



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:06 AM GMT

PDB ID : 4ERP  
Title : Crystal structure of a gemcitabine-diphosphateinhibited E. coli class Ia ribonucleotide reductase complex  
Authors : Zimanyi, C.M.; Drennan, C.L.  
Deposited on : 2012-04-20  
Resolution : 4.45 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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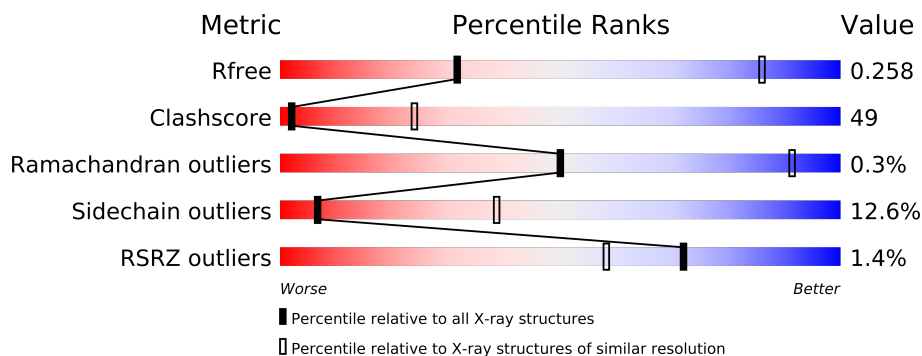
The following versions of software and data (see [references](#)) were used in the production of this report:

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 4.45 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	1020 (5.30-3.50)
Clashscore	79885	1285 (5.30-3.50)
Ramachandran outliers	78287	1214 (5.26-3.50)
Sidechain outliers	78261	1195 (5.26-3.50)
RSRZ outliers	66119	1020 (5.30-3.50)

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	761	
1	B	761	
1	C	761	
1	D	761	
2	E	375	
2	F	375	
2	G	375	
2	H	375	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 35205 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 Ribonucleoside-diphosphatereductase 1 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	734	Total	C	N	O	S	0	0	0
			5845	3712	1004	1105	24			
1	B	735	Total	C	N	O	S	0	0	0
			5850	3715	1005	1106	24			
1	C	733	Total	C	N	O	S	0	0	0
			5841	3710	1003	1104	24			
1	D	736	Total	C	N	O	S	0	0	0
			5859	3720	1007	1108	24			

- Molecule 2 is a protein called Ribonucleoside-diphosphatereductase 1 subunit beta.

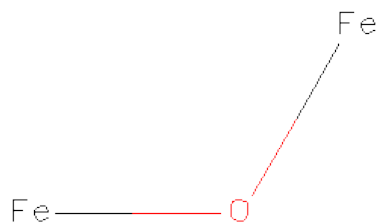
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	354	Total	C	N	O	S	0	0	0
			2900	1850	480	557	13			
2	F	358	Total	C	N	O	S	0	0	0
			2930	1867	486	564	13			
2	G	357	Total	C	N	O	S	0	0	0
			2922	1863	483	563	13			
2	H	356	Total	C	N	O	S	0	0	0
			2914	1857	483	561	13			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is MU-OXO-DIIRON (three-letter code: FEO) (formula:  $\text{Fe}_2\text{O}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	Fe	O	0	0
			3	2	1		
4	F	1	Total	Fe	O	0	0
			3	2	1		
4	G	1	Total	Fe	O	0	0
			3	2	1		
4	H	1	Total	Fe	O	0	0
			3	2	1		

- Molecule 5 is water.

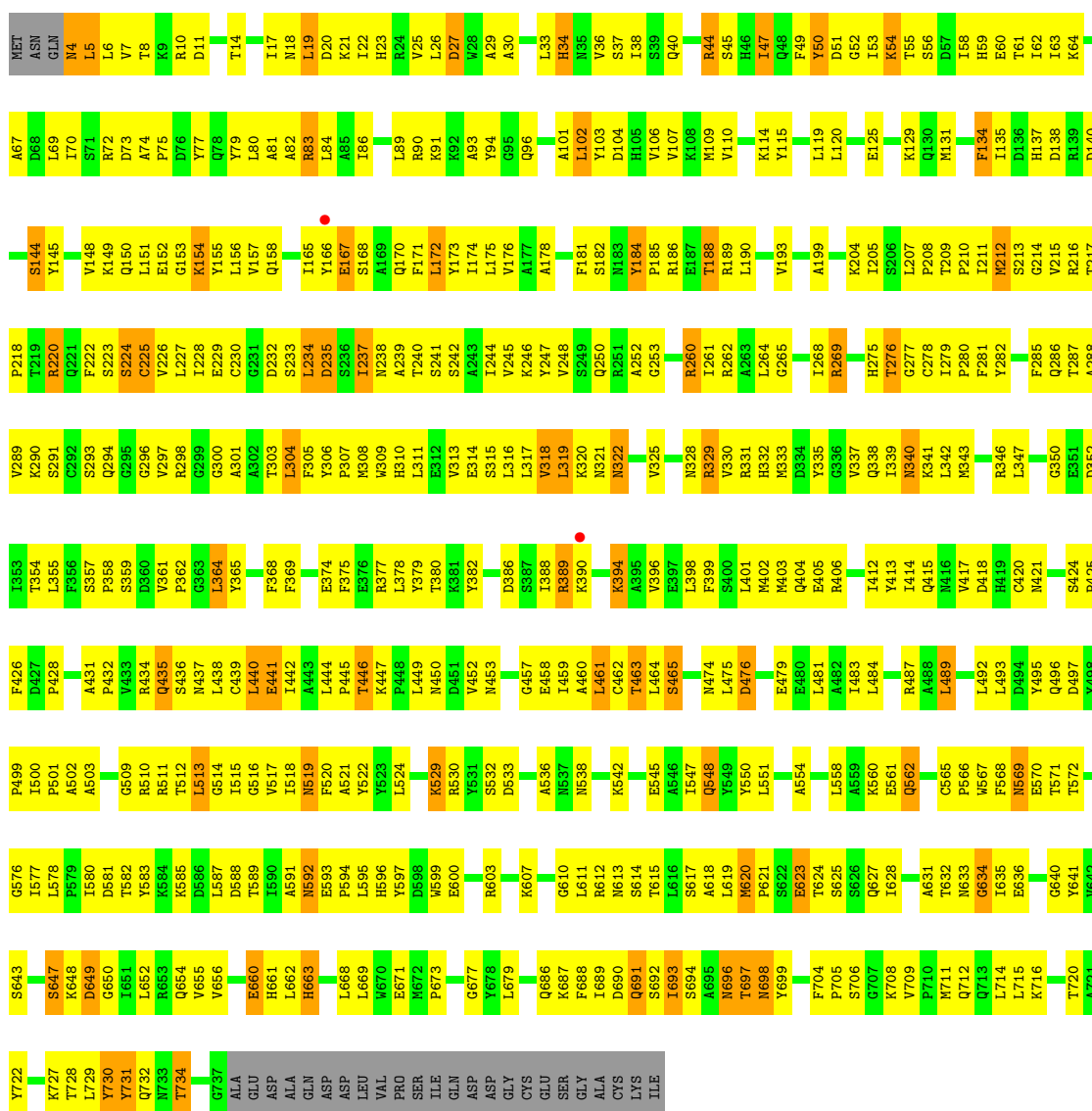
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	2	Total	O	0	0
			2	2		
5	F	2	Total	O	0	0
			2	2		
5	G	2	Total	O	0	0
			2	2		
5	H	2	Total	O	0	0
			2	2		

### 3 Residue-property plots

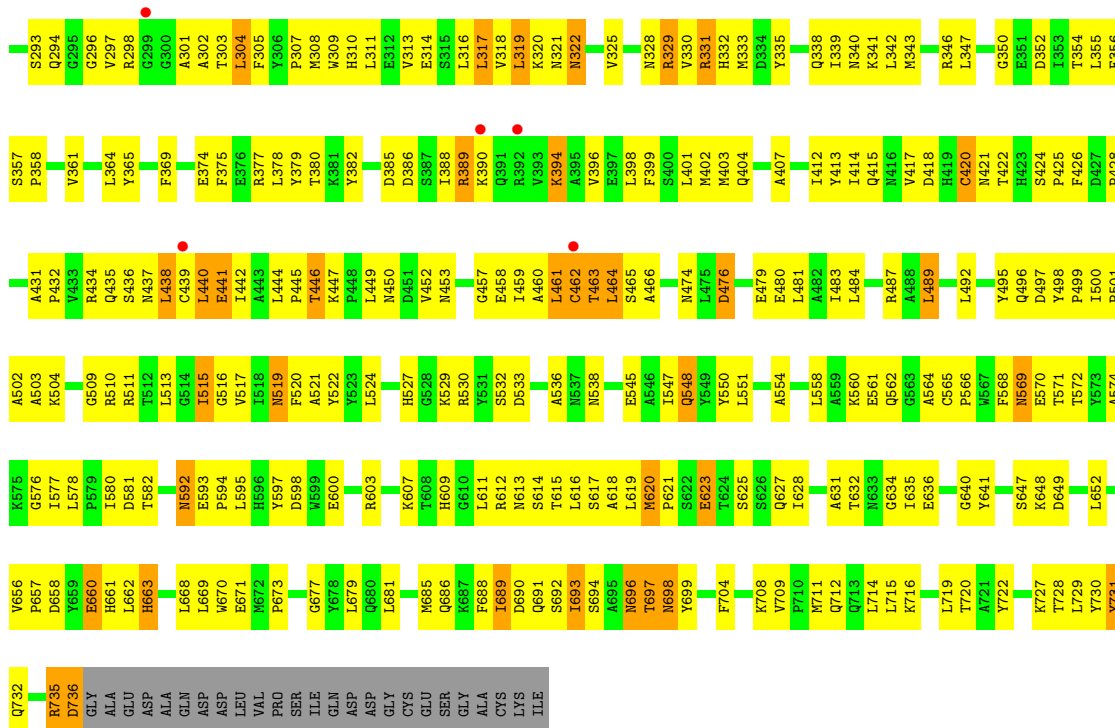
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Chain A:

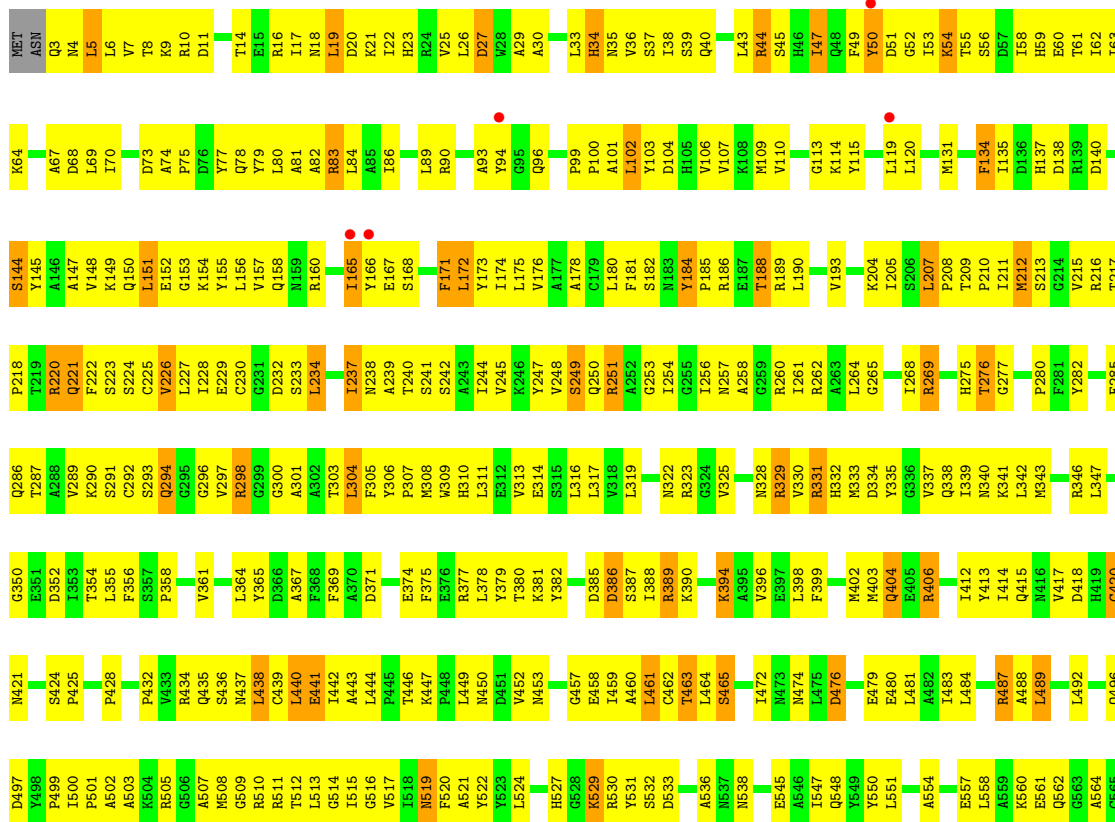




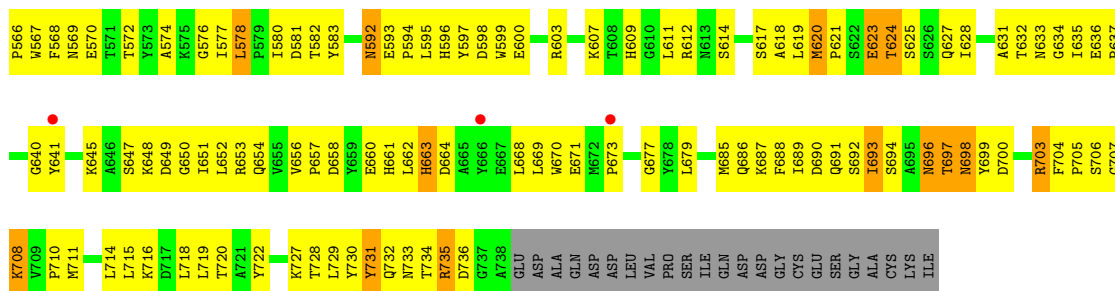


• Molecule 1: Ribonucleoside-diphosphatereductase 1 subunit alpha

Chain D:

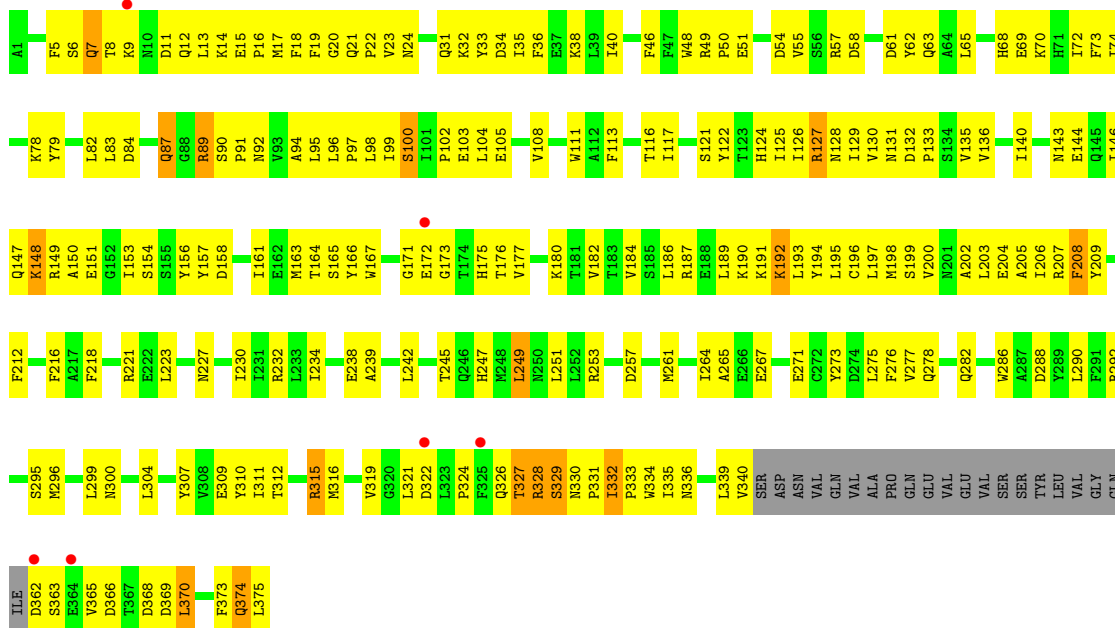






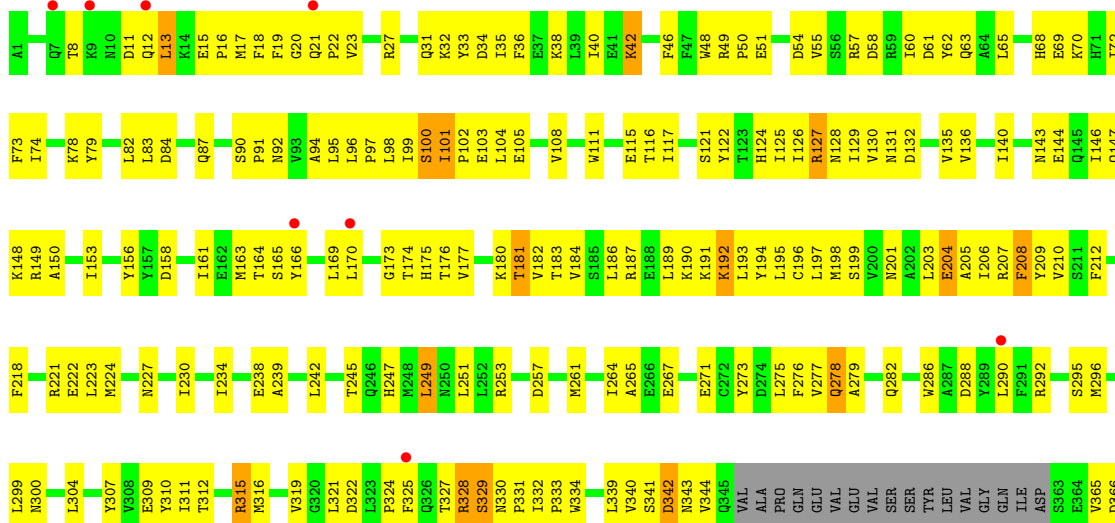
• Molecule 2: Ribonucleoside-diphosphatereductase 1 subunit beta

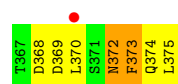
Chain E:



• Molecule 2: Ribonucleoside-diphosphatereductase 1 subunit beta

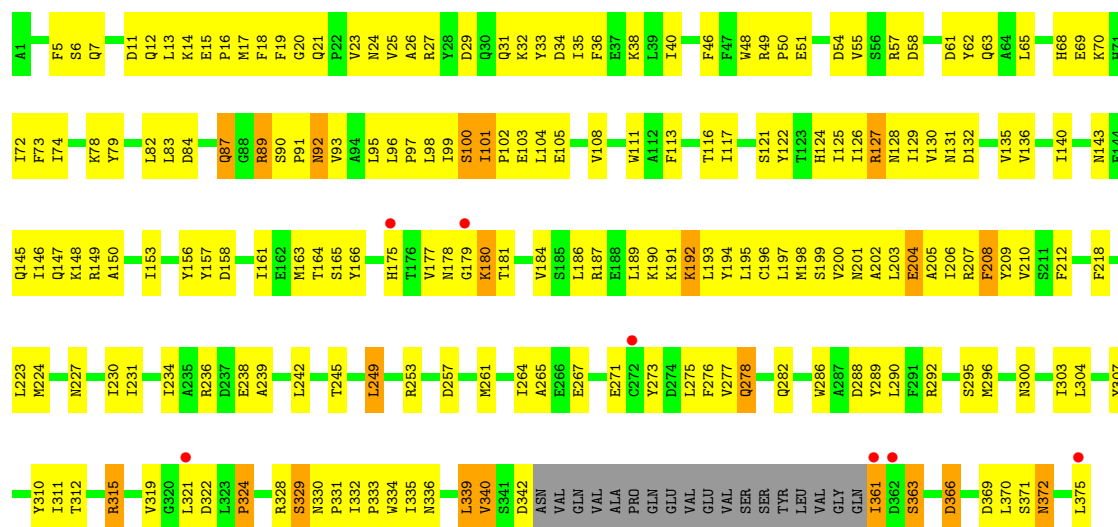
Chain F:





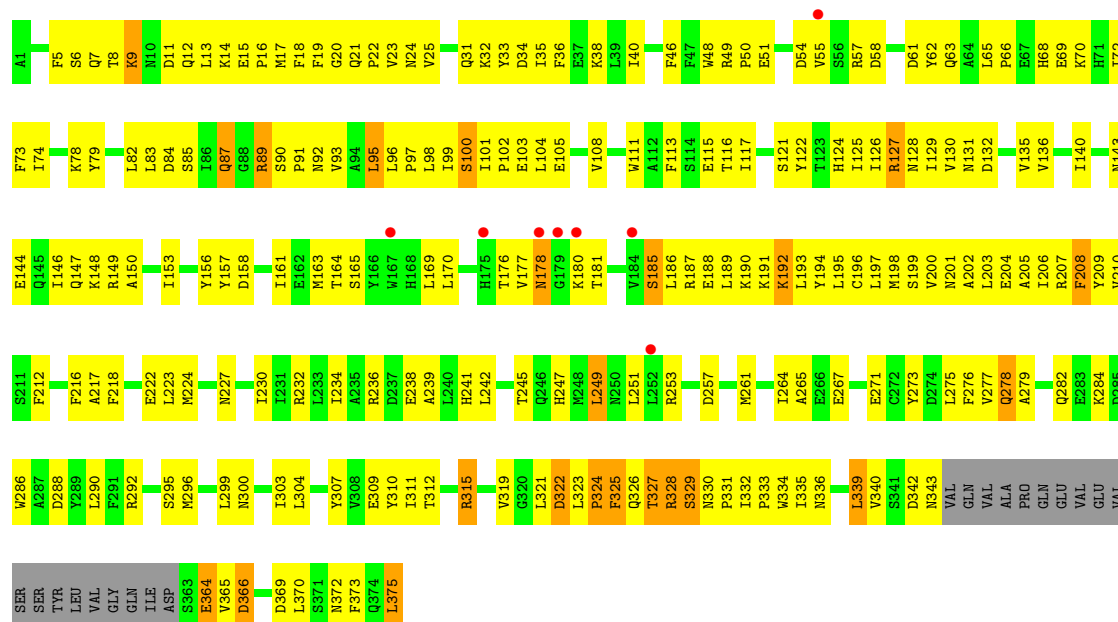
• Molecule 2: Ribonucleoside-diphosphatereductase 1 subunit beta

Chain G:



• Molecule 2: Ribonucleoside-diphosphatereductase 1 subunit beta

Chain H:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.67Å 398.91Å 319.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.45 49.54 – 4.44	Depositor EDS
% Data completeness (in resolution range)	82.3 (50.00-4.45) 81.9 (49.54-4.44)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.75 (at 4.45Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.233 , 0.267 0.226 , 0.258	Depositor DCC
$R_{free}$ test set	2128 reflections (5.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	108.8	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 118.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 46097 reflections	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	35205	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.31	0/5973	0.51	0/8090
1	B	0.31	0/5978	0.54	1/8097 (0.0%)
1	C	0.31	0/5969	0.55	0/8085
1	D	0.31	0/5987	0.53	0/8109
2	E	0.32	0/2964	0.49	1/4019 (0.0%)
2	F	0.34	0/2994	0.51	2/4060 (0.0%)
2	G	0.34	0/2986	0.51	2/4049 (0.0%)
2	H	0.33	0/2978	0.48	0/4038
All	All	0.32	0/35829	0.52	6/48547 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	324	PRO	N-CA-C	5.82	127.23	112.10
2	G	92	ASN	N-CA-C	5.57	126.03	111.00
1	B	360	ASP	O-C-N	-5.35	114.14	122.70
2	E	362	ASP	CB-CG-OD2	5.17	122.95	118.30
2	F	342	ASP	CB-CG-OD2	5.14	122.92	118.30
2	F	342	ASP	N-CA-C	5.13	124.85	111.00

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	5845	0	5770	637	0
1	B	5850	0	5774	647	0
1	C	5841	0	5767	626	0
1	D	5859	0	5783	649	0
2	E	2900	0	2826	238	0
2	F	2930	0	2854	232	0
2	G	2922	0	2846	239	0
2	H	2914	0	2837	275	0
3	A	31	0	12	4	0
3	B	31	0	12	9	0
3	C	31	0	11	15	0
3	D	31	0	12	10	0
4	E	3	0	0	0	0
4	F	3	0	0	0	0
4	G	3	0	0	0	0
4	H	3	0	0	0	0
5	E	2	0	0	1	0
5	F	2	0	0	1	0
5	G	2	0	0	1	0
5	H	2	0	0	0	0
All	All	35205	0	34504	3414	0

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 49.

All (3414) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:115:TYR:CE1	1:C:216:ARG:HD2	1.42	1.53
1:C:442:ILE:HD12	1:C:462:CYS:SG	1.48	1.51
1:D:114:LYS:HG3	1:D:166:TYR:CE2	1.45	1.50
1:B:222:PHE:CD2	1:B:492:LEU:HD11	1.44	1.49
1:A:5:LEU:HD12	1:A:17:ILE:CG1	1.41	1.49
1:D:89:LEU:CD2	1:D:152:GLU:HG3	1.53	1.38
2:H:232:ARG:HD3	2:H:342:ASP:CB	1.51	1.38
1:D:89:LEU:HD21	1:D:152:GLU:CG	1.52	1.38
2:F:38:LYS:HD3	2:F:344:VAL:CG1	1.53	1.36
1:D:172:LEU:HD23	1:D:216:ARG:NH2	1.37	1.34
1:D:215:VAL:O	1:D:216:ARG:HG2	1.25	1.33
1:B:258:ALA:HB3	1:B:282:TYR:CE2	1.62	1.32

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:172:LEU:HD23	1:A:216:ARG:CZ	1.60	1.32
2:H:55:VAL:HG21	2:H:128:ASN:ND2	1.39	1.31
1:A:5:LEU:CD1	1:A:17:ILE:HG12	1.59	1.30
2:E:322:ASP:O	2:E:324:PRO:HD3	1.27	1.29
1:B:258:ALA:HB3	1:B:282:TYR:CZ	1.70	1.26
2:H:232:ARG:CD	2:H:342:ASP:HB2	1.65	1.25
1:A:215:VAL:O	1:A:216:ARG:HG2	1.07	1.25
2:F:340:VAL:HG12	2:F:341:SER:OG	1.35	1.25
2:F:13:LEU:O	2:F:32:LYS:HD2	1.29	1.25
1:B:189:ARG:O	1:B:193:VAL:HG23	1.35	1.24
2:G:322:ASP:O	2:G:324:PRO:HD3	1.34	1.24
1:C:418:ASP:O	1:C:422:THR:HG23	1.32	1.23
1:C:442:ILE:CD1	1:C:462:CYS:SG	2.26	1.22
1:B:114:LYS:HE2	1:B:166:TYR:CE2	1.74	1.22
1:B:222:PHE:CD2	1:B:492:LEU:CD1	2.25	1.20
1:B:282:TYR:CE2	1:B:304:LEU:HD22	1.76	1.19
1:C:50:TYR:CE2	1:C:53:ILE:HB	1.79	1.18
1:C:115:TYR:CE1	1:C:216:ARG:CD	2.27	1.18
1:B:619:LEU:HD12	1:B:693:ILE:CG2	1.72	1.18
1:C:254:ILE:N	1:C:438:LEU:HD12	1.57	1.18
2:E:205:ALA:HB1	2:E:315:ARG:HD3	1.22	1.17
1:A:208:PRO:CG	1:A:211:ILE:HD13	1.72	1.17
1:B:619:LEU:HD12	1:B:693:ILE:HG22	1.26	1.17
1:B:711:MET:HB3	2:H:364:GLU:O	1.45	1.17
1:B:40:GLN:NE2	2:H:333:PRO:HG2	1.58	1.16
1:D:463:THR:O	1:D:464:LEU:HD23	1.43	1.16
1:A:317:LEU:HD12	1:A:401:LEU:HD23	1.25	1.15
1:C:17:ILE:HD12	3:C:801:ATP:C2	1.79	1.15
1:A:463:THR:CB	1:A:513:LEU:HD23	1.75	1.15
1:B:222:PHE:CE2	1:B:492:LEU:HD11	1.82	1.15
1:C:441:GLU:HG2	1:C:620:MET:CB	1.78	1.13
1:B:282:TYR:HE2	1:B:304:LEU:CD2	1.60	1.13
1:C:301:ALA:O	1:C:438:LEU:HD11	1.46	1.13
1:A:463:THR:OG1	1:A:513:LEU:HD23	1.47	1.13
1:C:617:SER:HB2	1:C:690:ASP:H	1.14	1.13
1:C:189:ARG:O	1:C:193:VAL:HG23	1.48	1.12
1:D:294:GLN:HB2	1:D:298:ARG:HG3	1.23	1.12
1:A:463:THR:O	1:A:464:LEU:HD23	1.47	1.12
1:B:735:ARG:HG3	1:B:735:ARG:O	1.43	1.12
1:C:515:ILE:HD12	1:C:551:LEU:HD13	1.28	1.12
1:D:254:ILE:N	1:D:438:LEU:HD12	1.64	1.11
1:A:215:VAL:O	1:A:216:ARG:CG	1.97	1.11

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:317:LEU:HD11	1:C:401:LEU:CD2	1.80	1.11
1:C:317:LEU:HD11	1:C:401:LEU:HD21	1.11	1.11
1:C:317:LEU:HD12	1:C:318:VAL:HG13	1.29	1.11
1:B:618:ALA:N	1:B:689:ILE:HD11	1.66	1.10
1:B:317:LEU:CD1	1:B:402:MET:HA	1.80	1.10
1:B:44:ARG:HG3	1:B:69:LEU:HD21	1.12	1.10
1:B:318:VAL:HG23	1:B:329:ARG:CZ	1.81	1.10
1:A:619:LEU:CB	1:A:693:ILE:HG22	1.82	1.10
1:B:621:PRO:HD3	1:B:694:SER:CB	1.81	1.10
1:D:172:LEU:HD23	1:D:216:ARG:CZ	1.81	1.09
1:B:282:TYR:CE2	1:B:304:LEU:CD2	2.34	1.09
1:C:369:PHE:CE2	1:C:434:ARG:HD3	1.86	1.09
1:B:619:LEU:CD1	1:B:693:ILE:HG22	1.81	1.09
1:C:293:SER:HB2	1:C:296:GLY:HA2	1.35	1.08
1:A:489:LEU:HD22	1:A:513:LEU:HD22	1.14	1.08
1:A:619:LEU:HB2	1:A:693:ILE:CG2	1.83	1.08
1:C:222:PHE:CD2	1:C:492:LEU:HD11	1.88	1.08
2:F:332:ILE:HG22	2:F:334:TRP:HE1	1.06	1.08
1:C:175:LEU:HD22	1:C:216:ARG:HD3	1.11	1.07
1:D:463:THR:C	1:D:464:LEU:HD23	1.73	1.07
1:D:157:VAL:HG12	1:D:166:TYR:HD2	1.14	1.07
1:B:258:ALA:CB	1:B:282:TYR:CE2	2.35	1.07
1:A:493:LEU:HD21	1:A:513:LEU:HD21	1.15	1.07
1:B:114:LYS:HE2	1:B:166:TYR:HE2	0.97	1.07
1:C:621:PRO:HD3	1:C:694:SER:HB2	1.33	1.07
1:D:301:ALA:O	1:D:438:LEU:HD11	1.55	1.07
1:C:735:ARG:O	1:C:736:ASP:HB3	1.53	1.06
1:D:44:ARG:HG3	1:D:69:LEU:HD21	1.30	1.06
1:A:647:SER:HB2	1:A:652:LEU:HG	1.37	1.06
1:D:150:GLN:HB3	1:D:154:LYS:HD3	1.38	1.06
1:C:441:GLU:HG2	1:C:620:MET:HB2	1.07	1.06
2:H:332:ILE:HG22	2:H:334:TRP:HE1	1.19	1.06
1:D:329:ARG:HD3	1:D:331:ARG:NH2	1.71	1.06
1:B:44:ARG:CG	1:B:69:LEU:HD21	1.86	1.06
1:A:692:SER:HB2	1:A:727:LYS:HB2	1.36	1.06
1:D:153:GLY:HA2	1:D:158:GLN:HE22	1.16	1.06
1:A:5:LEU:HD12	1:A:17:ILE:CD1	1.85	1.06
1:B:700:ASP:OD1	1:B:735:ARG:HD2	1.55	1.06
1:C:331:ARG:HG2	1:C:332:HIS:HD2	1.11	1.05
1:A:225:CYS:HB3	1:A:253:GLY:O	1.55	1.05
1:A:208:PRO:HG2	1:A:211:ILE:HD13	1.06	1.05
2:F:332:ILE:HG22	2:F:334:TRP:NE1	1.71	1.05

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:513:LEU:HD11	1:C:616:LEU:HD23	1.36	1.04
1:A:227:LEU:HB3	1:A:435:GLN:NE2	1.72	1.04
1:D:685:MET:O	1:D:689:ILE:HG13	1.57	1.04
1:D:44:ARG:HE	1:D:44:ARG:HA	0.88	1.04
1:C:44:ARG:HG3	1:C:69:LEU:HD21	1.34	1.04
2:H:336:ASN:HA	2:H:339:LEU:HD11	1.34	1.04
2:E:339:LEU:O	2:E:339:LEU:HD12	1.55	1.04
1:C:513:LEU:HD11	1:C:616:LEU:CD2	1.88	1.04
1:C:44:ARG:HA	1:C:44:ARG:HE	1.22	1.03
1:D:150:GLN:O	1:D:154:LYS:HG3	1.57	1.03
1:D:114:LYS:CG	1:D:166:TYR:CE2	2.41	1.03
1:D:617:SER:HB2	1:D:690:ASP:H	1.19	1.03
1:D:39:SER:HB3	2:G:332:ILE:HG22	1.40	1.03
1:C:167:GLU:OE2	1:C:172:LEU:HD12	1.57	1.02
1:B:220:ARG:O	1:B:496:GLN:HA	1.59	1.02
2:G:340:VAL:HG13	2:G:340:VAL:O	1.59	1.02
1:A:155:TYR:HD1	1:A:212:MET:CB	1.72	1.02
1:B:286:GLN:NE2	1:B:332:HIS:HB2	1.72	1.02
2:F:38:LYS:HD3	2:F:344:VAL:HG11	1.03	1.01
1:B:619:LEU:CG	1:B:693:ILE:HG22	1.90	1.01
1:C:294:GLN:OE1	1:C:298:ARG:HD3	1.60	1.01
1:A:172:LEU:CD2	1:A:216:ARG:NH1	2.23	1.01
1:C:175:LEU:CD2	1:C:216:ARG:HD3	1.90	1.01
1:B:621:PRO:HD3	1:B:694:SER:HB2	1.37	1.01
1:D:157:VAL:HG12	1:D:166:TYR:CD2	1.96	1.00
2:G:273:TYR:CE2	2:G:324:PRO:HG3	1.96	1.00
1:D:44:ARG:NE	1:D:44:ARG:HA	1.66	1.00
1:A:172:LEU:CD2	1:A:216:ARG:CZ	2.37	1.00
1:D:286:GLN:OE1	1:D:332:HIS:HB2	1.61	1.00
1:A:298:ARG:HE	1:C:6:LEU:HD21	1.25	1.00
1:C:17:ILE:HD12	3:C:801:ATP:H2	1.24	1.00
1:A:5:LEU:HB2	1:A:17:ILE:CG2	1.92	1.00
1:A:463:THR:C	1:A:464:LEU:HD23	1.81	1.00
1:B:258:ALA:CB	1:B:282:TYR:CZ	2.45	0.99
1:C:226:VAL:HG12	1:C:461:LEU:HD22	1.43	0.99
1:D:220:ARG:O	1:D:496:GLN:HA	1.62	0.99
1:C:157:VAL:HG23	1:C:216:ARG:HH12	1.26	0.99
1:B:286:GLN:HE21	1:B:332:HIS:HB2	1.21	0.99
1:D:711:MET:CB	2:G:363:SER:HB3	1.92	0.99
1:D:215:VAL:O	1:D:216:ARG:CG	2.11	0.99
1:B:466:ALA:HA	1:B:516:GLY:O	1.63	0.98
1:B:318:VAL:CG2	1:B:329:ARG:NH1	2.26	0.98

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:254:ILE:H	1:D:438:LEU:CD1	1.76	0.98
2:H:65:LEU:HD21	2:H:223:LEU:HD13	1.45	0.98
1:A:489:LEU:CD2	1:A:513:LEU:HD22	1.93	0.98
1:D:6:LEU:HB2	1:D:51:ASP:OD1	1.62	0.98
1:D:623:GLU:HG2	1:D:633:ASN:ND2	1.78	0.97
1:D:44:ARG:HE	1:D:44:ARG:CA	1.76	0.97
1:D:711:MET:HB3	2:G:363:SER:HB3	1.46	0.97
1:C:331:ARG:HG2	1:C:332:HIS:CD2	1.97	0.97
1:D:711:MET:H	2:G:363:SER:CB	1.76	0.97
1:A:208:PRO:HG2	1:A:211:ILE:CD1	1.94	0.97
2:H:55:VAL:CG2	2:H:128:ASN:ND2	2.27	0.97
1:C:369:PHE:HE2	1:C:434:ARG:HD3	1.22	0.97
1:D:316:LEU:O	1:D:319:LEU:HG	1.64	0.97
1:A:625:SER:O	1:A:628:ILE:HG22	1.65	0.96
2:E:65:LEU:HD21	2:E:223:LEU:HD13	1.47	0.96
1:B:109:MET:SD	1:B:166:TYR:HB3	2.05	0.96
1:D:37:SER:HB3	2:G:331:PRO:O	1.62	0.96
1:D:144:SER:O	1:D:148:VAL:HG23	1.65	0.96
1:A:317:LEU:HD12	1:A:401:LEU:CD2	1.96	0.96
2:F:92:ASN:HA	2:F:96:LEU:HD13	1.48	0.96
1:B:317:LEU:HD11	1:B:402:MET:HA	1.48	0.96
1:A:144:SER:O	1:A:148:VAL:HG23	1.66	0.96
1:A:341:LYS:HB2	1:A:722:TYR:OH	1.66	0.96
1:A:361:VAL:CG1	1:A:364:LEU:HB2	1.96	0.95
1:C:464:LEU:HD13	1:C:620:MET:SD	2.05	0.95
1:B:369:PHE:CD1	1:B:434:ARG:HA	2.02	0.95
2:F:322:ASP:O	2:F:324:PRO:HD3	1.65	0.95
1:C:207:LEU:HD11	1:C:212:MET:SD	2.05	0.95
1:A:618:ALA:HB2	1:A:691:GLN:HG3	1.46	0.95
2:G:149:ARG:HH12	2:G:286:TRP:HB2	1.32	0.95
2:F:12:GLN:HE21	2:F:23:VAL:HG13	1.30	0.95
1:A:227:LEU:CB	1:A:435:GLN:NE2	2.29	0.95
1:D:114:LYS:N	1:D:114:LYS:HD3	1.81	0.94
1:D:625:SER:O	1:D:628:ILE:HG22	1.67	0.94
1:A:109:MET:SD	1:A:166:TYR:HB3	2.07	0.94
2:F:149:ARG:HH12	2:F:286:TRP:HB2	1.33	0.94
1:A:369:PHE:CE2	1:A:434:ARG:HD3	2.01	0.94
1:C:157:VAL:CG2	1:C:216:ARG:HH12	1.81	0.94
1:C:320:LYS:HE2	1:C:333:MET:O	1.66	0.94
1:B:701:PRO:HD2	1:B:735:ARG:HG2	1.48	0.94
1:A:413:TYR:OH	1:A:731:TYR:HE2	1.50	0.94
1:D:172:LEU:CD2	1:D:216:ARG:NH2	2.31	0.94

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:38:LYS:CD	2:F:344:VAL:HG11	1.96	0.94
1:B:617:SER:CB	1:B:689:ILE:HD12	1.97	0.93
1:D:168:SER:OG	1:D:171:PHE:HB2	1.68	0.93
1:C:109:MET:SD	1:C:166:TYR:HB3	2.09	0.93
1:B:226:VAL:HG12	1:B:461:LEU:HD22	1.50	0.93
2:H:111:TRP:HZ2	2:H:204:GLU:OE2	1.49	0.93
1:C:625:SER:O	1:C:628:ILE:HG22	1.69	0.93
1:B:619:LEU:CB	1:B:693:ILE:HG22	1.97	0.93
1:D:254:ILE:H	1:D:438:LEU:HD12	1.29	0.93
1:C:420:CYS:O	1:C:424:SER:HB2	1.68	0.92
1:D:205:ILE:HD11	1:D:481:LEU:HB3	1.51	0.92
1:A:623:GLU:HG2	1:A:633:ASN:ND2	1.84	0.92
1:C:17:ILE:CD1	3:C:801:ATP:H2	1.81	0.92
1:D:294:GLN:HB2	1:D:298:ARG:CG	1.98	0.92
1:D:364:LEU:O	1:D:364:LEU:HD13	1.69	0.92
2:H:149:ARG:HH12	2:H:286:TRP:HB2	1.33	0.92
2:F:38:LYS:HD3	2:F:344:VAL:HG12	1.51	0.92
1:B:37:SER:HB3	2:H:331:PRO:O	1.69	0.92
2:E:205:ALA:HB1	2:E:315:ARG:CD	2.00	0.91
1:B:315:SER:O	1:B:318:VAL:HG13	1.70	0.91
1:C:254:ILE:H	1:C:438:LEU:CD1	1.82	0.91
1:B:317:LEU:HD12	1:B:402:MET:HA	1.50	0.91
1:B:619:LEU:HB2	1:B:693:ILE:HA	1.53	0.91
2:H:55:VAL:HG21	2:H:128:ASN:HD21	1.20	0.91
1:D:89:LEU:HD21	1:D:152:GLU:HG3	0.91	0.91
1:A:425:PRO:HG2	1:A:690:ASP:HB3	1.49	0.91
2:H:232:ARG:NH1	2:H:343:ASN:H	1.69	0.91
1:B:145:TYR:HE2	1:B:652:LEU:HD23	1.36	0.91
1:C:53:ILE:CD1	1:C:58:ILE:HG12	2.01	0.91
1:A:5:LEU:HB2	1:A:17:ILE:HG21	1.51	0.91
1:C:369:PHE:HD2	1:C:434:ARG:NH1	1.67	0.91
1:C:157:VAL:CG2	1:C:216:ARG:NH1	2.33	0.91
1:D:168:SER:HG	1:D:171:PHE:HD2	0.92	0.91
1:C:361:VAL:CG1	1:C:364:LEU:HB2	2.01	0.90
1:B:297:VAL:HB	1:B:298:ARG:HE	1.35	0.90
2:G:273:TYR:HE2	2:G:324:PRO:HG3	1.32	0.90
1:C:254:ILE:N	1:C:438:LEU:CD1	2.34	0.90
1:D:89:LEU:HD21	1:D:152:GLU:CD	1.89	0.90
1:D:157:VAL:O	1:D:166:TYR:HB2	1.72	0.90
1:D:294:GLN:CB	1:D:298:ARG:HG3	2.01	0.90
2:H:12:GLN:HG2	2:H:102:PRO:HD3	1.53	0.90
1:A:463:THR:HB	1:A:513:LEU:HD23	1.49	0.90

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:365:TYR:CZ	1:B:369:PHE:HE2	1.88	0.90
1:B:258:ALA:HB3	1:B:282:TYR:OH	1.72	0.90
1:C:685:MET:O	1:C:689:ILE:HG12	1.70	0.90
1:B:215:VAL:HG22	1:B:222:PHE:CZ	2.06	0.90
1:A:155:TYR:HD1	1:A:212:MET:HB3	1.35	0.90
2:F:340:VAL:CG1	2:F:341:SER:OG	2.20	0.90
1:D:716:LYS:HG2	2:G:370:LEU:HD21	1.54	0.90
2:G:92:ASN:HA	2:G:96:LEU:HD13	1.51	0.90
2:H:111:TRP:CZ2	2:H:204:GLU:OE2	2.25	0.89
1:C:447:LYS:HB2	1:C:458:GLU:H	1.36	0.89
2:H:236:ARG:HD3	2:H:342:ASP:OD1	1.73	0.89
1:C:254:ILE:H	1:C:438:LEU:HD12	1.38	0.89
1:B:282:TYR:HA	1:B:285:PHE:HD2	1.36	0.89
2:F:87:GLN:O	2:F:91:PRO:CD	2.20	0.89
1:A:207:LEU:HB2	1:A:212:MET:HE2	1.54	0.89
1:A:369:PHE:HD2	1:A:434:ARG:HH11	1.14	0.89
1:C:175:LEU:HD22	1:C:216:ARG:CD	2.01	0.89
1:B:689:ILE:HG13	1:B:691:GLN:O	1.73	0.89
1:B:619:LEU:CD1	1:B:693:ILE:CG2	2.43	0.89
1:C:89:LEU:HD21	1:C:152:GLU:HG3	1.54	0.89
1:B:205:ILE:HD11	1:B:481:LEU:HB3	1.55	0.89
2:G:87:GLN:O	2:G:91:PRO:CD	2.21	0.88
2:E:87:GLN:O	2:E:91:PRO:CD	2.21	0.88
1:C:317:LEU:CD1	1:C:401:LEU:HD21	2.02	0.88
2:H:87:GLN:O	2:H:91:PRO:CD	2.21	0.88
1:A:361:VAL:HG12	1:A:364:LEU:HB2	1.53	0.88
1:B:365:TYR:CE2	1:B:369:PHE:HE2	1.91	0.88
1:D:248:VAL:HG23	1:D:254:ILE:CG1	2.03	0.88
1:C:205:ILE:HD11	1:C:481:LEU:HB3	1.56	0.88
1:A:114:LYS:HE2	1:A:166:TYR:CE2	2.08	0.88
1:D:248:VAL:CG2	1:D:254:ILE:HG13	2.03	0.88
1:B:168:SER:OG	1:B:171:PHE:HB2	1.74	0.87
1:D:222:PHE:CD2	1:D:492:LEU:HD11	2.08	0.87
1:B:619:LEU:HD12	1:B:693:ILE:HG21	1.55	0.87
2:H:332:ILE:HG22	2:H:334:TRP:NE1	1.88	0.87
1:A:298:ARG:NE	1:C:6:LEU:HD21	1.89	0.87
1:C:81:ALA:HA	1:C:84:LEU:HD12	1.56	0.87
1:C:301:ALA:C	1:C:438:LEU:HD11	1.95	0.87
1:D:304:LEU:HD12	1:D:333:MET:SD	2.15	0.87
1:C:226:VAL:CG1	1:C:461:LEU:HD22	2.04	0.87
1:B:617:SER:HB2	1:B:690:ASP:H	1.38	0.87
2:H:206:ILE:O	2:H:210:VAL:HG23	1.75	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:712:GLN:HE21	2:F:370:LEU:HD23	1.40	0.86
1:D:81:ALA:HA	1:D:84:LEU:HD12	1.56	0.86
1:B:222:PHE:CG	1:B:492:LEU:HD11	2.09	0.86
1:B:617:SER:HB3	1:B:689:ILE:HD12	1.54	0.86
1:D:711:MET:H	2:G:363:SER:HB2	1.37	0.86
2:E:55:VAL:HG21	2:E:128:ASN:ND2	1.91	0.86
1:D:172:LEU:HD23	1:D:216:ARG:HH22	1.37	0.86
2:G:12:GLN:OE1	2:G:27:ARG:HD3	1.76	0.86
1:A:565:CYS:HB3	1:A:568:PHE:HB2	1.58	0.85
1:D:39:SER:CB	2:G:332:ILE:HG22	2.05	0.85
2:E:92:ASN:HA	2:E:96:LEU:HD13	1.58	0.85
2:F:332:ILE:CG2	2:F:334:TRP:NE1	2.40	0.85
1:B:522:TYR:CE1	1:B:662:LEU:HD11	2.10	0.85
1:B:109:MET:HE3	1:B:166:TYR:O	1.75	0.85
1:A:619:LEU:HB2	1:A:693:ILE:HG22	0.92	0.85
2:F:12:GLN:NE2	2:F:23:VAL:HG13	1.91	0.85
1:B:261:ILE:HB	1:B:278:CYS:SG	2.16	0.85
1:D:150:GLN:HB3	1:D:154:LYS:CD	2.07	0.85
1:B:114:LYS:CE	1:B:166:TYR:CE2	2.60	0.85
1:A:81:ALA:HA	1:A:84:LEU:HD12	1.59	0.85
1:B:686:GLN:HA	1:B:689:ILE:HG22	1.57	0.85
1:A:248:VAL:HG21	1:A:289:VAL:HA	1.59	0.85
1:D:50:TYR:CE2	1:D:53:ILE:HD12	2.11	0.85
1:C:463:THR:C	1:C:464:LEU:HD23	1.96	0.85
1:A:615:THR:HG21	1:A:691:GLN:NE2	1.91	0.85
1:C:317:LEU:CD1	1:C:401:LEU:CD2	2.53	0.85
1:D:37:SER:CB	2:G:331:PRO:O	2.25	0.84
1:D:5:LEU:HD12	1:D:17:ILE:HG12	1.59	0.84
1:C:258:ALA:HB1	1:C:261:ILE:HD12	1.58	0.84
1:C:441:GLU:CG	1:C:620:MET:HB2	2.01	0.84
2:F:13:LEU:O	2:F:32:LYS:CD	2.21	0.84
1:B:301:ALA:CB	1:B:438:LEU:CD2	2.56	0.84
2:F:187:ARG:HG2	2:F:191:LYS:HE3	1.60	0.84
1:C:568:PHE:CE2	1:C:574:ALA:HB2	2.12	0.84
2:E:322:ASP:O	2:E:324:PRO:CD	2.21	0.84
1:B:318:VAL:HG23	1:B:329:ARG:NH1	1.91	0.84
2:F:332:ILE:CG2	2:F:334:TRP:HE1	1.89	0.84
2:H:158:ASP:HA	2:H:161:ILE:HD12	1.59	0.84
1:D:157:VAL:H	1:D:167:GLU:HG2	1.42	0.84
1:A:689:ILE:CG2	1:A:691:GLN:O	2.25	0.84
1:C:560:LYS:HD3	1:C:609:HIS:CG	2.12	0.84
2:F:38:LYS:CD	2:F:344:VAL:CG1	2.48	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:615:THR:HG21	1:A:691:GLN:HE22	1.42	0.84
1:A:153:GLY:HA2	1:A:158:GLN:HE22	1.42	0.84
1:C:50:TYR:HE2	1:C:53:ILE:HB	1.39	0.84
1:D:172:LEU:CD2	1:D:216:ARG:CZ	2.56	0.84
1:B:248:VAL:HG11	1:B:289:VAL:HA	1.59	0.84
1:B:301:ALA:CB	1:B:438:LEU:HD21	2.08	0.84
2:E:177:VAL:HG23	2:E:180:LYS:O	1.78	0.84
2:G:177:VAL:HB	2:G:180:LYS:O	1.78	0.84
1:A:204:LYS:HE3	1:A:481:LEU:HD21	1.60	0.84
2:H:203:LEU:HA	2:H:207:ARG:HB2	1.58	0.84
2:H:187:ARG:HG2	2:H:191:LYS:HE3	1.59	0.84
1:B:222:PHE:CE2	1:B:492:LEU:CD1	2.52	0.83
1:B:318:VAL:HG21	1:B:329:ARG:NH1	1.91	0.83
1:D:248:VAL:HG23	1:D:254:ILE:HG13	1.59	0.83
1:A:562:GLN:HG3	1:A:562:GLN:O	1.77	0.83
1:A:155:TYR:CD1	1:A:212:MET:CB	2.59	0.83
2:H:206:ILE:HD11	2:H:315:ARG:HG2	1.57	0.83
1:B:618:ALA:CA	1:B:689:ILE:HD11	2.08	0.83
1:A:618:ALA:HB2	1:A:691:GLN:CG	2.08	0.83
1:C:369:PHE:CD2	1:C:434:ARG:HG2	2.13	0.83
1:A:689:ILE:HG22	1:A:691:GLN:O	1.79	0.83
1:C:316:LEU:O	1:C:319:LEU:HG	1.78	0.83
2:F:309:GLU:HG2	2:F:325:PHE:CD1	2.12	0.83
1:B:81:ALA:HA	1:B:84:LEU:HD12	1.60	0.83
1:D:114:LYS:HG3	1:D:166:TYR:CZ	2.13	0.83
1:D:329:ARG:HD3	1:D:331:ARG:HH21	1.40	0.83
1:C:317:LEU:HD13	1:C:401:LEU:HG	1.61	0.82
2:G:55:VAL:HG21	2:G:128:ASN:ND2	1.92	0.82
1:D:703:ARG:O	1:D:703:ARG:HG3	1.78	0.82
1:B:258:ALA:HB3	1:B:282:TYR:HE2	1.44	0.82
1:C:39:SER:HB3	2:E:332:ILE:HG22	1.60	0.82
2:G:322:ASP:O	2:G:324:PRO:CD	2.24	0.82
1:C:515:ILE:HD12	1:C:551:LEU:CD1	2.07	0.82
1:C:464:LEU:CD1	1:C:620:MET:SD	2.67	0.82
1:A:463:THR:CB	1:A:513:LEU:CD2	2.58	0.82
1:A:618:ALA:HB2	1:A:691:GLN:HB2	1.60	0.82
1:A:205:ILE:HD11	1:A:481:LEU:HB3	1.59	0.82
1:B:619:LEU:CG	1:B:693:ILE:CG2	2.57	0.82
1:A:172:LEU:HD23	1:A:216:ARG:NH2	1.93	0.82
1:A:615:THR:CB	1:A:691:GLN:NE2	2.43	0.82
2:E:339:LEU:HD13	2:E:340:VAL:HG23	1.62	0.82
1:C:37:SER:HB3	2:E:331:PRO:O	1.79	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:222:PHE:HB3	1:B:492:LEU:HD21	1.61	0.82
1:D:689:ILE:HD13	1:D:693:ILE:HG23	1.60	0.82
1:B:301:ALA:HB3	1:B:438:LEU:CD2	2.10	0.82
1:C:560:LYS:HD3	1:C:609:HIS:CE1	2.15	0.81
2:E:187:ARG:HG2	2:E:191:LYS:HE3	1.59	0.81
1:B:222:PHE:CB	1:B:492:LEU:HD21	2.11	0.81
1:C:317:LEU:HD12	1:C:318:VAL:CG1	2.09	0.81
1:A:569:ASN:HD22	1:A:570:GLU:H	1.28	0.81
1:A:207:LEU:HB2	1:A:212:MET:CE	2.09	0.81
1:C:50:TYR:O	1:C:53:ILE:HG22	1.80	0.81
1:D:316:LEU:HA	1:D:319:LEU:HD11	1.62	0.81
1:C:658:ASP:HB3	1:C:662:LEU:HD12	1.63	0.81
1:C:157:VAL:HG23	1:C:216:ARG:NH1	1.93	0.81
1:D:228:ILE:HD11	1:D:459:ILE:HG12	1.62	0.81
1:C:6:LEU:HD12	1:C:51:ASP:OD2	1.81	0.81
1:C:44:ARG:NE	1:C:44:ARG:HA	1.94	0.81
2:G:158:ASP:HA	2:G:161:ILE:HD12	1.62	0.81
1:D:207:LEU:HG	1:D:212:MET:SD	2.21	0.81
1:A:6:LEU:HD11	1:C:298:ARG:NE	1.95	0.81
1:C:293:SER:CB	1:C:296:GLY:HA2	2.09	0.81
1:C:513:LEU:HD12	1:C:616:LEU:HA	1.60	0.81
2:G:187:ARG:HG2	2:G:191:LYS:HE3	1.61	0.81
2:G:206:ILE:O	2:G:210:VAL:HG23	1.81	0.81
1:B:686:GLN:NE2	1:B:689:ILE:CG2	2.44	0.81
2:H:12:GLN:HE21	2:H:23:VAL:HG13	1.44	0.81
1:C:222:PHE:CD2	1:C:492:LEU:CD1	2.64	0.81
1:B:226:VAL:CG1	1:B:461:LEU:HD22	2.09	0.80
1:B:228:ILE:HD11	1:B:459:ILE:HG12	1.60	0.80
1:A:692:SER:CB	1:A:727:LYS:HB2	2.10	0.80
1:D:59:HIS:HB2	3:D:801:ATP:H5'1	1.61	0.80
1:D:244:ILE:O	1:D:248:VAL:HB	1.81	0.80
1:B:282:TYR:HE2	1:B:304:LEU:HD21	1.46	0.80
1:B:289:VAL:HG11	1:B:302:ALA:HB2	1.63	0.80
1:D:248:VAL:CG2	1:D:254:ILE:CG1	2.60	0.80
2:F:158:ASP:HA	2:F:161:ILE:HD12	1.64	0.80
1:C:153:GLY:HA2	1:C:158:GLN:HE22	1.45	0.80
1:D:447:LYS:HB2	1:D:458:GLU:H	1.46	0.80
1:A:6:LEU:CD1	1:C:298:ARG:CZ	2.60	0.80
2:F:206:ILE:HD11	2:F:315:ARG:HG2	1.62	0.80
1:B:37:SER:CB	2:H:331:PRO:O	2.29	0.80
1:C:361:VAL:HG11	1:C:364:LEU:HB2	1.64	0.80
1:C:316:LEU:HA	1:C:319:LEU:HD11	1.63	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:155:TYR:HD1	1:C:212:MET:HB2	1.47	0.80
1:D:93:ALA:HB2	1:D:165:ILE:O	1.82	0.80
1:D:93:ALA:HB2	1:D:165:ILE:HG22	1.62	0.80
1:C:290:LYS:HD2	1:C:296:GLY:O	1.81	0.80
1:A:369:PHE:CZ	1:A:434:ARG:HB3	2.17	0.80
1:B:625:SER:O	1:B:628:ILE:HG22	1.80	0.80
1:C:685:MET:O	1:C:689:ILE:CD1	2.30	0.80
1:B:282:TYR:CE2	1:B:304:LEU:HD21	2.17	0.80
1:D:309:TRP:CH2	1:D:364:LEU:HD12	2.17	0.80
1:C:712:GLN:HE21	2:E:370:LEU:HD21	1.47	0.80
1:A:617:SER:HB2	1:A:690:ASP:H	1.44	0.79
2:G:322:ASP:C	2:G:324:PRO:HD3	2.01	0.79
1:A:618:ALA:CB	1:A:691:GLN:HB2	2.11	0.79
1:A:6:LEU:O	1:A:7:VAL:HG23	1.82	0.79
2:E:205:ALA:CB	2:E:315:ARG:HD3	2.11	0.79
1:B:569:ASN:HD22	1:B:570:GLU:H	1.29	0.79
1:A:19:LEU:HD12	1:A:19:LEU:H	1.47	0.79
1:C:207:LEU:CD1	1:C:212:MET:SD	2.70	0.79
1:C:53:ILE:HD11	1:C:58:ILE:HG12	1.64	0.79
1:A:692:SER:CB	1:A:727:LYS:CB	2.61	0.79
2:E:339:LEU:CD1	2:E:340:VAL:HG23	2.12	0.79
2:G:12:GLN:HG2	2:G:102:PRO:HD3	1.64	0.79
2:E:203:LEU:HA	2:E:207:ARG:HB2	1.64	0.79
1:D:93:ALA:CB	1:D:165:ILE:O	2.29	0.79
1:C:228:ILE:HD11	1:C:459:ILE:HG12	1.63	0.79
1:D:301:ALA:C	1:D:438:LEU:HD11	2.01	0.79
1:C:561:GLU:HG2	1:C:562:GLN:HG3	1.65	0.79
1:A:447:LYS:HB2	1:A:458:GLU:H	1.47	0.79
1:C:44:ARG:CG	1:C:69:LEU:HD21	2.12	0.79
1:B:369:PHE:CE1	1:B:434:ARG:HA	2.16	0.79
2:G:179:GLY:O	2:G:180:LYS:CD	2.30	0.79
1:D:568:PHE:CE2	1:D:574:ALA:HB2	2.18	0.79
1:C:114:LYS:HG3	1:C:166:TYR:CD2	2.18	0.79
1:A:228:ILE:HD11	1:A:459:ILE:HG12	1.62	0.79
1:D:39:SER:HB3	2:G:332:ILE:CG2	2.12	0.79
1:C:341:LYS:HB2	1:C:722:TYR:OH	1.83	0.79
2:G:12:GLN:HE21	2:G:23:VAL:HG13	1.46	0.78
1:B:522:TYR:HE1	1:B:662:LEU:HD11	1.47	0.78
2:F:55:VAL:HG21	2:F:128:ASN:ND2	1.97	0.78
2:F:203:LEU:HA	2:F:207:ARG:HB2	1.65	0.78
1:D:463:THR:O	1:D:464:LEU:CD2	2.30	0.78
1:C:685:MET:O	1:C:689:ILE:CG1	2.30	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:258:ALA:HB1	1:D:261:ILE:HD12	1.65	0.78
1:B:686:GLN:CD	1:B:727:LYS:HG3	2.04	0.78
1:A:615:THR:HB	1:A:691:GLN:NE2	1.98	0.78
1:B:189:ARG:O	1:B:193:VAL:CG2	2.26	0.78
2:E:204:GLU:HG2	2:E:238:GLU:OE1	1.83	0.78
1:A:692:SER:HB2	1:A:727:LYS:CB	2.11	0.78
1:C:215:VAL:O	1:C:216:ARG:HB3	1.81	0.78
1:D:114:LYS:HG3	1:D:166:TYR:HE2	1.43	0.78
1:C:513:LEU:CD1	1:C:616:LEU:HD23	2.11	0.78
1:B:303:THR:OG1	1:B:438:LEU:HD12	1.83	0.78
1:C:569:ASN:HD22	1:C:570:GLU:H	1.27	0.78
1:A:420:CYS:O	1:A:424:SER:HB2	1.83	0.78
1:A:615:THR:CG2	1:A:691:GLN:NE2	2.47	0.78
1:C:301:ALA:O	1:C:438:LEU:CD1	2.29	0.78
1:D:329:ARG:CD	1:D:331:ARG:HH21	1.97	0.78
1:C:730:TYR:O	1:C:731:TYR:O	2.02	0.78
1:D:420:CYS:O	1:D:424:SER:HB2	1.83	0.78
1:A:167:GLU:OE1	1:A:172:LEU:HA	1.84	0.78
1:A:463:THR:HB	1:A:513:LEU:CD2	2.13	0.78
1:A:369:PHE:CE1	1:A:434:ARG:HA	2.19	0.78
2:E:12:GLN:HE21	2:E:23:VAL:HG13	1.48	0.78
1:A:322:ASN:HA	1:A:331:ARG:HE	1.49	0.78
1:C:621:PRO:HD3	1:C:694:SER:CB	2.13	0.78
1:B:93:ALA:HB2	1:B:165:ILE:O	1.82	0.78
2:E:322:ASP:C	2:E:324:PRO:HD3	2.04	0.78
2:H:339:LEU:HD13	2:H:339:LEU:H	1.47	0.78
1:A:565:CYS:HB2	1:A:611:LEU:O	1.82	0.78
2:G:206:ILE:HD11	2:G:315:ARG:HG2	1.65	0.78
1:B:619:LEU:HB2	1:B:693:ILE:HG22	1.64	0.78
1:A:172:LEU:HD21	1:A:216:ARG:NH1	1.97	0.78
1:B:145:TYR:CZ	1:B:149:LYS:HG2	2.19	0.78
2:E:87:GLN:O	2:E:91:PRO:HD2	1.83	0.78
1:B:19:LEU:HD22	2:H:295:SER:O	1.84	0.78
1:B:282:TYR:HA	1:B:285:PHE:CD2	2.19	0.78
2:G:340:VAL:CG1	2:G:340:VAL:O	2.30	0.78
1:B:93:ALA:CB	1:B:165:ILE:O	2.32	0.78
2:E:158:ASP:HA	2:E:161:ILE:HD12	1.66	0.78
2:F:206:ILE:O	2:F:210:VAL:HG23	1.84	0.77
1:D:248:VAL:HG23	1:D:254:ILE:CD1	2.14	0.77
2:G:87:GLN:O	2:G:91:PRO:HD2	1.83	0.77
1:D:560:LYS:HD3	1:D:609:HIS:CG	2.19	0.77
1:C:19:LEU:H	1:C:19:LEU:HD12	1.47	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:361:VAL:CG1	1:B:364:LEU:HB2	2.14	0.77
2:F:87:GLN:O	2:F:91:PRO:HD2	1.83	0.77
2:H:87:GLN:O	2:H:91:PRO:HD2	1.83	0.77
2:G:203:LEU:HA	2:G:207:ARG:HB2	1.65	0.77
1:A:275:HIS:CD2	1:A:277:GLY:H	2.03	0.77
1:D:730:TYR:O	1:D:731:TYR:O	2.03	0.77
1:C:560:LYS:HD3	1:C:609:HIS:ND1	2.00	0.77
1:D:561:GLU:HG2	1:D:562:GLN:HG3	1.65	0.77
1:D:297:VAL:O	1:D:297:VAL:HG12	1.83	0.77
1:B:301:ALA:HB3	1:B:438:LEU:HD22	1.66	0.77
1:A:619:LEU:HD12	1:A:693:ILE:HG21	1.66	0.77
1:D:227:LEU:HD23	1:D:435:GLN:HG3	1.66	0.77
1:B:275:HIS:CD2	1:B:277:GLY:H	2.03	0.77
2:H:92:ASN:HA	2:H:96:LEU:HD13	1.65	0.76
1:C:623:GLU:O	1:C:627:GLN:HG2	1.84	0.76
1:C:157:VAL:HG21	1:C:216:ARG:NH1	2.00	0.76
1:D:44:ARG:HG3	1:D:69:LEU:CD2	2.13	0.76
1:C:275:HIS:CD2	1:C:277:GLY:H	2.03	0.76
1:D:621:PRO:HD3	1:D:694:SER:CB	2.15	0.76
1:D:49:PHE:HD1	1:D:53:ILE:HD13	1.50	0.76
1:B:301:ALA:HB1	1:B:438:LEU:HD21	1.68	0.76
1:D:560:LYS:HE2	1:D:609:HIS:CE1	2.19	0.76
1:B:437:ASN:HD21	1:B:439:CYS:HB2	1.51	0.76
1:D:5:LEU:HB2	1:D:17:ILE:HG12	1.65	0.76
1:D:275:HIS:CD2	1:D:277:GLY:H	2.03	0.76
1:A:5:LEU:CG	1:A:17:ILE:HG12	2.16	0.76
1:C:313:VAL:O	1:C:317:LEU:HD23	1.86	0.76
1:B:59:HIS:HB2	3:B:801:ATP:H4'	1.65	0.76
1:B:730:TYR:O	1:B:731:TYR:O	2.03	0.76
1:C:428:PRO:O	1:C:432:PRO:HB3	1.85	0.76
1:B:155:TYR:HD1	1:B:212:MET:HB2	1.51	0.76
1:C:369:PHE:CE2	1:C:434:ARG:CD	2.66	0.76
2:H:336:ASN:CA	2:H:339:LEU:HD11	2.13	0.76
2:E:339:LEU:HD12	2:E:339:LEU:C	2.06	0.76
1:D:719:LEU:HD22	2:G:375:LEU:HD21	1.68	0.76
1:A:276:THR:HG23	1:A:280:PRO:HG2	1.66	0.76
1:B:466:ALA:CA	1:B:516:GLY:O	2.33	0.76
1:A:5:LEU:CD1	1:A:17:ILE:CD1	2.64	0.76
1:C:17:ILE:CD1	3:C:801:ATP:C2	2.60	0.76
1:A:440:LEU:HD12	1:A:728:THR:HB	1.68	0.76
1:D:421:ASN:O	1:D:428:PRO:HG3	1.86	0.76
1:D:89:LEU:HD22	1:D:152:GLU:HG3	1.64	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:489:LEU:HD22	1:D:513:LEU:HD22	1.68	0.75
1:A:167:GLU:OE1	1:A:172:LEU:HB2	1.86	0.75
1:B:40:GLN:HE22	2:H:333:PRO:HG2	1.51	0.75
1:D:175:LEU:HD22	1:D:216:ARG:HD2	1.67	0.75
2:H:309:GLU:HG2	2:H:325:PHE:CD1	2.22	0.75
2:G:179:GLY:O	2:G:180:LYS:HD3	1.86	0.75
1:D:406:ARG:NH1	1:D:697:THR:HG23	2.01	0.75
1:D:275:HIS:HD2	1:D:277:GLY:H	1.34	0.75
1:A:562:GLN:HG2	1:A:612:ARG:CZ	2.16	0.75
1:A:297:VAL:CG1	1:C:4:ASN:ND2	2.50	0.75
1:C:418:ASP:O	1:C:422:THR:CG2	2.27	0.75
1:C:53:ILE:HD13	1:C:58:ILE:HG12	1.67	0.75
1:A:529:LYS:HB3	1:A:536:ALA:HB2	1.66	0.75
1:C:94:TYR:HE2	1:C:168:SER:HB2	1.52	0.75
1:C:716:LYS:HG2	2:E:370:LEU:HD13	1.69	0.75
1:C:457:GLY:O	1:C:502:ALA:HB1	1.87	0.75
2:F:239:ALA:CB	2:F:342:ASP:OD2	2.35	0.75
1:D:168:SER:OG	1:D:171:PHE:HD2	1.67	0.74
1:B:464:LEU:HA	1:B:514:GLY:O	1.86	0.74
1:A:5:LEU:HD12	1:A:17:ILE:HG12	0.78	0.74
1:A:618:ALA:HB2	1:A:691:GLN:CB	2.16	0.74
1:B:365:TYR:CZ	1:B:369:PHE:CE2	2.75	0.74
1:C:437:ASN:HD21	1:C:439:CYS:HB2	1.52	0.74
1:B:275:HIS:HD2	1:B:277:GLY:H	1.34	0.74
1:A:227:LEU:HD23	1:A:435:GLN:HG2	1.70	0.74
2:H:336:ASN:HA	2:H:339:LEU:CD1	2.14	0.74
1:C:361:VAL:HG12	1:C:364:LEU:HB2	1.67	0.74
1:D:316:LEU:O	1:D:319:LEU:CG	2.34	0.74
1:A:489:LEU:HD22	1:A:513:LEU:CD2	2.07	0.74
1:A:716:LYS:HG2	2:F:370:LEU:HD11	1.69	0.74
1:B:19:LEU:HB2	2:H:295:SER:HB3	1.69	0.74
1:B:316:LEU:O	1:B:319:LEU:CD1	2.35	0.74
1:C:204:LYS:HE3	1:C:481:LEU:HD21	1.69	0.74
2:E:12:GLN:HG2	2:E:102:PRO:HD3	1.68	0.74
1:B:361:VAL:HG12	1:B:364:LEU:HB2	1.68	0.74
2:E:204:GLU:HG2	2:E:238:GLU:CD	2.08	0.74
1:A:647:SER:HB2	1:A:652:LEU:CG	2.17	0.74
1:A:437:ASN:HD21	1:A:439:CYS:HB2	1.52	0.74
1:D:364:LEU:C	1:D:364:LEU:HD13	2.07	0.74
2:G:201:ASN:O	2:G:205:ALA:HB3	1.87	0.74
1:D:19:LEU:HD22	2:G:295:SER:O	1.88	0.74
1:A:6:LEU:HD11	1:C:298:ARG:CZ	2.18	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:227:LEU:HD23	1:B:435:GLN:HG3	1.67	0.74
1:A:623:GLU:HG2	1:A:633:ASN:HD22	1.49	0.74
1:A:475:LEU:HD11	1:A:542:LYS:HE2	1.69	0.74
1:A:315:SER:O	1:A:318:VAL:CG2	2.35	0.74
1:D:157:VAL:CG1	1:D:166:TYR:HD2	1.97	0.74
1:D:623:GLU:HG2	1:D:633:ASN:HD22	1.50	0.74
1:B:208:PRO:HD3	1:B:464:LEU:O	1.88	0.74
1:B:700:ASP:OD1	1:B:735:ARG:CD	2.36	0.73
2:H:310:TYR:N	2:H:328:ARG:HD3	2.04	0.73
2:F:372:ASN:HD22	2:F:372:ASN:H	1.35	0.73
1:B:617:SER:C	1:B:689:ILE:CD1	2.57	0.73
2:H:85:SER:O	2:H:89:ARG:NH2	2.21	0.73
1:B:341:LYS:HB2	1:B:722:TYR:OH	1.88	0.73
1:B:286:GLN:NE2	1:B:332:HIS:CB	2.51	0.73
1:C:59:HIS:HB2	3:C:801:ATP:H5'2	1.68	0.73
1:B:40:GLN:NE2	2:H:333:PRO:CG	2.45	0.73
1:C:44:ARG:HG3	1:C:69:LEU:CD2	2.14	0.73
1:A:421:ASN:O	1:A:428:PRO:HG3	1.87	0.73
2:F:316:MET:SD	2:F:324:PRO:HG3	2.29	0.73
2:H:201:ASN:O	2:H:205:ALA:HB3	1.88	0.73
1:D:260:ARG:HG3	1:D:365:TYR:CZ	2.24	0.73
1:D:248:VAL:HG23	1:D:254:ILE:HD11	1.69	0.73
2:H:12:GLN:CG	2:H:102:PRO:HD3	2.19	0.73
2:G:65:LEU:HD21	2:G:223:LEU:HD13	1.69	0.73
1:B:145:TYR:HE2	1:B:652:LEU:CD2	2.02	0.73
1:A:89:LEU:HD21	1:A:152:GLU:HG3	1.70	0.73
1:C:425:PRO:HG2	1:C:690:ASP:HB3	1.69	0.73
1:A:625:SER:O	1:A:628:ILE:CG2	2.37	0.73
1:A:308:MET:HE2	1:A:398:LEU:HD23	1.69	0.73
2:F:201:ASN:O	2:F:205:ALA:HB3	1.89	0.73
1:C:6:LEU:HD12	1:C:51:ASP:CG	2.09	0.73
1:A:369:PHE:HD2	1:A:434:ARG:NH1	1.86	0.73
2:F:87:GLN:O	2:F:91:PRO:HD3	1.89	0.73
1:C:232:ASP:OD2	1:C:262:ARG:NE	2.20	0.73
2:E:310:TYR:N	2:E:328:ARG:HD3	2.04	0.73
1:C:94:TYR:CE2	1:C:168:SER:HB2	2.24	0.72
1:A:155:TYR:HD1	1:A:212:MET:HB2	1.54	0.72
2:E:316:MET:SD	2:E:324:PRO:HG2	2.28	0.72
1:C:560:LYS:HE2	1:C:609:HIS:CE1	2.24	0.72
1:A:319:LEU:HA	1:A:329:ARG:HG3	1.71	0.72
1:B:234:LEU:H	1:B:234:LEU:HD22	1.53	0.72
1:C:513:LEU:HD11	1:C:616:LEU:HD22	1.71	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:279:ILE:HD13	1:A:319:LEU:HD21	1.70	0.72
1:C:275:HIS:HD2	1:C:277:GLY:H	1.35	0.72
2:F:204:GLU:HG2	2:F:238:GLU:OE1	1.89	0.72
1:D:437:ASN:HD21	1:D:439:CYS:HB2	1.54	0.72
1:D:19:LEU:H	1:D:19:LEU:HD12	1.53	0.72
1:C:115:TYR:HE1	1:C:216:ARG:HD2	0.95	0.72
2:G:201:ASN:O	2:G:205:ALA:CB	2.37	0.72
1:A:275:HIS:HD2	1:A:277:GLY:H	1.35	0.72
1:A:167:GLU:OE1	1:A:172:LEU:CA	2.38	0.72
1:B:440:LEU:HD12	1:B:728:THR:HB	1.71	0.72
1:A:234:LEU:HD22	1:A:234:LEU:H	1.54	0.72
1:D:293:SER:OG	1:D:296:GLY:HA2	1.89	0.72
1:C:696:ASN:HD22	1:C:696:ASN:H	1.37	0.72
1:D:329:ARG:CG	1:D:331:ARG:HH21	2.03	0.72
1:C:369:PHE:O	1:C:421:ASN:CG	2.27	0.72
1:B:686:GLN:NE2	1:B:727:LYS:HE3	2.05	0.72
1:A:463:THR:HG1	1:A:513:LEU:HD23	1.51	0.72
1:A:320:LYS:HE2	1:A:333:MET:O	1.90	0.72
1:B:19:LEU:HD12	1:B:19:LEU:H	1.54	0.72
1:A:705:PRO:O	1:A:706:SER:HB2	1.90	0.71
1:C:106:VAL:O	1:C:110:VAL:HG23	1.89	0.71
2:F:312:THR:HB	2:F:325:PHE:CD2	2.24	0.71
1:D:34:HIS:O	1:D:35:ASN:HB2	1.91	0.71
1:C:735:ARG:O	1:C:736:ASP:CB	2.34	0.71
2:E:339:LEU:O	2:E:340:VAL:HB	1.91	0.71
2:H:176:THR:OG1	2:H:181:THR:HG22	1.89	0.71
2:F:65:LEU:HD21	2:F:223:LEU:HD13	1.72	0.71
2:H:232:ARG:HD3	2:H:342:ASP:HB2	0.75	0.71
1:A:227:LEU:HB3	1:A:435:GLN:HE22	1.52	0.71
1:C:316:LEU:O	1:C:319:LEU:CD1	2.38	0.71
1:C:248:VAL:HG21	1:C:289:VAL:HA	1.72	0.71
2:H:87:GLN:O	2:H:91:PRO:HD3	1.90	0.71
2:F:177:VAL:N	2:F:180:LYS:O	2.21	0.71
1:B:529:LYS:H	1:B:529:LYS:HD2	1.54	0.71
1:D:234:LEU:HD22	1:D:234:LEU:H	1.55	0.71
1:C:222:PHE:CE2	1:C:492:LEU:HD11	2.25	0.71
1:A:298:ARG:HH21	1:C:6:LEU:HD21	1.54	0.71
2:E:87:GLN:O	2:E:91:PRO:HD3	1.90	0.71
1:B:658:ASP:HB3	1:B:662:LEU:HD12	1.73	0.71
1:C:621:PRO:CD	1:C:694:SER:HB2	2.18	0.71
1:A:369:PHE:HE2	1:A:434:ARG:HD3	1.50	0.71
1:D:150:GLN:O	1:D:154:LYS:CG	2.35	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:54:LYS:O	1:B:58:ILE:HG13	1.91	0.71
1:B:308:MET:HE2	1:B:398:LEU:HD23	1.72	0.71
1:A:6:LEU:HD12	1:C:298:ARG:NH1	2.05	0.71
1:C:254:ILE:HG22	1:C:256:ILE:HG13	1.73	0.71
1:D:150:GLN:OE1	1:D:154:LYS:HD2	1.89	0.71
1:A:106:VAL:O	1:A:110:VAL:HG23	1.90	0.71
2:F:205:ALA:HB1	2:F:315:ARG:HD3	1.73	0.70
1:C:254:ILE:O	1:C:438:LEU:HG	1.91	0.70
1:D:254:ILE:N	1:D:438:LEU:CD1	2.40	0.70
1:C:4:ASN:HD22	1:C:4:ASN:N	1.89	0.70
1:C:545:GLU:HG3	1:C:595:LEU:HD23	1.73	0.70
1:C:663:HIS:ND1	1:C:663:HIS:N	2.39	0.70
2:G:87:GLN:O	2:G:91:PRO:HD3	1.89	0.70
2:H:201:ASN:O	2:H:205:ALA:CB	2.39	0.70
2:F:310:TYR:N	2:F:328:ARG:HD3	2.05	0.70
2:G:204:GLU:HG2	2:G:238:GLU:OE1	1.90	0.70
1:B:39:SER:HB2	2:H:303:ILE:HG21	1.71	0.70
1:A:692:SER:HB3	1:A:727:LYS:HD2	1.74	0.70
1:B:365:TYR:CE2	1:B:369:PHE:CE2	2.77	0.70
1:D:569:ASN:OD1	1:D:570:GLU:N	2.24	0.70
1:C:620:MET:O	1:C:620:MET:HG2	1.91	0.70
1:A:235:ASP:OD2	1:B:246:LYS:NZ	2.25	0.70
2:E:173:GLY:O	2:E:175:HIS:CE1	2.43	0.70
1:B:106:VAL:O	1:B:110:VAL:HG23	1.91	0.70
1:B:301:ALA:HB1	1:B:438:LEU:CD2	2.21	0.70
1:A:315:SER:O	1:A:318:VAL:HG23	1.92	0.70
1:B:617:SER:C	1:B:689:ILE:HD11	2.11	0.70
1:B:701:PRO:CD	1:B:735:ARG:HG2	2.20	0.70
2:G:205:ALA:HB1	2:G:315:ARG:HD3	1.74	0.70
1:D:114:LYS:HG3	1:D:166:TYR:CD2	2.19	0.70
1:C:114:LYS:N	1:C:114:LYS:HD3	2.06	0.70
1:A:6:LEU:HD12	1:C:298:ARG:CZ	2.21	0.70
1:D:282:TYR:CE2	1:D:304:LEU:HD22	2.26	0.70
2:H:339:LEU:HD13	2:H:339:LEU:N	2.06	0.70
1:A:5:LEU:HB2	1:A:17:ILE:HG23	1.71	0.69
1:A:279:ILE:HD13	1:A:319:LEU:CD2	2.22	0.69
1:A:545:GLU:HG3	1:A:595:LEU:HD23	1.73	0.69
1:B:572:THR:HB	1:B:577:ILE:HD12	1.74	0.69
1:D:167:GLU:OE2	1:D:216:ARG:NH2	2.24	0.69
1:B:696:ASN:H	1:B:696:ASN:HD22	1.37	0.69
2:E:82:LEU:HD13	2:E:140:ILE:HG22	1.75	0.69
1:A:222:PHE:CD2	1:A:492:LEU:HD11	2.27	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:13:LEU:O	2:H:32:LYS:HD2	1.92	0.69
1:D:50:TYR:CD2	1:D:50:TYR:N	2.55	0.69
2:H:232:ARG:NH1	2:H:343:ASN:N	2.40	0.69
1:A:572:THR:HB	1:A:577:ILE:HD12	1.74	0.69
1:C:115:TYR:CD1	1:C:216:ARG:CG	2.76	0.69
1:B:441:GLU:HB3	1:B:619:LEU:O	1.92	0.69
2:H:232:ARG:HH12	2:H:343:ASN:H	1.40	0.69
2:E:206:ILE:CD1	2:E:312:THR:HG23	2.23	0.69
1:D:329:ARG:CB	1:D:331:ARG:HH21	2.04	0.69
1:D:696:ASN:H	1:D:696:ASN:HD22	1.37	0.69
1:D:106:VAL:O	1:D:110:VAL:HG23	1.92	0.69
1:D:153:GLY:HA2	1:D:158:GLN:NE2	2.00	0.69
1:A:413:TYR:HH	1:A:731:TYR:HE2	0.73	0.69
2:H:89:ARG:HG2	2:H:90:SER:N	2.06	0.69
2:F:309:GLU:HG2	2:F:325:PHE:CE1	2.27	0.69
1:D:308:MET:HE2	1:D:398:LEU:HD23	1.72	0.69
2:H:309:GLU:OE2	2:H:325:PHE:CD1	2.46	0.69
1:B:301:ALA:CB	1:B:438:LEU:HD22	2.22	0.69
2:E:333:PRO:O	2:E:336:ASN:ND2	2.25	0.69
2:G:82:LEU:HD13	2:G:140:ILE:HG22	1.75	0.69
1:B:168:SER:HG	1:B:171:PHE:HD2	1.41	0.69
1:A:208:PRO:HG3	1:A:211:ILE:HD13	1.72	0.69
1:B:40:GLN:HE21	2:H:333:PRO:HG2	1.53	0.69
2:G:333:PRO:O	2:G:336:ASN:ND2	2.25	0.69
1:A:298:ARG:HH21	1:C:6:LEU:CD2	2.05	0.69
1:A:298:ARG:NH2	1:C:6:LEU:HD21	2.08	0.69
1:C:227:LEU:HD23	1:C:435:GLN:HG3	1.75	0.69
1:B:593:GLU:OE2	1:B:596:HIS:NE2	2.26	0.69
1:A:463:THR:O	1:A:464:LEU:CD2	2.34	0.69
1:C:369:PHE:CD2	1:C:434:ARG:HD3	2.26	0.69
1:D:49:PHE:CD1	1:D:53:ILE:HD13	2.27	0.69
1:A:510:ARG:HG3	1:A:567:TRP:HE3	1.58	0.69
1:A:135:ILE:HD11	1:A:174:ILE:HG21	1.74	0.69
1:A:181:PHE:O	1:A:184:TYR:HB2	1.93	0.69
2:H:232:ARG:HD3	2:H:342:ASP:HB3	1.70	0.69
1:C:692:SER:HB2	1:C:727:LYS:HB2	1.74	0.69
1:D:329:ARG:HD3	1:D:331:ARG:HH22	1.56	0.69
1:D:517:VAL:HG12	1:D:619:LEU:HD22	1.75	0.69
2:H:206:ILE:CD1	2:H:315:ARG:HG2	2.22	0.69
1:C:308:MET:HE2	1:C:398:LEU:HD23	1.75	0.69
1:D:241:SER:O	1:D:245:VAL:HG23	1.93	0.69
1:D:705:PRO:O	1:D:706:SER:HB2	1.93	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:465:SER:O	1:C:515:ILE:HA	1.92	0.68
2:G:92:ASN:O	2:G:96:LEU:HB2	1.93	0.68
1:B:441:GLU:HG2	1:B:620:MET:CB	2.23	0.68
1:C:685:MET:O	1:C:689:ILE:HD11	1.93	0.68
1:B:22:ILE:HD11	3:B:801:ATP:C2	2.28	0.68
1:D:567:TRP:O	1:D:569:ASN:N	2.26	0.68
2:H:277:VAL:HG22	2:H:324:PRO:HG3	1.76	0.68
2:F:197:LEU:HD12	2:F:198:MET:N	2.07	0.68
1:C:234:LEU:H	1:C:234:LEU:HD22	1.56	0.68
1:B:250:GLN:HE22	1:B:499:PRO:HG3	1.58	0.68
2:G:197:LEU:HD12	2:G:198:MET:N	2.08	0.68
1:B:711:MET:CB	2:H:364:GLU:O	2.33	0.68
1:A:226:VAL:CG1	1:A:461:LEU:HD22	2.22	0.68
1:A:309:TRP:CH2	1:A:364:LEU:HD12	2.27	0.68
1:B:239:ALA:HA	1:B:452:VAL:HG12	1.75	0.68
1:B:689:ILE:CG1	1:B:691:GLN:O	2.40	0.68
2:H:332:ILE:CG2	2:H:334:TRP:HE1	2.02	0.68
1:D:55:THR:HA	1:D:58:ILE:HD12	1.76	0.68
2:H:82:LEU:HD13	2:H:140:ILE:HG22	1.74	0.68
1:D:167:GLU:CD	1:D:172:LEU:HB2	2.14	0.68
1:D:286:GLN:CD	1:D:332:HIS:ND1	2.46	0.68
1:C:7:VAL:HG21	3:C:801:ATP:N1	2.09	0.68
1:A:232:ASP:CG	1:A:262:ARG:HE	1.97	0.68
1:C:135:ILE:HD11	1:C:174:ILE:HG21	1.76	0.68
1:B:735:ARG:CG	1:B:735:ARG:O	2.30	0.68
1:A:226:VAL:HG12	1:A:461:LEU:HD22	1.76	0.68
1:D:22:ILE:HD12	1:D:22:ILE:H	1.58	0.68
1:C:276:THR:HG21	1:D:291:SER:O	1.94	0.68
1:B:318:VAL:HG21	1:B:329:ARG:HH12	1.56	0.68
2:H:205:ALA:HB1	2:H:315:ARG:HD3	1.76	0.68
1:B:22:ILE:HD12	1:B:22:ILE:H	1.59	0.68
1:D:440:LEU:HD12	1:D:728:THR:HB	1.75	0.68
2:H:5:PHE:CD1	2:H:24:ASN:O	2.45	0.68
1:D:135:ILE:HD11	1:D:174:ILE:HG21	1.76	0.68
1:A:59:HIS:HB2	3:A:801:ATP:H4'	1.76	0.68
1:D:522:TYR:HE1	1:D:662:LEU:HD11	1.59	0.68
2:H:232:ARG:CD	2:H:342:ASP:CB	2.45	0.68
1:A:361:VAL:HG11	1:A:364:LEU:HG	1.74	0.68
1:C:420:CYS:O	1:C:424:SER:CB	2.42	0.68
1:B:145:TYR:CE2	1:B:652:LEU:HD23	2.26	0.68
2:E:197:LEU:HD12	2:E:198:MET:N	2.08	0.68
1:D:572:THR:HB	1:D:577:ILE:HD12	1.74	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:232:ASP:OD2	1:D:262:ARG:NE	2.23	0.67
1:B:155:TYR:CE1	1:B:212:MET:SD	2.87	0.67
1:B:510:ARG:HG3	1:B:567:TRP:HE3	1.59	0.67
1:A:696:ASN:H	1:A:696:ASN:HD22	1.43	0.67
1:A:232:ASP:OD2	1:A:262:ARG:NE	2.27	0.67
1:D:306:TYR:OH	1:D:317:LEU:HD23	1.94	0.67
1:B:208:PRO:HG2	1:B:211:ILE:HD13	1.77	0.67
1:D:316:LEU:O	1:D:319:LEU:CD1	2.42	0.67
1:D:150:GLN:OE1	1:D:154:LYS:HE2	1.94	0.67
2:E:65:LEU:CD2	2:E:223:LEU:HD13	2.24	0.67
2:H:185:SER:HB3	2:H:188:GLU:HB2	1.75	0.67
1:C:222:PHE:CG	1:C:492:LEU:HD11	2.28	0.67
1:C:305:PHE:CE1	1:C:436:SER:O	2.48	0.67
1:A:406:ARG:NH1	1:A:732:GLN:HG3	2.10	0.67
1:C:625:SER:O	1:C:628:ILE:CG2	2.41	0.67
1:D:44:ARG:CG	1:D:69:LEU:HD21	2.16	0.67
1:C:316:LEU:O	1:C:319:LEU:CG	2.43	0.67
2:F:204:GLU:HG2	2:F:238:GLU:CD	2.15	0.67
1:C:232:ASP:CG	1:C:262:ARG:HE	1.97	0.67
1:C:442:ILE:HD11	1:C:462:CYS:SG	2.34	0.67
1:B:286:GLN:HE21	1:B:332:HIS:CB	2.04	0.67
1:D:689:ILE:CD1	1:D:693:ILE:HG23	2.24	0.67
1:D:658:ASP:CG	1:D:658:ASP:O	2.32	0.67
1:D:181:PHE:O	1:D:184:TYR:HB2	1.94	0.67
1:C:241:SER:O	1:C:245:VAL:HG23	1.93	0.67
1:C:155:TYR:HD1	1:C:212:MET:CB	2.07	0.67
1:D:114:LYS:HE3	1:D:166:TYR:OH	1.95	0.67
1:D:711:MET:HB2	2:G:363:SER:HB3	1.75	0.67
2:E:177:VAL:CG2	2:E:180:LYS:O	2.42	0.67
1:D:406:ARG:HH11	1:D:697:THR:HG23	1.59	0.67
1:C:440:LEU:HD12	1:C:728:THR:HB	1.74	0.67
1:A:465:SER:HB2	1:A:489:LEU:CD1	2.24	0.67
2:G:12:GLN:CG	2:G:102:PRO:HD3	2.25	0.67
2:G:204:GLU:HG2	2:G:238:GLU:CD	2.15	0.67
2:H:197:LEU:HD12	2:H:198:MET:N	2.09	0.67
1:A:215:VAL:C	1:A:216:ARG:HG2	2.08	0.67
1:B:711:MET:HB3	2:H:364:GLU:C	2.15	0.67
1:B:565:CYS:HB3	1:B:568:PHE:HB2	1.76	0.67
1:C:114:LYS:HE2	1:C:166:TYR:CE2	2.29	0.66
1:B:258:ALA:CB	1:B:282:TYR:OH	2.41	0.66
1:C:254:ILE:HG21	1:C:256:ILE:HD11	1.75	0.66
2:E:206:ILE:HD13	2:E:312:THR:OG1	1.94	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:369:PHE:CD2	1:C:434:ARG:CG	2.77	0.66
1:D:168:SER:OG	1:D:171:PHE:CD2	2.44	0.66
2:H:307:TYR:O	2:H:311:ILE:HG22	1.96	0.66
2:H:332:ILE:CG2	2:H:334:TRP:NE1	2.57	0.66
1:C:686:GLN:HA	1:C:689:ILE:CG1	2.25	0.66
1:C:668:LEU:HB2	1:C:671:GLU:HG3	1.76	0.66
1:D:464:LEU:HD22	1:D:514:GLY:HA3	1.77	0.66
1:A:493:LEU:HD21	1:A:513:LEU:CD2	2.08	0.66
1:D:560:LYS:HD3	1:D:609:HIS:CE1	2.31	0.66
1:D:413:TYR:HH	1:D:731:TYR:HE2	1.43	0.66
1:A:155:TYR:CD1	1:A:212:MET:HB3	2.25	0.66
2:E:328:ARG:CZ	2:E:328:ARG:HB3	2.26	0.66
1:A:93:ALA:HB2	1:A:165:ILE:O	1.96	0.66
2:H:178:ASN:CG	2:H:178:ASN:O	2.33	0.66
1:D:211:ILE:O	1:D:215:VAL:HG23	1.96	0.66
1:A:155:TYR:CD1	1:A:212:MET:HB2	2.27	0.66
1:D:619:LEU:HB2	1:D:693:ILE:HG22	1.77	0.66
1:C:560:LYS:HD3	1:C:609:HIS:CD2	2.31	0.66
1:A:301:ALA:CB	1:A:438:LEU:HD21	2.25	0.66
1:A:239:ALA:HA	1:A:452:VAL:HG12	1.76	0.66
1:C:216:ARG:HG2	1:C:216:ARG:O	1.94	0.66
1:B:135:ILE:HD11	1:B:174:ILE:HG21	1.77	0.66
1:B:212:MET:O	1:B:216:ARG:NH1	2.29	0.66
2:H:124:HIS:HA	2:H:127:ARG:HD3	1.77	0.66
2:E:149:ARG:HH12	2:E:286:TRP:HB2	1.60	0.66
1:C:517:VAL:HG12	1:C:619:LEU:HD22	1.76	0.66
1:D:663:HIS:N	1:D:663:HIS:ND1	2.38	0.66
1:B:168:SER:OG	1:B:171:PHE:HD2	1.77	0.66
1:B:227:LEU:HD11	1:B:437:ASN:HB3	1.76	0.66
1:A:369:PHE:O	1:A:421:ASN:CG	2.34	0.66
1:C:712:GLN:HE21	2:E:370:LEU:CD2	2.08	0.66
1:A:522:TYR:HE1	1:A:662:LEU:HD11	1.59	0.66
1:B:168:SER:HG	1:B:171:PHE:HB2	1.60	0.66
1:A:512:THR:HB	1:A:615:THR:OG1	1.96	0.66
1:D:37:SER:HB2	1:D:40:GLN:HB2	1.77	0.66
1:A:369:PHE:CE2	1:A:434:ARG:HB3	2.31	0.66
2:F:307:TYR:O	2:F:311:ILE:HG22	1.95	0.66
1:A:40:GLN:NE2	2:F:333:PRO:HG2	2.10	0.66
1:A:241:SER:O	1:A:245:VAL:HG23	1.95	0.66
1:C:302:ALA:HA	1:C:438:LEU:HD11	1.78	0.66
1:B:425:PRO:HG2	1:B:690:ASP:HB3	1.78	0.65
1:A:517:VAL:HG12	1:A:619:LEU:HD22	1.78	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:181:PHE:O	1:C:184:TYR:HB2	1.94	0.65
2:E:12:GLN:CG	2:E:102:PRO:HD3	2.26	0.65
1:D:208:PRO:HG2	1:D:211:ILE:HD13	1.77	0.65
1:B:686:GLN:NE2	1:B:689:ILE:HG23	2.11	0.65
2:H:330:ASN:OD1	2:H:331:PRO:HD2	1.96	0.65
2:E:13:LEU:O	2:E:32:LYS:HD2	1.96	0.65
1:B:181:PHE:O	1:B:184:TYR:HB2	1.96	0.65
1:B:621:PRO:CD	1:B:694:SER:CB	2.69	0.65
2:F:35:ILE:HG23	2:F:36:PHE:H	1.61	0.65
1:A:493:LEU:HD11	1:A:513:LEU:HD11	1.77	0.65
1:D:286:GLN:OE1	1:D:332:HIS:CB	2.41	0.65
1:D:307:PRO:HG2	1:D:310:HIS:HB2	1.78	0.65
1:A:79:TYR:O	1:A:83:ARG:HG2	1.97	0.65
1:B:513:LEU:HG	1:B:613:ASN:ND2	2.11	0.65
1:B:464:LEU:CA	1:B:514:GLY:O	2.44	0.65
1:B:513:LEU:HG	1:B:613:ASN:HD22	1.61	0.65
1:D:154:LYS:HE2	1:D:624:THR:CG2	2.26	0.65
1:A:692:SER:HB3	1:A:727:LYS:CB	2.24	0.65
2:F:94:ALA:O	2:F:95:LEU:HD23	1.96	0.65
1:D:560:LYS:HE2	1:D:609:HIS:ND1	2.11	0.65
2:H:35:ILE:HG23	2:H:36:PHE:H	1.62	0.65
1:B:241:SER:O	1:B:245:VAL:HG23	1.95	0.65
1:A:297:VAL:O	1:A:297:VAL:CG1	2.44	0.65
2:F:372:ASN:H	2:F:372:ASN:ND2	1.95	0.65
1:D:239:ALA:HA	1:D:452:VAL:HG12	1.78	0.65
1:D:147:ALA:O	1:D:151:LEU:HG	1.97	0.65
1:D:167:GLU:OE2	1:D:172:LEU:HB2	1.97	0.65
1:B:516:GLY:HA3	1:B:620:MET:CE	2.26	0.65
1:D:184:TYR:O	1:D:189:ARG:NH2	2.29	0.65
1:C:513:LEU:O	1:C:513:LEU:HD12	1.96	0.65
1:B:167:GLU:HG3	1:B:168:SER:N	2.12	0.65
2:F:328:ARG:HB3	2:F:328:ARG:CZ	2.27	0.65
1:A:184:TYR:O	1:A:189:ARG:NH2	2.29	0.65
1:C:79:TYR:O	1:C:83:ARG:HG2	1.96	0.65
1:B:619:LEU:HB2	1:B:693:ILE:CG2	2.26	0.65
1:B:686:GLN:NE2	1:B:727:LYS:HG3	2.11	0.65
1:A:167:GLU:CD	1:A:172:LEU:HB2	2.17	0.64
1:C:322:ASN:HA	1:C:331:ARG:HH21	1.62	0.64
1:C:22:ILE:HD12	1:C:22:ILE:H	1.61	0.64
2:E:62:TYR:O	2:E:70:LYS:HE2	1.98	0.64
1:A:93:ALA:CB	1:A:165:ILE:O	2.45	0.64
2:E:20:GLY:CA	2:E:100:SER:HB3	2.27	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:153:GLY:CA	1:D:158:GLN:HE22	2.01	0.64
1:D:208:PRO:HD3	1:D:464:LEU:O	1.98	0.64
1:C:6:LEU:HD12	1:C:51:ASP:OD1	1.97	0.64
1:C:716:LYS:HG2	2:E:370:LEU:HD22	1.78	0.64
1:B:315:SER:O	1:B:318:VAL:CG1	2.45	0.64
2:H:328:ARG:HB3	2:H:328:ARG:CZ	2.28	0.64
1:A:298:ARG:CZ	1:C:6:LEU:HD21	2.27	0.64
1:C:232:ASP:OD2	1:C:262:ARG:NH2	2.29	0.64
1:D:625:SER:O	1:D:628:ILE:CG2	2.41	0.64
1:B:619:LEU:HG	1:B:693:ILE:CG2	2.28	0.64
1:D:227:LEU:HD11	1:D:437:ASN:HB3	1.80	0.64
1:B:215:VAL:HG22	1:B:222:PHE:HZ	1.63	0.64
1:B:464:LEU:CB	1:B:514:GLY:O	2.46	0.64
2:E:90:SER:HB2	2:E:91:PRO:HD3	1.79	0.64
1:D:560:LYS:HD3	1:D:609:HIS:CD2	2.33	0.64
2:E:35:ILE:HG23	2:E:36:PHE:H	1.62	0.64
2:G:361:ILE:N	2:G:361:ILE:HD13	2.13	0.64
2:G:372:ASN:OD1	2:G:372:ASN:N	2.30	0.64
1:C:617:SER:HB2	1:C:690:ASP:N	1.99	0.64
1:A:227:LEU:HB2	1:A:460:ALA:HB3	1.78	0.64
1:A:145:TYR:OH	1:A:149:LYS:HE3	1.98	0.64
1:D:145:TYR:OH	1:D:149:LYS:HE3	1.98	0.64
1:A:297:VAL:HG11	1:C:4:ASN:HD22	1.62	0.64
1:D:150:GLN:OE1	1:D:154:LYS:CD	2.45	0.64
1:A:329:ARG:HD3	1:A:331:ARG:NH1	2.13	0.64
1:D:558:LEU:HD11	1:D:562:GLN:NE2	2.12	0.64
2:H:177:VAL:O	2:H:178:ASN:ND2	2.30	0.64
1:C:572:THR:HB	1:C:577:ILE:HD12	1.79	0.64
1:B:307:PRO:HG2	1:B:310:HIS:HB2	1.79	0.64
1:C:209:THR:HB	1:C:210:PRO:HD3	1.80	0.64
2:G:366:ASP:O	2:G:366:ASP:CG	2.36	0.64
1:C:685:MET:C	1:C:689:ILE:HD11	2.19	0.63
1:A:686:GLN:CD	1:A:727:LYS:HG3	2.19	0.63
2:H:90:SER:HB2	2:H:91:PRO:HD3	1.79	0.63
2:E:177:VAL:HG21	2:E:182:VAL:HG23	1.78	0.63
1:D:297:VAL:O	1:D:297:VAL:CG1	2.45	0.63
2:F:369:ASP:O	2:F:372:ASN:ND2	2.31	0.63
2:G:307:TYR:O	2:G:311:ILE:HG22	1.97	0.63
1:C:109:MET:HE3	1:C:166:TYR:O	1.99	0.63
1:C:211:ILE:O	1:C:215:VAL:HG23	1.98	0.63
1:B:211:ILE:O	1:B:215:VAL:HG23	1.99	0.63
1:B:618:ALA:N	1:B:689:ILE:CD1	2.52	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:227:LEU:HB2	1:B:460:ALA:HB3	1.79	0.63
1:A:689:ILE:HG21	1:A:691:GLN:O	1.98	0.63
1:C:254:ILE:HG22	1:C:256:ILE:CG1	2.27	0.63
1:C:278:CYS:HB3	1:C:282:TYR:CE1	2.33	0.63
2:F:90:SER:HB2	2:F:91:PRO:HD3	1.81	0.63
1:B:19:LEU:HD22	2:H:295:SER:C	2.18	0.63
1:A:301:ALA:HB3	1:A:438:LEU:HD21	1.79	0.63
1:C:208:PRO:HG2	1:C:211:ILE:HD13	1.78	0.63
1:C:463:THR:CA	1:C:464:LEU:HD23	2.28	0.63
1:A:516:GLY:HA2	1:A:618:ALA:O	1.98	0.63
1:A:619:LEU:HD12	1:A:693:ILE:CG2	2.28	0.63
1:C:55:THR:HA	1:C:58:ILE:HD12	1.80	0.63
2:G:35:ILE:HG23	2:G:36:PHE:H	1.63	0.63
1:C:558:LEU:HD11	1:C:562:GLN:NE2	2.14	0.63
1:D:375:PHE:O	1:D:379:TYR:HB2	1.98	0.63
1:B:6:LEU:HB2	1:B:51:ASP:OD1	1.98	0.63
1:B:441:GLU:CB	1:B:619:LEU:O	2.46	0.63
2:F:12:GLN:NE2	2:F:23:VAL:CG1	2.60	0.63
1:C:228:ILE:C	1:C:435:GLN:HE22	2.01	0.63
1:A:94:TYR:HE2	1:A:168:SER:HB2	1.63	0.63
1:A:6:LEU:HD22	1:A:14:THR:HG22	1.81	0.63
1:B:37:SER:HB2	1:B:40:GLN:HB2	1.78	0.63
1:C:686:GLN:CD	1:C:727:LYS:HG3	2.19	0.63
1:C:465:SER:O	1:C:516:GLY:N	2.30	0.63
1:C:513:LEU:CD2	1:C:613:ASN:ND2	2.62	0.63
1:B:145:TYR:CE2	1:B:652:LEU:CD2	2.82	0.63
1:A:297:VAL:HG11	1:C:4:ASN:ND2	2.13	0.63
1:B:234:LEU:HA	1:B:237:ILE:HD12	1.80	0.63
1:A:463:THR:OG1	1:A:513:LEU:CD2	2.36	0.63
1:A:465:SER:HB2	1:A:489:LEU:HD11	1.80	0.63
2:H:65:LEU:CD2	2:H:223:LEU:HD13	2.23	0.63
1:A:341:LYS:HB2	1:A:722:TYR:HH	1.62	0.63
1:A:319:LEU:HB3	1:A:330:VAL:H	1.64	0.63
1:C:239:ALA:HA	1:C:452:VAL:HG12	1.80	0.63
1:A:307:PRO:HG2	1:A:310:HIS:HB2	1.81	0.63
1:D:441:GLU:HG2	1:D:620:MET:CB	2.29	0.63
1:B:232:ASP:CG	1:B:262:ARG:HB3	2.19	0.63
1:D:153:GLY:O	1:D:160:ARG:NH2	2.31	0.63
1:D:155:TYR:HE2	1:D:212:MET:CE	2.12	0.63
1:D:172:LEU:CD2	1:D:216:ARG:NH1	2.61	0.63
2:E:205:ALA:HB2	2:E:242:LEU:HD13	1.79	0.63
1:D:560:LYS:CE	1:D:609:HIS:ND1	2.62	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:62:TYR:O	2:F:70:LYS:HE2	1.99	0.63
1:A:522:TYR:CE1	1:A:662:LEU:HD11	2.34	0.63
1:B:318:VAL:CG2	1:B:329:ARG:CZ	2.62	0.63
1:D:686:GLN:CD	1:D:727:LYS:HG3	2.20	0.63
2:E:65:LEU:O	2:E:70:LYS:HG3	1.98	0.63
2:G:13:LEU:O	2:G:32:LYS:HD2	1.98	0.63
2:E:173:GLY:O	2:E:175:HIS:NE2	2.31	0.63
1:C:250:GLN:HE22	1:C:499:PRO:HG3	1.63	0.63
2:H:6:SER:OG	2:H:21:GLN:NE2	2.27	0.63
2:F:82:LEU:HD13	2:F:140:ILE:HG22	1.79	0.63
2:H:273:TYR:OH	2:H:324:PRO:HB3	1.99	0.62
1:A:474:ASN:ND2	1:A:476:ASP:HB2	2.14	0.62
1:B:558:LEU:HD12	1:B:561:GLU:HB3	1.81	0.62
1:D:155:TYR:HE1	1:D:209:THR:HG23	1.64	0.62
1:A:5:LEU:CD1	1:A:17:ILE:CG1	2.38	0.62
1:A:176:VAL:HG13	1:A:215:VAL:HG11	1.81	0.62
1:A:305:PHE:CE1	1:A:436:SER:O	2.53	0.62
1:C:361:VAL:HG11	1:C:364:LEU:CB	2.29	0.62
2:F:206:ILE:CD1	2:F:315:ARG:HG2	2.30	0.62
1:A:686:GLN:NE2	1:A:727:LYS:HE3	2.15	0.62
1:A:226:VAL:HG21	1:A:247:TYR:CD2	2.35	0.62
1:C:238:ASN:OD1	1:D:242:SER:HA	1.99	0.62
2:H:195:LEU:HD13	2:H:271:GLU:HG2	1.82	0.62
1:C:157:VAL:HG21	1:C:216:ARG:HH11	1.65	0.62
1:B:155:TYR:CD1	1:B:212:MET:HB2	2.31	0.62
1:A:232:ASP:OD2	1:A:262:ARG:NH2	2.31	0.62
2:F:239:ALA:HB2	2:F:342:ASP:OD2	1.99	0.62
1:A:227:LEU:HD11	1:A:437:ASN:HB3	1.81	0.62
1:D:234:LEU:HA	1:D:237:ILE:HD12	1.82	0.62
1:C:305:PHE:CZ	1:C:436:SER:O	2.52	0.62
1:B:305:PHE:CZ	1:B:436:SER:O	2.52	0.62
2:F:99:ILE:HD11	2:F:108:VAL:HG21	1.79	0.62
1:D:25:VAL:HG21	3:D:801:ATP:H3'	1.82	0.62
1:B:209:THR:HB	1:B:210:PRO:HD3	1.82	0.62
1:B:375:PHE:O	1:B:379:TYR:HB2	1.98	0.62
1:C:474:ASN:ND2	1:C:476:ASP:HB2	2.15	0.62
1:A:167:GLU:OE1	1:A:172:LEU:CB	2.47	0.62
1:B:317:LEU:HD11	1:B:402:MET:CA	2.28	0.62
2:H:62:TYR:O	2:H:70:LYS:HE2	1.99	0.62
2:F:12:GLN:OE1	2:F:27:ARG:HD3	1.99	0.62
2:G:90:SER:HB2	2:G:91:PRO:HD3	1.81	0.62
1:D:341:LYS:HB2	1:D:722:TYR:OH	2.00	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:278:CYS:HB3	1:B:282:TYR:CE1	2.35	0.62
1:A:227:LEU:CG	1:A:435:GLN:NE2	2.62	0.62
2:H:65:LEU:O	2:H:70:LYS:HG3	1.99	0.62
1:D:428:PRO:O	1:D:432:PRO:HB3	2.00	0.62
2:F:201:ASN:O	2:F:205:ALA:CB	2.47	0.62
1:C:330:VAL:HB	1:C:335:TYR:OH	1.99	0.62
1:C:522:TYR:HE1	1:C:662:LEU:HD11	1.63	0.62
1:C:227:LEU:HD11	1:C:437:ASN:HB3	1.81	0.62
1:C:569:ASN:HD22	1:C:570:GLU:N	1.96	0.62
1:A:234:LEU:HA	1:A:237:ILE:HD12	1.82	0.62
1:D:79:TYR:O	1:D:83:ARG:HG2	1.98	0.62
1:B:474:ASN:ND2	1:B:476:ASP:HB2	2.15	0.62
1:D:227:LEU:HB2	1:D:460:ALA:HB3	1.81	0.62
1:D:286:GLN:NE2	1:D:332:HIS:ND1	2.48	0.62
1:A:647:SER:O	1:A:650:GLY:N	2.33	0.62
1:C:560:LYS:CD	1:C:609:HIS:CE1	2.83	0.62
2:F:312:THR:HB	2:F:325:PHE:HD2	1.62	0.62
1:A:406:ARG:HH11	1:A:732:GLN:HG3	1.64	0.62
1:C:167:GLU:OE2	1:C:172:LEU:CD1	2.43	0.61
1:B:701:PRO:HD2	1:B:735:ARG:CG	2.25	0.61
1:B:702:SER:HB3	1:B:735:ARG:HD3	1.81	0.61
2:G:236:ARG:HG3	2:G:340:VAL:HG23	1.82	0.61
1:B:232:ASP:OD2	1:B:262:ARG:HB3	2.00	0.61
1:C:307:PRO:HG2	1:C:310:HIS:HB2	1.79	0.61
1:C:302:ALA:N	1:C:438:LEU:HD21	2.15	0.61
1:A:228:ILE:HG21	1:A:240:THR:HG23	1.81	0.61
1:B:369:PHE:CE1	1:B:434:ARG:CA	2.83	0.61
1:A:440:LEU:HD12	1:A:728:THR:CB	2.30	0.61
1:A:716:LYS:HG2	2:F:370:LEU:HD21	1.82	0.61
1:B:62:ILE:HD12	1:B:84:LEU:HD22	1.82	0.61
1:C:59:HIS:HB2	3:C:801:ATP:C5'	2.30	0.61
1:C:686:GLN:NE2	1:C:727:LYS:HE3	2.14	0.61
1:D:50:TYR:CD2	1:D:53:ILE:HD12	2.35	0.61
2:F:330:ASN:OD1	2:F:331:PRO:HD2	2.00	0.61
1:C:114:LYS:HG3	1:C:166:TYR:CE2	2.35	0.61
1:D:157:VAL:N	1:D:167:GLU:HG2	2.14	0.61
1:B:513:LEU:CD1	1:B:613:ASN:ND2	2.63	0.61
1:A:617:SER:O	1:A:691:GLN:HG2	1.99	0.61
2:H:55:VAL:HG21	2:H:128:ASN:CG	2.18	0.61
2:F:339:LEU:O	2:F:340:VAL:HG23	2.00	0.61
2:E:307:TYR:O	2:E:311:ILE:HG22	1.99	0.61
1:D:150:GLN:HE22	1:D:645:LYS:NZ	1.99	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:320:LYS:CE	1:C:333:MET:O	2.46	0.61
1:A:250:GLN:HE22	1:A:499:PRO:HG3	1.65	0.61
1:A:50:TYR:O	1:A:53:ILE:HB	2.00	0.61
1:A:49:PHE:HD1	1:A:53:ILE:HD13	1.65	0.61
1:B:82:ALA:O	1:B:86:ILE:HG12	1.99	0.61
1:C:375:PHE:O	1:C:379:TYR:HB2	2.00	0.61
1:D:158:GLN:HB3	1:D:165:ILE:CD1	2.30	0.61
1:D:465:SER:HB2	1:D:489:LEU:CD1	2.30	0.61
1:C:686:GLN:HA	1:C:689:ILE:HG13	1.83	0.61
1:A:569:ASN:HD22	1:A:570:GLU:N	1.97	0.61
1:C:305:PHE:CE2	1:C:436:SER:HB3	2.36	0.61
1:C:521:ALA:HB3	1:C:632:THR:HG21	1.82	0.61
1:B:663:HIS:ND1	1:B:663:HIS:N	2.47	0.61
1:D:114:LYS:CD	1:D:114:LYS:N	2.57	0.61
1:A:211:ILE:O	1:A:215:VAL:HG23	2.00	0.61
1:A:428:PRO:O	1:A:432:PRO:HB3	2.01	0.61
2:G:12:GLN:NE2	2:G:23:VAL:HG13	2.15	0.61
2:E:177:VAL:CB	2:E:180:LYS:O	2.49	0.61
1:D:290:LYS:NZ	1:D:300:GLY:O	2.30	0.61
2:H:232:ARG:HH11	2:H:343:ASN:N	1.99	0.61
1:B:569:ASN:HD22	1:B:570:GLU:N	1.98	0.61
1:C:227:LEU:HB2	1:C:460:ALA:HB3	1.82	0.61
2:H:99:ILE:HD11	2:H:108:VAL:HG21	1.83	0.61
1:A:150:GLN:O	1:A:154:LYS:HB2	2.00	0.61
1:D:696:ASN:H	1:D:696:ASN:ND2	1.99	0.61
1:B:262:ARG:NH1	1:B:267:PRO:O	2.33	0.61
1:A:209:THR:HB	1:A:210:PRO:HD3	1.83	0.61
1:D:511:ARG:HD3	1:D:612:ARG:O	2.01	0.61
2:H:310:TYR:CD2	2:H:330:ASN:OD1	2.54	0.61
1:A:225:CYS:CB	1:A:253:GLY:O	2.41	0.61
1:A:361:VAL:HG11	1:A:364:LEU:CG	2.31	0.61
1:D:59:HIS:O	1:D:62:ILE:HG12	2.01	0.61
2:G:62:TYR:O	2:G:70:LYS:HE2	2.01	0.61
1:C:711:MET:HG2	2:E:365:VAL:HG22	1.81	0.61
2:G:195:LEU:HD13	2:G:271:GLU:HG2	1.81	0.61
1:C:621:PRO:CD	1:C:694:SER:CB	2.79	0.60
1:A:305:PHE:CZ	1:A:436:SER:O	2.54	0.60
1:D:6:LEU:CB	1:D:51:ASP:OD1	2.44	0.60
1:A:361:VAL:HG11	1:A:364:LEU:HB2	1.81	0.60
1:D:522:TYR:CE1	1:D:662:LEU:HD11	2.36	0.60
1:B:428:PRO:O	1:B:432:PRO:HB3	2.01	0.60
2:E:89:ARG:HG2	2:E:90:SER:N	2.16	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:474:ASN:ND2	1:D:476:ASP:HB2	2.16	0.60
1:A:172:LEU:HD21	1:A:216:ARG:HH12	1.65	0.60
1:C:332:HIS:O	1:C:333:MET:CG	2.49	0.60
1:C:234:LEU:HA	1:C:237:ILE:HD12	1.83	0.60
2:H:20:GLY:CA	2:H:100:SER:HB3	2.31	0.60
1:A:375:PHE:O	1:A:379:TYR:HB2	2.01	0.60
1:B:587:LEU:HD23	1:B:590:ILE:HD11	1.84	0.60
1:D:623:GLU:HG2	1:D:633:ASN:HD21	1.63	0.60
1:C:515:ILE:HD13	1:C:551:LEU:HD22	1.82	0.60
1:D:39:SER:CB	2:G:332:ILE:CG2	2.74	0.60
1:A:567:TRP:O	1:A:569:ASN:ND2	2.34	0.60
1:A:82:ALA:O	1:A:86:ILE:HG12	2.02	0.60
2:E:104:LEU:O	2:E:108:VAL:HG23	2.02	0.60
1:D:696:ASN:N	1:D:696:ASN:HD22	1.99	0.60
1:D:521:ALA:HB3	1:D:632:THR:HG21	1.84	0.60
2:E:195:LEU:HD13	2:E:271:GLU:HG2	1.83	0.60
1:B:316:LEU:HA	1:B:319:LEU:HD11	1.83	0.60
1:A:208:PRO:CG	1:A:211:ILE:CD1	2.64	0.60
2:F:205:ALA:HB1	2:F:315:ARG:CD	2.31	0.60
1:D:330:VAL:HB	1:D:335:TYR:OH	2.01	0.60
1:A:369:PHE:CE2	1:A:434:ARG:CD	2.80	0.60
1:D:5:LEU:HD12	1:D:17:ILE:CG1	2.31	0.60
2:H:207:ARG:HH22	2:H:282:GLN:CD	2.04	0.60
1:C:17:ILE:HD12	3:C:801:ATP:N1	2.15	0.60
2:E:206:ILE:HD13	2:E:312:THR:CB	2.32	0.60
1:A:293:SER:HB2	1:A:298:ARG:O	2.01	0.60
1:C:714:LEU:HD22	1:C:732:GLN:HE22	1.67	0.60
1:B:319:LEU:HA	1:B:329:ARG:HG2	1.84	0.60
1:B:283:LYS:HG2	1:B:330:VAL:HG22	1.82	0.60
1:D:253:GLY:C	1:D:438:LEU:HD12	2.21	0.60
2:E:74:ILE:O	2:E:78:LYS:HG3	2.01	0.60
1:C:716:LYS:CG	2:E:370:LEU:HD22	2.32	0.60
1:D:560:LYS:HD3	1:D:609:HIS:ND1	2.17	0.60
1:A:663:HIS:N	1:A:663:HIS:ND1	2.39	0.60
1:C:155:TYR:CZ	1:C:628:ILE:HD12	2.37	0.60
1:B:282:TYR:CD2	1:B:304:LEU:CD2	2.84	0.60
2:H:91:PRO:O	2:H:95:LEU:HG	2.01	0.60
2:H:205:ALA:HB1	2:H:315:ARG:CD	2.32	0.60
1:D:82:ALA:O	1:D:86:ILE:HG12	2.02	0.60
1:C:167:GLU:HG2	1:C:168:SER:N	2.17	0.59
1:A:278:CYS:HB3	1:A:282:TYR:CE1	2.37	0.59
1:D:686:GLN:NE2	1:D:727:LYS:HE3	2.16	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:39:SER:CB	2:E:332:ILE:HG22	2.31	0.59
1:B:587:LEU:O	1:B:589:THR:N	2.34	0.59
1:A:521:ALA:HB3	1:A:632:THR:HG21	1.83	0.59
2:E:5:PHE:HE2	2:E:7:GLN:NE2	2.00	0.59
1:D:305:PHE:CZ	1:D:436:SER:O	2.54	0.59
1:D:209:THR:HB	1:D:210:PRO:HD3	1.83	0.59
2:E:99:ILE:HD11	2:E:108:VAL:HG21	1.83	0.59
1:B:656:VAL:O	1:B:657:PRO:C	2.40	0.59
2:E:12:GLN:NE2	2:E:23:VAL:HG13	2.17	0.59
2:H:104:LEU:O	2:H:108:VAL:HG23	2.02	0.59
1:D:147:ALA:HB2	1:D:627:GLN:O	2.02	0.59
1:B:228:ILE:HG21	1:B:240:THR:HG23	1.83	0.59
1:A:449:LEU:HD21	1:A:502:ALA:CB	2.33	0.59
1:D:6:LEU:HD12	1:D:51:ASP:OD1	2.02	0.59
1:A:22:ILE:O	1:A:26:LEU:HG	2.02	0.59
1:A:569:ASN:ND2	1:A:570:GLU:H	2.00	0.59
1:B:305:PHE:CE1	1:B:436:SER:O	2.55	0.59
2:E:167:TRP:NE1	2:E:172:GLU:OE2	2.34	0.59
1:C:207:LEU:N	1:C:207:LEU:HD23	2.17	0.59
1:B:286:GLN:NE2	1:B:332:HIS:ND1	2.50	0.59
2:G:205:ALA:HB1	2:G:315:ARG:CD	2.32	0.59
1:D:656:VAL:O	1:D:657:PRO:C	2.39	0.59
1:C:82:ALA:O	1:C:86:ILE:HG12	2.01	0.59
1:D:708:LYS:O	1:D:710:PRO:HD3	2.03	0.59
1:B:617:SER:O	1:B:691:GLN:HG3	2.03	0.59
1:A:303:THR:OG1	1:A:438:LEU:HD12	2.02	0.59
1:D:595:LEU:HD22	1:D:599:TRP:NE1	2.18	0.59
1:D:689:ILE:HG22	1:D:691:GLN:O	2.03	0.59
1:D:711:MET:CB	2:G:363:SER:CB	2.75	0.59
2:G:99:ILE:HD11	2:G:108:VAL:HG21	1.84	0.59
1:D:703:ARG:CG	1:D:703:ARG:O	2.51	0.59
1:B:262:ARG:HG2	1:B:275:HIS:CE1	2.38	0.59
1:C:216:ARG:CG	1:C:216:ARG:O	2.51	0.59
1:A:425:PRO:CG	1:A:690:ASP:HB3	2.27	0.59
1:C:59:HIS:O	1:C:62:ILE:HG12	2.03	0.59
1:D:361:VAL:CG1	1:D:364:LEU:HB2	2.33	0.59
1:B:414:ILE:HB	1:B:729:LEU:HD12	1.83	0.59
1:D:685:MET:O	1:D:689:ILE:CG1	2.44	0.59
1:D:5:LEU:HB2	1:D:17:ILE:CG1	2.32	0.59
2:G:206:ILE:CD1	2:G:315:ARG:HG2	2.32	0.59
1:D:207:LEU:HD23	1:D:207:LEU:N	2.18	0.59
2:F:38:LYS:CD	2:F:344:VAL:HG12	2.25	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:149:ARG:NH1	2:G:286:TRP:HB2	2.13	0.59
2:H:12:GLN:NE2	2:H:23:VAL:HG13	2.15	0.59
1:A:716:LYS:HA	2:F:370:LEU:HD11	1.84	0.59
2:E:193:LEU:O	2:E:197:LEU:HG	2.02	0.59
1:A:316:LEU:HA	1:A:319:LEU:HD11	1.85	0.59
2:G:20:GLY:CA	2:G:100:SER:HB3	2.33	0.59
1:B:37:SER:OG	2:H:331:PRO:O	2.20	0.59
1:C:670:TRP:CE2	1:C:735:ARG:HG3	2.38	0.59
2:G:334:TRP:O	2:G:335:ILE:C	2.42	0.59
1:C:569:ASN:ND2	1:C:570:GLU:H	1.98	0.59
1:C:696:ASN:H	1:C:696:ASN:ND2	2.00	0.59
2:E:147:GLN:O	2:E:150:ALA:HB3	2.03	0.59
1:A:6:LEU:HD11	1:C:298:ARG:CD	2.32	0.58
1:C:417:VAL:HG23	1:C:418:ASP:N	2.18	0.58
1:C:44:ARG:CA	1:C:44:ARG:HE	2.07	0.58
1:D:43:LEU:HD12	2:G:334:TRP:NE1	2.18	0.58
2:H:193:LEU:O	2:H:197:LEU:HG	2.03	0.58
1:C:619:LEU:HB2	1:C:693:ILE:HG22	1.85	0.58
1:C:529:LYS:HB3	1:C:536:ALA:HB2	1.84	0.58
2:F:73:PHE:HB2	2:F:218:PHE:CE2	2.38	0.58
1:D:617:SER:HB2	1:D:690:ASP:N	2.04	0.58
1:D:50:TYR:H	1:D:50:TYR:HD2	1.50	0.58
2:F:74:ILE:O	2:F:78:LYS:HG3	2.03	0.58
2:G:193:LEU:O	2:G:197:LEU:HG	2.03	0.58
2:H:6:SER:CB	2:H:21:GLN:HE21	2.16	0.58
1:D:305:PHE:CE1	1:D:436:SER:O	2.56	0.58
1:A:417:VAL:HG23	1:A:418:ASP:N	2.18	0.58
1:B:595:LEU:HD22	1:B:599:TRP:NE1	2.18	0.58
1:C:34:HIS:O	1:C:35:ASN:HB2	2.03	0.58
2:F:115:GLU:OE1	2:F:115:GLU:HA	2.03	0.58
2:H:55:VAL:CG2	2:H:128:ASN:CG	2.71	0.58
2:F:104:LEU:O	2:F:108:VAL:HG23	2.02	0.58
1:B:567:TRP:O	1:B:569:ASN:ND2	2.36	0.58
1:B:86:ILE:HG21	1:B:140:ASP:HB3	1.85	0.58
1:D:592:ASN:O	1:D:594:PRO:HD3	2.04	0.58
1:B:712:GLN:NE2	2:H:369:ASP:HB3	2.18	0.58
1:B:286:GLN:NE2	1:B:332:HIS:CG	2.71	0.58
1:B:521:ALA:HB3	1:B:632:THR:HG21	1.84	0.58
1:C:449:LEU:HD21	1:C:502:ALA:CB	2.33	0.58
2:E:167:TRP:CD1	2:E:172:GLU:OE2	2.57	0.58
1:B:276:THR:HG23	1:B:280:PRO:HG2	1.84	0.58
1:A:621:PRO:HD3	1:A:694:SER:CB	2.33	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:20:GLY:HA3	2:E:100:SER:HB3	1.85	0.58
1:B:511:ARG:HD3	1:B:612:ARG:O	2.03	0.58
1:D:597:TYR:O	1:D:598:ASP:C	2.41	0.58
1:B:592:ASN:O	1:B:594:PRO:HD3	2.03	0.58
2:F:195:LEU:HD13	2:F:271:GLU:HG2	1.84	0.58
1:A:227:LEU:CB	1:A:435:GLN:HE22	2.08	0.58
1:A:511:ARG:HD3	1:A:612:ARG:O	2.03	0.58
2:F:83:LEU:HD22	2:F:203:LEU:HG	1.85	0.58
2:H:309:GLU:HG2	2:H:325:PHE:CE1	2.38	0.58
1:D:692:SER:HB2	1:D:727:LYS:HB2	1.86	0.58
2:H:62:TYR:HB2	2:H:224:MET:HE1	1.86	0.58
2:G:74:ILE:O	2:G:78:LYS:HG3	2.04	0.58
1:A:176:VAL:HA	1:A:215:VAL:HG11	1.84	0.58
2:H:329:SER:O	2:H:330:ASN:C	2.40	0.58
1:D:329:ARG:CD	1:D:331:ARG:NH2	2.53	0.58
2:F:94:ALA:C	2:F:95:LEU:HD23	2.24	0.58
1:A:621:PRO:HD3	1:A:694:SER:HB2	1.86	0.58
1:B:10:ARG:H	1:B:55:THR:CG2	2.16	0.58
1:A:474:ASN:HD21	1:A:476:ASP:HB2	1.69	0.58
1:C:474:ASN:HD21	1:C:476:ASP:HB2	1.69	0.58
1:D:564:ALA:HA	1:D:611:LEU:O	2.03	0.58
1:B:412:ILE:HD12	1:B:412:ILE:N	2.19	0.58
2:H:336:ASN:O	2:H:340:VAL:HG23	2.03	0.58
1:B:440:LEU:HD12	1:B:728:THR:CB	2.33	0.58
1:C:545:GLU:HG3	1:C:595:LEU:CD2	2.33	0.58
1:A:513:LEU:O	1:A:615:THR:O	2.22	0.58
2:H:364:GLU:HA	2:H:364:GLU:OE1	2.04	0.58
2:F:92:ASN:O	2:F:96:LEU:HB2	2.04	0.58
1:A:22:ILE:HD12	1:A:22:ILE:H	1.68	0.58
1:A:10:ARG:H	1:A:55:THR:CG2	2.16	0.58
1:B:696:ASN:H	1:B:696:ASN:ND2	2.01	0.58
2:E:20:GLY:O	2:E:21:GLN:C	2.43	0.58
1:D:286:GLN:O	1:D:289:VAL:HG22	2.03	0.57
1:D:150:GLN:OE1	1:D:154:LYS:CE	2.52	0.57
1:B:10:ARG:CG	1:B:56:SER:HB2	2.34	0.57
1:C:435:GLN:CD	1:C:446:THR:HG21	2.24	0.57
2:E:273:TYR:O	2:E:277:VAL:HG23	2.04	0.57
2:E:191:LYS:HG2	2:E:264:ILE:HG23	1.87	0.57
1:C:522:TYR:CE1	1:C:662:LEU:HD11	2.39	0.57
1:D:406:ARG:HH11	1:D:697:THR:CG2	2.17	0.57
1:C:515:ILE:CD1	1:C:551:LEU:HD22	2.34	0.57
1:D:441:GLU:HG2	1:D:620:MET:HB3	1.86	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:191:LYS:HG2	2:G:264:ILE:HG23	1.86	0.57
1:B:245:VAL:O	1:B:249:SER:HB3	2.04	0.57
1:A:167:GLU:OE2	1:A:216:ARG:NH2	2.36	0.57
2:H:328:ARG:NH1	2:H:328:ARG:HB3	2.20	0.57
2:F:20:GLY:CA	2:F:100:SER:HB3	2.34	0.57
1:C:560:LYS:CE	1:C:609:HIS:CE1	2.87	0.57
1:B:59:HIS:O	1:B:62:ILE:HG12	2.04	0.57
2:E:334:TRP:O	2:E:335:ILE:C	2.43	0.57
1:A:520:PHE:CE2	1:A:524:LEU:HD11	2.39	0.57
1:A:86:ILE:HG21	1:A:140:ASP:HB3	1.85	0.57
1:D:207:LEU:CG	1:D:212:MET:SD	2.92	0.57
1:B:515:ILE:HB	1:B:616:LEU:O	2.05	0.57
1:C:260:ARG:HD3	1:C:365:TYR:CE2	2.39	0.57
2:G:331:PRO:C	2:G:333:PRO:HD3	2.25	0.57
1:A:696:ASN:H	1:A:696:ASN:ND2	2.02	0.57
1:A:414:ILE:HB	1:A:729:LEU:HD12	1.86	0.57
1:D:361:VAL:CG1	1:D:382:TYR:CE2	2.87	0.57
2:E:83:LEU:HD22	2:E:203:LEU:HG	1.86	0.57
2:H:230:ILE:O	2:H:234:ILE:HG12	2.04	0.57
1:D:152:GLU:HA	1:D:156:LEU:HD12	1.86	0.57
1:C:317:LEU:HD13	1:C:401:LEU:CG	2.34	0.57
1:D:62:ILE:HD12	1:D:84:LEU:HD22	1.86	0.57
1:B:309:TRP:CH2	1:B:364:LEU:HD12	2.39	0.57
1:B:413:TYR:HB3	1:B:729:LEU:O	2.04	0.57
1:A:576:GLY:HA3	1:A:607:LYS:HE2	1.87	0.57
2:F:230:ILE:O	2:F:234:ILE:HG12	2.05	0.57
2:G:132:ASP:OD2	2:G:135:VAL:HG13	2.05	0.57
1:B:207:LEU:N	1:B:207:LEU:HD23	2.19	0.57
1:D:316:LEU:CA	1:D:319:LEU:HD11	2.35	0.57
1:D:329:ARG:HB3	1:D:331:ARG:HE	1.70	0.57
1:C:513:LEU:CD1	1:C:616:LEU:HA	2.33	0.57
1:A:696:ASN:HD22	1:A:696:ASN:N	2.01	0.57
1:D:447:LYS:HB2	1:D:458:GLU:N	2.19	0.57
1:B:268:ILE:O	1:B:269:ARG:HB3	2.05	0.57
1:D:576:GLY:HA3	1:D:607:LYS:HE2	1.87	0.57
1:B:318:VAL:HG23	1:B:329:ARG:NH2	2.18	0.57
1:C:286:GLN:O	1:C:289:VAL:HG22	2.04	0.57
2:F:277:VAL:HG22	2:F:324:PRO:HB3	1.86	0.57
2:H:206:ILE:O	2:H:210:VAL:CG2	2.51	0.57
1:A:268:ILE:O	1:A:269:ARG:HB3	2.05	0.57
1:B:520:PHE:HB3	1:B:635:ILE:HA	1.87	0.57
1:D:86:ILE:HG21	1:D:140:ASP:HB3	1.87	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:276:THR:HG23	1:D:280:PRO:HG2	1.87	0.57
1:C:174:ILE:HG23	1:C:175:LEU:N	2.20	0.57
1:C:155:TYR:CD1	1:C:212:MET:HB2	2.35	0.57
1:A:317:LEU:CD1	1:A:401:LEU:HD23	2.16	0.57
1:A:435:GLN:HG2	1:A:436:SER:N	2.19	0.57
2:E:331:PRO:C	2:E:333:PRO:HD3	2.25	0.57
2:E:148:LYS:HG2	2:E:149:ARG:N	2.19	0.57
2:H:96:LEU:HA	2:H:99:ILE:HD12	1.86	0.57
1:D:268:ILE:O	1:D:269:ARG:HB3	2.05	0.57
2:F:72:ILE:HG23	2:F:290:LEU:HD23	1.87	0.57
1:C:10:ARG:CG	1:C:56:SER:HB2	2.35	0.57
1:D:254:ILE:H	1:D:438:LEU:HD11	1.64	0.57
1:C:369:PHE:CD2	1:C:434:ARG:CD	2.88	0.57
2:F:329:SER:O	2:F:330:ASN:C	2.40	0.57
1:C:511:ARG:HD3	1:C:612:ARG:O	2.05	0.57
2:E:132:ASP:OD2	2:E:135:VAL:HG13	2.05	0.57
1:B:515:ILE:HD13	1:B:551:LEU:CD1	2.35	0.56
1:A:6:LEU:O	1:A:7:VAL:CG2	2.52	0.56
1:B:316:LEU:O	1:B:319:LEU:HD12	2.05	0.56
1:A:615:THR:CG2	1:A:691:GLN:HE22	2.14	0.56
1:B:131:MET:HE3	1:B:193:VAL:HG11	1.87	0.56
2:G:273:TYR:O	2:G:277:VAL:HG23	2.05	0.56
1:D:294:GLN:CG	1:D:298:ARG:HG3	2.34	0.56
1:D:282:TYR:CD2	1:D:304:LEU:HD13	2.40	0.56
1:D:150:GLN:CB	1:D:154:LYS:CD	2.82	0.56
1:D:309:TRP:CZ2	1:D:364:LEU:CD1	2.88	0.56
2:G:83:LEU:HD22	2:G:203:LEU:HG	1.87	0.56
2:G:15:GLU:OE1	2:G:20:GLY:HA3	2.05	0.56
1:D:176:VAL:HG13	1:D:215:VAL:HG21	1.87	0.56
1:C:369:PHE:CE2	1:C:434:ARG:CG	2.88	0.56
1:A:712:GLN:HE21	2:F:370:LEU:CD2	2.15	0.56
1:B:10:ARG:NH2	3:B:801:ATP:O2A	2.34	0.56
2:E:328:ARG:HB3	2:E:328:ARG:NH1	2.20	0.56
1:A:182:SER:O	1:A:189:ARG:CZ	2.53	0.56
2:G:111:TRP:O	2:G:111:TRP:HD1	1.88	0.56
1:B:156:LEU:HD22	1:B:167:GLU:HG2	1.87	0.56
1:B:444:LEU:HD22	1:B:512:THR:HG21	1.87	0.56
2:F:42:LYS:HG3	2:F:344:VAL:HG23	1.87	0.56
1:C:10:ARG:H	1:C:55:THR:CG2	2.18	0.56
1:D:303:THR:HA	1:D:334:ASP:O	2.05	0.56
1:D:711:MET:N	2:G:363:SER:CB	2.59	0.56
2:H:74:ILE:O	2:H:78:LYS:HG3	2.04	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:369:PHE:CZ	1:A:434:ARG:CB	2.88	0.56
2:H:149:ARG:NH1	2:H:286:TRP:HB2	2.14	0.56
1:B:522:TYR:CD1	1:B:662:LEU:HD11	2.39	0.56
1:D:50:TYR:HE2	1:D:53:ILE:HD12	1.64	0.56
1:C:560:LYS:CD	1:C:609:HIS:ND1	2.68	0.56
1:B:625:SER:O	1:B:628:ILE:CG2	2.52	0.56
2:E:295:SER:OG	2:E:300:ASN:HB3	2.05	0.56
1:A:190:LEU:H	1:A:190:LEU:HD22	1.71	0.56
1:C:527:HIS:O	1:C:529:LYS:HD2	2.05	0.56
1:B:417:VAL:HG23	1:B:418:ASP:N	2.20	0.56
1:D:68:ASP:OD2	1:D:651:ILE:HG21	2.05	0.56
2:G:310:TYR:CE2	2:G:330:ASN:HB2	2.39	0.56
2:H:72:ILE:HG23	2:H:290:LEU:HD23	1.87	0.56
1:D:464:LEU:HD22	1:D:514:GLY:CA	2.35	0.56
2:H:309:GLU:OE2	2:H:325:PHE:HD1	1.89	0.56
1:A:459:ILE:HD11	1:A:502:ALA:HB3	1.86	0.56
1:D:5:LEU:CD1	1:D:17:ILE:HG12	2.34	0.56
1:D:55:THR:HA	1:D:58:ILE:CD1	2.35	0.56
2:F:191:LYS:HG2	2:F:264:ILE:HG23	1.87	0.56
2:E:207:ARG:HH22	2:E:282:GLN:CD	2.09	0.56
2:F:111:TRP:HZ2	2:F:204:GLU:OE2	1.89	0.56
1:D:474:ASN:HD21	1:D:476:ASP:HB2	1.70	0.56
1:C:592:ASN:O	1:C:594:PRO:HD3	2.05	0.56
1:A:668:LEU:HB2	1:A:671:GLU:HG3	1.87	0.56
1:C:222:PHE:HE2	1:C:495:TYR:CD2	2.24	0.56
2:G:104:LEU:O	2:G:108:VAL:HG23	2.04	0.56
1:D:222:PHE:HB2	1:D:492:LEU:HD21	1.86	0.56
1:A:59:HIS:O	1:A:62:ILE:HG12	2.06	0.56
1:C:230:CYS:SG	1:C:237:ILE:HA	2.46	0.56
1:C:440:LEU:HD12	1:C:728:THR:CB	2.34	0.56
1:C:576:GLY:HA3	1:C:607:LYS:HE2	1.87	0.56
1:B:669:LEU:HD11	1:B:698:ASN:ND2	2.21	0.56
1:A:592:ASN:O	1:A:594:PRO:HD3	2.04	0.56
1:C:115:TYR:CD1	1:C:216:ARG:CD	2.88	0.56
1:C:131:MET:HE3	1:C:193:VAL:HG11	1.86	0.56
1:D:74:ALA:HB1	1:D:77:TYR:HD2	1.70	0.56
1:D:154:LYS:HE2	1:D:624:THR:HG22	1.87	0.56
2:F:295:SER:OG	2:F:300:ASN:HB3	2.05	0.56
1:C:228:ILE:HG21	1:C:240:THR:HG23	1.87	0.56
2:H:96:LEU:HA	2:H:99:ILE:CD1	2.35	0.56
2:H:197:LEU:HD13	2:H:249:LEU:HG	1.87	0.56
1:C:242:SER:HA	1:D:238:ASN:OD1	2.06	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:310:TYR:CE2	2:H:330:ASN:CG	2.79	0.56
1:A:10:ARG:CG	1:A:56:SER:HB2	2.35	0.56
2:H:191:LYS:HG2	2:H:264:ILE:HG23	1.87	0.56
1:D:414:ILE:HB	1:D:729:LEU:HD12	1.88	0.56
2:H:5:PHE:CE1	2:H:24:ASN:O	2.59	0.56
1:D:190:LEU:HD22	1:D:190:LEU:H	1.70	0.56
1:D:147:ALA:CB	1:D:628:ILE:HA	2.36	0.56
1:C:317:LEU:CD1	1:C:401:LEU:CG	2.84	0.56
1:D:10:ARG:CG	1:D:56:SER:HB2	2.36	0.56
1:C:560:LYS:CE	1:C:609:HIS:ND1	2.69	0.56
1:C:268:ILE:O	1:C:269:ARG:HB3	2.05	0.56
1:B:449:LEU:HG	1:B:457:GLY:HA3	1.87	0.56
1:A:29:ALA:HB1	1:A:80:LEU:HD12	1.88	0.56
2:G:192:LYS:HE3	2:G:192:LYS:O	2.06	0.56
1:B:114:LYS:CE	1:B:166:TYR:HE2	1.91	0.56
1:B:316:LEU:O	1:B:319:LEU:HG	2.06	0.56
1:C:22:ILE:HD11	3:C:801:ATP:N3	2.21	0.56
1:C:254:ILE:CG2	1:C:256:ILE:HD11	2.36	0.56
1:D:228:ILE:HG21	1:D:240:THR:HG23	1.87	0.56
2:G:334:TRP:O	2:G:336:ASN:N	2.38	0.56
1:A:217:THR:HB	1:A:218:PRO:HD2	1.88	0.56
2:E:96:LEU:HA	2:E:99:ILE:CD1	2.36	0.56
2:F:111:TRP:CZ2	2:F:204:GLU:OE2	2.59	0.56
2:F:193:LEU:O	2:F:197:LEU:HG	2.05	0.56
2:G:230:ILE:O	2:G:234:ILE:HG12	2.06	0.56
1:A:618:ALA:O	1:A:619:LEU:HD23	2.06	0.56
2:F:273:TYR:O	2:F:277:VAL:HG23	2.05	0.56
1:C:247:TYR:CE1	1:C:499:PRO:HD2	2.41	0.56
2:H:132:ASP:OD2	2:H:135:VAL:HG13	2.06	0.56
1:A:538:ASN:ND2	1:A:593:GLU:HB2	2.20	0.56
2:G:6:SER:OG	2:G:24:ASN:HB3	2.06	0.56
2:E:31:GLN:N	2:E:31:GLN:CD	2.60	0.56
2:G:125:ILE:O	2:G:129:ILE:HG12	2.06	0.56
1:D:115:TYR:CE1	1:D:216:ARG:HD2	2.41	0.55
1:B:222:PHE:CD2	1:B:492:LEU:CG	2.89	0.55
1:B:617:SER:C	1:B:689:ILE:HD12	2.26	0.55
2:F:19:PHE:CE2	2:F:190:LYS:HG2	2.41	0.55
2:F:111:TRP:HD1	2:F:111:TRP:O	1.88	0.55
2:H:273:TYR:O	2:H:277:VAL:HG23	2.06	0.55
2:F:197:LEU:HD13	2:F:249:LEU:HG	1.88	0.55
2:E:15:GLU:OE1	2:E:20:GLY:HA3	2.06	0.55
1:D:417:VAL:HG23	1:D:418:ASP:N	2.21	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:217:THR:HB	1:D:218:PRO:HD2	1.87	0.55
1:C:62:ILE:HD12	1:C:84:LEU:HD22	1.87	0.55
1:A:228:ILE:N	1:A:435:GLN:HE22	2.04	0.55
2:H:15:GLU:OE1	2:H:20:GLY:HA3	2.05	0.55
2:E:111:TRP:O	2:E:111:TRP:HD1	1.89	0.55
1:D:172:LEU:HD13	1:D:173:TYR:N	2.21	0.55
1:C:17:ILE:HA	3:C:801:ATP:N1	2.22	0.55
1:D:86:ILE:O	1:D:90:ARG:HG3	2.06	0.55
1:A:641:TYR:CE2	1:A:668:LEU:HD11	2.42	0.55
2:E:72:ILE:HG23	2:E:290:LEU:HD23	1.89	0.55
1:B:172:LEU:HD23	1:B:216:ARG:CZ	2.36	0.55
1:B:215:VAL:O	1:B:216:ARG:CG	2.54	0.55
1:A:227:LEU:CA	1:A:435:GLN:HE22	2.19	0.55
2:G:179:GLY:C	2:G:180:LYS:HG2	2.26	0.55
2:H:20:GLY:O	2:H:21:GLN:C	2.43	0.55
1:A:669:LEU:HD11	1:A:698:ASN:ND2	2.21	0.55
1:D:303:THR:OG1	1:D:438:LEU:HA	2.07	0.55
1:D:150:GLN:CD	1:D:154:LYS:HD2	2.26	0.55
1:A:227:LEU:HD23	1:A:435:GLN:CG	2.36	0.55
2:H:335:ILE:O	2:H:339:LEU:CD1	2.55	0.55
2:G:339:LEU:O	2:G:340:VAL:HG12	2.06	0.55
2:F:20:GLY:O	2:F:21:GLN:C	2.42	0.55
1:B:647:SER:OG	1:B:652:LEU:HD11	2.05	0.55
1:D:420:CYS:O	1:D:424:SER:CB	2.53	0.55
1:D:19:LEU:HD22	2:G:295:SER:C	2.27	0.55
1:D:668:LEU:HB2	1:D:671:GLU:HG3	1.89	0.55
1:B:6:LEU:HD22	1:B:14:THR:HG22	1.88	0.55
2:H:73:PHE:HB2	2:H:218:PHE:CE2	2.41	0.55
1:B:94:TYR:CE2	1:B:168:SER:HB3	2.42	0.55
2:F:340:VAL:HG12	2:F:341:SER:CB	2.35	0.55
1:D:53:ILE:O	1:D:58:ILE:HD11	2.07	0.55
1:A:94:TYR:CE2	1:A:168:SER:HB2	2.41	0.55
1:B:587:LEU:C	1:B:589:THR:H	2.09	0.55
1:C:538:ASN:ND2	1:C:593:GLU:HB2	2.22	0.55
2:E:192:LYS:HE3	2:E:192:LYS:O	2.06	0.55
1:B:244:ILE:O	1:B:248:VAL:HG22	2.07	0.55
1:A:172:LEU:HD13	1:A:173:TYR:N	2.21	0.55
1:D:442:ILE:HG23	1:D:444:LEU:HG	1.88	0.55
1:C:317:LEU:CD1	1:C:401:LEU:HG	2.33	0.55
1:C:513:LEU:HD21	1:C:613:ASN:ND2	2.21	0.55
2:G:96:LEU:HA	2:G:99:ILE:CD1	2.36	0.55
2:E:177:VAL:HG21	2:E:182:VAL:CG2	2.36	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:83:LEU:HD22	2:H:203:LEU:HG	1.87	0.55
1:D:182:SER:O	1:D:189:ARG:CZ	2.55	0.55
1:B:474:ASN:HD21	1:B:476:ASP:HB2	1.69	0.55
1:B:708:LYS:O	1:B:709:VAL:C	2.45	0.55
2:H:31:GLN:CD	2:H:31:GLN:N	2.60	0.55
1:C:378:LEU:HB3	1:C:382:TYR:HE2	1.71	0.55
1:B:168:SER:OG	1:B:171:PHE:CD2	2.55	0.55
1:B:686:GLN:HA	1:B:689:ILE:CG2	2.32	0.55
1:B:260:ARG:O	1:B:261:ILE:C	2.41	0.55
1:D:516:GLY:HA2	1:D:618:ALA:O	2.07	0.55
2:F:15:GLU:OE1	2:F:20:GLY:HA3	2.06	0.55
2:G:95:LEU:O	2:G:99:ILE:HG13	2.06	0.55
2:F:16:PRO:HG2	2:F:18:PHE:O	2.07	0.55
1:C:93:ALA:HB2	1:C:165:ILE:O	2.07	0.55
1:A:4:ASN:OD1	1:C:297:VAL:CG1	2.54	0.55
1:D:74:ALA:HB1	1:D:77:TYR:CD2	2.42	0.55
1:D:364:LEU:C	1:D:364:LEU:CD1	2.76	0.55
2:G:96:LEU:HA	2:G:99:ILE:HD12	1.89	0.55
1:A:420:CYS:O	1:A:424:SER:CB	2.53	0.55
1:D:730:TYR:O	1:D:731:TYR:C	2.46	0.55
2:G:197:LEU:HD13	2:G:249:LEU:HG	1.88	0.55
1:B:597:TYR:O	1:B:598:ASP:C	2.42	0.55
2:G:16:PRO:HG2	2:G:18:PHE:O	2.07	0.55
1:B:174:ILE:HG23	1:B:175:LEU:N	2.22	0.55
1:B:115:TYR:CD1	1:B:216:ARG:HG3	2.42	0.55
1:D:619:LEU:HD12	1:D:693:ILE:CG2	2.37	0.55
1:D:223:SER:OG	1:D:461:LEU:HD11	2.07	0.55
2:E:334:TRP:O	2:E:336:ASN:N	2.40	0.55
2:E:197:LEU:HD13	2:E:249:LEU:HG	1.87	0.55
2:G:72:ILE:HG23	2:G:290:LEU:HD23	1.88	0.55
1:C:115:TYR:CE1	1:C:216:ARG:CG	2.90	0.54
1:D:158:GLN:HB3	1:D:165:ILE:HD12	1.87	0.54
1:D:465:SER:O	1:D:515:ILE:HA	2.07	0.54
1:D:293:SER:HB2	1:D:298:ARG:O	2.06	0.54
1:D:29:ALA:HB1	1:D:80:LEU:HD12	1.89	0.54
1:C:513:LEU:HD23	1:C:613:ASN:ND2	2.23	0.54
1:C:29:ALA:HB1	1:C:80:LEU:HD12	1.89	0.54
1:D:22:ILE:HD11	3:D:801:ATP:N3	2.21	0.54
1:D:52:GLY:C	1:D:53:ILE:HG22	2.28	0.54
1:D:568:PHE:CD2	1:D:574:ALA:HB2	2.41	0.54
1:B:730:TYR:O	1:B:731:TYR:C	2.46	0.54
1:C:86:ILE:HG21	1:C:140:ASP:HB3	1.89	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:20:GLY:O	2:G:21:GLN:C	2.42	0.54
2:G:125:ILE:HD13	2:G:227:ASN:ND2	2.22	0.54
2:E:122:TYR:HA	2:E:125:ILE:HD12	1.89	0.54
1:C:332:HIS:O	1:C:333:MET:HG2	2.07	0.54
2:F:328:ARG:NH1	2:F:328:ARG:HB3	2.22	0.54
1:B:569:ASN:ND2	1:B:570:GLU:H	2.00	0.54
1:B:440:LEU:HB2	1:B:730:TYR:CE1	2.42	0.54
1:C:714:LEU:CD2	1:C:732:GLN:HE22	2.19	0.54
1:D:412:ILE:HD12	1:D:412:ILE:N	2.23	0.54
1:C:217:THR:HB	1:C:218:PRO:HD2	1.88	0.54
2:E:205:ALA:O	2:E:209:TYR:HB2	2.07	0.54
1:C:369:PHE:CE2	1:C:434:ARG:HB3	2.43	0.54
1:A:696:ASN:HB2	1:A:731:TYR:O	2.08	0.54
2:E:207:ARG:HH22	2:E:282:GLN:NE2	2.05	0.54
1:B:230:CYS:SG	1:B:237:ILE:HA	2.47	0.54
1:B:529:LYS:HB3	1:B:536:ALA:HB2	1.89	0.54
1:A:290:LYS:NZ	1:A:300:GLY:O	2.37	0.54
2:E:73:PHE:HB2	2:E:218:PHE:CE2	2.42	0.54
1:D:520:PHE:CE2	1:D:524:LEU:HD11	2.42	0.54
2:H:65:LEU:HD21	2:H:223:LEU:CD1	2.30	0.54
2:F:322:ASP:O	2:F:324:PRO:CD	2.47	0.54
1:D:567:TRP:O	1:D:568:PHE:C	2.45	0.54
1:A:189:ARG:O	1:A:193:VAL:HG23	2.06	0.54
2:E:111:TRP:CD1	2:E:111:TRP:C	2.80	0.54
1:D:520:PHE:HB3	1:D:635:ILE:HA	1.88	0.54
1:A:44:ARG:HE	1:A:44:ARG:HA	1.73	0.54
1:C:464:LEU:HD12	1:C:620:MET:SD	2.47	0.54
1:B:286:GLN:O	1:B:289:VAL:HG22	2.07	0.54
1:A:212:MET:O	1:A:216:ARG:NH1	2.40	0.54
1:B:40:GLN:HE21	2:H:333:PRO:CG	2.16	0.54
1:C:278:CYS:O	1:C:282:TYR:HD1	1.90	0.54
2:E:84:ASP:HA	2:E:87:GLN:HB2	1.90	0.54
1:A:55:THR:HA	1:A:58:ILE:HD12	1.88	0.54
1:A:174:ILE:HG23	1:A:175:LEU:N	2.21	0.54
1:D:658:ASP:HB3	1:D:662:LEU:HD12	1.90	0.54
1:D:641:TYR:CE2	1:D:668:LEU:HD11	2.42	0.54
1:A:301:ALA:HB3	1:A:438:LEU:CD2	2.37	0.54
1:B:89:LEU:HD21	1:B:152:GLU:HG3	1.88	0.54
1:D:538:ASN:ND2	1:D:593:GLU:HB2	2.22	0.54
1:B:217:THR:HB	1:B:218:PRO:HD2	1.88	0.54
1:B:25:VAL:HG21	3:B:801:ATP:O2'	2.08	0.54
1:A:279:ILE:CD1	1:A:319:LEU:HD21	2.35	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:24:ASN:ND2	2:G:25:VAL:HG12	2.22	0.54
1:C:708:LYS:O	1:C:709:VAL:C	2.45	0.54
1:C:564:ALA:HA	1:C:611:LEU:O	2.07	0.54
1:B:261:ILE:HG21	1:B:278:CYS:HA	1.89	0.54
1:A:151:LEU:O	1:A:156:LEU:HG	2.07	0.54
1:C:25:VAL:HG21	3:C:801:ATP:O3'	2.08	0.54
1:C:686:GLN:HA	1:C:689:ILE:HG12	1.90	0.54
1:D:689:ILE:CG2	1:D:691:GLN:O	2.55	0.54
1:B:641:TYR:CE2	1:B:668:LEU:HD11	2.43	0.54
1:B:576:GLY:HA3	1:B:607:LYS:HE2	1.89	0.54
2:H:16:PRO:HG2	2:H:18:PHE:O	2.07	0.54
1:D:174:ILE:HG23	1:D:175:LEU:N	2.22	0.54
1:D:172:LEU:CD2	1:D:216:ARG:HH22	2.08	0.54
2:H:12:GLN:O	2:H:14:LYS:N	2.41	0.54
1:B:658:ASP:O	1:B:662:LEU:HB2	2.08	0.54
1:A:37:SER:HB3	1:A:40:GLN:HB2	1.89	0.54
1:D:568:PHE:CE2	1:D:574:ALA:CB	2.91	0.54
1:A:596:HIS:HB3	1:A:597:TYR:CE2	2.42	0.54
2:G:122:TYR:HA	2:G:125:ILE:HD12	1.88	0.54
2:G:31:GLN:N	2:G:31:GLN:CD	2.61	0.54
1:B:109:MET:CE	1:B:166:TYR:O	2.54	0.54
1:B:618:ALA:O	1:B:619:LEU:HD23	2.08	0.54
1:B:302:ALA:O	1:B:333:MET:HB3	2.08	0.54
1:B:36:VAL:HA	1:B:77:TYR:CE2	2.43	0.54
1:A:226:VAL:HB	1:A:459:ILE:HG22	1.90	0.54
1:D:719:LEU:HD12	2:G:370:LEU:HD22	1.90	0.54
1:D:5:LEU:CB	1:D:17:ILE:HG12	2.37	0.54
1:A:562:GLN:CG	1:A:612:ARG:CZ	2.85	0.54
1:B:55:THR:HA	1:B:58:ILE:HD12	1.90	0.54
2:F:207:ARG:HH22	2:F:282:GLN:CD	2.11	0.54
1:A:545:GLU:CD	1:A:596:HIS:H	2.11	0.54
1:A:509:GLY:O	1:A:566:PRO:HB2	2.07	0.54
1:A:693:ILE:HD12	1:A:693:ILE:N	2.23	0.54
1:C:21:LYS:O	1:C:25:VAL:HG23	2.08	0.54
1:B:702:SER:HB3	1:B:735:ARG:CD	2.38	0.54
1:D:516:GLY:HA2	1:D:619:LEU:HD23	1.90	0.54
1:A:49:PHE:CD1	1:A:53:ILE:HD13	2.44	0.54
1:B:22:ILE:HD12	1:B:22:ILE:N	2.23	0.54
1:B:569:ASN:HD22	1:B:569:ASN:N	2.06	0.54
1:D:621:PRO:HD3	1:D:694:SER:HB2	1.89	0.54
1:A:230:CYS:SG	1:A:237:ILE:HA	2.49	0.54
2:H:125:ILE:HG21	2:H:227:ASN:HD22	1.73	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:125:ILE:O	2:H:129:ILE:HG12	2.08	0.54
2:H:192:LYS:HE3	2:H:192:LYS:O	2.08	0.54
1:A:340:ASN:HB3	1:A:368:PHE:CE1	2.42	0.53
1:A:413:TYR:OH	1:A:731:TYR:CE2	2.39	0.53
1:D:22:ILE:HD12	1:D:22:ILE:N	2.24	0.53
2:G:73:PHE:HB2	2:G:218:PHE:CE2	2.43	0.53
1:B:686:GLN:HE21	1:B:727:LYS:HE3	1.71	0.53
2:H:330:ASN:ND2	2:H:332:ILE:O	2.42	0.53
1:C:617:SER:HB3	1:C:689:ILE:HA	1.89	0.53
1:D:711:MET:HB2	2:G:363:SER:CB	2.37	0.53
2:F:12:GLN:O	2:F:101:ILE:HG22	2.08	0.53
1:B:538:ASN:ND2	1:B:593:GLU:HB2	2.23	0.53
2:H:143:ASN:CG	2:H:146:ILE:HD13	2.28	0.53
1:D:509:GLY:O	1:D:566:PRO:HD2	2.07	0.53
1:B:4:ASN:ND2	1:B:5:LEU:HD22	2.24	0.53
2:F:192:LYS:HE3	2:F:192:LYS:O	2.07	0.53
1:B:689:ILE:HG23	1:B:689:ILE:O	2.08	0.53
1:C:62:ILE:HG13	1:C:63:ILE:N	2.23	0.53
2:E:96:LEU:HD12	2:E:108:VAL:HG11	1.91	0.53
1:D:53:ILE:O	1:D:53:ILE:CG1	2.55	0.53
1:B:364:LEU:O	1:B:364:LEU:HD13	2.07	0.53
1:A:131:MET:HE1	1:A:178:ALA:HB2	1.91	0.53
1:C:656:VAL:O	1:C:657:PRO:C	2.46	0.53
1:A:74:ALA:HB1	1:A:77:TYR:HD2	1.73	0.53
2:E:122:TYR:O	2:E:126:ILE:HG13	2.09	0.53
1:D:180:LEU:HD23	1:D:488:ALA:HB1	1.90	0.53
2:F:173:GLY:O	2:F:183:THR:HG23	2.08	0.53
2:G:34:ASP:O	2:G:38:LYS:HG3	2.09	0.53
2:F:31:GLN:CD	2:F:31:GLN:N	2.61	0.53
2:E:253:ARG:HG3	2:E:265:ALA:HB1	1.91	0.53
1:D:147:ALA:HB1	1:D:628:ILE:HA	1.91	0.53
1:B:215:VAL:O	1:B:216:ARG:CB	2.56	0.53
1:D:240:THR:HG22	1:D:244:ILE:HD11	1.90	0.53
2:F:95:LEU:O	2:F:99:ILE:HG13	2.08	0.53
2:F:96:LEU:HA	2:F:99:ILE:CD1	2.39	0.53
1:B:365:TYR:O	1:B:368:PHE:N	2.41	0.53
1:A:52:GLY:C	1:A:53:ILE:HG22	2.28	0.53
1:C:712:GLN:HG3	2:E:370:LEU:HD21	1.89	0.53
1:A:74:ALA:HB1	1:A:77:TYR:CD2	2.44	0.53
2:H:125:ILE:HD13	2:H:227:ASN:ND2	2.23	0.53
2:F:132:ASP:OD2	2:F:135:VAL:HG13	2.08	0.53
1:A:412:ILE:HD12	1:A:412:ILE:N	2.24	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:412:ILE:N	1:C:412:ILE:HD12	2.23	0.53
1:B:211:ILE:HA	1:B:222:PHE:CE1	2.43	0.53
1:B:464:LEU:HB2	1:B:514:GLY:O	2.08	0.53
1:B:283:LYS:HG2	1:B:330:VAL:CG2	2.38	0.53
2:E:273:TYR:HB2	2:E:321:LEU:HD22	1.90	0.53
2:E:273:TYR:CE2	2:E:324:PRO:HG3	2.43	0.53
1:D:154:LYS:HE2	1:D:624:THR:HG21	1.89	0.53
1:D:517:VAL:HG12	1:D:619:LEU:CD2	2.38	0.53
2:F:149:ARG:NH1	2:F:286:TRP:HB2	2.14	0.53
2:F:309:GLU:HA	2:F:325:PHE:CD2	2.44	0.53
1:C:730:TYR:O	1:C:731:TYR:C	2.46	0.53
1:B:520:PHE:CE2	1:B:524:LEU:HD11	2.44	0.53
2:E:195:LEU:HD11	2:E:275:LEU:HD11	1.90	0.53
2:G:125:ILE:HG21	2:G:227:ASN:HD22	1.73	0.53
2:E:125:ILE:O	2:E:129:ILE:HG12	2.08	0.53
1:B:378:LEU:HB3	1:B:382:TYR:HE2	1.73	0.53
1:B:290:LYS:NZ	1:B:299:GLY:O	2.37	0.53
1:B:176:VAL:HG13	1:B:215:VAL:HG21	1.90	0.53
1:A:441:GLU:HG2	1:A:620:MET:CB	2.39	0.53
1:A:227:LEU:HB3	1:A:435:GLN:CD	2.26	0.53
2:F:99:ILE:HD13	2:F:105:GLU:HA	1.90	0.53
1:A:447:LYS:HB2	1:A:458:GLU:N	2.20	0.53
2:H:92:ASN:O	2:H:96:LEU:HB2	2.07	0.53
2:F:177:VAL:HB	2:F:180:LYS:O	2.07	0.53
2:G:277:VAL:HG22	2:G:324:PRO:CG	2.39	0.53
1:C:10:ARG:HG3	1:C:56:SER:HB2	1.91	0.53
1:B:74:ALA:HB1	1:B:77:TYR:HD2	1.73	0.53
1:C:286:GLN:OE1	1:C:332:HIS:HB2	2.09	0.53
1:D:43:LEU:CD1	2:G:334:TRP:CE2	2.91	0.53
1:D:249:SER:HB2	1:D:292:CYS:SG	2.49	0.53
2:E:332:ILE:N	2:E:333:PRO:HD3	2.24	0.53
1:A:569:ASN:N	1:A:569:ASN:ND2	2.56	0.53
1:C:240:THR:HG22	1:C:244:ILE:HD11	1.91	0.53
1:A:542:LYS:HG3	1:A:596:HIS:CD2	2.43	0.53
2:E:310:TYR:CE2	2:E:330:ASN:HB2	2.43	0.53
1:C:237:ILE:HD13	1:C:281:PHE:CE2	2.44	0.53
1:A:378:LEU:HB3	1:A:382:TYR:HE2	1.74	0.53
2:E:230:ILE:O	2:E:234:ILE:HG12	2.07	0.53
1:B:711:MET:CB	2:H:364:GLU:H	2.22	0.53
1:C:226:VAL:CG1	1:C:461:LEU:CD2	2.84	0.53
1:D:711:MET:N	2:G:363:SER:HB2	2.17	0.53
2:E:95:LEU:O	2:E:99:ILE:HG13	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:308:MET:HB3	1:B:343:MET:HE2	1.91	0.53
1:D:519:ASN:HA	1:D:632:THR:OG1	2.09	0.53
1:B:86:ILE:O	1:B:90:ARG:HG3	2.09	0.53
2:H:122:TYR:HA	2:H:125:ILE:HD12	1.90	0.53
2:H:130:VAL:HG12	2:H:131:ASN:N	2.24	0.53
1:C:175:LEU:CD2	1:C:216:ARG:CD	2.75	0.53
1:A:425:PRO:HG2	1:A:690:ASP:CB	2.33	0.53
2:E:99:ILE:HD13	2:E:105:GLU:HA	1.91	0.53
1:B:668:LEU:HB2	1:B:671:GLU:HG3	1.90	0.53
1:A:62:ILE:HG13	1:A:63:ILE:N	2.24	0.53
1:C:449:LEU:HD21	1:C:502:ALA:HB2	1.91	0.53
1:B:712:GLN:HE21	2:H:369:ASP:HB3	1.72	0.53
2:G:328:ARG:HB3	2:G:328:ARG:NH1	2.23	0.53
1:D:20:ASP:HA	1:D:23:HIS:CD2	2.44	0.53
1:C:222:PHE:CE2	1:C:492:LEU:CD1	2.90	0.53
1:D:157:VAL:O	1:D:166:TYR:CB	2.52	0.53
1:B:172:LEU:HD13	1:B:173:TYR:N	2.23	0.53
2:F:96:LEU:HA	2:F:99:ILE:HD12	1.89	0.53
1:B:647:SER:HB2	1:B:652:LEU:HG	1.89	0.53
1:D:21:LYS:O	1:D:25:VAL:HG23	2.08	0.53
2:F:207:ARG:HH22	2:F:282:GLN:NE2	2.07	0.53
1:B:19:LEU:CD2	2:H:295:SER:O	2.57	0.53
1:B:269:ARG:HG3	1:B:269:ARG:O	2.09	0.53
1:A:96:GLN:NE2	1:D:386:ASP:OD2	2.42	0.53
1:B:706:SER:O	1:B:708:LYS:HG3	2.09	0.53
1:A:242:SER:HA	1:B:238:ASN:OD1	2.08	0.53
2:F:125:ILE:HD13	2:F:227:ASN:ND2	2.23	0.53
1:C:442:ILE:HG23	1:C:444:LEU:HG	1.92	0.52
1:B:94:TYR:HE2	1:B:168:SER:HB3	1.73	0.52
2:F:34:ASP:O	2:F:38:LYS:HG3	2.09	0.52
1:A:207:LEU:HB3	1:A:208:PRO:HD2	1.91	0.52
1:A:442:ILE:HG23	1:A:444:LEU:HG	1.91	0.52
1:D:378:LEU:HB3	1:D:382:TYR:HE2	1.73	0.52
1:C:361:VAL:CG1	1:C:364:LEU:CB	2.81	0.52
1:C:696:ASN:HD22	1:C:696:ASN:N	2.00	0.52
2:G:207:ARG:HH22	2:G:282:GLN:CD	2.13	0.52
1:D:230:CYS:SG	1:D:237:ILE:HA	2.49	0.52
1:B:6:LEU:HD12	1:B:51:ASP:OD1	2.08	0.52
2:H:253:ARG:HG3	2:H:265:ALA:HB1	1.91	0.52
1:C:463:THR:HG21	1:C:492:LEU:HD23	1.91	0.52
1:D:437:ASN:ND2	1:D:439:CYS:HB2	2.24	0.52
1:B:74:ALA:HB1	1:B:77:TYR:CD2	2.43	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:339:LEU:CD1	2:E:339:LEU:C	2.77	0.52
1:A:322:ASN:HA	1:A:331:ARG:NE	2.23	0.52
1:D:440:LEU:HD12	1:D:728:THR:CB	2.38	0.52
2:G:295:SER:OG	2:G:300:ASN:HB3	2.09	0.52
1:D:110:VAL:HG21	1:D:120:LEU:HD11	1.91	0.52
1:C:114:LYS:N	1:C:114:LYS:CD	2.73	0.52
1:D:215:VAL:O	1:D:216:ARG:CB	2.57	0.52
1:A:19:LEU:HD12	1:A:19:LEU:N	2.20	0.52
2:H:295:SER:OG	2:H:300:ASN:HB3	2.09	0.52
2:F:239:ALA:HA	2:F:242:LEU:HD21	1.92	0.52
1:D:519:ASN:HD21	1:D:657:PRO:HG2	1.74	0.52
1:D:668:LEU:O	1:D:671:GLU:N	2.41	0.52
1:D:149:LYS:HG3	1:D:652:LEU:HD21	1.91	0.52
1:A:668:LEU:O	1:A:671:GLU:N	2.42	0.52
1:B:50:TYR:CE2	1:B:53:ILE:HD12	2.45	0.52
2:G:130:VAL:HG12	2:G:131:ASN:N	2.25	0.52
1:B:215:VAL:O	1:B:216:ARG:NH1	2.41	0.52
2:F:209:TYR:HA	2:F:212:PHE:CD2	2.45	0.52
1:D:301:ALA:O	1:D:438:LEU:CD1	2.44	0.52
1:C:74:ALA:HB1	1:C:77:TYR:HD2	1.74	0.52
2:G:332:ILE:N	2:G:333:PRO:HD3	2.25	0.52
2:F:84:ASP:HA	2:F:87:GLN:HB2	1.91	0.52
1:A:22:ILE:HD11	3:A:801:ATP:C2	2.44	0.52
1:A:558:LEU:HD23	1:A:612:ARG:HG2	1.92	0.52
1:B:696:ASN:N	1:B:696:ASN:HD22	2.00	0.52
1:B:719:LEU:HD22	2:H:375:LEU:CD2	2.39	0.52
2:E:143:ASN:CG	2:E:146:ILE:HD13	2.29	0.52
2:H:6:SER:CB	2:H:21:GLN:NE2	2.71	0.52
2:E:5:PHE:CE2	2:E:7:GLN:NE2	2.77	0.52
2:E:16:PRO:HG2	2:E:18:PHE:O	2.09	0.52
2:H:34:ASP:O	2:H:38:LYS:HG3	2.09	0.52
1:A:286:GLN:O	1:A:289:VAL:HG22	2.08	0.52
1:A:449:LEU:HD21	1:A:502:ALA:HB2	1.91	0.52
2:H:336:ASN:O	2:H:339:LEU:HD22	2.10	0.52
1:C:6:LEU:CD1	1:C:51:ASP:OD2	2.56	0.52
2:F:273:TYR:HB2	2:F:321:LEU:HD22	1.90	0.52
2:H:195:LEU:HD11	2:H:275:LEU:HD11	1.91	0.52
1:D:592:ASN:ND2	1:D:592:ASN:H	2.08	0.52
1:B:592:ASN:H	1:B:592:ASN:ND2	2.07	0.52
2:H:169:LEU:O	2:H:170:LEU:HD23	2.09	0.52
1:B:70:ILE:O	1:B:653:ARG:HD2	2.10	0.52
1:C:444:LEU:HD21	1:C:691:GLN:OE1	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:619:LEU:HG	1:B:693:ILE:HG23	1.91	0.52
1:B:621:PRO:HD3	1:B:694:SER:OG	2.08	0.52
2:F:99:ILE:CD1	2:F:108:VAL:HG21	2.40	0.52
1:A:621:PRO:HG3	1:A:730:TYR:CE2	2.45	0.52
1:B:150:GLN:HE22	1:B:645:LYS:NZ	2.08	0.52
2:E:96:LEU:HA	2:E:99:ILE:HD12	1.91	0.52
1:A:62:ILE:HD12	1:A:84:LEU:HD22	1.91	0.52
1:B:21:LYS:O	1:B:25:VAL:HG23	2.10	0.52
1:C:269:ARG:HG3	1:C:269:ARG:O	2.09	0.52
1:D:103:TYR:O	1:D:107:VAL:HG23	2.10	0.52
2:G:143:ASN:CG	2:G:146:ILE:HD13	2.29	0.52
1:D:145:TYR:HE2	1:D:652:LEU:HD23	1.75	0.52
2:F:195:LEU:HD11	2:F:275:LEU:HD11	1.92	0.52
2:F:122:TYR:HA	2:F:125:ILE:HD12	1.91	0.52
1:C:110:VAL:HG21	1:C:120:LEU:HD11	1.92	0.52
1:A:227:LEU:HG	1:A:435:GLN:HE21	1.73	0.52
2:H:339:LEU:HD22	2:H:340:VAL:HG23	1.92	0.52
2:G:339:LEU:HD13	2:G:339:LEU:O	2.09	0.52
1:A:369:PHE:CE2	1:A:434:ARG:CB	2.93	0.52
2:H:79:TYR:HB2	2:H:286:TRP:CH2	2.45	0.52
1:B:519:ASN:ND2	1:B:632:THR:H	2.08	0.52
2:F:310:TYR:CE2	2:F:330:ASN:HB2	2.44	0.52
1:B:10:ARG:N	1:B:55:THR:HG22	2.25	0.52
1:B:62:ILE:HG13	1:B:63:ILE:N	2.24	0.52
1:A:269:ARG:HG3	1:A:269:ARG:O	2.09	0.52
2:F:238:GLU:O	2:F:242:LEU:HD23	2.10	0.52
1:D:189:ARG:O	1:D:193:VAL:HG23	2.09	0.52
2:F:166:TYR:HB3	2:F:184:VAL:HG21	1.90	0.52
1:A:278:CYS:O	1:A:282:TYR:HD1	1.93	0.52
1:D:220:ARG:O	1:D:496:GLN:CA	2.48	0.52
1:A:696:ASN:HB3	1:A:730:TYR:HB3	1.92	0.52
1:A:37:SER:HB2	2:F:333:PRO:HD3	1.92	0.52
2:E:191:LYS:HG2	2:E:264:ILE:CG2	2.40	0.52
1:A:330:VAL:HB	1:A:335:TYR:OH	2.10	0.52
1:A:238:ASN:OD1	1:B:242:SER:HA	2.10	0.52
1:C:308:MET:HB3	1:C:343:MET:HE2	1.91	0.52
1:C:520:PHE:HB3	1:C:635:ILE:HA	1.91	0.52
2:G:111:TRP:CD1	2:G:111:TRP:C	2.81	0.52
1:A:36:VAL:HA	1:A:77:TYR:CE2	2.45	0.52
2:F:125:ILE:HG21	2:F:227:ASN:HD22	1.75	0.52
1:D:225:CYS:H	1:D:462:CYS:HB3	1.75	0.52
1:B:180:LEU:HD23	1:B:488:ALA:HB1	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:215:VAL:O	1:B:216:ARG:HG2	2.09	0.52
2:E:339:LEU:O	2:E:340:VAL:CB	2.57	0.52
1:C:223:SER:HB2	1:C:461:LEU:HD11	1.92	0.52
1:A:53:ILE:CG1	1:A:53:ILE:O	2.55	0.52
1:A:237:ILE:HD13	1:A:281:PHE:CE2	2.44	0.52
1:D:595:LEU:HD22	1:D:599:TRP:HE1	1.75	0.52
1:D:338:GLN:HG2	1:D:415:GLN:NE2	2.25	0.52
1:C:26:LEU:HB2	1:C:38:ILE:HG23	1.91	0.52
1:C:444:LEU:HD11	1:C:462:CYS:SG	2.49	0.52
1:D:89:LEU:CD2	1:D:152:GLU:CG	2.38	0.52
1:B:442:ILE:HG23	1:B:444:LEU:HG	1.91	0.52
2:H:284:LYS:HE3	2:H:325:PHE:CZ	2.46	0.52
1:D:248:VAL:HG11	1:D:289:VAL:HA	1.91	0.52
1:C:313:VAL:O	1:C:317:LEU:CD2	2.56	0.52
2:G:89:ARG:HG2	2:G:90:SER:N	2.25	0.52
2:E:92:ASN:CA	2:E:96:LEU:HD13	2.35	0.52
1:D:25:VAL:HG21	3:D:801:ATP:C3'	2.40	0.52
1:A:10:ARG:N	1:A:55:THR:HG22	2.25	0.52
1:C:565:CYS:SG	1:C:568:PHE:HB2	2.50	0.52
1:C:316:LEU:O	1:C:319:LEU:HD12	2.09	0.52
1:B:458:GLU:OE2	1:B:510:ARG:NH1	2.43	0.52
1:B:509:GLY:O	1:B:566:PRO:HB2	2.10	0.52
1:C:569:ASN:N	1:C:569:ASN:HD22	2.08	0.52
1:A:595:LEU:HD22	1:A:599:TRP:NE1	2.25	0.52
1:B:595:LEU:HD22	1:B:599:TRP:HE1	1.75	0.52
2:E:6:SER:OG	2:E:24:ASN:HB3	2.09	0.52
1:B:406:ARG:NH1	1:B:732:GLN:HG3	2.25	0.52
1:C:103:TYR:O	1:C:107:VAL:HG23	2.10	0.51
1:D:465:SER:HB2	1:D:489:LEU:HD11	1.92	0.51
1:A:512:THR:HG22	1:A:614:SER:HB2	1.92	0.51
1:D:617:SER:O	1:D:691:GLN:HG3	2.09	0.51
1:C:44:ARG:HG3	1:C:69:LEU:HD11	1.91	0.51
1:C:74:ALA:HB1	1:C:77:TYR:CD2	2.44	0.51
1:A:569:ASN:N	1:A:569:ASN:HD22	2.08	0.51
1:A:20:ASP:HA	1:A:23:HIS:CD2	2.45	0.51
1:A:261:ILE:HD12	1:A:281:PHE:HD2	1.75	0.51
2:H:5:PHE:HD1	2:H:24:ASN:O	1.91	0.51
1:D:145:TYR:CE2	1:D:652:LEU:HD23	2.45	0.51
1:B:6:LEU:HD22	1:B:14:THR:CG2	2.39	0.51
2:F:143:ASN:CG	2:F:146:ILE:HD13	2.30	0.51
1:B:374:GLU:HG3	1:B:378:LEU:HD11	1.92	0.51
2:E:130:VAL:HG12	2:E:131:ASN:N	2.25	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:615:THR:HB	1:B:691:GLN:NE2	2.25	0.51
1:C:22:ILE:HD12	1:C:22:ILE:N	2.26	0.51
1:C:36:VAL:HA	1:C:77:TYR:CE2	2.45	0.51
2:F:12:GLN:HE21	2:F:23:VAL:CG1	2.12	0.51
1:D:309:TRP:CZ2	1:D:364:LEU:HD12	2.45	0.51
1:A:562:GLN:HG2	1:A:612:ARG:NE	2.26	0.51
2:E:171:GLY:O	2:E:175:HIS:CE1	2.63	0.51
1:C:519:ASN:ND2	1:C:632:THR:H	2.08	0.51
1:D:225:CYS:O	1:D:462:CYS:CB	2.59	0.51
1:A:338:GLN:HG2	1:A:415:GLN:NE2	2.24	0.51
1:B:110:VAL:HG21	1:B:120:LEU:HD11	1.91	0.51
1:D:36:VAL:HA	1:D:77:TYR:CE2	2.44	0.51
1:C:282:TYR:CE2	1:C:304:LEU:HD22	2.44	0.51
1:A:227:LEU:CA	1:A:435:GLN:NE2	2.73	0.51
1:D:6:LEU:HD22	1:D:14:THR:HG22	1.91	0.51
1:C:568:PHE:CE2	1:C:574:ALA:CB	2.89	0.51
1:C:459:ILE:HD11	1:C:502:ALA:HB3	1.92	0.51
2:F:111:TRP:C	2:F:111:TRP:CD1	2.83	0.51
1:A:475:LEU:CD1	1:A:542:LYS:HE2	2.39	0.51
1:A:655:VAL:HG12	1:A:656:VAL:O	2.10	0.51
1:B:282:TYR:CD2	1:B:304:LEU:HD22	2.37	0.51
1:D:619:LEU:HD12	1:D:693:ILE:HG22	1.91	0.51
1:A:308:MET:HB3	1:A:343:MET:HE2	1.92	0.51
2:G:175:HIS:O	2:G:177:VAL:HG23	2.11	0.51
1:C:517:VAL:HG12	1:C:619:LEU:CD2	2.39	0.51
1:C:86:ILE:O	1:C:90:ARG:HG3	2.11	0.51
1:B:20:ASP:HA	1:B:23:HIS:CD2	2.46	0.51
2:F:130:VAL:HG12	2:F:131:ASN:N	2.25	0.51
1:B:437:ASN:ND2	1:B:439:CYS:HB2	2.24	0.51
1:A:517:VAL:HG12	1:A:619:LEU:CD2	2.40	0.51
2:E:339:LEU:HD12	2:E:340:VAL:HG23	1.91	0.51
1:B:519:ASN:HD21	1:B:657:PRO:HG2	1.76	0.51
1:C:568:PHE:CD2	1:C:574:ALA:HB2	2.45	0.51
1:D:440:LEU:HB2	1:D:730:TYR:CE1	2.45	0.51
1:C:93:ALA:CB	1:C:165:ILE:O	2.59	0.51
2:G:33:TYR:OH	2:G:257:ASP:HB2	2.11	0.51
2:G:253:ARG:HG3	2:G:265:ALA:HB1	1.93	0.51
1:D:217:THR:HB	1:D:218:PRO:CD	2.41	0.51
1:D:465:SER:HB2	1:D:489:LEU:HD12	1.92	0.51
1:B:103:TYR:O	1:B:107:VAL:HG23	2.10	0.51
1:A:156:LEU:HB3	1:A:167:GLU:HG2	1.92	0.51
2:G:273:TYR:HB2	2:G:321:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:254:ILE:O	1:C:438:LEU:CG	2.59	0.51
2:H:209:TYR:HA	2:H:212:PHE:CD2	2.45	0.51
1:B:15:GLU:OE2	3:B:801:ATP:N6	2.41	0.51
2:E:12:GLN:O	2:E:14:LYS:N	2.44	0.51
1:B:262:ARG:HB2	1:B:359:SER:HB3	1.92	0.51
1:D:269:ARG:O	1:D:269:ARG:HG3	2.09	0.51
2:H:273:TYR:HB2	2:H:321:LEU:HD22	1.92	0.51
1:D:356:PHE:CE1	1:D:390:LYS:HB3	2.45	0.51
2:F:340:VAL:CG1	2:F:341:SER:N	2.74	0.51
1:C:50:TYR:CD2	1:C:53:ILE:HB	2.41	0.51
2:E:209:TYR:HA	2:E:212:PHE:CD2	2.46	0.51
1:D:8:THR:N	1:D:52:GLY:O	2.44	0.51
1:C:569:ASN:N	1:C:569:ASN:ND2	2.57	0.51
1:D:560:LYS:CE	1:D:609:HIS:CE1	2.92	0.51
2:F:372:ASN:N	2:F:372:ASN:HD22	1.98	0.51
1:D:234:LEU:O	1:D:237:ILE:HD12	2.11	0.51
1:D:519:ASN:ND2	1:D:632:THR:H	2.08	0.51
1:D:67:ALA:HA	1:D:70:ILE:HD11	1.92	0.51
1:B:263:ALA:HB3	1:B:357:SER:OG	2.11	0.51
1:C:441:GLU:OE1	1:C:442:ILE:HG12	2.11	0.51
1:B:325:VAL:HG13	1:B:328:ASN:HB3	1.93	0.51
1:D:282:TYR:HA	1:D:285:PHE:HD2	1.76	0.51
1:D:62:ILE:HG13	1:D:63:ILE:N	2.23	0.51
1:D:7:VAL:HG21	3:D:801:ATP:N1	2.26	0.51
1:B:569:ASN:ND2	1:B:569:ASN:N	2.56	0.51
2:E:153:ILE:HD11	2:E:207:ARG:HE	1.76	0.51
1:D:487:ARG:HD3	1:D:558:LEU:HD22	1.92	0.51
1:A:4:ASN:OD1	1:C:297:VAL:HG12	2.10	0.51
2:E:33:TYR:OH	2:E:257:ASP:HB2	2.11	0.51
1:D:157:VAL:C	1:D:166:TYR:HB2	2.30	0.51
1:B:319:LEU:HB3	1:B:330:VAL:H	1.76	0.51
1:D:374:GLU:HG3	1:D:378:LEU:HD11	1.93	0.51
2:G:99:ILE:HD13	2:G:105:GLU:HA	1.93	0.51
2:H:207:ARG:HH22	2:H:282:GLN:NE2	2.08	0.51
2:E:79:TYR:HB2	2:E:286:TRP:CH2	2.46	0.51
2:H:20:GLY:HA3	2:H:100:SER:HB3	1.92	0.51
2:F:125:ILE:O	2:F:129:ILE:HG12	2.10	0.51
1:A:708:LYS:O	1:A:709:VAL:C	2.45	0.51
1:A:403:MET:HG2	1:A:711:MET:HE1	1.92	0.51
1:B:515:ILE:HD13	1:B:551:LEU:CD2	2.40	0.51
1:B:516:GLY:CA	1:B:620:MET:CE	2.89	0.51
1:B:248:VAL:HG21	1:B:288:ALA:O	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:465:SER:HB2	1:A:489:LEU:HD12	1.93	0.51
1:B:131:MET:HA	1:B:134:PHE:CE2	2.46	0.51
1:C:8:THR:OG1	1:C:52:GLY:O	2.28	0.51
1:D:444:LEU:HD22	1:D:512:THR:HG21	1.93	0.51
1:B:519:ASN:HA	1:B:632:THR:OG1	2.11	0.51
1:A:22:ILE:HD11	3:A:801:ATP:N3	2.26	0.51
1:D:557:GLU:O	1:D:560:LYS:HB2	2.11	0.51
1:A:542:LYS:HE3	1:A:596:HIS:NE2	2.26	0.51
1:B:234:LEU:HA	1:B:237:ILE:CD1	2.41	0.51
1:B:26:LEU:HB2	1:B:38:ILE:HG23	1.92	0.51
2:H:319:VAL:HG23	2:H:321:LEU:H	1.76	0.51
1:B:587:LEU:C	1:B:589:THR:N	2.64	0.51
1:B:279:ILE:HB	1:B:280:PRO:HD3	1.93	0.51
2:G:329:SER:O	2:G:330:ASN:C	2.48	0.51
2:E:125:ILE:HG21	2:E:227:ASN:HD22	1.75	0.51
1:C:356:PHE:CE1	1:C:390:LYS:HB3	2.46	0.51
2:F:174:THR:CG2	2:F:181:THR:HB	2.41	0.51
1:B:515:ILE:HD13	1:B:551:LEU:HD13	1.92	0.50
1:A:224:SER:C	1:A:225:CYS:SG	2.89	0.50
1:A:623:GLU:O	1:A:627:GLN:HG2	2.10	0.50
1:B:467:PHE:HE1	1:B:481:LEU:HB3	1.75	0.50
1:A:712:GLN:HE22	2:F:366:ASP:HB3	1.76	0.50
1:A:8:THR:HB	1:A:54:LYS:HA	1.91	0.50
2:G:191:LYS:HG2	2:G:264:ILE:CG2	2.41	0.50
1:C:437:ASN:ND2	1:C:439:CYS:HB2	2.25	0.50
1:B:529:LYS:N	1:B:529:LYS:HD2	2.25	0.50
1:C:592:ASN:H	1:C:592:ASN:ND2	2.08	0.50
1:B:620:MET:SD	1:B:620:MET:O	2.69	0.50
1:B:258:ALA:HB1	1:B:282:TYR:CZ	2.45	0.50
1:C:10:ARG:N	1:C:55:THR:HG22	2.27	0.50
1:A:361:VAL:HG11	1:A:364:LEU:CB	2.41	0.50
1:A:369:PHE:CD2	1:A:434:ARG:HD3	2.45	0.50
1:A:623:GLU:HG2	1:A:633:ASN:HD21	1.72	0.50
1:D:8:THR:HB	1:D:54:LYS:HA	1.93	0.50
1:C:279:ILE:HD13	1:C:319:LEU:HD22	1.92	0.50
2:G:161:ILE:O	2:G:165:SER:HB2	2.11	0.50
2:E:149:ARG:NH1	2:E:286:TRP:HB2	2.26	0.50
1:B:593:GLU:OE2	1:B:596:HIS:CE1	2.64	0.50
1:C:576:GLY:CA	1:C:607:LYS:HE2	2.41	0.50
1:A:21:LYS:O	1:A:25:VAL:HG23	2.11	0.50
1:A:692:SER:HB3	1:A:727:LYS:HB3	1.93	0.50
1:A:224:SER:C	1:A:225:CYS:HG	2.15	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:513:LEU:O	1:C:615:THR:O	2.29	0.50
1:A:282:TYR:CD2	1:A:304:LEU:HD13	2.47	0.50
2:G:96:LEU:HD12	2:G:108:VAL:HG11	1.93	0.50
2:E:99:ILE:CD1	2:E:108:VAL:HG21	2.42	0.50
2:E:79:TYR:HB2	2:E:286:TRP:CZ2	2.46	0.50
1:B:262:ARG:HD3	1:B:266:SER:HB3	1.92	0.50
1:A:297:VAL:O	1:A:297:VAL:HG12	2.11	0.50
1:D:232:ASP:CG	1:D:262:ARG:HE	2.13	0.50
1:B:86:ILE:HG22	1:B:90:ARG:HD2	1.94	0.50
1:C:669:LEU:HD11	1:C:698:ASN:ND2	2.26	0.50
1:C:67:ALA:HA	1:C:70:ILE:HD11	1.94	0.50
1:D:449:LEU:HD21	1:D:502:ALA:CB	2.42	0.50
1:C:441:GLU:HG2	1:C:620:MET:HB3	1.87	0.50
1:B:217:THR:HB	1:B:218:PRO:CD	2.42	0.50
1:A:215:VAL:N	1:A:222:PHE:HE1	2.09	0.50
2:H:326:GLN:HG3	2:H:327:THR:O	2.11	0.50
2:G:166:TYR:HB3	2:G:184:VAL:HG21	1.93	0.50
1:D:325:VAL:HG13	1:D:328:ASN:HB3	1.93	0.50
1:C:176:VAL:HG13	1:C:215:VAL:HG21	1.93	0.50
1:C:217:THR:HB	1:C:218:PRO:CD	2.41	0.50
2:E:319:VAL:HG23	2:E:321:LEU:H	1.76	0.50
2:E:239:ALA:HA	2:E:242:LEU:HD21	1.93	0.50
1:C:185:PRO:O	1:C:189:ARG:CB	2.59	0.50
1:D:285:PHE:O	1:D:289:VAL:HG13	2.12	0.50
1:D:686:GLN:OE1	1:D:693:ILE:HG13	2.12	0.50
2:G:27:ARG:HB2	2:G:29:ASP:OD1	2.12	0.50
2:E:92:ASN:HA	2:E:96:LEU:CD1	2.37	0.50
2:H:206:ILE:HG21	2:H:312:THR:OG1	2.12	0.50
2:G:178:ASN:C	2:G:180:LYS:H	2.15	0.50
2:G:209:TYR:HA	2:G:212:PHE:CD2	2.47	0.50
1:B:147:ALA:CB	1:B:628:ILE:HA	2.41	0.50
1:A:19:LEU:HD22	2:F:295:SER:O	2.11	0.50
2:F:122:TYR:O	2:F:126:ILE:HG13	2.11	0.50
2:F:288:ASP:O	2:F:292:ARG:HB2	2.12	0.50
1:A:479:GLU:HA	1:A:550:TYR:HB3	1.94	0.50
1:D:333:MET:O	1:D:335:TYR:CE1	2.64	0.50
1:D:6:LEU:HD22	1:D:14:THR:CG2	2.42	0.50
2:G:36:PHE:O	2:G:40:ILE:HG13	2.12	0.50
1:B:522:TYR:CD1	1:B:662:LEU:CD1	2.95	0.50
1:C:279:ILE:HB	1:C:280:PRO:HD3	1.92	0.50
2:E:149:ARG:NH2	2:E:282:GLN:O	2.45	0.50
2:H:99:ILE:HD13	2:H:105:GLU:HA	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:131:MET:HE3	1:D:193:VAL:HG11	1.93	0.50
1:A:519:ASN:ND2	1:A:632:THR:H	2.09	0.50
2:E:288:ASP:O	2:E:292:ARG:HB2	2.12	0.50
1:D:669:LEU:HD11	1:D:698:ASN:ND2	2.26	0.50
1:A:647:SER:O	1:A:648:LYS:C	2.48	0.50
1:A:285:PHE:O	1:A:289:VAL:HG13	2.12	0.50
1:A:459:ILE:CD1	1:A:502:ALA:HB3	2.41	0.50
1:B:558:LEU:HD23	1:B:612:ARG:HG2	1.92	0.50
2:G:111:TRP:CD1	2:G:111:TRP:O	2.65	0.50
2:H:122:TYR:O	2:H:126:ILE:HG13	2.12	0.50
1:A:711:MET:HE2	1:A:711:MET:O	2.12	0.50
2:F:50:PRO:CG	2:F:121:SER:HB3	2.42	0.50
1:C:441:GLU:CD	1:C:442:ILE:HG12	2.32	0.50
2:F:96:LEU:HD12	2:F:108:VAL:HG11	1.93	0.50
1:A:10:ARG:HG3	1:A:56:SER:HB2	1.93	0.50
1:B:303:THR:OG1	1:B:438:LEU:CD1	2.56	0.50
1:C:4:ASN:ND2	1:C:4:ASN:N	2.59	0.50
2:F:194:TYR:CE1	2:F:249:LEU:HD23	2.47	0.50
1:D:522:TYR:HB2	1:D:657:PRO:HG2	1.94	0.50
2:F:33:TYR:OH	2:F:257:ASP:HB2	2.11	0.50
2:E:34:ASP:O	2:E:38:LYS:HG3	2.12	0.50
1:B:30:ALA:HA	1:B:33:LEU:HD12	1.92	0.50
1:B:640:GLY:HA2	1:B:668:LEU:HD13	1.94	0.50
1:A:332:HIS:O	1:A:333:MET:HG3	2.11	0.50
2:G:153:ILE:HD11	2:G:207:ARG:HE	1.77	0.50
1:D:696:ASN:HB2	1:D:731:TYR:O	2.12	0.50
2:E:365:VAL:HG12	2:E:366:ASP:N	2.26	0.50
1:D:576:GLY:CA	1:D:607:LYS:HE2	2.41	0.50
2:G:50:PRO:CG	2:G:121:SER:HB3	2.42	0.50
1:C:338:GLN:HG2	1:C:415:GLN:NE2	2.27	0.50
2:H:288:ASP:O	2:H:292:ARG:HB2	2.12	0.50
1:C:102:LEU:O	1:C:106:VAL:HG23	2.12	0.49
2:H:328:ARG:CB	2:H:328:ARG:CZ	2.90	0.49
1:D:30:ALA:HA	1:D:33:LEU:HD12	1.94	0.49
1:C:282:TYR:CD2	1:C:304:LEU:HD13	2.46	0.49
1:A:227:LEU:HG	1:A:435:GLN:NE2	2.27	0.49
1:D:685:MET:HB2	1:D:689:ILE:HD11	1.93	0.49
1:D:617:SER:HB3	1:D:689:ILE:HA	1.94	0.49
2:H:74:ILE:HG12	2:H:78:LYS:HE3	1.93	0.49
2:H:79:TYR:HB2	2:H:286:TRP:CZ2	2.46	0.49
2:H:161:ILE:O	2:H:165:SER:HB2	2.12	0.49
2:G:190:LYS:HB3	2:G:261:MET:SD	2.52	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:153:ILE:HG23	2:F:199:SER:OG	2.12	0.49
2:F:153:ILE:HD11	2:F:207:ARG:HE	1.77	0.49
1:C:86:ILE:HG22	1:C:90:ARG:HD2	1.93	0.49
2:E:125:ILE:HD13	2:E:227:ASN:ND2	2.27	0.49
1:C:597:TYR:O	1:C:598:ASP:C	2.47	0.49
1:B:102:LEU:O	1:B:106:VAL:HG23	2.11	0.49
1:B:700:ASP:OD2	1:B:735:ARG:NH1	2.44	0.49
2:E:74:ILE:HG12	2:E:78:LYS:HE3	1.94	0.49
1:A:109:MET:HE3	1:A:166:TYR:O	2.11	0.49
2:G:84:ASP:HA	2:G:87:GLN:HB2	1.94	0.49
2:H:19:PHE:CE2	2:H:190:LYS:HG2	2.47	0.49
1:C:37:SER:CB	2:E:331:PRO:O	2.57	0.49
2:F:161:ILE:O	2:F:165:SER:HB2	2.11	0.49
2:F:74:ILE:HG12	2:F:78:LYS:HE3	1.94	0.49
1:D:234:LEU:HA	1:D:237:ILE:CD1	2.42	0.49
2:G:204:GLU:HG3	5:G:601:HOH:O	2.12	0.49
1:A:592:ASN:ND2	1:A:592:ASN:H	2.09	0.49
1:D:319:LEU:O	1:D:329:ARG:HG2	2.12	0.49
1:B:29:ALA:HB1	1:B:80:LEU:HD12	1.93	0.49
1:C:670:TRP:CZ2	1:C:735:ARG:HA	2.47	0.49
2:E:326:GLN:HG3	2:E:327:THR:O	2.11	0.49
2:G:319:VAL:HG23	2:G:321:LEU:H	1.76	0.49
1:A:461:LEU:HD23	1:A:503:ALA:HB1	1.93	0.49
2:F:190:LYS:HB3	2:F:261:MET:SD	2.52	0.49
1:B:22:ILE:HD11	3:B:801:ATP:N3	2.27	0.49
2:H:96:LEU:HD12	2:H:108:VAL:HG11	1.95	0.49
1:D:640:GLY:HA2	1:D:668:LEU:HD13	1.95	0.49
1:B:278:CYS:HB3	1:B:282:TYR:HE1	1.77	0.49
2:F:319:VAL:HG23	2:F:321:LEU:H	1.77	0.49
2:E:92:ASN:O	2:E:96:LEU:HB2	2.12	0.49
2:F:372:ASN:HD22	2:F:373:PHE:H	1.61	0.49
2:E:36:PHE:O	2:E:40:ILE:HG13	2.12	0.49
2:G:311:ILE:HG23	2:G:312:THR:H	1.78	0.49
2:G:310:TYR:N	2:G:328:ARG:HD3	2.28	0.49
1:C:414:ILE:HB	1:C:729:LEU:HD12	1.93	0.49
1:D:119:LEU:N	1:D:119:LEU:HD12	2.26	0.49
1:B:175:LEU:HD22	1:B:216:ARG:HD2	1.94	0.49
1:B:222:PHE:CE2	1:B:492:LEU:HD12	2.46	0.49
1:B:19:LEU:HD13	2:H:295:SER:H	1.77	0.49
1:C:19:LEU:N	1:C:19:LEU:HD12	2.21	0.49
2:F:177:VAL:CB	2:F:180:LYS:O	2.61	0.49
1:D:658:ASP:O	1:D:658:ASP:OD2	2.31	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:131:MET:HA	1:D:134:PHE:CE2	2.48	0.49
1:D:670:TRP:HB3	1:D:735:ARG:HH12	1.78	0.49
2:H:238:GLU:O	2:H:242:LEU:HD23	2.13	0.49
2:G:277:VAL:HG22	2:G:324:PRO:HG2	1.94	0.49
1:B:700:ASP:HA	1:B:735:ARG:HB3	1.95	0.49
1:B:145:TYR:CZ	1:B:149:LYS:CG	2.94	0.49
2:G:201:ASN:O	2:G:205:ALA:HB2	2.13	0.49
2:E:161:ILE:O	2:E:165:SER:HB2	2.12	0.49
2:G:239:ALA:HA	2:G:242:LEU:HD21	1.94	0.49
1:B:242:SER:O	1:B:246:LYS:HG2	2.13	0.49
1:C:641:TYR:O	1:C:656:VAL:HG13	2.13	0.49
1:A:291:SER:O	1:B:280:PRO:HB3	2.12	0.49
2:H:33:TYR:OH	2:H:257:ASP:HB2	2.13	0.49
1:B:264:LEU:HD12	1:B:265:GLY:N	2.28	0.49
1:B:463:THR:HB	1:B:489:LEU:CD2	2.43	0.49
2:E:238:GLU:O	2:E:242:LEU:HD23	2.12	0.49
1:C:131:MET:HA	1:C:134:PHE:CE2	2.47	0.49
1:D:441:GLU:CD	1:D:442:ILE:HG12	2.33	0.49
1:C:285:PHE:O	1:C:289:VAL:HG13	2.12	0.49
1:A:240:THR:HG22	1:A:244:ILE:HD11	1.94	0.49
2:G:339:LEU:O	2:G:339:LEU:CD1	2.61	0.49
1:A:217:THR:HB	1:A:218:PRO:CD	2.42	0.49
1:B:297:VAL:HG21	1:B:298:ARG:HH21	1.77	0.49
1:D:10:ARG:HG3	1:D:56:SER:HB2	1.93	0.49
2:F:328:ARG:CB	2:F:328:ARG:CZ	2.90	0.49
1:B:10:ARG:HG3	1:B:56:SER:HB2	1.93	0.49
1:D:260:ARG:O	1:D:358:PRO:HG2	2.12	0.49
1:D:19:LEU:HD12	1:D:19:LEU:N	2.26	0.49
1:B:234:LEU:O	1:B:237:ILE:HD12	2.13	0.49
1:B:339:ILE:HD11	1:B:414:ILE:HD12	1.93	0.49
1:A:110:VAL:HG21	1:A:120:LEU:HD11	1.95	0.49
1:D:545:GLU:HG3	1:D:595:LEU:HD23	1.95	0.49
1:A:576:GLY:CA	1:A:607:LYS:HE2	2.42	0.49
2:G:122:TYR:O	2:G:126:ILE:HG13	2.12	0.49
1:C:426:PHE:HA	1:C:571:THR:HA	1.95	0.49
1:C:20:ASP:HA	1:C:23:HIS:CD2	2.48	0.49
1:C:119:LEU:HD12	1:C:119:LEU:N	2.28	0.49
1:D:109:MET:HB2	1:D:115:TYR:CD2	2.48	0.49
1:A:5:LEU:HB2	1:A:17:ILE:HG12	1.94	0.49
2:F:191:LYS:HG2	2:F:264:ILE:CG2	2.42	0.49
2:E:177:VAL:HB	2:E:180:LYS:O	2.11	0.49
1:C:276:THR:HG21	1:D:292:CYS:HA	1.93	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:37:SER:OG	2:F:331:PRO:O	2.27	0.49
2:G:207:ARG:HH22	2:G:282:GLN:NE2	2.11	0.49
2:E:329:SER:O	2:E:330:ASN:C	2.48	0.49
2:E:17:MET:HG2	2:E:257:ASP:OD2	2.13	0.49
1:D:700:ASP:OD1	1:D:735:ARG:HD2	2.13	0.49
1:A:264:LEU:HD12	1:A:265:GLY:N	2.28	0.49
1:B:479:GLU:HB3	1:B:550:TYR:CD1	2.48	0.49
1:C:394:LYS:HD3	1:C:394:LYS:H	1.78	0.49
1:D:26:LEU:HB2	1:D:38:ILE:HG23	1.94	0.49
1:B:222:PHE:CG	1:B:492:LEU:HD21	2.48	0.49
1:B:283:LYS:CG	1:B:330:VAL:HG22	2.43	0.49
1:C:254:ILE:O	1:C:438:LEU:CD1	2.61	0.49
1:B:297:VAL:HB	1:B:298:ARG:NE	2.16	0.49
2:G:179:GLY:C	2:G:180:LYS:CG	2.81	0.49
1:B:22:ILE:CD1	1:B:22:ILE:H	2.26	0.49
2:E:186:LEU:HG	2:E:190:LYS:HE3	1.95	0.49
2:G:238:GLU:O	2:G:242:LEU:HD23	2.13	0.49
1:D:86:ILE:HG22	1:D:90:ARG:HD2	1.93	0.49
1:B:530:ARG:HB2	1:B:533:ASP:OD2	2.13	0.49
1:C:109:MET:HB2	1:C:115:TYR:CD2	2.48	0.48
1:B:215:VAL:HG22	1:B:222:PHE:CE1	2.47	0.48
1:A:369:PHE:CE2	1:A:434:ARG:CG	2.96	0.48
2:H:84:ASP:HA	2:H:87:GLN:HB2	1.94	0.48
2:H:99:ILE:CD1	2:H:108:VAL:HG21	2.43	0.48
2:H:176:THR:HG23	2:H:181:THR:HG23	1.95	0.48
2:H:140:ILE:O	2:H:146:ILE:HG21	2.12	0.48
1:B:119:LEU:HD12	1:B:119:LEU:N	2.27	0.48
1:B:78:GLN:NE2	1:B:654:GLN:HA	2.28	0.48
1:B:109:MET:HB2	1:B:115:TYR:CD2	2.48	0.48
1:A:154:LYS:HB3	1:A:155:TYR:CD2	2.48	0.48
1:D:39:SER:HB2	2:G:303:ILE:HG21	1.95	0.48
1:B:522:TYR:HB2	1:B:657:PRO:HG2	1.94	0.48
1:C:232:ASP:OD2	1:C:262:ARG:CZ	2.61	0.48
2:E:328:ARG:CZ	2:E:328:ARG:CB	2.90	0.48
2:F:36:PHE:O	2:F:40:ILE:HG13	2.12	0.48
2:G:195:LEU:HD11	2:G:275:LEU:HD11	1.94	0.48
1:B:576:GLY:CA	1:B:607:LYS:HE2	2.44	0.48
1:A:246:LYS:HG3	1:A:500:ILE:HD11	1.95	0.48
1:A:6:LEU:HD22	1:A:14:THR:CG2	2.43	0.48
1:A:692:SER:HB3	1:A:727:LYS:CD	2.43	0.48
1:A:18:ASN:O	1:A:19:LEU:C	2.51	0.48
1:A:520:PHE:HB3	1:A:635:ILE:HA	1.94	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:36:PHE:O	2:H:40:ILE:HG13	2.14	0.48
1:A:86:ILE:HG22	1:A:90:ARG:HD2	1.95	0.48
2:E:50:PRO:CG	2:E:121:SER:HB3	2.44	0.48
1:C:151:LEU:O	1:C:156:LEU:HG	2.13	0.48
1:A:7:VAL:HG23	1:A:17:ILE:HG22	1.96	0.48
1:A:207:LEU:HD23	1:A:465:SER:OG	2.14	0.48
1:C:253:GLY:C	1:C:438:LEU:HD12	2.26	0.48
1:A:298:ARG:CZ	1:C:6:LEU:HD11	2.44	0.48
2:G:99:ILE:CD1	2:G:108:VAL:HG21	2.43	0.48
1:A:10:ARG:H	1:A:55:THR:HG21	1.78	0.48
1:A:234:LEU:O	1:A:237:ILE:HD12	2.13	0.48
2:F:46:PHE:O	2:F:48:TRP:HD1	1.97	0.48
1:B:350:GLY:HA2	1:B:396:VAL:CG2	2.43	0.48
1:A:220:ARG:O	1:A:496:GLN:HA	2.13	0.48
1:C:388:ILE:O	1:C:389:ARG:C	2.51	0.48
1:B:547:ILE:O	1:B:551:LEU:HG	2.12	0.48
1:A:208:PRO:HD3	1:A:464:LEU:O	2.13	0.48
1:D:339:ILE:HD11	1:D:414:ILE:HD12	1.94	0.48
2:H:178:ASN:OD1	2:H:178:ASN:O	2.30	0.48
2:G:130:VAL:HG12	2:G:131:ASN:H	1.79	0.48
1:C:264:LEU:HD12	1:C:265:GLY:N	2.28	0.48
2:E:156:TYR:HB3	2:E:196:CYS:SG	2.54	0.48
1:D:47:ILE:HD13	1:D:47:ILE:C	2.33	0.48
1:B:466:ALA:CB	1:B:516:GLY:O	2.62	0.48
2:E:206:ILE:HG22	2:E:206:ILE:O	2.14	0.48
1:D:685:MET:CB	1:D:689:ILE:HD11	2.44	0.48
1:A:625:SER:C	1:A:628:ILE:HG22	2.34	0.48
2:G:79:TYR:HB2	2:G:286:TRP:CH2	2.48	0.48
1:D:168:SER:OG	1:D:171:PHE:CB	2.52	0.48
1:D:309:TRP:CH2	1:D:364:LEU:CD1	2.92	0.48
1:D:222:PHE:CB	1:D:492:LEU:HD21	2.43	0.48
2:F:372:ASN:HD22	2:F:373:PHE:N	2.12	0.48
1:B:406:ARG:HD3	1:B:732:GLN:NE2	2.28	0.48
2:F:253:ARG:HG3	2:F:265:ALA:HB1	1.95	0.48
1:D:347:LEU:HD21	1:D:715:LEU:HD22	1.96	0.48
1:C:648:LYS:HE2	1:C:648:LYS:HB3	1.68	0.48
1:C:47:ILE:HG23	1:C:47:ILE:O	2.14	0.48
1:D:394:LYS:H	1:D:394:LYS:HD3	1.78	0.48
1:A:119:LEU:HD12	1:A:119:LEU:N	2.29	0.48
1:D:155:TYR:HE2	1:D:212:MET:HE1	1.79	0.48
2:E:311:ILE:HG23	2:E:312:THR:H	1.78	0.48
1:D:293:SER:CB	1:D:298:ARG:O	2.61	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:441:GLU:OE1	1:D:442:ILE:HG12	2.13	0.48
1:C:44:ARG:NE	1:C:44:ARG:CA	2.73	0.48
2:G:79:TYR:HB2	2:G:286:TRP:CZ2	2.49	0.48
2:G:12:GLN:O	2:G:14:LYS:N	2.47	0.48
1:A:54:LYS:HD3	1:A:56:SER:HB3	1.95	0.48
1:B:54:LYS:HD3	1:B:56:SER:HB3	1.96	0.48
2:G:69:GLU:HG2	2:G:296:MET:HG3	1.96	0.48
2:G:74:ILE:HG12	2:G:78:LYS:HE3	1.95	0.48
2:G:82:LEU:HD22	2:G:146:ILE:HG23	1.96	0.48
1:C:234:LEU:O	1:C:237:ILE:HD12	2.14	0.48
1:A:479:GLU:HB2	1:A:550:TYR:CD1	2.48	0.48
1:B:668:LEU:O	1:B:671:GLU:N	2.41	0.48
1:A:322:ASN:O	1:A:331:ARG:NH1	2.47	0.48
1:D:19:LEU:HB2	2:G:295:SER:HB3	1.96	0.48
2:H:239:ALA:HA	2:H:242:LEU:HD21	1.96	0.48
2:G:288:ASP:O	2:G:292:ARG:HB2	2.13	0.48
1:D:33:LEU:HB2	1:D:36:VAL:HG21	1.96	0.48
1:A:247:TYR:CE1	1:A:499:PRO:HD2	2.48	0.48
1:D:37:SER:OG	2:G:331:PRO:O	2.31	0.48
2:F:20:GLY:N	2:F:100:SER:HB3	2.29	0.48
2:E:92:ASN:O	2:E:96:LEU:HD13	2.14	0.48
1:C:712:GLN:HE21	2:E:370:LEU:CG	2.26	0.48
1:C:19:LEU:HD22	2:E:295:SER:O	2.12	0.48
1:D:406:ARG:NH1	1:D:697:THR:CG2	2.74	0.48
1:A:131:MET:HE3	1:A:193:VAL:HG11	1.96	0.48
2:G:20:GLY:N	2:G:100:SER:HB3	2.29	0.48
2:G:5:PHE:CD1	2:G:24:ASN:O	2.67	0.48
1:A:496:GLN:O	1:A:496:GLN:HG3	2.14	0.48
1:D:388:ILE:O	1:D:389:ARG:C	2.50	0.48
1:B:153:GLY:HA2	1:B:158:GLN:HE22	1.78	0.48
2:H:7:GLN:NE2	2:H:7:GLN:HA	2.29	0.48
1:D:156:LEU:HD22	1:D:167:GLU:HG3	1.95	0.48
1:A:464:LEU:HD22	1:A:514:GLY:O	2.14	0.48
1:A:615:THR:CG2	1:A:691:GLN:HE21	2.25	0.48
1:A:313:VAL:O	1:A:317:LEU:HG	2.14	0.48
1:D:294:GLN:HG2	1:D:298:ARG:HG3	1.96	0.48
1:D:248:VAL:HG21	1:D:289:VAL:HA	1.96	0.48
1:D:102:LEU:O	1:D:106:VAL:HG23	2.14	0.48
2:H:322:ASP:O	2:H:324:PRO:HD3	2.14	0.48
2:E:253:ARG:HG3	2:E:265:ALA:CB	2.44	0.48
1:D:323:ARG:HG3	2:F:292:ARG:CG	2.43	0.48
1:C:47:ILE:C	1:C:47:ILE:HD13	2.34	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:50:PRO:CG	2:H:121:SER:HB3	2.44	0.48
1:A:311:LEU:HA	1:A:355:LEU:HB3	1.96	0.48
1:B:489:LEU:HD22	1:B:513:LEU:HD22	1.95	0.47
1:B:513:LEU:CG	1:B:613:ASN:ND2	2.76	0.47
1:A:5:LEU:CB	1:A:17:ILE:HG12	2.43	0.47
1:B:316:LEU:O	1:B:319:LEU:CG	2.62	0.47
1:A:692:SER:CB	1:A:727:LYS:HB3	2.41	0.47
1:B:145:TYR:OH	1:B:149:LYS:CG	2.62	0.47
2:E:194:TYR:CE1	2:E:249:LEU:HD23	2.50	0.47
1:A:306:TYR:CD2	1:A:316:LEU:HD13	2.49	0.47
1:D:560:LYS:CD	1:D:609:HIS:CE1	2.97	0.47
2:G:194:TYR:CE1	2:G:249:LEU:HD23	2.49	0.47
1:A:86:ILE:O	1:A:90:ARG:HG3	2.14	0.47
1:A:30:ALA:HA	1:A:33:LEU:HD12	1.96	0.47
2:H:253:ARG:HG3	2:H:265:ALA:CB	2.44	0.47
1:A:325:VAL:HG13	1:A:328:ASN:HB3	1.94	0.47
1:A:350:GLY:HA2	1:A:396:VAL:CG2	2.44	0.47
1:C:320:LYS:NZ	1:C:331:ARG:O	2.45	0.47
2:F:374:GLN:O	2:F:375:LEU:OXT	2.31	0.47
1:B:144:SER:O	1:B:145:TYR:C	2.52	0.47
1:A:26:LEU:HB2	1:A:38:ILE:HG23	1.94	0.47
2:H:191:LYS:HG2	2:H:264:ILE:CG2	2.43	0.47
1:B:510:ARG:HA	1:B:565:CYS:SG	2.53	0.47
1:B:696:ASN:HB2	1:B:731:TYR:O	2.14	0.47
1:A:697:THR:HG1	1:A:699:TYR:HE1	1.60	0.47
1:C:618:ALA:O	1:C:619:LEU:HD23	2.14	0.47
2:F:17:MET:HG2	2:F:257:ASP:OD2	2.14	0.47
1:D:479:GLU:HA	1:D:550:TYR:HB3	1.96	0.47
2:E:374:GLN:O	2:E:375:LEU:HD23	2.14	0.47
1:D:264:LEU:HD12	1:D:265:GLY:N	2.28	0.47
1:A:6:LEU:HB2	1:A:51:ASP:OD1	2.15	0.47
1:A:441:GLU:OE1	1:A:442:ILE:HG12	2.13	0.47
1:A:339:ILE:HG22	1:A:340:ASN:N	2.29	0.47
2:F:310:TYR:CA	2:F:328:ARG:HD3	2.44	0.47
2:E:190:LYS:HB3	2:E:261:MET:SD	2.54	0.47
2:G:19:PHE:CE2	2:G:190:LYS:HG2	2.49	0.47
2:H:130:VAL:HG12	2:H:131:ASN:H	1.78	0.47
1:A:47:ILE:HD13	1:A:47:ILE:C	2.34	0.47
1:A:617:SER:CB	1:A:689:ILE:HA	2.44	0.47
1:A:617:SER:HB2	1:A:690:ASP:N	2.21	0.47
1:A:693:ILE:HD12	1:A:693:ILE:H	1.80	0.47
1:C:303:THR:OG1	1:C:438:LEU:HA	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:339:ILE:HD11	1:A:414:ILE:HD12	1.96	0.47
1:C:316:LEU:CA	1:C:319:LEU:HD11	2.37	0.47
1:A:699:TYR:CZ	1:A:714:LEU:HD23	2.49	0.47
1:A:301:ALA:HB1	1:A:438:LEU:HD21	1.95	0.47
1:C:699:TYR:CZ	1:C:714:LEU:HD23	2.50	0.47
1:B:4:ASN:HD22	1:B:5:LEU:HD22	1.80	0.47
1:B:479:GLU:HA	1:B:550:TYR:HB3	1.96	0.47
2:G:7:GLN:NE2	2:G:7:GLN:HA	2.30	0.47
1:B:167:GLU:OE2	1:B:172:LEU:HB2	2.15	0.47
1:A:615:THR:HB	1:A:691:GLN:HE21	1.76	0.47
1:A:516:GLY:HA3	1:A:620:MET:HE3	1.96	0.47
1:B:33:LEU:HB2	1:B:36:VAL:HG21	1.96	0.47
2:E:84:ASP:OD1	2:E:208:PHE:CE2	2.67	0.47
2:H:186:LEU:HG	2:H:190:LYS:HE3	1.96	0.47
1:B:147:ALA:HB2	1:B:627:GLN:O	2.14	0.47
2:H:69:GLU:HG2	2:H:296:MET:HG3	1.95	0.47
1:B:361:VAL:HG11	1:B:364:LEU:HB2	1.92	0.47
2:E:309:GLU:HB3	2:E:328:ARG:HD2	1.97	0.47
1:A:374:GLU:HG3	1:A:378:LEU:HD11	1.96	0.47
2:E:16:PRO:HA	2:E:257:ASP:OD1	2.15	0.47
1:B:356:PHE:CE1	1:B:390:LYS:HB3	2.50	0.47
2:F:58:ASP:O	2:F:61:ASP:HB2	2.15	0.47
1:C:172:LEU:HD23	1:C:212:MET:HE3	1.96	0.47
2:E:205:ALA:O	2:E:311:ILE:HD11	2.15	0.47
2:F:79:TYR:HB2	2:F:286:TRP:CH2	2.49	0.47
2:G:103:GLU:HG2	2:G:104:LEU:H	1.80	0.47
2:E:103:GLU:HG2	2:E:104:LEU:H	1.79	0.47
2:H:311:ILE:HG23	2:H:312:THR:H	1.79	0.47
2:E:19:PHE:CE2	2:E:190:LYS:HG2	2.49	0.47
2:F:204:GLU:HG3	5:F:602:HOH:O	2.13	0.47
2:G:140:ILE:O	2:G:146:ILE:HG21	2.14	0.47
1:A:660:GLU:H	1:A:660:GLU:HG2	1.49	0.47
1:B:47:ILE:O	1:B:47:ILE:HG23	2.14	0.47
1:D:152:GLU:O	1:D:158:GLN:NE2	2.48	0.47
1:B:285:PHE:O	1:B:289:VAL:HG13	2.14	0.47
1:A:214:GLY:HA3	1:A:222:PHE:CE1	2.50	0.47
2:H:124:HIS:O	2:H:128:ASN:ND2	2.47	0.47
2:E:206:ILE:HD13	2:E:312:THR:HG23	1.95	0.47
1:A:227:LEU:CD2	1:A:435:GLN:HG2	2.43	0.47
1:A:339:ILE:HG22	1:A:340:ASN:H	1.80	0.47
2:G:11:ASP:OD2	2:G:13:LEU:HB2	2.14	0.47
2:H:89:ARG:HE	2:H:89:ARG:HB3	1.50	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:53:ILE:HG12	1:D:58:ILE:HG12	1.97	0.47
2:G:186:LEU:HG	2:G:190:LYS:HE3	1.96	0.47
1:D:560:LYS:CD	1:D:609:HIS:ND1	2.77	0.47
1:A:545:GLU:HG3	1:A:595:LEU:CD2	2.42	0.47
2:E:82:LEU:HD22	2:E:146:ILE:HG23	1.96	0.47
2:H:194:TYR:CE1	2:H:249:LEU:HD23	2.50	0.47
1:D:647:SER:HB2	1:D:652:LEU:CD1	2.45	0.47
2:F:82:LEU:HD22	2:F:146:ILE:HG23	1.95	0.47
2:G:20:GLY:HA3	2:G:100:SER:HB3	1.96	0.47
1:B:545:GLU:HG3	1:B:595:LEU:HD23	1.96	0.47
2:H:116:THR:OG1	2:H:117:ILE:HD12	2.14	0.47
1:C:479:GLU:HA	1:C:550:TYR:HB3	1.96	0.47
1:C:347:LEU:HD13	1:C:399:PHE:HB2	1.95	0.47
1:B:64:LYS:HG3	1:B:649:ASP:OD2	2.15	0.47
2:H:9:LYS:H	2:H:9:LYS:HG3	1.60	0.47
1:A:67:ALA:HA	1:A:70:ILE:HD11	1.96	0.47
1:B:115:TYR:CE1	1:B:216:ARG:HG3	2.49	0.47
1:A:10:ARG:H	1:A:55:THR:HG22	1.79	0.47
1:A:234:LEU:HA	1:A:237:ILE:CD1	2.44	0.47
1:A:102:LEU:O	1:A:106:VAL:HG23	2.15	0.47
2:H:82:LEU:HD22	2:H:146:ILE:HG23	1.95	0.47
1:D:510:ARG:HB3	1:D:614:SER:OG	2.14	0.47
2:H:46:PHE:O	2:H:48:TRP:HD1	1.98	0.47
1:D:530:ARG:HB2	1:D:533:ASP:OD2	2.14	0.47
1:C:222:PHE:CB	1:C:492:LEU:HD21	2.44	0.47
1:C:496:GLN:HG3	1:C:496:GLN:O	2.15	0.47
1:D:114:LYS:O	1:D:217:THR:HG22	2.15	0.47
1:C:317:LEU:CD1	1:C:318:VAL:HG13	2.20	0.47
1:D:496:GLN:HG3	1:D:496:GLN:O	2.14	0.47
1:A:369:PHE:CD1	1:A:434:ARG:HA	2.48	0.47
2:E:84:ASP:OD1	2:E:208:PHE:HE2	1.96	0.47
2:F:69:GLU:HG2	2:F:296:MET:HG3	1.97	0.47
1:D:413:TYR:HB3	1:D:729:LEU:O	2.14	0.47
1:A:529:LYS:N	1:A:529:LYS:HD2	2.30	0.47
2:H:6:SER:HB2	2:H:21:GLN:NE2	2.29	0.47
1:C:519:ASN:CG	1:C:631:ALA:HB1	2.35	0.47
1:C:520:PHE:CE2	1:C:524:LEU:HD11	2.49	0.47
1:D:247:TYR:CZ	1:D:499:PRO:HD2	2.49	0.47
1:C:325:VAL:HG13	1:C:328:ASN:HB3	1.96	0.47
1:C:114:LYS:O	1:C:217:THR:HG22	2.15	0.47
1:D:157:VAL:O	1:D:166:TYR:N	2.46	0.47
1:B:114:LYS:HB3	1:B:157:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:228:ILE:C	1:B:435:GLN:HE22	2.18	0.47
1:A:435:GLN:CG	1:A:436:SER:N	2.78	0.47
1:B:369:PHE:O	1:B:421:ASN:ND2	2.48	0.47
1:C:696:ASN:HB2	1:C:731:TYR:O	2.15	0.47
2:F:111:TRP:CD1	2:F:111:TRP:O	2.67	0.47
2:H:68:HIS:O	2:H:72:ILE:HG13	2.15	0.47
2:E:68:HIS:O	2:E:72:ILE:HG13	2.15	0.47
2:G:16:PRO:HA	2:G:257:ASP:OD1	2.15	0.47
1:D:347:LEU:HD13	1:D:399:PHE:HB2	1.95	0.47
1:A:547:ILE:O	1:A:551:LEU:HG	2.15	0.47
2:G:58:ASP:O	2:G:61:ASP:HB2	2.15	0.47
1:D:167:GLU:CD	1:D:216:ARG:HH21	2.19	0.46
1:A:437:ASN:ND2	1:A:439:CYS:HB2	2.26	0.46
1:D:223:SER:OG	1:D:496:GLN:OE1	2.27	0.46
1:A:413:TYR:HE1	1:A:731:TYR:CD2	2.33	0.46
1:C:459:ILE:CD1	1:C:502:ALA:HB3	2.45	0.46
1:B:19:LEU:HD12	1:B:19:LEU:N	2.27	0.46
1:D:225:CYS:O	1:D:462:CYS:HB2	2.15	0.46
1:B:311:LEU:HA	1:B:355:LEU:HB3	1.96	0.46
2:H:153:ILE:HG23	2:H:199:SER:OG	2.15	0.46
1:A:648:LYS:HE2	1:A:648:LYS:HB3	1.76	0.46
2:H:201:ASN:O	2:H:205:ALA:HB2	2.15	0.46
1:D:185:PRO:O	1:D:189:ARG:HB2	2.16	0.46
1:C:403:MET:HG2	1:C:711:MET:HE1	1.97	0.46
2:F:16:PRO:HA	2:F:257:ASP:OD1	2.15	0.46
2:G:253:ARG:HG3	2:G:265:ALA:CB	2.45	0.46
1:D:483:ILE:HA	1:D:554:ALA:HB1	1.97	0.46
1:C:220:ARG:O	1:C:496:GLN:HA	2.15	0.46
1:D:623:GLU:CG	1:D:633:ASN:ND2	2.64	0.46
1:B:496:GLN:O	1:B:496:GLN:HG3	2.14	0.46
1:C:282:TYR:HA	1:C:285:PHE:HD2	1.79	0.46
1:A:282:TYR:CE2	1:A:304:LEU:HD22	2.50	0.46
2:H:90:SER:CB	2:H:91:PRO:HD3	2.46	0.46
1:D:339:ILE:HG22	1:D:340:ASN:N	2.31	0.46
2:G:242:LEU:HD23	2:G:242:LEU:H	1.80	0.46
1:A:185:PRO:O	1:A:189:ARG:HB2	2.16	0.46
1:A:519:ASN:HA	1:A:632:THR:OG1	2.15	0.46
1:D:47:ILE:HG23	1:D:47:ILE:O	2.15	0.46
1:A:357:SER:O	1:A:359:SER:N	2.48	0.46
1:C:350:GLY:HA2	1:C:396:VAL:CG2	2.45	0.46
1:A:588:ASP:O	1:A:591:ALA:O	2.34	0.46
1:B:207:LEU:HD12	1:B:211:ILE:CG2	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:515:ILE:HD13	1:B:551:LEU:HD22	1.97	0.46
2:E:311:ILE:HG23	2:E:312:THR:N	2.31	0.46
1:D:443:ALA:H	1:D:691:GLN:HB3	1.80	0.46
2:H:70:LYS:O	2:H:74:ILE:HG22	2.15	0.46
1:B:226:VAL:CG1	1:B:461:LEU:CD2	2.90	0.46
2:H:111:TRP:CD1	2:H:241:HIS:CD2	3.04	0.46
2:F:309:GLU:HA	2:F:325:PHE:CG	2.50	0.46
2:F:222:GLU:O	2:F:223:LEU:HD23	2.15	0.46
1:B:67:ALA:HA	1:B:70:ILE:HD11	1.97	0.46
1:C:339:ILE:HG22	1:C:340:ASN:N	2.31	0.46
1:C:339:ILE:HD11	1:C:414:ILE:HD12	1.96	0.46
1:A:260:ARG:HD3	1:A:365:TYR:CE2	2.50	0.46
1:B:45:SER:HB2	1:B:61:THR:HG22	1.96	0.46
1:A:483:ILE:HA	1:A:554:ALA:HB1	1.97	0.46
2:E:166:TYR:HB3	2:E:184:VAL:HG21	1.97	0.46
1:C:530:ARG:HB2	1:C:533:ASP:OD2	2.16	0.46
1:B:388:ILE:O	1:B:389:ARG:C	2.51	0.46
1:B:240:THR:HG22	1:B:244:ILE:HD11	1.98	0.46
1:B:306:TYR:CD2	1:B:316:LEU:HD13	2.50	0.46
1:A:620:MET:SD	1:A:620:MET:N	2.78	0.46
1:C:302:ALA:CA	1:C:438:LEU:HD11	2.46	0.46
1:A:309:TRP:CZ3	1:A:364:LEU:HD12	2.50	0.46
1:A:340:ASN:OD1	1:A:343:MET:HG2	2.16	0.46
1:B:641:TYR:O	1:B:656:VAL:HG13	2.15	0.46
1:D:369:PHE:O	1:D:421:ASN:CG	2.54	0.46
1:A:297:VAL:CG1	1:C:4:ASN:HD21	2.26	0.46
2:F:372:ASN:N	2:F:372:ASN:ND2	2.58	0.46
1:D:594:PRO:O	1:D:596:HIS:CD2	2.69	0.46
2:G:25:VAL:HG22	2:G:26:ALA:N	2.30	0.46
2:E:130:VAL:HG12	2:E:131:ASN:H	1.79	0.46
1:A:246:LYS:CG	1:A:500:ILE:HD11	2.45	0.46
2:E:58:ASP:O	2:E:61:ASP:HB2	2.15	0.46
1:D:151:LEU:HA	1:D:155:TYR:HB2	1.97	0.46
1:A:617:SER:C	1:A:689:ILE:HG23	2.36	0.46
1:A:647:SER:OG	1:A:652:LEU:HD11	2.16	0.46
1:C:30:ALA:HA	1:C:33:LEU:HD12	1.97	0.46
1:C:75:PRO:HB2	1:C:660:GLU:OE2	2.16	0.46
1:B:10:ARG:H	1:B:55:THR:HG21	1.78	0.46
2:E:11:ASP:OD2	2:E:13:LEU:HB2	2.16	0.46
2:F:70:LYS:O	2:F:74:ILE:HG22	2.14	0.46
2:H:277:VAL:CG2	2:H:324:PRO:HG3	2.44	0.46
2:H:17:MET:HG2	2:H:257:ASP:OD2	2.14	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:413:TYR:HB3	1:C:729:LEU:O	2.15	0.46
2:E:247:HIS:O	2:E:251:LEU:HG	2.16	0.46
2:F:221:ARG:HG3	2:F:221:ARG:HH11	1.80	0.46
1:B:208:PRO:CD	1:B:464:LEU:O	2.62	0.46
1:C:54:LYS:HG2	1:C:56:SER:H	1.80	0.46
2:E:206:ILE:CD1	2:E:312:THR:HA	2.46	0.46
1:D:329:ARG:HB2	1:D:331:ARG:HH21	1.79	0.46
1:A:361:VAL:CG1	1:A:364:LEU:CB	2.81	0.46
2:G:261:MET:SD	2:G:264:ILE:HD12	2.55	0.46
1:B:565:CYS:HA	1:B:566:PRO:HD3	1.83	0.46
2:E:69:GLU:HG2	2:E:296:MET:HG3	1.98	0.46
2:H:103:GLU:HG2	2:H:104:LEU:H	1.80	0.46
1:D:131:MET:HE1	1:D:178:ALA:HB2	1.98	0.46
2:F:68:HIS:O	2:F:72:ILE:HG13	2.16	0.46
1:B:457:GLY:C	1:B:502:ALA:HB1	2.36	0.46
2:G:124:HIS:HA	2:G:127:ARG:HD3	1.98	0.46
1:B:483:ILE:HA	1:B:554:ALA:HB1	1.96	0.46
1:B:513:LEU:O	1:B:615:THR:O	2.34	0.46
1:B:145:TYR:OH	1:B:149:LYS:HG2	2.16	0.46
1:A:204:LYS:HG2	1:A:481:LEU:HD11	1.96	0.46
2:F:312:THR:HB	2:F:325:PHE:CE2	2.50	0.46
1:D:260:ARG:HG3	1:D:365:TYR:CE2	2.50	0.46
1:A:103:TYR:O	1:A:107:VAL:HG23	2.16	0.46
1:D:647:SER:HB2	1:D:652:LEU:HD11	1.97	0.46
1:B:587:LEU:O	1:B:588:ASP:C	2.51	0.46
1:A:47:ILE:HG23	1:A:47:ILE:O	2.15	0.46
1:B:172:LEU:HD23	1:B:216:ARG:NH2	2.31	0.46
1:B:220:ARG:NH2	1:B:495:TYR:OH	2.48	0.46
1:C:33:LEU:HB2	1:C:36:VAL:HG21	1.98	0.46
1:C:225:CYS:O	1:C:226:VAL:HG13	2.15	0.46
2:F:79:TYR:HB2	2:F:286:TRP:CZ2	2.50	0.46
1:D:374:GLU:OE2	1:D:377:ARG:HD3	2.16	0.46
1:C:19:LEU:HB2	2:E:295:SER:HB3	1.98	0.46
2:F:242:LEU:H	2:F:242:LEU:HD23	1.81	0.46
2:E:310:TYR:CA	2:E:328:ARG:HD3	2.45	0.46
1:B:339:ILE:HG22	1:B:340:ASN:N	2.31	0.46
1:A:131:MET:HA	1:A:134:PHE:CE2	2.50	0.46
2:H:16:PRO:HA	2:H:257:ASP:OD1	2.16	0.46
1:C:483:ILE:HA	1:C:554:ALA:HB1	1.98	0.46
1:D:350:GLY:HA2	1:D:396:VAL:CG2	2.45	0.46
1:B:646:ALA:HB1	1:B:650:GLY:HA2	1.98	0.46
1:B:679:LEU:HD22	1:B:720:THR:HB	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:441:GLU:HG2	1:A:620:MET:HB3	1.98	0.46
1:B:711:MET:HB3	2:H:364:GLU:N	2.31	0.46
1:C:685:MET:CB	1:C:689:ILE:HD11	2.45	0.46
1:D:425:PRO:HG2	1:D:690:ASP:HB3	1.97	0.46
1:A:109:MET:HB2	1:A:115:TYR:CD2	2.51	0.46
2:G:205:ALA:O	2:G:209:TYR:HB2	2.16	0.46
1:A:315:SER:O	1:A:318:VAL:HG22	2.15	0.46
2:G:311:ILE:HG23	2:G:312:THR:N	2.31	0.46
1:C:374:GLU:HG3	1:C:378:LEU:HD11	1.98	0.46
2:F:130:VAL:HG12	2:F:131:ASN:H	1.80	0.46
1:C:480:GLU:OE2	1:C:484:LEU:HD11	2.16	0.46
2:E:46:PHE:O	2:E:48:TRP:HD1	1.98	0.46
1:C:311:LEU:HA	1:C:355:LEU:HB3	1.97	0.46
1:A:347:LEU:HD13	1:A:399:PHE:HB2	1.98	0.46
2:H:365:VAL:O	2:H:365:VAL:HG22	2.15	0.46
1:B:72:ARG:HB3	1:B:642:VAL:HG13	1.98	0.46
1:B:516:GLY:HA3	1:B:620:MET:SD	2.57	0.45
1:B:73:ASP:C	1:B:75:PRO:HD3	2.37	0.45
1:D:73:ASP:C	1:D:75:PRO:HD3	2.36	0.45
1:A:228:ILE:H	1:A:435:GLN:HE22	1.63	0.45
2:H:12:GLN:O	2:H:13:LEU:C	2.54	0.45
2:H:84:ASP:OD1	2:H:208:PHE:HE2	1.99	0.45
1:B:27:ASP:OD1	1:B:38:ILE:HD13	2.16	0.45
2:E:111:TRP:O	2:E:111:TRP:CD1	2.68	0.45
2:F:175:HIS:O	2:F:181:THR:HA	2.15	0.45
1:B:463:THR:HG21	1:B:492:LEU:HD23	1.98	0.45
1:A:5:LEU:C	1:A:17:ILE:HG23	2.37	0.45
2:E:264:ILE:HA	2:E:267:GLU:HG2	1.98	0.45
2:G:203:LEU:HA	2:G:207:ARG:HD2	1.97	0.45
2:E:140:ILE:O	2:E:146:ILE:HG21	2.16	0.45
1:C:234:LEU:HA	1:C:237:ILE:CD1	2.45	0.45
1:C:619:LEU:HD12	1:C:693:ILE:CG2	2.47	0.45
2:F:35:ILE:HG23	2:F:36:PHE:N	2.29	0.45
1:C:697:THR:HG1	1:C:699:TYR:HE1	1.63	0.45
1:A:73:ASP:C	1:A:75:PRO:HD3	2.36	0.45
2:G:49:ARG:HB3	2:G:51:GLU:OE1	2.16	0.45
2:G:116:THR:OG1	2:G:117:ILE:HD12	2.15	0.45
1:D:699:TYR:CZ	1:D:714:LEU:HD23	2.51	0.45
1:A:513:LEU:HD12	1:A:613:ASN:ND2	2.31	0.45
2:F:340:VAL:CG1	2:F:341:SER:CB	2.93	0.45
1:B:701:PRO:HD3	1:B:734:THR:HG22	1.98	0.45
1:A:298:ARG:HE	1:C:6:LEU:CD2	2.11	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:447:LYS:HB2	1:C:458:GLU:N	2.17	0.45
2:H:190:LYS:HB3	2:H:261:MET:SD	2.55	0.45
2:H:176:THR:HG23	2:H:180:LYS:C	2.37	0.45
2:H:242:LEU:HD23	2:H:242:LEU:H	1.81	0.45
2:G:127:ARG:H	2:G:127:ARG:HG2	1.60	0.45
1:C:144:SER:O	1:C:145:TYR:C	2.54	0.45
1:C:73:ASP:C	1:C:75:PRO:HD3	2.37	0.45
2:H:84:ASP:OD1	2:H:208:PHE:CE2	2.69	0.45
1:C:204:LYS:HG2	1:C:481:LEU:HD11	1.99	0.45
1:D:222:PHE:CD2	1:D:492:LEU:CD1	2.92	0.45
1:D:9:LYS:HB3	3:D:801:ATP:PG	2.57	0.45
2:E:203:LEU:HA	2:E:207:ARG:HD2	1.98	0.45
1:C:696:ASN:ND2	1:C:696:ASN:N	2.63	0.45
1:A:320:LYS:CE	1:A:331:ARG:O	2.65	0.45
2:H:136:VAL:O	2:H:140:ILE:HG13	2.17	0.45
2:H:24:ASN:ND2	2:H:25:VAL:HG12	2.32	0.45
1:C:519:ASN:HA	1:C:632:THR:OG1	2.15	0.45
1:B:152:GLU:HG2	1:B:152:GLU:O	2.17	0.45
2:H:9:LYS:NZ	2:H:9:LYS:HB2	2.31	0.45
1:D:367:ALA:O	1:D:371:ASP:O	2.34	0.45
1:A:600:GLU:HA	1:A:603:ARG:HB3	1.98	0.45
1:B:699:TYR:CZ	1:B:714:LEU:HD23	2.51	0.45
1:C:99:PRO:HA	1:C:100:PRO:HD3	1.73	0.45
1:D:114:LYS:CE	1:D:166:TYR:OH	2.62	0.45
1:B:211:ILE:HA	1:B:222:PHE:CD1	2.52	0.45
1:A:5:LEU:CB	1:A:17:ILE:HG21	2.36	0.45
1:A:6:LEU:CD1	1:C:298:ARG:NH1	2.73	0.45
1:C:55:THR:HA	1:C:58:ILE:CD1	2.46	0.45
1:C:254:ILE:O	1:C:302:ALA:HA	2.17	0.45
1:D:316:LEU:HA	1:D:319:LEU:CD1	2.41	0.45
1:A:229:GLU:CD	1:A:434:ARG:HD2	2.36	0.45
2:E:90:SER:HB3	2:E:157:TYR:CE1	2.52	0.45
2:H:90:SER:HB3	2:H:157:TYR:CE1	2.51	0.45
1:B:275:HIS:HD2	1:B:277:GLY:N	2.10	0.45
1:B:524:LEU:HD22	1:B:536:ALA:HB1	1.98	0.45
1:C:714:LEU:CD2	1:C:732:GLN:NE2	2.78	0.45
1:A:519:ASN:CG	1:A:631:ALA:HB1	2.37	0.45
2:G:68:HIS:O	2:G:72:ILE:HG13	2.16	0.45
1:B:313:VAL:HG13	1:B:314:GLU:N	2.31	0.45
1:C:221:GLN:HE21	1:C:221:GLN:HB2	1.58	0.45
2:E:242:LEU:HD23	2:E:242:LEU:H	1.82	0.45
1:A:282:TYR:HA	1:A:285:PHE:HD2	1.81	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:44:ARG:CD	1:C:69:LEU:HD21	2.47	0.45
2:H:311:ILE:HG23	2:H:312:THR:N	2.32	0.45
2:H:278:GLN:NE2	2:H:279:ALA:N	2.65	0.45
1:A:558:LEU:CD2	1:A:612:ARG:HG2	2.47	0.45
1:B:10:ARG:H	1:B:55:THR:HG22	1.80	0.45
1:B:719:LEU:HD22	2:H:375:LEU:HD21	1.99	0.45
1:B:592:ASN:N	1:B:592:ASN:ND2	2.64	0.45
1:B:697:THR:HG1	1:B:699:TYR:HE1	1.65	0.45
1:A:530:ARG:HB2	1:A:533:ASP:OD2	2.16	0.45
2:G:46:PHE:O	2:G:48:TRP:HD1	1.99	0.45
2:H:58:ASP:O	2:H:61:ASP:HB2	2.16	0.45
1:B:515:ILE:HG21	1:B:551:LEU:HD11	1.98	0.45
1:C:290:LYS:HB3	1:C:296:GLY:HA3	1.99	0.45
2:E:204:GLU:HG3	5:E:602:HOH:O	2.15	0.45
2:E:206:ILE:HD13	2:E:312:THR:HA	1.97	0.45
1:D:693:ILE:O	1:D:693:ILE:HD12	2.17	0.45
2:G:35:ILE:HG23	2:G:36:PHE:N	2.31	0.45
1:D:7:VAL:HG23	1:D:17:ILE:HG22	1.97	0.45
1:C:560:LYS:HD3	1:C:609:HIS:NE2	2.32	0.45
2:H:203:LEU:HD23	2:H:203:LEU:O	2.16	0.45
2:E:245:THR:O	2:E:249:LEU:HD12	2.16	0.45
1:A:268:ILE:HD11	1:A:275:HIS:HA	1.99	0.45
2:G:136:VAL:O	2:G:140:ILE:HG13	2.17	0.45
1:A:640:GLY:HA2	1:A:668:LEU:HD13	1.98	0.45
2:G:17:MET:HG2	2:G:257:ASP:OD2	2.17	0.45
1:D:67:ALA:HA	1:D:70:ILE:CD1	2.47	0.45
1:C:385:ASP:O	1:C:390:LYS:HE2	2.16	0.45
2:G:156:TYR:HB3	2:G:196:CYS:SG	2.57	0.45
1:D:99:PRO:HA	1:D:100:PRO:HD3	1.73	0.45
1:C:342:LEU:HD11	1:C:346:ARG:HE	1.82	0.45
1:C:207:LEU:HD12	1:C:211:ILE:CG2	2.46	0.45
1:D:316:LEU:C	1:D:319:LEU:HG	2.35	0.45
1:A:298:ARG:NH2	1:C:6:LEU:CG	2.80	0.45
1:A:568:PHE:CE2	1:A:610:GLY:HA2	2.52	0.45
1:B:55:THR:HG21	3:B:801:ATP:PB	2.57	0.45
2:E:153:ILE:HG23	2:E:199:SER:OG	2.17	0.45
2:G:153:ILE:HG23	2:G:199:SER:OG	2.16	0.45
1:C:268:ILE:HD11	1:C:275:HIS:HA	1.99	0.45
1:A:303:THR:OG1	1:A:438:LEU:HA	2.17	0.45
1:D:647:SER:O	1:D:650:GLY:N	2.50	0.45
2:F:140:ILE:O	2:F:146:ILE:HG21	2.16	0.45
1:C:519:ASN:HD22	1:C:519:ASN:HA	1.58	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:524:LEU:HD22	1:D:536:ALA:HB1	1.99	0.45
1:D:247:TYR:CE1	1:D:499:PRO:HD2	2.52	0.45
1:C:578:LEU:HD12	1:C:580:ILE:HD11	1.99	0.45
1:B:623:GLU:OE1	1:B:623:GLU:HA	2.17	0.45
1:C:114:LYS:HE2	1:C:166:TYR:HE2	1.80	0.45
1:B:516:GLY:HA3	1:B:620:MET:HE1	1.99	0.45
1:C:9:LYS:HE2	3:C:801:ATP:O3G	2.16	0.45
2:H:310:TYR:CA	2:H:328:ARG:HD3	2.47	0.45
1:D:150:GLN:NE2	1:D:645:LYS:NZ	2.63	0.45
1:D:39:SER:OG	2:G:332:ILE:HG22	2.17	0.45
2:F:103:GLU:HG2	2:F:104:LEU:H	1.81	0.45
1:A:730:TYR:O	1:A:731:TYR:C	2.54	0.45
2:G:84:ASP:OD1	2:G:208:PHE:HE2	2.00	0.45
2:F:186:LEU:HG	2:F:190:LYS:HE3	1.99	0.45
2:F:261:MET:SD	2:F:264:ILE:HD12	2.57	0.45
2:H:49:ARG:HB3	2:H:51:GLU:OE1	2.17	0.45
1:B:394:LYS:HD3	1:B:394:LYS:H	1.82	0.45
1:D:156:LEU:HD22	1:D:167:GLU:O	2.16	0.45
1:B:208:PRO:CG	1:B:211:ILE:HD13	2.46	0.45
1:B:617:SER:CA	1:B:689:ILE:HD12	2.45	0.45
1:A:689:ILE:HD13	1:A:693:ILE:HG23	1.99	0.45
1:C:7:VAL:HG11	3:C:801:ATP:C6	2.52	0.45
1:C:254:ILE:H	1:C:438:LEU:HD11	1.73	0.45
1:B:44:ARG:HA	1:B:44:ARG:HD3	1.41	0.45
1:A:224:SER:O	1:A:252:ALA:HB1	2.16	0.45
1:D:425:PRO:HG3	1:D:690:ASP:OD1	2.17	0.45
2:F:20:GLY:HA3	2:F:100:SER:HB3	1.98	0.45
2:G:90:SER:CB	2:G:91:PRO:HD3	2.46	0.45
2:F:311:ILE:HG23	2:F:312:THR:H	1.81	0.45
2:F:203:LEU:O	2:F:203:LEU:HD23	2.17	0.45
2:F:245:THR:O	2:F:249:LEU:HD12	2.17	0.45
1:D:545:GLU:OE2	1:D:597:TYR:CD2	2.69	0.45
1:A:33:LEU:HB2	1:A:36:VAL:HG21	1.99	0.45
1:C:27:ASP:OD1	1:C:38:ILE:HD13	2.17	0.45
1:B:47:ILE:HD13	1:B:47:ILE:C	2.37	0.45
1:B:600:GLU:HA	1:B:603:ARG:HB3	1.98	0.45
1:C:149:LYS:HG2	1:C:652:LEU:HD21	1.99	0.45
2:E:277:VAL:HG22	2:E:324:PRO:HB3	1.99	0.44
2:E:70:LYS:O	2:E:74:ILE:HG22	2.17	0.44
1:B:149:LYS:HA	1:B:149:LYS:HD3	1.87	0.44
2:G:84:ASP:OD1	2:G:208:PHE:CE2	2.70	0.44
2:H:205:ALA:O	2:H:209:TYR:HB2	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:5:LEU:HD12	1:D:17:ILE:CD1	2.47	0.44
1:D:17:ILE:HA	3:D:801:ATP:N1	2.32	0.44
2:G:178:ASN:C	2:G:180:LYS:N	2.70	0.44
2:E:370:LEU:N	2:E:370:LEU:HD23	2.32	0.44
1:B:268:ILE:HD11	1:B:275:HIS:HA	1.99	0.44
1:C:275:HIS:HD2	1:C:277:GLY:N	2.10	0.44
1:B:337:VAL:HB	1:B:414:ILE:HD13	1.99	0.44
1:C:34:HIS:O	1:C:35:ASN:CB	2.65	0.44
1:B:712:GLN:CD	2:H:366:ASP:OD1	2.56	0.44
1:B:643:SER:HB3	1:B:654:GLN:HB3	1.99	0.44
1:D:78:GLN:NE2	1:D:654:GLN:HA	2.32	0.44
1:C:600:GLU:HA	1:C:603:ARG:HB3	1.99	0.44
1:B:626:SER:OG	1:B:633:ASN:HA	2.18	0.44
2:F:299:LEU:HD11	2:F:304:LEU:HD13	1.99	0.44
1:D:229:GLU:CD	1:D:434:ARG:HD2	2.37	0.44
1:C:115:TYR:CD1	1:C:216:ARG:HG3	2.49	0.44
1:C:441:GLU:OE2	1:C:442:ILE:HG12	2.17	0.44
1:D:464:LEU:N	1:D:464:LEU:HD23	2.26	0.44
1:D:623:GLU:O	1:D:627:GLN:HG2	2.18	0.44
1:B:615:THR:HB	1:B:691:GLN:HE21	1.80	0.44
1:C:293:SER:HB2	1:C:296:GLY:CA	2.26	0.44
1:B:249:SER:HA	1:B:292:CYS:SG	2.57	0.44
1:B:289:VAL:O	1:B:300:GLY:HA3	2.16	0.44
1:C:10:ARG:NH2	1:C:91:LYS:HG2	2.32	0.44
1:A:27:ASP:OD1	1:A:38:ILE:HD13	2.18	0.44
1:D:53:ILE:O	1:D:54:LYS:C	2.55	0.44
1:C:18:ASN:O	1:C:19:LEU:C	2.56	0.44
1:A:232:ASP:OD2	1:A:262:ARG:CZ	2.64	0.44
1:A:102:LEU:HG	1:A:135:ILE:CD1	2.47	0.44
2:E:124:HIS:HA	2:E:127:ARG:HD3	2.00	0.44
1:C:222:PHE:HB3	1:C:492:LEU:HD21	1.99	0.44
1:D:207:LEU:HD12	1:D:211:ILE:CG2	2.47	0.44
1:B:441:GLU:HG2	1:B:620:MET:HB3	1.96	0.44
1:C:294:GLN:C	1:C:296:GLY:N	2.71	0.44
1:B:328:ASN:O	1:B:329:ARG:HG3	2.17	0.44
1:D:319:LEU:HB3	1:D:330:VAL:H	1.83	0.44
1:D:44:ARG:HG3	1:D:69:LEU:HD11	1.99	0.44
1:A:298:ARG:HH21	1:C:6:LEU:CG	2.30	0.44
2:F:277:VAL:HG22	2:F:324:PRO:CB	2.47	0.44
1:D:204:LYS:HE3	1:D:481:LEU:HD21	1.98	0.44
1:D:22:ILE:CD1	1:D:22:ILE:H	2.27	0.44
1:B:519:ASN:CG	1:B:631:ALA:HB1	2.38	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:261:MET:SD	2:H:264:ILE:HD12	2.57	0.44
1:D:260:ARG:O	1:D:261:ILE:C	2.55	0.44
2:G:70:LYS:O	2:G:74:ILE:HG22	2.16	0.44
1:A:699:TYR:O	1:A:734:THR:HG22	2.17	0.44
1:C:679:LEU:HD22	1:C:720:THR:HB	1.99	0.44
1:D:578:LEU:HD12	1:D:580:ILE:HD11	1.99	0.44
1:B:556:ASN:O	1:B:559:ALA:HB3	2.17	0.44
1:B:102:LEU:HG	1:B:135:ILE:CD1	2.48	0.44
1:C:692:SER:HB2	1:C:727:LYS:CB	2.45	0.44
1:C:320:LYS:CE	1:C:331:ARG:O	2.66	0.44
2:H:339:LEU:N	2:H:339:LEU:CD1	2.77	0.44
1:D:361:VAL:HG11	1:D:364:LEU:HB2	1.99	0.44
1:A:510:ARG:HG2	1:A:567:TRP:HB2	1.99	0.44
1:D:340:ASN:OD1	1:D:343:MET:HG2	2.18	0.44
1:B:39:SER:CB	2:H:303:ILE:HG21	2.43	0.44
2:G:25:VAL:CG2	2:G:26:ALA:N	2.81	0.44
2:F:49:ARG:HB3	2:F:51:GLU:OE1	2.18	0.44
1:D:207:LEU:CD1	1:D:212:MET:SD	3.05	0.44
1:B:711:MET:CB	2:H:364:GLU:N	2.80	0.44
1:D:248:VAL:HG21	1:D:254:ILE:HG13	1.95	0.44
1:D:319:LEU:HA	1:D:329:ARG:HG3	1.98	0.44
1:D:442:ILE:CG2	1:D:444:LEU:HG	2.48	0.44
2:E:90:SER:HB3	2:E:157:TYR:CZ	2.52	0.44
1:B:55:THR:HG21	3:B:801:ATP:O2B	2.18	0.44
1:A:262:ARG:CG	1:A:275:HIS:CE1	3.01	0.44
1:D:308:MET:HB3	1:D:343:MET:HE2	1.99	0.44
1:D:337:VAL:HB	1:D:414:ILE:HD13	1.99	0.44
2:H:176:THR:HA	2:H:180:LYS:O	2.17	0.44
2:F:62:TYR:HA	2:F:65:LEU:HD12	2.00	0.44
2:G:143:ASN:HB3	2:G:146:ILE:HB	2.00	0.44
1:D:310:HIS:ND1	1:D:311:LEU:N	2.66	0.44
1:C:378:LEU:HB3	1:C:382:TYR:CE2	2.52	0.44
1:C:532:SER:CB	1:C:673:PRO:HD2	2.48	0.44
1:B:367:ALA:O	1:B:371:ASP:O	2.36	0.44
1:B:7:VAL:HG23	1:B:17:ILE:HG22	2.00	0.44
1:A:176:VAL:HA	1:A:215:VAL:CG1	2.46	0.44
1:A:464:LEU:HD13	1:A:620:MET:HE2	1.98	0.44
2:F:205:ALA:O	2:F:209:TYR:HB2	2.17	0.44
2:F:15:GLU:HB2	2:F:101:ILE:HG23	1.99	0.44
1:D:9:LYS:HB3	3:D:801:ATP:O3G	2.17	0.44
1:C:19:LEU:HD22	2:E:295:SER:C	2.37	0.44
1:A:189:ARG:O	1:A:190:LEU:C	2.56	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:177:VAL:HG22	2:H:177:VAL:O	2.18	0.44
1:C:140:ASP:CG	1:C:169:ALA:HB3	2.38	0.44
1:A:74:ALA:N	1:A:75:PRO:HD3	2.33	0.44
1:C:208:PRO:CG	1:C:211:ILE:HD13	2.47	0.44
1:D:148:VAL:HA	1:D:151:LEU:CD1	2.47	0.44
1:B:168:SER:HG	1:B:171:PHE:CB	2.29	0.44
1:B:257:ASN:HD22	1:B:435:GLN:HB3	1.81	0.44
1:C:185:PRO:O	1:C:189:ARG:HB3	2.18	0.44
1:C:369:PHE:O	1:C:421:ASN:OD1	2.36	0.44
1:A:337:VAL:HB	1:A:414:ILE:HD13	2.00	0.44
2:H:90:SER:HB3	2:H:157:TYR:CZ	2.52	0.44
1:A:22:ILE:HD12	1:A:22:ILE:N	2.33	0.44
2:E:12:GLN:O	2:E:13:LEU:C	2.56	0.44
1:A:297:VAL:O	1:A:297:VAL:HG13	2.17	0.44
1:C:711:MET:CE	1:C:715:LEU:HG	2.48	0.44
1:C:711:MET:O	1:C:711:MET:HE2	2.18	0.44
1:D:545:GLU:HG3	1:D:595:LEU:CD2	2.48	0.44
1:B:50:TYR:HE2	1:B:53:ILE:CG1	2.30	0.44
2:E:221:ARG:HG3	2:E:221:ARG:HH11	1.83	0.44
1:B:441:GLU:OE1	1:B:442:ILE:HG12	2.17	0.44
1:B:689:ILE:CG2	1:B:689:ILE:O	2.64	0.44
1:C:302:ALA:HA	1:C:438:LEU:CD1	2.46	0.44
1:C:547:ILE:O	1:C:551:LEU:HG	2.17	0.44
1:C:365:TYR:CE2	1:C:369:PHE:CE2	3.05	0.44
1:A:293:SER:OG	1:A:296:GLY:HA2	2.17	0.44
1:D:461:LEU:HD23	1:D:503:ALA:HB1	1.99	0.44
2:H:111:TRP:CD1	2:H:241:HIS:CE1	3.05	0.44
1:B:205:ILE:HG12	1:B:467:PHE:CD1	2.53	0.44
1:D:54:LYS:HD3	1:D:56:SER:HB3	1.99	0.44
2:E:203:LEU:HD23	2:E:203:LEU:O	2.18	0.44
1:D:268:ILE:HD11	1:D:275:HIS:HA	1.99	0.44
1:D:275:HIS:HD2	1:D:277:GLY:N	2.10	0.44
2:F:177:VAL:HG21	2:F:182:VAL:HG23	2.00	0.44
2:F:98:LEU:CD1	2:F:193:LEU:HD13	2.48	0.44
1:B:263:ALA:HB3	1:B:357:SER:CB	2.48	0.44
2:F:253:ARG:HG3	2:F:265:ALA:CB	2.47	0.44
1:C:45:SER:HB2	1:C:61:THR:HG22	1.99	0.44
2:G:278:GLN:HB3	2:G:278:GLN:HE21	1.63	0.44
1:D:221:GLN:HE21	1:D:221:GLN:HB2	1.54	0.44
1:C:102:LEU:HG	1:C:135:ILE:CD1	2.48	0.44
1:C:464:LEU:HD23	1:C:464:LEU:N	2.32	0.44
1:B:99:PRO:HA	1:B:100:PRO:HD3	1.73	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:209:TYR:CE2	2:F:339:LEU:CD2	3.01	0.44
1:B:711:MET:HE2	1:B:711:MET:O	2.17	0.44
1:D:441:GLU:OE2	1:D:442:ILE:HG12	2.17	0.44
2:F:8:THR:HB	2:F:21:GLN:NE2	2.32	0.44
2:F:90:SER:CB	2:F:91:PRO:HD3	2.45	0.44
2:E:90:SER:CB	2:E:91:PRO:HD3	2.46	0.44
1:A:510:ARG:HG3	1:A:567:TRP:CE3	2.46	0.44
1:C:716:LYS:HG2	2:E:370:LEU:CD1	2.45	0.44
2:F:203:LEU:HA	2:F:207:ARG:HD2	2.00	0.44
2:E:35:ILE:HG23	2:E:36:PHE:N	2.31	0.44
2:G:15:GLU:HB2	2:G:101:ILE:HG23	2.00	0.44
1:C:524:LEU:HB3	1:C:529:LYS:O	2.18	0.44
1:D:600:GLU:HA	1:D:603:ARG:HB3	1.99	0.44
1:A:578:LEU:HD12	1:A:580:ILE:HD11	2.00	0.44
1:B:330:VAL:HB	1:B:335:TYR:OH	2.18	0.43
1:A:441:GLU:CD	1:A:442:ILE:HG12	2.38	0.43
1:A:617:SER:HB3	1:A:689:ILE:HA	2.00	0.43
1:C:10:ARG:H	1:C:55:THR:HG21	1.81	0.43
2:H:309:GLU:HG2	2:H:325:PHE:CG	2.53	0.43
1:D:286:GLN:CD	1:D:332:HIS:HB2	2.32	0.43
1:D:257:ASN:HD22	1:D:435:GLN:HB3	1.83	0.43
1:C:77:TYR:HA	1:C:80:LEU:HB3	2.00	0.43
1:A:114:LYS:HB3	1:A:157:VAL:HG11	2.00	0.43
1:B:144:SER:O	1:B:146:ALA:N	2.50	0.43
1:C:309:TRP:CH2	1:C:364:LEU:HD12	2.52	0.43
2:G:90:SER:HB3	2:G:157:TYR:CZ	2.53	0.43
1:D:50:TYR:CD2	1:D:53:ILE:HB	2.53	0.43
2:F:311:ILE:HG23	2:F:312:THR:N	2.33	0.43
1:B:147:ALA:HB1	1:B:628:ILE:HA	2.00	0.43
1:A:18:ASN:O	1:A:20:ASP:N	2.51	0.43
1:B:250:GLN:NE2	1:B:499:PRO:HG3	2.31	0.43
1:A:592:ASN:N	1:A:592:ASN:ND2	2.66	0.43
2:F:164:THR:OG1	2:F:189:LEU:HD11	2.17	0.43
1:C:172:LEU:CD2	1:C:212:MET:CE	2.96	0.43
1:B:465:SER:O	1:B:515:ILE:HA	2.18	0.43
1:A:5:LEU:HD12	1:A:17:ILE:HD13	1.90	0.43
1:C:17:ILE:HD11	3:C:801:ATP:H2	1.77	0.43
1:A:227:LEU:HD23	1:A:435:GLN:CD	2.38	0.43
1:D:618:ALA:O	1:D:619:LEU:HD23	2.18	0.43
1:C:89:LEU:CD2	1:C:152:GLU:HG3	2.37	0.43
1:B:522:TYR:CE1	1:B:662:LEU:CD1	2.94	0.43
1:B:657:PRO:O	1:B:662:LEU:HD12	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:447:LYS:HB3	1:D:457:GLY:HA2	2.00	0.43
1:A:322:ASN:C	1:A:331:ARG:HH11	2.21	0.43
1:A:134:PHE:N	1:A:134:PHE:CD1	2.86	0.43
1:D:232:ASP:OD2	1:D:262:ARG:NH2	2.51	0.43
2:H:98:LEU:CD1	2:H:193:LEU:HD13	2.48	0.43
2:F:136:VAL:O	2:F:140:ILE:HG13	2.18	0.43
1:B:374:GLU:OE2	1:B:377:ARG:HD3	2.17	0.43
1:C:67:ALA:HA	1:C:70:ILE:CD1	2.48	0.43
1:B:72:ARG:HG2	1:B:72:ARG:H	1.63	0.43
2:H:156:TYR:HB3	2:H:196:CYS:SG	2.58	0.43
2:G:200:VAL:C	2:G:202:ALA:N	2.70	0.43
1:D:648:LYS:HE2	1:D:648:LYS:HB3	1.61	0.43
2:F:60:ILE:H	2:F:60:ILE:HG13	1.66	0.43
1:C:174:ILE:HG23	1:C:175:LEU:H	1.83	0.43
1:C:172:LEU:CD2	1:C:212:MET:HE3	2.48	0.43
1:B:248:VAL:HG11	1:B:289:VAL:CA	2.41	0.43
1:A:465:SER:O	1:A:515:ILE:HA	2.19	0.43
1:B:510:ARG:CG	1:B:567:TRP:HE3	2.27	0.43
1:A:178:ALA:O	1:A:182:SER:N	2.51	0.43
1:D:658:ASP:OD2	1:D:662:LEU:HD12	2.19	0.43
1:A:93:ALA:HB1	1:A:165:ILE:O	2.18	0.43
1:B:4:ASN:ND2	1:B:5:LEU:H	2.15	0.43
1:A:374:GLU:OE2	1:A:377:ARG:HD3	2.19	0.43
1:D:27:ASP:OD1	1:D:38:ILE:HD13	2.18	0.43
1:C:719:LEU:HB3	2:E:375:LEU:CD2	2.49	0.43
1:B:342:LEU:HD11	1:B:346:ARG:HE	1.83	0.43
1:D:313:VAL:HG13	1:D:314:GLU:N	2.33	0.43
1:B:107:VAL:O	1:B:110:VAL:HB	2.19	0.43
1:C:52:GLY:O	1:C:53:ILE:C	2.56	0.43
1:D:316:LEU:O	1:D:319:LEU:HD12	2.17	0.43
1:D:228:ILE:C	1:D:435:GLN:HE22	2.22	0.43
1:C:313:VAL:HG13	1:C:314:GLU:N	2.34	0.43
2:F:92:ASN:CA	2:F:96:LEU:HD13	2.35	0.43
1:D:8:THR:O	1:D:54:LYS:HA	2.19	0.43
1:A:447:LYS:HB3	1:A:457:GLY:HA2	2.01	0.43
1:D:365:TYR:CE2	1:D:369:PHE:HE2	2.36	0.43
1:D:189:ARG:O	1:D:190:LEU:C	2.57	0.43
2:E:21:GLN:HA	2:E:22:PRO:HD3	1.85	0.43
1:B:558:LEU:CD2	1:B:612:ARG:HG2	2.48	0.43
1:A:90:ARG:NH2	1:A:137:HIS:HB3	2.33	0.43
1:C:592:ASN:ND2	1:C:592:ASN:N	2.65	0.43
1:A:711:MET:CE	1:A:715:LEU:HG	2.49	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:116:THR:OG1	2:E:117:ILE:HD12	2.16	0.43
1:C:510:ARG:HB3	1:C:614:SER:OG	2.18	0.43
1:D:207:LEU:HD12	1:D:211:ILE:HG21	2.01	0.43
1:B:513:LEU:HD11	1:B:613:ASN:ND2	2.34	0.43
1:B:319:LEU:HG	1:B:319:LEU:H	1.46	0.43
1:D:620:MET:SD	1:D:620:MET:N	2.79	0.43
2:H:11:ASP:OD2	2:H:13:LEU:HB2	2.19	0.43
2:F:83:LEU:HD22	2:F:203:LEU:CG	2.47	0.43
2:G:203:LEU:HD23	2:G:203:LEU:O	2.18	0.43
1:D:18:ASN:O	1:D:19:LEU:C	2.56	0.43
1:B:719:LEU:HD22	2:H:375:LEU:HD22	2.01	0.43
1:D:185:PRO:HB2	1:D:188:THR:OG1	2.18	0.43
1:A:519:ASN:HD22	1:A:519:ASN:HA	1.59	0.43
1:D:595:LEU:HD13	1:D:599:TRP:CD1	2.54	0.43
1:D:714:LEU:HD22	1:D:732:GLN:NE2	2.34	0.43
1:B:500:ILE:HG23	1:B:501:PRO:HD2	2.01	0.43
2:G:164:THR:OG1	2:G:189:LEU:HD11	2.19	0.43
1:C:498:TYR:HB2	1:C:504:LYS:HB2	2.01	0.43
1:D:342:LEU:HD11	1:D:346:ARG:HE	1.83	0.43
1:D:150:GLN:HE22	1:D:645:LYS:HZ2	1.65	0.43
1:C:74:ALA:N	1:C:75:PRO:HD3	2.33	0.43
1:B:150:GLN:NE2	1:B:645:LYS:NZ	2.67	0.43
1:B:54:LYS:CD	1:B:56:SER:HB3	2.49	0.43
1:B:510:ARG:HG2	1:B:567:TRP:HB2	2.00	0.43
1:C:545:GLU:HA	1:C:688:PHE:CD1	2.53	0.43
1:C:394:LYS:HD3	1:C:394:LYS:N	2.33	0.43
1:A:342:LEU:HD11	1:A:346:ARG:HE	1.82	0.43
1:B:532:SER:HA	1:B:677:GLY:HA3	2.01	0.43
1:A:388:ILE:O	1:A:389:ARG:C	2.57	0.43
1:B:190:LEU:HD22	1:B:190:LEU:N	2.33	0.43
1:C:122:ASP:O	1:C:189:ARG:NH2	2.50	0.43
1:D:403:MET:HG2	1:D:711:MET:HE1	2.01	0.43
1:D:361:VAL:HG12	1:D:364:LEU:HB2	2.00	0.43
1:C:361:VAL:HG11	1:C:364:LEU:HG	2.00	0.43
2:F:84:ASP:OD1	2:F:208:PHE:CE2	2.71	0.43
2:H:85:SER:O	2:H:89:ARG:CZ	2.66	0.43
1:D:311:LEU:HA	1:D:355:LEU:HB3	1.99	0.43
1:D:714:LEU:HD22	1:D:732:GLN:HE22	1.83	0.43
1:A:101:ALA:HB3	1:A:104:ASP:OD2	2.19	0.43
1:D:527:HIS:O	1:D:529:LYS:HD2	2.19	0.43
1:B:207:LEU:HD12	1:B:211:ILE:HG21	2.00	0.43
1:B:441:GLU:CD	1:B:442:ILE:HG12	2.39	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:342:ASP:O	2:H:342:ASP:OD1	2.37	0.43
1:A:617:SER:O	1:A:691:GLN:CG	2.65	0.43
1:C:670:TRP:CD2	1:C:735:ARG:HG3	2.54	0.43
1:D:154:LYS:CE	1:D:624:THR:HG21	2.49	0.43
2:H:95:LEU:N	2:H:95:LEU:HD23	2.34	0.43
2:E:191:LYS:HE2	2:E:267:GLU:OE2	2.19	0.43
1:B:568:PHE:CE2	1:B:610:GLY:HA2	2.54	0.43
2:F:295:SER:OG	2:F:296:MET:N	2.52	0.43
1:D:34:HIS:O	1:D:35:ASN:CB	2.65	0.43
2:E:136:VAL:O	2:E:140:ILE:HG13	2.19	0.43
1:D:641:TYR:O	1:D:656:VAL:HG13	2.18	0.43
1:C:519:ASN:HD21	1:C:657:PRO:HG2	1.83	0.43
1:B:50:TYR:HE2	1:B:53:ILE:HD12	1.82	0.43
1:A:357:SER:O	1:A:358:PRO:C	2.57	0.43
1:C:321:ASN:O	1:C:329:ARG:HG2	2.19	0.43
1:A:583:TYR:CG	1:A:687:LYS:HG3	2.53	0.43
1:D:547:ILE:O	1:D:551:LEU:HG	2.19	0.43
1:A:532:SER:CB	1:A:673:PRO:HD2	2.48	0.43
2:F:340:VAL:HG12	2:F:341:SER:HG	1.70	0.43
2:G:277:VAL:HG22	2:G:324:PRO:CB	2.49	0.43
1:C:617:SER:CB	1:C:689:ILE:HA	2.49	0.43
1:C:685:MET:C	1:C:689:ILE:CG1	2.87	0.43
1:C:515:ILE:HD13	1:C:551:LEU:CD2	2.48	0.43
1:A:722:TYR:HD2	2:F:375:LEU:HD22	1.84	0.43
1:D:50:TYR:HD2	1:D:53:ILE:HB	1.83	0.43
2:F:309:GLU:HB3	2:F:328:ARG:HD2	2.01	0.43
2:E:98:LEU:CD1	2:E:193:LEU:HD13	2.49	0.43
2:G:206:ILE:O	2:G:210:VAL:CG2	2.61	0.43
2:H:20:GLY:N	2:H:100:SER:HB3	2.32	0.43
1:A:291:SER:O	1:B:280:PRO:CB	2.67	0.43
1:D:385:ASP:OD1	1:D:387:SER:OG	2.31	0.43
1:A:45:SER:HB2	1:A:61:THR:HG22	2.00	0.43
2:F:116:THR:OG1	2:F:117:ILE:HD12	2.18	0.43
1:D:165:ILE:HA	1:D:165:ILE:HD13	1.78	0.43
1:A:516:GLY:HA3	1:A:620:MET:CE	2.49	0.43
1:C:686:GLN:CA	1:C:689:ILE:HG12	2.48	0.43
1:B:734:THR:HG22	1:B:735:ARG:H	1.83	0.43
1:C:229:GLU:CD	1:C:434:ARG:HD2	2.39	0.43
1:B:229:GLU:CD	1:B:434:ARG:HD2	2.40	0.43
2:G:91:PRO:HA	2:G:95:LEU:CD1	2.49	0.43
2:E:94:ALA:O	2:E:97:PRO:HD2	2.19	0.43
2:E:369:ASP:OD2	2:E:370:LEU:HD23	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:18:ASN:O	1:B:19:LEU:C	2.56	0.43
1:A:237:ILE:HG13	1:A:237:ILE:H	1.51	0.43
1:D:237:ILE:H	1:D:237:ILE:HG13	1.51	0.43
1:A:452:VAL:HG23	1:A:453:ASN:ND2	2.33	0.43
1:A:75:PRO:HB2	1:A:660:GLU:OE2	2.19	0.43
2:G:117:ILE:HD12	2:G:117:ILE:N	2.34	0.43
1:B:578:LEU:HD12	1:B:580:ILE:HD11	2.01	0.43
1:C:115:TYR:CD1	1:C:216:ARG:HG2	2.53	0.42
1:B:114:LYS:O	1:B:217:THR:HG22	2.18	0.42
1:A:172:LEU:CD2	1:A:216:ARG:NH2	2.68	0.42
2:E:277:VAL:HG22	2:E:324:PRO:CG	2.49	0.42
1:C:466:ALA:HA	1:C:516:GLY:O	2.19	0.42
1:D:150:GLN:CB	1:D:154:LYS:HD2	2.49	0.42
2:G:332:ILE:O	2:G:332:ILE:HD12	2.18	0.42
1:C:258:ALA:HB1	1:C:261:ILE:CD1	2.38	0.42
1:A:447:LYS:CB	1:A:457:GLY:HA2	2.49	0.42
1:B:440:LEU:HB2	1:B:730:TYR:CD1	2.54	0.42
1:B:374:GLU:HG3	1:B:378:LEU:CD1	2.49	0.42
2:H:117:ILE:HD12	2:H:117:ILE:N	2.34	0.42
1:D:531:TYR:CE2	1:D:637:PRO:HD3	2.53	0.42
1:B:617:SER:HB2	1:B:690:ASP:N	2.20	0.42
1:A:513:LEU:HD12	1:A:613:ASN:HD22	1.83	0.42
2:H:309:GLU:HB3	2:H:328:ARG:HD2	2.00	0.42
1:C:369:PHE:O	1:C:421:ASN:ND2	2.52	0.42
1:A:114:LYS:O	1:A:217:THR:HG22	2.19	0.42
2:E:177:VAL:N	2:E:180:LYS:O	2.50	0.42
1:C:276:THR:HG23	1:C:280:PRO:HG2	2.00	0.42
1:D:107:VAL:O	1:D:110:VAL:HB	2.19	0.42
1:A:714:LEU:HD22	1:A:732:GLN:NE2	2.35	0.42
1:D:134:PHE:CD1	1:D:134:PHE:N	2.86	0.42
2:H:21:GLN:HA	2:H:22:PRO:HD3	1.85	0.42
1:C:524:LEU:HD22	1:C:536:ALA:HB1	2.01	0.42
1:A:417:VAL:HG23	1:A:418:ASP:H	1.83	0.42
1:D:700:ASP:CG	1:D:735:ARG:HD2	2.39	0.42
1:A:215:VAL:N	1:A:222:PHE:CE1	2.86	0.42
1:D:74:ALA:N	1:D:75:PRO:HD3	2.35	0.42
2:H:336:ASN:HA	2:H:339:LEU:HD21	2.00	0.42
2:G:90:SER:HB3	2:G:157:TYR:CE1	2.54	0.42
2:F:264:ILE:HA	2:F:267:GLU:HG2	2.00	0.42
1:B:147:ALA:O	1:B:151:LEU:HG	2.19	0.42
1:A:320:LYS:HE2	1:A:331:ARG:O	2.19	0.42
1:A:524:LEU:HD22	1:A:536:ALA:HB1	2.00	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:357:SER:O	1:B:358:PRO:C	2.57	0.42
1:B:153:GLY:O	1:B:160:ARG:NH2	2.46	0.42
2:H:9:LYS:NZ	2:H:9:LYS:CB	2.83	0.42
1:C:500:ILE:HG23	1:C:501:PRO:HD2	2.00	0.42
1:B:34:HIS:ND1	1:B:34:HIS:N	2.65	0.42
1:C:167:GLU:CG	1:C:168:SER:N	2.82	0.42
1:C:212:MET:O	1:C:216:ARG:NH2	2.52	0.42
1:C:220:ARG:NH2	1:C:495:TYR:OH	2.52	0.42
1:D:113:GLY:C	1:D:114:LYS:HD3	2.38	0.42
1:B:222:PHE:H	1:B:496:GLN:HB2	1.85	0.42
1:C:69:LEU:HB2	1:C:77:TYR:CD1	2.54	0.42
2:F:21:GLN:HA	2:F:22:PRO:HD3	1.85	0.42
1:A:204:LYS:HG2	1:A:481:LEU:CD1	2.49	0.42
1:C:279:ILE:HD13	1:C:319:LEU:CD2	2.49	0.42
2:E:143:ASN:HB3	2:E:146:ILE:HB	2.02	0.42
1:C:407:ALA:CA	1:C:732:GLN:OE1	2.67	0.42
1:D:90:ARG:NH2	1:D:137:HIS:HB3	2.34	0.42
1:B:545:GLU:HG3	1:B:595:LEU:CD2	2.50	0.42
2:G:310:TYR:HB2	2:G:328:ARG:HG3	2.01	0.42
2:G:113:PHE:HA	2:G:116:THR:HG23	2.02	0.42
2:H:247:HIS:O	2:H:251:LEU:HG	2.19	0.42
1:A:288:ALA:HB2	1:B:284:HIS:CE1	2.55	0.42
1:A:548:GLN:HE21	1:A:548:GLN:CA	2.32	0.42
1:A:313:VAL:HG13	1:A:314:GLU:N	2.33	0.42
1:C:178:ALA:O	1:C:182:SER:N	2.52	0.42
1:D:256:ILE:HB	1:D:304:LEU:HG	2.00	0.42
1:B:77:TYR:HA	1:B:80:LEU:HB3	2.00	0.42
1:B:467:PHE:CE1	1:B:481:LEU:HB3	2.55	0.42
1:B:519:ASN:CB	1:B:631:ALA:HB1	2.50	0.42
1:A:53:ILE:O	1:A:58:ILE:HD11	2.19	0.42
2:E:261:MET:SD	2:E:264:ILE:HD12	2.59	0.42
2:H:217:ALA:HB1	2:H:296:MET:HE1	2.02	0.42
2:H:96:LEU:CB	2:H:97:PRO:HD3	2.50	0.42
2:G:62:TYR:HA	2:G:65:LEU:HD12	2.00	0.42
1:D:519:ASN:CB	1:D:631:ALA:HB1	2.49	0.42
1:D:385:ASP:O	1:D:390:LYS:HE2	2.20	0.42
1:C:357:SER:O	1:C:358:PRO:C	2.57	0.42
1:B:462:CYS:SG	1:B:462:CYS:O	2.77	0.42
1:B:583:TYR:CG	1:B:687:LYS:HG3	2.54	0.42
1:B:185:PRO:O	1:B:189:ARG:CB	2.67	0.42
1:C:685:MET:HB3	1:C:689:ILE:HD11	2.01	0.42
1:D:293:SER:OG	1:D:296:GLY:CA	2.65	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:670:TRP:CE2	1:C:735:ARG:CG	3.02	0.42
2:G:334:TRP:C	2:G:336:ASN:N	2.71	0.42
2:H:222:GLU:O	2:H:223:LEU:HD23	2.20	0.42
2:F:96:LEU:CB	2:F:97:PRO:HD3	2.49	0.42
2:F:84:ASP:OD1	2:F:208:PHE:HE2	2.02	0.42
2:E:99:ILE:HG21	2:E:105:GLU:HB2	2.01	0.42
1:A:10:ARG:NH2	1:A:91:LYS:HG2	2.35	0.42
2:H:264:ILE:HA	2:H:267:GLU:HG2	2.01	0.42
2:G:295:SER:OG	2:G:296:MET:N	2.53	0.42
2:G:366:ASP:OD1	2:G:369:ASP:HB3	2.19	0.42
1:A:378:LEU:HB3	1:A:382:TYR:CE2	2.54	0.42
1:D:347:LEU:HD22	1:D:399:PHE:CG	2.54	0.42
1:C:347:LEU:HD22	1:C:399:PHE:CG	2.54	0.42
1:D:532:SER:CB	1:D:673:PRO:HD2	2.49	0.42
2:E:164:THR:OG1	2:E:189:LEU:HD11	2.19	0.42
1:B:385:ASP:OD1	1:B:387:SER:OG	2.31	0.42
1:A:34:HIS:N	1:A:34:HIS:ND1	2.65	0.42
2:E:206:ILE:HD13	2:E:312:THR:CG2	2.50	0.42
2:E:295:SER:OG	2:E:296:MET:N	2.52	0.42
1:D:519:ASN:CG	1:D:631:ALA:HB1	2.40	0.42
2:H:245:THR:O	2:H:249:LEU:HD12	2.19	0.42
1:D:394:LYS:HD3	1:D:394:LYS:N	2.35	0.42
1:B:532:SER:CB	1:B:673:PRO:HD2	2.50	0.42
1:B:704:PHE:O	1:B:707:GLY:N	2.51	0.42
1:B:347:LEU:HD13	1:B:399:PHE:HB2	2.01	0.42
1:C:548:GLN:CA	1:C:548:GLN:HE21	2.33	0.42
1:C:167:GLU:OE1	1:C:172:LEU:HA	2.20	0.42
1:C:301:ALA:C	1:C:438:LEU:CD1	2.78	0.42
1:C:184:TYR:HB3	1:C:189:ARG:HB2	2.02	0.42
1:C:369:PHE:CE2	1:C:434:ARG:CB	3.03	0.42
1:D:37:SER:OG	2:G:333:PRO:HD3	2.19	0.42
1:A:298:ARG:NH2	1:C:6:LEU:HG	2.35	0.42
1:A:52:GLY:O	1:A:53:ILE:CG2	2.68	0.42
1:D:447:LYS:CB	1:D:457:GLY:HA2	2.50	0.42
1:D:621:PRO:HD3	1:D:694:SER:OG	2.20	0.42
2:G:98:LEU:CD1	2:G:193:LEU:HD13	2.49	0.42
2:H:143:ASN:HB3	2:H:146:ILE:HB	2.00	0.42
1:C:452:VAL:HG23	1:C:453:ASN:ND2	2.34	0.42
1:C:374:GLU:OE2	1:C:377:ARG:HD3	2.20	0.42
1:A:532:SER:HA	1:A:677:GLY:HA3	2.01	0.42
1:A:199:ALA:HB2	1:A:484:LEU:HD13	2.01	0.42
1:A:394:LYS:H	1:A:394:LYS:HD3	1.84	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:584:LYS:HG3	1:B:586:ASP:H	1.85	0.42
1:C:207:LEU:HD12	1:C:211:ILE:HG21	2.01	0.42
1:B:441:GLU:HG2	1:B:620:MET:HB2	1.99	0.42
1:B:515:ILE:O	1:B:618:ALA:O	2.37	0.42
1:B:282:TYR:O	1:B:285:PHE:HB2	2.20	0.42
1:C:22:ILE:CD1	1:C:22:ILE:H	2.29	0.42
1:D:52:GLY:O	1:D:53:ILE:CG2	2.68	0.42
1:C:319:LEU:HB3	1:C:330:VAL:H	1.85	0.42
1:B:55:THR:HG21	3:B:801:ATP:O1B	2.20	0.42
2:G:264:ILE:HA	2:G:267:GLU:HG2	2.01	0.42
2:H:295:SER:OG	2:H:296:MET:N	2.52	0.42
1:B:696:ASN:N	1:B:696:ASN:ND2	2.63	0.42
1:A:714:LEU:HD22	1:A:732:GLN:HE22	1.84	0.42
1:B:545:GLU:HA	1:B:688:PHE:CD1	2.54	0.42
2:G:73:PHE:CE2	2:G:224:MET:HE3	2.55	0.42
1:D:500:ILE:HG23	1:D:501:PRO:HD2	2.01	0.42
1:C:450:ASN:N	1:C:450:ASN:ND2	2.67	0.42
1:B:134:PHE:HB3	1:B:194:LYS:HG3	2.02	0.42
1:C:131:MET:HE3	1:C:193:VAL:CG1	2.50	0.42
1:B:621:PRO:CD	1:B:694:SER:OG	2.67	0.42
2:G:336:ASN:HA	2:G:339:LEU:HD11	2.01	0.42
1:B:369:PHE:CE1	1:B:434:ARG:O	2.72	0.42
2:G:36:PHE:CE1	2:G:104:LEU:HD13	2.55	0.42
2:G:83:LEU:HD22	2:G:203:LEU:CG	2.49	0.42
1:D:452:VAL:HG23	1:D:453:ASN:ND2	2.34	0.42
1:C:519:ASN:HD22	1:C:632:THR:H	1.66	0.42
1:B:50:TYR:HE2	1:B:53:ILE:CD1	2.33	0.42
1:B:50:TYR:HE2	1:B:53:ILE:HG13	1.84	0.42
1:A:500:ILE:HG23	1:A:501:PRO:HD2	2.01	0.42
1:C:479:GLU:HG3	1:C:550:TYR:CD1	2.54	0.42
1:A:643:SER:HB3	1:A:654:GLN:HB3	2.02	0.42
1:D:250:GLN:O	1:D:251:ARG:C	2.58	0.42
2:F:156:TYR:HB3	2:F:196:CYS:SG	2.60	0.42
1:C:131:MET:HA	1:C:134:PHE:CD2	2.55	0.41
1:D:286:GLN:CD	1:D:332:HIS:CG	2.93	0.41
1:D:77:TYR:HA	1:D:80:LEU:HB3	2.02	0.41
1:A:413:TYR:HB3	1:A:729:LEU:O	2.19	0.41
2:H:203:LEU:HA	2:H:207:ARG:HD2	2.02	0.41
1:A:320:LYS:NZ	1:A:331:ARG:O	2.53	0.41
2:G:245:THR:O	2:G:249:LEU:HD12	2.20	0.41
1:D:545:GLU:HA	1:D:688:PHE:CD1	2.55	0.41
1:A:69:LEU:HB2	1:A:77:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:583:TYR:HB3	1:B:687:LYS:HG3	2.02	0.41
1:D:45:SER:HB2	1:D:61:THR:HG22	2.01	0.41
2:F:124:HIS:HA	2:F:127:ARG:HD3	2.00	0.41
1:B:463:THR:HB	1:B:489:LEU:HD21	2.02	0.41
1:B:686:GLN:OE1	1:B:727:LYS:HG3	2.19	0.41
1:A:696:ASN:N	1:A:696:ASN:ND2	2.64	0.41
1:A:730:TYR:O	1:A:731:TYR:O	2.37	0.41
2:G:92:ASN:CA	2:G:96:LEU:HD13	2.37	0.41
1:D:55:THR:CG2	1:D:56:SER:N	2.84	0.41
1:D:545:GLU:OE2	1:D:597:TYR:HD2	2.03	0.41
2:E:132:ASP:HA	2:E:133:PRO:HD3	1.91	0.41
1:A:77:TYR:HA	1:A:80:LEU:HB3	2.02	0.41
1:A:426:PHE:HA	1:A:571:THR:HA	2.01	0.41
2:E:49:ARG:HB3	2:E:51:GLU:OE1	2.20	0.41
1:B:178:ALA:O	1:B:182:SER:N	2.53	0.41
2:F:147:GLN:HA	2:F:150:ALA:HB3	2.02	0.41
1:D:463:THR:HB	1:D:489:LEU:CD2	2.51	0.41
1:C:254:ILE:CG2	1:C:256:ILE:CG1	2.95	0.41
1:C:134:PHE:N	1:C:134:PHE:CD1	2.86	0.41
1:D:69:LEU:HB2	1:D:77:TYR:CD1	2.55	0.41
1:A:244:ILE:O	1:A:248:VAL:HG23	2.19	0.41
2:F:102:PRO:HG2	2:F:103:GLU:H	1.86	0.41
2:H:111:TRP:CD1	2:H:241:HIS:NE2	2.88	0.41
1:D:3:GLN:N	1:D:5:LEU:HD21	2.35	0.41
2:E:12:GLN:C	2:E:14:LYS:N	2.73	0.41
1:B:38:ILE:HB	2:H:303:ILE:HD11	2.02	0.41
1:A:185:PRO:HB2	1:A:188:THR:OG1	2.21	0.41
1:A:94:TYR:C	1:A:96:GLN:H	2.23	0.41
1:A:220:ARG:NH2	1:A:495:TYR:OH	2.53	0.41
1:B:101:ALA:HB3	1:B:104:ASP:OD2	2.20	0.41
1:D:101:ALA:HB3	1:D:104:ASP:OD2	2.19	0.41
2:E:216:PHE:HZ	2:E:232:ARG:HA	1.85	0.41
2:H:200:VAL:C	2:H:202:ALA:N	2.72	0.41
2:H:164:THR:OG1	2:H:189:LEU:HD11	2.20	0.41
1:D:505:ARG:HG2	1:D:505:ARG:HH11	1.86	0.41
1:C:94:TYR:C	1:C:96:GLN:H	2.24	0.41
1:B:220:ARG:CZ	1:B:495:TYR:CE1	3.03	0.41
1:A:214:GLY:C	1:A:222:PHE:HE1	2.24	0.41
1:B:134:PHE:CD1	1:B:134:PHE:N	2.86	0.41
1:B:131:MET:HA	1:B:134:PHE:CD2	2.56	0.41
1:A:435:GLN:OE1	1:A:446:THR:HG21	2.20	0.41
1:D:685:MET:C	1:D:689:ILE:HG13	2.33	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:37:SER:OG	2:G:333:PRO:CD	2.68	0.41
1:A:440:LEU:HB2	1:A:730:TYR:CE1	2.55	0.41
1:D:5:LEU:HD23	1:D:5:LEU:N	2.35	0.41
1:B:569:ASN:ND2	1:B:570:GLU:N	2.65	0.41
1:D:718:LEU:HD13	1:D:729:LEU:HD11	2.02	0.41
1:A:276:THR:HG21	1:B:291:SER:O	2.20	0.41
1:C:519:ASN:CB	1:C:631:ALA:HB1	2.51	0.41
1:B:595:LEU:HD13	1:B:599:TRP:CD1	2.55	0.41
1:A:67:ALA:HA	1:A:70:ILE:CD1	2.50	0.41
1:D:532:SER:HA	1:D:677:GLY:HA3	2.01	0.41
2:F:169:LEU:HB2	2:F:170:LEU:HG	2.02	0.41
1:A:125:GLU:HG2	1:A:129:LYS:HD2	2.02	0.41
1:C:107:VAL:O	1:C:110:VAL:HB	2.20	0.41
1:B:617:SER:HB3	1:B:689:ILE:CD1	2.39	0.41
1:A:5:LEU:O	1:A:17:ILE:HG23	2.20	0.41
1:B:245:VAL:HA	1:B:248:VAL:HG22	2.02	0.41
1:B:122:ASP:O	1:B:189:ARG:NH2	2.50	0.41
1:C:681:LEU:O	1:C:685:MET:HG3	2.21	0.41
1:B:700:ASP:OD1	1:B:735:ARG:CG	2.68	0.41
1:B:74:ALA:N	1:B:75:PRO:HD3	2.34	0.41
1:C:304:LEU:HD12	1:C:333:MET:SD	2.60	0.41
2:G:102:PRO:HG2	2:G:103:GLU:H	1.86	0.41
1:B:722:TYR:HD2	2:H:375:LEU:HB3	1.85	0.41
1:A:107:VAL:O	1:A:110:VAL:HB	2.19	0.41
1:D:178:ALA:O	1:D:182:SER:N	2.54	0.41
1:C:407:ALA:HB2	1:C:732:GLN:OE1	2.20	0.41
1:A:4:ASN:CG	1:C:297:VAL:HG11	2.41	0.41
1:B:263:ALA:HB3	1:B:357:SER:HB2	2.02	0.41
1:B:263:ALA:CB	1:B:357:SER:OG	2.67	0.41
1:B:347:LEU:HD21	1:B:715:LEU:HD22	2.03	0.41
1:D:94:TYR:C	1:D:96:GLN:H	2.23	0.41
1:B:548:GLN:HE21	1:B:548:GLN:CA	2.34	0.41
1:C:155:TYR:O	1:C:172:LEU:HD11	2.20	0.41
1:C:625:SER:C	1:C:628:ILE:HG22	2.37	0.41
2:G:96:LEU:CB	2:G:97:PRO:HD3	2.50	0.41
1:D:9:LYS:HE2	3:D:801:ATP:O1G	2.21	0.41
1:A:52:GLY:C	1:A:53:ILE:CG2	2.89	0.41
1:B:510:ARG:HB3	1:B:614:SER:OG	2.21	0.41
1:A:279:ILE:HD13	1:A:319:LEU:HD22	2.02	0.41
1:D:519:ASN:HD22	1:D:632:THR:H	1.66	0.41
1:C:407:ALA:HA	1:C:732:GLN:OE1	2.20	0.41
1:C:532:SER:HA	1:C:677:GLY:HA3	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:278:GLN:NE2	2:F:279:ALA:N	2.69	0.41
1:D:679:LEU:HD22	1:D:720:THR:HB	2.02	0.41
2:H:299:LEU:HD11	2:H:304:LEU:HD13	2.02	0.41
2:H:236:ARG:HD3	2:H:342:ASP:CG	2.40	0.41
1:A:442:ILE:CG2	1:A:444:LEU:HG	2.50	0.41
1:D:286:GLN:OE1	1:D:332:HIS:CG	2.74	0.41
1:D:444:LEU:HD12	1:D:460:ALA:HB1	2.03	0.41
1:D:378:LEU:HB3	1:D:382:TYR:CE2	2.52	0.41
2:G:12:GLN:O	2:G:13:LEU:C	2.57	0.41
2:G:99:ILE:HG21	2:G:105:GLU:HB2	2.03	0.41
2:E:91:PRO:HA	2:E:95:LEU:CD1	2.50	0.41
1:B:62:ILE:CD1	1:B:84:LEU:HD22	2.48	0.41
2:E:191:LYS:C	2:E:193:LEU:H	2.24	0.41
1:D:131:MET:HA	1:D:134:PHE:CD2	2.56	0.41
1:D:310:HIS:O	1:D:355:LEU:HD22	2.21	0.41
1:A:83:ARG:HG2	1:A:83:ARG:H	1.63	0.41
1:B:712:GLN:OE1	2:H:366:ASP:OD1	2.38	0.41
1:C:207:LEU:CG	1:C:212:MET:SD	3.09	0.41
1:D:172:LEU:HD11	1:D:212:MET:HG2	2.03	0.41
1:B:220:ARG:CZ	1:B:495:TYR:HE1	2.34	0.41
1:B:689:ILE:HA	1:B:689:ILE:HD12	1.91	0.41
1:C:10:ARG:N	3:C:801:ATP:O2G	2.54	0.41
1:A:298:ARG:NH2	1:C:6:LEU:CD2	2.74	0.41
1:B:365:TYR:O	1:B:366:ASP:C	2.57	0.41
1:A:369:PHE:CD2	1:A:434:ARG:HG2	2.55	0.41
1:D:374:GLU:HG3	1:D:378:LEU:CD1	2.51	0.41
1:A:716:LYS:HG2	2:F:370:LEU:CD1	2.44	0.41
1:A:8:THR:O	1:A:54:LYS:HA	2.21	0.41
2:G:177:VAL:HG12	2:G:178:ASN:N	2.36	0.41
2:E:83:LEU:HD22	2:E:203:LEU:CG	2.48	0.41
1:C:640:GLY:HA2	1:C:668:LEU:HD13	2.03	0.41
1:B:712:GLN:NE2	2:H:366:ASP:OD1	2.53	0.41
1:B:67:ALA:HA	1:B:70:ILE:CD1	2.51	0.41
1:C:578:LEU:HB2	1:C:580:ILE:HG12	2.02	0.41
1:A:321:ASN:HB2	1:A:405:GLU:OE1	2.20	0.41
1:D:4:ASN:HB3	1:D:16:ARG:NH1	2.35	0.41
1:C:125:GLU:HG2	1:C:129:LYS:HD2	2.03	0.41
1:D:583:TYR:CG	1:D:687:LYS:HG3	2.55	0.41
1:B:450:ASN:ND2	1:B:450:ASN:N	2.66	0.41
1:C:115:TYR:HE1	1:C:216:ARG:HH11	1.67	0.41
1:D:148:VAL:HA	1:D:151:LEU:HD12	2.03	0.41
1:D:151:LEU:HG	1:D:151:LEU:H	1.63	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:617:SER:HB2	1:B:689:ILE:HD12	1.94	0.41
2:H:216:PHE:HZ	2:H:232:ARG:HA	1.86	0.41
1:B:131:MET:HE3	1:B:193:VAL:CG1	2.49	0.41
1:C:278:CYS:O	1:C:282:TYR:CD1	2.71	0.41
1:D:617:SER:CB	1:D:689:ILE:HA	2.50	0.41
1:A:369:PHE:CZ	1:A:434:ARG:CA	3.04	0.41
1:B:645:LYS:O	1:B:652:LEU:HB2	2.21	0.41
1:C:361:VAL:HG11	1:C:364:LEU:CG	2.50	0.41
2:E:96:LEU:CB	2:E:97:PRO:HD3	2.51	0.41
2:G:179:GLY:O	2:G:180:LYS:HD2	2.17	0.41
2:H:278:GLN:HB3	2:H:278:GLN:HE21	1.64	0.41
1:A:40:GLN:HE21	2:F:333:PRO:HG2	1.82	0.41
1:B:510:ARG:NH1	1:B:567:TRP:CZ3	2.89	0.41
1:A:545:GLU:HA	1:A:688:PHE:CD1	2.56	0.41
2:G:65:LEU:CD2	2:G:223:LEU:HD13	2.47	0.41
1:A:699:TYR:HB2	1:A:734:THR:HG22	2.03	0.41
2:F:143:ASN:HB3	2:F:146:ILE:HB	2.03	0.41
1:B:90:ARG:NH2	1:B:137:HIS:HB3	2.36	0.41
1:A:519:ASN:HD22	1:A:632:THR:H	1.69	0.41
1:D:707:GLY:O	1:D:708:LYS:HD2	2.21	0.41
2:F:73:PHE:CE2	2:F:224:MET:HE3	2.56	0.41
2:G:231:ILE:O	2:G:234:ILE:HB	2.21	0.41
1:D:417:VAL:HG23	1:D:418:ASP:H	1.86	0.41
2:E:50:PRO:HB3	2:E:121:SER:HB3	2.02	0.41
1:A:223:SER:OG	1:A:496:GLN:OE1	2.33	0.41
2:E:113:PHE:HA	2:E:116:THR:HG23	2.03	0.41
1:A:431:ALA:HB1	1:A:445:PRO:CG	2.51	0.41
2:H:147:GLN:HA	2:H:150:ALA:HB3	2.02	0.41
2:E:151:GLU:HA	2:E:154:SER:HG	1.85	0.41
1:D:450:ASN:ND2	1:D:450:ASN:N	2.66	0.41
1:A:450:ASN:ND2	1:A:450:ASN:N	2.67	0.41
2:G:304:LEU:HA	2:G:304:LEU:HD12	1.93	0.41
1:B:333:MET:O	1:B:335:TYR:CE1	2.74	0.41
1:A:465:SER:HB3	1:A:515:ILE:HG23	2.03	0.41
1:C:417:VAL:HG23	1:C:418:ASP:H	1.85	0.41
1:C:417:VAL:CG2	1:C:418:ASP:N	2.83	0.41
1:A:647:SER:C	1:A:649:ASP:N	2.72	0.41
1:C:461:LEU:HD23	1:C:503:ALA:HB1	2.03	0.41
1:A:633:ASN:O	1:A:634:GLY:C	2.59	0.41
1:C:228:ILE:CD1	1:C:459:ILE:HG12	2.42	0.41
1:D:529:LYS:H	1:D:529:LYS:HD2	1.86	0.41
1:D:480:GLU:OE2	1:D:484:LEU:HD11	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:68:ASP:OD2	1:B:651:ILE:HG21	2.21	0.41
1:A:5:LEU:CD1	1:A:17:ILE:HD13	2.47	0.40
2:E:273:TYR:HE2	2:E:324:PRO:HG3	1.85	0.40
1:C:302:ALA:CA	1:C:438:LEU:HD21	2.51	0.40
1:D:226:VAL:HG12	1:D:461:LEU:HD22	2.03	0.40
1:D:7:VAL:HG11	3:D:801:ATP:C6	2.56	0.40
2:H:191:LYS:HE2	2:H:267:GLU:OE2	2.22	0.40
1:A:596:HIS:CB	1:A:597:TYR:CE2	3.04	0.40
1:B:340:ASN:OD1	1:B:343:MET:HG2	2.20	0.40
1:C:305:PHE:CZ	1:C:436:SER:HB3	2.57	0.40
1:C:247:TYR:CZ	1:C:499:PRO:HD2	2.55	0.40
2:H:113:PHE:HA	2:H:116:THR:HG23	2.03	0.40
2:F:127:ARG:HG2	2:F:127:ARG:H	1.59	0.40
1:D:583:TYR:HB3	1:D:687:LYS:HG3	2.03	0.40
1:D:208:PRO:CG	1:D:211:ILE:HD13	2.47	0.40
1:C:254:ILE:CA	1:C:438:LEU:HD12	2.43	0.40
1:D:253:GLY:CA	1:D:438:LEU:CD1	3.00	0.40
1:D:150:GLN:O	1:D:154:LYS:N	2.49	0.40
1:D:403:MET:HG2	1:D:711:MET:CE	2.50	0.40
1:A:369:PHE:CE1	1:A:434:ARG:CA	2.99	0.40
2:G:177:VAL:CB	2:G:180:LYS:O	2.59	0.40
1:C:569:ASN:ND2	1:C:570:GLU:N	2.65	0.40
1:C:19:LEU:H	1:C:19:LEU:CD1	2.16	0.40
2:H:99:ILE:HG21	2:H:105:GLU:HB2	2.03	0.40
1:A:699:TYR:HB2	1:A:734:THR:CG2	2.51	0.40
1:B:487:ARG:HD3	1:B:558:LEU:HD22	2.03	0.40
1:D:325:VAL:HG13	1:D:328:ASN:CB	2.51	0.40
1:C:199:ALA:HB2	1:C:484:LEU:HD13	2.04	0.40
1:B:321:ASN:HB2	1:B:405:GLU:OE1	2.20	0.40
2:E:299:LEU:HD11	2:E:304:LEU:HD13	2.03	0.40
1:C:463:THR:HB	1:C:489:LEU:CD2	2.50	0.40
1:D:208:PRO:HG2	1:D:211:ILE:CD1	2.50	0.40
1:B:208:PRO:HG2	1:B:211:ILE:CD1	2.49	0.40
1:B:286:GLN:HE22	1:B:332:HIS:CG	2.35	0.40
1:B:316:LEU:CA	1:B:319:LEU:HD11	2.48	0.40
1:A:517:VAL:HG22	1:A:518:ILE:N	2.36	0.40
1:C:131:MET:HE1	1:C:178:ALA:HB2	2.04	0.40
2:G:336:ASN:O	2:G:339:LEU:HD12	2.21	0.40
2:F:277:VAL:CG2	2:F:324:PRO:HB3	2.50	0.40
2:E:334:TRP:C	2:E:336:ASN:N	2.72	0.40
1:A:569:ASN:ND2	1:A:570:GLU:N	2.65	0.40
1:C:558:LEU:HD23	1:C:612:ARG:HG2	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:592:ASN:ND2	1:D:592:ASN:N	2.65	0.40
1:D:670:TRP:HB3	1:D:735:ARG:NH1	2.36	0.40
1:C:144:SER:O	1:C:146:ALA:N	2.55	0.40
1:D:578:LEU:HB2	1:D:580:ILE:HG12	2.03	0.40
2:G:147:GLN:HA	2:G:150:ALA:HB3	2.03	0.40
1:C:509:GLY:O	1:C:566:PRO:HD2	2.22	0.40
1:C:431:ALA:HB1	1:C:445:PRO:CG	2.52	0.40
1:D:404:GLN:HE21	1:D:404:GLN:HB2	1.69	0.40
2:F:247:HIS:O	2:F:251:LEU:HG	2.21	0.40
1:B:513:LEU:HD11	1:B:613:ASN:HD21	1.86	0.40
1:B:94:TYR:CD1	1:B:100:PRO:HD2	2.57	0.40
1:B:228:ILE:CD1	1:B:459:ILE:HG12	2.41	0.40
1:A:155:TYR:CE1	1:A:212:MET:HG2	2.55	0.40
2:H:332:ILE:O	2:H:332:ILE:HG13	2.21	0.40
1:C:185:PRO:O	1:C:189:ARG:HB2	2.22	0.40
1:B:69:LEU:HB2	1:B:77:TYR:CD1	2.56	0.40
2:E:339:LEU:CD1	2:E:340:VAL:CG2	2.90	0.40
2:H:65:LEU:HA	2:H:66:PRO:HD3	1.86	0.40
1:D:378:LEU:O	1:D:381:LYS:HB3	2.22	0.40
1:D:361:VAL:HG13	1:D:382:TYR:CE2	2.57	0.40
1:C:204:LYS:HG2	1:C:481:LEU:CD1	2.52	0.40
1:B:519:ASN:HD22	1:B:632:THR:H	1.69	0.40
1:A:55:THR:HG21	3:A:801:ATP:O2B	2.22	0.40
2:H:279:ALA:HA	2:H:282:GLN:OE1	2.21	0.40
1:A:711:MET:HE1	1:A:715:LEU:HG	2.03	0.40
2:F:117:ILE:N	2:F:117:ILE:HD12	2.37	0.40
1:A:288:ALA:HB2	1:B:284:HIS:HE1	1.85	0.40
1:B:125:GLU:HG2	1:B:129:LYS:HD2	2.04	0.40
2:E:200:VAL:C	2:E:202:ALA:N	2.71	0.40
2:G:145:GLN:HG2	2:G:289:TYR:CG	2.57	0.40
1:D:507:ALA:O	1:D:508:MET:C	2.60	0.40
1:A:585:LYS:C	1:A:587:LEU:H	2.24	0.40
2:H:115:GLU:OE1	2:H:115:GLU:HA	2.22	0.40
1:D:207:LEU:HD11	1:D:212:MET:SD	2.62	0.40
2:F:11:ASP:OD1	2:F:13:LEU:HD12	2.22	0.40
2:H:13:LEU:O	2:H:32:LYS:CD	2.66	0.40
1:B:507:ALA:C	1:B:509:GLY:N	2.74	0.40
1:A:596:HIS:HB3	1:A:597:TYR:CD2	2.57	0.40
2:E:310:TYR:CZ	2:E:330:ASN:HB2	2.57	0.40
1:D:67:ALA:O	1:D:653:ARG:HG3	2.22	0.40
2:H:370:LEU:O	2:H:372:ASN:N	2.55	0.40
1:A:679:LEU:HD22	1:A:720:THR:HB	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	732/761 (96%)	672 (92%)	57 (8%)	3 (0%)	43	90
1	B	733/761 (96%)	679 (93%)	50 (7%)	4 (0%)	38	88
1	C	731/761 (96%)	681 (93%)	48 (7%)	2 (0%)	50	91
1	D	734/761 (96%)	673 (92%)	59 (8%)	2 (0%)	50	91
2	E	350/375 (93%)	325 (93%)	25 (7%)	0	100	100
2	F	354/375 (94%)	326 (92%)	28 (8%)	0	100	100
2	G	353/375 (94%)	328 (93%)	25 (7%)	0	100	100
2	H	352/375 (94%)	327 (93%)	24 (7%)	1 (0%)	50	91
All	All	4339/4544 (96%)	4011 (92%)	316 (7%)	12 (0%)	50	91

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	731	TYR
1	C	731	TYR
1	D	731	TYR
1	B	300	GLY
2	H	324	PRO
1	A	634	GLY
1	A	731	TYR
1	B	634	GLY
1	D	634	GLY
1	C	634	GLY
1	B	362	PRO
1	A	362	PRO

### 5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	629/651 (97%)	532 (85%)	97 (15%)	4	28
1	B	629/651 (97%)	545 (87%)	84 (13%)	6	35
1	C	629/651 (97%)	542 (86%)	87 (14%)	5	34
1	D	630/651 (97%)	537 (85%)	93 (15%)	4	30
2	E	321/340 (94%)	292 (91%)	29 (9%)	14	56
2	F	325/340 (96%)	297 (91%)	28 (9%)	15	59
2	G	324/340 (95%)	295 (91%)	29 (9%)	14	56
2	H	323/340 (95%)	289 (90%)	34 (10%)	10	48
All	All	3810/3964 (96%)	3329 (87%)	481 (13%)	7	38

All (481) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	5	LEU
1	A	11	ASP
1	A	19	LEU
1	A	27	ASP
1	A	34	HIS
1	A	44	ARG
1	A	47	ILE
1	A	50	TYR
1	A	54	LYS
1	A	60	GLU
1	A	64	LYS
1	A	72	ARG
1	A	83	ARG
1	A	102	LEU
1	A	134	PHE
1	A	138	ASP
1	A	144	SER
1	A	154	LYS
1	A	167	GLU
1	A	170	GLN

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Mol	Chain	Res	Type
1	A	171	PHE
1	A	172	LEU
1	A	184	TYR
1	A	186	ARG
1	A	188	THR
1	A	212	MET
1	A	213	SER
1	A	220	ARG
1	A	224	SER
1	A	225	CYS
1	A	233	SER
1	A	234	LEU
1	A	235	ASP
1	A	237	ILE
1	A	260	ARG
1	A	269	ARG
1	A	276	THR
1	A	287	THR
1	A	294	GLN
1	A	304	LEU
1	A	318	VAL
1	A	319	LEU
1	A	322	ASN
1	A	329	ARG
1	A	340	ASN
1	A	352	ASP
1	A	354	THR
1	A	364	LEU
1	A	380	THR
1	A	386	ASP
1	A	389	ARG
1	A	390	LYS
1	A	394	LYS
1	A	402	MET
1	A	404	GLN
1	A	435	GLN
1	A	440	LEU
1	A	441	GLU
1	A	446	THR
1	A	461	LEU
1	A	462	CYS
1	A	463	THR

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Mol	Chain	Res	Type
1	A	465	SER
1	A	476	ASP
1	A	487	ARG
1	A	489	LEU
1	A	497	ASP
1	A	513	LEU
1	A	519	ASN
1	A	529	LYS
1	A	548	GLN
1	A	560	LYS
1	A	561	GLU
1	A	562	GLN
1	A	569	ASN
1	A	581	ASP
1	A	582	THR
1	A	589	THR
1	A	592	ASN
1	A	620	MET
1	A	623	GLU
1	A	624	THR
1	A	636	GLU
1	A	647	SER
1	A	649	ASP
1	A	660	GLU
1	A	661	HIS
1	A	663	HIS
1	A	691	GLN
1	A	693	ILE
1	A	696	ASN
1	A	697	THR
1	A	698	ASN
1	A	704	PHE
1	A	730	TYR
1	A	734	THR
1	B	4	ASN
1	B	5	LEU
1	B	11	ASP
1	B	19	LEU
1	B	27	ASP
1	B	34	HIS
1	B	44	ARG
1	B	47	ILE

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Mol	Chain	Res	Type
1	B	50	TYR
1	B	60	GLU
1	B	64	LYS
1	B	102	LEU
1	B	134	PHE
1	B	138	ASP
1	B	167	GLU
1	B	171	PHE
1	B	172	LEU
1	B	184	TYR
1	B	186	ARG
1	B	189	ARG
1	B	207	LEU
1	B	220	ARG
1	B	221	GLN
1	B	226	VAL
1	B	233	SER
1	B	234	LEU
1	B	237	ILE
1	B	249	SER
1	B	260	ARG
1	B	262	ARG
1	B	269	ARG
1	B	276	THR
1	B	283	LYS
1	B	286	GLN
1	B	287	THR
1	B	297	VAL
1	B	298	ARG
1	B	304	LEU
1	B	317	LEU
1	B	318	VAL
1	B	319	LEU
1	B	322	ASN
1	B	331	ARG
1	B	352	ASP
1	B	354	THR
1	B	380	THR
1	B	386	ASP
1	B	389	ARG
1	B	394	LYS
1	B	402	MET

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Mol	Chain	Res	Type
1	B	404	GLN
1	B	440	LEU
1	B	441	GLU
1	B	446	THR
1	B	461	LEU
1	B	463	THR
1	B	476	ASP
1	B	479	GLU
1	B	487	ARG
1	B	489	LEU
1	B	497	ASP
1	B	519	ASN
1	B	548	GLN
1	B	569	ASN
1	B	581	ASP
1	B	582	THR
1	B	592	ASN
1	B	620	MET
1	B	623	GLU
1	B	636	GLU
1	B	647	SER
1	B	649	ASP
1	B	660	GLU
1	B	661	HIS
1	B	663	HIS
1	B	693	ILE
1	B	696	ASN
1	B	697	THR
1	B	698	ASN
1	B	702	SER
1	B	732	GLN
1	B	733	ASN
1	B	735	ARG
1	B	736	ASP
1	C	4	ASN
1	C	5	LEU
1	C	6	LEU
1	C	11	ASP
1	C	19	LEU
1	C	27	ASP
1	C	34	HIS
1	C	37	SER

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Mol	Chain	Res	Type
1	C	44	ARG
1	C	47	ILE
1	C	50	TYR
1	C	53	ILE
1	C	60	GLU
1	C	64	LYS
1	C	83	ARG
1	C	102	LEU
1	C	114	LYS
1	C	134	PHE
1	C	138	ASP
1	C	171	PHE
1	C	184	TYR
1	C	186	ARG
1	C	189	ARG
1	C	207	LEU
1	C	213	SER
1	C	216	ARG
1	C	220	ARG
1	C	221	GLN
1	C	226	VAL
1	C	233	SER
1	C	234	LEU
1	C	237	ILE
1	C	246	LYS
1	C	260	ARG
1	C	269	ARG
1	C	276	THR
1	C	287	THR
1	C	304	LEU
1	C	317	LEU
1	C	319	LEU
1	C	322	ASN
1	C	329	ARG
1	C	331	ARG
1	C	352	ASP
1	C	354	THR
1	C	380	THR
1	C	386	ASP
1	C	389	ARG
1	C	394	LYS
1	C	402	MET

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Mol	Chain	Res	Type
1	C	404	GLN
1	C	420	CYS
1	C	438	LEU
1	C	440	LEU
1	C	441	GLU
1	C	446	THR
1	C	461	LEU
1	C	462	CYS
1	C	463	THR
1	C	464	LEU
1	C	476	ASP
1	C	487	ARG
1	C	489	LEU
1	C	497	ASP
1	C	515	ILE
1	C	519	ASN
1	C	548	GLN
1	C	569	ASN
1	C	581	ASP
1	C	582	THR
1	C	592	ASN
1	C	620	MET
1	C	623	GLU
1	C	636	GLU
1	C	647	SER
1	C	649	ASP
1	C	660	GLU
1	C	661	HIS
1	C	663	HIS
1	C	689	ILE
1	C	693	ILE
1	C	696	ASN
1	C	697	THR
1	C	698	ASN
1	C	704	PHE
1	C	735	ARG
1	C	736	ASP
1	D	5	LEU
1	D	11	ASP
1	D	19	LEU
1	D	27	ASP
1	D	34	HIS

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Mol	Chain	Res	Type
1	D	44	ARG
1	D	47	ILE
1	D	50	TYR
1	D	54	LYS
1	D	60	GLU
1	D	64	LYS
1	D	83	ARG
1	D	102	LEU
1	D	134	PHE
1	D	138	ASP
1	D	144	SER
1	D	151	LEU
1	D	165	ILE
1	D	171	PHE
1	D	172	LEU
1	D	184	TYR
1	D	186	ARG
1	D	188	THR
1	D	207	LEU
1	D	212	MET
1	D	213	SER
1	D	220	ARG
1	D	221	GLN
1	D	224	SER
1	D	226	VAL
1	D	233	SER
1	D	234	LEU
1	D	237	ILE
1	D	249	SER
1	D	251	ARG
1	D	269	ARG
1	D	276	THR
1	D	287	THR
1	D	294	GLN
1	D	298	ARG
1	D	304	LEU
1	D	322	ASN
1	D	329	ARG
1	D	331	ARG
1	D	352	ASP
1	D	354	THR
1	D	380	THR

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Mol	Chain	Res	Type
1	D	386	ASP
1	D	389	ARG
1	D	394	LYS
1	D	402	MET
1	D	404	GLN
1	D	406	ARG
1	D	420	CYS
1	D	438	LEU
1	D	440	LEU
1	D	441	GLU
1	D	446	THR
1	D	461	LEU
1	D	463	THR
1	D	465	SER
1	D	472	ILE
1	D	476	ASP
1	D	487	ARG
1	D	489	LEU
1	D	497	ASP
1	D	519	ASN
1	D	529	LYS
1	D	548	GLN
1	D	578	LEU
1	D	581	ASP
1	D	582	THR
1	D	592	ASN
1	D	620	MET
1	D	623	GLU
1	D	624	THR
1	D	636	GLU
1	D	649	ASP
1	D	660	GLU
1	D	661	HIS
1	D	663	HIS
1	D	664	ASP
1	D	693	ILE
1	D	696	ASN
1	D	697	THR
1	D	698	ASN
1	D	703	ARG
1	D	704	PHE
1	D	708	LYS

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Mol	Chain	Res	Type
1	D	733	ASN
1	D	734	THR
1	D	735	ARG
1	D	736	ASP
2	E	7	GLN
2	E	8	THR
2	E	9	LYS
2	E	54	ASP
2	E	57	ARG
2	E	63	GLN
2	E	87	GLN
2	E	89	ARG
2	E	100	SER
2	E	127	ARG
2	E	144	GLU
2	E	148	LYS
2	E	163	MET
2	E	176	THR
2	E	192	LYS
2	E	208	PHE
2	E	249	LEU
2	E	276	PHE
2	E	278	GLN
2	E	315	ARG
2	E	327	THR
2	E	328	ARG
2	E	329	SER
2	E	332	ILE
2	E	363	SER
2	E	368	ASP
2	E	370	LEU
2	E	373	PHE
2	E	374	GLN
2	F	13	LEU
2	F	42	LYS
2	F	54	ASP
2	F	57	ARG
2	F	63	GLN
2	F	100	SER
2	F	101	ILE
2	F	127	ARG
2	F	144	GLU

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Mol	Chain	Res	Type
2	F	148	LYS
2	F	163	MET
2	F	176	THR
2	F	181	THR
2	F	192	LYS
2	F	204	GLU
2	F	208	PHE
2	F	249	LEU
2	F	276	PHE
2	F	278	GLN
2	F	315	ARG
2	F	327	THR
2	F	328	ARG
2	F	329	SER
2	F	343	ASN
2	F	365	VAL
2	F	368	ASP
2	F	372	ASN
2	F	373	PHE
2	G	54	ASP
2	G	57	ARG
2	G	63	GLN
2	G	87	GLN
2	G	89	ARG
2	G	93	VAL
2	G	100	SER
2	G	101	ILE
2	G	127	ARG
2	G	148	LYS
2	G	163	MET
2	G	180	LYS
2	G	181	THR
2	G	192	LYS
2	G	204	GLU
2	G	208	PHE
2	G	249	LEU
2	G	276	PHE
2	G	278	GLN
2	G	315	ARG
2	G	329	SER
2	G	339	LEU
2	G	340	VAL

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Mol	Chain	Res	Type
2	G	342	ASP
2	G	361	ILE
2	G	363	SER
2	G	366	ASP
2	G	371	SER
2	G	372	ASN
2	H	8	THR
2	H	9	LYS
2	H	54	ASP
2	H	57	ARG
2	H	63	GLN
2	H	87	GLN
2	H	89	ARG
2	H	93	VAL
2	H	95	LEU
2	H	100	SER
2	H	101	ILE
2	H	127	ARG
2	H	144	GLU
2	H	148	LYS
2	H	163	MET
2	H	178	ASN
2	H	185	SER
2	H	192	LYS
2	H	208	PHE
2	H	249	LEU
2	H	276	PHE
2	H	278	GLN
2	H	315	ARG
2	H	322	ASP
2	H	323	LEU
2	H	325	PHE
2	H	327	THR
2	H	328	ARG
2	H	329	SER
2	H	339	LEU
2	H	364	GLU
2	H	366	ASP
2	H	373	PHE
2	H	375	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	46	HIS
1	A	78	GLN
1	A	130	GLN
1	A	150	GLN
1	A	158	GLN
1	A	221	GLN
1	A	250	GLN
1	A	275	HIS
1	A	321	ASN
1	A	328	ASN
1	A	338	GLN
1	A	404	GLN
1	A	415	GLN
1	A	435	GLN
1	A	450	ASN
1	A	519	ASN
1	A	569	ASN
1	A	592	ASN
1	A	613	ASN
1	A	630	ASN
1	A	686	GLN
1	A	691	GLN
1	A	696	ASN
1	A	698	ASN
1	A	712	GLN
1	A	713	GLN
1	B	4	ASN
1	B	78	GLN
1	B	130	GLN
1	B	150	GLN
1	B	158	GLN
1	B	221	GLN
1	B	250	GLN
1	B	257	ASN
1	B	275	HIS
1	B	286	GLN
1	B	328	ASN
1	B	338	GLN
1	B	404	GLN
1	B	415	GLN
1	B	450	ASN
1	B	453	ASN
1	B	519	ASN

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Mol	Chain	Res	Type
1	B	569	ASN
1	B	592	ASN
1	B	613	ASN
1	B	686	GLN
1	B	691	GLN
1	B	696	ASN
1	B	698	ASN
1	B	713	GLN
1	C	4	ASN
1	C	78	GLN
1	C	130	GLN
1	C	150	GLN
1	C	158	GLN
1	C	221	GLN
1	C	250	GLN
1	C	275	HIS
1	C	321	ASN
1	C	328	ASN
1	C	332	HIS
1	C	338	GLN
1	C	404	GLN
1	C	415	GLN
1	C	450	ASN
1	C	453	ASN
1	C	519	ASN
1	C	562	GLN
1	C	569	ASN
1	C	592	ASN
1	C	613	ASN
1	C	630	ASN
1	C	696	ASN
1	C	698	ASN
1	C	712	GLN
1	C	713	GLN
1	D	78	GLN
1	D	130	GLN
1	D	150	GLN
1	D	158	GLN
1	D	221	GLN
1	D	257	ASN
1	D	275	HIS
1	D	321	ASN

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Mol	Chain	Res	Type
1	D	328	ASN
1	D	338	GLN
1	D	404	GLN
1	D	415	GLN
1	D	450	ASN
1	D	519	ASN
1	D	562	GLN
1	D	592	ASN
1	D	613	ASN
1	D	627	GLN
1	D	630	ASN
1	D	696	ASN
1	D	713	GLN
2	E	7	GLN
2	E	76	ASN
2	E	227	ASN
2	E	246	GLN
2	E	278	GLN
2	E	336	ASN
2	F	7	GLN
2	F	21	GLN
2	F	76	ASN
2	F	227	ASN
2	F	246	GLN
2	F	278	GLN
2	F	372	ASN
2	G	7	GLN
2	G	76	ASN
2	G	227	ASN
2	G	246	GLN
2	G	278	GLN
2	G	336	ASN
2	H	7	GLN
2	H	76	ASN
2	H	128	ASN
2	H	227	ASN
2	H	246	GLN
2	H	278	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 ⓘ

8 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	ATP	A	801	-	33,33,33	1.98	8 (24%)	52,52,52	2.55	15 (28%)
3	ATP	B	801	-	33,33,33	1.98	8 (24%)	52,52,52	2.55	15 (28%)
3	ATP	C	801	-	33,33,33	1.90	8 (24%)	52,52,52	2.41	16 (30%)
3	ATP	D	801	-	33,33,33	1.95	9 (27%)	52,52,52	2.44	12 (23%)
4	FEO	E	501	2,5	0,2,2	0.00	-	0,1,1	0.00	-
4	FEO	F	501	2,5	0,2,2	0.00	-	0,1,1	0.00	-
4	FEO	G	501	2,5	0,2,2	0.00	-	0,1,1	0.00	-
4	FEO	H	501	2,5	0,2,2	0.00	-	0,1,1	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	801	-	-	0/22/38/38	0/1/3/3
3	ATP	B	801	-	-	0/22/38/38	0/1/3/3
3	ATP	C	801	-	-	0/22/38/38	0/1/3/3
3	ATP	D	801	-	-	0/22/38/38	0/1/3/3
4	FEO	E	501	2,5	-	0/0/0/0	0/0/0/0
4	FEO	F	501	2,5	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FEO	G	501	2,5	-	0/0/0/0	0/0/0/0
4	FEO	H	501	2,5	-	0/0/0/0	0/0/0/0

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	801	ATP	O4'-C1'	4.86	1.48	1.41
3	D	801	ATP	O4'-C1'	4.79	1.48	1.41
3	B	801	ATP	O4'-C1'	4.76	1.48	1.41
3	A	801	ATP	O4'-C1'	4.73	1.48	1.41
3	D	801	ATP	C6-N6	4.68	1.50	1.35
3	B	801	ATP	C6-N6	4.65	1.50	1.35
3	A	801	ATP	C6-N6	4.63	1.50	1.35
3	C	801	ATP	C6-N6	4.62	1.49	1.35
3	A	801	ATP	C2'-C1'	-4.40	1.47	1.53
3	B	801	ATP	C2'-C1'	-4.36	1.47	1.53
3	C	801	ATP	C2'-C3'	-4.33	1.41	1.53
3	D	801	ATP	C2'-C3'	-4.32	1.41	1.53
3	A	801	ATP	C2'-C3'	-4.32	1.41	1.53
3	B	801	ATP	C2'-C3'	-4.31	1.41	1.53
3	D	801	ATP	C2'-C1'	-3.60	1.48	1.53
3	C	801	ATP	O4'-C4'	-2.72	1.38	1.45
3	B	801	ATP	O4'-C4'	-2.67	1.38	1.45
3	A	801	ATP	O4'-C4'	-2.64	1.38	1.45
3	C	801	ATP	O3'-C3'	-2.57	1.36	1.43
3	D	801	ATP	O4'-C4'	-2.54	1.39	1.45
3	D	801	ATP	O3'-C3'	-2.51	1.36	1.43
3	B	801	ATP	O3'-C3'	-2.47	1.37	1.43
3	A	801	ATP	O3'-C3'	-2.47	1.37	1.43
3	C	801	ATP	C2'-C1'	-2.29	1.50	1.53
3	B	801	ATP	C4-N9	-2.18	1.34	1.37
3	A	801	ATP	C4-N9	-2.18	1.34	1.37
3	B	801	ATP	C8-N9	-2.14	1.33	1.36
3	D	801	ATP	C4-N9	-2.12	1.34	1.37
3	A	801	ATP	C8-N9	-2.10	1.33	1.36
3	C	801	ATP	C4-N9	-2.08	1.34	1.37
3	D	801	ATP	PA-O3A	-2.06	1.56	1.59
3	D	801	ATP	PB-O3A	-2.06	1.56	1.59
3	C	801	ATP	PB-O3A	-2.05	1.56	1.59

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	ATP	O4'-C1'-N9	10.79	118.47	108.44
3	B	801	ATP	O4'-C1'-N9	10.78	118.47	108.44
3	C	801	ATP	N3-C2-N1	-8.92	121.25	128.71
3	D	801	ATP	O4'-C1'-N9	8.79	116.61	108.44
3	B	801	ATP	N3-C2-N1	-8.71	121.43	128.71
3	A	801	ATP	N3-C2-N1	-8.70	121.44	128.71
3	D	801	ATP	N3-C2-N1	-8.69	121.44	128.71
3	C	801	ATP	O4'-C1'-N9	7.92	115.80	108.44
3	D	801	ATP	PB-O3B-PG	-4.95	117.16	131.68
3	D	801	ATP	N3-C4-N9	4.74	134.00	125.43
3	C	801	ATP	N3-C4-N9	4.71	133.94	125.43
3	A	801	ATP	N3-C4-N9	4.64	133.81	125.43
3	B	801	ATP	N3-C4-N9	4.63	133.80	125.43
3	C	801	ATP	PA-O3A-PB	-4.53	118.40	131.68
3	D	801	ATP	PA-O3A-PB	-4.51	118.46	131.68
3	C	801	ATP	PB-O3B-PG	-3.86	120.37	131.68
3	C	801	ATP	C2'-C1'-N9	-3.82	103.46	113.27
3	B	801	ATP	PA-O3A-PB	-3.66	120.95	131.68
3	A	801	ATP	PA-O3A-PB	-3.65	120.97	131.68
3	D	801	ATP	O3A-PB-O3B	3.59	108.95	101.66
3	A	801	ATP	C3'-C2'-C1'	3.46	106.32	100.91
3	B	801	ATP	C3'-C2'-C1'	3.45	106.30	100.91
3	B	801	ATP	O3A-PB-O3B	3.39	108.55	101.66
3	A	801	ATP	O3A-PB-O3B	3.38	108.53	101.66
3	B	801	ATP	PB-O3B-PG	-3.00	122.89	131.68
3	A	801	ATP	PB-O3B-PG	-2.99	122.90	131.68
3	C	801	ATP	O3A-PB-O3B	2.93	107.61	101.66
3	D	801	ATP	C5-C4-N3	-2.90	119.38	125.70
3	B	801	ATP	C5-C4-N3	-2.87	119.46	125.70
3	A	801	ATP	C5-C4-N3	-2.86	119.46	125.70
3	B	801	ATP	O2'-C2'-C1'	-2.81	102.72	111.23
3	C	801	ATP	C5-C4-N3	-2.80	119.60	125.70
3	A	801	ATP	O2'-C2'-C1'	-2.80	102.77	111.23
3	C	801	ATP	C3'-C2'-C1'	2.73	105.19	100.91
3	D	801	ATP	C4'-O4'-C1'	-2.73	106.78	109.75
3	C	801	ATP	C8-N9-C4	2.60	108.88	106.90
3	D	801	ATP	C8-N9-C4	2.53	108.83	106.90
3	B	801	ATP	O5'-C5'-C4'	2.48	118.03	108.94
3	A	801	ATP	O5'-C5'-C4'	2.47	118.00	108.94
3	B	801	ATP	O3A-PA-O5'	2.46	114.38	103.41
3	A	801	ATP	O3A-PA-O5'	2.45	114.36	103.41
3	A	801	ATP	C8-N9-C4	2.40	108.73	106.90
3	D	801	ATP	O3A-PA-O5'	2.39	114.09	103.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	ATP	C8-N9-C4	2.38	108.72	106.90
3	D	801	ATP	C2-N3-C4	2.34	120.67	114.01
3	C	801	ATP	O3A-PA-O5'	2.31	113.75	103.41
3	A	801	ATP	C2-N3-C4	2.30	120.57	114.01
3	C	801	ATP	C2-N3-C4	2.30	120.55	114.01
3	B	801	ATP	C2-N3-C4	2.29	120.52	114.01
3	D	801	ATP	O5'-C5'-C4'	2.28	117.32	108.94
3	C	801	ATP	C4'-O4'-C1'	-2.25	107.30	109.75
3	C	801	ATP	O2'-C2'-C1'	-2.15	104.72	111.23
3	A	801	ATP	C2'-C3'-C4'	2.13	106.89	102.65
3	B	801	ATP	C2'-C3'-C4'	2.12	106.88	102.65
3	A	801	ATP	C4'-O4'-C1'	-2.11	107.45	109.75
3	B	801	ATP	C4'-O4'-C1'	-2.09	107.48	109.75
3	C	801	ATP	C2'-C3'-C4'	2.07	106.78	102.65
3	C	801	ATP	O3'-C3'-C4'	-2.04	105.07	111.08

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	734/761 (96%)	0.11	2 (0%) 91 86	62, 120, 165, 251	0
1	B	735/761 (96%)	0.34	15 (2%) 62 49	76, 152, 200, 256	0
1	C	733/761 (96%)	0.17	6 (0%) 83 71	63, 128, 171, 261	0
1	D	736/761 (96%)	0.24	8 (1%) 77 63	68, 133, 187, 253	0
2	E	354/375 (94%)	0.34	6 (1%) 67 54	77, 152, 210, 243	0
2	F	358/375 (95%)	0.45	9 (2%) 54 44	74, 151, 209, 256	0
2	G	357/375 (95%)	0.25	7 (1%) 62 49	96, 162, 207, 255	0
2	H	356/375 (94%)	0.27	8 (2%) 59 47	117, 172, 208, 267	0
All	All	4363/4544 (96%)	0.25	61 (1%) 72 58	62, 141, 198, 267	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	166	TYR	4.4
1	B	295	GLY	3.7
1	C	225	CYS	3.2
1	C	392	ARG	3.1
2	F	9	LYS	3.0
1	B	72	ARG	3.0
1	D	165	ILE	2.8
1	B	296	GLY	2.8
1	B	49	PHE	2.8
2	F	170	LEU	2.7
2	E	9	LYS	2.6
2	E	322	ASP	2.5
2	G	361	ILE	2.5
2	E	362	ASP	2.5
2	G	375	LEU	2.5
1	B	275	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	12	GLN	2.4
1	B	269	ARG	2.4
2	E	172	GLU	2.4
2	G	179	GLY	2.3
1	B	166	TYR	2.3
2	E	364	GLU	2.3
2	H	180	LYS	2.3
1	B	100	PRO	2.3
2	H	178	ASN	2.3
2	G	321	LEU	2.3
1	B	99	PRO	2.3
1	A	166	TYR	2.2
1	B	272	GLU	2.2
2	E	325	PHE	2.2
2	H	184	VAL	2.2
1	C	390	LYS	2.2
1	D	119	LEU	2.2
2	F	7	GLN	2.2
2	F	290	LEU	2.1
2	G	362	ASP	2.1
2	H	179	GLY	2.1
1	B	190	LEU	2.1
1	B	294	GLN	2.1
1	C	299	GLY	2.1
1	B	641	TYR	2.1
2	F	166	TYR	2.1
1	A	390	LYS	2.1
1	D	94	TYR	2.1
1	C	439	CYS	2.1
2	H	55	VAL	2.1
1	D	673	PRO	2.1
2	G	272	CYS	2.1
2	F	325	PHE	2.1
2	F	370	LEU	2.1
2	G	175	HIS	2.1
1	C	462	CYS	2.1
1	D	50	TYR	2.1
2	H	167	TRP	2.0
1	B	262	ARG	2.0
1	D	666	TYR	2.0
2	F	21	GLN	2.0
2	H	175	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	641	TYR	2.0
1	B	651	ILE	2.0
2	H	252	LEU	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	ATP	C	801	31/31	0.30	0.55	138,138,138,138	0
3	ATP	B	801	31/31	0.46	0.36	225,225,225,225	0
3	ATP	D	801	31/31	0.37	0.15	195,195,195,195	0
3	ATP	A	801	31/31	0.29	-0.27	126,126,126,126	0
4	FEO	F	501	3/3	0.22	-1.03	106,106,106,106	0
4	FEO	G	501	3/3	0.14	-1.50	124,124,124,124	0
4	FEO	H	501	3/3	0.11	-1.84	133,133,133,133	0
4	FEO	E	501	3/3	0.16	-1.96	119,119,119,119	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.