG	UNP P0A6H5
I	-3	HIS	-	EXPRESSION TAG	UNP P0A6H5
I	-2	HIS	-	EXPRESSION TAG	UNP P0A6H5
I	-1	HIS	-	EXPRESSION TAG	UNP P0A6H5
I	0	HIS	-	EXPRESSION TAG	UNP P0A6H5
I	1	HIS	-	EXPRESSION TAG	UNP P0A6H5

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

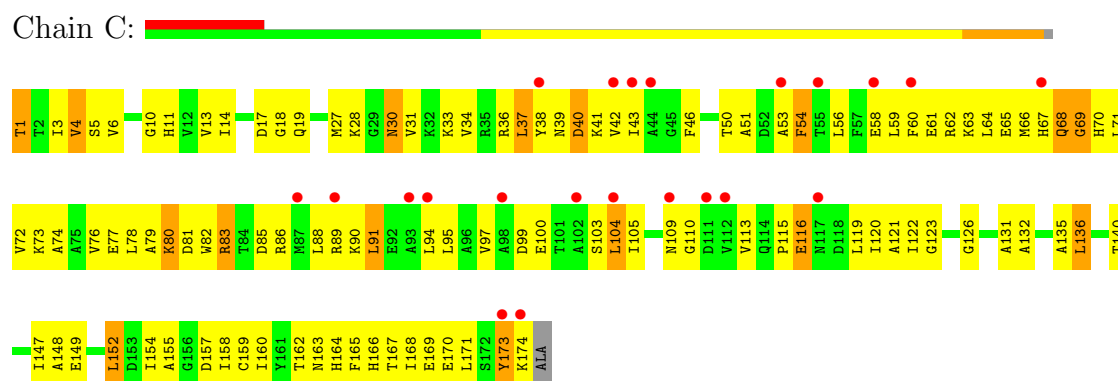


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

### 3 Residue-property plots

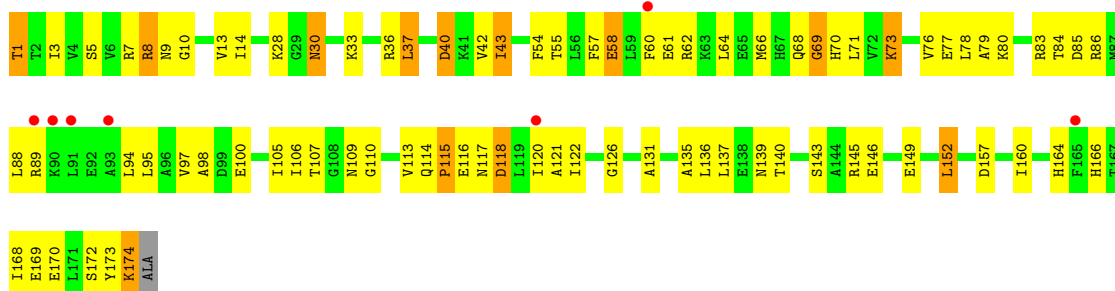
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

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



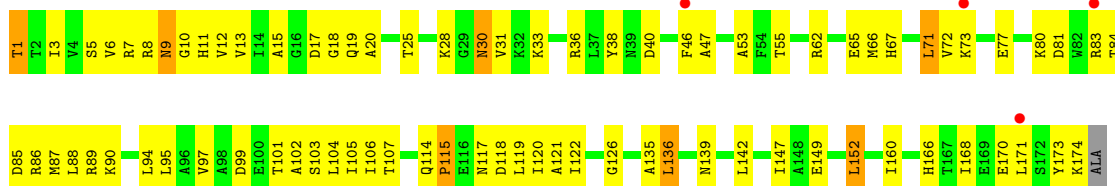
- Molecule 1: HEAT SHOCK LOCUS HSLV

Chain X:



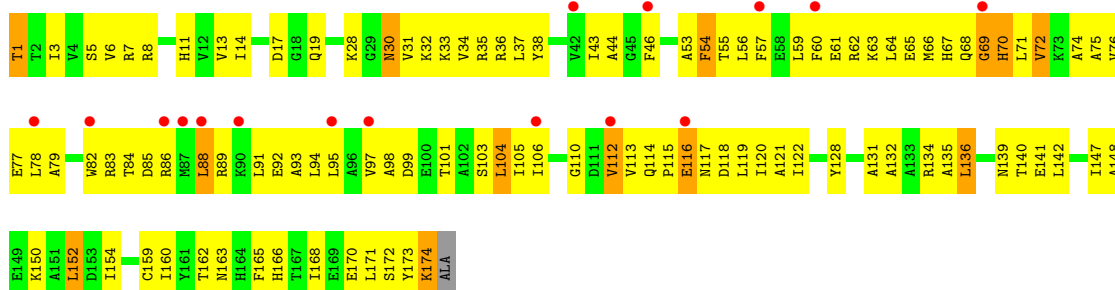
- Molecule 1: HEAT SHOCK LOCUS HSLV

Chain A:



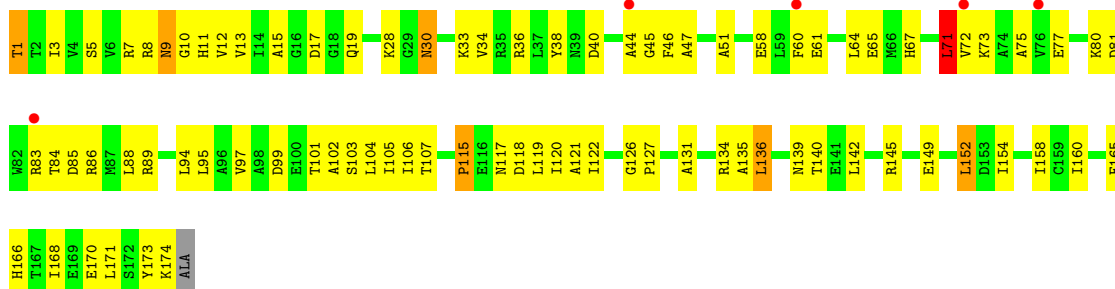
- Molecule 1: HEAT SHOCK LOCUS HSLV

Chain B:



- Molecule 1: HEAT SHOCK LOCUS HSLV

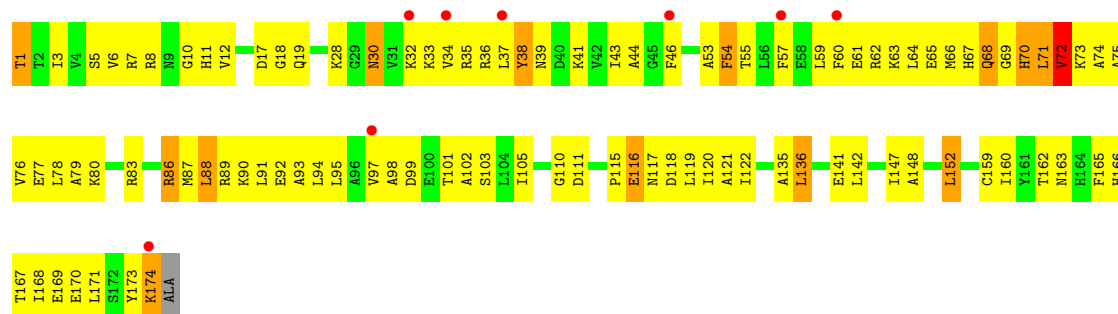
Chain Z:



- Molecule 1: HEAT SHOCK LOCUS HSLV

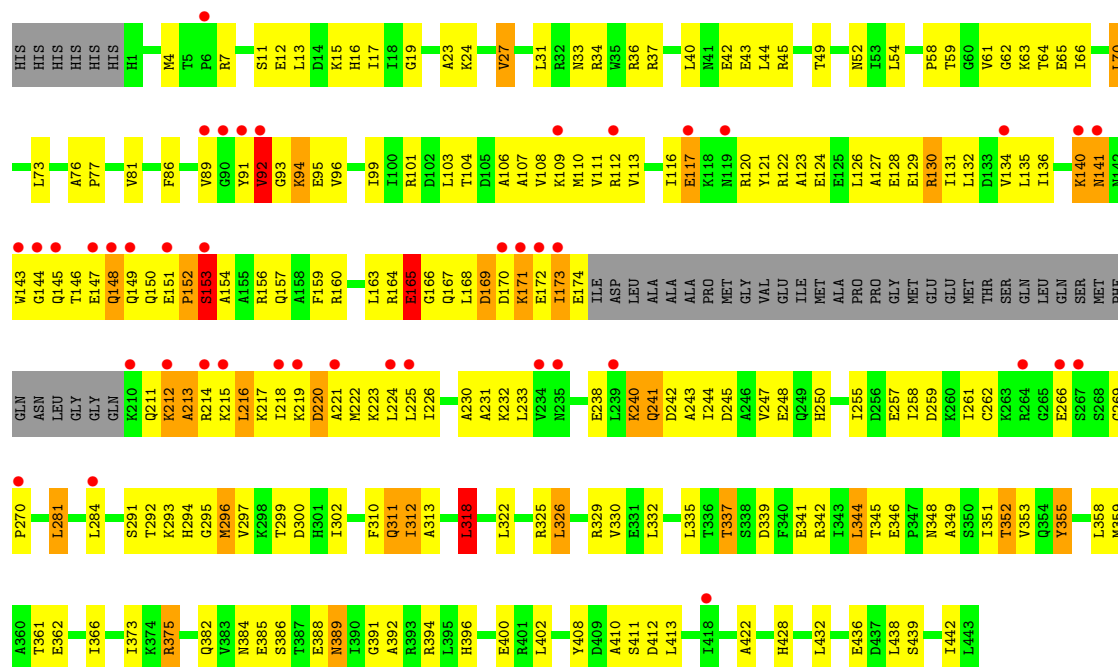
Chain Y:





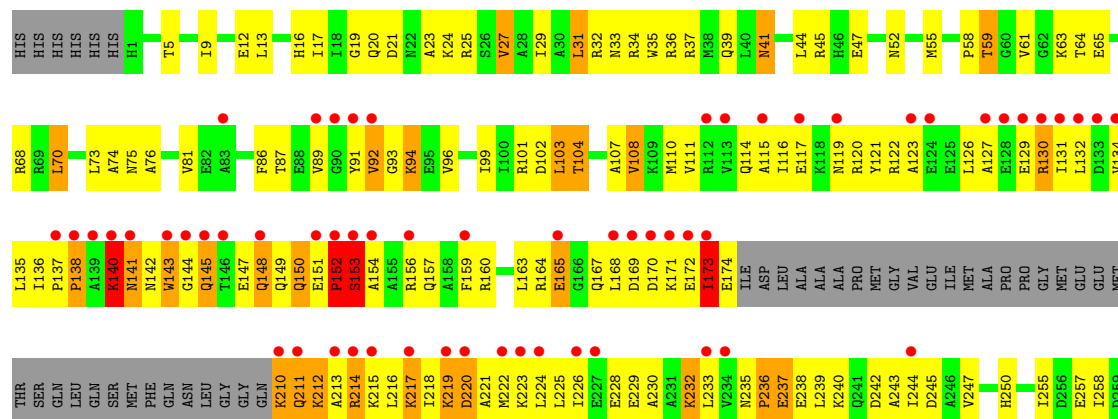
• Molecule 2: HEAT SHOCK LOCUS HSLU

Chain E:

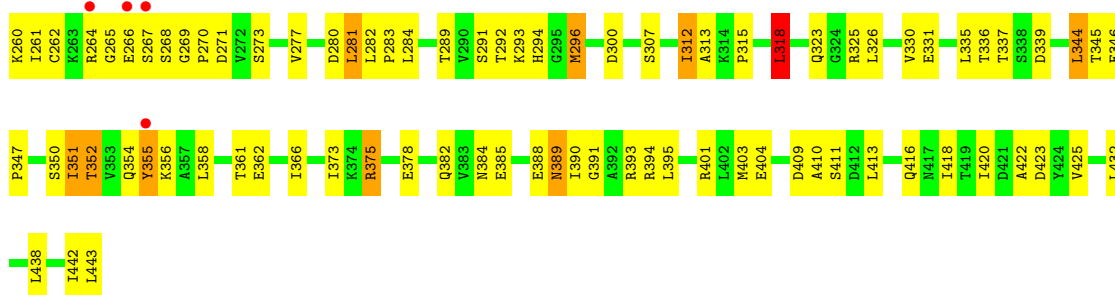


• Molecule 2: HEAT SHOCK LOCUS HSLU

Chain F:

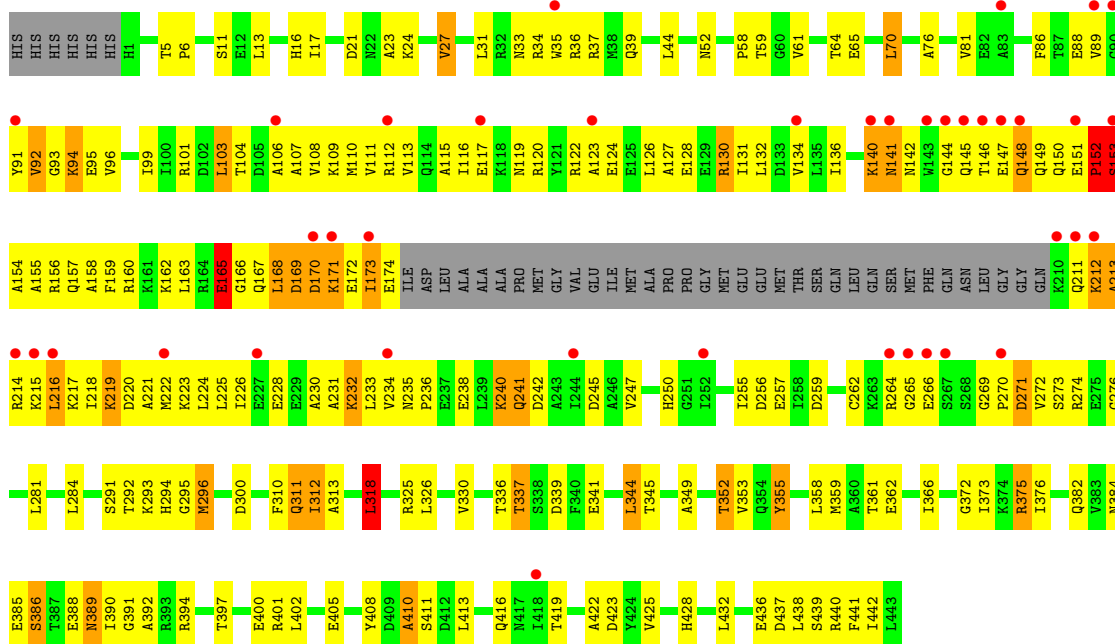






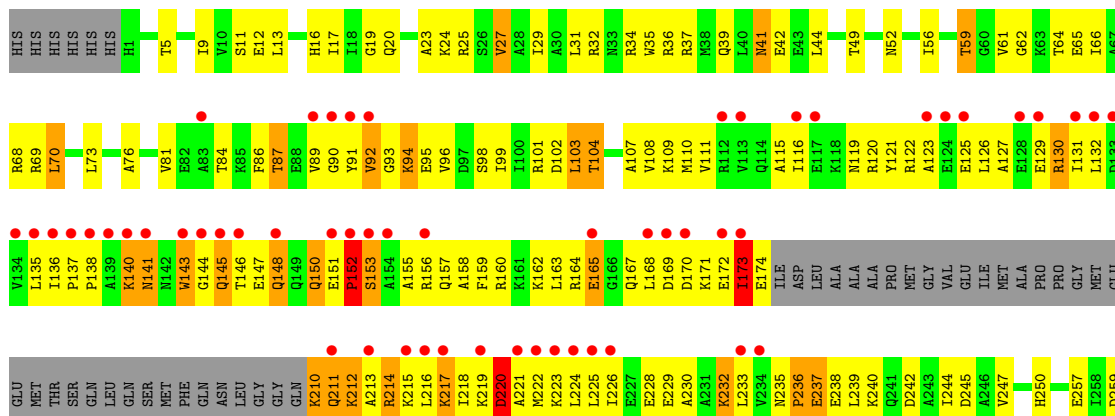
• Molecule 2: HEAT SHOCK LOCUS HSLU

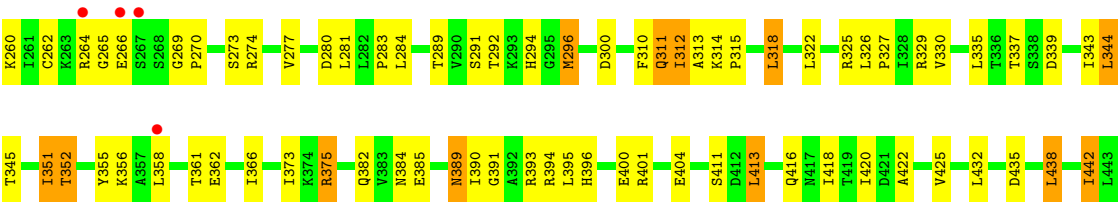
Chain G:



• Molecule 2: HEAT SHOCK LOCUS HSLU

Chain I:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	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, $R_{free}$	0.261 , 0.309 0.257 , 0.305	Depositor DCC
$R_{free}$ test set	10933 reflections (11.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.6	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 32.7	EDS
Estimated twinning fraction	0.499 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	3 of 119676 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	23636	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	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 60.98 % 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 1.4024e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.46	0/1345	0.72	0/1817
1	B	0.41	0/1345	0.66	0/1817
1	C	0.44	0/1345	0.66	0/1817
1	D	0.37	0/1345	0.65	0/1817
1	V	0.45	0/1345	0.64	0/1817
1	X	0.36	0/1345	0.64	0/1817
1	Y	0.41	0/1345	0.67	0/1817
1	Z	0.46	0/1345	0.72	0/1817
2	E	0.42	0/3266	0.69	3/4400 (0.1%)
2	F	0.45	1/3266 (0.0%)	0.69	2/4400 (0.0%)
2	G	0.43	1/3266 (0.0%)	0.69	4/4400 (0.1%)
2	I	0.42	0/3266	0.68	2/4400 (0.0%)
All	All	0.43	2/23824 (0.0%)	0.68	11/32136 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	219	LYS	C-N	5.58	1.46	1.34
2	F	152	PRO	CA-C	-5.43	1.42	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	318	LEU	CA-CB-CG	6.46	130.16	115.30
2	I	220	ASP	CB-CA-C	-6.40	97.59	110.40
2	G	318	LEU	CA-CB-CG	6.35	129.90	115.30
2	G	152	PRO	C-N-CA	-5.99	106.72	121.70
2	F	152	PRO	CA-N-CD	-5.91	103.23	111.50
2	G	153	SER	C-N-CA	5.65	135.82	121.70
2	E	152	PRO	CA-N-CD	-5.51	103.79	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	152	PRO	CA-N-CD	-5.29	104.10	111.50
2	E	153	SER	CB-CA-C	5.29	120.14	110.10
2	I	152	PRO	CA-N-CD	-5.28	104.10	111.50
2	F	318	LEU	CA-CB-CG	5.20	127.27	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1328	0	1348	96	0
1	B	1328	0	1348	126	0
1	C	1328	0	1348	140	0
1	D	1328	0	1348	87	0
1	V	1328	0	1348	143	0
1	X	1328	0	1348	98	0
1	Y	1328	0	1348	121	0
1	Z	1328	0	1348	101	0
2	E	3226	0	3294	260	1
2	F	3226	0	3293	265	1
2	G	3226	0	3294	280	0
2	I	3226	0	3293	303	0
3	E	27	0	12	3	0
3	F	27	0	12	3	0
3	G	27	0	12	3	0
3	I	27	0	12	4	0
All	All	23636	0	24006	1871	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 39.

All (1871) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:152:PRO:O	2:E:154:ALA:CA	1.83	1.25
2:E:152:PRO:C	2:E:154:ALA:H	1.27	1.15
2:E:152:PRO:C	2:E:154:ALA:N	1.80	1.12
1:B:135:ALA:HB1	1:Z:136:LEU:HD13	1.21	1.12
2:F:216:LEU:HG	2:F:221:ALA:HB2	1.25	1.11
1:D:83:ARG:HB3	1:D:83:ARG:NH1	1.71	1.06
2:E:152:PRO:O	2:E:153:SER:C	1.88	1.04
1:X:83:ARG:NH1	1:X:83:ARG:HB3	1.71	1.04
1:C:115:PRO:HG3	1:C:120:ILE:HG12	1.38	1.02
1:C:105:ILE:HD11	1:C:120:ILE:CG2	1.91	1.01
1:Y:83:ARG:HD2	1:Y:110:GLY:HA3	1.39	1.01
1:A:160:ILE:HD11	1:Z:19:GLN:NE2	1.75	1.01
2:G:152:PRO:HB2	2:G:156:ARG:HB2	1.36	1.00
2:E:174:GLU:HB3	2:E:211:GLN:HG3	1.44	1.00
2:E:212:LYS:HD3	2:E:216:LEU:HD21	1.40	0.99
2:E:152:PRO:HB2	2:E:156:ARG:HB2	1.42	0.99
1:V:15:ALA:HB2	1:V:168:ILE:HG23	1.47	0.97
2:E:170:ASP:HA	2:E:217:LYS:HA	1.46	0.97
2:F:217:LYS:O	2:F:221:ALA:N	1.98	0.96
2:G:130:ARG:HB2	2:G:130:ARG:NH2	1.80	0.96
1:Z:80:LYS:HA	1:Z:83:ARG:NH1	1.79	0.96
2:E:312:ILE:HD13	2:E:312:ILE:H	1.31	0.96
2:E:104:THR:HG21	2:E:292:THR:HG21	1.48	0.96
2:F:27:VAL:HG13	2:F:70:LEU:HG	1.48	0.96
2:G:174:GLU:HB3	2:G:211:GLN:HG3	1.47	0.95
1:X:83:ARG:HB3	1:X:83:ARG:HH11	1.23	0.95
2:E:130:ARG:HD2	2:E:225:LEU:HD11	1.49	0.95
2:E:130:ARG:HB2	2:E:130:ARG:NH2	1.82	0.94
2:G:92:VAL:HG21	2:I:92:VAL:HA	1.49	0.94
1:V:105:ILE:HD11	1:V:120:ILE:CG2	1.98	0.93
2:F:216:LEU:CG	2:F:221:ALA:HB2	1.98	0.92
2:G:212:LYS:HD3	2:G:216:LEU:HD21	1.51	0.92
1:C:105:ILE:HD11	1:C:120:ILE:HG21	1.49	0.92
2:I:122:ARG:HH11	2:I:126:LEU:HD23	1.32	0.92
2:G:168:LEU:HG	2:G:219:LYS:HD3	1.48	0.92
1:X:30:ASN:H	1:X:30:ASN:HD22	1.17	0.92
2:I:91:TYR:O	2:I:92:VAL:HG13	1.71	0.91
2:I:312:ILE:H	2:I:312:ILE:HD13	1.32	0.91
1:A:83:ARG:HH11	1:A:83:ARG:HG2	1.33	0.91
1:V:79:ALA:HB1	1:V:110:GLY:HA2	1.53	0.91
2:I:148:GLN:HA	2:I:151:GLU:HG3	1.53	0.90
1:V:152:LEU:HD13	1:V:166:HIS:ND1	1.85	0.90
1:D:174:LYS:HA	1:D:174:LYS:NZ	1.87	0.90

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:152:PRO:O	2:E:154:ALA:N	0.76	0.90
1:A:90:LYS:NZ	1:B:89:ARG:NH2	2.20	0.90
1:C:13:VAL:HG12	1:C:170:GLU:HA	1.52	0.89
2:G:94:LYS:HA	2:G:94:LYS:HE2	1.54	0.89
1:D:135:ALA:HB1	1:V:136:LEU:HD13	1.54	0.89
1:B:104:LEU:HD12	1:B:112:VAL:HG12	1.55	0.89
1:V:105:ILE:HD11	1:V:120:ILE:HG23	1.53	0.88
2:F:171:LYS:NZ	2:F:218:ILE:HD11	1.88	0.88
2:E:132:LEU:HD11	2:E:160:ARG:HG3	1.55	0.88
2:E:145:GLN:HB2	2:E:148:GLN:HB2	1.55	0.88
1:Z:10:GLY:HA3	1:Z:174:LYS:HA	1.55	0.88
1:B:140:THR:CG2	1:Z:140:THR:HG22	2.04	0.88
2:G:312:ILE:H	2:G:312:ILE:HD13	1.39	0.88
1:Y:63:LYS:HA	1:Y:66:MET:HE3	1.56	0.87
1:Z:80:LYS:HA	1:Z:83:ARG:HH12	1.36	0.87
1:C:136:LEU:HD13	1:X:135:ALA:HB1	1.54	0.87
2:F:94:LYS:HE2	2:F:94:LYS:HA	1.54	0.87
1:C:158:ILE:O	1:V:25:THR:HA	1.73	0.87
1:C:152:LEU:HD13	1:C:166:HIS:ND1	1.90	0.86
1:X:174:LYS:HA	1:X:174:LYS:NZ	1.90	0.86
2:E:94:LYS:HE2	2:E:94:LYS:HA	1.55	0.86
2:E:299:THR:HA	2:E:302:ILE:HD13	1.57	0.86
1:B:136:LEU:HD13	1:Z:135:ALA:HB1	1.58	0.86
1:B:86:ARG:HA	1:B:89:ARG:NE	1.90	0.86
2:E:153:SER:HA	2:E:157:GLN:HG2	1.58	0.85
1:B:1:THR:HB	1:B:33:LYS:HZ3	1.39	0.85
1:A:19:GLN:NE2	1:Z:160:ILE:HD11	1.90	0.85
2:I:217:LYS:O	2:I:221:ALA:HB2	1.77	0.85
1:D:83:ARG:HB3	1:D:83:ARG:HH11	1.36	0.85
2:G:104:THR:HG21	2:G:292:THR:HG21	1.59	0.84
2:E:89:VAL:HG12	2:E:93:GLY:HA3	1.60	0.84
2:F:122:ARG:HH11	2:F:126:LEU:HD23	1.41	0.84
2:G:211:GLN:HG2	2:G:212:LYS:H	1.41	0.84
1:Y:72:VAL:O	1:Y:76:VAL:HG23	1.77	0.84
1:A:85:ASP:O	1:A:89:ARG:HB2	1.77	0.84
2:I:174:GLU:HA	2:I:213:ALA:H	1.43	0.83
1:C:71:LEU:HG	1:C:99:ASP:OD1	1.76	0.83
1:B:140:THR:HG22	1:Z:140:THR:HG22	1.61	0.83
2:I:351:ILE:HD13	2:I:351:ILE:H	1.40	0.83
1:B:135:ALA:HB1	1:Z:136:LEU:CD1	2.08	0.83
2:I:224:LEU:O	2:I:228:GLU:HB2	1.78	0.83
2:F:312:ILE:H	2:F:312:ILE:HD13	1.42	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:356:LYS:HG3	2:I:366:ILE:HG22	1.61	0.82
2:I:217:LYS:O	2:I:221:ALA:CB	2.27	0.82
1:B:72:VAL:O	1:B:76:VAL:HG23	1.79	0.82
2:F:145:GLN:HB2	2:F:148:GLN:HG2	1.61	0.82
2:I:132:LEU:HD11	2:I:160:ARG:HG3	1.60	0.82
1:C:158:ILE:CG2	1:V:25:THR:HB	2.08	0.82
1:B:1:THR:HB	1:B:33:LYS:NZ	1.94	0.82
1:D:136:LEU:HD13	1:V:135:ALA:HB1	1.58	0.82
1:B:86:ARG:HA	1:B:89:ARG:CZ	2.09	0.82
1:C:86:ARG:HA	1:C:89:ARG:NH1	1.95	0.81
2:G:109:LYS:HD3	2:I:296:MET:HB3	1.61	0.81
1:A:160:ILE:HD11	1:Z:19:GLN:HE22	1.45	0.81
1:D:43:ILE:H	1:D:43:ILE:HD13	1.45	0.81
2:F:91:TYR:O	2:F:92:VAL:HG13	1.81	0.81
2:G:150:GLN:O	2:G:153:SER:HB2	1.81	0.81
1:B:63:LYS:HA	1:B:66:MET:HE3	1.62	0.81
2:I:171:LYS:NZ	2:I:218:ILE:HD11	1.95	0.81
1:Y:60:PHE:CD1	1:Y:78:LEU:HD22	2.16	0.81
2:E:211:GLN:HG2	2:E:212:LYS:H	1.45	0.81
2:I:27:VAL:HG13	2:I:70:LEU:HG	1.62	0.81
2:G:174:GLU:HA	2:G:212:LYS:HB3	1.62	0.80
2:G:92:VAL:CG2	2:I:92:VAL:HA	2.12	0.80
1:B:57:PHE:O	1:B:61:GLU:HG3	1.82	0.80
1:V:115:PRO:HG3	1:V:120:ILE:HG13	1.64	0.80
1:A:1:THR:HB	1:A:33:LYS:HZ3	1.47	0.80
1:C:54:PHE:O	1:C:58:GLU:HB2	1.82	0.80
2:F:224:LEU:O	2:F:228:GLU:HB2	1.82	0.80
1:D:28:LYS:HE2	1:D:30:ASN:ND2	1.97	0.80
1:A:80:LYS:HA	1:A:83:ARG:NH1	1.98	0.79
2:I:19:GLY:O	2:I:24:LYS:HE3	1.83	0.79
2:G:92:VAL:HG21	2:I:92:VAL:HG12	1.63	0.79
2:E:344:LEU:O	2:E:352:THR:HB	1.82	0.79
2:E:389:ASN:C	2:E:389:ASN:HD22	1.85	0.79
1:A:90:LYS:HZ1	1:B:89:ARG:NH2	1.80	0.79
2:G:344:LEU:O	2:G:352:THR:HB	1.82	0.79
1:Z:10:GLY:HA2	1:Z:173:TYR:CE1	2.17	0.79
2:F:384:ASN:ND2	2:F:394:ARG:HE	1.81	0.79
1:C:28:LYS:HE2	1:C:30:ASN:ND2	1.97	0.79
2:I:172:GLU:HB3	2:I:215:LYS:HD2	1.65	0.79
2:F:151:GLU:HB2	2:F:152:PRO:CD	2.13	0.79
2:I:312:ILE:CD1	2:I:312:ILE:H	1.96	0.78
1:B:134:ARG:HG2	1:Z:154:ILE:HD12	1.65	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:130:ARG:HH21	2:G:130:ARG:HB2	1.43	0.78
1:C:115:PRO:HB2	1:C:119:LEU:O	1.83	0.78
1:Y:1:THR:HB	1:Y:33:LYS:NZ	1.99	0.78
2:F:312:ILE:H	2:F:312:ILE:CD1	1.96	0.78
1:Y:170:GLU:HG2	1:Y:171:LEU:H	1.47	0.78
2:I:108:VAL:HA	2:I:111:VAL:HG22	1.64	0.78
2:G:173:ILE:HG12	2:G:212:LYS:HD2	1.65	0.78
2:F:351:ILE:HD13	2:F:351:ILE:H	1.46	0.78
2:F:211:GLN:HE21	2:F:212:LYS:H	1.29	0.77
1:D:139:ASN:HD22	1:V:136:LEU:HD11	1.49	0.77
1:A:10:GLY:HA2	1:A:173:TYR:CE1	2.19	0.77
2:E:174:GLU:HA	2:E:212:LYS:HB3	1.65	0.77
2:F:389:ASN:ND2	2:F:391:GLY:H	1.83	0.77
2:E:103:LEU:HD22	2:E:247:VAL:HG22	1.65	0.77
2:F:135:LEU:HG	2:F:171:LYS:HE2	1.67	0.77
1:X:60:PHE:HB2	1:X:78:LEU:HD22	1.67	0.77
2:I:89:VAL:HG12	2:I:93:GLY:HA3	1.67	0.77
1:Y:105:ILE:HD11	1:Y:120:ILE:HG23	1.67	0.77
2:F:393:ARG:HG2	2:F:393:ARG:HH11	1.49	0.77
1:B:28:LYS:NZ	1:B:30:ASN:HD21	1.82	0.77
2:E:147:GLU:HA	2:E:150:GLN:HG3	1.67	0.77
2:F:130:ARG:HG2	2:F:225:LEU:HD11	1.66	0.76
2:F:375:ARG:CZ	2:F:422:ALA:HB1	2.14	0.76
2:F:174:GLU:HA	2:F:213:ALA:H	1.49	0.76
2:F:64:THR:HB	3:F:1450:ADP:O2A	1.84	0.76
2:I:147:GLU:HG2	2:I:150:GLN:NE2	2.00	0.76
2:G:173:ILE:HD11	2:G:221:ALA:HB1	1.68	0.76
2:E:91:TYR:O	2:E:92:VAL:HG13	1.86	0.76
2:G:152:PRO:HB3	2:G:156:ARG:H	1.49	0.76
1:D:30:ASN:H	1:D:30:ASN:HD22	1.31	0.76
1:A:67:HIS:HD2	1:A:73:LYS:HD2	1.49	0.76
1:V:27:MET:SD	1:X:113:VAL:HG21	2.25	0.76
1:X:13:VAL:HG12	1:X:170:GLU:HG3	1.66	0.76
2:G:89:VAL:HA	2:G:93:GLY:N	2.00	0.75
2:G:389:ASN:ND2	2:G:391:GLY:H	1.84	0.75
2:G:397:THR:HG22	2:I:327:PRO:HA	1.66	0.75
1:A:13:VAL:HG12	1:A:170:GLU:HG3	1.67	0.75
1:B:71:LEU:HG	1:B:99:ASP:OD1	1.86	0.75
2:G:145:GLN:HB2	2:G:148:GLN:HB2	1.67	0.75
2:E:130:ARG:HB2	2:E:130:ARG:HH21	1.51	0.75
1:C:71:LEU:HD21	1:C:97:VAL:HG11	1.69	0.75
2:F:171:LYS:HZ2	2:F:218:ILE:HD11	1.52	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:173:ILE:HG12	2:F:212:LYS:HD2	1.68	0.75
2:F:218:ILE:C	2:F:220:ASP:H	1.89	0.75
2:E:116:ILE:O	2:E:120:ARG:HB2	1.87	0.75
2:F:123:ALA:HA	2:F:127:ALA:HB3	1.68	0.74
1:C:105:ILE:HD11	1:C:120:ILE:HG23	1.68	0.74
2:E:291:SER:HA	2:E:296:MET:HE2	1.69	0.74
2:E:64:THR:HB	3:E:450:ADP:O2A	1.87	0.74
2:F:235:ASN:OD1	2:F:238:GLU:HB2	1.87	0.74
2:F:172:GLU:HB3	2:F:215:LYS:HD2	1.68	0.74
1:X:30:ASN:ND2	1:X:30:ASN:H	1.85	0.74
2:G:312:ILE:H	2:G:312:ILE:CD1	2.00	0.74
1:X:37:LEU:HD23	1:X:57:PHE:HB3	1.69	0.74
1:V:115:PRO:HB2	1:V:119:LEU:O	1.87	0.74
1:C:135:ALA:HB1	1:X:136:LEU:HD13	1.69	0.74
2:F:217:LYS:HB2	2:F:217:LYS:NZ	2.03	0.74
2:I:94:LYS:HE2	2:I:94:LYS:HA	1.69	0.74
1:B:60:PHE:CD1	1:B:78:LEU:HD22	2.22	0.74
1:X:43:ILE:HD13	1:X:43:ILE:H	1.53	0.74
2:E:171:LYS:HG3	2:E:218:ILE:HD11	1.70	0.74
2:I:389:ASN:ND2	2:I:391:GLY:H	1.86	0.74
1:Z:67:HIS:CD2	1:Z:73:LYS:HD2	2.22	0.74
2:E:152:PRO:CB	2:E:156:ARG:HB2	2.17	0.74
2:E:384:ASN:ND2	2:E:394:ARG:HE	1.86	0.74
2:I:153:SER:HB3	2:I:157:GLN:OE1	1.88	0.74
1:X:105:ILE:HD11	1:X:120:ILE:HG23	1.69	0.74
1:C:160:ILE:HG23	1:V:160:ILE:HG23	1.70	0.74
2:E:312:ILE:CD1	2:E:312:ILE:H	1.98	0.74
2:G:92:VAL:HG21	2:I:92:VAL:CG1	2.17	0.73
2:G:291:SER:HA	2:G:296:MET:HE2	1.69	0.73
2:G:150:GLN:C	2:G:153:SER:OG	2.27	0.73
2:I:217:LYS:HG3	2:I:218:ILE:H	1.51	0.73
1:C:71:LEU:HD21	1:C:97:VAL:CG1	2.17	0.73
1:V:132:ALA:HB2	1:V:154:ILE:HG21	1.70	0.73
2:G:389:ASN:HD22	2:G:389:ASN:C	1.91	0.73
2:G:169:ASP:OD1	2:G:218:ILE:HD12	1.88	0.73
1:V:138:GLU:C	1:V:139:ASN:HD22	1.92	0.73
2:F:223:LYS:HA	2:F:226:ILE:HG12	1.70	0.73
2:G:345:THR:CG2	2:G:373:ILE:HD13	2.18	0.73
1:X:95:LEU:HB2	1:X:106:ILE:HB	1.69	0.73
1:C:132:ALA:HB2	1:C:154:ILE:HG21	1.70	0.73
1:B:17:ASP:HA	1:B:165:PHE:O	1.89	0.73
2:F:81:VAL:HG11	2:F:99:ILE:HG12	1.71	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Y:71:LEU:HG	1:Y:99:ASP:OD1	1.89	0.72
1:C:86:ARG:HG3	1:C:89:ARG:HH22	1.52	0.72
2:I:344:LEU:O	2:I:352:THR:HB	1.89	0.72
2:I:81:VAL:HG11	2:I:99:ILE:HG12	1.71	0.72
1:B:28:LYS:HZ2	1:B:30:ASN:HD21	1.35	0.72
2:G:122:ARG:CZ	2:G:126:LEU:HD21	2.20	0.72
2:G:64:THR:HB	3:G:2450:ADP:O2A	1.88	0.72
1:A:90:LYS:HZ2	1:B:89:ARG:NH2	1.88	0.72
1:D:28:LYS:HE2	1:D:30:ASN:HD21	1.54	0.72
1:V:54:PHE:O	1:V:58:GLU:HB2	1.90	0.72
1:C:70:HIS:CE1	1:C:72:VAL:HB	2.25	0.72
2:I:345:THR:CG2	2:I:373:ILE:HD13	2.20	0.72
2:G:91:TYR:HD1	2:I:91:TYR:CD2	2.08	0.72
1:A:83:ARG:NH1	1:A:83:ARG:HG2	1.99	0.72
1:A:10:GLY:HA3	1:A:174:LYS:HA	1.69	0.72
2:G:140:LYS:O	2:G:141:ASN:HB2	1.89	0.72
1:X:152:LEU:HD13	1:X:166:HIS:ND1	2.04	0.72
1:Y:57:PHE:O	1:Y:61:GLU:HG3	1.89	0.72
2:E:359:MET:HG3	2:E:366:ILE:HG13	1.71	0.72
2:G:432:LEU:HD12	2:G:432:LEU:H	1.55	0.72
1:Y:86:ARG:HA	1:Y:89:ARG:CZ	2.20	0.72
2:E:345:THR:CG2	2:E:373:ILE:HD13	2.19	0.72
1:V:90:LYS:HZ1	1:X:89:ARG:NH1	1.88	0.72
1:C:158:ILE:HG22	1:V:25:THR:HB	1.72	0.72
1:C:46:PHE:CE2	1:C:53:ALA:HB2	2.25	0.72
1:Y:36:ARG:O	1:Y:37:LEU:HD23	1.89	0.71
2:I:41:ASN:HD22	2:I:41:ASN:C	1.92	0.71
1:D:60:PHE:HB2	1:D:78:LEU:HD22	1.69	0.71
1:V:71:LEU:HG	1:V:99:ASP:OD1	1.89	0.71
2:I:108:VAL:HG21	2:I:294:HIS:HD2	1.55	0.71
1:C:160:ILE:CG2	1:V:160:ILE:HG23	2.19	0.71
1:Z:85:ASP:O	1:Z:89:ARG:HB2	1.89	0.71
2:I:384:ASN:ND2	2:I:394:ARG:HE	1.87	0.71
2:I:173:ILE:HG12	2:I:212:LYS:HD2	1.72	0.71
1:C:136:LEU:HD11	1:X:139:ASN:HD22	1.56	0.71
2:F:148:GLN:OE1	2:F:151:GLU:HG3	1.91	0.71
1:D:37:LEU:HD13	1:D:57:PHE:HB3	1.70	0.71
1:C:80:LYS:HB3	1:C:80:LYS:HZ2	1.55	0.71
2:G:168:LEU:HA	2:G:219:LYS:HB3	1.73	0.71
1:B:104:LEU:CD1	1:B:112:VAL:HG12	2.19	0.71
2:E:312:ILE:HG12	2:E:313:ALA:H	1.56	0.71
1:B:134:ARG:HG2	1:Z:154:ILE:CD1	2.21	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:117:GLU:HG3	2:E:120:ARG:NH2	2.04	0.71
2:G:150:GLN:CA	2:G:153:SER:OG	2.39	0.71
2:G:130:ARG:HD2	2:G:225:LEU:HD11	1.71	0.71
1:C:17:ASP:HA	1:C:165:PHE:O	1.91	0.71
2:E:389:ASN:ND2	2:E:391:GLY:H	1.89	0.70
1:Y:86:ARG:HA	1:Y:89:ARG:NE	2.05	0.70
2:E:27:VAL:HG13	2:E:70:LEU:HG	1.71	0.70
1:Y:28:LYS:NZ	1:Y:30:ASN:ND2	2.39	0.70
2:I:242:ASP:HA	2:I:245:ASP:OD1	1.91	0.70
2:F:89:VAL:HG11	2:F:94:LYS:O	1.90	0.70
2:F:257:GLU:HB2	2:F:260:LYS:HG3	1.74	0.70
1:B:152:LEU:HD13	1:B:166:HIS:ND1	2.07	0.70
2:G:170:ASP:HA	2:G:217:LYS:HA	1.72	0.70
2:E:216:LEU:HD23	2:E:216:LEU:H	1.57	0.70
1:D:30:ASN:H	1:D:30:ASN:ND2	1.90	0.70
1:D:174:LYS:HZ2	1:D:174:LYS:HA	1.56	0.69
2:F:152:PRO:HB2	2:F:156:ARG:HB2	1.72	0.69
1:A:90:LYS:HZ1	1:B:89:ARG:HH22	1.37	0.69
1:V:51:ALA:HB3	1:X:110:GLY:O	1.91	0.69
2:G:108:VAL:HG21	2:G:294:HIS:CD2	2.26	0.69
2:F:315:PRO:O	2:F:318:LEU:HB2	1.91	0.69
2:I:151:GLU:HB2	2:I:152:PRO:CD	2.23	0.69
1:C:94:LEU:HB3	1:C:122:ILE:HD12	1.73	0.69
1:D:95:LEU:HB2	1:D:106:ILE:HB	1.72	0.69
1:Z:1:THR:HB	1:Z:33:LYS:HZ3	1.57	0.69
2:G:132:LEU:HD11	2:G:160:ARG:HG2	1.74	0.69
1:Y:28:LYS:NZ	1:Y:30:ASN:HD21	1.89	0.69
2:I:64:THR:HB	3:I:3450:ADP:O2A	1.92	0.69
1:A:28:LYS:HD2	1:B:113:VAL:HG13	1.75	0.69
2:G:150:GLN:O	2:G:153:SER:CB	2.41	0.69
2:G:150:GLN:HA	2:G:153:SER:OG	1.93	0.69
2:E:124:GLU:HA	2:E:127:ALA:HB3	1.72	0.69
1:Z:117:ASN:O	1:Z:118:ASP:HB2	1.93	0.69
1:V:3:ILE:HD12	1:V:122:ILE:HD11	1.73	0.69
2:F:242:ASP:HA	2:F:245:ASP:OD1	1.91	0.69
2:E:169:ASP:OD1	2:E:218:ILE:HD12	1.93	0.69
2:I:170:ASP:HA	2:I:217:LYS:HA	1.75	0.69
2:G:345:THR:HG21	2:G:373:ILE:HD13	1.75	0.69
2:E:219:LYS:O	2:E:223:LYS:HG3	1.93	0.68
2:G:91:TYR:O	2:G:92:VAL:HG13	1.92	0.68
2:I:236:PRO:HG2	2:I:237:GLU:H	1.58	0.68
2:F:130:ARG:NH2	2:F:229:GLU:HG3	2.07	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:293:LYS:HG3	2:E:294:HIS:CD2	2.28	0.68
1:V:79:ALA:HB1	1:V:110:GLY:CA	2.24	0.68
2:I:223:LYS:HA	2:I:226:ILE:HG12	1.75	0.68
2:E:173:ILE:N	2:E:173:ILE:HD13	2.08	0.68
2:I:239:LEU:HD23	2:I:240:LYS:N	2.07	0.68
2:I:174:GLU:HB3	2:I:211:GLN:HB2	1.75	0.68
2:G:124:GLU:HA	2:G:127:ALA:HB3	1.74	0.68
2:G:173:ILE:N	2:G:173:ILE:HD13	2.08	0.68
2:I:163:LEU:HD11	2:I:222:MET:CE	2.24	0.68
2:E:214:ARG:HG2	2:E:215:LYS:N	2.09	0.68
2:E:108:VAL:HG21	2:E:294:HIS:ND1	2.07	0.68
1:C:79:ALA:HB1	1:C:110:GLY:HA2	1.76	0.68
2:F:96:VAL:HG11	2:F:281:LEU:HD12	1.74	0.68
2:G:122:ARG:O	2:G:126:LEU:HD23	1.93	0.68
1:Z:77:GLU:O	1:Z:80:LYS:HB2	1.93	0.68
1:X:86:ARG:HA	1:X:89:ARG:NH1	2.09	0.68
2:G:220:ASP:HA	2:G:223:LYS:HD2	1.75	0.68
1:D:10:GLY:HA2	1:D:173:TYR:CE1	2.29	0.68
1:A:8:ARG:NH1	1:A:142:LEU:O	2.24	0.68
2:F:25:ARG:O	2:F:29:ILE:HG12	1.92	0.68
2:E:150:GLN:O	2:E:153:SER:OG	2.12	0.68
1:A:80:LYS:HA	1:A:83:ARG:HH12	1.57	0.68
1:A:135:ALA:HB1	1:Y:136:LEU:HD13	1.75	0.68
1:C:158:ILE:HG23	1:V:25:THR:HB	1.74	0.67
2:E:375:ARG:CZ	2:E:422:ALA:HB1	2.23	0.67
1:X:55:THR:O	1:X:58:GLU:HB2	1.94	0.67
2:G:223:LYS:HA	2:G:226:ILE:HG12	1.76	0.67
1:B:28:LYS:NZ	1:B:30:ASN:ND2	2.42	0.67
1:V:30:ASN:ND2	1:V:30:ASN:H	1.92	0.67
2:F:344:LEU:O	2:F:352:THR:HB	1.94	0.67
1:X:36:ARG:NH1	1:X:40:ASP:O	2.28	0.67
2:E:153:SER:CA	2:E:157:GLN:HG2	2.25	0.67
2:E:131:ILE:HD11	2:E:218:ILE:HG12	1.75	0.67
2:G:216:LEU:HD23	2:G:216:LEU:H	1.60	0.67
2:G:171:LYS:HB2	2:G:218:ILE:HG13	1.76	0.67
2:G:52:ASN:HB2	2:G:325:ARG:O	1.94	0.67
1:Y:8:ARG:NH1	1:Y:142:LEU:O	2.26	0.67
2:I:291:SER:HA	2:I:296:MET:HE2	1.76	0.67
1:C:73:LYS:HD3	1:C:76:VAL:HG11	1.77	0.67
1:D:174:LYS:HZ3	1:D:174:LYS:HA	1.56	0.67
2:I:108:VAL:HG21	2:I:294:HIS:CD2	2.30	0.67
1:C:51:ALA:HB3	1:D:110:GLY:O	1.95	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:136:ILE:O	2:E:136:ILE:HG22	1.94	0.67
1:D:143:SER:OG	1:D:146:GLU:HG3	1.94	0.67
1:B:8:ARG:NH1	1:B:142:LEU:O	2.27	0.67
1:D:36:ARG:NH1	1:D:40:ASP:O	2.24	0.67
2:G:152:PRO:HB2	2:G:156:ARG:CB	2.19	0.67
2:F:151:GLU:HB2	2:F:152:PRO:HD2	1.76	0.66
2:G:174:GLU:HA	2:G:213:ALA:H	1.60	0.66
2:E:122:ARG:O	2:E:126:LEU:HD23	1.95	0.66
2:E:174:GLU:CB	2:E:211:GLN:HG3	2.23	0.66
2:F:389:ASN:HD22	2:F:391:GLY:H	1.41	0.66
2:F:236:PRO:HG2	2:F:237:GLU:H	1.60	0.66
1:V:73:LYS:HA	1:V:76:VAL:HG12	1.77	0.66
1:C:27:MET:SD	1:D:113:VAL:HG21	2.36	0.66
1:Z:51:ALA:CB	1:Y:111:ASP:OD2	2.43	0.66
1:V:83:ARG:HG3	1:V:83:ARG:HH11	1.60	0.66
1:Y:65:GLU:HG2	2:I:143:TRP:CD1	2.30	0.66
2:G:174:GLU:HB3	2:G:211:GLN:CG	2.22	0.66
1:B:56:LEU:HD13	1:B:95:LEU:HD11	1.77	0.66
2:E:361:THR:HG21	2:F:36:ARG:HA	1.78	0.66
2:E:147:GLU:HA	2:E:150:GLN:CG	2.24	0.66
1:D:83:ARG:HB3	1:D:83:ARG:CZ	2.26	0.66
1:V:37:LEU:HD23	1:V:37:LEU:N	2.10	0.66
1:X:143:SER:OG	1:X:146:GLU:HG3	1.95	0.66
2:I:217:LYS:NZ	2:I:217:LYS:HB2	2.11	0.66
1:A:1:THR:HB	1:A:33:LYS:NZ	2.10	0.66
2:G:432:LEU:HD12	2:G:432:LEU:N	2.10	0.66
2:G:242:ASP:HA	2:G:245:ASP:OD1	1.96	0.66
2:G:91:TYR:HB2	2:I:90:GLY:O	1.96	0.66
2:E:89:VAL:HA	2:E:93:GLY:N	2.11	0.66
1:A:19:GLN:HE22	1:Z:160:ILE:HD11	1.59	0.65
1:X:174:LYS:HA	1:X:174:LYS:HZ3	1.60	0.65
1:C:86:ARG:HA	1:C:89:ARG:HH12	1.59	0.65
2:G:92:VAL:HG21	2:I:92:VAL:CA	2.26	0.65
1:Y:65:GLU:HG2	2:I:143:TRP:NE1	2.12	0.65
1:Y:17:ASP:HA	1:Y:165:PHE:O	1.96	0.65
2:G:131:ILE:HD11	2:G:218:ILE:HG12	1.78	0.65
2:G:131:ILE:HD11	2:G:218:ILE:CD1	2.25	0.65
2:G:136:ILE:O	2:G:136:ILE:HG22	1.96	0.65
1:V:3:ILE:HB	1:V:122:ILE:HG12	1.79	0.65
2:I:135:LEU:CD2	2:I:171:LYS:HE2	2.27	0.65
2:E:103:LEU:HD13	2:E:247:VAL:HG13	1.78	0.65
2:I:262:CYS:SG	2:I:318:LEU:HD13	2.37	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:218:ILE:C	2:F:220:ASP:N	2.50	0.65
2:E:174:GLU:HB3	2:E:211:GLN:CG	2.24	0.65
2:E:312:ILE:HG12	2:E:313:ALA:N	2.11	0.65
2:E:293:LYS:HG3	2:E:294:HIS:HD2	1.62	0.65
1:A:86:ARG:HA	1:A:89:ARG:CZ	2.26	0.65
1:Z:67:HIS:HD2	1:Z:73:LYS:HD2	1.60	0.65
1:D:64:LEU:O	1:D:69:GLY:N	2.30	0.65
1:A:67:HIS:CD2	1:A:73:LYS:HD2	2.31	0.65
1:Y:28:LYS:HZ2	1:Y:30:ASN:HD21	1.43	0.65
2:F:174:GLU:HB3	2:F:211:GLN:HB2	1.77	0.65
2:I:235:ASN:HB2	2:I:236:PRO:HD2	1.79	0.65
1:X:174:LYS:HZ2	1:X:174:LYS:HA	1.60	0.65
2:I:257:GLU:HB2	2:I:260:LYS:HG3	1.78	0.65
2:F:211:GLN:HE21	2:F:212:LYS:N	1.95	0.64
2:F:27:VAL:CG1	2:F:70:LEU:HG	2.25	0.64
1:A:28:LYS:NZ	1:A:30:ASN:ND2	2.45	0.64
2:F:130:ARG:HH21	2:F:229:GLU:HG3	1.61	0.64
1:C:6:VAL:HG21	1:C:147:ILE:HG22	1.80	0.64
2:F:375:ARG:HB3	2:F:425:VAL:HG11	1.80	0.64
1:Z:65:GLU:OE1	2:G:141:ASN:HB3	1.96	0.64
2:G:384:ASN:ND2	2:G:394:ARG:HE	1.95	0.64
2:G:103:LEU:HD22	2:G:247:VAL:HG22	1.79	0.64
2:E:211:GLN:HG2	2:E:212:LYS:N	2.12	0.64
1:A:65:GLU:HG2	2:E:143:TRP:HE1	1.62	0.64
2:I:130:ARG:NH2	2:I:229:GLU:HG3	2.12	0.64
1:V:3:ILE:HD11	1:V:46:PHE:O	1.98	0.64
1:V:30:ASN:HD22	1:V:30:ASN:H	1.43	0.64
2:F:108:VAL:C	2:F:110:MET:H	2.01	0.64
1:A:87:MET:CE	1:B:84:THR:HG23	2.27	0.64
1:Z:13:VAL:HG12	1:Z:170:GLU:HG3	1.80	0.64
1:B:59:LEU:HG	1:B:78:LEU:CD1	2.28	0.64
1:B:105:ILE:HD11	1:B:120:ILE:HG23	1.79	0.64
2:I:122:ARG:NH1	2:I:126:LEU:HD23	2.10	0.64
2:E:89:VAL:HG12	2:E:93:GLY:CA	2.27	0.64
1:D:1:THR:HB	1:D:33:LYS:HZ3	1.61	0.64
1:C:56:LEU:HD13	1:C:95:LEU:HD11	1.80	0.64
1:Y:152:LEU:HD13	1:Y:166:HIS:ND1	2.12	0.64
1:Z:84:THR:HG23	1:Z:85:ASP:H	1.62	0.64
2:G:211:GLN:HG2	2:G:212:LYS:N	2.11	0.64
1:V:71:LEU:HD21	1:V:97:VAL:CG1	2.28	0.64
2:F:41:ASN:C	2:F:41:ASN:HD22	2.01	0.64
2:F:135:LEU:HD13	2:F:159:PHE:HD2	1.63	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:211:GLN:NE2	2:F:212:LYS:H	1.96	0.63
2:I:147:GLU:CG	2:I:150:GLN:NE2	2.61	0.63
2:F:151:GLU:CB	2:F:152:PRO:CD	2.74	0.63
1:V:17:ASP:O	1:V:33:LYS:HD2	1.97	0.63
1:Z:105:ILE:CD1	1:Z:120:ILE:HG23	2.29	0.63
2:E:214:ARG:HD3	2:E:216:LEU:HD22	1.80	0.63
2:G:91:TYR:O	2:G:92:VAL:HG22	1.99	0.63
2:G:89:VAL:HG12	2:G:93:GLY:C	2.19	0.63
1:Y:60:PHE:HD1	1:Y:78:LEU:HD22	1.63	0.63
1:A:77:GLU:O	1:A:80:LYS:HB2	1.98	0.63
2:E:345:THR:HG21	2:E:373:ILE:HD13	1.81	0.63
2:I:96:VAL:HG11	2:I:281:LEU:HD12	1.80	0.63
2:G:152:PRO:CB	2:G:156:ARG:H	2.10	0.63
2:G:359:MET:HG3	2:G:366:ILE:HG13	1.80	0.63
2:I:140:LYS:H	2:I:140:LYS:HD3	1.63	0.63
1:C:83:ARG:HG3	1:C:83:ARG:HH11	1.64	0.63
2:E:168:LEU:HD23	2:E:219:LYS:HB3	1.81	0.63
2:I:86:PHE:O	2:I:89:VAL:HG22	1.98	0.63
2:I:123:ALA:HA	2:I:127:ALA:HB3	1.80	0.63
2:I:223:LYS:HD2	2:I:223:LYS:N	2.14	0.63
1:Y:136:LEU:HB3	1:Y:147:ILE:CD1	2.28	0.63
2:G:174:GLU:CB	2:G:211:GLN:HG3	2.25	0.63
2:I:20:GLN:O	2:I:24:LYS:HG3	1.99	0.63
2:E:130:ARG:CD	2:E:225:LEU:HD11	2.26	0.63
1:Y:70:HIS:HE1	1:Y:72:VAL:HB	1.64	0.63
2:F:351:ILE:N	2:F:351:ILE:HD13	2.14	0.63
2:F:140:LYS:H	2:F:140:LYS:HD3	1.63	0.63
1:C:36:ARG:NE	1:C:169:GLU:OE1	2.31	0.63
1:B:38:TYR:HB2	1:B:64:LEU:HD12	1.81	0.63
1:V:105:ILE:HD11	1:V:120:ILE:HG21	1.81	0.62
2:G:171:LYS:HG3	2:G:218:ILE:HD11	1.81	0.62
2:G:147:GLU:HA	2:G:150:GLN:HG3	1.81	0.62
2:I:212:LYS:NZ	2:I:212:LYS:HB2	2.14	0.62
1:D:136:LEU:CD1	1:V:135:ALA:HB1	2.29	0.62
2:F:131:ILE:HG21	2:F:222:MET:HE1	1.81	0.62
2:F:312:ILE:HD13	2:F:312:ILE:N	2.14	0.62
1:Y:28:LYS:HZ1	1:Y:30:ASN:ND2	1.97	0.62
2:E:122:ARG:CZ	2:E:126:LEU:HD21	2.30	0.62
1:D:152:LEU:HD13	1:D:166:HIS:CE1	2.35	0.62
2:F:218:ILE:O	2:F:222:MET:HB3	1.98	0.62
1:C:170:GLU:HG3	1:C:171:LEU:H	1.65	0.62
1:X:149:GLU:HG2	1:X:168:ILE:HD11	1.82	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:V:86:ARG:HA	1:V:89:ARG:CZ	2.29	0.62
2:G:170:ASP:HB3	2:G:217:LYS:HD3	1.79	0.62
1:V:6:VAL:HG21	1:V:147:ILE:HG22	1.80	0.62
2:I:153:SER:C	2:I:157:GLN:HB2	2.19	0.62
1:X:73:LYS:HZ1	1:X:77:GLU:HG3	1.64	0.62
2:G:214:ARG:HD3	2:G:216:LEU:HD22	1.80	0.62
1:B:131:ALA:HB3	1:Z:131:ALA:HB3	1.80	0.62
1:A:47:ALA:HB3	1:A:94:LEU:HB2	1.82	0.62
2:I:12:GLU:HG2	2:I:73:LEU:HD13	1.82	0.62
1:A:117:ASN:O	1:A:118:ASP:HB2	1.99	0.62
2:E:173:ILE:HD11	2:E:221:ALA:CB	2.30	0.62
2:F:393:ARG:HG2	2:F:393:ARG:NH1	2.13	0.62
2:G:440:ARG:HD3	2:I:314:LYS:HD3	1.81	0.62
1:B:154:ILE:CD1	1:Z:134:ARG:HG2	2.29	0.62
2:F:89:VAL:HA	2:F:92:VAL:C	2.19	0.61
1:X:62:ARG:O	1:X:66:MET:HB2	1.99	0.61
2:F:220:ASP:O	2:F:224:LEU:HD23	2.00	0.61
2:E:140:LYS:O	2:E:141:ASN:HB2	1.98	0.61
1:V:34:VAL:HB	1:V:167:THR:HG22	1.82	0.61
1:Z:80:LYS:O	1:Z:84:THR:HG22	1.99	0.61
2:F:102:ASP:C	2:F:104:THR:H	2.03	0.61
1:Y:53:ALA:O	1:Y:55:THR:N	2.33	0.61
2:F:167:GLN:O	2:F:168:LEU:HB3	2.00	0.61
2:I:132:LEU:HA	2:I:135:LEU:HD12	1.83	0.61
1:Z:10:GLY:HA3	1:Z:174:LYS:CA	2.27	0.61
2:G:375:ARG:CZ	2:G:422:ALA:HB1	2.30	0.61
2:I:432:LEU:N	2:I:432:LEU:HD12	2.15	0.61
2:I:375:ARG:HB3	2:I:425:VAL:HG11	1.82	0.61
2:I:132:LEU:HD23	2:I:135:LEU:HD12	1.83	0.61
1:C:38:TYR:CG	1:C:64:LEU:HD13	2.35	0.61
2:E:292:THR:HG22	2:E:294:HIS:H	1.66	0.61
2:I:217:LYS:HG3	2:I:218:ILE:N	2.16	0.61
1:C:64:LEU:HD23	1:C:74:ALA:CB	2.30	0.61
1:V:47:ALA:HB3	1:V:94:LEU:HB2	1.83	0.61
1:Y:141:GLU:HA	1:Y:141:GLU:OE2	1.99	0.61
1:Y:1:THR:HB	1:Y:33:LYS:HZ2	1.64	0.61
1:X:60:PHE:CZ	1:X:97:VAL:HG11	2.35	0.61
1:V:70:HIS:HE1	1:V:72:VAL:HB	1.66	0.61
1:A:15:ALA:HB1	1:A:152:LEU:HD12	1.80	0.61
1:B:136:LEU:CD1	1:Z:135:ALA:HB1	2.31	0.61
1:V:71:LEU:HD21	1:V:97:VAL:HG11	1.81	0.61
1:V:46:PHE:HB3	1:V:57:PHE:CZ	2.36	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:116:ILE:O	2:I:120:ARG:HB2	2.00	0.61
2:E:58:PRO:HG2	2:E:61:VAL:HG11	1.81	0.61
1:D:94:LEU:CD2	1:D:107:THR:HG22	2.29	0.61
1:C:152:LEU:HB3	1:C:166:HIS:CE1	2.35	0.61
2:E:109:LYS:HG3	2:E:109:LYS:O	2.01	0.61
1:A:136:LEU:HD13	1:Y:135:ALA:HB1	1.82	0.61
2:F:116:ILE:O	2:F:120:ARG:HB2	2.01	0.61
2:E:432:LEU:H	2:E:432:LEU:HD12	1.66	0.61
2:F:103:LEU:CD1	2:F:247:VAL:HG13	2.31	0.61
2:I:389:ASN:HD22	2:I:391:GLY:H	1.47	0.61
1:Z:1:THR:HB	1:Z:33:LYS:NZ	2.15	0.61
2:G:362:GLU:HG2	2:G:410:ALA:HB1	1.81	0.61
1:V:28:LYS:HE2	1:V:30:ASN:ND2	2.15	0.60
2:G:91:TYR:CD1	2:I:91:TYR:CD2	2.89	0.60
1:Y:1:THR:HB	1:Y:33:LYS:HZ3	1.64	0.60
2:E:432:LEU:N	2:E:432:LEU:HD12	2.15	0.60
2:F:147:GLU:O	2:F:151:GLU:HG2	2.00	0.60
2:F:108:VAL:HA	2:F:111:VAL:HG22	1.83	0.60
2:I:269:GLY:N	2:I:270:PRO:HD2	2.16	0.60
2:F:127:ALA:HA	2:F:130:ARG:NH2	2.16	0.60
1:B:115:PRO:HG3	1:B:120:ILE:HG12	1.82	0.60
2:G:262:CYS:SG	2:G:318:LEU:HD13	2.41	0.60
1:C:59:LEU:HD11	1:C:63:LYS:HE2	1.84	0.60
2:I:389:ASN:C	2:I:389:ASN:HD22	2.05	0.60
1:V:81:ASP:HB3	1:V:88:LEU:CD1	2.31	0.60
1:D:105:ILE:HD11	1:D:120:ILE:HG23	1.83	0.60
2:G:96:VAL:HG11	2:G:281:LEU:HD12	1.84	0.60
2:G:140:LYS:H	2:G:140:LYS:HD3	1.67	0.60
2:F:291:SER:HA	2:F:296:MET:HE2	1.82	0.60
2:F:413:LEU:O	2:F:416:GLN:HG3	2.00	0.60
2:F:217:LYS:O	2:F:220:ASP:HB2	2.02	0.60
2:G:152:PRO:CB	2:G:156:ARG:HB2	2.22	0.60
2:I:344:LEU:HD13	2:I:395:LEU:HD13	1.82	0.60
2:F:262:CYS:SG	2:F:318:LEU:HD13	2.42	0.60
2:E:311:GLN:HE21	2:E:311:GLN:CA	2.12	0.60
2:F:101:ARG:O	2:F:104:THR:HB	2.02	0.60
2:F:358:LEU:O	2:F:361:THR:HB	2.01	0.60
2:F:432:LEU:N	2:F:432:LEU:HD12	2.16	0.60
2:E:151:GLU:HB2	2:E:152:PRO:CD	2.30	0.59
2:F:220:ASP:O	2:F:224:LEU:N	2.27	0.59
1:V:5:SER:HB3	1:V:120:ILE:HB	1.83	0.59
2:I:108:VAL:C	2:I:110:MET:H	2.03	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:V:17:ASP:HA	1:V:165:PHE:O	2.02	0.59
1:D:152:LEU:HD13	1:D:166:HIS:ND1	2.17	0.59
1:B:141:GLU:OE2	1:B:141:GLU:HA	2.02	0.59
2:E:152:PRO:O	2:E:154:ALA:C	2.39	0.59
1:C:10:GLY:HA3	1:C:174:LYS:HA	1.84	0.59
2:E:173:ILE:HG12	2:E:212:LYS:HD2	1.84	0.59
2:G:173:ILE:HD11	2:G:221:ALA:CB	2.31	0.59
1:B:170:GLU:HG2	1:B:171:LEU:H	1.67	0.59
1:C:86:ARG:HG3	1:C:89:ARG:NH2	2.17	0.59
1:A:87:MET:HE1	1:B:84:THR:HG23	1.82	0.59
2:E:169:ASP:O	2:E:218:ILE:HG13	2.03	0.59
2:G:88:GLU:CD	2:I:90:GLY:HA2	2.23	0.59
1:C:37:LEU:N	1:C:37:LEU:HD23	2.16	0.59
1:Y:86:ARG:HA	1:Y:89:ARG:NH1	2.16	0.59
1:X:79:ALA:HB1	1:X:110:GLY:HA2	1.83	0.59
1:B:64:LEU:HD23	1:B:74:ALA:CB	2.32	0.59
2:G:142:ASN:CB	2:G:149:GLN:HE22	2.15	0.59
1:Y:53:ALA:C	1:Y:55:THR:H	2.04	0.59
2:F:123:ALA:HA	2:F:127:ALA:CB	2.31	0.59
1:Y:67:HIS:CD2	1:Y:73:LYS:HD2	2.38	0.59
1:V:86:ARG:HA	1:V:89:ARG:NH1	2.17	0.59
1:X:152:LEU:HD22	1:X:166:HIS:HE1	1.68	0.59
2:I:375:ARG:CZ	2:I:422:ALA:HB1	2.33	0.59
2:I:214:ARG:HE	2:I:216:LEU:HB3	1.67	0.59
2:E:389:ASN:HD22	2:E:391:GLY:H	1.48	0.59
1:C:3:ILE:O	1:C:121:ALA:HA	2.03	0.59
2:G:116:ILE:O	2:G:120:ARG:HB2	2.02	0.59
2:F:170:ASP:HB3	2:F:217:LYS:HD3	1.84	0.58
2:E:131:ILE:O	2:E:134:VAL:HG12	2.03	0.58
2:G:168:LEU:HD12	2:G:219:LYS:HB3	1.84	0.58
2:G:27:VAL:HG13	2:G:70:LEU:HG	1.85	0.58
2:E:257:GLU:O	2:E:257:GLU:HG3	2.03	0.58
2:E:167:GLN:NE2	2:E:168:LEU:HG	2.18	0.58
2:I:217:LYS:O	2:I:221:ALA:HB3	2.01	0.58
2:I:130:ARG:HH21	2:I:229:GLU:HG3	1.68	0.58
1:C:132:ALA:CB	1:C:154:ILE:HG21	2.33	0.58
1:D:37:LEU:N	1:D:37:LEU:HD23	2.18	0.58
2:F:52:ASN:HB2	2:F:325:ARG:O	2.04	0.58
2:F:132:LEU:HD11	2:F:160:ARG:HG2	1.85	0.58
2:F:232:LYS:N	2:F:232:LYS:HZ1	2.01	0.58
2:I:101:ARG:O	2:I:104:THR:HB	2.02	0.58
2:I:312:ILE:HG12	2:I:313:ALA:N	2.19	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:86:PHE:O	2:E:89:VAL:HG22	2.03	0.58
1:C:28:LYS:HD3	1:C:31:VAL:HG22	1.84	0.58
1:V:73:LYS:NZ	1:V:77:GLU:HG2	2.18	0.58
1:B:154:ILE:HD12	1:Z:134:ARG:CG	2.33	0.58
2:G:122:ARG:NH1	2:G:126:LEU:HD21	2.19	0.58
2:G:174:GLU:CA	2:G:212:LYS:HB3	2.34	0.58
2:I:12:GLU:HG2	2:I:73:LEU:CD1	2.34	0.58
1:D:62:ARG:O	1:D:66:MET:HB2	2.04	0.58
1:Z:88:LEU:HD12	1:Z:88:LEU:H	1.69	0.58
2:I:217:LYS:CG	2:I:218:ILE:H	2.11	0.58
1:Z:86:ARG:HA	1:Z:89:ARG:NH2	2.18	0.58
1:D:64:LEU:HB3	1:D:69:GLY:HA2	1.85	0.58
1:C:157:ASP:OD2	1:C:164:HIS:NE2	2.34	0.58
1:B:36:ARG:O	1:B:37:LEU:HD23	2.03	0.58
1:Y:168:ILE:N	1:Y:168:ILE:HD12	2.18	0.58
2:I:135:LEU:HD23	2:I:171:LYS:HE2	1.86	0.58
1:Y:60:PHE:HE1	1:Y:75:ALA:HA	1.69	0.58
2:G:231:ALA:C	2:G:233:LEU:H	2.06	0.58
2:I:130:ARG:HG2	2:I:225:LEU:HD11	1.84	0.58
2:I:27:VAL:CG1	2:I:70:LEU:HG	2.33	0.58
1:V:54:PHE:HD1	1:X:76:VAL:HG21	1.69	0.58
2:G:214:ARG:HG2	2:G:215:LYS:N	2.19	0.57
1:V:70:HIS:CE1	1:V:72:VAL:HB	2.39	0.57
1:A:152:LEU:HD13	1:A:166:HIS:ND1	2.19	0.57
2:E:337:THR:O	2:E:341:GLU:HG3	2.03	0.57
2:I:89:VAL:HG11	2:I:94:LYS:O	2.03	0.57
1:V:136:LEU:HB3	1:V:147:ILE:CD1	2.34	0.57
1:Y:72:VAL:O	1:Y:75:ALA:HB3	2.03	0.57
2:G:389:ASN:HD22	2:G:391:GLY:H	1.49	0.57
2:F:235:ASN:HB2	2:F:236:PRO:HD2	1.86	0.57
1:V:139:ASN:HD22	1:V:139:ASN:N	2.02	0.57
2:I:103:LEU:CD1	2:I:247:VAL:HG13	2.34	0.57
1:X:100:GLU:OE2	1:X:173:TYR:HB2	2.04	0.57
2:I:127:ALA:HA	2:I:130:ARG:NH2	2.18	0.57
1:Y:46:PHE:CE2	1:Y:53:ALA:HB2	2.39	0.57
2:E:4:MET:HE1	2:E:73:LEU:HD11	1.86	0.57
1:C:159:CYS:HB3	1:C:162:THR:HB	1.86	0.57
2:G:359:MET:CE	2:I:36:ARG:NH1	2.67	0.57
2:I:401:ARG:NH2	2:I:442:ILE:HG13	2.19	0.57
2:E:134:VAL:CG1	2:E:171:LYS:HD3	2.34	0.57
1:C:168:ILE:N	1:C:168:ILE:HD12	2.19	0.57
2:F:108:VAL:HG21	2:F:294:HIS:HD2	1.69	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:356:LYS:HA	2:F:366:ILE:HG22	1.86	0.57
2:G:312:ILE:N	2:G:312:ILE:HD13	2.15	0.57
1:C:73:LYS:O	1:C:76:VAL:HG12	2.05	0.57
1:V:170:GLU:HG3	1:V:171:LEU:H	1.70	0.57
2:I:168:LEU:O	2:I:217:LYS:HD2	2.04	0.57
1:B:46:PHE:CE2	1:B:53:ALA:HB2	2.40	0.57
2:E:147:GLU:CA	2:E:150:GLN:HG3	2.34	0.57
2:I:89:VAL:HA	2:I:92:VAL:C	2.24	0.57
2:I:219:LYS:HA	2:I:219:LYS:HE3	1.85	0.57
1:C:73:LYS:HA	1:C:76:VAL:HG12	1.87	0.57
1:Z:12:VAL:HG12	1:Z:171:LEU:HB3	1.86	0.57
1:Z:152:LEU:HD13	1:Z:166:HIS:CE1	2.40	0.57
2:G:122:ARG:NE	2:G:126:LEU:HD21	2.20	0.57
2:F:151:GLU:HB2	2:F:152:PRO:HD3	1.87	0.57
1:B:128:TYR:O	1:Z:131:ALA:HB1	2.05	0.57
1:C:17:ASP:O	1:C:33:LYS:HD2	2.05	0.57
2:I:89:VAL:HA	2:I:92:VAL:O	2.04	0.57
2:F:174:GLU:HA	2:F:212:LYS:HB3	1.86	0.56
1:X:30:ASN:N	1:X:30:ASN:HD22	1.86	0.56
1:Z:51:ALA:HB2	1:Y:111:ASP:OD2	2.05	0.56
2:F:239:LEU:HD23	2:F:240:LYS:N	2.19	0.56
2:G:312:ILE:HG12	2:G:313:ALA:N	2.20	0.56
1:Y:99:ASP:OD2	1:Y:101:THR:HB	2.04	0.56
2:G:441:PHE:HD1	2:I:56:ILE:HD13	1.69	0.56
1:Z:115:PRO:HG3	1:Z:120:ILE:HG12	1.87	0.56
2:F:58:PRO:HG2	2:F:61:VAL:HG11	1.87	0.56
1:A:55:THR:OG1	1:B:83:ARG:NH2	2.36	0.56
1:A:88:LEU:H	1:A:88:LEU:CD1	2.18	0.56
2:F:210:LYS:N	2:F:210:LYS:HD3	2.19	0.56
1:V:39:ASN:O	1:V:41:LYS:HG3	2.06	0.56
2:E:262:CYS:SG	2:E:318:LEU:HD13	2.45	0.56
2:F:217:LYS:HZ2	2:F:217:LYS:HB2	1.69	0.56
2:F:229:GLU:OE2	2:F:232:LYS:HD2	2.05	0.56
2:E:130:ARG:HB2	2:E:130:ARG:CZ	2.35	0.56
2:G:88:GLU:HB3	2:I:90:GLY:HA2	1.87	0.56
2:E:389:ASN:ND2	2:E:389:ASN:C	2.58	0.56
1:C:67:HIS:NE2	1:C:77:GLU:HG3	2.20	0.56
1:X:152:LEU:HD13	1:X:166:HIS:CE1	2.40	0.56
2:G:432:LEU:CD1	2:G:432:LEU:H	2.17	0.56
1:D:10:GLY:HA2	1:D:173:TYR:CZ	2.40	0.56
1:Z:36:ARG:NH1	1:Z:40:ASP:O	2.38	0.56
2:E:12:GLU:OE1	2:E:15:LYS:HE2	2.06	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:130:ARG:CD	2:G:225:LEU:HD11	2.35	0.56
2:G:91:TYR:HB3	2:I:91:TYR:HA	1.88	0.56
2:F:108:VAL:C	2:F:110:MET:N	2.59	0.56
1:Z:105:ILE:HD11	1:Z:120:ILE:HG23	1.86	0.56
2:F:76:ALA:HB1	2:F:250:HIS:O	2.04	0.56
2:E:52:ASN:HB2	2:E:325:ARG:O	2.05	0.56
2:I:210:LYS:N	2:I:210:LYS:HD3	2.20	0.56
2:F:65:GLU:HG3	3:F:1450:ADP:H2'	1.87	0.56
1:D:1:THR:HB	1:D:33:LYS:NZ	2.20	0.56
2:G:361:THR:HG21	2:I:36:ARG:HA	1.86	0.56
2:I:76:ALA:HB1	2:I:250:HIS:O	2.06	0.56
1:Y:62:ARG:HA	1:Y:65:GLU:HG3	1.88	0.56
2:E:77:PRO:HB2	2:E:103:LEU:HD21	1.88	0.56
1:Z:88:LEU:CD1	1:Z:88:LEU:H	2.19	0.56
2:G:34:ARG:CZ	2:G:250:HIS:HA	2.36	0.56
1:Y:38:TYR:HB2	1:Y:64:LEU:HD12	1.87	0.56
2:I:96:VAL:HG12	2:I:284:LEU:HD11	1.88	0.56
2:E:216:LEU:N	2:E:216:LEU:HD23	2.21	0.56
1:C:64:LEU:HA	1:C:74:ALA:CB	2.36	0.56
1:B:19:GLN:HB2	1:B:163:ASN:ND2	2.21	0.56
2:I:158:ALA:HB1	2:I:162:LYS:NZ	2.21	0.56
2:G:145:GLN:C	2:G:147:GLU:H	2.09	0.56
2:G:88:GLU:CD	2:I:90:GLY:CA	2.74	0.56
1:B:154:ILE:HD12	1:Z:134:ARG:HB3	1.87	0.56
1:A:36:ARG:NH1	1:A:40:ASP:O	2.36	0.56
2:G:311:GLN:CA	2:G:311:GLN:HE21	2.19	0.56
2:F:173:ILE:HD13	2:F:173:ILE:N	2.20	0.56
2:F:163:LEU:HD11	2:F:222:MET:CE	2.35	0.56
1:X:105:ILE:CD1	1:X:120:ILE:HG23	2.36	0.56
2:E:232:LYS:NZ	2:E:232:LYS:HB3	2.21	0.56
2:E:152:PRO:HB3	2:E:156:ARG:H	1.72	0.55
1:V:136:LEU:HB3	1:V:147:ILE:HD12	1.88	0.55
1:B:62:ARG:O	1:B:66:MET:HG3	2.06	0.55
1:Z:149:GLU:HG2	1:Z:168:ILE:HD11	1.88	0.55
1:Y:98:ALA:CB	1:Y:103:SER:HB3	2.36	0.55
1:X:86:ARG:CG	1:X:89:ARG:HH22	2.19	0.55
1:B:154:ILE:HD12	1:Z:134:ARG:HG2	1.86	0.55
2:I:103:LEU:HD13	2:I:247:VAL:HG22	1.88	0.55
2:G:58:PRO:HG2	2:G:61:VAL:HG11	1.89	0.55
2:E:151:GLU:CB	2:E:152:PRO:CD	2.84	0.55
2:F:135:LEU:HD22	2:F:159:PHE:CE2	2.41	0.55
2:E:173:ILE:HD11	2:E:221:ALA:HB1	1.88	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:221:ALA:O	2:I:225:LEU:HD23	2.05	0.55
2:E:27:VAL:CG1	2:E:70:LEU:HG	2.36	0.55
1:D:55:THR:O	1:D:58:GLU:HB3	2.07	0.55
1:D:83:ARG:CB	1:D:83:ARG:HH11	2.14	0.55
2:G:147:GLU:HA	2:G:150:GLN:CG	2.35	0.55
2:G:130:ARG:CG	2:G:225:LEU:HD11	2.36	0.55
2:I:135:LEU:HB3	2:I:159:PHE:CD2	2.41	0.55
1:C:85:ASP:O	1:C:89:ARG:HB2	2.06	0.55
1:D:28:LYS:HG2	1:D:31:VAL:HG22	1.89	0.55
1:V:63:LYS:HD2	1:V:77:GLU:HB3	1.88	0.55
1:Z:15:ALA:HB1	1:Z:152:LEU:HD12	1.87	0.55
1:A:6:VAL:HG21	1:A:147:ILE:HG22	1.86	0.55
2:F:216:LEU:CD2	2:F:221:ALA:HB2	2.36	0.55
2:F:225:LEU:HA	2:F:228:GLU:CB	2.37	0.55
1:B:72:VAL:O	1:B:75:ALA:HB3	2.06	0.55
2:F:153:SER:N	2:F:156:ARG:HB3	2.21	0.55
1:V:132:ALA:CB	1:V:154:ILE:HG21	2.35	0.55
2:E:269:GLY:N	2:E:270:PRO:HD2	2.21	0.55
2:I:25:ARG:O	2:I:29:ILE:HG12	2.07	0.55
2:F:345:THR:CG2	2:F:373:ILE:HD12	2.36	0.55
2:E:92:VAL:HG21	2:F:91:TYR:C	2.27	0.55
1:A:28:LYS:HZ2	1:A:30:ASN:ND2	2.04	0.55
2:F:32:ARG:O	2:F:36:ARG:HG3	2.07	0.55
1:X:10:GLY:HA2	1:X:173:TYR:CE1	2.42	0.55
2:F:269:GLY:N	2:F:270:PRO:HD2	2.21	0.55
2:I:151:GLU:HB2	2:I:152:PRO:HD3	1.89	0.55
2:G:109:LYS:HB2	2:I:296:MET:HG2	1.87	0.55
2:I:235:ASN:OD1	2:I:238:GLU:HB2	2.07	0.55
1:D:6:VAL:HG21	1:D:147:ILE:HG22	1.88	0.55
2:G:147:GLU:O	2:G:150:GLN:HG3	2.07	0.55
1:V:63:LYS:HA	1:V:66:MET:HE3	1.89	0.55
1:V:67:HIS:CD2	1:V:73:LYS:HE2	2.42	0.55
1:V:83:ARG:CG	1:V:83:ARG:HH11	2.19	0.55
2:E:96:VAL:HG12	2:E:284:LEU:HD11	1.89	0.55
2:G:382:GLN:O	2:G:386:SER:HB3	2.07	0.55
1:X:83:ARG:CZ	1:X:83:ARG:HB3	2.36	0.55
2:E:174:GLU:HA	2:E:213:ALA:H	1.72	0.55
2:I:122:ARG:CZ	2:I:122:ARG:HA	2.37	0.55
2:I:167:GLN:O	2:I:168:LEU:HB3	2.05	0.55
2:F:89:VAL:HG12	2:F:93:GLY:CA	2.36	0.55
2:I:393:ARG:NH2	3:I:3450:ADP:O1B	2.40	0.55
2:F:270:PRO:O	2:F:273:SER:HB3	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:1:THR:HB	1:X:33:LYS:NZ	2.22	0.55
1:Z:28:LYS:NZ	1:Z:30:ASN:ND2	2.55	0.55
1:Z:8:ARG:NH1	1:Z:142:LEU:O	2.32	0.55
2:E:131:ILE:HD11	2:E:218:ILE:CD1	2.37	0.54
2:G:124:GLU:HA	2:G:127:ALA:CB	2.37	0.54
2:I:140:LYS:O	2:I:141:ASN:HB3	2.07	0.54
2:I:432:LEU:H	2:I:432:LEU:HD12	1.71	0.54
2:E:150:GLN:O	2:E:153:SER:CB	2.54	0.54
1:B:140:THR:CG2	1:Z:140:THR:CG2	2.84	0.54
1:A:28:LYS:HD2	1:B:113:VAL:CG1	2.36	0.54
1:B:168:ILE:HD12	1:B:168:ILE:N	2.23	0.54
1:X:86:ARG:HG2	1:X:89:ARG:HH22	1.71	0.54
1:X:85:ASP:HB3	1:X:88:LEU:HB2	1.88	0.54
1:V:38:TYR:N	1:V:61:GLU:OE1	2.40	0.54
1:V:83:ARG:CZ	1:V:83:ARG:HB3	2.37	0.54
1:X:64:LEU:O	1:X:69:GLY:N	2.36	0.54
2:E:312:ILE:N	2:E:312:ILE:HD13	2.12	0.54
1:Y:70:HIS:CE1	1:Y:73:LYS:H	2.25	0.54
2:F:91:TYR:O	2:F:92:VAL:HG22	2.07	0.54
2:G:131:ILE:HD11	2:G:218:ILE:CG1	2.38	0.54
2:E:140:LYS:HD3	2:E:140:LYS:H	1.72	0.54
2:G:358:LEU:O	2:G:361:THR:HB	2.08	0.54
2:F:59:THR:O	2:F:61:VAL:HG13	2.07	0.54
1:B:99:ASP:OD2	1:B:101:THR:HB	2.07	0.54
1:X:1:THR:HB	1:X:33:LYS:HZ3	1.73	0.54
2:F:35:TRP:O	2:F:39:GLN:HG2	2.08	0.54
2:E:112:ARG:HG3	2:E:112:ARG:HH11	1.72	0.54
2:F:131:ILE:HD11	2:F:218:ILE:HD13	1.88	0.54
2:I:214:ARG:NE	2:I:216:LEU:HB3	2.23	0.54
2:I:171:LYS:HZ3	2:I:218:ILE:HD11	1.73	0.54
2:I:108:VAL:C	2:I:110:MET:N	2.61	0.54
1:A:152:LEU:HD13	1:A:166:HIS:CE1	2.42	0.54
1:Z:88:LEU:HD12	1:Z:88:LEU:N	2.21	0.54
1:B:53:ALA:O	1:B:55:THR:N	2.40	0.54
1:Y:43:ILE:HG12	1:Y:98:ALA:O	2.07	0.54
2:F:264:ARG:NE	2:F:265:GLY:H	2.05	0.54
2:E:63:LYS:HD3	2:E:332:LEU:HD13	1.88	0.54
2:F:212:LYS:NZ	2:F:212:LYS:HB2	2.23	0.54
2:E:108:VAL:C	2:E:110:MET:H	2.11	0.54
2:G:86:PHE:O	2:G:89:VAL:HG22	2.07	0.54
1:C:3:ILE:HD11	1:C:46:PHE:O	2.08	0.54
2:E:408:TYR:HD1	2:F:29:ILE:HD11	1.73	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:V:90:LYS:NZ	1:X:89:ARG:NH1	2.56	0.54
2:F:292:THR:C	2:F:294:HIS:H	2.11	0.54
1:Z:95:LEU:HB2	1:Z:106:ILE:HB	1.90	0.54
1:B:6:VAL:HG12	1:B:7:ARG:N	2.22	0.54
2:F:135:LEU:CG	2:F:171:LYS:HE2	2.35	0.54
2:F:103:LEU:O	2:F:107:ALA:HB2	2.08	0.54
2:I:358:LEU:O	2:I:361:THR:HB	2.06	0.54
1:B:86:ARG:HA	1:B:89:ARG:NH1	2.23	0.53
1:C:6:VAL:HG21	1:C:147:ILE:CG2	2.38	0.53
1:Y:98:ALA:HB2	1:Y:103:SER:HB3	1.90	0.53
1:V:159:CYS:HB3	1:V:162:THR:HB	1.90	0.53
2:E:230:ALA:O	2:E:233:LEU:HB3	2.08	0.53
1:V:141:GLU:OE2	1:V:141:GLU:HA	2.07	0.53
1:A:10:GLY:HA3	1:A:174:LYS:CA	2.37	0.53
1:X:14:ILE:HD12	1:X:43:ILE:HG12	1.90	0.53
2:I:393:ARG:HH11	2:I:393:ARG:HG2	1.72	0.53
2:F:223:LYS:HD2	2:F:223:LYS:N	2.23	0.53
2:E:167:GLN:HE22	2:E:168:LEU:HG	1.73	0.53
2:G:217:LYS:HG3	2:G:219:LYS:HZ3	1.72	0.53
2:E:344:LEU:HD23	2:E:373:ILE:HG23	1.89	0.53
1:C:154:ILE:HG22	1:C:155:ALA:N	2.23	0.53
1:V:1:THR:HB	1:V:33:LYS:NZ	2.23	0.53
1:A:88:LEU:H	1:A:88:LEU:HD12	1.74	0.53
1:A:12:VAL:HG12	1:A:171:LEU:HB3	1.90	0.53
2:F:147:GLU:HG2	2:F:150:GLN:HE21	1.72	0.53
1:Y:115:PRO:HG3	1:Y:120:ILE:HG12	1.90	0.53
1:Y:64:LEU:HD23	1:Y:74:ALA:CB	2.38	0.53
2:G:257:GLU:O	2:G:257:GLU:HG3	2.08	0.53
2:F:257:GLU:HB2	2:F:260:LYS:CG	2.39	0.53
1:X:73:LYS:NZ	1:X:77:GLU:HG3	2.23	0.53
2:G:408:TYR:HB2	2:I:29:ILE:HD11	1.91	0.53
2:F:23:ALA:HB1	2:F:55:MET:HE3	1.90	0.53
1:X:86:ARG:HA	1:X:89:ARG:HH12	1.73	0.53
2:F:151:GLU:CB	2:F:152:PRO:HD3	2.39	0.53
2:G:116:ILE:O	2:G:116:ILE:HG22	2.08	0.53
2:I:103:LEU:O	2:I:107:ALA:HB2	2.09	0.53
2:G:173:ILE:HG12	2:G:212:LYS:CD	2.38	0.53
2:F:89:VAL:HG12	2:F:93:GLY:HA3	1.90	0.53
1:B:60:PHE:HD1	1:B:78:LEU:HD22	1.73	0.53
1:V:71:LEU:HD13	1:V:71:LEU:C	2.29	0.53
1:V:3:ILE:HB	1:V:122:ILE:CG1	2.37	0.53
2:F:135:LEU:HB3	2:F:159:PHE:CD2	2.43	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:109:ASN:O	1:X:110:GLY:C	2.46	0.53
1:V:94:LEU:HB3	1:V:122:ILE:HD12	1.89	0.53
1:Z:60:PHE:CE2	1:Z:97:VAL:HG21	2.44	0.53
1:V:86:ARG:HA	1:V:89:ARG:NH2	2.24	0.53
1:V:6:VAL:HG21	1:V:147:ILE:CG2	2.39	0.53
1:Y:10:GLY:HA2	1:Y:173:TYR:CZ	2.44	0.53
1:Y:79:ALA:O	1:Y:83:ARG:HG2	2.09	0.53
2:I:345:THR:CG2	2:I:373:ILE:CD1	2.87	0.53
2:F:140:LYS:O	2:F:141:ASN:HB3	2.09	0.53
2:E:322:LEU:O	2:E:326:LEU:HD22	2.09	0.53
2:G:150:GLN:O	2:G:153:SER:OG	2.27	0.52
2:G:126:LEU:O	2:G:130:ARG:NH2	2.40	0.52
2:I:130:ARG:CG	2:I:225:LEU:HD11	2.39	0.52
2:I:173:ILE:N	2:I:173:ILE:HD13	2.25	0.52
1:V:28:LYS:CE	1:V:30:ASN:ND2	2.72	0.52
2:F:108:VAL:HG21	2:F:294:HIS:CD2	2.44	0.52
1:Y:10:GLY:HA2	1:Y:173:TYR:CE1	2.44	0.52
2:G:232:LYS:NZ	2:G:232:LYS:HB3	2.24	0.52
1:X:115:PRO:HG3	1:X:120:ILE:HG12	1.91	0.52
1:Z:38:TYR:HE1	1:Z:65:GLU:HG2	1.73	0.52
1:Z:149:GLU:OE1	1:Z:168:ILE:HD11	2.09	0.52
1:C:13:VAL:HG12	1:C:170:GLU:CA	2.33	0.52
2:E:172:GLU:HG3	2:E:214:ARG:O	2.08	0.52
2:I:312:ILE:N	2:I:312:ILE:HD13	2.12	0.52
2:F:86:PHE:O	2:F:89:VAL:HG22	2.08	0.52
1:C:36:ARG:C	1:C:37:LEU:HD23	2.29	0.52
2:E:358:LEU:O	2:E:361:THR:HB	2.08	0.52
2:F:432:LEU:H	2:F:432:LEU:HD12	1.74	0.52
1:V:64:LEU:HD23	1:V:74:ALA:CB	2.39	0.52
2:E:217:LYS:HG3	2:E:219:LYS:NZ	2.24	0.52
2:G:292:THR:HG22	2:G:293:LYS:N	2.24	0.52
1:A:10:GLY:HA2	1:A:173:TYR:CZ	2.43	0.52
2:G:134:VAL:HG21	2:G:172:GLU:O	2.08	0.52
1:V:148:ALA:O	1:V:152:LEU:HB2	2.10	0.52
2:I:366:ILE:HG13	2:I:420:ILE:CD1	2.39	0.52
2:E:140:LYS:HD3	2:E:140:LYS:N	2.25	0.52
2:G:359:MET:HE1	2:I:36:ARG:NH1	2.24	0.52
2:E:257:GLU:O	2:E:257:GLU:CG	2.57	0.52
2:F:366:ILE:HD12	2:F:418:ILE:HB	1.90	0.52
2:F:21:ASP:HA	2:F:24:LYS:HD2	1.91	0.52
2:I:211:GLN:NE2	2:I:212:LYS:H	2.08	0.52
1:C:168:ILE:HG22	1:C:169:GLU:N	2.25	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Z:7:ARG:HB2	1:Z:12:VAL:HG23	1.91	0.52
2:G:401:ARG:NH2	2:I:329:ARG:O	2.42	0.52
1:D:85:ASP:HB3	1:D:88:LEU:HB2	1.92	0.52
2:I:362:GLU:HG3	2:I:411:SER:HA	1.90	0.52
1:C:140:THR:HG22	1:X:140:THR:HG22	1.92	0.52
1:Z:10:GLY:HA2	1:Z:173:TYR:CZ	2.44	0.52
1:B:136:LEU:HB3	1:B:147:ILE:CD1	2.39	0.52
2:G:292:THR:HB	2:G:295:GLY:O	2.10	0.52
2:G:128:GLU:O	2:G:131:ILE:HG22	2.10	0.52
1:V:36:ARG:C	1:V:37:LEU:HD23	2.30	0.52
2:I:140:LYS:HD3	2:I:140:LYS:N	2.25	0.52
2:F:362:GLU:HG3	2:F:411:SER:HA	1.92	0.52
2:E:131:ILE:HD11	2:E:218:ILE:CG1	2.40	0.52
2:I:174:GLU:HA	2:I:212:LYS:HB3	1.92	0.52
1:A:33:LYS:HA	1:A:46:PHE:CE1	2.45	0.52
2:G:362:GLU:HG2	2:G:410:ALA:CB	2.39	0.52
2:E:311:GLN:NE2	2:E:311:GLN:CA	2.72	0.52
2:F:356:LYS:HA	2:F:366:ILE:CG2	2.40	0.52
2:G:405:GLU:HG3	2:G:428:HIS:CE1	2.45	0.52
2:E:76:ALA:HB1	2:E:250:HIS:O	2.09	0.52
2:G:130:ARG:HB2	2:G:130:ARG:CZ	2.40	0.52
1:A:149:GLU:HG2	1:A:168:ILE:HD11	1.91	0.52
1:V:13:VAL:HG12	1:V:170:GLU:HA	1.92	0.52
1:A:88:LEU:N	1:A:88:LEU:HD12	2.25	0.52
1:A:105:ILE:CD1	1:A:120:ILE:HG23	2.40	0.52
1:V:90:LYS:HZ1	1:X:89:ARG:HH11	1.58	0.52
1:V:152:LEU:HD13	1:V:166:HIS:CE1	2.45	0.52
2:E:122:ARG:NH1	2:E:126:LEU:HD21	2.24	0.52
1:X:70:HIS:ND1	1:X:73:LYS:HB2	2.24	0.52
2:E:311:GLN:N	2:E:311:GLN:HE21	2.08	0.52
2:F:23:ALA:HA	2:F:330:VAL:HG21	1.92	0.52
2:F:136:ILE:HD11	2:F:159:PHE:CZ	2.45	0.51
1:Z:8:ARG:O	1:Z:11:HIS:HB2	2.10	0.51
2:E:151:GLU:HB2	2:E:152:PRO:HD2	1.91	0.51
2:G:151:GLU:CB	2:G:152:PRO:CD	2.88	0.51
2:I:89:VAL:HG12	2:I:93:GLY:CA	2.38	0.51
1:B:30:ASN:C	1:B:30:ASN:HD22	2.13	0.51
1:A:66:MET:HB3	1:A:67:HIS:ND1	2.25	0.51
2:E:168:LEU:HD22	2:E:219:LYS:HD3	1.92	0.51
2:I:147:GLU:O	2:I:151:GLU:HG2	2.10	0.51
2:F:147:GLU:CG	2:F:150:GLN:NE2	2.73	0.51
2:I:132:LEU:HD11	2:I:160:ARG:CG	2.36	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:136:ILE:HD11	2:I:159:PHE:CZ	2.46	0.51
1:B:128:TYR:CE1	1:Z:127:PRO:HB2	2.45	0.51
2:E:432:LEU:H	2:E:432:LEU:CD1	2.23	0.51
2:G:96:VAL:CG1	2:G:281:LEU:HD12	2.40	0.51
2:G:269:GLY:N	2:G:270:PRO:HD2	2.25	0.51
1:D:70:HIS:ND1	1:D:73:LYS:HB2	2.25	0.51
2:F:135:LEU:CD2	2:F:171:LYS:HE2	2.40	0.51
2:F:225:LEU:HA	2:F:228:GLU:HB3	1.91	0.51
1:V:90:LYS:NZ	1:X:84:THR:O	2.44	0.51
2:I:102:ASP:C	2:I:104:THR:H	2.14	0.51
2:I:211:GLN:HE21	2:I:212:LYS:N	2.09	0.51
2:G:89:VAL:HG12	2:G:93:GLY:CA	2.41	0.51
2:G:108:VAL:HG21	2:G:294:HIS:HD2	1.73	0.51
2:I:315:PRO:O	2:I:318:LEU:HB2	2.10	0.51
2:I:158:ALA:HB1	2:I:162:LYS:HZ2	1.73	0.51
2:E:95:GLU:H	2:E:95:GLU:CD	2.14	0.51
2:I:62:GLY:O	2:I:66:ILE:HG13	2.11	0.51
2:E:132:LEU:HB3	2:E:156:ARG:NH1	2.26	0.51
2:F:168:LEU:O	2:F:217:LYS:HD2	2.11	0.51
2:F:384:ASN:HD21	2:F:390:ILE:HG12	1.76	0.51
1:A:10:GLY:HA2	1:A:173:TYR:CD1	2.44	0.51
1:B:60:PHE:CE2	1:B:97:VAL:HG21	2.45	0.51
2:G:171:LYS:HE3	2:G:172:GLU:N	2.26	0.51
1:A:28:LYS:HE2	1:B:114:GLN:O	2.10	0.51
1:C:90:LYS:HE2	1:D:89:ARG:CZ	2.40	0.51
1:A:95:LEU:HB2	1:A:106:ILE:HB	1.91	0.51
1:Y:95:LEU:HD12	1:Y:95:LEU:N	2.25	0.51
2:I:211:GLN:HE21	2:I:212:LYS:H	1.56	0.51
2:I:163:LEU:HD11	2:I:222:MET:HE3	1.92	0.51
1:C:136:LEU:HB3	1:C:147:ILE:CD1	2.41	0.51
1:D:105:ILE:CD1	1:D:120:ILE:HG23	2.39	0.51
2:I:311:GLN:CA	2:I:311:GLN:HE21	2.23	0.51
1:C:5:SER:HA	1:C:13:VAL:O	2.11	0.51
2:I:108:VAL:HA	2:I:111:VAL:CG2	2.37	0.51
1:C:73:LYS:CD	1:C:76:VAL:HG11	2.40	0.51
2:G:212:LYS:CD	2:G:216:LEU:HD21	2.33	0.51
2:I:123:ALA:HA	2:I:127:ALA:CB	2.40	0.51
1:Y:19:GLN:HB2	1:Y:163:ASN:ND2	2.26	0.51
1:D:109:ASN:O	1:D:110:GLY:C	2.49	0.51
1:X:94:LEU:CD2	1:X:107:THR:HG22	2.40	0.51
1:D:30:ASN:ND2	1:D:30:ASN:N	2.54	0.50
1:Z:5:SER:HB3	1:Z:120:ILE:HB	1.92	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:63:LYS:HG2	2:E:332:LEU:HD22	1.92	0.50
2:F:218:ILE:O	2:F:220:ASP:N	2.45	0.50
1:V:103:SER:HB3	1:V:120:ILE:HD11	1.93	0.50
1:B:154:ILE:CD1	1:Z:134:ARG:CG	2.89	0.50
1:C:62:ARG:HA	1:C:65:GLU:OE2	2.11	0.50
2:G:337:THR:O	2:G:341:GLU:HG3	2.11	0.50
1:B:79:ALA:HB1	1:B:110:GLY:HA2	1.93	0.50
2:I:163:LEU:HD11	2:I:222:MET:HE1	1.93	0.50
2:F:143:TRP:HB2	2:F:148:GLN:HE21	1.76	0.50
2:G:112:ARG:HH11	2:G:112:ARG:HG3	1.76	0.50
1:C:28:LYS:CE	1:C:30:ASN:ND2	2.70	0.50
2:E:259:ASP:HB3	2:E:310:PHE:CZ	2.46	0.50
1:A:115:PRO:CG	1:A:119:LEU:O	2.60	0.50
2:G:234:VAL:O	2:G:236:PRO:HD3	2.11	0.50
1:C:103:SER:HB3	1:C:120:ILE:HD11	1.94	0.50
1:Z:149:GLU:OE2	1:Z:166:HIS:HD2	1.94	0.50
1:Y:3:ILE:HB	1:Y:122:ILE:CG1	2.42	0.50
2:F:134:VAL:HG21	2:F:172:GLU:O	2.12	0.50
1:X:64:LEU:HB3	1:X:69:GLY:HA2	1.94	0.50
1:D:73:LYS:NZ	1:D:77:GLU:HG2	2.27	0.50
2:F:17:ILE:N	2:F:17:ILE:HD12	2.26	0.50
2:E:171:LYS:HE3	2:E:172:GLU:N	2.26	0.50
2:I:217:LYS:HB2	2:I:217:LYS:HZ3	1.76	0.50
1:D:43:ILE:HD13	1:D:43:ILE:N	2.21	0.50
2:F:389:ASN:HD22	2:F:389:ASN:C	2.14	0.50
2:F:401:ARG:NH2	2:F:442:ILE:HG13	2.26	0.50
2:I:216:LEU:HD11	2:I:221:ALA:HA	1.94	0.50
1:X:149:GLU:CG	1:X:168:ILE:HD11	2.42	0.50
2:I:432:LEU:H	2:I:432:LEU:CD1	2.25	0.50
2:F:362:GLU:HG2	2:F:410:ALA:CB	2.42	0.50
2:I:164:ARG:O	2:I:165:GLU:HB3	2.11	0.50
1:A:103:SER:O	1:A:104:LEU:HB3	2.12	0.50
1:A:102:ALA:HB1	1:A:114:GLN:OE1	2.11	0.50
2:E:147:GLU:O	2:E:150:GLN:HG3	2.11	0.50
2:G:91:TYR:C	2:G:92:VAL:HG22	2.32	0.50
2:I:130:ARG:CD	2:I:225:LEU:HD11	2.42	0.50
1:B:65:GLU:OE2	2:F:143:TRP:CD1	2.65	0.50
1:Y:12:VAL:HG12	1:Y:171:LEU:HB3	1.94	0.50
2:G:382:GLN:HA	2:G:382:GLN:NE2	2.27	0.50
2:G:165:GLU:HG2	2:G:166:GLY:N	2.26	0.50
1:Z:77:GLU:HA	1:Z:80:LYS:HD2	1.94	0.50
2:I:94:LYS:HZ2	2:I:98:SER:HB3	1.76	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:145:GLN:CA	2:I:145:GLN:HE21	2.24	0.50
1:C:63:LYS:HA	1:C:66:MET:HE3	1.94	0.50
1:B:59:LEU:HD12	1:B:59:LEU:O	2.12	0.50
1:C:1:THR:HB	1:C:33:LYS:NZ	2.27	0.50
1:Z:17:ASP:HA	1:Z:165:PHE:O	2.12	0.50
2:E:408:TYR:HB2	2:F:29:ILE:HD11	1.93	0.50
1:Z:51:ALA:HB3	1:Y:111:ASP:OD2	2.11	0.50
1:X:68:GLN:O	1:X:70:HIS:N	2.45	0.50
2:I:119:ASN:ND2	2:I:233:LEU:HD23	2.27	0.50
1:D:149:GLU:HG2	1:D:168:ILE:HD11	1.94	0.50
2:F:89:VAL:HG12	2:F:93:GLY:C	2.32	0.49
1:A:65:GLU:HG2	2:E:143:TRP:NE1	2.26	0.49
1:V:11:HIS:HA	1:V:171:LEU:O	2.12	0.49
1:D:140:THR:HG22	1:V:140:THR:CG2	2.42	0.49
1:C:173:TYR:CD2	1:C:173:TYR:N	2.80	0.49
2:I:95:GLU:H	2:I:95:GLU:CD	2.16	0.49
1:Z:84:THR:HG23	1:Z:85:ASP:N	2.26	0.49
2:F:147:GLU:HG2	2:F:150:GLN:NE2	2.27	0.49
1:B:28:LYS:HD3	1:B:31:VAL:HG22	1.94	0.49
1:Y:35:ARG:O	1:Y:169:GLU:HG3	2.13	0.49
1:C:80:LYS:HB3	1:C:80:LYS:NZ	2.26	0.49
1:V:28:LYS:HD3	1:V:31:VAL:HG22	1.94	0.49
2:I:73:LEU:HG	2:I:73:LEU:O	2.12	0.49
2:I:115:ALA:O	2:I:119:ASN:HB2	2.13	0.49
2:F:130:ARG:CG	2:F:225:LEU:HD11	2.39	0.49
2:E:170:ASP:HB3	2:E:217:LYS:HD3	1.95	0.49
2:I:169:ASP:O	2:I:218:ILE:HG13	2.11	0.49
1:C:37:LEU:HD23	1:C:42:VAL:O	2.12	0.49
1:D:14:ILE:HD12	1:D:43:ILE:HG12	1.92	0.49
2:I:345:THR:HG21	2:I:373:ILE:CD1	2.43	0.49
2:G:361:THR:HG22	2:I:35:TRP:CZ3	2.47	0.49
2:I:35:TRP:O	2:I:39:GLN:HG2	2.12	0.49
2:F:258:ILE:HG22	2:F:307:SER:O	2.12	0.49
1:B:92:GLU:O	1:B:93:ALA:HB2	2.12	0.49
1:X:86:ARG:HA	1:X:89:ARG:CZ	2.42	0.49
2:G:65:GLU:HG3	3:G:2450:ADP:H2'	1.94	0.49
1:D:71:LEU:HD21	1:D:97:VAL:CG1	2.42	0.49
1:Y:39:ASN:O	1:Y:41:LYS:HG3	2.12	0.49
1:D:117:ASN:O	1:D:118:ASP:HB2	2.10	0.49
2:F:123:ALA:CA	2:F:127:ALA:HB3	2.38	0.49
2:E:292:THR:HB	2:E:295:GLY:O	2.12	0.49
2:I:132:LEU:HD23	2:I:135:LEU:CD1	2.42	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:393:ARG:NH2	3:F:1450:ADP:O1B	2.45	0.49
2:E:124:GLU:HA	2:E:127:ALA:CB	2.39	0.49
2:I:270:PRO:O	2:I:274:ARG:HD2	2.12	0.49
2:F:119:ASN:ND2	2:F:233:LEU:HD23	2.27	0.49
2:F:132:LEU:HD11	2:F:160:ARG:CG	2.41	0.49
2:I:171:LYS:O	2:I:215:LYS:HD2	2.12	0.49
2:I:212:LYS:HB2	2:I:212:LYS:HZ2	1.78	0.49
2:G:93:GLY:O	2:G:94:LYS:C	2.51	0.49
1:D:150:LYS:HD3	1:V:139:ASN:OD1	2.13	0.49
2:I:103:LEU:HD13	2:I:247:VAL:HG13	1.94	0.49
2:I:34:ARG:CZ	2:I:250:HIS:HA	2.42	0.49
1:B:82:TRP:HE1	1:B:91:LEU:HB2	1.78	0.49
1:B:88:LEU:HD12	1:B:91:LEU:HD11	1.93	0.49
1:X:89:ARG:HH11	1:X:89:ARG:HB2	1.77	0.49
2:I:366:ILE:HD12	2:I:418:ILE:HB	1.93	0.49
1:C:54:PHE:CD1	1:D:76:VAL:HG21	2.47	0.49
1:C:94:LEU:HD13	1:C:122:ILE:HB	1.93	0.49
1:A:8:ARG:O	1:A:11:HIS:HB2	2.13	0.49
2:E:408:TYR:CD1	2:F:29:ILE:HD11	2.46	0.49
1:X:117:ASN:O	1:X:118:ASP:HB2	2.12	0.49
2:E:134:VAL:HG13	2:E:171:LYS:HD3	1.94	0.49
2:I:220:ASP:O	2:I:224:LEU:HD23	2.12	0.49
1:B:86:ARG:HA	1:B:89:ARG:HE	1.75	0.49
2:G:89:VAL:HA	2:G:93:GLY:CA	2.42	0.49
1:Y:6:VAL:HG12	1:Y:7:ARG:N	2.28	0.49
2:F:86:PHE:HB2	2:F:277:VAL:HG13	1.94	0.49
2:E:255:ILE:HD13	2:E:281:LEU:HD21	1.93	0.49
2:G:436:GLU:O	2:G:439:SER:HB2	2.12	0.49
2:I:413:LEU:O	2:I:416:GLN:HG3	2.12	0.49
1:X:83:ARG:HH11	1:X:83:ARG:CB	2.10	0.49
1:A:160:ILE:HG13	1:Z:160:ILE:O	2.12	0.49
1:Z:86:ARG:HG2	1:Z:89:ARG:HH22	1.77	0.49
2:I:122:ARG:NE	2:I:122:ARG:HA	2.28	0.49
2:I:229:GLU:OE2	2:I:232:LYS:HD2	2.12	0.49
1:C:71:LEU:HD21	1:C:97:VAL:HG12	1.93	0.49
2:E:77:PRO:HB3	2:E:107:ALA:HB2	1.95	0.49
1:B:69:GLY:O	1:B:71:LEU:N	2.45	0.49
2:G:131:ILE:CD1	2:G:218:ILE:HG12	2.42	0.49
2:G:140:LYS:O	2:G:141:ASN:CB	2.59	0.49
1:V:59:LEU:HD11	1:V:63:LYS:HE2	1.95	0.49
2:G:23:ALA:HA	2:G:330:VAL:HG21	1.95	0.49
2:G:33:ASN:ND2	2:G:36:ARG:HD2	2.27	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:435:ASP:CG	2:I:438:LEU:HB2	2.33	0.49
1:Z:34:VAL:HG13	1:Z:44:ALA:O	2.13	0.49
2:E:211:GLN:O	2:E:212:LYS:HB2	2.13	0.49
2:E:173:ILE:HD11	2:E:221:ALA:HB2	1.95	0.49
1:Y:36:ARG:NE	1:Y:169:GLU:OE2	2.44	0.49
2:I:32:ARG:O	2:I:36:ARG:HG3	2.13	0.49
1:X:73:LYS:NZ	1:X:77:GLU:CG	2.75	0.49
2:F:218:ILE:HG23	2:F:222:MET:HB2	1.95	0.48
2:I:171:LYS:HZ2	2:I:218:ILE:HD11	1.72	0.48
1:D:61:GLU:O	1:D:65:GLU:HG2	2.12	0.48
1:B:117:ASN:O	1:B:118:ASP:HB2	2.13	0.48
1:V:157:ASP:OD2	1:V:164:HIS:NE2	2.33	0.48
2:E:150:GLN:O	2:E:153:SER:HB2	2.14	0.48
2:F:172:GLU:O	2:F:173:ILE:HG23	2.13	0.48
2:G:88:GLU:CG	2:I:90:GLY:HA2	2.43	0.48
2:I:135:LEU:HD22	2:I:159:PHE:CD2	2.48	0.48
1:Y:170:GLU:CG	1:Y:171:LEU:H	2.23	0.48
1:V:73:LYS:HD2	1:V:76:VAL:CG1	2.43	0.48
2:G:264:ARG:NE	2:G:265:GLY:H	2.11	0.48
1:Z:3:ILE:HB	1:Z:122:ILE:HG12	1.95	0.48
2:I:396:HIS:O	2:I:400:GLU:HB2	2.14	0.48
1:X:30:ASN:ND2	1:X:30:ASN:N	2.50	0.48
1:A:80:LYS:O	1:A:81:ASP:C	2.50	0.48
2:I:151:GLU:CB	2:I:152:PRO:CD	2.88	0.48
1:Y:170:GLU:HG2	1:Y:171:LEU:N	2.21	0.48
1:B:28:LYS:HZ1	1:B:30:ASN:ND2	2.10	0.48
1:B:44:ALA:HB2	1:B:97:VAL:HG23	1.94	0.48
2:E:408:TYR:HA	2:F:29:ILE:CD1	2.43	0.48
1:D:5:SER:HB3	1:D:120:ILE:HB	1.95	0.48
2:E:222:MET:O	2:E:226:ILE:HG12	2.14	0.48
2:G:270:PRO:HB2	2:G:274:ARG:HD2	1.95	0.48
1:D:131:ALA:HB3	1:V:131:ALA:HB3	1.95	0.48
2:F:12:GLU:HG2	2:F:73:LEU:HD11	1.94	0.48
2:E:23:ALA:HA	2:E:330:VAL:HG21	1.94	0.48
2:G:130:ARG:HD2	2:G:225:LEU:CD1	2.42	0.48
1:B:85:ASP:O	1:B:89:ARG:HG3	2.14	0.48
1:Y:7:ARG:NE	1:Y:118:ASP:OD2	2.42	0.48
1:B:132:ALA:HB1	1:Z:135:ALA:HB2	1.93	0.48
2:G:231:ALA:C	2:G:233:LEU:N	2.67	0.48
2:I:311:GLN:NE2	2:I:311:GLN:HA	2.28	0.48
2:F:12:GLU:HG2	2:F:73:LEU:CD1	2.42	0.48
2:E:160:ARG:HH12	2:E:164:ARG:NH2	2.11	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:11:HIS:HE1	1:C:174:LYS:NZ	2.11	0.48
2:G:222:MET:O	2:G:226:ILE:HG12	2.13	0.48
2:G:108:VAL:HA	2:G:111:VAL:HG22	1.96	0.48
2:F:153:SER:HA	2:F:157:GLN:H	1.79	0.48
2:G:109:LYS:O	2:G:113:VAL:HG23	2.14	0.48
1:X:43:ILE:HD11	1:X:98:ALA:HB3	1.96	0.48
1:X:5:SER:HB3	1:X:120:ILE:HB	1.95	0.48
1:A:7:ARG:HB2	1:A:12:VAL:HG23	1.95	0.48
2:F:115:ALA:O	2:F:119:ASN:HB2	2.13	0.48
2:F:268:SER:HA	2:F:271:ASP:OD2	2.12	0.48
2:E:174:GLU:CA	2:E:212:LYS:HB3	2.40	0.48
2:I:216:LEU:HG	2:I:221:ALA:HB2	1.96	0.48
1:B:98:ALA:CB	1:B:103:SER:HB3	2.42	0.48
1:D:30:ASN:HD22	1:D:30:ASN:N	1.96	0.48
2:F:351:ILE:CD1	2:F:351:ILE:H	2.24	0.48
1:B:94:LEU:HB3	1:B:122:ILE:HD12	1.95	0.48
2:I:335:LEU:HD22	2:I:339:ASP:HB3	1.96	0.48
2:E:342:ARG:NH2	2:E:346:GLU:OE2	2.37	0.48
2:E:153:SER:C	2:E:157:GLN:HG2	2.33	0.48
2:F:223:LYS:HA	2:F:226:ILE:CG1	2.41	0.48
2:I:223:LYS:HA	2:I:226:ILE:CG1	2.43	0.48
2:E:408:TYR:CB	2:F:29:ILE:HD11	2.43	0.48
2:G:103:LEU:HD13	2:G:247:VAL:HG13	1.96	0.48
2:E:258:ILE:O	2:E:261:ILE:HG12	2.14	0.48
1:Z:121:ALA:HB1	1:Z:126:GLY:O	2.14	0.48
2:F:163:LEU:HD21	2:F:222:MET:HE1	1.94	0.48
2:E:292:THR:HG22	2:E:293:LYS:N	2.27	0.48
1:B:38:TYR:HB2	1:B:64:LEU:CD1	2.43	0.48
1:Y:3:ILE:HB	1:Y:122:ILE:HG12	1.96	0.48
1:V:80:LYS:C	1:V:80:LYS:HD2	2.34	0.48
1:Z:86:ARG:HA	1:Z:89:ARG:CZ	2.43	0.48
2:F:152:PRO:CB	2:F:156:ARG:HB2	2.41	0.48
1:X:145:ARG:NE	1:X:170:GLU:OE1	2.40	0.48
1:X:37:LEU:N	1:X:37:LEU:HD12	2.28	0.48
1:C:115:PRO:CB	1:C:119:LEU:O	2.57	0.48
2:G:312:ILE:HG12	2:G:313:ALA:H	1.79	0.48
1:A:139:ASN:HD22	1:Y:136:LEU:HD11	1.78	0.48
2:E:91:TYR:C	2:E:92:VAL:HG22	2.33	0.48
1:C:70:HIS:HE1	1:C:72:VAL:HB	1.73	0.48
1:X:10:GLY:HA2	1:X:173:TYR:CZ	2.48	0.48
2:F:34:ARG:CZ	2:F:250:HIS:HA	2.44	0.48
1:A:5:SER:HB3	1:A:120:ILE:HB	1.96	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:8:ARG:HG2	1:X:9:ASN:ND2	2.29	0.48
1:V:8:ARG:HG2	1:V:9:ASN:ND2	2.29	0.48
2:I:151:GLU:HB2	2:I:152:PRO:HD2	1.96	0.47
1:B:98:ALA:HB2	1:B:103:SER:HB3	1.95	0.47
1:C:136:LEU:CD1	1:X:135:ALA:HB1	2.36	0.47
2:I:59:THR:O	2:I:61:VAL:HG13	2.14	0.47
1:C:83:ARG:HH11	1:C:83:ARG:CG	2.25	0.47
1:A:121:ALA:HB1	1:A:126:GLY:O	2.14	0.47
2:G:372:GLY:O	2:G:376:ILE:HG13	2.14	0.47
2:E:212:LYS:NZ	2:E:212:LYS:HB2	2.29	0.47
1:Y:136:LEU:HB3	1:Y:147:ILE:HD12	1.94	0.47
1:Y:44:ALA:HB2	1:Y:97:VAL:HG23	1.96	0.47
1:Y:62:ARG:O	1:Y:66:MET:HG3	2.14	0.47
2:F:102:ASP:C	2:F:104:THR:N	2.67	0.47
2:F:103:LEU:HD13	2:F:247:VAL:HG22	1.96	0.47
1:B:71:LEU:HD13	1:B:71:LEU:C	2.34	0.47
2:I:219:LYS:O	2:I:223:LYS:HD3	2.14	0.47
1:B:13:VAL:HG12	1:B:170:GLU:HG3	1.96	0.47
2:I:23:ALA:HA	2:I:330:VAL:HG21	1.95	0.47
1:C:14:ILE:O	1:C:34:VAL:HG11	2.14	0.47
2:G:148:GLN:HA	2:G:151:GLU:HG2	1.95	0.47
1:C:68:GLN:O	1:C:70:HIS:N	2.48	0.47
2:F:267:SER:O	2:F:271:ASP:OD2	2.31	0.47
1:D:8:ARG:O	1:D:11:HIS:HB2	2.14	0.47
1:V:146:GLU:O	1:V:150:LYS:HG3	2.14	0.47
2:E:348:ASN:O	2:E:349:ALA:HB3	2.15	0.47
2:E:19:GLY:O	2:E:24:LYS:HE3	2.14	0.47
2:F:160:ARG:HG2	2:F:160:ARG:HH11	1.80	0.47
2:E:86:PHE:HA	2:E:89:VAL:HG13	1.95	0.47
1:C:59:LEU:HG	1:C:78:LEU:HD13	1.95	0.47
1:Y:33:LYS:HA	1:Y:46:PHE:CE1	2.50	0.47
2:I:344:LEU:CD1	2:I:395:LEU:HD13	2.43	0.47
1:B:64:LEU:HD23	1:B:74:ALA:HB3	1.95	0.47
1:V:85:ASP:HB3	1:V:88:LEU:HD12	1.96	0.47
2:I:17:ILE:HD12	2:I:17:ILE:N	2.29	0.47
2:F:211:GLN:O	2:F:212:LYS:HB2	2.15	0.47
2:G:130:ARG:HG2	2:G:225:LEU:HD11	1.97	0.47
1:V:115:PRO:CB	1:V:119:LEU:O	2.61	0.47
1:V:30:ASN:N	1:V:30:ASN:HD22	2.04	0.47
1:D:15:ALA:HB1	1:D:152:LEU:HD12	1.97	0.47
2:E:109:LYS:O	2:E:113:VAL:HG23	2.15	0.47
1:D:86:ARG:HA	1:D:89:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:362:GLU:HG3	2:E:411:SER:HA	1.95	0.47
1:A:25:THR:HA	1:Z:158:ILE:O	2.14	0.47
2:F:335:LEU:HD22	2:F:339:ASP:HB3	1.95	0.47
2:I:163:LEU:HD21	2:I:222:MET:HE1	1.96	0.47
1:C:69:GLY:O	1:C:71:LEU:N	2.48	0.47
2:F:312:ILE:HG12	2:F:313:ALA:N	2.29	0.47
1:A:18:GLY:HA2	1:A:33:LYS:HE3	1.97	0.47
2:E:108:VAL:C	2:E:110:MET:N	2.68	0.47
2:I:167:GLN:HB2	2:I:218:ILE:CG2	2.44	0.47
1:C:60:PHE:HB2	1:C:78:LEU:HD22	1.96	0.47
1:B:70:HIS:HE1	1:B:72:VAL:HB	1.80	0.47
1:C:64:LEU:HA	1:C:74:ALA:HB2	1.97	0.47
1:A:62:ARG:CD	2:E:141:ASN:HD21	2.28	0.47
1:A:65:GLU:OE1	2:E:143:TRP:NE1	2.47	0.47
2:G:359:MET:HE3	2:I:36:ARG:NH1	2.30	0.47
2:I:270:PRO:O	2:I:273:SER:HB3	2.15	0.47
1:V:170:GLU:CG	1:V:171:LEU:N	2.78	0.47
1:B:3:ILE:HB	1:B:122:ILE:HG12	1.97	0.47
2:F:142:ASN:ND2	2:F:149:GLN:NE2	2.63	0.47
2:E:442:ILE:CG2	2:E:442:ILE:O	2.63	0.47
1:Y:92:GLU:O	1:Y:93:ALA:HB2	2.14	0.47
1:V:173:TYR:CD2	1:V:173:TYR:N	2.83	0.47
1:Y:34:VAL:HB	1:Y:167:THR:HG22	1.97	0.47
2:E:149:GLN:C	2:E:151:GLU:H	2.17	0.47
2:F:169:ASP:O	2:F:218:ILE:HG13	2.15	0.47
2:G:170:ASP:CB	2:G:217:LYS:HD3	2.45	0.47
1:C:60:PHE:CZ	1:C:97:VAL:HG11	2.50	0.47
2:F:153:SER:CA	2:F:156:ARG:HB3	2.45	0.47
1:D:28:LYS:CE	1:D:30:ASN:HD21	2.27	0.47
2:F:318:LEU:O	2:F:323:GLN:NE2	2.41	0.47
2:F:280:ASP:O	2:F:283:PRO:HD2	2.14	0.47
1:A:99:ASP:OD1	1:A:101:THR:N	2.42	0.47
2:E:62:GLY:O	2:E:66:ILE:HG13	2.15	0.47
2:I:280:ASP:O	2:I:283:PRO:HD2	2.15	0.47
2:F:219:LYS:C	2:F:223:LYS:HD3	2.35	0.47
1:V:7:ARG:HH21	1:V:103:SER:N	2.13	0.47
1:Y:60:PHE:CE2	1:Y:97:VAL:HG21	2.50	0.47
1:B:70:HIS:CE1	1:B:72:VAL:HB	2.50	0.47
2:I:389:ASN:HD22	2:I:390:ILE:N	2.12	0.47
2:G:131:ILE:O	2:G:134:VAL:HG12	2.15	0.47
1:V:83:ARG:NH1	1:V:83:ARG:CG	2.78	0.47
1:D:152:LEU:HD22	1:D:166:HIS:HE1	1.80	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:121:ALA:HB1	1:X:126:GLY:O	2.15	0.47
2:G:211:GLN:O	2:G:212:LYS:HB2	2.14	0.47
2:I:155:ALA:O	2:I:159:PHE:HD1	1.97	0.47
2:G:108:VAL:C	2:G:110:MET:N	2.68	0.47
2:G:344:LEU:HD23	2:G:373:ILE:HG23	1.97	0.47
1:A:30:ASN:ND2	1:A:30:ASN:H	2.13	0.47
2:I:236:PRO:O	2:I:238:GLU:N	2.41	0.47
2:G:336:THR:O	2:G:339:ASP:HB2	2.15	0.47
1:C:81:ASP:HB3	1:C:88:LEU:CD1	2.45	0.47
2:E:152:PRO:HB2	2:E:156:ARG:CB	2.27	0.46
2:F:145:GLN:HB2	2:F:148:GLN:CG	2.40	0.46
1:A:28:LYS:HZ3	1:A:30:ASN:ND2	2.12	0.46
1:D:86:ARG:O	1:D:90:LYS:HE3	2.15	0.46
1:Z:71:LEU:HD21	1:Z:99:ASP:HB3	1.97	0.46
1:V:91:LEU:O	1:V:91:LEU:HD12	2.14	0.46
1:V:169:GLU:OE1	1:V:169:GLU:HA	2.15	0.46
2:F:174:GLU:CA	2:F:212:LYS:HB3	2.44	0.46
2:I:211:GLN:O	2:I:212:LYS:HB2	2.15	0.46
2:G:362:GLU:HG3	2:G:411:SER:HA	1.97	0.46
2:F:432:LEU:CD1	2:F:432:LEU:H	2.28	0.46
2:E:12:GLU:CD	2:E:15:LYS:HE2	2.35	0.46
1:C:4:VAL:HA	1:C:120:ILE:O	2.16	0.46
1:Y:79:ALA:HB1	1:Y:110:GLY:HA2	1.96	0.46
2:F:148:GLN:HA	2:F:151:GLU:CG	2.45	0.46
1:V:71:LEU:HD21	1:V:97:VAL:HG12	1.97	0.46
1:Z:152:LEU:HD13	1:Z:166:HIS:ND1	2.31	0.46
1:Z:30:ASN:ND2	1:Z:30:ASN:H	2.14	0.46
1:Y:174:LYS:HD2	1:Y:174:LYS:N	2.30	0.46
2:I:220:ASP:O	2:I:224:LEU:HB2	2.16	0.46
1:Y:70:HIS:CE1	1:Y:72:VAL:HB	2.48	0.46
1:B:136:LEU:HD11	1:Z:139:ASN:HD22	1.79	0.46
2:G:108:VAL:C	2:G:110:MET:H	2.19	0.46
2:F:122:ARG:CZ	2:F:122:ARG:HA	2.46	0.46
2:G:392:ALA:HB3	3:G:2450:ADP:C8	2.50	0.46
1:C:67:HIS:CE1	1:C:77:GLU:HG3	2.50	0.46
2:G:165:GLU:HG2	2:G:166:GLY:H	1.81	0.46
1:D:168:ILE:HG22	1:D:169:GLU:N	2.30	0.46
2:G:147:GLU:CA	2:G:150:GLN:HG3	2.44	0.46
2:I:129:GLU:HB2	2:I:130:ARG:NH1	2.31	0.46
1:Y:63:LYS:HD2	1:Y:77:GLU:HB3	1.96	0.46
1:X:60:PHE:HZ	1:X:97:VAL:HG11	1.77	0.46
1:Z:17:ASP:O	1:Z:33:LYS:HD2	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:264:ARG:CZ	2:F:265:GLY:H	2.28	0.46
1:B:79:ALA:HB2	1:B:106:ILE:HG23	1.97	0.46
2:E:382:GLN:O	2:E:386:SER:HB3	2.16	0.46
2:F:346:GLU:HB2	2:F:347:PRO:HD3	1.98	0.46
2:G:145:GLN:HB2	2:G:148:GLN:CB	2.41	0.46
2:I:174:GLU:CA	2:I:212:LYS:HB3	2.46	0.46
2:G:89:VAL:HG12	2:G:93:GLY:HA3	1.98	0.46
1:C:136:LEU:HB3	1:C:147:ILE:HD12	1.97	0.46
1:C:64:LEU:HD23	1:C:74:ALA:HB3	1.97	0.46
1:V:58:GLU:O	1:V:61:GLU:HB2	2.16	0.46
1:Z:149:GLU:HG2	1:Z:168:ILE:CD1	2.45	0.46
1:D:149:GLU:CD	1:D:168:ILE:HD11	2.36	0.46
1:C:18:GLY:C	1:C:163:ASN:HD21	2.19	0.46
2:F:388:GLU:OE2	2:F:388:GLU:N	2.49	0.46
1:V:90:LYS:HZ1	1:X:89:ARG:HD3	1.80	0.46
1:C:170:GLU:CG	1:C:171:LEU:H	2.28	0.46
2:I:102:ASP:C	2:I:104:THR:N	2.69	0.46
1:C:64:LEU:HA	1:C:74:ALA:HB1	1.97	0.46
1:X:13:VAL:CG1	1:X:170:GLU:HG3	2.43	0.46
1:X:37:LEU:H	1:X:37:LEU:HD12	1.81	0.46
2:F:255:ILE:HD13	2:F:281:LEU:HD21	1.97	0.46
2:G:255:ILE:HD13	2:G:281:LEU:HD21	1.97	0.46
2:F:63:LYS:HE2	2:F:307:SER:OG	2.15	0.46
2:G:152:PRO:HB3	2:G:156:ARG:N	2.26	0.46
1:Y:68:GLN:O	1:Y:70:HIS:N	2.49	0.46
2:I:292:THR:C	2:I:294:HIS:H	2.20	0.46
2:F:344:LEU:HD21	2:F:395:LEU:HD22	1.98	0.46
1:A:87:MET:HE3	1:B:84:THR:HG23	1.96	0.46
1:B:53:ALA:C	1:B:55:THR:H	2.19	0.46
2:F:164:ARG:O	2:F:165:GLU:HB3	2.16	0.46
2:G:212:LYS:NZ	2:G:212:LYS:HB2	2.30	0.46
1:B:103:SER:C	1:B:104:LEU:HD23	2.36	0.46
1:B:34:VAL:HG13	1:B:44:ALA:O	2.15	0.46
1:D:115:PRO:HG3	1:D:120:ILE:HG12	1.98	0.46
1:Z:149:GLU:CG	1:Z:168:ILE:HD11	2.46	0.46
2:G:259:ASP:HB3	2:G:310:PHE:CZ	2.51	0.46
1:C:67:HIS:O	1:C:68:GLN:C	2.54	0.46
1:C:121:ALA:HB1	1:C:126:GLY:O	2.15	0.46
2:E:34:ARG:CZ	2:E:250:HIS:HA	2.45	0.46
1:Y:88:LEU:HD12	1:Y:91:LEU:HD11	1.97	0.46
2:G:217:LYS:CB	2:G:219:LYS:HZ3	2.28	0.45
2:I:356:LYS:CG	2:I:366:ILE:HG22	2.40	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:145:GLN:CA	2:F:145:GLN:HE21	2.28	0.45
1:V:68:GLN:O	1:V:70:HIS:N	2.49	0.45
1:B:117:ASN:C	1:B:119:LEU:N	2.69	0.45
1:D:67:HIS:O	1:D:68:GLN:C	2.54	0.45
1:D:86:ARG:HA	1:D:89:ARG:NH2	2.31	0.45
1:C:34:VAL:HB	1:C:167:THR:HG22	1.98	0.45
2:E:135:LEU:O	2:E:136:ILE:HG12	2.16	0.45
2:I:96:VAL:HG12	2:I:284:LEU:CD1	2.46	0.45
1:C:83:ARG:HG3	1:C:109:ASN:O	2.17	0.45
2:G:311:GLN:HA	2:G:311:GLN:HE21	1.81	0.45
2:E:355:TYR:HE2	2:E:400:GLU:OE2	2.00	0.45
2:E:145:GLN:HG3	2:E:148:GLN:HG3	1.98	0.45
2:I:135:LEU:HD22	2:I:159:PHE:HD2	1.80	0.45
1:Y:6:VAL:HG21	1:Y:147:ILE:HG22	1.98	0.45
2:I:420:ILE:HD12	2:I:420:ILE:N	2.31	0.45
2:E:388:GLU:O	2:E:394:ARG:NH2	2.49	0.45
1:Z:33:LYS:HA	1:Z:46:PHE:CE1	2.52	0.45
1:D:86:ARG:HA	1:D:89:ARG:CZ	2.46	0.45
1:Y:5:SER:HB3	1:Y:120:ILE:HB	1.98	0.45
1:B:154:ILE:HD12	1:Z:134:ARG:CB	2.47	0.45
2:E:311:GLN:HA	2:E:311:GLN:NE2	2.32	0.45
1:V:64:LEU:HD23	1:V:74:ALA:HB2	1.98	0.45
1:Y:95:LEU:H	1:Y:95:LEU:HD12	1.82	0.45
2:E:81:VAL:HG11	2:E:99:ILE:HG12	1.97	0.45
2:E:335:LEU:HD22	2:E:339:ASP:HB3	1.96	0.45
1:C:170:GLU:CG	1:C:171:LEU:N	2.80	0.45
1:Y:63:LYS:HD3	1:Y:66:MET:CE	2.46	0.45
1:Y:71:LEU:HD13	1:Y:72:VAL:N	2.32	0.45
1:B:63:LYS:HD2	1:B:77:GLU:HB3	1.98	0.45
2:I:65:GLU:HG3	3:I:3450:ADP:H2'	1.99	0.45
1:V:154:ILE:HG22	1:V:155:ALA:N	2.30	0.45
1:V:134:ARG:HD2	1:V:138:GLU:OE1	2.16	0.45
1:D:60:PHE:CZ	1:D:97:VAL:HG11	2.51	0.45
1:Z:145:ARG:NE	1:Z:170:GLU:OE1	2.43	0.45
1:C:56:LEU:HD21	1:C:91:LEU:HD13	1.98	0.45
2:G:142:ASN:HB2	2:G:149:GLN:NE2	2.32	0.45
1:C:39:ASN:O	1:C:41:LYS:N	2.50	0.45
2:I:52:ASN:HB2	2:I:325:ARG:O	2.17	0.45
1:B:11:HIS:CE1	1:B:172:SER:OG	2.69	0.45
2:F:31:LEU:HD11	2:F:74:ALA:HB2	1.98	0.45
2:E:217:LYS:HG3	2:E:219:LYS:HZ1	1.80	0.45
1:Y:53:ALA:C	1:Y:55:THR:N	2.70	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:57:PHE:O	1:X:61:GLU:HB2	2.16	0.45
1:B:148:ALA:O	1:B:152:LEU:HB2	2.16	0.45
1:V:73:LYS:O	1:V:77:GLU:HB2	2.17	0.45
1:D:84:THR:O	1:D:89:ARG:NH1	2.49	0.45
2:I:311:GLN:CA	2:I:311:GLN:NE2	2.80	0.45
2:E:382:GLN:HA	2:E:382:GLN:NE2	2.31	0.45
2:G:272:VAL:O	2:G:276:GLY:N	2.50	0.45
1:Y:59:LEU:O	1:Y:59:LEU:HD12	2.16	0.45
2:F:129:GLU:HB2	2:F:130:ARG:NH1	2.31	0.45
2:G:91:TYR:HD1	2:I:91:TYR:HD2	1.62	0.45
1:C:148:ALA:O	1:C:152:LEU:HB2	2.16	0.45
1:B:5:SER:HB3	1:B:120:ILE:HB	1.98	0.45
1:D:73:LYS:HZ2	1:D:77:GLU:HG2	1.82	0.45
2:I:16:HIS:HB2	2:I:17:ILE:HD12	1.98	0.45
1:B:159:CYS:HB3	1:B:162:THR:HB	1.98	0.45
2:E:165:GLU:HG2	2:E:166:GLY:N	2.32	0.45
2:E:244:ILE:HG22	2:E:245:ASP:N	2.32	0.45
2:G:91:TYR:CB	2:I:91:TYR:HA	2.47	0.45
2:I:130:ARG:HD2	2:I:225:LEU:HD11	1.99	0.45
1:Y:70:HIS:ND1	1:Y:73:LYS:HB2	2.32	0.45
2:F:104:THR:HA	2:F:107:ALA:HB3	1.98	0.45
1:X:152:LEU:HD23	1:X:152:LEU:O	2.17	0.45
2:G:76:ALA:HB1	2:G:250:HIS:O	2.17	0.45
1:B:117:ASN:C	1:B:119:LEU:H	2.20	0.45
2:E:242:ASP:HA	2:E:245:ASP:OD1	2.16	0.45
2:F:216:LEU:HG	2:F:221:ALA:CB	2.18	0.45
2:F:232:LYS:N	2:F:232:LYS:NZ	2.64	0.45
2:G:174:GLU:HB3	2:G:211:GLN:HB2	1.99	0.45
2:I:129:GLU:HB2	2:I:130:ARG:HH11	1.81	0.45
2:G:219:LYS:O	2:G:223:LYS:HE3	2.17	0.45
2:I:145:GLN:C	2:I:147:GLU:H	2.20	0.45
2:G:432:LEU:CD1	2:G:432:LEU:N	2.78	0.45
1:Y:152:LEU:HD13	1:Y:166:HIS:CE1	2.51	0.45
2:F:356:LYS:HG3	2:F:366:ILE:HG22	1.99	0.45
2:G:271:ASP:HA	2:G:274:ARG:HB2	1.98	0.45
2:E:355:TYR:CE2	2:E:400:GLU:OE2	2.70	0.45
2:I:322:LEU:HD12	2:I:322:LEU:HA	1.84	0.45
1:X:37:LEU:CD2	1:X:57:PHE:HB3	2.43	0.45
1:B:95:LEU:N	1:B:95:LEU:HD12	2.31	0.45
2:G:441:PHE:HA	2:I:315:PRO:HG2	1.99	0.45
1:A:149:GLU:HG2	1:A:168:ILE:CD1	2.47	0.45
2:F:350:SER:O	2:F:354:GLN:HG3	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:81:VAL:HG11	2:G:99:ILE:HG12	1.99	0.45
2:E:170:ASP:CB	2:E:217:LYS:HD3	2.47	0.44
2:G:109:LYS:HG3	2:G:109:LYS:O	2.15	0.44
2:F:375:ARG:NH2	2:F:422:ALA:HB1	2.32	0.44
1:Z:33:LYS:O	1:Z:45:GLY:HA2	2.17	0.44
2:I:12:GLU:CG	2:I:73:LEU:HD13	2.47	0.44
2:I:432:LEU:N	2:I:432:LEU:CD1	2.80	0.44
1:Y:38:TYR:CD2	1:Y:41:LYS:HD2	2.52	0.44
2:G:33:ASN:HD22	2:G:36:ARG:HD2	1.82	0.44
2:I:435:ASP:OD1	2:I:438:LEU:HD12	2.17	0.44
2:G:442:ILE:CG2	2:G:442:ILE:O	2.65	0.44
2:G:153:SER:N	2:G:156:ARG:HB3	2.32	0.44
2:G:216:LEU:HD23	2:G:216:LEU:N	2.29	0.44
2:G:92:VAL:CG2	2:I:92:VAL:CG1	2.92	0.44
2:I:132:LEU:HB3	2:I:156:ARG:CZ	2.47	0.44
1:B:150:LYS:O	1:B:154:ILE:HG12	2.18	0.44
2:G:153:SER:HA	2:G:157:GLN:HG3	1.99	0.44
1:A:84:THR:HG23	1:A:85:ASP:N	2.33	0.44
2:G:101:ARG:O	2:G:104:THR:HB	2.17	0.44
2:F:153:SER:HA	2:F:156:ARG:HB3	1.98	0.44
2:G:134:VAL:CG1	2:G:171:LYS:HD3	2.46	0.44
1:Y:8:ARG:HH12	1:Y:141:GLU:C	2.20	0.44
2:I:119:ASN:CG	2:I:233:LEU:HD23	2.37	0.44
2:G:16:HIS:HB2	2:G:17:ILE:HD12	1.99	0.44
2:E:240:LYS:HD3	2:E:241:GLN:N	2.32	0.44
1:V:5:SER:HB3	1:V:120:ILE:HD13	1.97	0.44
2:I:217:LYS:CG	2:I:218:ILE:N	2.78	0.44
1:C:38:TYR:N	1:C:61:GLU:OE1	2.48	0.44
1:Y:19:GLN:N	1:Y:163:ASN:ND2	2.66	0.44
1:Z:13:VAL:CG1	1:Z:170:GLU:HG3	2.44	0.44
2:F:21:ASP:O	2:F:24:LYS:HB2	2.17	0.44
2:G:270:PRO:O	2:G:273:SER:N	2.51	0.44
2:G:35:TRP:O	2:G:39:GLN:HG2	2.17	0.44
2:G:95:GLU:H	2:G:95:GLU:CD	2.20	0.44
1:Y:32:LYS:HE3	1:Y:32:LYS:HB2	1.74	0.44
2:I:218:ILE:C	2:I:220:ASP:N	2.70	0.44
2:I:312:ILE:CG1	2:I:313:ALA:N	2.80	0.44
1:Y:6:VAL:HG21	1:Y:147:ILE:CG2	2.47	0.44
1:V:35:ARG:HD3	1:V:57:PHE:CD2	2.52	0.44
1:D:8:ARG:HG2	1:D:9:ASN:ND2	2.33	0.44
1:C:19:GLN:HB2	1:C:163:ASN:ND2	2.32	0.44
1:V:98:ALA:HA	1:V:102:ALA:O	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:148:GLN:OE1	2:E:151:GLU:HG3	2.18	0.44
1:C:5:SER:HB3	1:C:120:ILE:HB	2.00	0.44
2:G:151:GLU:HB2	2:G:152:PRO:HD2	1.99	0.44
2:I:159:PHE:O	2:I:163:LEU:HB2	2.18	0.44
2:F:94:LYS:NZ	2:F:101:ARG:HH12	2.15	0.44
2:G:292:THR:HG22	2:G:294:HIS:H	1.83	0.44
2:E:89:VAL:HG12	2:E:93:GLY:C	2.37	0.44
1:C:62:ARG:O	1:C:65:GLU:HB2	2.18	0.44
1:D:121:ALA:HB1	1:D:126:GLY:O	2.17	0.44
1:B:32:LYS:HE3	1:B:32:LYS:HB2	1.76	0.44
2:E:128:GLU:O	2:E:129:GLU:C	2.56	0.44
2:I:131:ILE:HD11	2:I:218:ILE:HD13	2.00	0.44
1:X:28:LYS:HG2	1:X:30:ASN:ND2	2.32	0.44
2:F:122:ARG:NE	2:F:122:ARG:HA	2.33	0.44
2:I:41:ASN:HD21	2:I:44:LEU:H	1.66	0.44
1:C:73:LYS:HA	1:C:76:VAL:CG1	2.47	0.44
2:E:140:LYS:O	2:E:141:ASN:CB	2.65	0.44
2:I:269:GLY:N	2:I:270:PRO:CD	2.81	0.44
1:X:10:GLY:O	1:X:172:SER:HA	2.18	0.44
2:E:436:GLU:O	2:E:439:SER:HB2	2.18	0.44
1:V:5:SER:O	1:V:119:LEU:HD12	2.18	0.44
2:I:123:ALA:C	2:I:127:ALA:HB3	2.38	0.44
1:Y:66:MET:C	1:Y:67:HIS:ND1	2.71	0.44
1:Y:71:LEU:CD1	1:Y:72:VAL:N	2.80	0.44
2:F:389:ASN:HD22	2:F:390:ILE:N	2.16	0.44
2:F:96:VAL:HG12	2:F:284:LEU:HD11	1.99	0.44
2:F:96:VAL:HG21	2:F:280:ASP:HB3	2.00	0.44
2:G:358:LEU:CD2	2:I:36:ARG:HB3	2.48	0.44
2:G:231:ALA:O	2:G:233:LEU:N	2.51	0.44
1:A:101:THR:O	1:A:102:ALA:HB2	2.18	0.44
1:Z:47:ALA:HB3	1:Z:94:LEU:HB2	1.99	0.44
2:F:167:GLN:O	2:F:168:LEU:CB	2.66	0.44
2:F:219:LYS:HE3	2:F:219:LYS:HA	1.99	0.44
2:E:214:ARG:CG	2:E:215:LYS:N	2.81	0.44
2:I:220:ASP:HB3	2:I:224:LEU:HD23	2.00	0.44
1:Y:63:LYS:CA	1:Y:66:MET:HE3	2.37	0.44
1:C:6:VAL:HG11	1:C:147:ILE:HG21	1.99	0.44
1:C:86:ARG:HA	1:C:89:ARG:CZ	2.48	0.44
2:G:358:LEU:HD22	2:I:36:ARG:HB2	1.99	0.44
1:A:149:GLU:OE1	1:A:168:ILE:HD11	2.18	0.44
1:V:170:GLU:HG3	1:V:171:LEU:N	2.32	0.44
2:E:442:ILE:O	2:E:442:ILE:HG22	2.16	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:106:ALA:O	2:E:110:MET:HB2	2.18	0.43
2:I:289:THR:CG2	2:I:296:MET:HG3	2.48	0.43
1:V:18:GLY:O	1:V:31:VAL:HG23	2.17	0.43
2:E:312:ILE:CG1	2:E:313:ALA:H	2.28	0.43
2:I:123:ALA:O	2:I:127:ALA:HB3	2.18	0.43
2:I:312:ILE:HG12	2:I:313:ALA:H	1.82	0.43
1:C:37:LEU:HD11	1:C:60:PHE:HD2	1.82	0.43
1:C:38:TYR:CE1	1:C:64:LEU:HB3	2.53	0.43
1:C:28:LYS:HE2	1:C:30:ASN:HD22	1.76	0.43
2:F:375:ARG:HA	2:F:378:GLU:HB2	2.00	0.43
2:I:240:LYS:HE2	2:I:240:LYS:HB3	1.85	0.43
2:E:135:LEU:HB3	2:E:159:PHE:CD2	2.53	0.43
1:Z:36:ARG:HD3	1:Z:40:ASP:OD1	2.19	0.43
2:E:438:LEU:O	2:E:438:LEU:HD23	2.18	0.43
2:F:244:ILE:HD12	2:F:244:ILE:N	2.33	0.43
2:E:132:LEU:HB3	2:E:156:ARG:CZ	2.48	0.43
2:F:217:LYS:HB2	2:F:217:LYS:HZ3	1.82	0.43
1:V:86:ARG:HG3	1:V:89:ARG:NH2	2.33	0.43
2:G:215:LYS:O	2:G:215:LYS:HG3	2.19	0.43
2:G:355:TYR:HE2	2:G:400:GLU:OE2	2.01	0.43
1:Y:86:ARG:HA	1:Y:89:ARG:HE	1.80	0.43
1:A:65:GLU:OE1	2:E:141:ASN:O	2.35	0.43
2:F:108:VAL:HA	2:F:111:VAL:CG2	2.47	0.43
1:B:7:ARG:NE	1:B:118:ASP:OD2	2.45	0.43
2:E:231:ALA:C	2:E:233:LEU:H	2.20	0.43
2:E:362:GLU:HG2	2:E:410:ALA:CB	2.49	0.43
2:G:88:GLU:CB	2:I:90:GLY:HA2	2.49	0.43
1:B:65:GLU:HB3	2:F:143:TRP:HA	2.01	0.43
2:G:106:ALA:HB2	2:I:289:THR:HB	2.00	0.43
2:G:358:LEU:HD23	2:I:36:ARG:HB3	1.98	0.43
2:G:163:LEU:O	2:G:163:LEU:HG	2.18	0.43
1:C:60:PHE:HZ	1:C:71:LEU:CD2	2.32	0.43
1:V:37:LEU:N	1:V:37:LEU:CD2	2.80	0.43
1:V:37:LEU:HD11	1:V:60:PHE:HD2	1.84	0.43
2:E:322:LEU:HD12	2:E:322:LEU:HA	1.87	0.43
2:F:16:HIS:HB2	2:F:17:ILE:HD12	2.01	0.43
2:G:155:ALA:O	2:G:159:PHE:HD1	2.01	0.43
1:A:3:ILE:HB	1:A:122:ILE:HG12	2.00	0.43
2:F:131:ILE:HG23	2:F:132:LEU:N	2.34	0.43
2:E:212:LYS:C	2:E:214:ARG:H	2.22	0.43
2:I:123:ALA:CA	2:I:127:ALA:HB3	2.45	0.43
2:I:160:ARG:HH11	2:I:160:ARG:HG2	1.82	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:43:ILE:HD13	1:D:98:ALA:O	2.19	0.43
1:A:1:THR:HA	1:A:17:ASP:OD1	2.18	0.43
1:X:149:GLU:OE1	1:X:166:HIS:CD2	2.72	0.43
2:I:235:ASN:HB2	2:I:236:PRO:CD	2.47	0.43
2:F:96:VAL:CG1	2:F:281:LEU:HD12	2.45	0.43
2:F:41:ASN:C	2:F:41:ASN:ND2	2.71	0.43
1:Y:98:ALA:HB2	1:Y:103:SER:CB	2.48	0.43
2:G:224:LEU:O	2:G:228:GLU:HG3	2.19	0.43
1:X:89:ARG:CB	1:X:89:ARG:HH11	2.32	0.43
2:G:223:LYS:HA	2:G:226:ILE:CG1	2.45	0.43
1:V:152:LEU:HB3	1:V:166:HIS:CE1	2.53	0.43
1:C:54:PHE:HD1	1:D:76:VAL:HG21	1.82	0.43
2:G:355:TYR:CE2	2:G:400:GLU:OE2	2.71	0.43
2:I:384:ASN:HD21	2:I:390:ILE:HG12	1.84	0.43
2:I:390:ILE:HG13	2:I:393:ARG:HB2	2.01	0.43
1:A:38:TYR:HE1	1:A:65:GLU:HG2	1.84	0.43
2:F:108:VAL:O	2:F:110:MET:N	2.52	0.43
1:Z:115:PRO:CG	1:Z:119:LEU:O	2.67	0.43
1:Y:90:LYS:HD2	1:Y:90:LYS:H	1.84	0.43
2:E:217:LYS:CB	2:E:219:LYS:HZ3	2.31	0.43
1:Y:73:LYS:O	1:Y:73:LYS:HD3	2.18	0.43
1:B:136:LEU:HD11	1:Z:135:ALA:O	2.18	0.43
1:C:160:ILE:CG2	1:V:160:ILE:CG2	2.93	0.43
1:X:168:ILE:HG22	1:X:169:GLU:N	2.33	0.43
1:B:152:LEU:HD13	1:B:166:HIS:CE1	2.54	0.43
2:I:223:LYS:N	2:I:223:LYS:CD	2.82	0.43
1:B:95:LEU:H	1:B:95:LEU:HD12	1.83	0.43
2:G:361:THR:CG2	2:I:35:TRP:CZ3	3.02	0.43
2:E:109:LYS:HD3	2:F:296:MET:HB3	2.01	0.43
2:F:20:GLN:O	2:F:24:LYS:HG3	2.18	0.43
1:D:86:ARG:HG2	1:D:89:ARG:HH22	1.83	0.43
2:F:336:THR:O	2:F:339:ASP:HB2	2.18	0.43
1:Z:61:GLU:HA	1:Z:64:LEU:HD12	2.00	0.43
2:E:128:GLU:O	2:E:131:ILE:HG22	2.19	0.43
2:I:94:LYS:NZ	2:I:101:ARG:HH12	2.16	0.43
1:C:63:LYS:HD3	1:C:66:MET:HE1	2.01	0.43
1:B:63:LYS:CA	1:B:66:MET:HE3	2.41	0.43
2:F:432:LEU:CD1	2:F:432:LEU:N	2.81	0.43
2:G:34:ARG:NH2	2:G:250:HIS:HA	2.34	0.43
1:D:149:GLU:CG	1:D:168:ILE:HD11	2.49	0.43
2:I:259:ASP:HB3	2:I:310:PHE:CZ	2.54	0.43
1:Z:81:ASP:HA	1:Z:84:THR:CG2	2.48	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Y:78:LEU:C	1:Y:80:LYS:N	2.72	0.43
1:B:65:GLU:HG2	2:F:143:TRP:CD1	2.54	0.43
1:V:73:LYS:HZ1	1:V:77:GLU:HG2	1.82	0.43
1:V:17:ASP:OD1	1:V:33:LYS:NZ	2.45	0.43
1:D:102:ALA:HB1	1:D:114:GLN:OE1	2.19	0.43
2:G:311:GLN:HA	2:G:311:GLN:NE2	2.33	0.43
2:I:5:THR:O	2:I:9:ILE:HG12	2.19	0.43
2:F:136:ILE:O	2:F:138:PRO:HD3	2.19	0.42
2:G:126:LEU:N	2:G:126:LEU:HD22	2.34	0.42
2:I:125:GLU:C	2:I:127:ALA:H	2.23	0.42
1:Y:61:GLU:O	1:Y:65:GLU:HG3	2.20	0.42
1:A:46:PHE:CD2	1:A:53:ALA:HB2	2.54	0.42
2:E:65:GLU:HG3	3:E:450:ADP:H2'	2.00	0.42
1:A:94:LEU:CD2	1:A:107:THR:HG22	2.50	0.42
2:I:339:ASP:O	2:I:343:ILE:HG13	2.18	0.42
2:G:240:LYS:HD3	2:G:241:GLN:N	2.34	0.42
2:I:84:THR:O	2:I:87:THR:OG1	2.35	0.42
2:F:5:THR:O	2:F:9:ILE:HG12	2.18	0.42
1:B:173:TYR:O	1:B:174:LYS:HB2	2.19	0.42
1:Z:101:THR:O	1:Z:102:ALA:HB2	2.19	0.42
2:E:168:LEU:CD2	2:E:219:LYS:HD3	2.49	0.42
2:I:148:GLN:C	2:I:150:GLN:H	2.23	0.42
2:G:256:ASP:O	2:G:257:GLU:HG2	2.20	0.42
1:A:99:ASP:C	1:A:99:ASP:OD1	2.57	0.42
2:E:16:HIS:HB2	2:E:17:ILE:HD12	2.01	0.42
2:E:150:GLN:C	2:E:153:SER:OG	2.57	0.42
2:F:145:GLN:C	2:F:147:GLU:H	2.22	0.42
2:I:264:ARG:NE	2:I:265:GLY:H	2.17	0.42
1:V:14:ILE:HD12	1:V:44:ALA:HA	2.00	0.42
1:X:157:ASP:OD2	1:X:164:HIS:NE2	2.52	0.42
2:E:148:GLN:HA	2:E:151:GLU:HG2	2.02	0.42
1:C:11:HIS:HA	1:C:171:LEU:O	2.19	0.42
2:E:131:ILE:CD1	2:E:218:ILE:HG12	2.47	0.42
1:C:168:ILE:CG2	1:C:169:GLU:N	2.83	0.42
2:G:389:ASN:C	2:G:389:ASN:ND2	2.63	0.42
1:X:152:LEU:HD22	1:X:166:HIS:CE1	2.50	0.42
2:E:123:ALA:O	2:E:127:ALA:HB2	2.20	0.42
1:D:114:GLN:HA	1:D:115:PRO:HD2	1.86	0.42
2:G:17:ILE:HD12	2:G:17:ILE:N	2.34	0.42
1:D:22:LEU:HD23	1:D:22:LEU:C	2.40	0.42
1:B:98:ALA:HB2	1:B:103:SER:CB	2.49	0.42
1:D:57:PHE:O	1:D:61:GLU:HB2	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:437:ASP:OD2	2:I:314:LYS:HE3	2.19	0.42
1:C:131:ALA:HB3	1:X:131:ALA:HB3	2.02	0.42
1:Y:94:LEU:HA	1:Y:94:LEU:HD23	1.91	0.42
2:I:109:LYS:O	2:I:109:LYS:HG3	2.19	0.42
2:F:225:LEU:HA	2:F:228:GLU:HB2	2.02	0.42
1:A:160:ILE:O	1:Z:160:ILE:HG13	2.20	0.42
2:E:101:ARG:O	2:E:104:THR:HB	2.19	0.42
1:A:86:ARG:HA	1:A:89:ARG:NH2	2.35	0.42
2:I:145:GLN:HA	2:I:145:GLN:NE2	2.34	0.42
2:E:77:PRO:HB2	2:E:103:LEU:CD2	2.49	0.42
2:E:116:ILE:HG22	2:E:116:ILE:O	2.19	0.42
2:G:134:VAL:HG13	2:G:171:LYS:HD3	2.02	0.42
2:F:33:ASN:ND2	2:F:36:ARG:HD2	2.34	0.42
1:Y:148:ALA:O	1:Y:152:LEU:HB2	2.19	0.42
1:B:13:VAL:HG12	1:B:170:GLU:HA	2.01	0.42
2:E:220:ASP:O	2:E:224:LEU:HD23	2.20	0.42
1:X:89:ARG:CB	1:X:89:ARG:NH1	2.83	0.42
1:Y:79:ALA:HB1	1:Y:110:GLY:O	2.20	0.42
2:I:170:ASP:HB2	2:I:216:LEU:O	2.19	0.42
1:Y:63:LYS:HD3	1:Y:66:MET:HE3	2.00	0.42
1:D:136:LEU:HD11	1:V:135:ALA:O	2.19	0.42
1:V:35:ARG:C	1:V:36:ARG:HG3	2.39	0.42
1:Y:168:ILE:HD12	1:Y:168:ILE:H	1.84	0.42
2:G:230:ALA:O	2:G:233:LEU:HB3	2.20	0.42
2:E:326:LEU:O	2:E:329:ARG:NE	2.48	0.42
1:Y:117:ASN:C	1:Y:119:LEU:N	2.71	0.42
2:F:167:GLN:HE22	2:F:219:LYS:HD2	1.84	0.42
2:G:168:LEU:HD12	2:G:219:LYS:CB	2.48	0.42
1:A:81:ASP:HA	1:A:84:THR:CG2	2.49	0.42
2:I:147:GLU:HG2	2:I:150:GLN:HE21	1.83	0.42
1:C:42:VAL:HG11	1:C:60:PHE:HE2	1.84	0.42
2:G:113:VAL:C	2:G:115:ALA:H	2.22	0.42
2:G:400:GLU:HG3	2:I:327:PRO:HB2	2.02	0.42
2:I:384:ASN:ND2	2:I:390:ILE:H	2.18	0.42
1:Y:87:MET:O	1:Y:89:ARG:N	2.53	0.42
1:C:46:PHE:CD2	1:C:53:ALA:HB2	2.54	0.42
1:C:82:TRP:CZ3	1:C:95:LEU:HD13	2.55	0.42
1:V:156:GLY:HA2	1:V:162:THR:HG22	2.02	0.42
1:A:105:ILE:HD11	1:A:120:ILE:HG23	2.02	0.42
1:B:3:ILE:O	1:B:121:ALA:HA	2.19	0.42
1:D:80:LYS:HE3	1:D:80:LYS:HB3	1.93	0.42
2:E:215:LYS:HG3	2:E:215:LYS:O	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:173:ILE:N	2:G:173:ILE:CD1	2.78	0.42
2:G:174:GLU:HB3	2:G:211:GLN:CB	2.49	0.42
2:G:167:GLN:OE1	2:G:168:LEU:N	2.52	0.42
2:F:150:GLN:O	2:F:153:SER:OG	2.38	0.42
1:C:58:GLU:O	1:C:61:GLU:HB2	2.19	0.42
2:E:392:ALA:HB3	3:E:450:ADP:C8	2.55	0.42
2:I:393:ARG:HG2	2:I:393:ARG:NH1	2.33	0.42
1:X:105:ILE:HD12	1:X:122:ILE:CG2	2.50	0.42
1:V:134:ARG:HH11	1:V:134:ARG:HG2	1.84	0.42
2:G:349:ALA:HB1	2:I:44:LEU:HD23	2.02	0.42
2:E:240:LYS:HD3	2:E:240:LYS:C	2.40	0.42
2:E:40:LEU:O	2:E:45:ARG:NH1	2.53	0.42
1:V:90:LYS:NZ	1:X:83:ARG:O	2.49	0.42
2:G:147:GLU:HG3	2:G:150:GLN:CD	2.40	0.42
1:Y:7:ARG:NH2	1:Y:102:ALA:C	2.74	0.42
1:C:71:LEU:HD13	1:C:71:LEU:C	2.40	0.42
2:F:148:GLN:HA	2:F:151:GLU:HG2	2.01	0.42
2:I:344:LEU:HD11	2:I:395:LEU:HD22	2.01	0.42
2:I:345:THR:HG23	2:I:373:ILE:HD13	2.02	0.42
1:C:123:GLY:O	1:C:126:GLY:N	2.43	0.42
1:Y:169:GLU:HA	1:Y:169:GLU:OE2	2.20	0.42
2:G:358:LEU:HD22	2:I:36:ARG:CB	2.50	0.42
1:B:6:VAL:HG12	1:B:7:ARG:H	1.82	0.42
1:D:68:GLN:O	1:D:70:HIS:N	2.53	0.42
2:F:258:ILE:HD12	2:F:261:ILE:HD11	2.01	0.42
1:Z:71:LEU:O	1:Z:75:ALA:N	2.49	0.42
2:F:214:ARG:HE	2:F:216:LEU:HB3	1.85	0.41
2:E:212:LYS:CD	2:E:216:LEU:HD21	2.29	0.41
1:B:43:ILE:HG12	1:B:98:ALA:O	2.19	0.41
1:Y:65:GLU:CG	2:I:143:TRP:CD1	3.02	0.41
1:Y:18:GLY:HA2	1:Y:33:LYS:HE3	2.01	0.41
1:X:3:ILE:HB	1:X:122:ILE:HG12	2.01	0.41
2:G:103:LEU:O	2:G:107:ALA:HB2	2.20	0.41
1:V:56:LEU:HD11	1:V:91:LEU:HD13	2.01	0.41
2:G:442:ILE:HG22	2:G:442:ILE:O	2.20	0.41
2:E:42:GLU:HA	2:E:45:ARG:NH2	2.35	0.41
1:Z:103:SER:O	1:Z:104:LEU:HB3	2.20	0.41
2:G:217:LYS:CG	2:G:219:LYS:HZ3	2.32	0.41
2:E:89:VAL:CG1	2:E:93:GLY:HA3	2.41	0.41
2:F:147:GLU:HA	2:F:150:GLN:HB3	2.01	0.41
1:A:17:ASP:O	1:A:33:LYS:HD2	2.20	0.41
2:E:117:GLU:OE2	2:E:120:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:42:VAL:HG13	1:X:98:ALA:O	2.20	0.41
1:C:46:PHE:HA	1:C:94:LEU:O	2.20	0.41
2:E:33:ASN:ND2	2:E:36:ARG:HD2	2.35	0.41
2:F:114:GLN:HA	2:F:117:GLU:HG2	2.01	0.41
2:F:282:LEU:HA	2:F:282:LEU:HD12	1.84	0.41
2:E:160:ARG:HH12	2:E:164:ARG:HH22	1.68	0.41
1:B:139:ASN:HD22	1:Z:136:LEU:HD11	1.85	0.41
2:E:168:LEU:HA	2:E:219:LYS:HB3	2.01	0.41
2:G:92:VAL:HG23	2:G:92:VAL:O	2.20	0.41
2:I:135:LEU:HD13	2:I:159:PHE:HB3	2.01	0.41
1:Y:18:GLY:C	1:Y:163:ASN:HD21	2.23	0.41
1:V:134:ARG:HG2	1:V:134:ARG:NH1	2.35	0.41
2:E:231:ALA:C	2:E:233:LEU:N	2.74	0.41
2:E:43:GLU:O	2:E:45:ARG:N	2.53	0.41
1:Y:159:CYS:HB3	1:Y:162:THR:HB	2.02	0.41
1:X:84:THR:O	1:X:89:ARG:NH1	2.54	0.41
2:G:145:GLN:O	2:G:147:GLU:N	2.54	0.41
2:E:312:ILE:CG1	2:E:313:ALA:N	2.81	0.41
2:I:86:PHE:HB2	2:I:277:VAL:HG13	2.02	0.41
1:Y:65:GLU:HB3	2:I:143:TRP:HA	2.01	0.41
1:V:20:ALA:HB2	1:V:31:VAL:HG21	2.02	0.41
2:G:384:ASN:HD21	2:G:390:ILE:HG12	1.86	0.41
2:G:27:VAL:CG1	2:G:70:LEU:HG	2.50	0.41
2:F:269:GLY:N	2:F:270:PRO:CD	2.84	0.41
2:I:17:ILE:HD11	2:I:69:ARG:HG3	2.02	0.41
2:E:402:LEU:HD12	2:E:428:HIS:HB2	2.03	0.41
1:V:10:GLY:HA3	1:V:174:LYS:HA	2.01	0.41
2:F:355:TYR:CE1	2:F:403:MET:HE3	2.55	0.41
1:C:50:THR:HG22	1:C:50:THR:O	2.20	0.41
2:E:160:ARG:HH11	2:E:160:ARG:HG2	1.86	0.41
2:E:173:ILE:N	2:E:173:ILE:CD1	2.78	0.41
2:G:112:ARG:O	2:G:115:ALA:HB3	2.21	0.41
2:E:432:LEU:N	2:E:432:LEU:CD1	2.81	0.41
1:X:7:ARG:O	1:X:8:ARG:HB2	2.20	0.41
1:X:160:ILE:HA	1:X:160:ILE:HD13	1.87	0.41
2:G:212:LYS:O	2:G:214:ARG:N	2.54	0.41
1:V:30:ASN:N	1:V:30:ASN:ND2	2.57	0.41
1:A:104:LEU:HD12	1:A:104:LEU:O	2.20	0.41
2:F:403:MET:SD	2:F:420:ILE:HD13	2.61	0.41
2:F:47:GLU:OE1	2:F:47:GLU:HA	2.20	0.41
2:F:167:GLN:NE2	2:F:219:LYS:HD2	2.35	0.41
1:V:86:ARG:O	1:V:90:LYS:HG2	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:134:VAL:HG11	2:E:171:LYS:HD3	2.03	0.41
2:I:130:ARG:HD2	2:I:225:LEU:CD1	2.51	0.41
2:F:91:TYR:O	2:F:92:VAL:CG1	2.60	0.41
1:X:43:ILE:N	1:X:43:ILE:HD13	2.28	0.41
2:I:345:THR:HG21	2:I:373:ILE:HD13	1.98	0.41
2:G:123:ALA:O	2:G:127:ALA:HB2	2.21	0.41
1:V:11:HIS:CE1	1:V:172:SER:OG	2.73	0.41
2:E:151:GLU:CB	2:E:152:PRO:HD3	2.50	0.41
2:F:216:LEU:HD11	2:F:221:ALA:HA	2.03	0.41
2:E:173:ILE:O	2:E:212:LYS:HD2	2.21	0.41
2:I:145:GLN:HA	2:I:145:GLN:HE21	1.85	0.41
2:G:312:ILE:CG1	2:G:313:ALA:N	2.83	0.41
1:B:63:LYS:HD3	1:B:63:LYS:HA	1.90	0.41
1:B:131:ALA:HA	1:Z:154:ILE:HG21	2.03	0.41
1:A:173:TYR:O	1:A:174:LYS:C	2.58	0.41
1:C:17:ASP:OD1	1:C:33:LYS:NZ	2.50	0.41
1:V:35:ARG:HB2	1:V:36:ARG:H	1.69	0.41
1:A:149:GLU:OE2	1:A:166:HIS:CD2	2.74	0.41
1:C:100:GLU:OE2	1:C:173:TYR:HD1	2.04	0.41
1:X:8:ARG:NH2	1:X:137:LEU:HD12	2.35	0.41
2:G:5:THR:O	2:G:6:PRO:C	2.59	0.41
2:F:45:ARG:HH11	2:F:45:ARG:HG3	1.86	0.41
2:F:171:LYS:O	2:F:172:GLU:HB3	2.21	0.41
2:G:145:GLN:C	2:G:147:GLU:N	2.73	0.41
2:G:91:TYR:CE1	2:I:91:TYR:CE2	3.09	0.41
2:G:171:LYS:HB2	2:G:218:ILE:CG1	2.47	0.41
2:E:159:PHE:O	2:E:163:LEU:HB2	2.21	0.41
2:I:257:GLU:HB2	2:I:260:LYS:CG	2.48	0.41
2:F:108:VAL:HG23	2:F:243:ALA:CB	2.51	0.41
2:G:142:ASN:HB2	2:G:149:GLN:HE22	1.83	0.41
1:Y:38:TYR:HB2	1:Y:64:LEU:CD1	2.51	0.41
1:D:6:VAL:HG21	1:D:147:ILE:CG2	2.49	0.41
1:Y:3:ILE:O	1:Y:121:ALA:HA	2.21	0.41
2:E:255:ILE:HD13	2:E:281:LEU:CD2	2.51	0.41
2:E:165:GLU:HG2	2:E:166:GLY:H	1.86	0.41
1:V:123:GLY:O	1:V:126:GLY:N	2.43	0.41
1:A:20:ALA:HB2	1:A:31:VAL:HG21	2.03	0.41
2:G:402:LEU:HD11	2:G:425:VAL:HA	2.03	0.41
2:G:158:ALA:O	2:G:162:LYS:HG3	2.21	0.41
1:X:80:LYS:HE3	1:X:80:LYS:HB3	1.94	0.41
1:C:43:ILE:HG23	1:C:171:LEU:HD13	2.03	0.41
2:G:174:GLU:HG3	2:G:213:ALA:CA	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:89:VAL:HA	2:G:93:GLY:HA3	2.03	0.41
2:G:86:PHE:HA	2:G:89:VAL:HG13	2.03	0.41
1:V:97:VAL:HB	1:V:104:LEU:CD1	2.50	0.41
2:G:358:LEU:CD2	2:I:36:ARG:CB	2.99	0.41
2:G:119:ASN:OD1	2:G:234:VAL:HG22	2.21	0.41
2:E:362:GLU:HG2	2:E:410:ALA:HB1	2.02	0.41
2:F:135:LEU:HD22	2:F:159:PHE:HE2	1.83	0.40
2:F:219:LYS:O	2:F:223:LYS:HD3	2.21	0.40
2:E:171:LYS:HB3	2:E:172:GLU:H	1.63	0.40
1:B:104:LEU:N	1:B:104:LEU:HD23	2.35	0.40
1:Y:101:THR:HG22	1:Y:102:ALA:N	2.35	0.40
1:C:86:ARG:CA	1:C:89:ARG:HH12	2.29	0.40
2:I:244:ILE:HD11	2:I:294:HIS:O	2.21	0.40
1:V:67:HIS:O	1:V:68:GLN:C	2.58	0.40
1:A:149:GLU:CG	1:A:168:ILE:HD11	2.52	0.40
1:Z:88:LEU:CD1	1:Z:88:LEU:N	2.82	0.40
1:A:6:VAL:HG21	1:A:147:ILE:CG2	2.50	0.40
2:E:34:ARG:NH2	2:E:250:HIS:HA	2.36	0.40
2:F:134:VAL:HG13	2:F:171:LYS:HD2	2.03	0.40
1:Z:173:TYR:O	1:Z:174:LYS:C	2.59	0.40
2:F:150:GLN:C	2:F:153:SER:OG	2.59	0.40
1:C:28:LYS:CE	1:C:30:ASN:HD21	2.34	0.40
1:B:14:ILE:HD12	1:B:44:ALA:HA	2.03	0.40
2:I:344:LEU:HA	2:I:344:LEU:HD12	1.84	0.40
1:V:99:ASP:N	1:V:99:ASP:OD1	2.55	0.40
2:G:362:GLU:OE2	2:I:32:ARG:NH2	2.34	0.40
1:Z:10:GLY:HA3	1:Z:174:LYS:N	2.37	0.40
1:A:139:ASN:ND2	1:Y:136:LEU:HD11	2.36	0.40
1:C:71:LEU:HD11	1:C:104:LEU:HD11	2.04	0.40
1:Y:11:HIS:HA	1:Y:171:LEU:O	2.22	0.40
2:I:236:PRO:C	2:I:238:GLU:H	2.21	0.40
1:D:64:LEU:CB	1:D:69:GLY:HA2	2.52	0.40
2:G:388:GLU:O	2:G:394:ARG:NH2	2.52	0.40
1:A:62:ARG:HD2	2:E:141:ASN:HD21	1.86	0.40
2:E:226:ILE:O	2:E:230:ALA:HB2	2.22	0.40
2:E:54:LEU:HB3	2:E:329:ARG:HD3	2.03	0.40
2:G:413:LEU:O	2:G:416:GLN:HG3	2.21	0.40
2:E:169:ASP:O	2:E:218:ILE:CG1	2.69	0.40
1:Y:65:GLU:OE1	2:I:143:TRP:CE2	2.74	0.40
1:B:66:MET:O	1:B:67:HIS:ND1	2.54	0.40
2:F:41:ASN:HD21	2:F:44:LEU:H	1.69	0.40
2:G:96:VAL:HG12	2:G:284:LEU:HD11	2.02	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:19:GLY:O	2:F:24:LYS:HE3	2.21	0.40
2:F:74:ALA:O	2:F:75:ASN:C	2.60	0.40
2:G:21:ASP:HA	2:G:24:LYS:HD2	2.02	0.40
1:V:21:THR:HG22	1:V:22:LEU:N	2.36	0.40
2:F:443:LEU:HD23	2:F:443:LEU:HA	1.91	0.40
2:E:164:ARG:NH1	2:E:164:ARG:HG2	2.36	0.40
2:I:125:GLU:HB3	2:I:126:LEU:H	1.73	0.40
2:I:172:GLU:O	2:I:173:ILE:HG23	2.22	0.40
2:I:174:GLU:C	2:I:212:LYS:HB3	2.42	0.40
2:I:218:ILE:HA	2:I:221:ALA:HB3	2.04	0.40
2:I:147:GLU:HA	2:I:150:GLN:HB3	2.04	0.40
2:I:61:VAL:C	3:I:3450:ADP:N7	2.75	0.40
1:X:114:GLN:HA	1:X:115:PRO:HD2	1.87	0.40
1:C:160:ILE:HG21	1:V:160:ILE:HG23	2.01	0.40
2:E:121:TYR:C	2:E:123:ALA:H	2.24	0.40
2:I:96:VAL:CG1	2:I:281:LEU:HD12	2.50	0.40
2:F:289:THR:CG2	2:F:296:MET:HG3	2.51	0.40
1:V:11:HIS:HE1	1:V:172:SER:OG	2.04	0.40
2:G:270:PRO:O	2:G:271:ASP:C	2.60	0.40
2:E:248:GLU:HG2	2:E:297:VAL:HG13	2.04	0.40
2:E:111:VAL:HG21	2:E:243:ALA:HB2	2.04	0.40
2:E:351:ILE:HD13	2:E:396:HIS:ND1	2.37	0.40

All (1) 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	Distance(Å)	Clash(Å)
2:E:7:ARG:NH2	2:F:409:ASP:OD2[2_665]	2.06	0.14

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	172/175 (98%)	151 (88%)	17 (10%)	4 (2%)	10	31
1	B	172/175 (98%)	138 (80%)	27 (16%)	7 (4%)	4	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	172/175 (98%)	140 (81%)	27 (16%)	5 (3%)	7	23
1	D	172/175 (98%)	146 (85%)	23 (13%)	3 (2%)	14	42
1	V	172/175 (98%)	144 (84%)	25 (14%)	3 (2%)	14	42
1	X	172/175 (98%)	148 (86%)	20 (12%)	4 (2%)	10	31
1	Y	172/175 (98%)	136 (79%)	26 (15%)	10 (6%)	3	7
1	Z	172/175 (98%)	150 (87%)	18 (10%)	4 (2%)	10	31
2	E	404/449 (90%)	349 (86%)	46 (11%)	9 (2%)	10	32
2	F	404/449 (90%)	343 (85%)	45 (11%)	16 (4%)	5	14
2	G	404/449 (90%)	344 (85%)	45 (11%)	15 (4%)	5	16
2	I	404/449 (90%)	347 (86%)	43 (11%)	14 (4%)	6	18
All	All	2992/3196 (94%)	2536 (85%)	362 (12%)	94 (3%)	7	21

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	116	GLU
1	V	116	GLU
1	Y	54	PHE
1	Y	68	GLN
1	Y	71	LEU
1	Y	72	VAL
2	E	92	VAL
2	E	144	GLY
2	E	153	SER
2	F	92	VAL
2	F	153	SER
2	F	165	GLU
2	F	212	LYS
2	F	236	PRO
2	G	92	VAL
2	G	153	SER
2	I	92	VAL
2	I	153	SER
2	I	165	GLU
2	I	212	LYS
2	I	236	PRO
2	I	237	GLU
1	C	40	ASP

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Mol	Chain	Res	Type
1	C	68	GLN
1	C	69	GLY
1	V	68	GLN
1	V	69	GLY
1	X	69	GLY
1	X	116	GLU
1	A	9	ASN
1	B	54	PHE
1	B	69	GLY
1	B	70	HIS
1	B	116	GLU
1	Z	71	LEU
1	Y	69	GLY
1	Y	116	GLU
2	E	44	LEU
2	E	165	GLU
2	E	212	LYS
2	F	143	TRP
2	F	230	ALA
2	G	141	ASN
2	G	144	GLY
2	G	165	GLU
2	G	170	ASP
2	G	212	LYS
2	G	213	ALA
2	I	230	ALA
1	C	113	VAL
1	D	115	PRO
1	X	115	PRO
1	A	71	LEU
1	Z	9	ASN
1	Y	70	HIS
1	Y	88	LEU
2	E	146	THR
2	F	154	ALA
2	F	237	GLU
2	F	300	ASP
2	G	44	LEU
2	G	146	THR
2	G	154	ALA
2	G	410	ALA
2	I	138	PRO

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Mol	Chain	Res	Type
2	I	143	TRP
2	I	146	THR
1	A	115	PRO
1	B	68	GLN
1	B	88	LEU
2	E	213	ALA
2	F	137	PRO
2	F	138	PRO
2	F	293	LYS
2	G	232	LYS
2	I	137	PRO
1	D	116	GLU
1	X	8	ARG
1	Z	115	PRO
1	Y	38	TYR
1	Y	86	ARG
2	E	141	ASN
2	F	140	LYS
2	G	271	ASP
2	I	42	GLU
2	I	144	GLY
1	D	69	GLY
1	Z	72	VAL
1	B	72	VAL
2	F	144	GLY
1	A	72	VAL
2	G	235	ASN
2	I	173	ILE
2	F	173	ILE

### 5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	136/136 (100%)	129 (95%)	7 (5%)	33	69
1	B	136/136 (100%)	125 (92%)	11 (8%)	17	43
1	C	136/136 (100%)	121 (89%)	15 (11%)	9	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	136/136 (100%)	124 (91%)	12 (9%)	14	38
1	V	136/136 (100%)	119 (88%)	17 (12%)	7	19
1	X	136/136 (100%)	124 (91%)	12 (9%)	14	38
1	Y	136/136 (100%)	127 (93%)	9 (7%)	24	56
1	Z	136/136 (100%)	128 (94%)	8 (6%)	28	62
2	E	350/383 (91%)	308 (88%)	42 (12%)	7	21
2	F	350/383 (91%)	301 (86%)	49 (14%)	5	15
2	G	350/383 (91%)	307 (88%)	43 (12%)	7	20
2	I	350/383 (91%)	301 (86%)	49 (14%)	5	15
All	All	2488/2620 (95%)	2214 (89%)	274 (11%)	9	26

All (274) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1	THR
1	C	4	VAL
1	C	30	ASN
1	C	37	LEU
1	C	40	ASP
1	C	54	PHE
1	C	80	LYS
1	C	83	ARG
1	C	91	LEU
1	C	104	LEU
1	C	116	GLU
1	C	136	LEU
1	C	149	GLU
1	C	152	LEU
1	C	173	TYR
1	D	1	THR
1	D	30	ASN
1	D	37	LEU
1	D	43	ILE
1	D	54	PHE
1	D	71	LEU
1	D	73	LYS
1	D	118	ASP
1	D	136	LEU
1	D	152	LEU

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Mol	Chain	Res	Type
1	D	160	ILE
1	D	174	LYS
1	V	1	THR
1	V	30	ASN
1	V	37	LEU
1	V	54	PHE
1	V	73	LYS
1	V	77	GLU
1	V	83	ARG
1	V	104	LEU
1	V	111	ASP
1	V	114	GLN
1	V	136	LEU
1	V	139	ASN
1	V	152	LEU
1	V	154	ILE
1	V	160	ILE
1	V	168	ILE
1	V	173	TYR
1	X	1	THR
1	X	30	ASN
1	X	37	LEU
1	X	40	ASP
1	X	43	ILE
1	X	54	PHE
1	X	58	GLU
1	X	71	LEU
1	X	73	LYS
1	X	118	ASP
1	X	152	LEU
1	X	174	LYS
1	A	1	THR
1	A	9	ASN
1	A	30	ASN
1	A	71	LEU
1	A	97	VAL
1	A	136	LEU
1	A	152	LEU
1	B	1	THR
1	B	30	ASN
1	B	35	ARG
1	B	54	PHE

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Mol	Chain	Res	Type
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
1	Z	1	THR
1	Z	9	ASN
1	Z	30	ASN
1	Z	58	GLU
1	Z	71	LEU
1	Z	107	THR
1	Z	136	LEU
1	Z	152	LEU
1	Y	1	THR
1	Y	30	ASN
1	Y	54	PHE
1	Y	72	VAL
1	Y	116	GLU
1	Y	136	LEU
1	Y	152	LEU
1	Y	160	ILE
1	Y	174	LYS
2	E	11	SER
2	E	13	LEU
2	E	27	VAL
2	E	31	LEU
2	E	37	ARG
2	E	49	THR
2	E	59	THR
2	E	70	LEU
2	E	92	VAL
2	E	94	LYS
2	E	117	GLU
2	E	130	ARG
2	E	140	LYS
2	E	148	GLN
2	E	153	SER
2	E	165	GLU
2	E	169	ASP
2	E	171	LYS

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Mol	Chain	Res	Type
2	E	173	ILE
2	E	216	LEU
2	E	220	ASP
2	E	238	GLU
2	E	240	LYS
2	E	241	GLN
2	E	266	GLU
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	344	LEU
2	E	352	THR
2	E	353	VAL
2	E	355	TYR
2	E	375	ARG
2	E	385	GLU
2	E	389	ASN
2	E	412	ASP
2	E	413	LEU
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

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Mol	Chain	Res	Type
2	F	148	GLN
2	F	150	GLN
2	F	152	PRO
2	F	153	SER
2	F	173	ILE
2	F	210	LYS
2	F	211	GLN
2	F	214	ARG
2	F	217	LYS
2	F	219	LYS
2	F	220	ASP
2	F	232	LYS
2	F	266	GLU
2	F	281	LEU
2	F	296	MET
2	F	312	ILE
2	F	318	LEU
2	F	326	LEU
2	F	331	GLU
2	F	337	THR
2	F	344	LEU
2	F	351	ILE
2	F	352	THR
2	F	355	TYR
2	F	375	ARG
2	F	382	GLN
2	F	385	GLU
2	F	389	ASN
2	F	404	GLU
2	F	423	ASP
2	F	438	LEU
2	G	11	SER
2	G	13	LEU
2	G	27	VAL
2	G	31	LEU
2	G	37	ARG
2	G	59	THR
2	G	70	LEU
2	G	94	LYS
2	G	103	LEU
2	G	117	GLU
2	G	130	ARG

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Mol	Chain	Res	Type
2	G	140	LYS
2	G	148	GLN
2	G	152	PRO
2	G	153	SER
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	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	375	ARG
2	G	385	GLU
2	G	386	SER
2	G	389	ASN
2	G	419	THR
2	G	423	ASP
2	G	438	LEU
2	I	11	SER
2	I	13	LEU
2	I	27	VAL
2	I	31	LEU
2	I	37	ARG
2	I	41	ASN
2	I	49	THR
2	I	59	THR
2	I	68	ARG
2	I	70	LEU

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Mol	Chain	Res	Type
2	I	87	THR
2	I	94	LYS
2	I	103	LEU
2	I	104	THR
2	I	121	TYR
2	I	130	ARG
2	I	140	LYS
2	I	141	ASN
2	I	145	GLN
2	I	148	GLN
2	I	150	GLN
2	I	152	PRO
2	I	173	ILE
2	I	210	LYS
2	I	211	GLN
2	I	214	ARG
2	I	217	LYS
2	I	220	ASP
2	I	232	LYS
2	I	266	GLU
2	I	296	MET
2	I	300	ASP
2	I	311	GLN
2	I	312	ILE
2	I	318	LEU
2	I	326	LEU
2	I	337	THR
2	I	344	LEU
2	I	351	ILE
2	I	352	THR
2	I	355	TYR
2	I	375	ARG
2	I	382	GLN
2	I	385	GLU
2	I	389	ASN
2	I	404	GLU
2	I	413	LEU
2	I	438	LEU
2	I	442	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	9	ASN
1	C	30	ASN
1	C	114	GLN
1	D	9	ASN
1	D	30	ASN
1	D	139	ASN
1	V	9	ASN
1	V	11	HIS
1	V	30	ASN
1	V	114	GLN
1	X	9	ASN
1	X	30	ASN
1	X	114	GLN
1	X	139	ASN
1	A	30	ASN
1	A	39	ASN
1	A	68	GLN
1	A	109	ASN
1	A	139	ASN
1	B	11	HIS
1	B	30	ASN
1	B	109	ASN
1	B	114	GLN
1	Z	30	ASN
1	Z	39	ASN
1	Z	109	ASN
1	Y	11	HIS
1	Y	30	ASN
1	Y	109	ASN
1	Y	114	GLN
1	Y	130	GLN
2	E	22	ASN
2	E	33	ASN
2	E	75	ASN
2	E	114	GLN
2	E	141	ASN
2	E	145	GLN
2	E	149	GLN
2	E	150	GLN
2	E	241	GLN
2	E	311	GLN
2	E	348	ASN
2	E	382	GLN

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Mol	Chain	Res	Type
2	E	384	ASN
2	E	389	ASN
2	E	416	GLN
2	E	428	HIS
2	F	22	ASN
2	F	33	ASN
2	F	41	ASN
2	F	114	GLN
2	F	141	ASN
2	F	142	ASN
2	F	145	GLN
2	F	149	GLN
2	F	150	GLN
2	F	157	GLN
2	F	211	GLN
2	F	348	ASN
2	F	365	ASN
2	F	384	ASN
2	F	389	ASN
2	F	416	GLN
2	F	417	ASN
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	311	GLN
2	G	348	ASN
2	G	382	GLN
2	G	384	ASN
2	G	389	ASN
2	G	416	GLN
2	G	428	HIS
2	I	22	ASN
2	I	41	ASN
2	I	75	ASN
2	I	114	GLN
2	I	142	ASN
2	I	145	GLN
2	I	149	GLN

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Mol	Chain	Res	Type
2	I	150	GLN
2	I	211	GLN
2	I	311	GLN
2	I	348	ASN
2	I	384	ASN
2	I	389	ASN
2	I	416	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

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	-	29,29,29	1.54	8 (27%)	45,45,45	1.55	6 (13%)
3	ADP	F	1450	-	29,29,29	1.52	5 (17%)	45,45,45	1.56	6 (13%)
3	ADP	G	2450	-	29,29,29	1.56	8 (27%)	45,45,45	1.59	7 (15%)
3	ADP	I	3450	-	29,29,29	1.51	6 (20%)	45,45,45	1.58	6 (13%)

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	-	-	0/16/32/32	0/1/3/3
3	ADP	F	1450	-	-	0/16/32/32	0/1/3/3
3	ADP	G	2450	-	-	0/16/32/32	0/1/3/3
3	ADP	I	3450	-	-	0/16/32/32	0/1/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2450	ADP	C8-N7	-3.76	1.27	1.34
3	E	450	ADP	C8-N7	-3.70	1.27	1.34
3	F	1450	ADP	C8-N7	-3.69	1.27	1.34
3	I	3450	ADP	C8-N7	-3.61	1.27	1.34
3	G	2450	ADP	C2'-C1'	2.72	1.57	1.53
3	F	1450	ADP	C4-N3	2.61	1.39	1.35
3	E	450	ADP	PB-O3A	-2.60	1.55	1.60
3	I	3450	ADP	C1'-N9	2.53	1.56	1.48
3	I	3450	ADP	C4-N3	2.52	1.39	1.35
3	G	2450	ADP	PB-O3A	-2.48	1.55	1.60
3	E	450	ADP	C2'-C1'	2.45	1.56	1.53
3	E	450	ADP	C1'-N9	2.34	1.56	1.48
3	F	1450	ADP	C1'-N9	2.30	1.55	1.48
3	G	2450	ADP	C4-N3	2.22	1.39	1.35
3	E	450	ADP	PA-O1A	-2.20	1.43	1.51
3	E	450	ADP	C4-N3	2.16	1.38	1.35
3	F	1450	ADP	C2-N3	2.14	1.36	1.32
3	G	2450	ADP	PA-O1A	-2.11	1.43	1.51
3	G	2450	ADP	C1'-N9	2.10	1.55	1.48
3	E	450	ADP	PA-O2A	-2.07	1.45	1.55
3	I	3450	ADP	PA-O2A	-2.05	1.45	1.55
3	G	2450	ADP	PA-O2A	-2.04	1.45	1.55
3	I	3450	ADP	PA-O1A	-2.03	1.43	1.51
3	I	3450	ADP	C2-N3	2.03	1.36	1.32
3	G	2450	ADP	PB-O3B	-2.03	1.47	1.54
3	F	1450	ADP	PA-O3A	2.01	1.63	1.59
3	E	450	ADP	PB-O3B	-2.00	1.47	1.54

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	3450	ADP	C4'-O4'-C1'	6.51	116.82	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2450	ADP	C4'-O4'-C1'	6.40	116.70	109.75
3	E	450	ADP	C4'-O4'-C1'	6.29	116.58	109.75
3	F	1450	ADP	C4'-O4'-C1'	6.27	116.56	109.75
3	F	1450	ADP	N3-C2-N1	-4.59	124.87	128.71
3	G	2450	ADP	N3-C2-N1	-4.53	124.92	128.71
3	I	3450	ADP	N3-C2-N1	-4.41	125.02	128.71
3	E	450	ADP	N3-C2-N1	-4.18	125.21	128.71
3	G	2450	ADP	C2'-C3'-C4'	3.06	108.75	102.65
3	E	450	ADP	C2'-C3'-C4'	3.02	108.67	102.65
3	I	3450	ADP	C2'-C3'-C4'	2.99	108.61	102.65
3	F	1450	ADP	C2'-C3'-C4'	2.97	108.58	102.65
3	I	3450	ADP	C3'-C2'-C1'	2.93	105.49	100.91
3	E	450	ADP	C3'-C2'-C1'	2.89	105.42	100.91
3	G	2450	ADP	C3'-C2'-C1'	2.83	105.33	100.91
3	F	1450	ADP	C3'-C2'-C1'	2.79	105.27	100.91
3	I	3450	ADP	N3-C4-N9	2.51	129.96	125.43
3	F	1450	ADP	N3-C4-N9	2.44	129.83	125.43
3	G	2450	ADP	N3-C4-N9	2.42	129.81	125.43
3	E	450	ADP	N3-C4-N9	2.32	129.63	125.43
3	F	1450	ADP	C5-C4-N9	-2.19	104.00	107.16
3	G	2450	ADP	C5-C4-N9	-2.15	104.06	107.16
3	G	2450	ADP	C2'-C1'-N9	-2.15	107.76	113.27
3	E	450	ADP	C5-C4-N9	-2.06	104.19	107.16
3	I	3450	ADP	C5-C4-N9	-2.06	104.19	107.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.57	4 (2%) 57 58	30, 54, 89, 98	0
1	B	174/175 (99%)	0.69	16 (9%) 9 7	36, 68, 101, 102	0
1	C	174/175 (99%)	0.73	22 (12%) 4 3	54, 81, 100, 102	0
1	D	174/175 (99%)	0.57	10 (5%) 23 23	49, 71, 97, 100	0
1	V	174/175 (99%)	0.63	15 (8%) 11 9	54, 80, 98, 102	0
1	X	174/175 (99%)	0.51	7 (4%) 36 37	51, 70, 98, 101	0
1	Y	174/175 (99%)	0.62	8 (4%) 31 31	36, 68, 100, 102	0
1	Z	174/175 (99%)	0.55	5 (2%) 49 50	30, 55, 90, 97	0
2	E	408/449 (90%)	0.73	42 (10%) 7 6	32, 59, 102, 102	0
2	F	408/449 (90%)	1.01	63 (15%) 3 2	33, 61, 102, 102	0
2	G	408/449 (90%)	0.75	40 (9%) 8 6	32, 59, 102, 102	0
2	I	408/449 (90%)	0.96	59 (14%) 3 3	32, 60, 102, 102	0
All	All	3024/3196 (94%)	0.75	291 (9%) 8 7	30, 63, 102, 102	0

All (291) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	90	GLY	10.8
2	G	144	GLY	9.9
2	F	90	GLY	9.6
2	F	141	ASN	8.4
2	F	144	GLY	8.2
2	I	145	GLN	7.8
2	I	141	ASN	7.8
2	F	146	THR	7.0
2	F	123	ALA	7.0
2	I	154	ALA	6.9
2	E	89	VAL	6.8

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Mol	Chain	Res	Type	RSRZ
2	E	140	LYS	6.7
2	F	134	VAL	6.4
2	F	165	GLU	6.3
2	F	226	ILE	6.3
2	I	226	ILE	6.2
2	I	143	TRP	6.2
2	G	214	ARG	6.1
2	F	267	SER	6.1
2	I	132	LEU	5.9
2	G	89	VAL	5.9
2	I	134	VAL	5.8
2	E	148	GLN	5.7
2	G	267	SER	5.6
2	I	140	LYS	5.4
2	F	153	SER	5.3
2	F	170	ASP	5.2
2	F	117	GLU	5.2
2	F	173	ILE	5.2
2	G	265	GLY	5.1
2	F	89	VAL	5.1
2	F	151	GLU	5.0
2	G	146	THR	4.9
2	F	133	ASP	4.9
2	I	219	LYS	4.9
2	E	145	GLN	4.9
2	E	215	LYS	4.8
2	I	165	GLU	4.8
2	I	91	TYR	4.8
2	I	152	PRO	4.8
2	I	123	ALA	4.8
2	I	92	VAL	4.8
1	Y	60	PHE	4.7
2	I	131	ILE	4.7
2	I	170	ASP	4.7
2	I	222	MET	4.7
2	F	222	MET	4.6
2	F	91	TYR	4.6
2	E	143	TRP	4.6
2	F	138	PRO	4.5
2	I	173	ILE	4.5
2	G	171	LYS	4.5
2	I	144	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
2	G	148	GLN	4.5
2	F	140	LYS	4.4
1	B	60	PHE	4.4
2	G	140	LYS	4.4
2	G	134	VAL	4.4
2	E	92	VAL	4.4
2	I	221	ALA	4.3
2	F	264	ARG	4.3
2	F	266	GLU	4.3
2	G	210	LYS	4.3
2	I	117	GLU	4.2
2	E	173	ILE	4.2
1	V	34	VAL	4.1
2	F	124	GLU	4.1
1	V	93	ALA	4.1
2	G	143	TRP	4.1
2	F	219	LYS	4.1
2	I	139	ALA	4.1
1	X	93	ALA	4.0
2	G	117	GLU	3.9
2	G	153	SER	3.9
2	E	221	ALA	3.9
2	I	211	GLN	3.9
2	I	89	VAL	3.9
1	X	91	LEU	3.9
2	G	91	TYR	3.8
2	I	266	GLU	3.8
2	E	91	TYR	3.8
2	F	169	ASP	3.7
2	I	113	VAL	3.7
2	G	264	ARG	3.7
2	G	141	ASN	3.6
2	I	168	LEU	3.6
2	I	216	LEU	3.6
2	E	267	SER	3.6
2	F	227	GLU	3.6
2	F	152	PRO	3.6
2	E	270	PRO	3.6
1	D	93	ALA	3.6
2	F	211	GLN	3.5
2	I	217	LYS	3.5
2	E	266	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
2	I	146	THR	3.5
2	E	134	VAL	3.5
1	V	94	LEU	3.5
2	F	234	VAL	3.5
1	Z	83	ARG	3.4
2	F	112	ARG	3.4
1	X	90	LYS	3.4
2	I	264	ARG	3.4
2	G	212	LYS	3.4
2	E	214	ARG	3.3
2	F	129	GLU	3.3
1	A	83	ARG	3.3
2	I	137	PRO	3.2
2	F	139	ALA	3.2
2	I	223	LYS	3.2
2	I	128	GLU	3.2
2	E	144	GLY	3.2
2	I	90	GLY	3.2
2	G	234	VAL	3.2
2	E	141	ASN	3.2
1	V	174	LYS	3.1
2	G	227	GLU	3.1
2	E	170	ASP	3.1
1	B	86	ARG	3.1
2	F	233	LEU	3.1
1	C	67	HIS	3.1
1	C	174	LYS	3.1
2	I	213	ALA	3.1
2	E	239	LEU	3.1
2	E	212	LYS	3.0
1	V	42	VAL	3.0
2	F	214	ARG	3.0
2	I	224	LEU	3.0
1	V	35	ARG	3.0
1	C	42	VAL	3.0
2	I	83	ALA	3.0
1	V	44	ALA	3.0
1	Y	57	PHE	3.0
2	I	151	GLU	3.0
2	G	215	LYS	3.0
2	F	154	ALA	2.9
2	I	169	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	42	VAL	2.9
1	C	93	ALA	2.9
1	B	78	LEU	2.9
1	C	53	ALA	2.8
2	I	148	GLN	2.8
2	F	143	TRP	2.8
2	F	244	ILE	2.8
2	F	119	ASN	2.8
2	F	92	VAL	2.8
2	I	116	ILE	2.8
1	C	98	ALA	2.8
2	F	215	LYS	2.8
2	F	130	ARG	2.8
2	E	151	GLU	2.8
1	C	112	VAL	2.8
2	F	113	VAL	2.8
2	G	83	ALA	2.8
2	I	138	PRO	2.7
2	G	151	GLU	2.7
2	I	234	VAL	2.7
1	A	46	PHE	2.7
2	E	153	SER	2.7
2	G	173	ILE	2.7
2	I	136	ILE	2.7
2	F	115	ALA	2.7
2	I	133	ASP	2.7
2	E	219	LYS	2.7
2	F	224	LEU	2.7
2	G	266	GLU	2.7
2	F	223	LYS	2.7
2	I	153	SER	2.7
1	D	89	ARG	2.7
2	E	264	ARG	2.7
2	G	123	ALA	2.7
2	F	168	LEU	2.7
1	B	46	PHE	2.7
1	B	95	LEU	2.6
2	I	267	SER	2.6
1	C	102	ALA	2.6
2	E	218	ILE	2.6
1	V	90	LYS	2.6
2	F	137	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	70	HIS	2.6
1	A	73	LYS	2.6
1	Y	97	VAL	2.6
2	E	147	GLU	2.6
2	E	225	LEU	2.6
1	C	60	PHE	2.6
1	C	89	ARG	2.6
2	F	83	ALA	2.6
1	Z	60	PHE	2.6
2	I	156	ARG	2.6
2	E	210	LYS	2.5
1	V	60	PHE	2.5
1	V	51	ALA	2.5
2	E	171	LYS	2.5
2	F	172	GLU	2.5
2	I	172	GLU	2.5
2	E	90	GLY	2.5
2	G	147	GLU	2.5
2	E	149	GLN	2.5
1	V	43	ILE	2.5
1	B	82	TRP	2.5
2	G	170	ASP	2.5
2	F	128	GLU	2.5
1	C	109	ASN	2.4
2	I	112	ARG	2.4
2	I	215	LYS	2.4
1	D	113	VAL	2.4
2	I	129	GLU	2.4
1	V	173	TYR	2.4
2	G	216	LEU	2.4
1	C	38	TYR	2.4
1	B	112	VAL	2.4
2	G	35	TRP	2.4
1	C	43	ILE	2.4
2	F	220	ASP	2.4
2	E	224	LEU	2.4
1	B	57	PHE	2.4
1	B	90	LYS	2.4
1	Z	44	ALA	2.4
1	B	87	MET	2.4
2	F	156	ARG	2.4
2	F	213	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	G	222	MET	2.4
2	E	117	GLU	2.3
2	E	6	PRO	2.3
2	F	355	TYR	2.3
2	G	112	ARG	2.3
2	F	159	PHE	2.3
1	D	91	LEU	2.3
2	E	284	LEU	2.3
1	C	44	ALA	2.3
1	B	116	GLU	2.3
2	F	217	LYS	2.3
2	I	225	LEU	2.3
1	D	103	SER	2.3
1	C	55	THR	2.3
1	B	97	VAL	2.3
1	Z	72	VAL	2.3
2	G	145	GLN	2.2
1	X	60	PHE	2.2
2	I	124	GLU	2.2
1	C	94	LEU	2.2
2	G	418	ILE	2.2
2	E	112	ARG	2.2
2	E	109	LYS	2.2
2	I	233	LEU	2.2
1	V	98	ALA	2.2
1	Y	37	LEU	2.2
2	F	171	LYS	2.2
1	B	88	LEU	2.2
2	F	132	LEU	2.2
2	G	270	PRO	2.2
2	E	234	VAL	2.2
1	X	89	ARG	2.2
2	F	145	GLN	2.2
1	C	58	GLU	2.2
1	C	173	TYR	2.2
1	B	69	GLY	2.2
2	E	235	ASN	2.2
1	Y	46	PHE	2.1
2	I	125	GLU	2.1
1	V	97	VAL	2.1
1	Z	76	VAL	2.1
1	D	97	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	G	106	ALA	2.1
1	X	120	ILE	2.1
2	E	418	ILE	2.1
1	C	104	LEU	2.1
1	A	171	LEU	2.1
1	V	112	VAL	2.1
1	D	79	ALA	2.1
1	C	117	ASN	2.1
2	E	172	GLU	2.1
2	F	210	LYS	2.1
2	I	358	LEU	2.1
1	C	87	MET	2.1
1	Y	34	VAL	2.1
1	B	106	ILE	2.1
2	G	244	ILE	2.1
2	I	135	LEU	2.1
2	F	127	ALA	2.1
2	G	211	GLN	2.1
1	Y	32	LYS	2.1
2	F	131	ILE	2.0
1	D	158	ILE	2.0
2	G	252	ILE	2.0
1	X	165	PHE	2.0
1	C	111	ASP	2.0
2	F	148	GLN	2.0
1	D	47	ALA	2.0
1	Y	174	LYS	2.0
2	E	119	ASN	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ADP	G	2450	27/27	0.26	0.99	38,46,58,59	0
3	ADP	F	1450	27/27	0.26	0.89	47,51,56,58	0
3	ADP	E	450	27/27	0.25	0.64	40,46,58,58	0
3	ADP	I	3450	27/27	0.23	0.37	45,49,54,55	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.