Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:24 am BST

PDB ID	:	3N6R
Title	:	CRYSTAL STRUCTURE OF the holoenzyme of PROPIONYL-COA CARBOXYLASE (PCC)
Authors	:	Huang, C.S.; Sadre-Bazzaz, K.; Tong, L.
Deposited on	:	2010-05-26
Resolution	:	3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

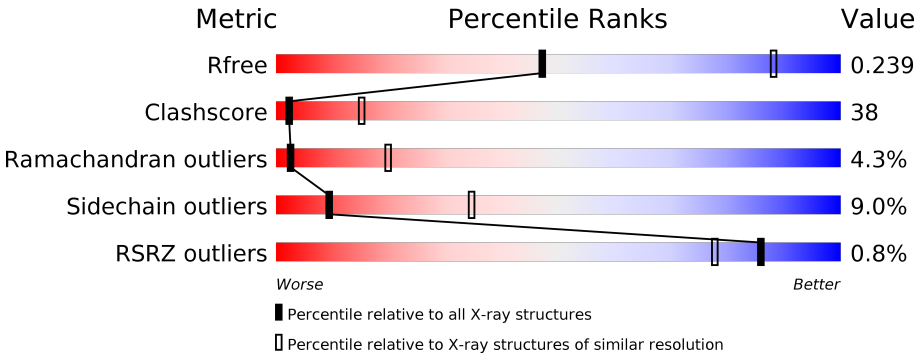
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	681	33% 44% 9% • 13%
1	C	681	31% 45% 10% 13%
1	E	681	2% 32% 44% 10% 13%
1	G	681	35% 50% 9% • 5%
1	I	681	35% 50% 10% • 5%
1	K	681	2% 35% 50% 9% 5%

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Mol	Chain	Length	Quality of chain
2	B	531	
2	D	531	
2	F	531	
2	H	531	
2	J	531	
2	L	531	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 51921 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Propionyl-CoA carboxylase, alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	591	Total	C	N	O	S	0	0	0
			4507	2828	794	857	28			
1	C	591	Total	C	N	O	S	0	0	0
			4507	2828	794	857	28			
1	E	591	Total	C	N	O	S	0	0	0
			4507	2828	794	857	28			
1	G	646	Total	C	N	O	S	0	0	0
			4950	3108	869	942	31			
1	I	646	Total	C	N	O	S	0	0	0
			4950	3108	869	942	31			
1	K	646	Total	C	N	O	S	0	0	0
			4950	3108	869	942	31			

- Molecule 2 is a protein called Propionyl-CoA carboxylase, beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	506	Total	C	N	O	S	0	0	0
			3910	2462	683	744	21			
2	D	506	Total	C	N	O	S	0	0	0
			3910	2462	683	744	21			
2	F	506	Total	C	N	O	S	0	0	0
			3910	2462	683	744	21			
2	H	506	Total	C	N	O	S	0	0	0
			3910	2462	683	744	21			
2	J	506	Total	C	N	O	S	0	0	0
			3910	2462	683	744	21			
2	L	506	Total	C	N	O	S	0	0	0
			3910	2462	683	744	21			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	11	MET	-	EXPRESSION TAG	UNP Q168G2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	12	GLY	-	EXPRESSION TAG	UNP Q168G2
B	13	SER	-	EXPRESSION TAG	UNP Q168G2
B	14	SER	-	EXPRESSION TAG	UNP Q168G2
B	15	HIS	-	EXPRESSION TAG	UNP Q168G2
B	16	HIS	-	EXPRESSION TAG	UNP Q168G2
B	17	HIS	-	EXPRESSION TAG	UNP Q168G2
B	18	HIS	-	EXPRESSION TAG	UNP Q168G2
B	19	HIS	-	EXPRESSION TAG	UNP Q168G2
B	20	HIS	-	EXPRESSION TAG	UNP Q168G2
B	21	SER	-	EXPRESSION TAG	UNP Q168G2
B	22	SER	-	EXPRESSION TAG	UNP Q168G2
B	23	GLY	-	EXPRESSION TAG	UNP Q168G2
B	24	LEU	-	EXPRESSION TAG	UNP Q168G2
B	25	VAL	-	EXPRESSION TAG	UNP Q168G2
B	26	PRO	-	EXPRESSION TAG	UNP Q168G2
B	27	ARG	-	EXPRESSION TAG	UNP Q168G2
B	28	GLY	-	EXPRESSION TAG	UNP Q168G2
B	29	SER	-	EXPRESSION TAG	UNP Q168G2
B	30	HIS	-	EXPRESSION TAG	UNP Q168G2
B	31	MET	-	EXPRESSION TAG	UNP Q168G2
D	11	MET	-	EXPRESSION TAG	UNP Q168G2
D	12	GLY	-	EXPRESSION TAG	UNP Q168G2
D	13	SER	-	EXPRESSION TAG	UNP Q168G2
D	14	SER	-	EXPRESSION TAG	UNP Q168G2
D	15	HIS	-	EXPRESSION TAG	UNP Q168G2
D	16	HIS	-	EXPRESSION TAG	UNP Q168G2
D	17	HIS	-	EXPRESSION TAG	UNP Q168G2
D	18	HIS	-	EXPRESSION TAG	UNP Q168G2
D	19	HIS	-	EXPRESSION TAG	UNP Q168G2
D	20	HIS	-	EXPRESSION TAG	UNP Q168G2
D	21	SER	-	EXPRESSION TAG	UNP Q168G2
D	22	SER	-	EXPRESSION TAG	UNP Q168G2
D	23	GLY	-	EXPRESSION TAG	UNP Q168G2
D	24	LEU	-	EXPRESSION TAG	UNP Q168G2
D	25	VAL	-	EXPRESSION TAG	UNP Q168G2
D	26	PRO	-	EXPRESSION TAG	UNP Q168G2
D	27	ARG	-	EXPRESSION TAG	UNP Q168G2
D	28	GLY	-	EXPRESSION TAG	UNP Q168G2
D	29	SER	-	EXPRESSION TAG	UNP Q168G2
D	30	HIS	-	EXPRESSION TAG	UNP Q168G2
D	31	MET	-	EXPRESSION TAG	UNP Q168G2
F	11	MET	-	EXPRESSION TAG	UNP Q168G2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	12	GLY	-	EXPRESSION TAG	UNP Q168G2
F	13	SER	-	EXPRESSION TAG	UNP Q168G2
F	14	SER	-	EXPRESSION TAG	UNP Q168G2
F	15	HIS	-	EXPRESSION TAG	UNP Q168G2
F	16	HIS	-	EXPRESSION TAG	UNP Q168G2
F	17	HIS	-	EXPRESSION TAG	UNP Q168G2
F	18	HIS	-	EXPRESSION TAG	UNP Q168G2
F	19	HIS	-	EXPRESSION TAG	UNP Q168G2
F	20	HIS	-	EXPRESSION TAG	UNP Q168G2
F	21	SER	-	EXPRESSION TAG	UNP Q168G2
F	22	SER	-	EXPRESSION TAG	UNP Q168G2
F	23	GLY	-	EXPRESSION TAG	UNP Q168G2
F	24	LEU	-	EXPRESSION TAG	UNP Q168G2
F	25	VAL	-	EXPRESSION TAG	UNP Q168G2
F	26	PRO	-	EXPRESSION TAG	UNP Q168G2
F	27	ARG	-	EXPRESSION TAG	UNP Q168G2
F	28	GLY	-	EXPRESSION TAG	UNP Q168G2
F	29	SER	-	EXPRESSION TAG	UNP Q168G2
F	30	HIS	-	EXPRESSION TAG	UNP Q168G2
F	31	MET	-	EXPRESSION TAG	UNP Q168G2
H	11	MET	-	EXPRESSION TAG	UNP Q168G2
H	12	GLY	-	EXPRESSION TAG	UNP Q168G2
H	13	SER	-	EXPRESSION TAG	UNP Q168G2
H	14	SER	-	EXPRESSION TAG	UNP Q168G2
H	15	HIS	-	EXPRESSION TAG	UNP Q168G2
H	16	HIS	-	EXPRESSION TAG	UNP Q168G2
H	17	HIS	-	EXPRESSION TAG	UNP Q168G2
H	18	HIS	-	EXPRESSION TAG	UNP Q168G2
H	19	HIS	-	EXPRESSION TAG	UNP Q168G2
H	20	HIS	-	EXPRESSION TAG	UNP Q168G2
H	21	SER	-	EXPRESSION TAG	UNP Q168G2
H	22	SER	-	EXPRESSION TAG	UNP Q168G2
H	23	GLY	-	EXPRESSION TAG	UNP Q168G2
H	24	LEU	-	EXPRESSION TAG	UNP Q168G2
H	25	VAL	-	EXPRESSION TAG	UNP Q168G2
H	26	PRO	-	EXPRESSION TAG	UNP Q168G2
H	27	ARG	-	EXPRESSION TAG	UNP Q168G2
H	28	GLY	-	EXPRESSION TAG	UNP Q168G2
H	29	SER	-	EXPRESSION TAG	UNP Q168G2
H	30	HIS	-	EXPRESSION TAG	UNP Q168G2
H	31	MET	-	EXPRESSION TAG	UNP Q168G2
J	11	MET	-	EXPRESSION TAG	UNP Q168G2

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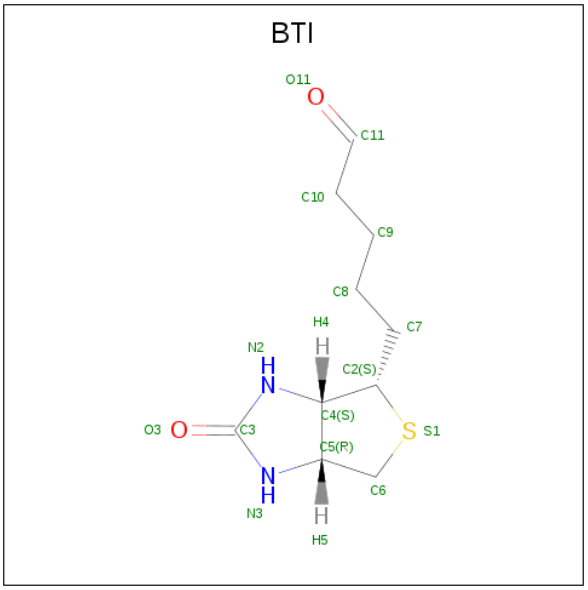
Chain	Residue	Modelled	Actual	Comment	Reference
J	12	GLY	-	EXPRESSION TAG	UNP Q168G2
J	13	SER	-	EXPRESSION TAG	UNP Q168G2
J	14	SER	-	EXPRESSION TAG	UNP Q168G2
J	15	HIS	-	EXPRESSION TAG	UNP Q168G2
J	16	HIS	-	EXPRESSION TAG	UNP Q168G2
J	17	HIS	-	EXPRESSION TAG	UNP Q168G2
J	18	HIS	-	EXPRESSION TAG	UNP Q168G2
J	19	HIS	-	EXPRESSION TAG	UNP Q168G2
J	20	HIS	-	EXPRESSION TAG	UNP Q168G2
J	21	SER	-	EXPRESSION TAG	UNP Q168G2
J	22	SER	-	EXPRESSION TAG	UNP Q168G2
J	23	GLY	-	EXPRESSION TAG	UNP Q168G2
J	24	LEU	-	EXPRESSION TAG	UNP Q168G2
J	25	VAL	-	EXPRESSION TAG	UNP Q168G2
J	26	PRO	-	EXPRESSION TAG	UNP Q168G2
J	27	ARG	-	EXPRESSION TAG	UNP Q168G2
J	28	GLY	-	EXPRESSION TAG	UNP Q168G2
J	29	SER	-	EXPRESSION TAG	UNP Q168G2
J	30	HIS	-	EXPRESSION TAG	UNP Q168G2
J	31	MET	-	EXPRESSION TAG	UNP Q168G2
L	11	MET	-	EXPRESSION TAG	UNP Q168G2
L	12	GLY	-	EXPRESSION TAG	UNP Q168G2
L	13	SER	-	EXPRESSION TAG	UNP Q168G2
L	14	SER	-	EXPRESSION TAG	UNP Q168G2
L	15	HIS	-	EXPRESSION TAG	UNP Q168G2
L	16	HIS	-	EXPRESSION TAG	UNP Q168G2
L	17	HIS	-	EXPRESSION TAG	UNP Q168G2
L	18	HIS	-	EXPRESSION TAG	UNP Q168G2
L	19	HIS	-	EXPRESSION TAG	UNP Q168G2
L	20	HIS	-	EXPRESSION TAG	UNP Q168G2
L	21	SER	-	EXPRESSION TAG	UNP Q168G2
L	22	SER	-	EXPRESSION TAG	UNP Q168G2
L	23	GLY	-	EXPRESSION TAG	UNP Q168G2
L	24	LEU	-	EXPRESSION TAG	UNP Q168G2
L	25	VAL	-	EXPRESSION TAG	UNP Q168G2
L	26	PRO	-	EXPRESSION TAG	UNP Q168G2
L	27	ARG	-	EXPRESSION TAG	UNP Q168G2
L	28	GLY	-	EXPRESSION TAG	UNP Q168G2
L	29	SER	-	EXPRESSION TAG	UNP Q168G2
L	30	HIS	-	EXPRESSION TAG	UNP Q168G2
L	31	MET	-	EXPRESSION TAG	UNP Q168G2

- Molecule 3 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL

(three-letter code: BTI) (formula: $C_{10}H_{16}N_2O_2S$).

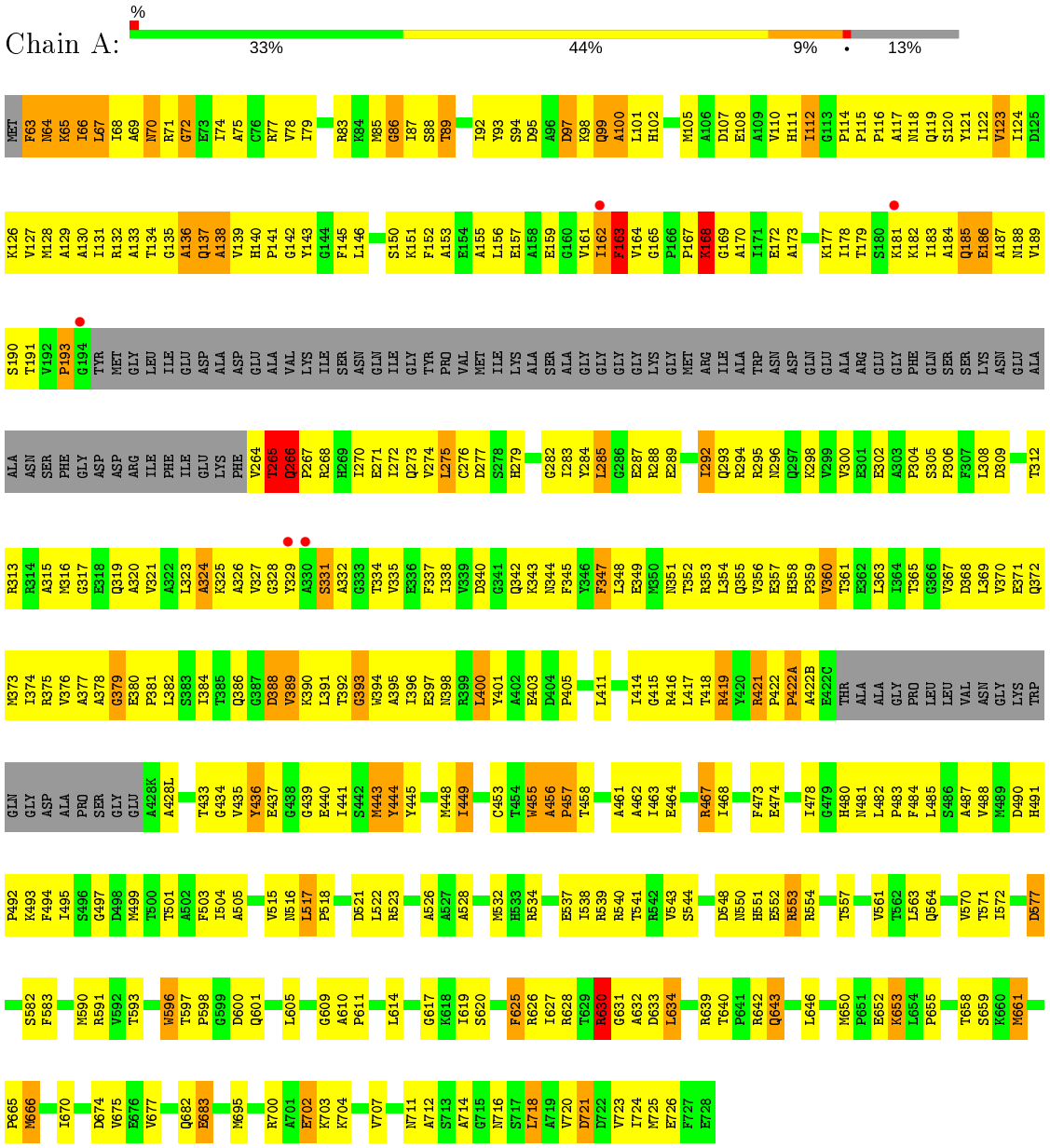


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	C	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	E	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	G	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	I	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	K	1	Total	C	N	O	S	0	0
			15	10	2	2	1		

3 Residue-property plots (i)

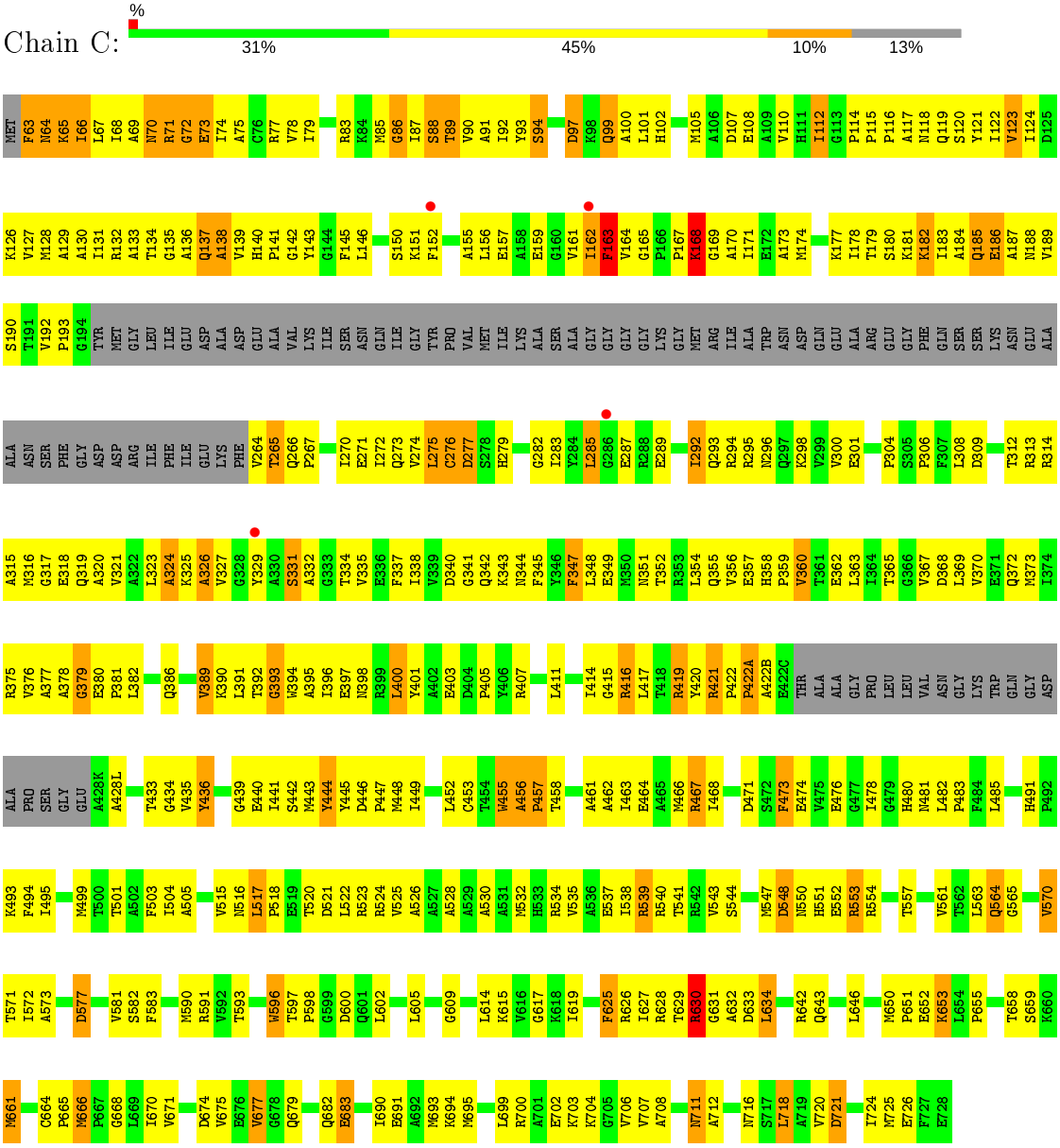
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Propionyl-CoA carboxylase, alpha subunit



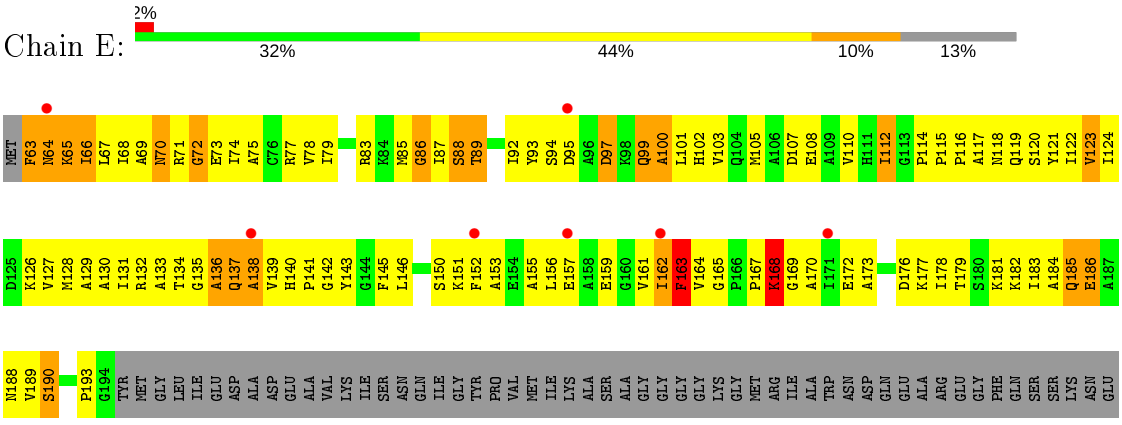
- Molecule 1: Propionyl-CoA carboxylase, alpha subunit

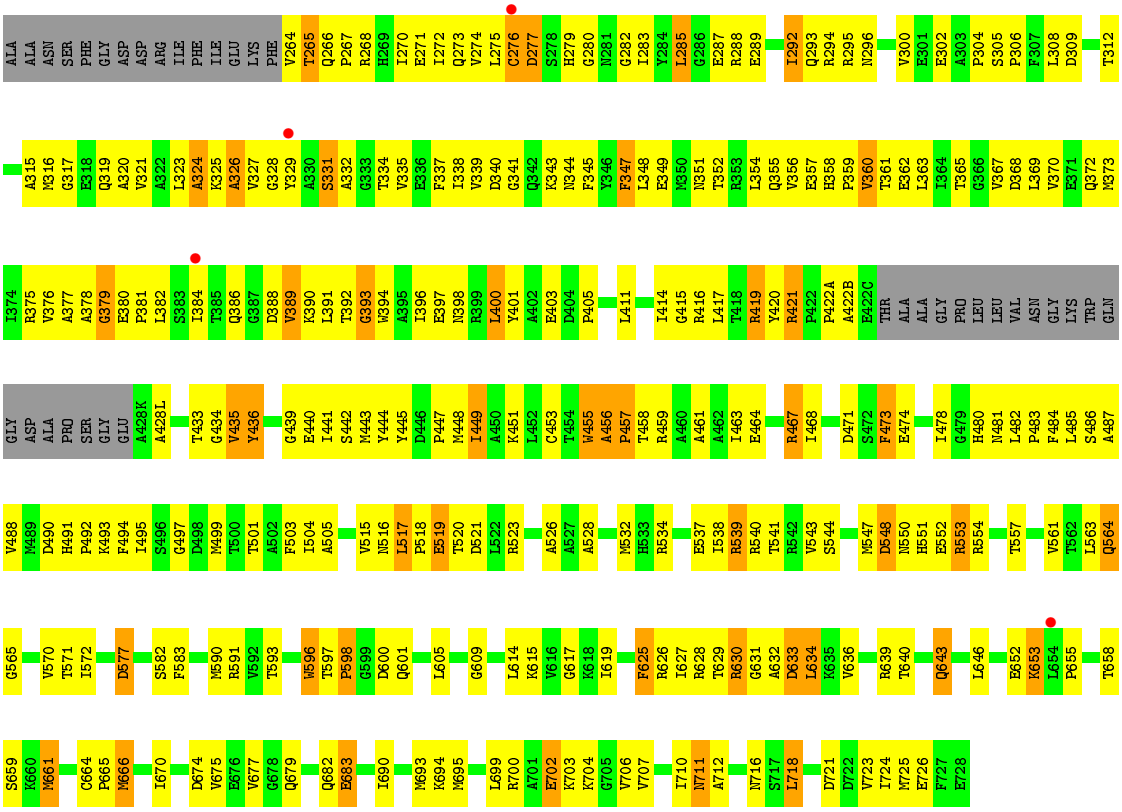
Chain C:



• Molecule 1: Propionyl-CoA carboxylase, alpha subunit

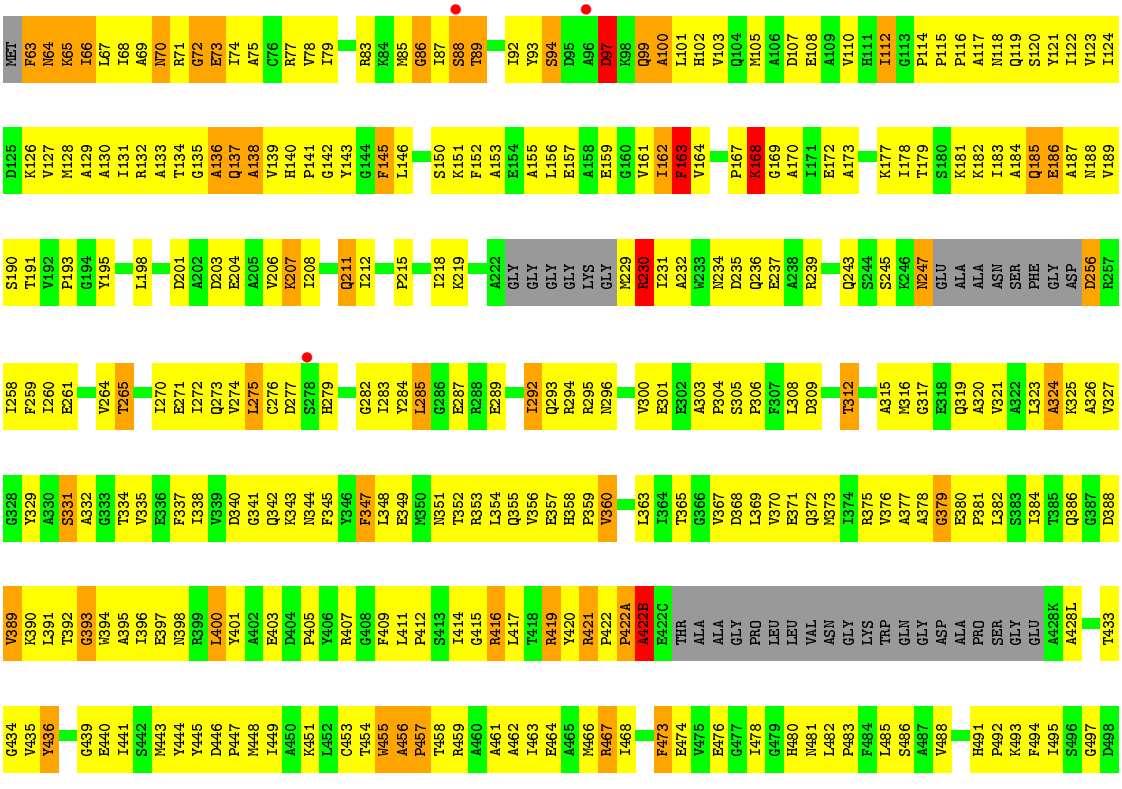
Chain E:

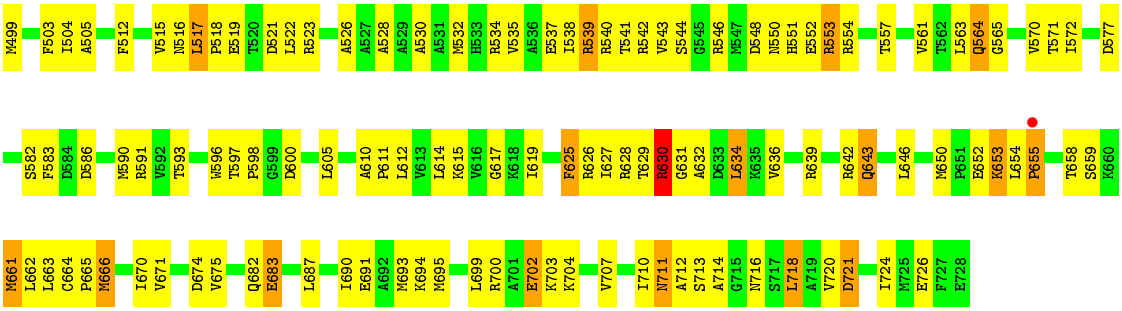




• Molecule 1: Propionyl-CoA carboxylase, alpha subunit

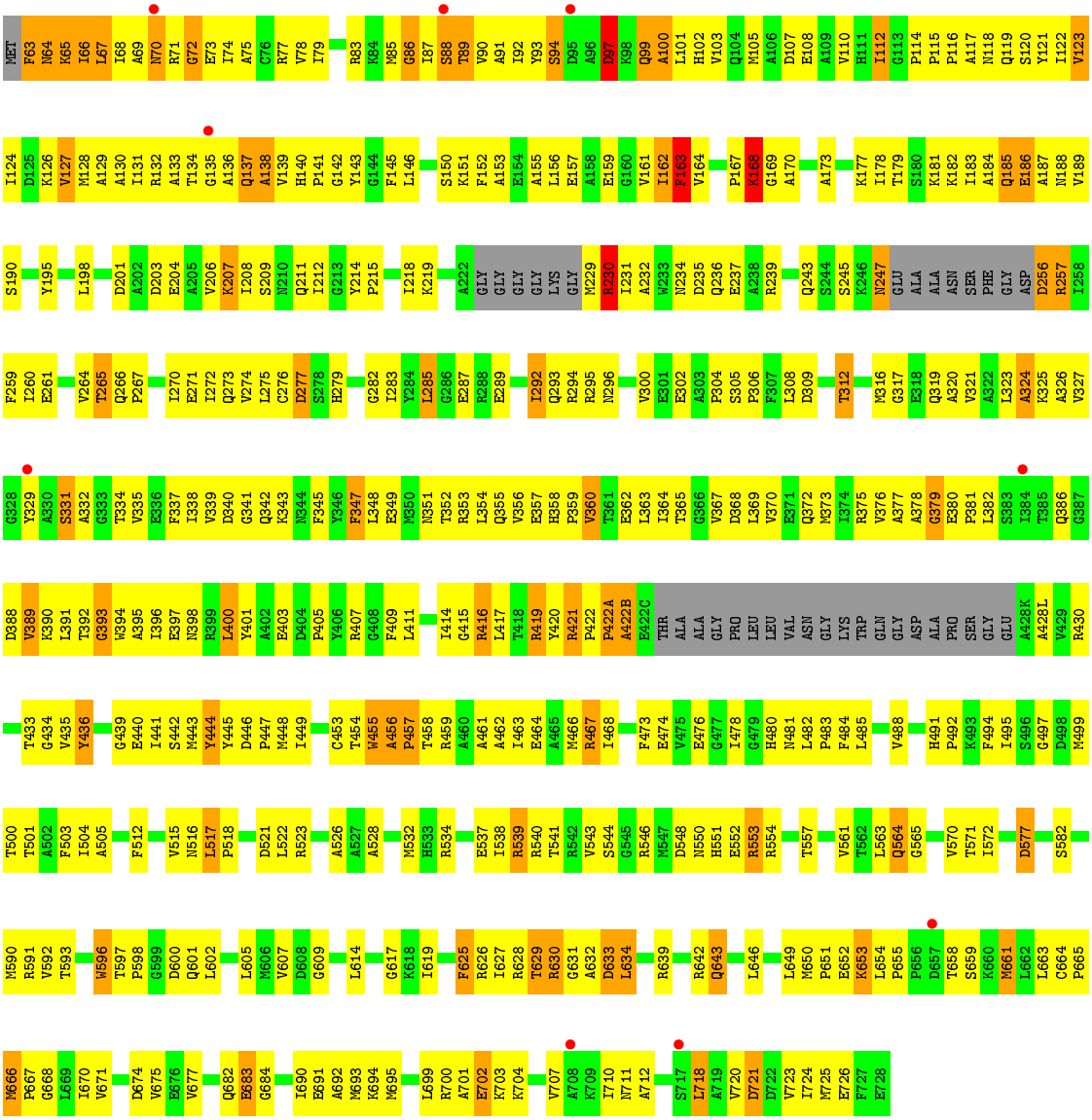
Chain G:





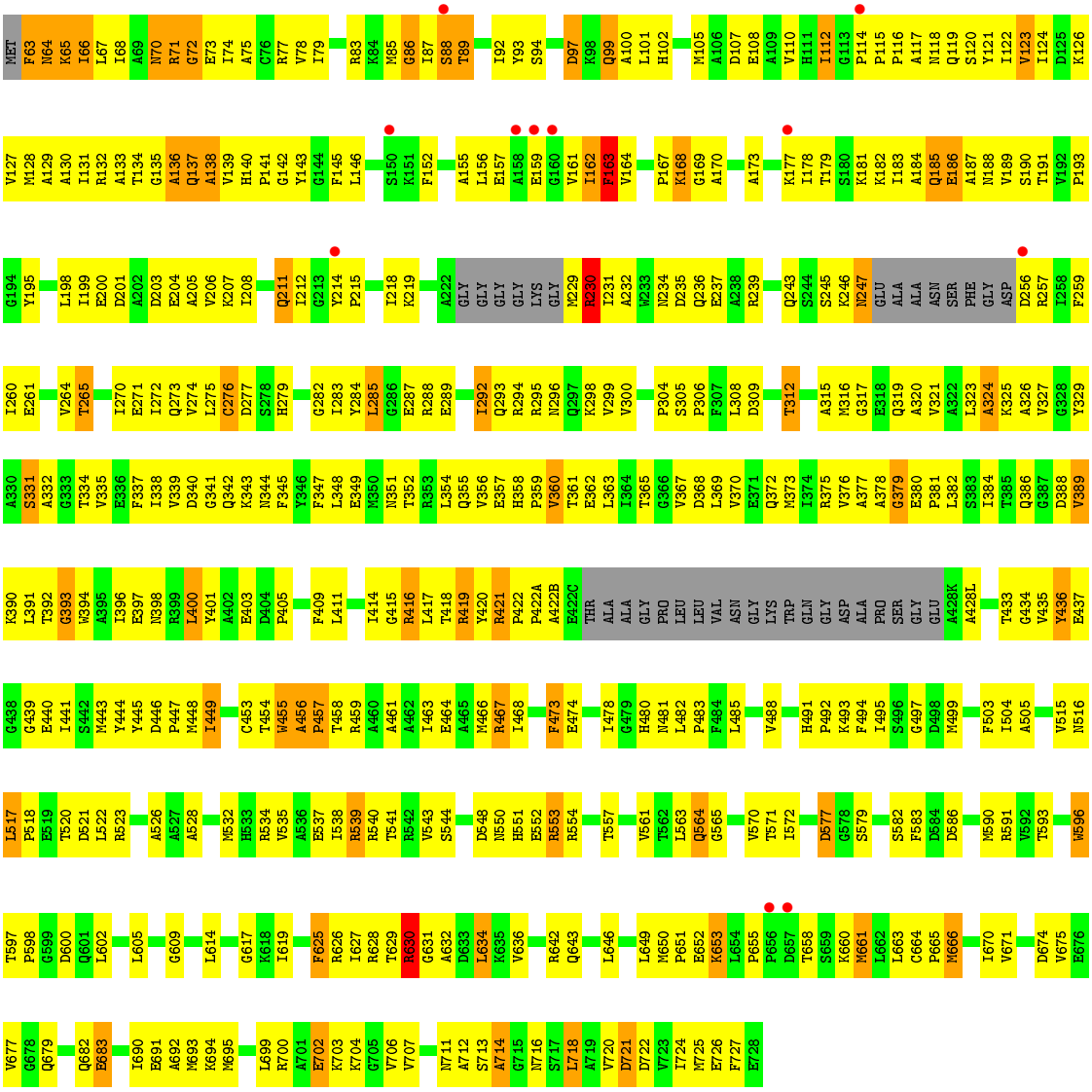
• Molecule 1: Propionyl-CoA carboxylase, alpha subunit

Chain I:



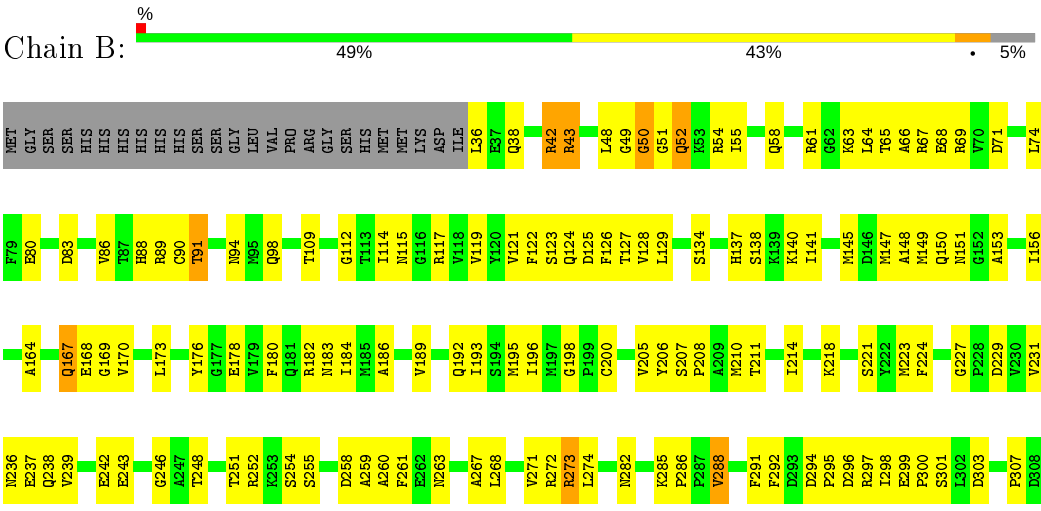
• Molecule 1: Propionyl-CoA carboxylase, alpha subunit

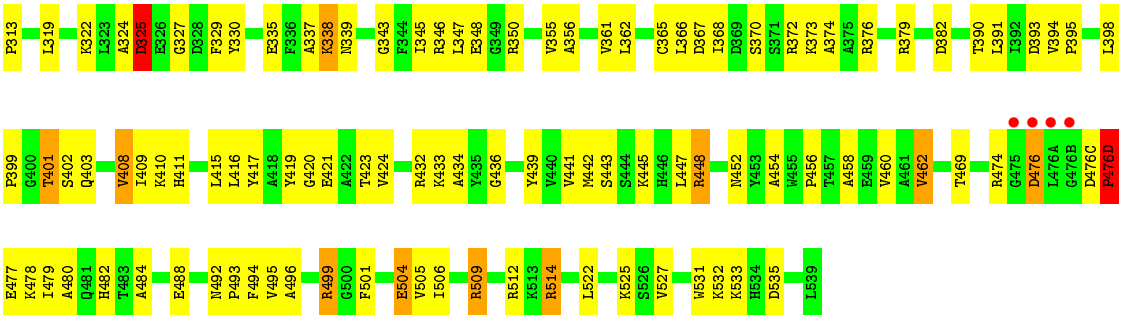
Chain K:



• Molecule 2: Propionyl-CoA carboxylase, beta subunit

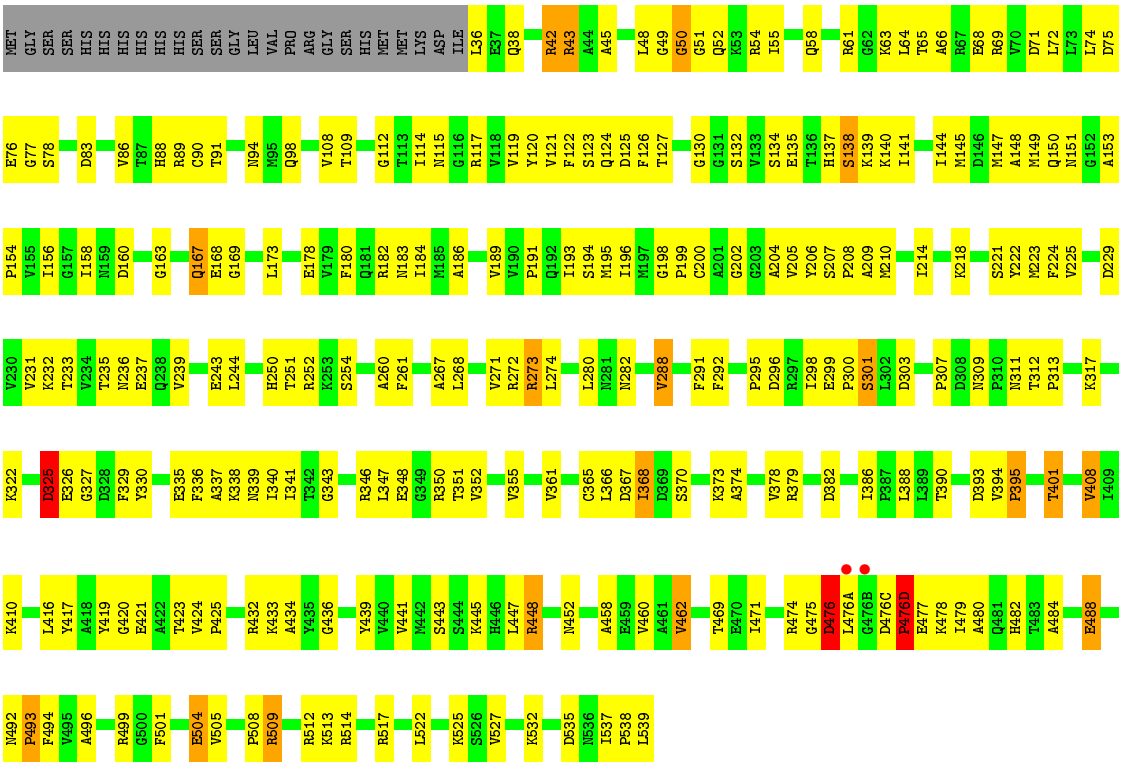
Chain B:





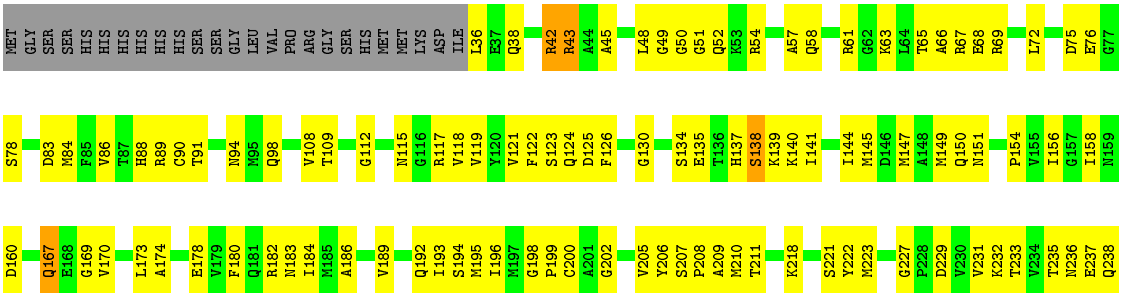
• Molecule 2: Propionyl-CoA carboxylase, beta subunit

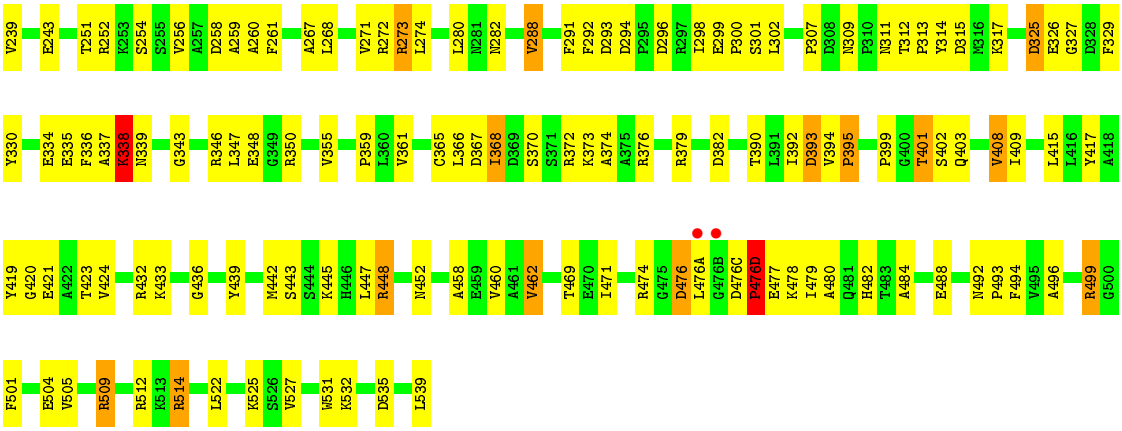
Chain D:



• Molecule 2: Propionyl-CoA carboxylase, beta subunit

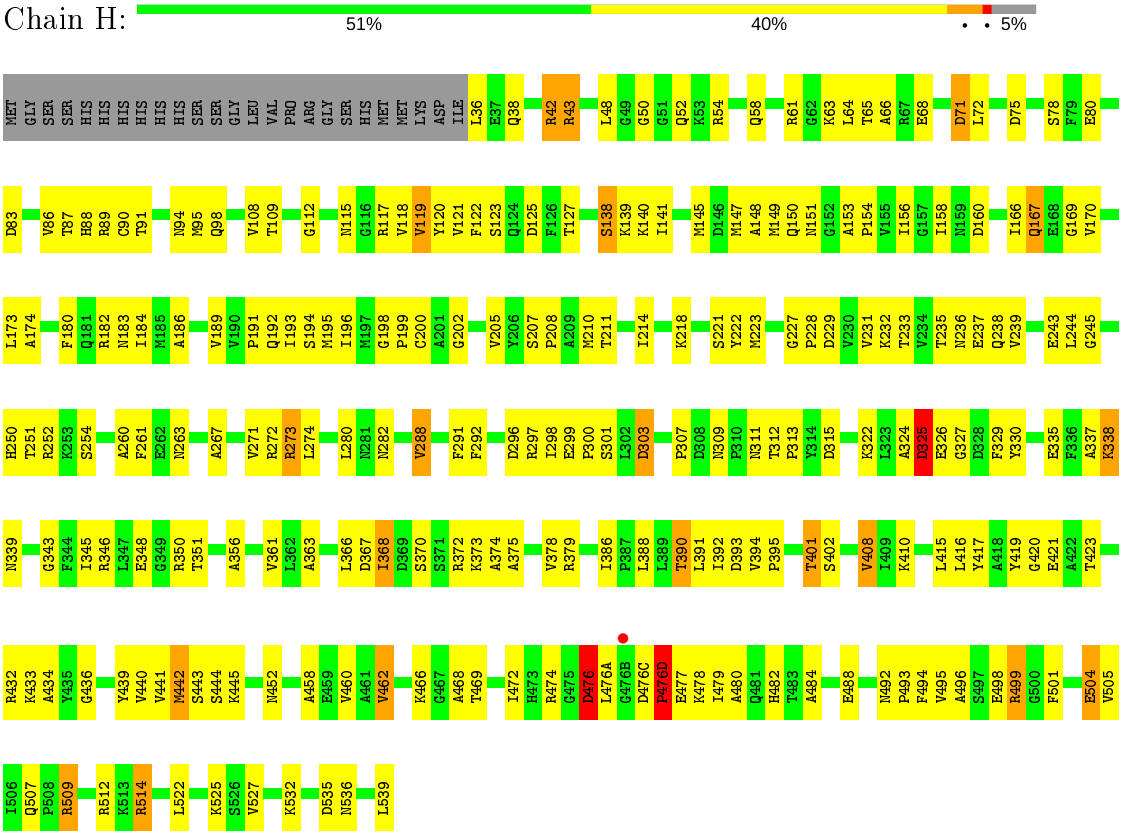
Chain F:





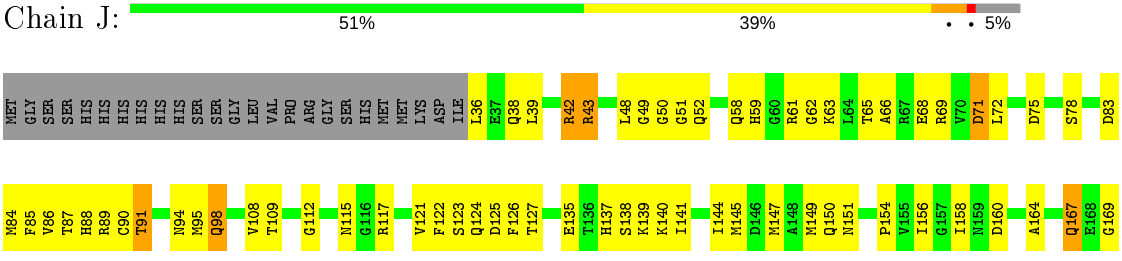
• Molecule 2: Propionyl-CoA carboxylase, beta subunit

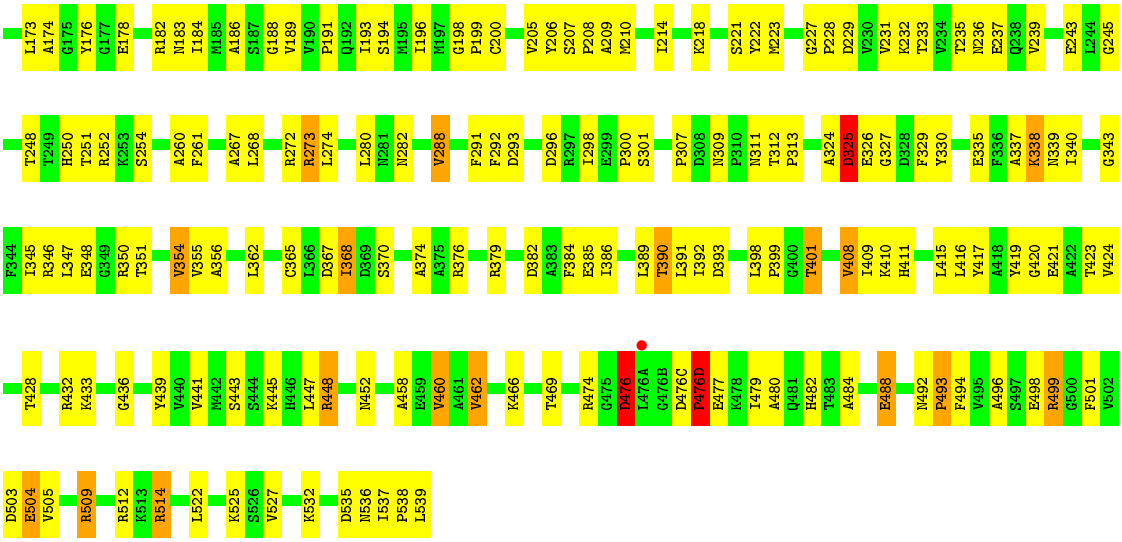
Chain H:



• Molecule 2: Propionyl-CoA carboxylase, beta subunit

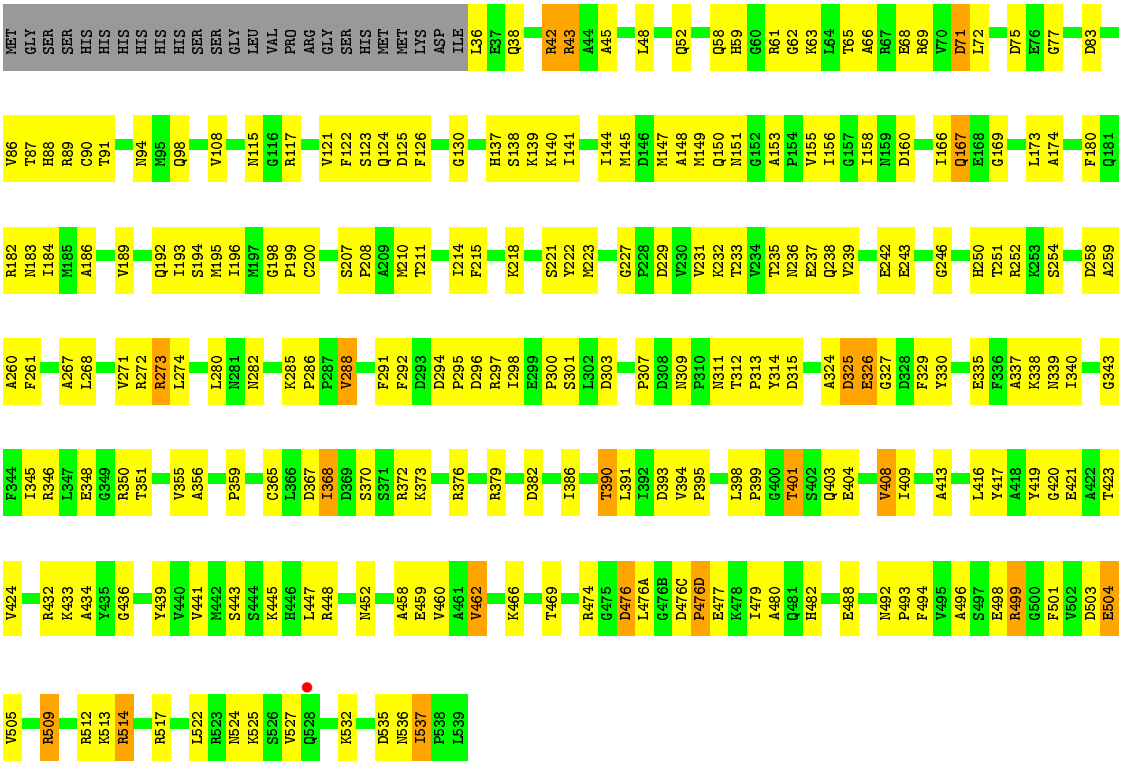
Chain J:





• Molecule 2: Propionyl-CoA carboxylase, beta subunit

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	133.89Å 159.17Å 153.74Å 113.87° 101.03° 108.99°	Depositor
Resolution (Å)	29.36 – 3.20 29.36 – 3.14	Depositor EDS
% Data completeness (in resolution range)	92.4 (29.36-3.20) 90.6 (29.36-3.14)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 3.11Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.212 , 0.245 0.206 , 0.239	Depositor DCC
R_{free} test set	12641 reflections (7.45%)	wwPDB-VP
Wilson B-factor (Å^2)	44.8	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 51.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.017 for -h,h+k+l,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	51921	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.51	0/4586	0.73	1/6209 (0.0%)
1	C	0.51	0/4586	0.74	1/6209 (0.0%)
1	E	0.52	0/4586	0.74	1/6209 (0.0%)
1	G	0.52	0/5036	0.74	1/6811 (0.0%)
1	I	0.51	0/5036	0.74	1/6811 (0.0%)
1	K	0.51	0/5036	0.73	1/6811 (0.0%)
2	B	0.62	1/3990 (0.0%)	0.81	0/5399
2	D	0.61	1/3990 (0.0%)	0.82	0/5399
2	F	0.61	1/3990 (0.0%)	0.82	0/5399
2	H	0.61	0/3990	0.80	0/5399
2	J	0.61	0/3990	0.82	0/5399
2	L	0.61	0/3990	0.81	0/5399
All	All	0.56	3/52806 (0.0%)	0.77	6/71454 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	E	0	1
1	G	0	1
1	I	0	1
1	K	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	365	CYS	CB-SG	-6.58	1.71	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	365	CYS	CB-SG	-5.84	1.72	1.81
2	F	365	CYS	CB-SG	-5.36	1.73	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	422(B)	ALA	N-CA-C	5.95	127.07	111.00
1	K	422(B)	ALA	N-CA-C	5.46	125.75	111.00
1	G	422(B)	ALA	N-CA-C	5.44	125.69	111.00
1	I	422(B)	ALA	N-CA-C	5.36	125.48	111.00
1	E	422(B)	ALA	N-CA-C	5.19	125.01	111.00
1	C	422(B)	ALA	N-CA-C	5.12	124.83	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	420	TYR	Sidechain
1	E	420	TYR	Sidechain
1	G	420	TYR	Sidechain
1	I	420	TYR	Sidechain
1	K	420	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4507	0	4511	424	0
1	C	4507	0	4512	449	0
1	E	4507	0	4512	449	0
1	G	4950	0	4944	491	0
1	I	4950	0	4943	486	0
1	K	4950	0	4943	474	0
2	B	3910	0	3851	260	0
2	D	3910	0	3851	251	0
2	F	3910	0	3851	229	0
2	H	3910	0	3851	239	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	3910	0	3851	233	0
2	L	3910	0	3851	230	0
3	A	15	0	15	1	0
3	C	15	0	15	0	0
3	E	15	0	15	1	0
3	G	15	0	15	0	0
3	I	15	0	15	2	0
3	K	15	0	15	0	0
All	All	51921	0	51561	3984	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 38.

All (3984) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:338:ILE:HD11	1:E:348:LEU:HB2	1.25	1.17
1:A:338:ILE:HD11	1:A:348:LEU:HB2	1.26	1.16
1:C:115:PRO:HG2	1:C:116:PRO:HD3	1.29	1.14
1:A:433:THR:HG22	1:A:435:VAL:H	1.06	1.11
1:G:400:LEU:HD13	1:G:449:ILE:HD11	1.33	1.11
1:K:338:ILE:HD11	1:K:348:LEU:HB2	1.22	1.10
1:I:400:LEU:HD13	1:I:449:ILE:HD11	1.32	1.10
1:C:338:ILE:HD11	1:C:348:LEU:HB2	1.25	1.09
1:I:338:ILE:HD11	1:I:348:LEU:HB2	1.23	1.09
2:L:167:GLN:N	2:L:167:GLN:HE21	1.51	1.09
1:I:433:THR:HG22	1:I:435:VAL:H	1.10	1.09
1:E:400:LEU:HD13	1:E:449:ILE:HD11	1.35	1.08
2:L:167:GLN:H	2:L:167:GLN:NE2	1.51	1.08
1:A:79:ILE:HG23	1:A:89:THR:HG21	1.36	1.07
1:E:433:THR:HG22	1:E:435:VAL:H	1.12	1.07
2:H:167:GLN:N	2:H:167:GLN:HE21	1.53	1.06
1:A:400:LEU:HD13	1:A:449:ILE:HD11	1.34	1.06
1:G:338:ILE:HD11	1:G:348:LEU:HB2	1.35	1.06
1:C:400:LEU:HD13	1:C:449:ILE:HD11	1.34	1.06
1:E:115:PRO:HG2	1:E:116:PRO:HD3	1.34	1.04
1:A:115:PRO:HG2	1:A:116:PRO:HD3	1.37	1.04
1:G:433:THR:HG22	1:G:435:VAL:H	1.23	1.04
1:K:433:THR:HG22	1:K:435:VAL:H	1.19	1.04
1:E:79:ILE:HG23	1:E:89:THR:HG21	1.38	1.03
1:C:433:THR:HG22	1:C:435:VAL:H	1.16	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:115:PRO:HG2	1:K:116:PRO:HD3	1.39	1.03
1:I:115:PRO:HG2	1:I:116:PRO:HD3	1.36	1.02
1:I:653:LYS:HD3	1:I:653:LYS:H	1.20	1.01
1:C:292:ILE:H	1:C:292:ILE:HD12	1.25	1.01
1:C:653:LYS:HD3	1:C:653:LYS:H	1.23	1.01
2:B:167:GLN:NE2	2:B:167:GLN:H	1.58	1.01
1:E:653:LYS:HD3	1:E:653:LYS:H	1.25	1.01
2:H:167:GLN:NE2	2:H:167:GLN:H	1.58	1.01
2:B:167:GLN:N	2:B:167:GLN:HE21	1.60	0.99
2:J:167:GLN:HE21	2:J:167:GLN:N	1.60	0.99
1:E:162:ILE:HG21	1:E:377:ALA:O	1.62	0.99
1:G:292:ILE:HD12	1:G:292:ILE:H	1.27	0.99
1:G:653:LYS:H	1:G:653:LYS:HD3	1.26	0.99
1:G:309:ASP:OD1	1:G:312:THR:HG22	1.63	0.98
1:E:308:LEU:HD22	1:E:316:MET:SD	2.03	0.98
1:I:309:ASP:OD1	1:I:312:THR:HG22	1.64	0.98
2:F:167:GLN:HE21	2:F:167:GLN:N	1.59	0.98
1:G:79:ILE:HG23	1:G:89:THR:HG21	1.44	0.98
1:A:653:LYS:H	1:A:653:LYS:HD3	1.23	0.98
1:C:79:ILE:HG23	1:C:89:THR:HG21	1.46	0.98
2:D:167:GLN:H	2:D:167:GLN:HE21	0.98	0.98
1:G:115:PRO:HG2	1:G:116:PRO:HD3	1.42	0.98
2:F:167:GLN:NE2	2:F:167:GLN:H	1.61	0.98
1:E:419:ARG:HD2	1:E:601:GLN:OE1	1.63	0.97
1:E:670:ILE:HG13	1:E:718:LEU:HD21	1.45	0.97
1:C:66:ILE:HD12	1:C:87:ILE:HG22	1.46	0.97
1:K:162:ILE:HG21	1:K:377:ALA:O	1.63	0.97
1:I:473:PHE:HB3	1:I:482:LEU:HD21	1.46	0.97
1:K:653:LYS:H	1:K:653:LYS:HD3	1.28	0.97
1:C:178:ILE:H	1:C:178:ILE:HD12	1.30	0.96
1:G:178:ILE:H	1:G:178:ILE:HD12	1.30	0.96
1:K:540:ARG:O	1:K:543:VAL:HG23	1.65	0.96
2:J:167:GLN:H	2:J:167:GLN:NE2	1.62	0.96
1:I:670:ILE:HG13	1:I:718:LEU:HD21	1.48	0.95
1:E:665:PRO:HG2	1:E:666:MET:HE1	1.45	0.95
1:G:162:ILE:HG21	1:G:377:ALA:O	1.67	0.95
1:K:292:ILE:H	1:K:292:ILE:HD12	1.30	0.95
1:K:400:LEU:HD13	1:K:449:ILE:HD11	1.45	0.95
1:I:528:ALA:O	1:I:532:MET:HG3	1.67	0.95
1:E:617:GLY:O	1:E:625:PHE:HB3	1.67	0.94
1:I:540:ARG:O	1:I:543:VAL:HG23	1.66	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:456:ALA:HB1	1:E:457:PRO:HD2	1.47	0.94
1:A:178:ILE:HD12	1:A:178:ILE:H	1.32	0.94
1:K:456:ALA:HB1	1:K:457:PRO:HD2	1.48	0.94
1:C:456:ALA:HB1	1:C:457:PRO:HD2	1.50	0.94
1:I:162:ILE:HG21	1:I:377:ALA:O	1.66	0.94
1:K:617:GLY:O	1:K:625:PHE:HB3	1.68	0.94
1:K:178:ILE:H	1:K:178:ILE:HD12	1.31	0.94
1:E:178:ILE:HD12	1:E:178:ILE:H	1.29	0.93
1:A:162:ILE:HG21	1:A:377:ALA:O	1.66	0.93
1:G:66:ILE:HD12	1:G:87:ILE:HG22	1.50	0.93
1:I:131:ILE:HG22	1:I:136:ALA:HB2	1.50	0.93
1:I:136:ALA:HB1	1:I:161:VAL:HG13	1.51	0.93
1:G:131:ILE:HG22	1:G:136:ALA:HB2	1.50	0.93
1:C:540:ARG:O	1:C:543:VAL:HG23	1.69	0.93
1:I:178:ILE:HD12	1:I:178:ILE:H	1.31	0.93
1:I:292:ILE:H	1:I:292:ILE:HD12	1.33	0.93
2:F:325:ASP:HA	2:F:512:ARG:HH12	1.32	0.93
1:A:670:ILE:HG13	1:A:718:LEU:HD21	1.51	0.93
1:K:309:ASP:OD1	1:K:312:THR:HG22	1.68	0.93
1:I:456:ALA:HB1	1:I:457:PRO:HD2	1.51	0.92
1:E:540:ARG:O	1:E:543:VAL:HG23	1.68	0.92
1:A:136:ALA:HB1	1:A:161:VAL:HG13	1.51	0.92
1:K:308:LEU:HD22	1:K:316:MET:SD	2.08	0.92
1:K:264:VAL:HG13	1:K:340:ASP:HB3	1.52	0.92
1:C:162:ILE:HG21	1:C:377:ALA:O	1.70	0.92
1:G:540:ARG:O	1:G:543:VAL:HG23	1.68	0.92
1:K:131:ILE:HG22	1:K:136:ALA:HB2	1.52	0.92
1:K:528:ALA:O	1:K:532:MET:HG3	1.67	0.92
1:C:308:LEU:HD22	1:C:316:MET:SD	2.10	0.91
2:F:207:SER:HB3	2:F:208:PRO:HD3	1.50	0.91
1:K:136:ALA:HB1	1:K:161:VAL:HG13	1.51	0.91
2:L:479:ILE:HD12	2:L:480:ALA:N	1.84	0.91
1:I:79:ILE:HG23	1:I:89:THR:HG21	1.52	0.91
1:E:528:ALA:O	1:E:532:MET:HG3	1.71	0.91
1:K:66:ILE:HD12	1:K:87:ILE:HG22	1.53	0.91
2:F:499:ARG:HG2	2:F:499:ARG:HH11	1.34	0.91
1:I:523:ARG:HB3	1:I:590:MET:HE1	1.53	0.91
1:A:665:PRO:HG2	1:A:666:MET:HE1	1.53	0.91
1:E:66:ILE:HD12	1:E:87:ILE:HG22	1.53	0.91
1:E:136:ALA:HB1	1:E:161:VAL:HG13	1.51	0.91
2:F:420:GLY:HA3	2:H:184:ILE:HD12	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:LEU:HD22	2:B:38:GLN:HG3	1.53	0.90
2:D:167:GLN:HE21	2:D:167:GLN:N	1.69	0.90
1:A:66:ILE:HD12	1:A:87:ILE:HG22	1.54	0.90
2:J:479:ILE:HD12	2:J:480:ALA:N	1.85	0.90
1:A:265:THR:O	1:A:267:PRO:HD3	1.72	0.90
1:C:457:PRO:HG2	1:C:458:THR:H	1.37	0.90
2:D:325:ASP:HA	2:D:512:ARG:HH12	1.37	0.90
1:G:456:ALA:HB1	1:G:457:PRO:HD2	1.51	0.90
1:A:617:GLY:O	1:A:625:PHE:HB3	1.72	0.89
2:B:88:HIS:HD2	2:B:90:CYS:H	1.17	0.89
2:F:83:ASP:HB2	2:F:140:LYS:HE3	1.52	0.89
2:B:325:ASP:HA	2:B:512:ARG:HH12	1.38	0.89
1:A:292:ILE:HD12	1:A:292:ILE:H	1.36	0.89
2:F:167:GLN:H	2:F:167:GLN:HE21	0.92	0.89
1:G:264:VAL:HG13	1:G:340:ASP:HB3	1.52	0.88
1:G:457:PRO:HG2	1:G:458:THR:H	1.38	0.88
1:G:390:LYS:HD3	1:G:391:LEU:N	1.87	0.88
1:G:136:ALA:HB1	1:G:161:VAL:HG13	1.55	0.88
2:L:207:SER:HB3	2:L:208:PRO:HD3	1.55	0.88
1:A:456:ALA:HB1	1:A:457:PRO:HD2	1.55	0.88
1:C:136:ALA:HB1	1:C:161:VAL:HG13	1.55	0.88
2:H:325:ASP:HA	2:H:512:ARG:HH12	1.36	0.88
2:H:499:ARG:HH21	2:J:89:ARG:HH11	1.21	0.88
1:G:528:ALA:O	1:G:532:MET:HG3	1.74	0.88
2:H:499:ARG:HG2	2:H:499:ARG:HH11	1.39	0.88
2:J:499:ARG:HH11	2:J:499:ARG:HG2	1.39	0.88
2:D:167:GLN:H	2:D:167:GLN:NE2	1.70	0.88
2:B:207:SER:HB3	2:B:208:PRO:HD3	1.56	0.88
1:C:617:GLY:O	1:C:625:PHE:HB3	1.73	0.88
1:G:127:VAL:HG12	1:G:131:ILE:HD11	1.55	0.88
1:E:457:PRO:HG2	1:E:458:THR:H	1.40	0.87
1:I:390:LYS:HD3	1:I:391:LEU:N	1.89	0.87
1:G:557:THR:HG23	1:G:572:ILE:O	1.74	0.87
1:K:665:PRO:HG2	1:K:666:MET:HE1	1.57	0.87
1:A:127:VAL:HG12	1:A:131:ILE:HD11	1.56	0.87
2:B:189:VAL:HA	2:B:282:ASN:ND2	1.89	0.87
2:H:207:SER:HB3	2:H:208:PRO:HD3	1.55	0.86
1:I:66:ILE:HD12	1:I:87:ILE:HG22	1.55	0.86
2:B:151:ASN:HD21	2:D:522:LEU:HD23	1.37	0.86
2:F:184:ILE:HD12	2:H:420:GLY:HA3	1.57	0.86
1:C:390:LYS:HD3	1:C:391:LEU:N	1.90	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:479:ILE:HD12	2:H:480:ALA:N	1.90	0.86
1:I:127:VAL:HG12	1:I:131:ILE:HD11	1.58	0.86
1:K:390:LYS:HD3	1:K:391:LEU:N	1.90	0.86
1:A:665:PRO:HG2	1:A:666:MET:CE	2.06	0.86
2:B:479:ILE:HD12	2:B:480:ALA:N	1.90	0.86
2:B:499:ARG:HH21	2:F:89:ARG:HH11	1.23	0.86
1:A:433:THR:HG22	1:A:435:VAL:N	1.91	0.85
1:I:400:LEU:HB3	1:I:449:ILE:HG12	1.58	0.85
1:A:517:LEU:HD22	1:A:517:LEU:H	1.38	0.85
2:J:499:ARG:HH21	2:L:89:ARG:HH11	1.23	0.85
1:A:131:ILE:HG22	1:A:136:ALA:HB2	1.58	0.85
1:A:308:LEU:HD22	1:A:316:MET:SD	2.16	0.85
1:C:517:LEU:HD22	1:C:517:LEU:H	1.40	0.85
1:E:665:PRO:HG2	1:E:666:MET:CE	2.06	0.85
2:L:504:GLU:HG3	2:L:505:VAL:N	1.89	0.85
1:E:131:ILE:HG22	1:E:136:ALA:HB2	1.56	0.85
1:E:156:LEU:HD12	1:E:163:PHE:HB2	1.59	0.85
1:G:396:ILE:HG12	1:G:463:ILE:HD13	1.58	0.84
1:E:557:THR:HG23	1:E:572:ILE:O	1.77	0.84
1:C:309:ASP:OD1	1:C:312:THR:HG22	1.76	0.84
2:B:499:ARG:HH11	2:B:499:ARG:HG2	1.41	0.84
2:H:417:TYR:OH	2:H:535:ASP:HB2	1.76	0.84
1:K:517:LEU:H	1:K:517:LEU:HD22	1.40	0.84
1:A:309:ASP:OD1	1:A:312:THR:HG22	1.78	0.84
1:E:421:ARG:HB3	1:E:474:GLU:HB2	1.59	0.84
1:C:131:ILE:HG22	1:C:136:ALA:HB2	1.56	0.84
1:K:112:ILE:HG13	1:K:120:SER:HB2	1.59	0.84
1:A:528:ALA:O	1:A:532:MET:HG3	1.78	0.84
2:J:207:SER:HB3	2:J:208:PRO:HD3	1.59	0.84
2:D:420:GLY:HA3	2:L:184:ILE:HD12	1.59	0.84
2:B:420:GLY:HA3	2:J:184:ILE:HD12	1.59	0.83
2:J:417:TYR:OH	2:J:535:ASP:HB2	1.76	0.83
1:K:457:PRO:HG2	1:K:458:THR:H	1.43	0.83
1:G:665:PRO:HG2	1:G:666:MET:HE1	1.61	0.83
2:J:91:THR:HA	2:J:98:GLN:HG3	1.60	0.83
1:E:596:TRP:CZ3	1:E:600:ASP:O	2.32	0.83
1:G:665:PRO:HG2	1:G:666:MET:CE	2.09	0.83
1:G:400:LEU:HB3	1:G:449:ILE:HG12	1.59	0.83
2:J:36:LEU:HD22	2:J:38:GLN:HG3	1.60	0.83
2:J:42:ARG:HG2	2:J:42:ARG:HH11	1.42	0.83
1:K:665:PRO:HG2	1:K:666:MET:CE	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:GLN:H	2:B:167:GLN:HE21	0.85	0.83
1:C:357:GLU:O	1:C:360:VAL:HG23	1.78	0.83
1:E:292:ILE:H	1:E:292:ILE:HD12	1.44	0.83
2:L:499:ARG:HH11	2:L:499:ARG:HG2	1.42	0.83
1:K:79:ILE:HG23	1:K:89:THR:HG21	1.60	0.83
1:G:670:ILE:HG13	1:G:718:LEU:HD21	1.61	0.82
2:J:325:ASP:HA	2:J:512:ARG:HH12	1.44	0.82
1:K:321:VAL:O	1:K:324:ALA:HB3	1.79	0.82
2:F:479:ILE:HD12	2:F:480:ALA:N	1.94	0.82
1:G:473:PHE:HB3	1:G:482:LEU:HD21	1.61	0.82
1:A:419:ARG:HH11	1:A:421:ARG:HB2	1.45	0.82
1:I:112:ILE:HG13	1:I:120:SER:HB2	1.62	0.82
1:G:112:ILE:HG13	1:G:120:SER:HB2	1.62	0.82
1:C:127:VAL:HG12	1:C:131:ILE:HD11	1.61	0.82
1:C:528:ALA:O	1:C:532:MET:HG3	1.79	0.82
1:K:198:LEU:HD13	1:K:256:ASP:O	1.79	0.82
1:C:665:PRO:HG2	1:C:666:MET:CE	2.10	0.81
1:C:718:LEU:HD23	1:C:718:LEU:N	1.95	0.81
1:G:321:VAL:O	1:G:324:ALA:HB3	1.81	0.81
1:I:357:GLU:O	1:I:360:VAL:HG23	1.81	0.81
1:I:517:LEU:HD22	1:I:517:LEU:H	1.45	0.81
1:K:473:PHE:HB3	1:K:482:LEU:HD21	1.61	0.81
1:C:294:ARG:HB2	1:C:504:ILE:HG12	1.63	0.81
1:C:321:VAL:O	1:C:324:ALA:HB3	1.80	0.81
1:E:127:VAL:HG12	1:E:131:ILE:HD11	1.61	0.81
1:C:156:LEU:HD12	1:C:163:PHE:HB2	1.62	0.81
1:A:338:ILE:CD1	1:A:348:LEU:HB2	2.09	0.81
1:G:123:VAL:O	1:G:127:VAL:HG23	1.80	0.81
2:F:184:ILE:HD13	2:H:417:TYR:HA	1.61	0.81
1:A:321:VAL:O	1:A:324:ALA:HB3	1.81	0.81
1:K:596:TRP:CZ3	1:K:600:ASP:O	2.34	0.81
2:D:88:HIS:HD2	2:D:90:CYS:H	1.27	0.81
1:C:523:ARG:HB3	1:C:590:MET:HE1	1.63	0.80
1:E:321:VAL:O	1:E:324:ALA:HB3	1.79	0.80
1:E:516:ASN:HB2	1:E:564:GLN:NE2	1.97	0.80
2:D:151:ASN:HD21	2:F:522:LEU:HD23	1.45	0.80
1:K:338:ILE:CD1	1:K:348:LEU:HB2	2.08	0.80
1:E:294:ARG:HB2	1:E:504:ILE:HG12	1.64	0.80
1:G:614:LEU:HD22	1:G:627:ILE:CG2	2.10	0.80
1:C:557:THR:HG23	1:C:572:ILE:O	1.80	0.80
1:E:718:LEU:N	1:E:718:LEU:HD23	1.97	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:293:GLN:O	1:I:504:ILE:HG21	1.80	0.80
1:C:156:LEU:CD1	1:C:163:PHE:HB2	2.12	0.80
1:I:156:LEU:HD12	1:I:163:PHE:HB2	1.62	0.80
1:E:517:LEU:HD22	1:E:517:LEU:H	1.47	0.80
1:I:321:VAL:O	1:I:324:ALA:HB3	1.81	0.80
1:E:156:LEU:CD1	1:E:163:PHE:HB2	2.12	0.80
1:E:596:TRP:HZ3	1:E:600:ASP:O	1.63	0.79
1:K:419:ARG:HH11	1:K:421:ARG:HB2	1.47	0.79
1:K:480:HIS:CD2	1:K:482:LEU:HB2	2.18	0.79
1:A:357:GLU:O	1:A:360:VAL:HG23	1.80	0.79
2:D:499:ARG:HH11	2:D:499:ARG:HG2	1.48	0.79
1:I:308:LEU:HD22	1:I:316:MET:SD	2.22	0.79
1:I:665:PRO:HG2	1:I:666:MET:CE	2.12	0.79
1:E:130:ALA:HA	1:E:133:ALA:HB3	1.63	0.79
1:I:94:SER:HB2	1:I:114:PRO:O	1.82	0.79
1:A:540:ARG:O	1:A:543:VAL:HG23	1.82	0.79
1:K:294:ARG:HB2	1:K:504:ILE:HG12	1.65	0.79
2:D:207:SER:HB3	2:D:208:PRO:HD3	1.65	0.79
1:K:421:ARG:HB3	1:K:474:GLU:HB2	1.64	0.79
1:I:123:VAL:O	1:I:127:VAL:HG23	1.81	0.79
1:I:198:LEU:HD13	1:I:256:ASP:O	1.82	0.79
1:K:557:THR:HG23	1:K:572:ILE:O	1.83	0.79
1:E:596:TRP:CZ3	1:E:600:ASP:HB2	2.17	0.79
1:I:419:ARG:HH11	1:I:421:ARG:HB2	1.47	0.78
1:I:421:ARG:HB3	1:I:474:GLU:HB2	1.63	0.78
1:K:614:LEU:HD22	1:K:627:ILE:CG2	2.13	0.78
1:C:115:PRO:CG	1:C:116:PRO:HD3	2.11	0.78
2:D:479:ILE:HD12	2:D:480:ALA:N	1.97	0.78
2:L:251:THR:HG21	2:L:260:ALA:HB2	1.64	0.78
1:A:396:ILE:HG12	1:A:463:ILE:HD13	1.66	0.78
2:H:88:HIS:HD2	2:H:90:CYS:H	1.32	0.78
2:B:409:ILE:HD13	2:J:205:VAL:HB	1.64	0.78
2:J:504:GLU:HG3	2:J:505:VAL:N	1.97	0.78
1:C:665:PRO:HG2	1:C:666:MET:HE1	1.65	0.78
1:E:400:LEU:HB3	1:E:449:ILE:HG12	1.65	0.78
1:G:163:PHE:O	1:G:163:PHE:HD1	1.67	0.78
2:L:36:LEU:HD22	2:L:38:GLN:HG3	1.64	0.78
1:A:419:ARG:NH1	1:A:421:ARG:HB2	1.96	0.78
2:F:460:VAL:HG21	2:F:496:ALA:HB2	1.65	0.78
1:G:517:LEU:H	1:G:517:LEU:HD22	1.46	0.78
1:I:433:THR:HG22	1:I:435:VAL:N	1.95	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:337:ALA:HB3	2:F:373:LYS:HD2	1.65	0.78
1:K:123:VAL:O	1:K:127:VAL:HG23	1.84	0.78
1:A:433:THR:CG2	1:A:435:VAL:HG12	2.13	0.78
1:A:557:THR:HG23	1:A:572:ILE:O	1.82	0.78
1:A:614:LEU:HD22	1:A:627:ILE:CG2	2.13	0.78
1:C:400:LEU:HB3	1:C:449:ILE:HG12	1.66	0.78
1:E:433:THR:CG2	1:E:435:VAL:HG12	2.13	0.78
1:C:516:ASN:HB2	1:C:564:GLN:NE2	1.99	0.78
1:E:419:ARG:NH1	1:E:421:ARG:HB2	1.98	0.78
2:B:88:HIS:CD2	2:B:90:CYS:H	2.00	0.78
1:E:653:LYS:N	1:E:653:LYS:HD3	1.98	0.78
1:G:419:ARG:HH11	1:G:421:ARG:HB2	1.48	0.78
1:K:357:GLU:O	1:K:360:VAL:HG23	1.84	0.78
1:K:433:THR:HG23	1:K:449:ILE:O	1.83	0.78
2:L:417:TYR:OH	2:L:535:ASP:HB2	1.83	0.78
2:D:89:ARG:HH11	2:F:499:ARG:HH21	1.31	0.77
1:I:457:PRO:HG2	1:I:458:THR:H	1.49	0.77
1:A:400:LEU:HB3	1:A:449:ILE:HG12	1.65	0.77
2:B:460:VAL:HG21	2:B:496:ALA:HB2	1.66	0.77
2:B:83:ASP:HB2	2:B:140:LYS:HE3	1.65	0.77
2:F:210:MET:HE2	2:H:417:TYR:HB2	1.66	0.77
1:A:390:LYS:HD3	1:A:391:LEU:N	1.98	0.77
2:D:36:LEU:HD22	2:D:38:GLN:HG3	1.65	0.77
1:E:309:ASP:OD1	1:E:312:THR:HG22	1.83	0.77
1:E:77:ARG:NH1	1:E:370:VAL:HG21	2.00	0.77
1:I:557:THR:HG23	1:I:572:ILE:O	1.83	0.77
1:I:596:TRP:CZ3	1:I:600:ASP:O	2.37	0.77
1:E:390:LYS:HD3	1:E:391:LEU:N	2.00	0.77
2:D:83:ASP:HB2	2:D:140:LYS:HE3	1.66	0.77
2:J:339:ASN:HD21	2:J:370:SER:HB3	1.49	0.77
1:C:130:ALA:HA	1:C:133:ALA:HB3	1.67	0.77
2:D:88:HIS:CD2	2:D:90:CYS:H	2.02	0.77
1:G:293:GLN:O	1:G:504:ILE:HG21	1.85	0.77
1:G:523:ARG:HB3	1:G:590:MET:HE1	1.64	0.77
1:K:523:ARG:HB3	1:K:590:MET:HE1	1.67	0.77
2:J:88:HIS:HD2	2:J:90:CYS:H	1.32	0.77
1:C:264:VAL:HG13	1:C:340:ASP:HB3	1.67	0.77
2:F:189:VAL:HG23	2:H:532:LYS:HE2	1.67	0.77
1:G:94:SER:HB2	1:G:114:PRO:O	1.85	0.77
1:I:653:LYS:HD3	1:I:653:LYS:N	2.00	0.77
1:E:115:PRO:CG	1:E:116:PRO:HD3	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:433:THR:CG2	1:C:435:VAL:HG12	2.15	0.76
2:D:184:ILE:HD13	2:L:417:TYR:HA	1.67	0.76
1:I:617:GLY:O	1:I:625:PHE:HB3	1.84	0.76
1:K:334:THR:HG21	1:K:355:GLN:NE2	2.01	0.76
1:A:163:PHE:O	1:A:163:PHE:HD1	1.67	0.76
1:I:156:LEU:CD1	1:I:163:PHE:HB2	2.15	0.76
1:G:334:THR:HG21	1:G:355:GLN:NE2	1.99	0.76
1:G:433:THR:CG2	1:G:435:VAL:HG12	2.16	0.76
1:I:264:VAL:HG13	1:I:340:ASP:HB3	1.65	0.76
1:K:397:GLU:HG3	1:K:453:CYS:SG	2.25	0.76
1:E:163:PHE:HD1	1:E:163:PHE:O	1.69	0.76
1:G:308:LEU:HD22	1:G:316:MET:SD	2.25	0.76
2:D:492:ASN:HD22	2:D:494:PHE:H	1.34	0.76
1:K:419:ARG:NH1	1:K:421:ARG:HB2	2.01	0.76
1:K:433:THR:HG22	1:K:435:VAL:N	1.98	0.76
1:A:130:ALA:HA	1:A:133:ALA:HB3	1.68	0.76
1:A:467:ARG:HB3	1:A:467:ARG:HH11	1.51	0.76
1:I:130:ALA:HA	1:I:133:ALA:HB3	1.66	0.76
2:J:189:VAL:HA	2:J:282:ASN:ND2	2.00	0.76
1:E:523:ARG:HB3	1:E:590:MET:HE1	1.66	0.76
1:E:94:SER:HB2	1:E:114:PRO:O	1.86	0.75
1:G:198:LEU:HD13	1:G:256:ASP:O	1.85	0.75
1:I:491:HIS:O	1:I:495:ILE:HG13	1.85	0.75
1:E:123:VAL:O	1:E:127:VAL:HG23	1.87	0.75
1:E:357:GLU:O	1:E:360:VAL:HG23	1.87	0.75
1:C:101:LEU:O	1:C:105:MET:HG3	1.87	0.75
1:G:130:ALA:HA	1:G:133:ALA:HB3	1.68	0.75
2:D:504:GLU:HG3	2:D:505:VAL:N	2.02	0.75
1:I:163:PHE:HD1	1:I:163:PHE:O	1.69	0.75
1:K:658:THR:HB	1:K:703:LYS:HD3	1.69	0.75
1:C:614:LEU:HD22	1:C:627:ILE:CG2	2.16	0.75
1:C:670:ILE:HG13	1:C:718:LEU:HD21	1.68	0.75
1:K:456:ALA:HB1	1:K:457:PRO:CD	2.16	0.75
1:A:294:ARG:HB2	1:A:504:ILE:HG12	1.69	0.75
1:C:596:TRP:CZ3	1:C:600:ASP:O	2.40	0.75
1:G:653:LYS:N	1:G:653:LYS:HD3	2.02	0.75
2:B:184:ILE:HD12	2:J:420:GLY:HA3	1.69	0.75
1:G:101:LEU:O	1:G:105:MET:HG3	1.87	0.75
1:G:398:ASN:HB3	1:G:485:LEU:HD13	1.68	0.75
1:G:614:LEU:HD22	1:G:627:ILE:HG23	1.67	0.75
2:H:288:VAL:HG13	2:H:350:ARG:HG3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:316:MET:HE3	1:I:337:PHE:HD1	1.52	0.75
2:J:492:ASN:HD22	2:J:494:PHE:H	1.33	0.75
1:A:128:MET:HA	1:A:131:ILE:HD12	1.69	0.74
2:B:522:LEU:HD23	2:F:151:ASN:HD21	1.52	0.74
1:I:66:ILE:HB	1:I:138:ALA:O	1.86	0.74
2:J:348:GLU:OE1	1:K:550:ASN:HB2	1.86	0.74
1:G:334:THR:HG21	1:G:355:GLN:HE21	1.49	0.74
1:A:115:PRO:CG	1:A:116:PRO:HD3	2.17	0.74
1:C:123:VAL:O	1:C:127:VAL:HG23	1.86	0.74
1:C:127:VAL:O	1:C:131:ILE:HG13	1.87	0.74
1:C:661:MET:HE2	1:C:726:GLU:HA	1.68	0.74
1:E:334:THR:HG21	1:E:355:GLN:NE2	2.02	0.74
1:I:596:TRP:HZ3	1:I:600:ASP:O	1.71	0.74
2:H:251:THR:HG21	2:H:260:ALA:HB2	1.69	0.74
2:D:417:TYR:HA	2:L:184:ILE:HD13	1.70	0.74
1:G:516:ASN:HB2	1:G:564:GLN:NE2	2.03	0.74
2:J:251:THR:HG21	2:J:260:ALA:HB2	1.70	0.74
1:K:234:ASN:ND2	1:K:236:GLN:HB2	2.03	0.74
1:K:401:TYR:HE2	1:K:448:MET:HB2	1.51	0.74
2:B:288:VAL:HG13	2:B:350:ARG:HG3	1.70	0.74
1:C:94:SER:HB2	1:C:114:PRO:O	1.88	0.74
2:D:173:LEU:HD21	2:L:436:GLY:HA2	1.68	0.74
1:I:528:ALA:HB1	1:I:605:LEU:HD22	1.69	0.74
1:A:661:MET:HE2	1:A:726:GLU:HA	1.70	0.74
1:C:66:ILE:HD12	1:C:87:ILE:CG2	2.18	0.74
1:G:294:ARG:HB2	1:G:504:ILE:HG12	1.69	0.74
1:I:338:ILE:CD1	1:I:348:LEU:HB2	2.12	0.74
2:J:445:LYS:HE2	2:J:452:ASN:OD1	1.88	0.74
1:G:421:ARG:HB3	1:G:474:GLU:HB2	1.70	0.73
1:A:428(L):ALA:HB3	1:A:455:TRP:HD1	1.53	0.73
1:E:115:PRO:HB2	1:E:444:TYR:CD2	2.24	0.73
2:F:296:ASP:O	2:F:298:ILE:HD12	1.88	0.73
2:F:504:GLU:HG3	2:F:505:VAL:N	2.03	0.73
1:I:419:ARG:NH1	1:I:421:ARG:HB2	2.04	0.73
1:I:516:ASN:HB2	1:I:564:GLN:NE2	2.03	0.73
1:I:661:MET:HE2	1:I:726:GLU:HA	1.71	0.73
1:K:334:THR:HG21	1:K:355:GLN:HE21	1.54	0.73
1:K:94:SER:HB2	1:K:114:PRO:O	1.87	0.73
2:L:88:HIS:HD2	2:L:90:CYS:H	1.34	0.73
1:A:653:LYS:N	1:A:653:LYS:HD3	2.01	0.73
1:C:115:PRO:HB2	1:C:444:TYR:CD2	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:PHE:HD1	1:C:163:PHE:O	1.71	0.73
1:C:433:THR:HG22	1:C:435:VAL:N	1.99	0.73
1:C:658:THR:HB	1:C:703:LYS:HD3	1.71	0.73
2:F:83:ASP:HB3	2:F:86:VAL:CG2	2.18	0.73
1:A:264:VAL:HG13	1:A:340:ASP:HB3	1.71	0.73
1:A:115:PRO:HB2	1:A:444:TYR:CD2	2.23	0.73
2:D:75:ASP:OD1	2:D:272:ARG:NH2	2.20	0.73
1:E:189:VAL:HG21	1:E:323:LEU:HB2	1.69	0.73
1:E:433:THR:HG22	1:E:435:VAL:N	1.97	0.73
1:A:473:PHE:HB3	1:A:482:LEU:HD21	1.68	0.73
1:I:614:LEU:HD22	1:I:627:ILE:HG23	1.70	0.73
1:C:419:ARG:HH11	1:C:421:ARG:HB2	1.54	0.73
2:F:65:THR:HG23	2:F:68:GLU:OE1	1.89	0.73
2:L:460:VAL:HG21	2:L:496:ALA:HB2	1.71	0.73
2:L:58:GLN:OE1	2:L:63:LYS:HE3	1.89	0.73
1:A:614:LEU:HD22	1:A:627:ILE:HG23	1.71	0.73
1:C:159:GLU:HB2	1:C:161:VAL:HG23	1.71	0.73
1:C:110:VAL:HG21	1:C:130:ALA:HB1	1.71	0.72
1:E:419:ARG:HH11	1:E:421:ARG:HB2	1.52	0.72
2:F:36:LEU:HD22	2:F:38:GLN:HG3	1.71	0.72
1:G:74:ILE:HD13	1:G:143:TYR:CE2	2.23	0.72
2:F:379:ARG:NH2	2:H:535:ASP:OD2	2.22	0.72
1:I:159:GLU:HB2	1:I:161:VAL:HG23	1.71	0.72
2:H:36:LEU:HD22	2:H:38:GLN:HG3	1.70	0.72
1:K:122:ILE:HA	1:K:146:LEU:HD11	1.70	0.72
1:K:127:VAL:HG12	1:K:131:ILE:HD11	1.69	0.72
1:K:163:PHE:O	1:K:163:PHE:HD1	1.71	0.72
1:K:415:GLY:O	1:K:440:GLU:HG3	1.88	0.72
1:K:417:LEU:HD21	1:K:478:ILE:HD13	1.70	0.72
1:G:283:ILE:HD12	1:G:389:VAL:HG21	1.69	0.72
1:G:550:ASN:HB2	2:L:348:GLU:OE1	1.88	0.72
2:H:504:GLU:HG3	2:H:505:VAL:N	2.03	0.72
2:H:65:THR:HG23	2:H:68:GLU:OE1	1.89	0.72
1:I:276:CYS:HA	1:I:282:GLY:HA2	1.72	0.72
2:F:288:VAL:HG13	2:F:350:ARG:HG3	1.72	0.72
1:G:494:PHE:HA	1:G:499:MET:HE2	1.69	0.72
1:I:494:PHE:HA	1:I:499:MET:HE1	1.71	0.72
1:I:665:PRO:HG2	1:I:666:MET:HE1	1.72	0.72
1:A:718:LEU:HD23	1:A:718:LEU:N	2.04	0.72
1:C:653:LYS:HD3	1:C:653:LYS:N	2.03	0.72
1:G:480:HIS:CD2	1:G:482:LEU:HB2	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:596:TRP:HZ3	1:K:600:ASP:O	1.71	0.72
1:E:473:PHE:HB3	1:E:482:LEU:HD21	1.70	0.72
1:G:456:ALA:HB1	1:G:457:PRO:CD	2.19	0.72
1:I:115:PRO:CG	1:I:116:PRO:HD3	2.16	0.72
1:K:66:ILE:H	1:K:66:ILE:HD13	1.52	0.72
1:E:419:ARG:CD	1:E:601:GLN:OE1	2.38	0.72
2:F:417:TYR:HA	2:H:184:ILE:HD13	1.70	0.72
2:J:83:ASP:HB2	2:J:140:LYS:HE3	1.70	0.72
1:A:596:TRP:CZ3	1:A:600:ASP:HB2	2.24	0.72
2:D:417:TYR:OH	2:D:535:ASP:HB2	1.89	0.72
1:G:338:ILE:CD1	1:G:348:LEU:HB2	2.17	0.72
2:F:532:LYS:HE2	2:H:189:VAL:HG23	1.72	0.72
1:C:419:ARG:NH1	1:C:421:ARG:HB2	2.04	0.72
1:C:522:LEU:HD22	1:C:563:LEU:HD13	1.71	0.72
1:G:66:ILE:HD12	1:G:87:ILE:CG2	2.20	0.72
1:I:658:THR:HB	1:I:703:LYS:HD3	1.71	0.72
1:A:112:ILE:HG13	1:A:120:SER:HB2	1.72	0.71
1:A:457:PRO:HG2	1:A:458:THR:H	1.54	0.71
2:B:504:GLU:HG3	2:B:505:VAL:N	2.03	0.71
1:E:112:ILE:HG13	1:E:120:SER:HB2	1.71	0.71
1:E:66:ILE:HD13	1:E:66:ILE:H	1.55	0.71
1:G:419:ARG:NH1	1:G:421:ARG:HB2	2.05	0.71
1:I:101:LEU:O	1:I:105:MET:HG3	1.89	0.71
1:I:718:LEU:HD23	1:I:718:LEU:N	2.05	0.71
2:B:462:VAL:CG2	2:J:169:GLY:HA2	2.19	0.71
1:C:596:TRP:HZ3	1:C:600:ASP:O	1.73	0.71
1:G:156:LEU:CD1	1:G:163:PHE:HB2	2.20	0.71
1:G:156:LEU:HD12	1:G:163:PHE:HB2	1.72	0.71
1:K:400:LEU:HB3	1:K:449:ILE:HG12	1.71	0.71
2:F:492:ASN:HD22	2:F:494:PHE:H	1.36	0.71
1:E:338:ILE:CD1	1:E:348:LEU:HB2	2.15	0.71
2:J:123:SER:HA	2:J:158:ILE:HB	1.73	0.71
1:I:219:LYS:HE2	1:I:229:MET:N	2.06	0.71
1:I:334:THR:HG21	1:I:355:GLN:NE2	2.05	0.71
1:K:293:GLN:O	1:K:504:ILE:HG21	1.90	0.71
1:C:550:ASN:HB2	2:F:348:GLU:OE1	1.90	0.71
1:K:115:PRO:HB2	1:K:444:TYR:CD2	2.25	0.71
1:A:179:THR:HG22	1:A:183:ILE:HD11	1.73	0.71
1:C:646:LEU:HD12	2:D:72:LEU:HD21	1.73	0.71
1:I:329:TYR:HE2	1:I:352:THR:HG22	1.56	0.71
1:K:66:ILE:HB	1:K:138:ALA:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:292:ILE:H	1:K:292:ILE:CD1	2.00	0.71
1:A:127:VAL:O	1:A:131:ILE:HG13	1.91	0.71
1:E:456:ALA:HB1	1:E:457:PRO:CD	2.20	0.71
1:E:596:TRP:CE3	1:E:600:ASP:HB2	2.25	0.71
1:E:658:THR:HB	1:E:703:LYS:HD3	1.71	0.71
1:E:85:MET:O	1:E:87:ILE:HG13	1.91	0.71
1:K:433:THR:CG2	1:K:435:VAL:HG12	2.20	0.71
1:C:112:ILE:HG13	1:C:120:SER:HB2	1.72	0.70
1:C:480:HIS:CD2	1:C:482:LEU:HB2	2.26	0.70
2:F:462:VAL:CG2	2:H:169:GLY:HA2	2.21	0.70
1:I:294:ARG:HB2	1:I:504:ILE:HG12	1.72	0.70
1:C:293:GLN:O	1:C:504:ILE:HG21	1.90	0.70
1:C:396:ILE:HG12	1:C:463:ILE:HD13	1.71	0.70
1:C:467:ARG:HB3	1:C:467:ARG:HH11	1.56	0.70
2:F:156:ILE:HD12	2:F:156:ILE:N	2.06	0.70
1:I:695:MET:SD	2:J:313:PRO:HG3	2.31	0.70
2:J:88:HIS:CD2	2:J:90:CYS:H	2.08	0.70
2:D:288:VAL:HG13	2:D:350:ARG:HG3	1.72	0.70
2:F:83:ASP:HB3	2:F:86:VAL:HG21	1.71	0.70
1:I:83:ARG:HG2	1:I:83:ARG:HH11	1.55	0.70
1:K:661:MET:HE2	1:K:726:GLU:HA	1.73	0.70
2:F:499:ARG:HG2	2:F:499:ARG:NH1	2.02	0.70
2:J:42:ARG:NH1	2:J:42:ARG:HG2	2.05	0.70
2:D:189:VAL:HG23	2:L:532:LYS:HE2	1.73	0.70
1:G:329:TYR:HE2	1:G:352:THR:HG22	1.56	0.70
1:G:718:LEU:HD23	1:G:718:LEU:N	2.06	0.70
2:H:348:GLU:OE1	1:I:550:ASN:HB2	1.91	0.70
1:K:614:LEU:HD22	1:K:627:ILE:HG23	1.73	0.70
1:A:596:TRP:CZ3	1:A:600:ASP:O	2.45	0.70
1:C:456:ALA:HB1	1:C:457:PRO:CD	2.20	0.70
1:C:596:TRP:CZ3	1:C:600:ASP:HB2	2.27	0.70
2:D:460:VAL:HG21	2:D:496:ALA:HB2	1.72	0.70
1:K:130:ALA:HA	1:K:133:ALA:HB3	1.73	0.70
1:K:219:LYS:HE2	1:K:229:MET:N	2.05	0.70
2:D:532:LYS:HE2	2:L:189:VAL:CG2	2.22	0.70
2:F:417:TYR:OH	2:F:535:ASP:HB2	1.91	0.70
1:G:464:GLU:O	1:G:468:ILE:HG13	1.92	0.70
1:I:396:ILE:HG12	1:I:463:ILE:HD13	1.73	0.70
1:C:85:MET:O	1:C:87:ILE:HG13	1.92	0.70
1:K:543:VAL:HG11	2:L:117:ARG:HD2	1.74	0.70
1:E:110:VAL:HG21	1:E:130:ALA:HB1	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:234:ASN:ND2	1:G:236:GLN:HB2	2.07	0.70
1:I:329:TYR:CE2	1:I:352:THR:HG22	2.26	0.70
1:K:204:GLU:O	1:K:208:ILE:HG13	1.92	0.70
2:B:348:GLU:OE1	1:E:550:ASN:HB2	1.91	0.69
1:K:670:ILE:HG13	1:K:718:LEU:HD21	1.73	0.69
1:A:123:VAL:O	1:A:127:VAL:HG23	1.92	0.69
1:K:218:ILE:HD12	1:K:260:ILE:HG12	1.73	0.69
1:C:494:PHE:HA	1:C:499:MET:HE2	1.73	0.69
2:D:379:ARG:NH2	2:L:535:ASP:OD2	2.25	0.69
1:E:639:ARG:HB3	1:E:643:GLN:HB3	1.74	0.69
1:G:617:GLY:O	1:G:625:PHE:HB3	1.93	0.69
2:B:210:MET:HE2	2:J:417:TYR:HB2	1.74	0.69
1:A:658:THR:HB	1:A:703:LYS:HD3	1.74	0.69
1:E:66:ILE:HB	1:E:138:ALA:O	1.92	0.69
1:G:66:ILE:H	1:G:66:ILE:HD13	1.58	0.69
1:A:523:ARG:HB3	1:A:590:MET:HE1	1.74	0.69
2:H:499:ARG:HG2	2:H:499:ARG:NH1	2.06	0.69
1:I:534:ARG:HG3	1:I:534:ARG:HH11	1.56	0.69
2:L:65:THR:HG23	2:L:68:GLU:OE1	1.91	0.69
2:B:89:ARG:HH11	2:D:499:ARG:HH21	1.40	0.69
1:E:467:ARG:HB3	1:E:467:ARG:HH11	1.58	0.69
1:I:614:LEU:HD22	1:I:627:ILE:CG2	2.21	0.69
1:A:334:THR:HG21	1:A:355:GLN:NE2	2.08	0.69
1:A:550:ASN:HB2	2:D:348:GLU:OE1	1.93	0.69
1:E:159:GLU:HB2	1:E:161:VAL:HG23	1.73	0.69
1:E:614:LEU:HD22	1:E:627:ILE:CG2	2.21	0.69
1:G:159:GLU:HB2	1:G:161:VAL:HG23	1.75	0.69
1:G:219:LYS:HE2	1:G:229:MET:N	2.06	0.69
1:G:433:THR:HG22	1:G:435:VAL:N	2.03	0.69
1:K:695:MET:SD	2:L:313:PRO:HG3	2.33	0.69
1:A:516:ASN:HB2	1:A:564:GLN:NE2	2.07	0.69
1:A:66:ILE:HD13	1:A:66:ILE:H	1.57	0.69
1:C:122:ILE:HA	1:C:146:LEU:HD11	1.74	0.69
1:E:337:PHE:C	1:E:338:ILE:HD12	2.13	0.69
2:F:445:LYS:HE2	2:F:452:ASN:OD1	1.92	0.69
1:G:74:ILE:HD13	1:G:143:TYR:HE2	1.57	0.69
1:G:596:TRP:CZ3	1:G:600:ASP:O	2.46	0.69
2:B:417:TYR:OH	2:B:535:ASP:HB2	1.93	0.69
1:E:128:MET:HA	1:E:131:ILE:HD12	1.74	0.69
2:L:42:ARG:HH11	2:L:42:ARG:HG2	1.57	0.69
2:B:499:ARG:HH21	2:F:89:ARG:NH1	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:THR:HG22	1:C:183:ILE:HD11	1.73	0.69
1:E:117:ALA:HB1	1:E:121:TYR:HB2	1.75	0.69
1:G:658:THR:HB	1:G:703:LYS:HD3	1.75	0.69
1:A:74:ILE:HD13	1:A:143:TYR:CE2	2.27	0.69
1:C:338:ILE:CD1	1:C:348:LEU:HB2	2.13	0.69
1:C:538:ILE:O	1:C:541:THR:HB	1.93	0.69
2:B:184:ILE:HD13	2:J:417:TYR:HA	1.74	0.69
1:K:201:ASP:OD1	1:K:203:ASP:HB2	1.92	0.69
2:L:83:ASP:HB2	2:L:140:LYS:HE3	1.74	0.69
2:L:189:VAL:HA	2:L:282:ASN:ND2	2.08	0.69
2:L:445:LYS:HE2	2:L:452:ASN:OD1	1.93	0.69
1:A:334:THR:HG21	1:A:355:GLN:HE21	1.58	0.68
1:A:670:ILE:CG1	1:A:718:LEU:HD21	2.23	0.68
1:E:101:LEU:O	1:E:105:MET:HG3	1.93	0.68
2:L:149:MET:SD	2:L:186:ALA:HB2	2.32	0.68
1:A:110:VAL:HG21	1:A:130:ALA:HB1	1.73	0.68
1:A:156:LEU:CD1	1:A:163:PHE:HB2	2.22	0.68
2:B:50:GLY:O	2:B:54:ARG:HD2	1.94	0.68
1:G:661:MET:HE2	1:G:726:GLU:HA	1.74	0.68
1:I:74:ILE:O	1:I:77:ARG:HB3	1.93	0.68
1:K:115:PRO:CG	1:K:116:PRO:HD3	2.21	0.68
1:E:396:ILE:HG12	1:E:463:ILE:HD13	1.73	0.68
1:G:357:GLU:O	1:G:360:VAL:HG23	1.94	0.68
1:A:159:GLU:HB2	1:A:161:VAL:HG23	1.75	0.68
1:A:417:LEU:HD21	1:A:478:ILE:HD13	1.74	0.68
2:B:445:LYS:HE2	2:B:452:ASN:OD1	1.93	0.68
1:C:66:ILE:HD13	1:C:66:ILE:H	1.58	0.68
1:I:117:ALA:HB1	1:I:121:TYR:HB2	1.75	0.68
1:K:235:ASP:O	1:K:239:ARG:HG2	1.93	0.68
2:H:329:PHE:CE1	2:H:343:GLY:HA3	2.28	0.68
1:I:129:ALA:O	1:I:133:ALA:HB2	1.93	0.68
1:I:456:ALA:HB1	1:I:457:PRO:CD	2.23	0.68
1:A:122:ILE:HA	1:A:146:LEU:HD11	1.74	0.68
1:A:140:HIS:CE1	1:A:142:GLY:H	2.12	0.68
2:B:65:THR:HG23	2:B:68:GLU:OE1	1.93	0.68
2:H:445:LYS:HE2	2:H:452:ASN:OD1	1.94	0.68
2:J:339:ASN:ND2	2:J:370:SER:HB3	2.08	0.68
1:K:159:GLU:HB2	1:K:161:VAL:HG23	1.76	0.68
2:D:65:THR:HG23	2:D:68:GLU:OE1	1.94	0.68
1:I:433:THR:CG2	1:I:435:VAL:HG12	2.24	0.68
1:I:538:ILE:O	1:I:541:THR:HB	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:179:THR:HG22	1:K:183:ILE:HD11	1.76	0.68
2:B:368:ILE:HG13	2:B:408:VAL:HG13	1.76	0.68
1:E:312:THR:O	1:E:316:MET:HG3	1.93	0.68
2:F:189:VAL:HA	2:F:282:ASN:ND2	2.08	0.68
1:I:596:TRP:CZ3	1:I:600:ASP:HB2	2.29	0.68
2:D:42:ARG:HH11	2:D:42:ARG:HG2	1.58	0.67
2:D:476(C):ASP:O	2:D:477:GLU:N	2.27	0.67
1:G:112:ILE:HD12	1:G:120:SER:O	1.93	0.67
1:I:464:GLU:O	1:I:468:ILE:HG13	1.95	0.67
1:A:77:ARG:NH1	1:A:370:VAL:HG21	2.09	0.67
1:E:397:GLU:HG3	1:E:453:CYS:SG	2.34	0.67
1:G:329:TYR:CE2	1:G:352:THR:HG22	2.30	0.67
2:J:499:ARG:NH1	2:J:499:ARG:HG2	2.06	0.67
1:K:140:HIS:CE1	1:K:142:GLY:H	2.12	0.67
1:K:276:CYS:HA	1:K:282:GLY:HA2	1.76	0.67
1:K:718:LEU:HD23	1:K:718:LEU:N	2.08	0.67
2:L:65:THR:OG1	2:L:68:GLU:HG3	1.93	0.67
1:A:480:HIS:CD2	1:A:482:LEU:HB2	2.30	0.67
2:B:83:ASP:HB3	2:B:86:VAL:CG2	2.24	0.67
1:G:115:PRO:CG	1:G:116:PRO:HD3	2.21	0.67
2:F:532:LYS:HE2	2:H:189:VAL:CG2	2.25	0.67
1:I:66:ILE:HD13	1:I:66:ILE:H	1.59	0.67
1:I:670:ILE:CG1	1:I:718:LEU:HD21	2.22	0.67
2:B:416:LEU:HG	2:J:210:MET:HE1	1.76	0.67
1:K:156:LEU:CD1	1:K:163:PHE:HB2	2.25	0.67
2:B:91:THR:HG21	2:L:91:THR:HG21	1.76	0.67
1:E:661:MET:HE2	1:E:726:GLU:HA	1.75	0.67
1:G:264:VAL:HG13	1:G:340:ASP:CB	2.23	0.67
1:G:528:ALA:HB1	1:G:605:LEU:HD22	1.75	0.67
2:J:167:GLN:H	2:J:167:GLN:HE21	0.79	0.67
1:A:642:ARG:HH11	2:B:71:ASP:HB3	1.60	0.67
2:F:476(C):ASP:O	2:F:477:GLU:N	2.26	0.67
1:I:122:ILE:HA	1:I:146:LEU:HD11	1.76	0.67
2:J:58:GLN:OE1	2:J:63:LYS:HE3	1.94	0.67
1:A:66:ILE:HB	1:A:138:ALA:O	1.95	0.67
1:E:464:GLU:O	1:E:468:ILE:HG13	1.94	0.67
1:I:334:THR:HG21	1:I:355:GLN:HE21	1.57	0.67
2:B:83:ASP:HB3	2:B:86:VAL:HG21	1.76	0.67
1:I:204:GLU:O	1:I:208:ILE:HG13	1.95	0.67
1:A:329:TYR:HE2	1:A:352:THR:HG22	1.59	0.67
1:C:276:CYS:HA	1:C:282:GLY:HA2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:169:GLY:HA2	2:L:462:VAL:CG2	2.24	0.67
2:D:329:PHE:CE1	2:D:343:GLY:HA3	2.30	0.67
1:G:117:ALA:HB1	1:G:121:TYR:HB2	1.76	0.67
2:L:423:THR:O	2:L:525:LYS:HE2	1.95	0.67
1:A:83:ARG:HH11	1:A:83:ARG:HG2	1.59	0.67
1:G:64:ASN:O	1:G:66:ILE:HG23	1.93	0.67
2:J:121:VAL:HG22	2:J:122:PHE:N	2.09	0.67
1:I:235:ASP:O	1:I:239:ARG:HG2	1.95	0.67
2:J:43:ARG:HH11	2:J:43:ARG:HG2	1.60	0.67
1:K:101:LEU:O	1:K:105:MET:HG3	1.95	0.67
1:K:401:TYR:CE2	1:K:448:MET:HB2	2.30	0.67
1:K:396:ILE:HG12	1:K:463:ILE:HD13	1.76	0.67
1:A:101:LEU:O	1:A:105:MET:HG3	1.94	0.66
2:H:492:ASN:HD22	2:H:494:PHE:H	1.41	0.66
1:I:92:ILE:HB	1:I:112:ILE:HG21	1.77	0.66
1:K:189:VAL:HG21	1:K:323:LEU:HB2	1.76	0.66
1:A:117:ALA:C	1:A:119:GLN:H	1.96	0.66
1:A:397:GLU:HG3	1:A:453:CYS:SG	2.35	0.66
1:A:64:ASN:O	1:A:66:ILE:HG23	1.95	0.66
1:C:443:MET:HG3	1:C:444:TYR:CD1	2.30	0.66
2:H:368:ILE:HG13	2:H:408:VAL:HG13	1.77	0.66
2:L:141:ILE:O	2:L:145:MET:HG3	1.96	0.66
2:D:462:VAL:CG2	2:L:169:GLY:HA2	2.26	0.66
1:C:329:TYR:HE2	1:C:352:THR:HG22	1.59	0.66
1:E:64:ASN:O	1:E:66:ILE:HG23	1.95	0.66
1:K:516:ASN:HB2	1:K:564:GLN:NE2	2.10	0.66
2:L:499:ARG:HG2	2:L:499:ARG:NH1	2.11	0.66
2:H:151:ASN:HD21	2:L:522:LEU:HD23	1.61	0.66
2:H:150:GLN:HG2	2:L:527:VAL:HG22	1.77	0.66
1:I:397:GLU:HG3	1:I:453:CYS:SG	2.35	0.66
1:C:358:HIS:ND1	1:C:359:PRO:HD3	2.11	0.66
2:D:291:PHE:CE1	2:D:348:GLU:HA	2.30	0.66
1:E:122:ILE:HA	1:E:146:LEU:HD11	1.78	0.66
1:G:110:VAL:HG21	1:G:130:ALA:HB1	1.77	0.66
2:J:368:ILE:HG13	2:J:408:VAL:HG13	1.77	0.66
1:A:156:LEU:HD12	1:A:163:PHE:HB2	1.76	0.66
1:G:232:ALA:HA	1:G:237:GLU:HG2	1.76	0.66
2:H:324:ALA:HA	2:H:345:ILE:HD12	1.78	0.66
1:C:140:HIS:CE1	1:C:142:GLY:H	2.13	0.66
1:C:614:LEU:HD22	1:C:627:ILE:HG23	1.77	0.66
2:D:339:ASN:HB3	2:D:361:VAL:HG12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:129:ALA:O	1:G:133:ALA:HB2	1.95	0.66
1:G:276:CYS:HA	1:G:282:GLY:HA2	1.78	0.66
1:K:264:VAL:HG13	1:K:340:ASP:CB	2.23	0.66
1:A:456:ALA:HB1	1:A:457:PRO:CD	2.26	0.66
1:E:398:ASN:HB3	1:E:485:LEU:HD13	1.78	0.66
1:K:117:ALA:HB1	1:K:121:TYR:HB2	1.77	0.66
1:K:400:LEU:HD11	1:K:482:LEU:HD13	1.78	0.66
1:A:312:THR:O	1:A:316:MET:HG3	1.96	0.66
1:K:265:THR:HB	1:K:341:GLY:H	1.61	0.66
2:D:210:MET:HE2	2:L:417:TYR:HB2	1.78	0.66
2:H:231:VAL:O	2:H:235:THR:HB	1.96	0.66
2:B:231:VAL:O	2:B:235:THR:HB	1.96	0.65
1:C:117:ALA:C	1:C:119:GLN:H	1.98	0.65
1:E:270:ILE:HG12	1:E:289:GLU:HG3	1.76	0.65
1:E:276:CYS:HA	1:E:282:GLY:HA2	1.78	0.65
1:E:433:THR:HG21	1:E:435:VAL:HG12	1.77	0.65
1:G:235:ASP:O	1:G:239:ARG:HG2	1.96	0.65
2:L:339:ASN:HD21	2:L:370:SER:HB3	1.60	0.65
1:C:337:PHE:C	1:C:338:ILE:HD12	2.16	0.65
2:D:445:LYS:HE2	2:D:452:ASN:OD1	1.95	0.65
2:D:58:GLN:HE21	2:D:61:ARG:HH21	1.43	0.65
1:E:92:ILE:HB	1:E:112:ILE:HG21	1.79	0.65
1:I:115:PRO:HB2	1:I:444:TYR:CD2	2.31	0.65
1:I:480:HIS:CD2	1:I:482:LEU:HB2	2.31	0.65
1:K:596:TRP:CZ3	1:K:600:ASP:HB2	2.31	0.65
1:A:464:GLU:O	1:A:468:ILE:HG13	1.96	0.65
1:A:276:CYS:HA	1:A:282:GLY:HA2	1.77	0.65
1:C:117:ALA:HB1	1:C:121:TYR:HB2	1.76	0.65
2:D:123:SER:HA	2:D:158:ILE:HB	1.77	0.65
2:D:416:LEU:HB2	2:D:441:VAL:HG22	1.79	0.65
1:E:504:ILE:HG23	1:E:505:ALA:N	2.11	0.65
1:G:443:MET:HG3	1:G:444:TYR:CD1	2.32	0.65
1:K:232:ALA:HA	1:K:237:GLU:HG2	1.79	0.65
1:K:522:LEU:HD22	1:K:563:LEU:HD13	1.79	0.65
1:A:143:TYR:CZ	1:A:356:VAL:HG22	2.31	0.65
1:E:177:LYS:HB3	1:E:181:LYS:NZ	2.12	0.65
1:E:670:ILE:CG1	1:E:718:LEU:HD21	2.24	0.65
1:I:77:ARG:NH1	1:I:370:VAL:HG21	2.10	0.65
1:I:401:TYR:HE2	1:I:448:MET:HB2	1.61	0.65
1:I:634:LEU:N	1:I:634:LEU:HD23	2.11	0.65
1:I:411:LEU:HD22	1:I:682:GLN:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:110:VAL:HG21	1:K:130:ALA:HB1	1.77	0.65
2:F:199:PRO:HB3	2:F:222:TYR:CZ	2.31	0.65
2:F:189:VAL:CG2	2:H:532:LYS:HE2	2.26	0.65
1:C:428(L):ALA:HB3	1:C:455:TRP:HD1	1.61	0.65
1:E:107:ASP:O	1:E:108:GLU:HG3	1.97	0.65
1:G:265:THR:HB	1:G:341:GLY:H	1.61	0.65
2:B:156:ILE:HD12	2:B:156:ILE:N	2.12	0.65
2:D:532:LYS:HE2	2:L:189:VAL:HG23	1.78	0.65
1:E:117:ALA:C	1:E:119:GLN:H	2.00	0.65
2:F:123:SER:HA	2:F:158:ILE:HB	1.79	0.65
2:H:189:VAL:HA	2:H:282:ASN:ND2	2.12	0.65
1:K:312:THR:HG21	1:K:343:LYS:HD3	1.79	0.65
1:C:66:ILE:HB	1:C:138:ALA:O	1.96	0.65
1:E:480:HIS:CD2	1:E:482:LEU:HB2	2.32	0.65
1:G:179:THR:HG22	1:G:183:ILE:HD11	1.78	0.65
2:H:65:THR:OG1	2:H:68:GLU:HG3	1.97	0.65
2:L:288:VAL:HG13	2:L:350:ARG:HG3	1.79	0.65
2:F:231:VAL:O	2:F:235:THR:HB	1.97	0.65
1:I:400:LEU:HD11	1:I:482:LEU:HD13	1.78	0.65
2:J:229:ASP:O	2:J:233:THR:HG23	1.97	0.65
1:A:94:SER:HB2	1:A:114:PRO:O	1.97	0.64
2:F:325:ASP:HA	2:F:512:ARG:NH1	2.10	0.64
2:H:88:HIS:CD2	2:H:90:CYS:H	2.14	0.64
1:I:234:ASN:ND2	1:I:236:GLN:HB2	2.11	0.64
1:K:283:ILE:HD12	1:K:389:VAL:HG21	1.77	0.64
1:K:308:LEU:CD2	1:K:316:MET:SD	2.84	0.64
2:L:121:VAL:O	2:L:144:ILE:HD13	1.96	0.64
1:A:421:ARG:HB3	1:A:474:GLU:HB2	1.78	0.64
2:B:416:LEU:HB2	2:B:441:VAL:HG22	1.79	0.64
1:C:304:PRO:O	1:C:394:TRP:CH2	2.50	0.64
1:C:433:THR:HG23	1:C:449:ILE:O	1.97	0.64
2:D:296:ASP:O	2:D:298:ILE:HD12	1.97	0.64
1:E:293:GLN:O	1:E:504:ILE:HG21	1.96	0.64
1:E:634:LEU:HD23	1:E:634:LEU:N	2.12	0.64
2:H:83:ASP:HB2	2:H:140:LYS:HE3	1.78	0.64
1:I:308:LEU:HD12	1:I:308:LEU:O	1.97	0.64
2:D:401:THR:HB	2:L:237:GLU:OE1	1.98	0.64
2:L:325:ASP:HA	2:L:512:ARG:HH12	1.62	0.64
1:C:338:ILE:N	1:C:338:ILE:HD12	2.13	0.64
1:C:397:GLU:HG3	1:C:453:CYS:SG	2.37	0.64
1:E:127:VAL:O	1:E:131:ILE:HG13	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:ARG:HH11	1:E:83:ARG:HG2	1.61	0.64
2:F:291:PHE:CE1	2:F:348:GLU:HA	2.32	0.64
1:K:117:ALA:C	1:K:119:GLN:H	1.99	0.64
1:A:163:PHE:O	1:A:163:PHE:CD1	2.49	0.64
2:D:251:THR:HG21	2:D:260:ALA:HB2	1.79	0.64
2:F:227:GLY:O	2:F:231:VAL:HG23	1.98	0.64
2:H:460:VAL:HG21	2:H:496:ALA:HB2	1.78	0.64
1:K:443:MET:HG3	1:K:444:TYR:CD1	2.32	0.64
1:A:528:ALA:HB1	1:A:605:LEU:HD22	1.77	0.64
1:E:443:MET:HG3	1:E:444:TYR:CD1	2.32	0.64
2:F:88:HIS:CD2	2:F:90:CYS:H	2.15	0.64
1:G:66:ILE:HB	1:G:138:ALA:O	1.96	0.64
1:G:181:LYS:O	1:G:185:GLN:HG3	1.98	0.64
2:F:169:GLY:HA2	2:H:462:VAL:CG2	2.27	0.64
1:A:630:ARG:C	1:A:632:ALA:H	2.01	0.64
2:B:382:ASP:OD1	2:B:424:VAL:HG13	1.98	0.64
1:C:421:ARG:HB3	1:C:474:GLU:HB2	1.79	0.64
1:E:308:LEU:CD2	1:E:316:MET:SD	2.83	0.64
1:K:526:ALA:HA	1:K:561:VAL:HG11	1.79	0.64
1:E:358:HIS:ND1	1:E:359:PRO:HD3	2.12	0.64
1:G:178:ILE:CD1	1:G:178:ILE:H	2.07	0.64
1:K:234:ASN:HD22	1:K:236:GLN:HB2	1.62	0.64
1:A:596:TRP:CE3	1:A:600:ASP:HB2	2.32	0.64
1:A:66:ILE:HD12	1:A:87:ILE:CG2	2.26	0.64
2:F:346:ARG:HA	2:F:350:ARG:O	1.98	0.64
1:G:164:VAL:HG23	1:G:377:ALA:HB2	1.80	0.64
1:I:128:MET:HA	1:I:131:ILE:HD12	1.78	0.64
2:L:329:PHE:CE1	2:L:343:GLY:HA3	2.32	0.64
2:B:124:GLN:HE21	2:B:137:HIS:CE1	2.16	0.64
2:B:261:PHE:CD1	2:B:267:ALA:HA	2.33	0.64
1:C:83:ARG:HG2	1:C:83:ARG:HH11	1.63	0.64
1:E:338:ILE:N	1:E:338:ILE:HD12	2.13	0.64
2:F:346:ARG:HH11	2:F:346:ARG:HG3	1.61	0.64
2:F:419:TYR:CE1	2:F:443:SER:HB2	2.33	0.64
1:G:163:PHE:CD1	1:G:163:PHE:O	2.49	0.64
1:I:143:TYR:CZ	1:I:356:VAL:HG22	2.33	0.64
1:A:265:THR:O	1:A:267:PRO:CD	2.46	0.64
2:B:123:SER:HA	2:B:158:ILE:HB	1.78	0.64
1:C:189:VAL:HG21	1:C:323:LEU:HB2	1.79	0.64
2:F:339:ASN:HD21	2:F:370:SER:HB3	1.61	0.64
1:I:337:PHE:C	1:I:338:ILE:HD12	2.19	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:443:MET:HG3	1:I:444:TYR:CD1	2.33	0.64
1:I:97:ASP:OD1	1:I:102:HIS:HE1	1.81	0.64
1:K:275:LEU:HD23	1:K:331:SER:O	1.98	0.64
2:B:476(C):ASP:O	2:B:477:GLU:N	2.31	0.63
1:C:329:TYR:CE2	1:C:352:THR:HG22	2.33	0.63
2:F:307:PRO:O	2:F:432:ARG:NH2	2.30	0.63
1:I:630:ARG:C	1:I:632:ALA:H	2.00	0.63
2:J:65:THR:HG23	2:J:68:GLU:OE1	1.98	0.63
1:K:329:TYR:HE2	1:K:352:THR:HG22	1.62	0.63
2:L:379:ARG:HD2	2:L:421:GLU:OE2	1.98	0.63
2:L:88:HIS:CD2	2:L:90:CYS:H	2.16	0.63
2:D:49:GLY:C	2:D:51:GLY:H	2.00	0.63
2:F:382:ASP:OD1	2:F:424:VAL:HG13	1.98	0.63
1:G:128:MET:HA	1:G:131:ILE:HD12	1.80	0.63
2:B:169:GLY:HA2	2:J:462:VAL:CG2	2.28	0.63
2:D:200:CYS:HB3	2:D:223:MET:HB3	1.79	0.63
2:H:273:ARG:HD2	2:H:330:TYR:HD1	1.64	0.63
1:I:110:VAL:HG21	1:I:130:ALA:HB1	1.81	0.63
1:A:85:MET:O	1:A:87:ILE:HG13	1.98	0.63
1:C:473:PHE:HB3	1:C:482:LEU:HD21	1.81	0.63
2:D:91:THR:HG21	2:H:91:THR:HG21	1.80	0.63
1:E:124:ILE:HG23	1:E:152:PHE:HD2	1.64	0.63
1:E:66:ILE:HD12	1:E:87:ILE:CG2	2.28	0.63
1:K:275:LEU:HG	1:K:332:ALA:HB2	1.81	0.63
1:K:329:TYR:CE2	1:K:352:THR:HG22	2.32	0.63
2:L:193:ILE:HD13	2:L:274:LEU:HD23	1.80	0.63
2:L:476(C):ASP:O	2:L:477:GLU:N	2.32	0.63
1:A:329:TYR:CE2	1:A:352:THR:HG22	2.33	0.63
2:B:532:LYS:HE2	2:J:189:VAL:CG2	2.28	0.63
1:C:143:TYR:CZ	1:C:356:VAL:HG22	2.33	0.63
1:C:64:ASN:O	1:C:66:ILE:HG23	1.98	0.63
1:E:163:PHE:CD1	1:E:163:PHE:O	2.49	0.63
1:E:411:LEU:HD22	1:E:682:GLN:HB2	1.81	0.63
1:G:177:LYS:HB3	1:G:181:LYS:NZ	2.14	0.63
1:G:414:ILE:HD11	1:G:443:MET:N	2.14	0.63
2:H:476(C):ASP:O	2:H:477:GLU:N	2.30	0.63
2:J:58:GLN:HE21	2:J:61:ARG:HH21	1.46	0.63
2:L:242:GLU:OE2	2:L:246:GLY:HA3	1.99	0.63
1:I:231:ILE:HD12	1:I:231:ILE:H	1.64	0.63
1:I:316:MET:CE	1:I:337:PHE:HD1	2.11	0.63
1:K:517:LEU:N	1:K:564:GLN:HE22	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:695:MET:SD	2:D:313:PRO:HG3	2.39	0.63
1:E:308:LEU:HD12	1:E:308:LEU:O	1.99	0.63
1:K:156:LEU:HD12	1:K:163:PHE:HB2	1.81	0.63
2:B:65:THR:OG1	2:B:68:GLU:HG3	1.98	0.63
1:C:517:LEU:N	1:C:564:GLN:HE22	1.95	0.63
1:E:334:THR:HG21	1:E:355:GLN:HE21	1.63	0.63
1:E:526:ALA:HA	1:E:561:VAL:HG11	1.80	0.63
1:G:467:ARG:HH11	1:G:467:ARG:HB3	1.64	0.63
2:H:167:GLN:HE21	2:H:167:GLN:H	0.75	0.63
2:H:89:ARG:HH11	2:L:499:ARG:HH21	1.46	0.63
2:B:151:ASN:ND2	2:D:522:LEU:HD23	2.12	0.62
1:E:630:ARG:C	1:E:632:ALA:H	2.00	0.62
2:F:91:THR:HG21	2:J:91:THR:HG21	1.80	0.62
1:G:433:THR:HG23	1:G:449:ILE:O	1.98	0.62
1:G:522:LEU:HD22	1:G:563:LEU:HD13	1.81	0.62
1:I:398:ASN:HB3	1:I:485:LEU:HD13	1.81	0.62
1:I:64:ASN:O	1:I:66:ILE:HG23	1.99	0.62
2:J:419:TYR:CE1	2:J:443:SER:HB2	2.34	0.62
1:K:467:ARG:HB3	1:K:467:ARG:HH11	1.63	0.62
1:K:653:LYS:HD3	1:K:653:LYS:N	2.08	0.62
2:D:300:PRO:HA	2:D:509:ARG:NH1	2.14	0.62
2:F:58:GLN:CD	2:F:63:LYS:HE3	2.20	0.62
2:H:527:VAL:HG22	2:J:150:GLN:HG2	1.81	0.62
1:I:259:PHE:CE2	1:I:261:GLU:HB2	2.34	0.62
1:I:66:ILE:HD12	1:I:87:ILE:CG2	2.28	0.62
1:E:304:PRO:HG2	1:E:394:TRP:CZ2	2.33	0.62
1:E:329:TYR:HE2	1:E:352:THR:HG22	1.65	0.62
1:E:304:PRO:O	1:E:394:TRP:CH2	2.51	0.62
1:E:78:VAL:HG13	1:E:79:ILE:N	2.14	0.62
1:I:177:LYS:HB3	1:I:181:LYS:NZ	2.14	0.62
2:J:43:ARG:NH1	2:J:43:ARG:HG2	2.13	0.62
1:A:433:THR:HG23	1:A:449:ILE:O	1.99	0.62
2:D:189:VAL:CG2	2:L:532:LYS:HE2	2.28	0.62
2:D:193:ILE:HD13	2:D:274:LEU:HD23	1.81	0.62
1:E:143:TYR:CZ	1:E:356:VAL:HG22	2.34	0.62
1:I:232:ALA:HA	1:I:237:GLU:HG2	1.80	0.62
2:B:499:ARG:NH1	2:B:499:ARG:HG2	2.07	0.62
1:E:179:THR:HG22	1:E:183:ILE:HD11	1.80	0.62
1:E:517:LEU:HD21	1:E:632:ALA:CB	2.30	0.62
1:G:292:ILE:HD13	1:G:300:VAL:O	1.99	0.62
1:I:146:LEU:HD23	1:I:152:PHE:CG	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:264:VAL:HG13	1:I:340:ASP:CB	2.29	0.62
1:K:181:LYS:O	1:K:185:GLN:HG3	2.00	0.62
1:K:517:LEU:HD21	1:K:632:ALA:CB	2.28	0.62
1:A:337:PHE:C	1:A:338:ILE:HD12	2.19	0.62
1:G:259:PHE:CE2	1:G:261:GLU:HB2	2.35	0.62
1:G:400:LEU:HD11	1:G:482:LEU:HD13	1.82	0.62
1:G:596:TRP:CZ3	1:G:600:ASP:HB2	2.35	0.62
2:J:231:VAL:O	2:J:235:THR:HB	2.00	0.62
2:J:288:VAL:HG13	2:J:350:ARG:HG3	1.81	0.62
1:K:64:ASN:O	1:K:66:ILE:HG23	2.00	0.62
1:K:66:ILE:HD12	1:K:87:ILE:CG2	2.26	0.62
1:K:83:ARG:HG2	1:K:83:ARG:HH11	1.64	0.62
1:A:74:ILE:HD13	1:A:143:TYR:HE2	1.64	0.62
1:E:186:GLU:C	1:E:188:ASN:H	2.02	0.62
1:E:433:THR:HG23	1:E:449:ILE:O	2.00	0.62
1:G:170:ALA:O	1:G:173:ALA:HB3	1.99	0.62
2:D:492:ASN:HB2	2:D:493:PRO:HD2	1.82	0.62
2:F:368:ILE:HG13	2:F:408:VAL:HG13	1.79	0.62
2:H:379:ARG:HD2	2:H:421:GLU:OE2	1.99	0.62
1:I:112:ILE:HD12	1:I:120:SER:O	2.00	0.62
1:I:275:LEU:HD23	1:I:276:CYS:N	2.14	0.62
1:K:480:HIS:HD2	1:K:482:LEU:HB2	1.65	0.62
1:A:124:ILE:HG23	1:A:152:PHE:HD2	1.65	0.62
1:A:181:LYS:O	1:A:185:GLN:HG3	1.99	0.62
1:C:186:GLU:C	1:C:188:ASN:H	2.02	0.62
1:C:334:THR:HG21	1:C:355:GLN:NE2	2.14	0.62
2:D:499:ARG:NH1	2:D:499:ARG:HG2	2.12	0.62
1:G:397:GLU:HG3	1:G:453:CYS:SG	2.39	0.62
1:I:140:HIS:CE1	1:I:142:GLY:H	2.18	0.62
1:I:414:ILE:HD11	1:I:443:MET:N	2.14	0.62
1:I:665:PRO:HG2	1:I:666:MET:HE2	1.81	0.62
1:C:128:MET:HA	1:C:131:ILE:HD12	1.82	0.62
1:C:401:TYR:HE2	1:C:448:MET:HB2	1.65	0.62
1:C:417:LEU:HD21	1:C:478:ILE:HD13	1.82	0.62
1:E:323:LEU:O	1:E:326:ALA:HB3	1.99	0.62
2:J:527:VAL:HG22	2:L:150:GLN:HG2	1.81	0.62
1:C:661:MET:HE1	1:C:726:GLU:HB3	1.81	0.61
1:C:75:ALA:O	1:C:78:VAL:HG12	1.99	0.61
2:D:89:ARG:NH1	2:F:499:ARG:HH21	1.98	0.61
2:F:88:HIS:HD2	2:F:90:CYS:H	1.47	0.61
1:G:275:LEU:HG	1:G:332:ALA:HB2	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:403:GLU:O	1:G:405:PRO:HD3	1.99	0.61
2:H:325:ASP:HA	2:H:512:ARG:NH1	2.12	0.61
1:A:293:GLN:O	1:A:504:ILE:HG21	2.00	0.61
1:C:163:PHE:CD1	1:C:163:PHE:O	2.53	0.61
1:C:320:ALA:HB1	1:C:335:VAL:HG21	1.82	0.61
2:F:42:ARG:HG2	2:F:42:ARG:HH11	1.65	0.61
1:G:292:ILE:CD1	1:G:292:ILE:H	1.97	0.61
1:A:292:ILE:CD1	1:A:292:ILE:H	2.05	0.61
1:A:358:HIS:ND1	1:A:359:PRO:HD3	2.16	0.61
2:B:346:ARG:HA	2:B:350:ARG:O	2.00	0.61
2:B:88:HIS:HD2	2:B:90:CYS:N	1.95	0.61
1:G:642:ARG:HH11	2:H:71:ASP:HB3	1.66	0.61
1:G:74:ILE:O	1:G:77:ARG:HB3	1.99	0.61
2:H:229:ASP:O	2:H:233:THR:HG23	2.00	0.61
2:B:532:LYS:HE2	2:J:189:VAL:HG23	1.82	0.61
2:J:499:ARG:HH21	2:L:89:ARG:NH1	1.95	0.61
2:J:83:ASP:HB3	2:J:86:VAL:CG2	2.30	0.61
1:K:596:TRP:CE3	1:K:600:ASP:HB2	2.35	0.61
1:A:117:ALA:HB1	1:A:121:TYR:HB2	1.81	0.61
2:D:58:GLN:OE1	2:D:63:LYS:HE3	2.00	0.61
1:C:275:LEU:HG	1:C:332:ALA:HB2	1.83	0.61
1:C:283:ILE:HD12	1:C:389:VAL:HG21	1.82	0.61
1:G:189:VAL:HA	1:G:319:GLN:OE1	2.01	0.61
2:J:83:ASP:HB3	2:J:86:VAL:HG21	1.81	0.61
1:A:596:TRP:HZ3	1:A:600:ASP:O	1.82	0.61
1:C:78:VAL:HG13	1:C:79:ILE:N	2.15	0.61
2:F:65:THR:OG1	2:F:68:GLU:HG3	2.00	0.61
2:H:499:ARG:HH21	2:J:89:ARG:NH1	1.95	0.61
1:K:74:ILE:O	1:K:77:ARG:HB3	2.00	0.61
1:K:97:ASP:OD1	1:K:102:HIS:HE1	1.84	0.61
2:L:339:ASN:ND2	2:L:370:SER:HB3	2.15	0.61
2:D:184:ILE:HD12	2:L:420:GLY:HA3	1.83	0.61
1:A:275:LEU:HD11	1:A:372:GLN:HB2	1.82	0.61
2:F:184:ILE:CD1	2:H:417:TYR:HA	2.30	0.61
1:G:122:ILE:HA	1:G:146:LEU:HD11	1.81	0.61
1:G:229:MET:HG3	1:G:229:MET:O	2.01	0.61
2:H:156:ILE:HD12	2:H:156:ILE:N	2.14	0.61
1:K:538:ILE:O	1:K:541:THR:HB	2.00	0.61
1:I:163:PHE:CD1	1:I:163:PHE:O	2.52	0.61
1:I:400:LEU:HD23	1:I:481:ASN:OD1	2.00	0.61
1:K:497:GLY:HA2	1:K:499:MET:HE3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:346:ARG:HH11	2:L:346:ARG:HG3	1.64	0.61
1:A:184:ALA:HB1	1:A:189:VAL:HB	1.83	0.61
1:C:129:ALA:O	1:C:133:ALA:HB2	2.01	0.61
1:C:275:LEU:HD11	1:C:372:GLN:HB2	1.83	0.61
1:C:596:TRP:CE3	1:C:600:ASP:HB2	2.35	0.61
1:E:164:VAL:HG23	1:E:377:ALA:HB2	1.82	0.61
1:G:77:ARG:NH1	1:G:370:VAL:HG21	2.16	0.61
2:F:535:ASP:OD2	2:H:379:ARG:NH2	2.33	0.61
1:A:661:MET:HE1	1:A:726:GLU:HB3	1.83	0.61
1:C:433:THR:HG21	1:C:435:VAL:HG12	1.83	0.61
2:D:50:GLY:O	2:D:54:ARG:HD2	2.01	0.61
1:E:66:ILE:O	1:E:66:ILE:HG12	2.00	0.61
2:F:329:PHE:CE1	2:F:343:GLY:HA3	2.35	0.61
1:G:115:PRO:HB2	1:G:444:TYR:CD2	2.36	0.61
1:I:67:LEU:HG	1:I:68:ILE:H	1.64	0.61
1:K:376:VAL:C	1:K:378:ALA:H	2.04	0.61
2:L:123:SER:HA	2:L:158:ILE:HB	1.82	0.61
2:B:42:ARG:HH11	2:B:42:ARG:HG2	1.66	0.60
1:C:630:ARG:C	1:C:632:ALA:H	2.02	0.60
1:E:75:ALA:O	1:E:78:VAL:HG12	2.00	0.60
1:G:365:THR:HG22	1:G:391:LEU:CD2	2.31	0.60
1:I:201:ASP:OD1	1:I:203:ASP:HB2	2.01	0.60
2:J:460:VAL:HG21	2:J:496:ALA:HB2	1.82	0.60
2:L:324:ALA:HA	2:L:345:ILE:HD12	1.82	0.60
1:A:164:VAL:HG23	1:A:377:ALA:HB2	1.83	0.60
1:A:464:GLU:OE2	1:A:464:GLU:HA	2.01	0.60
1:A:411:LEU:HD22	1:A:682:GLN:HB2	1.83	0.60
2:F:409:ILE:HD13	2:H:205:VAL:HB	1.82	0.60
1:G:458:THR:O	1:G:461:ALA:HB3	2.02	0.60
1:I:74:ILE:HD13	1:I:143:TYR:CE2	2.36	0.60
1:K:658:THR:OG1	1:K:702:GLU:HG2	2.00	0.60
2:D:307:PRO:O	2:D:432:ARG:NH2	2.34	0.60
2:D:436:GLY:HA2	2:L:173:LEU:HD21	1.82	0.60
1:E:74:ILE:O	1:E:77:ARG:HB3	2.01	0.60
1:G:401:TYR:HE2	1:G:448:MET:HB2	1.66	0.60
2:H:337:ALA:HB1	2:H:370:SER:HA	1.83	0.60
2:H:423:THR:O	2:H:525:LYS:HE2	2.01	0.60
1:I:189:VAL:HG21	1:I:323:LEU:HB2	1.83	0.60
1:K:127:VAL:O	1:K:131:ILE:HG13	2.01	0.60
1:K:77:ARG:NH1	1:K:370:VAL:HG21	2.16	0.60
1:K:596:TRP:CG	1:K:597:THR:N	2.69	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:619:ILE:HD12	1:K:625:PHE:C	2.21	0.60
2:D:417:TYR:HB2	2:L:210:MET:HE2	1.83	0.60
2:D:535:ASP:OD2	2:L:379:ARG:NH2	2.34	0.60
1:C:467:ARG:HE	1:C:630:ARG:HG3	1.66	0.60
1:E:181:LYS:O	1:E:185:GLN:HG3	2.00	0.60
1:E:329:TYR:CE2	1:E:352:THR:HG22	2.37	0.60
1:I:215:PRO:HB2	1:I:231:ILE:CG2	2.32	0.60
1:I:492:PRO:HA	1:I:495:ILE:HD12	1.83	0.60
1:I:526:ALA:HA	1:I:561:VAL:HG11	1.83	0.60
2:B:173:LEU:HD21	2:J:436:GLY:HA2	1.83	0.60
1:K:414:ILE:HD11	1:K:443:MET:N	2.15	0.60
1:K:517:LEU:H	1:K:564:GLN:HE22	1.46	0.60
2:L:231:VAL:O	2:L:235:THR:HB	2.01	0.60
1:C:504:ILE:HG23	1:C:505:ALA:N	2.15	0.60
1:C:653:LYS:H	1:C:653:LYS:CD	2.08	0.60
2:D:156:ILE:HD12	2:D:156:ILE:N	2.16	0.60
1:E:517:LEU:N	1:E:564:GLN:HE22	2.00	0.60
1:A:283:ILE:HD12	1:A:389:VAL:HG21	1.83	0.60
1:C:400:LEU:HD21	1:C:482:LEU:HD13	1.83	0.60
1:G:275:LEU:HD23	1:G:331:SER:O	2.01	0.60
1:G:417:LEU:HD21	1:G:478:ILE:HD13	1.83	0.60
1:G:538:ILE:O	1:G:541:THR:HB	2.02	0.60
1:G:670:ILE:CG1	1:G:718:LEU:HD21	2.29	0.60
2:F:417:TYR:HB2	2:H:210:MET:HE2	1.82	0.60
1:I:186:GLU:C	1:I:188:ASN:H	2.04	0.60
1:I:543:VAL:HG12	1:I:544:SER:O	2.02	0.60
2:L:156:ILE:HD12	2:L:156:ILE:N	2.15	0.60
1:E:494:PHE:HA	1:E:499:MET:HE2	1.84	0.60
2:B:237:GLU:OE1	2:J:401:THR:HB	2.01	0.60
1:A:304:PRO:O	1:A:394:TRP:CH2	2.54	0.60
1:C:92:ILE:HB	1:C:112:ILE:HG21	1.83	0.60
1:E:97:ASP:OD1	1:E:102:HIS:HE1	1.85	0.60
1:E:265:THR:HG22	1:E:266:GLN:HG2	1.83	0.60
2:F:169:GLY:HA2	2:H:462:VAL:HG22	1.82	0.60
1:A:480:HIS:HD2	1:A:482:LEU:HB2	1.67	0.60
1:A:74:ILE:O	1:A:77:ARG:HB3	2.02	0.60
2:D:58:GLN:CD	2:D:63:LYS:HE3	2.22	0.60
1:E:403:GLU:O	1:E:405:PRO:HD3	2.02	0.60
2:F:339:ASN:ND2	2:F:370:SER:HB3	2.17	0.60
2:B:169:GLY:HA2	2:J:462:VAL:HG22	1.83	0.60
1:A:276:CYS:O	1:A:382:LEU:HD21	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:460:VAL:CG2	2:B:496:ALA:HB2	2.32	0.60
1:C:414:ILE:HD11	1:C:443:MET:N	2.16	0.60
1:C:464:GLU:O	1:C:468:ILE:HG13	2.02	0.60
2:D:337:ALA:HB3	2:D:373:LYS:HD2	1.84	0.60
1:G:97:ASP:OD1	1:G:102:HIS:HE1	1.85	0.60
1:K:128:MET:HA	1:K:131:ILE:HD12	1.83	0.60
1:K:163:PHE:O	1:K:163:PHE:CD1	2.54	0.60
1:C:276:CYS:O	1:C:382:LEU:HD21	2.01	0.59
1:C:392:THR:O	1:C:455:TRP:HZ3	1.84	0.59
1:E:118:ASN:HD21	1:E:119:GLN:HE21	1.50	0.59
2:L:124:GLN:HE21	2:L:137:HIS:CE1	2.19	0.59
2:L:337:ALA:HB3	2:L:373:LYS:HD2	1.84	0.59
2:L:42:ARG:NH1	2:L:42:ARG:HG2	2.17	0.59
1:A:267:PRO:O	1:A:501:THR:HG23	2.02	0.59
2:B:348:GLU:OE2	1:E:551:HIS:HE1	1.85	0.59
2:D:261:PHE:CD1	2:D:267:ALA:HA	2.37	0.59
1:E:129:ALA:O	1:E:133:ALA:HB2	2.01	0.59
2:F:50:GLY:O	2:F:54:ARG:HD2	2.01	0.59
2:D:151:ASN:ND2	2:F:522:LEU:HD23	2.15	0.59
2:H:273:ARG:HD2	2:H:330:TYR:CD1	2.37	0.59
2:H:83:ASP:HB3	2:H:86:VAL:CG2	2.32	0.59
2:J:476(C):ASP:O	2:J:477:GLU:N	2.35	0.59
2:L:193:ILE:CD1	2:L:274:LEU:HD23	2.33	0.59
1:E:414:ILE:HD11	1:E:443:MET:N	2.18	0.59
2:B:121:VAL:HG22	2:B:122:PHE:N	2.17	0.59
1:A:695:MET:SD	2:B:313:PRO:HG3	2.43	0.59
1:C:265:THR:HB	1:C:341:GLY:H	1.67	0.59
1:E:459:ARG:O	1:E:463:ILE:HG12	2.03	0.59
2:B:417:TYR:HA	2:J:184:ILE:HD13	1.83	0.59
2:D:237:GLU:OE1	2:L:401:THR:HB	2.03	0.59
1:C:679:GLN:O	1:C:706:VAL:HG13	2.02	0.59
1:E:275:LEU:HG	1:E:332:ALA:HB2	1.84	0.59
1:E:619:ILE:HD12	1:E:625:PHE:C	2.23	0.59
2:F:239:VAL:HG22	2:F:243:GLU:HB2	1.84	0.59
2:H:149:MET:SD	2:H:186:ALA:HB2	2.43	0.59
2:H:42:ARG:HH11	2:H:42:ARG:HG2	1.67	0.59
1:I:164:VAL:HG23	1:I:377:ALA:HB2	1.84	0.59
2:J:160:ASP:OD1	2:J:198:GLY:HA3	2.03	0.59
1:K:178:ILE:CD1	1:K:178:ILE:H	2.07	0.59
1:K:577:ASP:HB2	1:K:591:ARG:NH2	2.16	0.59
2:D:160:ASP:OD1	2:D:198:GLY:HA3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:THR:O	1:E:183:ILE:HG13	2.02	0.59
2:F:173:LEU:HD21	2:H:436:GLY:HA2	1.84	0.59
1:G:83:ARG:HH11	1:G:83:ARG:HG2	1.66	0.59
2:H:291:PHE:CE1	2:H:348:GLU:HA	2.36	0.59
2:J:65:THR:OG1	2:J:68:GLU:HG3	2.03	0.59
1:K:528:ALA:HB1	1:K:605:LEU:HD22	1.84	0.59
1:K:467:ARG:HE	1:K:630:ARG:HG3	1.67	0.59
2:L:325:ASP:C	2:L:327:GLY:H	2.06	0.59
2:B:462:VAL:HG22	2:J:169:GLY:HA2	1.85	0.59
2:B:527:VAL:HG22	2:F:150:GLN:HG2	1.84	0.59
2:B:54:ARG:HH11	2:B:54:ARG:HG2	1.67	0.59
2:D:83:ASP:HB3	2:D:86:VAL:CG2	2.32	0.59
1:G:167:PRO:O	1:G:169:GLY:N	2.36	0.59
1:G:189:VAL:HG21	1:G:323:LEU:HB2	1.83	0.59
1:G:275:LEU:HD23	1:G:276:CYS:N	2.18	0.59
2:J:492:ASN:HB2	2:J:493:PRO:HD2	1.83	0.59
1:K:598:PRO:HD2	2:L:292:PHE:CE1	2.38	0.59
2:B:61:ARG:HB2	2:B:63:LYS:HG3	1.85	0.59
1:E:334:THR:HG22	1:E:351:ASN:HB2	1.84	0.59
1:E:614:LEU:HD22	1:E:627:ILE:HG23	1.84	0.59
2:F:334:GLU:O	2:F:338:LYS:HD2	2.02	0.59
2:F:462:VAL:HG22	2:H:169:GLY:HA2	1.84	0.59
2:F:460:VAL:CG2	2:F:496:ALA:HB2	2.33	0.59
1:G:131:ILE:CG2	1:G:136:ALA:HB2	2.27	0.59
1:G:634:LEU:HD23	1:G:634:LEU:N	2.17	0.59
2:H:346:ARG:HA	2:H:350:ARG:O	2.03	0.59
1:I:634:LEU:H	1:I:634:LEU:HD23	1.67	0.59
1:I:543:VAL:HG11	2:J:117:ARG:HD2	1.85	0.59
1:K:428(L):ALA:HB3	1:K:455:TRP:HD1	1.67	0.59
1:A:619:ILE:HD12	1:A:625:PHE:C	2.23	0.59
1:G:543:VAL:HG12	1:G:544:SER:O	2.03	0.59
1:I:117:ALA:C	1:I:119:GLN:H	2.03	0.59
1:K:358:HIS:ND1	1:K:359:PRO:HD3	2.18	0.59
1:A:433:THR:HG22	1:A:434:GLY:N	2.18	0.59
2:D:121:VAL:HG22	2:D:122:PHE:N	2.18	0.59
2:D:368:ILE:HG13	2:D:408:VAL:HG13	1.85	0.59
1:E:275:LEU:HD11	1:E:372:GLN:HB2	1.85	0.59
2:F:261:PHE:CD1	2:F:267:ALA:HA	2.38	0.59
1:G:234:ASN:HD22	1:G:236:GLN:HB2	1.66	0.59
1:K:400:LEU:HD23	1:K:481:ASN:OD1	2.02	0.59
1:C:181:LYS:O	1:C:185:GLN:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:436:GLY:HA2	2:H:173:LEU:HD21	1.85	0.58
1:G:117:ALA:C	1:G:119:GLN:H	2.06	0.58
1:G:132:ARG:HD3	1:G:159:GLU:OE1	2.03	0.58
1:G:392:THR:O	1:G:455:TRP:HZ3	1.86	0.58
1:K:259:PHE:CE2	1:K:261:GLU:HB2	2.38	0.58
1:K:275:LEU:HD11	1:K:372:GLN:HB2	1.84	0.58
1:K:642:ARG:HH11	2:L:71:ASP:HB3	1.68	0.58
1:A:320:ALA:HB1	1:A:335:VAL:HG21	1.85	0.58
2:B:325:ASP:HA	2:B:512:ARG:NH1	2.15	0.58
1:C:178:ILE:H	1:C:178:ILE:CD1	2.08	0.58
2:D:436:GLY:O	2:D:439:TYR:HB3	2.03	0.58
1:E:492:PRO:HA	1:E:495:ILE:HD12	1.84	0.58
1:G:596:TRP:HZ3	1:G:600:ASP:O	1.86	0.58
1:I:338:ILE:N	1:I:338:ILE:HD12	2.19	0.58
1:I:78:VAL:HG23	1:I:370:VAL:CG1	2.33	0.58
1:I:653:LYS:H	1:I:653:LYS:CD	2.06	0.58
2:J:324:ALA:HA	2:J:345:ILE:HD12	1.85	0.58
1:K:365:THR:HG22	1:K:391:LEU:CD2	2.33	0.58
2:L:298:ILE:HG23	2:L:509:ARG:HB2	1.83	0.58
1:A:112:ILE:HD12	1:A:120:SER:O	2.03	0.58
1:A:189:VAL:HG21	1:A:323:LEU:HB2	1.85	0.58
1:A:433:THR:HG21	1:A:435:VAL:HG12	1.83	0.58
1:A:517:LEU:N	1:A:564:GLN:HE22	2.01	0.58
1:C:398:ASN:HB3	1:C:485:LEU:HD13	1.84	0.58
2:F:58:GLN:OE1	2:F:63:LYS:HE3	2.03	0.58
1:G:124:ILE:HG23	1:G:152:PHE:HD2	1.68	0.58
2:H:43:ARG:HG2	2:H:43:ARG:HH11	1.69	0.58
1:I:170:ALA:O	1:I:173:ALA:HB3	2.03	0.58
1:I:181:LYS:O	1:I:185:GLN:HG3	2.02	0.58
1:K:411:LEU:HD22	1:K:682:GLN:HB2	1.85	0.58
1:C:308:LEU:CD2	1:C:316:MET:SD	2.90	0.58
1:I:467:ARG:HE	1:I:630:ARG:HG3	1.68	0.58
2:J:199:PRO:HB3	2:J:222:TYR:CZ	2.38	0.58
1:K:128:MET:SD	1:K:131:ILE:HD12	2.44	0.58
1:K:186:GLU:C	1:K:188:ASN:H	2.07	0.58
1:A:724:ILE:HG22	1:A:725:MET:HG3	1.85	0.58
1:C:365:THR:HG22	1:C:391:LEU:HD22	1.85	0.58
1:C:66:ILE:CD1	1:C:87:ILE:HG22	2.29	0.58
1:E:400:LEU:HD21	1:E:482:LEU:HD13	1.84	0.58
2:H:348:GLU:OE2	1:I:551:HIS:HE1	1.86	0.58
1:I:467:ARG:HH11	1:I:467:ARG:HB3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:553:ARG:NH1	2:J:115:ASN:OD1	2.37	0.58
1:A:78:VAL:HG13	1:A:79:ILE:N	2.18	0.58
1:C:264:VAL:CG1	1:C:340:ASP:HB3	2.34	0.58
1:C:526:ALA:HA	1:C:561:VAL:HG11	1.85	0.58
2:F:182:ARG:HG3	2:F:182:ARG:HH11	1.69	0.58
1:G:140:HIS:CE1	1:G:142:GLY:H	2.21	0.58
1:I:157:GLU:C	1:I:159:GLU:H	2.06	0.58
1:K:552:GLU:H	1:K:552:GLU:CD	2.07	0.58
2:L:149:MET:CE	2:L:189:VAL:HG11	2.33	0.58
1:A:363:LEU:HD13	1:A:455:TRP:HB3	1.85	0.58
2:B:329:PHE:CE1	2:B:343:GLY:HA3	2.38	0.58
1:C:598:PRO:HD2	2:D:292:PHE:CE1	2.38	0.58
2:D:337:ALA:HB1	2:D:370:SER:HA	1.85	0.58
2:D:416:LEU:HG	2:L:210:MET:HE1	1.85	0.58
2:F:346:ARG:NH1	2:F:346:ARG:HG3	2.18	0.58
1:G:528:ALA:HB1	1:G:605:LEU:CD2	2.32	0.58
1:I:179:THR:O	1:I:183:ILE:HG13	2.04	0.58
1:I:335:VAL:O	1:I:335:VAL:HG23	2.04	0.58
1:K:304:PRO:O	1:K:394:TRP:CH2	2.57	0.58
1:K:543:VAL:HG12	1:K:544:SER:O	2.04	0.58
1:A:128:MET:SD	1:A:131:ILE:HD12	2.44	0.58
1:C:312:THR:O	1:C:316:MET:HG3	2.03	0.58
1:C:577:ASP:HB2	1:C:591:ARG:NH2	2.19	0.58
1:C:634:LEU:HD23	1:C:634:LEU:N	2.18	0.58
2:D:150:GLN:HG2	2:F:527:VAL:HG22	1.86	0.58
1:E:140:HIS:CE1	1:E:142:GLY:H	2.20	0.58
1:G:218:ILE:HD12	1:G:260:ILE:HG12	1.86	0.58
1:G:396:ILE:HG12	1:G:463:ILE:CD1	2.31	0.58
1:K:212:ILE:HD12	1:K:260:ILE:HG22	1.86	0.58
2:L:346:ARG:HG3	2:L:346:ARG:NH1	2.16	0.58
1:C:74:ILE:HD13	1:C:143:TYR:CE2	2.39	0.58
2:D:195:MET:SD	2:D:271:VAL:HG21	2.43	0.58
2:D:199:PRO:HB3	2:D:222:TYR:CZ	2.39	0.58
2:D:42:ARG:NH1	2:D:42:ARG:HG2	2.18	0.58
1:E:170:ALA:O	1:E:173:ALA:HB3	2.04	0.58
1:G:146:LEU:HD23	1:G:152:PHE:CG	2.38	0.58
1:G:143:TYR:CZ	1:G:356:VAL:HG22	2.39	0.58
2:H:43:ARG:NH1	2:H:43:ARG:HG2	2.18	0.58
1:I:128:MET:SD	1:I:131:ILE:HD12	2.44	0.58
1:K:78:VAL:HG23	1:K:370:VAL:CG1	2.33	0.58
1:A:380:GLU:CG	1:A:381:PRO:HD2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:ILE:HB	1:C:335:VAL:HG23	1.85	0.58
1:C:365:THR:HG22	1:C:391:LEU:CD2	2.34	0.58
1:G:204:GLU:O	1:G:208:ILE:HG13	2.04	0.58
2:H:148:ALA:HB1	2:H:153:ALA:O	2.04	0.58
2:H:87:THR:HG23	2:L:498:GLU:HG2	1.86	0.58
1:I:179:THR:HG22	1:I:183:ILE:HD11	1.85	0.58
1:I:275:LEU:HG	1:I:332:ALA:HB2	1.86	0.58
1:I:365:THR:HG22	1:I:391:LEU:CD2	2.34	0.58
2:B:170:VAL:HG11	2:J:460:VAL:HG23	1.86	0.58
1:A:504:ILE:HG23	1:A:505:ALA:N	2.19	0.57
1:E:543:VAL:HG12	1:E:544:SER:O	2.04	0.57
1:G:231:ILE:H	1:G:231:ILE:HD12	1.69	0.57
1:G:596:TRP:CE3	1:G:600:ASP:HB2	2.39	0.57
1:G:658:THR:OG1	1:G:702:GLU:HG2	2.04	0.57
1:K:92:ILE:HB	1:K:112:ILE:HG21	1.86	0.57
1:K:184:ALA:HB1	1:K:189:VAL:HB	1.85	0.57
1:K:67:LEU:HG	1:K:68:ILE:H	1.69	0.57
2:L:300:PRO:HA	2:L:509:ARG:NH1	2.18	0.57
1:C:304:PRO:HG2	1:C:394:TRP:CZ2	2.39	0.57
1:K:74:ILE:HD13	1:K:143:TYR:CE2	2.39	0.57
1:K:415:GLY:C	1:K:440:GLU:HG3	2.24	0.57
1:C:124:ILE:HG23	1:C:152:PHE:HD2	1.69	0.57
2:F:178:GLU:O	2:F:182:ARG:HG3	2.04	0.57
1:G:128:MET:SD	1:G:131:ILE:HD12	2.44	0.57
1:G:358:HIS:HB2	1:G:369:LEU:HD12	1.85	0.57
2:L:58:GLN:HE21	2:L:61:ARG:HH21	1.52	0.57
2:B:401:THR:HB	2:J:237:GLU:OE1	2.04	0.57
1:C:157:GLU:C	1:C:159:GLU:H	2.06	0.57
1:C:74:ILE:O	1:C:77:ARG:HB3	2.03	0.57
1:A:551:HIS:HE1	2:D:348:GLU:OE2	1.86	0.57
1:E:630:ARG:C	1:E:632:ALA:N	2.57	0.57
1:G:275:LEU:HD11	1:G:372:GLN:HB2	1.85	0.57
1:I:596:TRP:CE3	1:I:600:ASP:HB2	2.39	0.57
1:I:630:ARG:C	1:I:632:ALA:N	2.55	0.57
1:A:275:LEU:HD23	1:A:331:SER:O	2.04	0.57
1:E:279:HIS:NE2	1:E:380:GLU:N	2.52	0.57
1:G:304:PRO:HG2	1:G:394:TRP:CZ2	2.40	0.57
2:F:401:THR:HB	2:H:237:GLU:OE1	2.04	0.57
1:I:137:GLN:O	1:I:138:ALA:HB2	2.03	0.57
1:I:670:ILE:HD11	1:I:718:LEU:HD11	1.85	0.57
2:J:307:PRO:O	2:J:432:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:230:ARG:HG2	1:K:230:ARG:HH11	1.69	0.57
1:K:398:ASN:HB3	1:K:485:LEU:HD13	1.86	0.57
1:K:464:GLU:O	1:K:468:ILE:HG13	2.05	0.57
1:K:504:ILE:HG23	1:K:505:ALA:N	2.19	0.57
1:A:400:LEU:HD21	1:A:482:LEU:HD13	1.85	0.57
1:A:491:HIS:O	1:A:495:ILE:HG13	2.04	0.57
1:A:517:LEU:HD22	1:A:517:LEU:N	2.15	0.57
1:A:526:ALA:HA	1:A:561:VAL:HG11	1.85	0.57
2:B:251:THR:HG21	2:B:260:ALA:HB2	1.86	0.57
2:B:501:PHE:CE1	2:J:174:ALA:HB2	2.40	0.57
1:C:279:HIS:NE2	1:C:380:GLU:N	2.53	0.57
2:D:193:ILE:CD1	2:D:274:LEU:HD23	2.35	0.57
1:E:131:ILE:CG2	1:E:136:ALA:HB2	2.32	0.57
2:L:419:TYR:CE1	2:L:443:SER:HB2	2.39	0.57
1:A:157:GLU:C	1:A:159:GLU:H	2.05	0.57
1:A:634:LEU:N	1:A:634:LEU:HD23	2.19	0.57
1:C:619:ILE:HD12	1:C:625:PHE:C	2.25	0.57
1:E:365:THR:HG22	1:E:391:LEU:HD22	1.86	0.57
1:G:400:LEU:HD21	1:G:482:LEU:HD13	1.85	0.57
2:H:75:ASP:OD1	2:H:272:ARG:NH2	2.38	0.57
1:I:121:TYR:HE2	1:I:445:TYR:HH	1.53	0.57
1:I:189:VAL:HA	1:I:319:GLN:OE1	2.04	0.57
1:I:78:VAL:HG13	1:I:79:ILE:N	2.19	0.57
1:K:137:GLN:O	1:K:138:ALA:HB2	2.04	0.57
1:K:177:LYS:O	1:K:181:LYS:HG2	2.04	0.57
1:C:164:VAL:HG23	1:C:377:ALA:HB2	1.86	0.57
2:F:207:SER:HB3	2:F:208:PRO:CD	2.26	0.57
1:G:276:CYS:O	1:G:382:LEU:HD21	2.05	0.57
1:G:85:MET:O	1:G:87:ILE:HG13	2.05	0.57
1:K:337:PHE:C	1:K:338:ILE:HD12	2.24	0.57
2:B:160:ASP:OD1	2:B:198:GLY:HA3	2.04	0.57
1:E:117:ALA:CB	1:E:121:TYR:HB2	2.35	0.57
1:E:264:VAL:CG1	1:E:340:ASP:HB3	2.35	0.57
1:E:417:LEU:HD21	1:E:478:ILE:HD13	1.87	0.57
1:G:400:LEU:HD23	1:G:481:ASN:OD1	2.05	0.57
1:G:683:GLU:HB2	1:G:704:LYS:HG3	1.86	0.57
1:I:283:ILE:HA	1:I:386:GLN:NE2	2.19	0.57
1:K:348:LEU:O	1:K:348:LEU:HD23	2.05	0.57
1:A:123:VAL:HG12	1:A:126:LYS:H	1.70	0.57
1:A:365:THR:HG22	1:A:391:LEU:CD2	2.35	0.57
1:E:137:GLN:O	1:E:138:ALA:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:200:CYS:HB3	2:F:223:MET:HB3	1.86	0.57
1:G:201:ASP:OD1	1:G:203:ASP:HB2	2.05	0.57
1:G:395:ALA:C	1:G:396:ILE:HD12	2.25	0.57
1:I:85:MET:O	1:I:87:ILE:HG13	2.05	0.57
1:K:112:ILE:HD12	1:K:120:SER:O	2.05	0.57
1:K:218:ILE:CD1	1:K:260:ILE:HG12	2.35	0.57
1:K:400:LEU:HD21	1:K:482:LEU:HD13	1.86	0.57
1:K:492:PRO:HA	1:K:495:ILE:HD12	1.85	0.57
1:C:270:ILE:HG12	1:C:289:GLU:HG3	1.87	0.56
1:E:190:SER:N	1:E:319:GLN:OE1	2.34	0.56
1:I:146:LEU:HD23	1:I:152:PHE:CD2	2.40	0.56
1:I:279:HIS:NE2	1:I:380:GLU:N	2.53	0.56
2:J:458:ALA:HB3	2:J:493:PRO:HB3	1.86	0.56
1:K:215:PRO:HB2	1:K:231:ILE:CG2	2.35	0.56
1:K:457:PRO:CG	1:K:458:THR:H	2.17	0.56
1:K:642:ARG:NH1	2:L:71:ASP:OD2	2.38	0.56
2:B:492:ASN:HB2	2:B:493:PRO:HD2	1.86	0.56
1:C:137:GLN:O	1:C:138:ALA:HB2	2.05	0.56
2:D:83:ASP:HB3	2:D:86:VAL:HG21	1.87	0.56
1:E:400:LEU:HD11	1:E:482:LEU:HD13	1.86	0.56
2:F:58:GLN:HE21	2:F:61:ARG:HH21	1.52	0.56
1:G:207:LYS:O	1:G:211:GLN:HB2	2.04	0.56
1:G:308:LEU:HD12	1:G:308:LEU:O	2.05	0.56
1:I:74:ILE:HD13	1:I:143:TYR:HE2	1.70	0.56
1:G:712:ALA:HA	1:G:716:ASN:ND2	2.20	0.56
1:G:92:ILE:HB	1:G:112:ILE:HG21	1.88	0.56
1:I:401:TYR:CE2	1:I:448:MET:HB2	2.40	0.56
1:I:66:ILE:HG12	1:I:66:ILE:O	2.05	0.56
2:L:83:ASP:HB3	2:L:86:VAL:HG21	1.87	0.56
2:B:74:LEU:HD13	2:B:112:GLY:HA3	1.87	0.56
1:E:634:LEU:HD23	1:E:634:LEU:H	1.69	0.56
2:F:237:GLU:OE1	2:H:401:THR:HB	2.06	0.56
2:H:141:ILE:O	2:H:145:MET:HG3	2.06	0.56
2:H:337:ALA:HB3	2:H:373:LYS:HD2	1.86	0.56
1:K:675:VAL:CG1	1:K:707:VAL:HG21	2.35	0.56
1:A:598:PRO:HD2	2:B:292:PHE:CE1	2.40	0.56
1:C:292:ILE:HD13	1:C:300:VAL:O	2.04	0.56
2:D:458:ALA:HB3	2:D:493:PRO:HB3	1.87	0.56
2:D:484:ALA:O	2:D:488:GLU:OE1	2.24	0.56
1:G:517:LEU:HB3	1:G:521:ASP:HB3	1.87	0.56
1:I:275:LEU:HD23	1:I:331:SER:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:167:PRO:O	1:K:169:GLY:N	2.38	0.56
1:A:275:LEU:HG	1:A:332:ALA:HB2	1.88	0.56
2:B:447:LEU:C	2:B:448:ARG:HG2	2.25	0.56
2:B:492:ASN:HD22	2:B:494:PHE:H	1.53	0.56
1:C:457:PRO:CG	1:C:458:THR:H	2.13	0.56
1:E:380:GLU:CG	1:E:381:PRO:HD2	2.36	0.56
1:I:127:VAL:O	1:I:131:ILE:HG13	2.05	0.56
1:I:354:LEU:HD11	1:I:358:HIS:CE1	2.41	0.56
1:I:675:VAL:CG1	1:I:707:VAL:HG21	2.36	0.56
1:K:553:ARG:NH1	2:L:115:ASN:OD1	2.39	0.56
2:L:291:PHE:CE1	2:L:348:GLU:HA	2.40	0.56
1:A:522:LEU:HD22	1:A:563:LEU:HD13	1.87	0.56
1:E:157:GLU:C	1:E:159:GLU:H	2.08	0.56
1:E:287:GLU:OE2	1:E:305:SER:N	2.38	0.56
1:E:358:HIS:HB2	1:E:369:LEU:HD12	1.87	0.56
1:G:335:VAL:HG23	1:G:335:VAL:O	2.06	0.56
1:G:441:ILE:HD12	1:G:478:ILE:HD13	1.88	0.56
2:J:75:ASP:OD1	2:J:272:ARG:NH2	2.37	0.56
1:K:74:ILE:HD13	1:K:143:TYR:HE2	1.69	0.56
2:B:479:ILE:C	2:B:479:ILE:HD12	2.26	0.56
2:B:501:PHE:N	2:B:501:PHE:CD2	2.69	0.56
1:C:272:ILE:HB	1:C:335:VAL:CG2	2.36	0.56
1:E:428(L):ALA:HB3	1:E:455:TRP:HD1	1.71	0.56
1:E:400:LEU:HD23	1:E:481:ASN:OD1	2.05	0.56
1:I:92:ILE:HB	1:I:112:ILE:CG2	2.34	0.56
2:J:149:MET:SD	2:J:186:ALA:HB2	2.45	0.56
2:L:250:HIS:HA	2:L:254:SER:OG	2.06	0.56
1:A:152:PHE:CE1	1:A:156:LEU:HD11	2.41	0.56
1:A:67:LEU:HG	1:A:68:ILE:H	1.71	0.56
2:D:339:ASN:HD21	2:D:370:SER:HB3	1.71	0.56
1:G:337:PHE:C	1:G:338:ILE:HD12	2.26	0.56
2:H:154:PRO:HG3	2:H:191:PRO:HD2	1.88	0.56
2:H:296:ASP:O	2:H:298:ILE:HD12	2.06	0.56
1:A:639:ARG:HB3	1:A:643:GLN:HB3	1.88	0.56
2:B:189:VAL:CG2	2:J:532:LYS:HE2	2.36	0.56
1:E:324:ALA:O	1:E:327:VAL:HG12	2.05	0.56
1:E:552:GLU:H	1:E:552:GLU:CD	2.09	0.56
2:H:121:VAL:HG22	2:H:122:PHE:N	2.20	0.56
1:K:157:GLU:C	1:K:159:GLU:H	2.07	0.56
1:K:517:LEU:HD21	1:K:632:ALA:HB1	1.87	0.56
2:L:460:VAL:CG2	2:L:496:ALA:HB2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ILE:HB	1:A:112:ILE:HG21	1.86	0.56
2:B:148:ALA:HB1	2:B:153:ALA:O	2.05	0.56
1:C:70:ASN:ND2	1:C:145:PHE:CD1	2.74	0.56
1:E:363:LEU:HD13	1:E:455:TRP:HB3	1.88	0.56
2:F:436:GLY:O	2:F:439:TYR:HB3	2.05	0.56
1:G:157:GLU:C	1:G:159:GLU:H	2.09	0.56
1:G:186:GLU:C	1:G:188:ASN:H	2.07	0.56
1:G:683:GLU:H	1:G:704:LYS:HG2	1.71	0.56
2:H:492:ASN:ND2	2:H:494:PHE:H	2.03	0.56
1:I:117:ALA:CB	1:I:121:TYR:HB2	2.36	0.56
1:K:354:LEU:C	1:K:354:LEU:HD13	2.26	0.56
1:K:497:GLY:O	1:K:499:MET:HG2	2.05	0.56
1:K:537:GLU:HG3	1:K:553:ARG:NH2	2.21	0.56
1:C:630:ARG:C	1:C:632:ALA:N	2.58	0.55
2:D:432:ARG:HG2	2:D:433:LYS:N	2.21	0.55
1:E:123:VAL:HG12	1:E:126:LYS:H	1.71	0.55
1:E:335:VAL:O	1:E:335:VAL:HG23	2.07	0.55
1:E:283:ILE:HG22	1:E:386:GLN:HG2	1.87	0.55
1:E:646:LEU:HD12	2:F:72:LEU:HD21	1.88	0.55
1:G:433:THR:HG22	1:G:434:GLY:N	2.21	0.55
1:G:670:ILE:CD1	1:G:718:LEU:HD21	2.36	0.55
1:I:283:ILE:HD12	1:I:389:VAL:HG21	1.88	0.55
1:A:70:ASN:ND2	1:A:145:PHE:CD1	2.75	0.55
1:A:443:MET:HG3	1:A:444:TYR:CD1	2.41	0.55
2:B:189:VAL:HA	2:B:282:ASN:HD22	1.67	0.55
1:C:66:ILE:O	1:C:66:ILE:HG12	2.05	0.55
1:G:137:GLN:O	1:G:138:ALA:HB2	2.06	0.55
1:G:528:ALA:CB	1:G:605:LEU:HD22	2.36	0.55
1:G:70:ASN:ND2	1:G:145:PHE:CD1	2.74	0.55
1:K:177:LYS:HB3	1:K:181:LYS:NZ	2.21	0.55
2:L:307:PRO:HG3	2:L:312:THR:O	2.06	0.55
1:A:129:ALA:O	1:A:133:ALA:HB2	2.06	0.55
1:A:177:LYS:HB3	1:A:181:LYS:NZ	2.21	0.55
1:A:272:ILE:HB	1:A:335:VAL:CG2	2.35	0.55
1:A:538:ILE:O	1:A:541:THR:HB	2.06	0.55
1:A:630:ARG:C	1:A:632:ALA:N	2.58	0.55
1:A:75:ALA:O	1:A:78:VAL:HG12	2.06	0.55
1:E:421:ARG:HD2	1:E:474:GLU:HG3	1.87	0.55
1:E:484:PHE:O	1:E:487:ALA:HB3	2.06	0.55
2:H:78:SER:O	2:H:112:GLY:HA2	2.07	0.55
1:I:185:GLN:O	1:I:188:ASN:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:517:LEU:HD21	1:I:632:ALA:CB	2.36	0.55
1:K:394:TRP:CE3	1:K:459:ARG:HG3	2.41	0.55
1:K:75:ALA:O	1:K:78:VAL:HG12	2.06	0.55
1:A:338:ILE:N	1:A:338:ILE:HD12	2.21	0.55
1:A:683:GLU:H	1:A:704:LYS:HG2	1.70	0.55
2:F:492:ASN:HB2	2:F:493:PRO:HD2	1.88	0.55
1:G:380:GLU:CG	1:G:381:PRO:HD2	2.36	0.55
1:G:283:ILE:HD12	1:G:389:VAL:CG2	2.37	0.55
1:K:491:HIS:O	1:K:495:ILE:HG13	2.07	0.55
1:A:517:LEU:HD21	1:A:632:ALA:CB	2.37	0.55
1:A:78:VAL:HA	1:A:370:VAL:HG11	1.88	0.55
2:B:419:TYR:CE1	2:B:443:SER:HB2	2.42	0.55
2:D:307:PRO:HG3	2:D:312:THR:O	2.07	0.55
2:D:346:ARG:HA	2:D:350:ARG:O	2.06	0.55
1:E:275:LEU:HD23	1:E:331:SER:O	2.06	0.55
1:G:92:ILE:HD12	1:G:112:ILE:HD13	1.87	0.55
1:G:443:MET:HG3	1:G:444:TYR:CE1	2.41	0.55
1:G:534:ARG:HG3	1:G:534:ARG:HH11	1.70	0.55
1:I:598:PRO:HD2	2:J:292:PHE:CE1	2.42	0.55
1:A:324:ALA:O	1:A:327:VAL:HG12	2.06	0.55
2:D:65:THR:OG1	2:D:68:GLU:HG3	2.07	0.55
2:F:379:ARG:HD2	2:F:421:GLU:OE2	2.07	0.55
1:G:127:VAL:O	1:G:131:ILE:HG13	2.06	0.55
1:G:215:PRO:HB2	1:G:231:ILE:CG2	2.36	0.55
1:G:324:ALA:O	1:G:327:VAL:HG12	2.06	0.55
1:G:78:VAL:HG23	1:G:370:VAL:CG1	2.36	0.55
1:G:401:TYR:CD2	1:G:448:MET:HA	2.42	0.55
1:G:661:MET:HE1	1:G:726:GLU:HB3	1.88	0.55
1:I:124:ILE:O	1:I:128:MET:HB2	2.05	0.55
1:K:229:MET:O	1:K:229:MET:HG3	2.06	0.55
1:A:186:GLU:C	1:A:188:ASN:H	2.09	0.55
1:C:123:VAL:HG12	1:C:126:LYS:H	1.70	0.55
2:D:154:PRO:HG3	2:D:191:PRO:HD2	1.89	0.55
2:F:160:ASP:OD1	2:F:198:GLY:HA3	2.06	0.55
2:F:196:ILE:HG22	2:F:221:SER:HB2	1.89	0.55
1:G:504:ILE:HG23	1:G:505:ALA:N	2.20	0.55
1:I:528:ALA:HB1	1:I:605:LEU:CD2	2.35	0.55
1:K:392:THR:O	1:K:455:TRP:HZ3	1.89	0.55
2:B:398:LEU:O	2:B:403:GLN:HG3	2.07	0.55
1:E:156:LEU:HD22	1:E:161:VAL:HB	1.89	0.55
1:G:517:LEU:HD21	1:G:632:ALA:CB	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:250:HIS:HA	2:J:254:SER:OG	2.07	0.55
1:A:358:HIS:HB2	1:A:369:LEU:HD12	1.88	0.55
1:C:334:THR:HG22	1:C:351:ASN:HB2	1.87	0.55
1:C:443:MET:HG3	1:C:444:TYR:CE1	2.42	0.55
1:E:275:LEU:HD23	1:E:276:CYS:N	2.21	0.55
1:E:401:TYR:HE2	1:E:448:MET:HB2	1.72	0.55
1:G:179:THR:O	1:G:183:ILE:HG13	2.07	0.55
1:G:401:TYR:HD2	1:G:448:MET:HA	1.71	0.55
1:G:464:GLU:HA	1:G:464:GLU:OE2	2.05	0.55
1:K:517:LEU:N	1:K:517:LEU:HD22	2.17	0.55
2:B:235:THR:HG22	2:B:237:GLU:HB2	1.88	0.55
2:B:307:PRO:O	2:B:432:ARG:NH2	2.39	0.55
1:C:539:ARG:NH2	2:D:326:GLU:OE2	2.40	0.55
2:D:43:ARG:HH11	2:D:43:ARG:HG2	1.72	0.55
1:I:417:LEU:HD21	1:I:478:ILE:HD13	1.88	0.55
1:I:602:LEU:HD12	1:I:614:LEU:O	2.06	0.55
2:H:498:GLU:HG2	2:J:87:THR:HG23	1.89	0.55
2:J:94:ASN:HA	2:J:98:GLN:OE1	2.06	0.55
1:K:433:THR:HG21	1:K:435:VAL:HG12	1.88	0.55
2:L:121:VAL:HG22	2:L:122:PHE:N	2.22	0.55
2:L:229:ASP:O	2:L:233:THR:HG23	2.06	0.55
2:L:382:ASP:OD1	2:L:424:VAL:HG13	2.06	0.55
2:B:324:ALA:HA	2:B:345:ILE:HD12	1.89	0.54
1:C:316:MET:CE	1:C:337:PHE:HD1	2.19	0.54
1:C:275:LEU:HD23	1:C:331:SER:O	2.06	0.54
1:C:598:PRO:HD2	2:D:292:PHE:CD1	2.42	0.54
2:D:309:ASN:HD21	2:D:311:ASN:HB2	1.72	0.54
1:E:405:PRO:HG2	1:E:481:ASN:HA	1.89	0.54
1:G:358:HIS:ND1	1:G:359:PRO:HD3	2.22	0.54
1:G:376:VAL:C	1:G:378:ALA:H	2.09	0.54
1:G:480:HIS:HD2	1:G:482:LEU:HB2	1.72	0.54
1:I:276:CYS:O	1:I:382:LEU:HD21	2.07	0.54
2:L:117:ARG:HH21	2:L:280:LEU:HG	1.72	0.54
1:A:264:VAL:HG13	1:A:340:ASP:CB	2.37	0.54
1:A:376:VAL:C	1:A:378:ALA:N	2.59	0.54
1:A:97:ASP:OD1	1:A:102:HIS:HE1	1.90	0.54
2:B:182:ARG:HG3	2:B:182:ARG:HH11	1.72	0.54
1:E:73:GLU:OE1	1:E:451:LYS:NZ	2.37	0.54
3:I:801:BTI:H63	2:J:399:PRO:HD3	1.89	0.54
1:K:563:LEU:O	1:K:565:GLY:N	2.40	0.54
2:J:522:LEU:HD23	2:L:151:ASN:HD21	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:VAL:HG12	1:A:544:SER:O	2.08	0.54
2:B:434:ALA:HB3	2:B:460:VAL:HG12	1.87	0.54
1:C:266:GLN:HG2	1:C:341:GLY:CA	2.38	0.54
2:D:43:ARG:HG2	2:D:43:ARG:NH1	2.22	0.54
1:E:365:THR:HG22	1:E:391:LEU:CD2	2.38	0.54
1:G:517:LEU:N	1:G:564:GLN:HE22	2.05	0.54
1:G:526:ALA:HA	1:G:561:VAL:HG11	1.90	0.54
1:G:646:LEU:HD12	2:H:72:LEU:HD11	1.89	0.54
1:I:458:THR:O	1:I:461:ALA:HB3	2.07	0.54
1:K:231:ILE:H	1:K:231:ILE:HD12	1.72	0.54
1:K:532:MET:O	1:K:535:VAL:HB	2.07	0.54
2:L:207:SER:HB3	2:L:208:PRO:CD	2.32	0.54
2:L:75:ASP:OD1	2:L:272:ARG:NH2	2.39	0.54
2:L:492:ASN:ND2	2:L:494:PHE:HB2	2.22	0.54
1:A:92:ILE:HD12	1:A:112:ILE:HD13	1.89	0.54
1:E:577:ASP:HB2	1:E:591:ARG:NH2	2.23	0.54
2:F:293:ASP:OD1	2:F:325:ASP:O	2.25	0.54
1:G:491:HIS:O	1:G:495:ILE:HG13	2.06	0.54
1:G:66:ILE:HD13	1:G:88:SER:O	2.06	0.54
1:G:78:VAL:HG13	1:G:79:ILE:N	2.21	0.54
2:J:156:ILE:HD12	2:J:156:ILE:N	2.21	0.54
1:K:335:VAL:HG23	1:K:335:VAL:O	2.08	0.54
1:K:304:PRO:HG2	1:K:394:TRP:CZ2	2.43	0.54
2:D:169:GLY:HA2	2:L:462:VAL:HG22	1.90	0.54
1:A:287:GLU:OE2	1:A:305:SER:N	2.36	0.54
1:C:411:LEU:HD22	1:C:682:GLN:HB2	1.90	0.54
2:D:492:ASN:ND2	2:D:494:PHE:H	2.01	0.54
2:F:83:ASP:HB3	2:F:86:VAL:HG23	1.90	0.54
1:G:75:ALA:O	1:G:78:VAL:HG12	2.07	0.54
1:K:376:VAL:C	1:K:378:ALA:N	2.60	0.54
1:K:378:ALA:O	1:K:379:GLY:C	2.46	0.54
2:B:141:ILE:O	2:B:145:MET:HG3	2.06	0.54
2:B:200:CYS:HB3	2:B:223:MET:HB3	1.88	0.54
2:B:291:PHE:CE1	2:B:348:GLU:HA	2.43	0.54
2:B:436:GLY:O	2:B:439:TYR:HB3	2.07	0.54
1:G:312:THR:O	1:G:316:MET:HG3	2.08	0.54
1:I:670:ILE:HD12	1:I:712:ALA:HB1	1.88	0.54
1:C:380:GLU:CG	1:C:381:PRO:HD2	2.38	0.54
1:E:178:ILE:H	1:E:178:ILE:CD1	2.06	0.54
2:F:193:ILE:CD1	2:F:274:LEU:HD23	2.37	0.54
1:G:316:MET:CE	1:G:337:PHE:HD1	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:378:ALA:O	1:G:379:GLY:C	2.46	0.54
1:I:683:GLU:HB2	1:I:704:LYS:HG3	1.88	0.54
2:J:296:ASP:O	2:J:298:ILE:HD12	2.08	0.54
1:K:444:TYR:O	1:K:445:TYR:CG	2.61	0.54
2:L:325:ASP:O	2:L:327:GLY:N	2.40	0.54
1:A:376:VAL:C	1:A:378:ALA:H	2.10	0.54
1:C:184:ALA:HB1	1:C:189:VAL:HB	1.90	0.54
1:C:401:TYR:CE2	1:C:448:MET:HB2	2.43	0.54
1:C:543:VAL:HG12	1:C:544:SER:O	2.08	0.54
2:D:49:GLY:O	2:D:51:GLY:N	2.41	0.54
1:E:74:ILE:HD13	1:E:143:TYR:CE2	2.42	0.54
2:F:374:ALA:HB3	2:F:415:LEU:HD13	1.90	0.54
1:G:347:PHE:CD1	1:G:347:PHE:O	2.61	0.54
2:H:307:PRO:O	2:H:432:ARG:NH2	2.41	0.54
1:I:518:PRO:HD2	1:I:521:ASP:HB2	1.89	0.54
1:K:123:VAL:HG12	1:K:126:LYS:H	1.73	0.54
2:L:239:VAL:HG22	2:L:243:GLU:HB2	1.89	0.54
1:A:392:THR:O	1:A:455:TRP:HZ3	1.90	0.54
1:A:534:ARG:HG3	1:A:534:ARG:HH11	1.72	0.54
1:C:444:TYR:CD1	1:C:444:TYR:N	2.76	0.54
2:D:298:ILE:HG23	2:D:509:ARG:HB2	1.90	0.54
1:E:189:VAL:CG2	1:E:323:LEU:HB2	2.36	0.54
1:E:491:HIS:CE1	1:E:493:LYS:HB2	2.43	0.54
1:G:695:MET:SD	2:H:313:PRO:HG3	2.48	0.54
1:I:324:ALA:O	1:I:327:VAL:HG12	2.08	0.54
1:I:358:HIS:ND1	1:I:359:PRO:HD3	2.21	0.54
2:J:149:MET:CE	2:J:189:VAL:HG11	2.38	0.54
1:K:190:SER:N	1:K:319:GLN:OE1	2.34	0.54
2:L:285:LYS:HB3	2:L:286:PRO:HD2	1.89	0.54
1:C:464:GLU:OE2	1:C:464:GLU:HA	2.08	0.54
1:E:92:ILE:HB	1:E:112:ILE:CG2	2.37	0.54
1:E:283:ILE:CG2	1:E:386:GLN:HG2	2.38	0.54
2:F:337:ALA:HB1	2:F:370:SER:HA	1.90	0.54
1:G:66:ILE:HG12	1:G:66:ILE:O	2.06	0.54
1:I:155:ALA:O	1:I:159:GLU:HG2	2.08	0.54
1:I:367:VAL:HG12	1:I:368:ASP:N	2.22	0.54
1:K:245:SER:C	1:K:247:ASN:H	2.11	0.54
1:K:441:ILE:HD12	1:K:478:ILE:HD13	1.89	0.54
1:A:444:TYR:CD1	1:A:444:TYR:N	2.76	0.53
2:B:298:ILE:N	2:B:298:ILE:HD12	2.23	0.53
1:C:267:PRO:O	1:C:501:THR:HG23	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:517:LEU:H	1:C:564:GLN:HE22	1.55	0.53
2:D:42:ARG:O	2:D:45:ALA:HB3	2.08	0.53
1:E:517:LEU:HD21	1:E:632:ALA:HB1	1.90	0.53
1:E:63:PHE:N	1:E:63:PHE:CD1	2.76	0.53
1:G:304:PRO:O	1:G:394:TRP:CH2	2.61	0.53
1:G:619:ILE:HD12	1:G:625:PHE:C	2.29	0.53
2:H:83:ASP:HB3	2:H:86:VAL:HG21	1.88	0.53
1:I:354:LEU:HD11	1:I:358:HIS:ND1	2.23	0.53
1:I:670:ILE:CD1	1:I:718:LEU:HD21	2.38	0.53
2:J:200:CYS:HB3	2:J:223:MET:HB3	1.90	0.53
1:K:143:TYR:CZ	1:K:356:VAL:HG22	2.43	0.53
1:K:670:ILE:CD1	1:K:718:LEU:HD21	2.38	0.53
2:L:436:GLY:O	2:L:439:TYR:HB3	2.07	0.53
1:A:99:GLN:HB2	1:A:436:TYR:OH	2.08	0.53
2:B:109:THR:HG22	2:B:122:PHE:CB	2.38	0.53
1:C:358:HIS:HB2	1:C:369:LEU:HD12	1.90	0.53
1:C:400:LEU:HD11	1:C:482:LEU:HD13	1.90	0.53
1:E:283:ILE:HD12	1:E:389:VAL:HG21	1.89	0.53
1:E:457:PRO:CG	1:E:458:THR:H	2.14	0.53
1:E:534:ARG:HH11	1:E:534:ARG:HG3	1.73	0.53
1:G:218:ILE:CD1	1:G:260:ILE:HG12	2.38	0.53
1:G:518:PRO:O	1:G:521:ASP:N	2.36	0.53
2:H:193:ILE:CD1	2:H:274:LEU:HD23	2.38	0.53
1:K:129:ALA:O	1:K:133:ALA:HB2	2.07	0.53
1:K:537:GLU:HG3	1:K:553:ARG:HH21	1.72	0.53
1:A:463:ILE:HD12	1:A:494:PHE:CE1	2.44	0.53
1:E:276:CYS:O	1:E:382:LEU:HD21	2.08	0.53
1:E:272:ILE:HB	1:E:335:VAL:CG2	2.38	0.53
1:G:312:THR:HG21	1:G:343:LYS:HD3	1.90	0.53
1:G:457:PRO:HG2	1:G:458:THR:N	2.17	0.53
2:H:346:ARG:HH11	2:H:346:ARG:HG3	1.72	0.53
1:I:378:ALA:O	1:I:379:GLY:C	2.46	0.53
1:K:66:ILE:O	1:K:66:ILE:HG12	2.08	0.53
1:K:670:ILE:HD12	1:K:712:ALA:HB1	1.90	0.53
2:L:43:ARG:HG2	2:L:43:ARG:HH11	1.74	0.53
2:B:299:GLU:HG3	2:B:322:LYS:HB3	1.89	0.53
2:B:94:ASN:HA	2:B:98:GLN:OE1	2.08	0.53
2:D:339:ASN:ND2	2:D:370:SER:HB3	2.24	0.53
1:E:136:ALA:HB1	1:E:161:VAL:CG1	2.33	0.53
1:E:334:THR:CG2	1:E:351:ASN:HB2	2.39	0.53
1:E:543:VAL:HG11	2:F:117:ARG:HD2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:625:PHE:CD1	1:E:625:PHE:N	2.76	0.53
1:G:177:LYS:O	1:G:181:LYS:HG2	2.08	0.53
2:H:149:MET:CE	2:H:189:VAL:HG11	2.39	0.53
1:I:285:LEU:N	1:I:285:LEU:HD12	2.23	0.53
1:I:304:PRO:O	1:I:394:TRP:CH2	2.61	0.53
1:I:304:PRO:HG2	1:I:394:TRP:CZ2	2.44	0.53
1:K:71:ARG:HG3	1:K:72:GLY:N	2.24	0.53
1:A:295:ARG:O	1:A:296:ASN:HB2	2.09	0.53
1:A:272:ILE:HB	1:A:335:VAL:HG23	1.90	0.53
1:A:683:GLU:HB2	1:A:704:LYS:HG3	1.90	0.53
2:B:460:VAL:HG21	2:B:496:ALA:CB	2.35	0.53
1:C:334:THR:HG21	1:C:355:GLN:HE21	1.72	0.53
2:D:145:MET:HE3	2:D:183:ASN:HD21	1.73	0.53
2:D:337:ALA:HB3	2:D:373:LYS:CD	2.39	0.53
1:E:312:THR:O	1:E:315:ALA:HB3	2.09	0.53
1:I:184:ALA:HB1	1:I:189:VAL:HB	1.91	0.53
1:I:78:VAL:HG23	1:I:370:VAL:HG11	1.90	0.53
1:I:392:THR:O	1:I:455:TRP:HZ3	1.91	0.53
1:I:661:MET:HE1	1:I:726:GLU:HB3	1.91	0.53
1:K:132:ARG:HD3	1:K:159:GLU:OE1	2.08	0.53
1:K:338:ILE:N	1:K:338:ILE:HD12	2.23	0.53
1:A:380:GLU:HG2	1:A:381:PRO:HD2	1.90	0.53
1:A:400:LEU:HD11	1:A:482:LEU:HD13	1.90	0.53
1:A:494:PHE:HA	1:A:499:MET:HE1	1.90	0.53
1:A:670:ILE:HD12	1:A:712:ALA:HB1	1.90	0.53
1:E:283:ILE:HA	1:E:386:GLN:NE2	2.24	0.53
1:E:443:MET:HG3	1:E:444:TYR:CE1	2.44	0.53
1:E:292:ILE:HG23	1:E:503:PHE:CD2	2.43	0.53
1:E:67:LEU:HG	1:E:68:ILE:H	1.72	0.53
2:F:251:THR:HG21	2:F:260:ALA:HB2	1.90	0.53
2:F:54:ARG:O	2:F:57:ALA:HB3	2.07	0.53
1:G:552:GLU:CD	1:G:552:GLU:H	2.12	0.53
1:G:598:PRO:HD2	2:H:292:PHE:CE1	2.44	0.53
1:G:642:ARG:NH1	2:H:71:ASP:OD2	2.41	0.53
1:K:292:ILE:HD13	1:K:300:VAL:O	2.09	0.53
1:A:66:ILE:O	1:A:66:ILE:HG12	2.08	0.53
2:B:149:MET:CE	2:B:189:VAL:HG11	2.39	0.53
2:B:346:ARG:HH11	2:B:346:ARG:HG3	1.74	0.53
1:C:444:TYR:O	1:C:445:TYR:CG	2.62	0.53
1:E:279:HIS:HD2	1:E:380:GLU:O	1.92	0.53
2:F:469:THR:HG23	2:F:482:HIS:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:484:ALA:O	2:F:488:GLU:OE1	2.27	0.53
1:I:376:VAL:C	1:I:378:ALA:H	2.12	0.53
2:J:346:ARG:HA	2:J:350:ARG:O	2.08	0.53
1:K:279:HIS:NE2	1:K:380:GLU:N	2.57	0.53
2:D:184:ILE:CD1	2:L:417:TYR:HA	2.39	0.53
1:A:137:GLN:O	1:A:138:ALA:HB2	2.08	0.53
1:A:140:HIS:ND1	1:A:141:PRO:HD2	2.24	0.53
1:A:458:THR:O	1:A:461:ALA:HB3	2.09	0.53
1:C:128:MET:SD	1:C:131:ILE:HD12	2.48	0.53
1:E:155:ALA:O	1:E:159:GLU:HG2	2.09	0.53
2:H:346:ARG:HG3	2:H:346:ARG:NH1	2.23	0.53
1:I:131:ILE:CG2	1:I:136:ALA:HB2	2.29	0.53
2:J:379:ARG:HD2	2:J:421:GLU:OE2	2.09	0.53
1:A:308:LEU:HD12	1:A:308:LEU:O	2.09	0.53
1:C:289:GLU:OE1	1:C:306:PRO:HD2	2.08	0.53
1:C:534:ARG:HG3	1:C:534:ARG:HH11	1.74	0.53
1:E:70:ASN:OD1	1:E:74:ILE:HG21	2.09	0.53
1:G:338:ILE:N	1:G:338:ILE:HD12	2.23	0.53
1:G:444:TYR:O	1:G:445:TYR:CG	2.62	0.53
1:G:675:VAL:CG1	1:G:707:VAL:HG21	2.38	0.53
1:I:411:LEU:HD22	1:I:682:GLN:CB	2.38	0.53
1:I:504:ILE:HG23	1:I:505:ALA:N	2.24	0.53
1:I:528:ALA:CB	1:I:605:LEU:HD22	2.36	0.53
2:J:109:THR:HG22	2:J:122:PHE:HB2	1.91	0.53
1:K:85:MET:O	1:K:87:ILE:HG13	2.09	0.53
2:L:501:PHE:CD2	2:L:501:PHE:N	2.75	0.53
2:L:83:ASP:HB3	2:L:86:VAL:CG2	2.38	0.53
1:C:114:PRO:HB2	1:C:115:PRO:HD2	1.91	0.53
1:C:156:LEU:HD22	1:C:161:VAL:HB	1.91	0.53
1:C:393:GLY:HA2	1:C:457:PRO:O	2.09	0.53
1:G:146:LEU:HD23	1:G:152:PHE:CD2	2.43	0.53
1:G:66:ILE:CD1	1:G:87:ILE:HG22	2.33	0.53
2:H:160:ASP:OD1	2:H:198:GLY:HA3	2.09	0.53
2:H:325:ASP:C	2:H:327:GLY:H	2.12	0.53
2:H:390:THR:HG23	2:H:419:TYR:OH	2.09	0.53
1:I:444:TYR:O	1:I:445:TYR:CG	2.62	0.53
1:K:124:ILE:O	1:K:128:MET:HB2	2.09	0.53
1:K:78:VAL:HG13	1:K:79:ILE:N	2.24	0.53
2:B:469:THR:HG23	2:B:482:HIS:HB3	1.91	0.52
2:B:58:GLN:HE21	2:B:61:ARG:HH21	1.58	0.52
1:C:335:VAL:O	1:C:335:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:114:ILE:O	2:D:115:ASN:HB2	2.08	0.52
1:E:272:ILE:HB	1:E:335:VAL:HG23	1.90	0.52
1:E:78:VAL:CG1	1:E:79:ILE:N	2.72	0.52
2:F:458:ALA:HB3	2:F:493:PRO:HB3	1.90	0.52
1:G:71:ARG:HG3	1:G:72:GLY:N	2.24	0.52
2:H:58:GLN:HE21	2:H:61:ARG:HH21	1.57	0.52
1:I:112:ILE:O	1:I:120:SER:HA	2.09	0.52
1:I:517:LEU:HD21	1:I:632:ALA:HB1	1.92	0.52
1:I:65:LYS:HE2	1:I:134:THR:O	2.10	0.52
1:I:66:ILE:HD13	1:I:88:SER:O	2.09	0.52
2:J:207:SER:HB3	2:J:208:PRO:CD	2.34	0.52
2:J:501:PHE:N	2:J:501:PHE:CD2	2.75	0.52
1:K:271:GLU:O	1:K:287:GLU:HB2	2.10	0.52
1:K:393:GLY:HA2	1:K:457:PRO:O	2.09	0.52
2:B:297:ARG:HG2	2:B:297:ARG:HH11	1.74	0.52
2:B:535:ASP:OD2	2:J:379:ARG:NH2	2.41	0.52
1:C:517:LEU:HD22	1:C:517:LEU:N	2.17	0.52
1:E:289:GLU:OE1	1:E:306:PRO:HD2	2.09	0.52
2:F:394:VAL:HG23	2:F:395:PRO:HD2	1.92	0.52
2:F:300:PRO:HA	2:F:509:ARG:NH1	2.24	0.52
2:H:484:ALA:O	2:H:488:GLU:OE1	2.28	0.52
1:I:132:ARG:HD3	1:I:159:GLU:OE1	2.09	0.52
1:I:275:LEU:HD11	1:I:372:GLN:HB2	1.90	0.52
1:I:390:LYS:HD3	1:I:391:LEU:H	1.71	0.52
2:J:178:GLU:HB3	2:J:182:ARG:NH1	2.24	0.52
1:K:122:ILE:HA	1:K:146:LEU:CD1	2.39	0.52
1:K:312:THR:O	1:K:316:MET:HG3	2.09	0.52
1:K:543:VAL:CG1	2:L:117:ARG:HD2	2.37	0.52
1:K:528:ALA:HB1	1:K:605:LEU:CD2	2.39	0.52
1:K:670:ILE:CG1	1:K:718:LEU:HD21	2.39	0.52
2:L:416:LEU:HB2	2:L:441:VAL:HG22	1.91	0.52
1:A:132:ARG:HD3	1:A:159:GLU:OE1	2.09	0.52
1:A:658:THR:OG1	1:A:702:GLU:HG2	2.10	0.52
1:C:189:VAL:HA	1:C:319:GLN:OE1	2.09	0.52
1:C:317:GLY:O	1:C:321:VAL:HG12	2.10	0.52
2:D:239:VAL:HG22	2:D:243:GLU:HB2	1.91	0.52
1:E:186:GLU:C	1:E:188:ASN:N	2.63	0.52
1:E:393:GLY:HA3	1:E:455:TRP:CZ3	2.45	0.52
1:G:283:ILE:HA	1:G:386:GLN:NE2	2.24	0.52
2:H:239:VAL:HG22	2:H:243:GLU:HB2	1.92	0.52
1:I:646:LEU:HD12	2:J:72:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:464:GLU:HA	1:K:464:GLU:OE2	2.10	0.52
1:K:70:ASN:ND2	1:K:145:PHE:CD1	2.78	0.52
2:L:149:MET:CE	2:L:189:VAL:CG1	2.87	0.52
1:A:78:VAL:HG23	1:A:370:VAL:CG1	2.40	0.52
2:D:367:ASP:O	2:D:368:ILE:C	2.46	0.52
1:E:444:TYR:CD1	1:E:444:TYR:N	2.78	0.52
2:F:141:ILE:O	2:F:145:MET:HG3	2.08	0.52
2:F:193:ILE:HD13	2:F:274:LEU:HD23	1.90	0.52
1:G:316:MET:HE3	1:G:337:PHE:HD1	1.74	0.52
2:H:123:SER:HA	2:H:158:ILE:HB	1.91	0.52
1:I:358:HIS:N	1:I:359:PRO:CD	2.72	0.52
2:J:492:ASN:ND2	2:J:494:PHE:H	2.06	0.52
1:K:458:THR:O	1:K:461:ALA:HB3	2.09	0.52
1:A:401:TYR:HE2	1:A:448:MET:HB2	1.74	0.52
1:A:543:VAL:HG11	2:B:117:ARG:HD2	1.91	0.52
2:B:192:GLN:O	2:B:211:THR:HB	2.10	0.52
2:B:296:ASP:O	2:B:298:ILE:HD12	2.09	0.52
1:C:177:LYS:O	1:C:181:LYS:HG2	2.10	0.52
1:C:614:LEU:HD22	1:C:627:ILE:HG21	1.91	0.52
1:C:68:ILE:HG22	1:C:70:ASN:H	1.74	0.52
1:C:646:LEU:HD13	2:D:64:LEU:HD13	1.92	0.52
2:F:309:ASN:HD21	2:F:311:ASN:HB2	1.74	0.52
1:I:401:TYR:CD2	1:I:448:MET:HA	2.44	0.52
1:A:335:VAL:O	1:A:335:VAL:HG23	2.10	0.52
1:A:316:MET:CE	1:A:337:PHE:HD1	2.23	0.52
1:C:292:ILE:H	1:C:292:ILE:CD1	1.96	0.52
1:C:92:ILE:HB	1:C:112:ILE:CG2	2.38	0.52
1:E:628:ARG:HG3	1:E:633:ASP:HA	1.90	0.52
1:E:70:ASN:ND2	1:E:145:PHE:CD1	2.77	0.52
1:E:78:VAL:HG23	1:E:370:VAL:CG1	2.39	0.52
2:F:254:SER:OG	2:F:256:VAL:HG23	2.10	0.52
1:G:405:PRO:HG2	1:G:481:ASN:HA	1.90	0.52
1:I:140:HIS:ND1	1:I:141:PRO:HD2	2.25	0.52
1:I:295:ARG:O	1:I:296:ASN:HB2	2.10	0.52
1:I:428(L):ALA:HB3	1:I:455:TRP:HD1	1.75	0.52
1:I:480:HIS:HD2	1:I:482:LEU:HB2	1.73	0.52
1:A:283:ILE:HA	1:A:386:GLN:NE2	2.24	0.52
1:A:517:LEU:H	1:A:564:GLN:HE22	1.58	0.52
2:B:42:ARG:NH1	2:B:42:ARG:HG2	2.24	0.52
1:C:376:VAL:C	1:C:378:ALA:H	2.13	0.52
1:C:543:VAL:HG11	2:D:117:ARG:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:712:ALA:HA	1:C:716:ASN:ND2	2.25	0.52
1:E:189:VAL:HA	1:E:319:GLN:OE1	2.09	0.52
1:E:362:GLU:HG2	1:E:367:VAL:O	2.09	0.52
2:F:42:ARG:NH1	2:F:42:ARG:HG2	2.24	0.52
2:H:492:ASN:HB2	2:H:493:PRO:HD2	1.91	0.52
1:I:75:ALA:O	1:I:78:VAL:HG12	2.10	0.52
1:K:99:GLN:HB2	1:K:436:TYR:OH	2.09	0.52
1:K:494:PHE:CD2	1:K:499:MET:HE1	2.45	0.52
1:A:66:ILE:HD13	1:A:88:SER:O	2.09	0.52
1:C:117:ALA:CB	1:C:121:TYR:HB2	2.40	0.52
1:C:131:ILE:CG2	1:C:136:ALA:HB2	2.34	0.52
1:C:156:LEU:HD13	1:C:163:PHE:HB2	1.91	0.52
1:C:164:VAL:HG23	1:C:373:MET:O	2.09	0.52
2:D:109:THR:HG22	2:D:122:PHE:HB2	1.90	0.52
2:D:180:PHE:O	2:D:184:ILE:HG13	2.09	0.52
2:D:189:VAL:HA	2:D:282:ASN:ND2	2.24	0.52
2:D:417:TYR:HA	2:L:184:ILE:CD1	2.39	0.52
2:D:51:GLY:O	2:D:55:ILE:HG13	2.10	0.52
1:E:504:ILE:CG2	1:E:505:ALA:N	2.73	0.52
1:G:444:TYR:CD1	1:G:444:TYR:N	2.77	0.52
2:H:200:CYS:HB3	2:H:223:MET:HB3	1.92	0.52
1:I:596:TRP:CG	1:I:597:THR:N	2.77	0.52
1:K:463:ILE:HD12	1:K:494:PHE:CE1	2.44	0.52
1:K:634:LEU:HD23	1:K:634:LEU:N	2.24	0.52
1:C:177:LYS:HB3	1:C:181:LYS:NZ	2.25	0.52
1:C:185:GLN:O	1:C:188:ASN:N	2.41	0.52
2:D:124:GLN:HE21	2:D:137:HIS:CE1	2.27	0.52
2:D:231:VAL:O	2:D:235:THR:HB	2.10	0.52
1:E:320:ALA:HB1	1:E:335:VAL:HG21	1.91	0.52
2:F:117:ARG:HH21	2:F:280:LEU:HG	1.74	0.52
2:H:261:PHE:CD1	2:H:267:ALA:HA	2.45	0.52
1:I:395:ALA:C	1:I:396:ILE:HD12	2.30	0.52
1:K:140:HIS:ND1	1:K:141:PRO:HD2	2.24	0.52
1:K:534:ARG:HH11	1:K:534:ARG:HG3	1.74	0.52
2:L:261:PHE:CD1	2:L:267:ALA:HA	2.44	0.52
1:A:83:ARG:HB3	1:A:83:ARG:CZ	2.40	0.52
1:C:93:TYR:HA	1:C:121:TYR:OH	2.10	0.52
1:E:71:ARG:HG3	1:E:72:GLY:N	2.24	0.52
2:F:501:PHE:N	2:F:501:PHE:CD2	2.74	0.52
1:G:457:PRO:CG	1:G:458:THR:H	2.14	0.52
1:G:577:ASP:HB2	1:G:591:ARG:NH2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:630:ARG:C	1:G:632:ALA:H	2.11	0.52
2:H:335:GLU:HA	2:H:338:LYS:HE2	1.91	0.52
1:K:289:GLU:OE1	1:K:306:PRO:HD2	2.10	0.52
2:B:51:GLY:O	2:B:55:ILE:HG13	2.09	0.51
2:B:78:SER:O	2:B:112:GLY:HA2	2.10	0.51
2:D:182:ARG:HH11	2:D:182:ARG:HG3	1.73	0.51
1:E:354:LEU:HD11	1:E:358:HIS:ND1	2.25	0.51
1:I:316:MET:HB3	1:I:337:PHE:CE1	2.44	0.51
1:I:403:GLU:O	1:I:405:PRO:HD3	2.09	0.51
2:J:340:ILE:HD13	2:J:374:ALA:HB2	1.92	0.51
1:K:189:VAL:HA	1:K:319:GLN:OE1	2.09	0.51
2:L:368:ILE:HG13	2:L:408:VAL:HG13	1.92	0.51
1:A:190:SER:N	1:A:319:GLN:OE1	2.33	0.51
1:A:378:ALA:O	1:A:379:GLY:C	2.49	0.51
1:A:393:GLY:HA3	1:A:455:TRP:CZ3	2.45	0.51
1:A:653:LYS:H	1:A:653:LYS:CD	2.09	0.51
2:B:232:LYS:O	2:B:236:ASN:N	2.37	0.51
2:B:458:ALA:HB3	2:B:493:PRO:HB3	1.93	0.51
2:D:145:MET:CE	2:D:183:ASN:ND2	2.74	0.51
1:E:146:LEU:HD23	1:E:152:PHE:CD2	2.44	0.51
1:G:117:ALA:CB	1:G:121:TYR:HB2	2.39	0.51
1:G:376:VAL:C	1:G:378:ALA:N	2.62	0.51
1:G:363:LEU:HD13	1:G:455:TRP:HB3	1.92	0.51
1:I:177:LYS:O	1:I:181:LYS:HG2	2.09	0.51
2:J:222:TYR:HB2	2:J:245:GLY:O	2.10	0.51
1:A:275:LEU:HD23	1:A:276:CYS:N	2.25	0.51
1:A:497:GLY:O	1:A:499:MET:HG2	2.11	0.51
2:B:300:PRO:HA	2:B:509:ARG:NH1	2.26	0.51
1:C:186:GLU:C	1:C:188:ASN:N	2.63	0.51
1:C:665:PRO:HG2	1:C:666:MET:HE2	1.91	0.51
1:E:538:ILE:O	1:E:541:THR:HB	2.11	0.51
2:F:94:ASN:HA	2:F:98:GLN:OE1	2.11	0.51
2:H:42:ARG:HG2	2:H:42:ARG:NH1	2.24	0.51
1:I:415:GLY:C	1:I:440:GLU:HG3	2.30	0.51
1:I:639:ARG:HB3	1:I:643:GLN:HB3	1.90	0.51
1:I:71:ARG:HG3	1:I:72:GLY:N	2.25	0.51
2:J:382:ASP:OD1	2:J:424:VAL:HG13	2.10	0.51
2:J:445:LYS:HE3	2:J:503:ASP:OD1	2.10	0.51
1:K:124:ILE:HG23	1:K:152:PHE:HD2	1.74	0.51
1:K:189:VAL:CG2	1:K:323:LEU:HB2	2.40	0.51
1:K:63:PHE:N	1:K:63:PHE:CD1	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:ARG:HD2	1:A:467:ARG:O	2.11	0.51
2:B:522:LEU:HD23	2:F:151:ASN:ND2	2.24	0.51
1:C:347:PHE:CD1	1:C:347:PHE:O	2.63	0.51
1:E:464:GLU:HA	1:E:464:GLU:OE2	2.10	0.51
1:E:517:LEU:N	1:E:517:LEU:HD22	2.22	0.51
1:E:517:LEU:H	1:E:564:GLN:HE22	1.58	0.51
1:E:661:MET:HE1	1:E:726:GLU:HB3	1.91	0.51
1:I:400:LEU:HD21	1:I:482:LEU:HD13	1.92	0.51
2:J:273:ARG:HD2	2:J:330:TYR:HD1	1.75	0.51
2:B:376:ARG:HH11	2:J:410:LYS:HZ2	1.58	0.51
1:K:380:GLU:CG	1:K:381:PRO:HD2	2.40	0.51
1:K:563:LEU:HD23	1:K:636:VAL:HG22	1.92	0.51
2:L:367:ASP:O	2:L:368:ILE:C	2.49	0.51
2:B:207:SER:HB3	2:B:208:PRO:CD	2.35	0.51
1:C:528:ALA:HB1	1:C:605:LEU:HD22	1.92	0.51
2:B:89:ARG:NH1	2:D:499:ARG:HH21	2.08	0.51
1:E:401:TYR:CE2	1:E:448:MET:HB2	2.46	0.51
1:G:123:VAL:HG12	1:G:126:LYS:H	1.76	0.51
1:G:163:PHE:CD1	1:G:163:PHE:C	2.84	0.51
1:G:400:LEU:HD11	1:G:482:LEU:CD1	2.39	0.51
1:I:186:GLU:C	1:I:188:ASN:N	2.64	0.51
1:I:441:ILE:HD12	1:I:478:ILE:HD13	1.91	0.51
1:I:658:THR:OG1	1:I:702:GLU:HG2	2.11	0.51
1:K:319:GLN:NE2	1:K:345:PHE:CE1	2.78	0.51
1:K:358:HIS:N	1:K:359:PRO:CD	2.74	0.51
1:A:189:VAL:HA	1:A:319:GLN:OE1	2.10	0.51
1:A:71:ARG:HG3	1:A:72:GLY:N	2.25	0.51
2:B:178:GLU:HB3	2:B:182:ARG:NH1	2.25	0.51
1:C:275:LEU:HD23	1:C:276:CYS:N	2.26	0.51
1:C:403:GLU:O	1:C:405:PRO:HD3	2.11	0.51
2:B:150:GLN:HG2	2:D:527:VAL:HG22	1.93	0.51
1:G:303:ALA:HB3	1:G:360:VAL:HG12	1.93	0.51
2:J:108:VAL:O	2:J:122:PHE:HA	2.09	0.51
1:K:207:LYS:O	1:K:207:LYS:HD2	2.11	0.51
1:K:679:GLN:O	1:K:706:VAL:HG13	2.11	0.51
2:L:43:ARG:HG2	2:L:43:ARG:NH1	2.25	0.51
1:C:304:PRO:HD2	1:C:394:TRP:CE2	2.46	0.51
1:C:433:THR:HG22	1:C:434:GLY:N	2.24	0.51
1:C:551:HIS:HE1	2:F:348:GLU:OE2	1.94	0.51
2:H:196:ILE:HD13	2:H:214:ILE:HG23	1.93	0.51
1:K:418:THR:O	1:K:437:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:ARG:HD2	2:B:421:GLU:OE2	2.11	0.51
1:C:362:GLU:HG2	1:C:367:VAL:O	2.11	0.51
1:C:400:LEU:HD21	1:C:482:LEU:CD1	2.41	0.51
2:D:501:PHE:CD2	2:D:501:PHE:N	2.77	0.51
1:E:124:ILE:O	1:E:128:MET:HB2	2.11	0.51
1:E:140:HIS:ND1	1:E:141:PRO:HD2	2.26	0.51
1:E:264:VAL:O	1:E:267:PRO:HD3	2.11	0.51
1:E:392:THR:O	1:E:455:TRP:HZ3	1.94	0.51
1:G:177:LYS:HB3	1:G:181:LYS:HZ1	1.76	0.51
1:G:665:PRO:HG2	1:G:666:MET:HE2	1.91	0.51
2:H:356:ALA:CB	2:H:391:LEU:HB2	2.41	0.51
1:I:415:GLY:O	1:I:440:GLU:HG3	2.10	0.51
1:I:444:TYR:N	1:I:444:TYR:CD1	2.78	0.51
1:K:206:VAL:HG13	1:K:235:ASP:HB3	1.93	0.51
1:K:363:LEU:HD13	1:K:455:TRP:HB3	1.93	0.51
1:A:517:LEU:CD2	1:A:517:LEU:H	2.15	0.51
1:A:614:LEU:HD22	1:A:627:ILE:HG21	1.92	0.51
2:B:75:ASP:OD1	2:B:272:ARG:NH2	2.43	0.51
1:C:324:ALA:O	1:C:327:VAL:HG12	2.11	0.51
1:C:279:HIS:HD2	1:C:380:GLU:O	1.93	0.51
1:E:458:THR:O	1:E:461:ALA:HB3	2.10	0.51
1:E:517:LEU:CD2	1:E:517:LEU:H	2.21	0.51
2:F:43:ARG:NH1	2:F:43:ARG:HG2	2.26	0.51
2:H:416:LEU:HB2	2:H:441:VAL:HG22	1.92	0.51
2:J:307:PRO:HG3	2:J:312:THR:O	2.10	0.51
1:K:179:THR:O	1:K:183:ILE:HG13	2.11	0.51
1:K:316:MET:O	1:K:320:ALA:HB2	2.11	0.51
1:K:365:THR:HG22	1:K:391:LEU:HD22	1.92	0.51
1:K:403:GLU:O	1:K:405:PRO:HD3	2.10	0.51
1:A:139:VAL:O	1:A:164:VAL:HG12	2.11	0.51
1:A:515:VAL:HG21	1:A:631:GLY:HA3	1.93	0.51
1:C:97:ASP:OD1	1:C:102:HIS:HE1	1.94	0.51
1:E:164:VAL:HG23	1:E:373:MET:O	2.10	0.51
1:E:378:ALA:O	1:E:379:GLY:C	2.50	0.51
1:G:320:ALA:HB1	1:G:335:VAL:HG21	1.94	0.51
2:F:539:LEU:OXT	2:H:372:ARG:NH2	2.44	0.51
2:H:50:GLY:O	2:H:54:ARG:HD2	2.11	0.51
1:I:283:ILE:HG22	1:I:386:GLN:HG2	1.93	0.51
1:I:362:GLU:HG2	1:I:367:VAL:O	2.11	0.51
1:I:693:MET:O	1:I:694:LYS:HB2	2.11	0.51
1:K:283:ILE:HA	1:K:386:GLN:NE2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:346:ARG:HA	2:L:350:ARG:O	2.10	0.51
1:A:393:GLY:HA2	1:A:457:PRO:O	2.11	0.50
1:A:537:GLU:HG3	1:A:553:ARG:NH2	2.26	0.50
1:C:71:ARG:HG3	1:C:72:GLY:N	2.26	0.50
2:D:178:GLU:O	2:D:182:ARG:HG3	2.10	0.50
3:E:801:BTI:H63	2:F:399:PRO:HD3	1.92	0.50
1:G:100:ALA:HB3	1:G:103:VAL:HG23	1.93	0.50
1:G:275:LEU:HD23	1:G:276:CYS:H	1.75	0.50
1:G:400:LEU:HD21	1:G:482:LEU:CD1	2.40	0.50
2:F:210:MET:HE1	2:H:416:LEU:HG	1.94	0.50
1:I:272:ILE:HB	1:I:335:VAL:CG2	2.41	0.50
1:I:405:PRO:HG2	1:I:481:ASN:HA	1.92	0.50
1:K:206:VAL:HG13	1:K:235:ASP:CB	2.41	0.50
1:K:400:LEU:HD11	1:K:482:LEU:CD1	2.41	0.50
2:D:462:VAL:HG22	2:L:169:GLY:HA2	1.93	0.50
2:L:149:MET:HE1	2:L:189:VAL:HG11	1.91	0.50
2:B:58:GLN:CD	2:B:63:LYS:HE3	2.31	0.50
1:C:295:ARG:O	1:C:296:ASN:HB2	2.11	0.50
1:C:348:LEU:O	1:C:348:LEU:HD23	2.11	0.50
1:C:334:THR:CG2	1:C:351:ASN:HB2	2.41	0.50
1:C:376:VAL:C	1:C:378:ALA:N	2.63	0.50
1:E:185:GLN:O	1:E:188:ASN:N	2.42	0.50
1:E:292:ILE:HD13	1:E:300:VAL:O	2.11	0.50
1:G:139:VAL:O	1:G:164:VAL:HG12	2.12	0.50
2:H:232:LYS:O	2:H:236:ASN:N	2.36	0.50
1:I:348:LEU:O	1:I:349:GLU:HB3	2.11	0.50
1:I:625:PHE:CD1	1:I:625:PHE:N	2.79	0.50
1:K:316:MET:CE	1:K:337:PHE:HD1	2.24	0.50
2:L:148:ALA:HB1	2:L:153:ALA:O	2.11	0.50
1:A:334:THR:HG22	1:A:351:ASN:HB2	1.93	0.50
1:A:634:LEU:HD23	1:A:634:LEU:H	1.76	0.50
1:C:363:LEU:HD13	1:C:455:TRP:HB3	1.93	0.50
1:C:74:ILE:HD13	1:C:143:TYR:HE2	1.77	0.50
2:D:273:ARG:HD2	2:D:330:TYR:CD1	2.47	0.50
1:E:177:LYS:HB3	1:E:181:LYS:HZ3	1.74	0.50
1:E:693:MET:O	1:E:694:LYS:HB2	2.11	0.50
1:G:92:ILE:CD1	1:G:112:ILE:HD13	2.42	0.50
1:G:380:GLU:HG2	1:G:381:PRO:HD2	1.93	0.50
1:I:577:ASP:HB2	1:I:591:ARG:NH2	2.26	0.50
1:I:671:VAL:CG2	1:I:691:GLU:HB2	2.41	0.50
1:K:276:CYS:O	1:K:382:LEU:HD21	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:405:PRO:HG2	1:K:481:ASN:HA	1.93	0.50
1:K:683:GLU:HB2	1:K:704:LYS:HG3	1.92	0.50
2:L:66:ALA:HB2	2:L:125:ASP:HA	1.93	0.50
2:L:94:ASN:HA	2:L:98:GLN:OE1	2.11	0.50
1:C:155:ALA:O	1:C:159:GLU:HG2	2.11	0.50
1:E:433:THR:HG22	1:E:434:GLY:N	2.23	0.50
1:E:515:VAL:CG2	1:E:631:GLY:HA3	2.41	0.50
1:E:675:VAL:CG1	1:E:707:VAL:HG21	2.41	0.50
2:F:156:ILE:CD1	2:F:156:ILE:N	2.73	0.50
1:G:112:ILE:O	1:G:120:SER:HA	2.12	0.50
1:G:287:GLU:HG3	1:G:308:LEU:HD21	1.93	0.50
1:G:74:ILE:HG23	1:G:75:ALA:N	2.27	0.50
1:I:348:LEU:O	1:I:348:LEU:HD23	2.11	0.50
1:K:317:GLY:O	1:K:321:VAL:HG12	2.11	0.50
1:K:283:ILE:HG22	1:K:386:GLN:HG2	1.93	0.50
1:K:400:LEU:HD13	1:K:449:ILE:CD1	2.32	0.50
1:K:664:CYS:SG	1:K:690:ILE:HD13	2.51	0.50
1:K:78:VAL:HG23	1:K:370:VAL:HG11	1.93	0.50
1:A:304:PRO:HG2	1:A:394:TRP:CZ2	2.46	0.50
1:A:665:PRO:HG2	1:A:666:MET:HE2	1.89	0.50
2:D:469:THR:HG23	2:D:482:HIS:HB3	1.92	0.50
1:E:74:ILE:HD13	1:E:143:TYR:HE2	1.76	0.50
1:G:354:LEU:HD11	1:G:358:HIS:ND1	2.27	0.50
1:G:99:GLN:HB2	1:G:436:TYR:OH	2.10	0.50
1:G:467:ARG:HE	1:G:630:ARG:HG3	1.76	0.50
1:G:67:LEU:HG	1:G:68:ILE:H	1.77	0.50
1:I:167:PRO:O	1:I:169:GLY:N	2.45	0.50
2:J:121:VAL:O	2:J:144:ILE:HD13	2.11	0.50
2:J:196:ILE:HG22	2:J:221:SER:HB2	1.93	0.50
2:J:423:THR:O	2:J:525:LYS:HE2	2.11	0.50
1:K:380:GLU:HG2	1:K:381:PRO:HD2	1.93	0.50
1:K:393:GLY:HA3	1:K:455:TRP:CZ3	2.47	0.50
1:K:92:ILE:HB	1:K:112:ILE:CG2	2.42	0.50
1:A:117:ALA:C	1:A:119:GLN:N	2.65	0.50
1:A:83:ARG:CG	1:A:83:ARG:HH11	2.23	0.50
2:B:356:ALA:CB	2:B:391:LEU:HB2	2.42	0.50
1:C:163:PHE:C	1:C:163:PHE:CD1	2.85	0.50
2:F:229:ASP:O	2:F:233:THR:HG23	2.12	0.50
2:F:367:ASP:O	2:F:368:ILE:C	2.48	0.50
1:I:380:GLU:CG	1:I:381:PRO:HD2	2.41	0.50
1:I:292:ILE:HG23	1:I:503:PHE:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:312:THR:O	1:K:315:ALA:HB3	2.10	0.50
1:K:65:LYS:HE2	1:K:134:THR:O	2.11	0.50
1:A:95:ASP:OD2	1:A:114:PRO:HA	2.12	0.50
1:A:365:THR:HG22	1:A:391:LEU:HD22	1.93	0.50
1:A:625:PHE:N	1:A:625:PHE:CD1	2.77	0.50
2:B:335:GLU:HA	2:B:338:LYS:HE2	1.94	0.50
2:B:346:ARG:NH1	2:B:346:ARG:HG3	2.27	0.50
2:B:54:ARG:HG2	2:B:54:ARG:NH1	2.27	0.50
1:C:312:THR:O	1:C:315:ALA:HB3	2.12	0.50
1:C:671:VAL:CG2	1:C:691:GLU:HB2	2.42	0.50
2:D:379:ARG:HD2	2:D:421:GLU:OE2	2.12	0.50
2:D:49:GLY:C	2:D:51:GLY:N	2.65	0.50
1:E:415:GLY:C	1:E:440:GLU:HG3	2.32	0.50
1:E:414:ILE:HD12	1:E:441:ILE:O	2.12	0.50
1:G:306:PRO:HG3	1:G:394:TRP:CH2	2.46	0.50
1:G:334:THR:HG22	1:G:351:ASN:HB2	1.93	0.50
2:H:207:SER:HB3	2:H:208:PRO:CD	2.33	0.50
1:I:433:THR:HG22	1:I:434:GLY:N	2.26	0.50
1:I:83:ARG:CG	1:I:83:ARG:HH11	2.22	0.50
2:J:91:THR:HA	2:J:98:GLN:CG	2.39	0.50
1:K:358:HIS:HB2	1:K:369:LEU:HD12	1.92	0.50
1:K:456:ALA:CB	1:K:457:PRO:CD	2.90	0.50
1:K:579:SER:O	1:K:591:ARG:HD2	2.12	0.50
1:K:661:MET:HE1	1:K:726:GLU:HB3	1.93	0.50
2:L:335:GLU:HA	2:L:338:LYS:HE2	1.94	0.50
1:A:293:GLN:HB3	1:A:298:LYS:HA	1.94	0.50
1:A:63:PHE:N	1:A:63:PHE:CD1	2.79	0.50
1:C:124:ILE:O	1:C:128:MET:HB2	2.12	0.50
2:D:474:ARG:O	2:D:476:ASP:N	2.45	0.50
1:E:167:PRO:O	1:E:169:GLY:N	2.44	0.50
1:E:369:LEU:O	1:E:373:MET:HB2	2.12	0.50
1:G:517:LEU:CD2	1:G:517:LEU:H	2.22	0.50
1:I:265:THR:HB	1:I:341:GLY:H	1.76	0.50
1:A:92:ILE:HB	1:A:112:ILE:CG2	2.42	0.50
1:A:185:GLN:O	1:A:188:ASN:N	2.44	0.50
1:A:376:VAL:HG23	1:A:377:ALA:N	2.26	0.50
1:A:405:PRO:HG2	1:A:481:ASN:HA	1.94	0.50
2:B:239:VAL:HG22	2:B:243:GLU:HB2	1.93	0.50
2:B:69:ARG:HA	2:B:268:LEU:HD11	1.94	0.50
1:A:646:LEU:HD13	2:B:64:LEU:HD13	1.94	0.50
1:C:380:GLU:HG2	1:C:381:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:642:ARG:HH11	2:D:71:ASP:HB3	1.77	0.50
1:E:184:ALA:HB1	1:E:189:VAL:HB	1.93	0.50
1:I:114:PRO:HB2	1:I:115:PRO:HD2	1.94	0.50
1:I:312:THR:O	1:I:316:MET:HG3	2.12	0.50
1:I:320:ALA:HB1	1:I:335:VAL:HG21	1.94	0.50
1:I:376:VAL:C	1:I:378:ALA:N	2.64	0.50
2:J:49:GLY:C	2:J:51:GLY:H	2.16	0.50
1:K:170:ALA:O	1:K:173:ALA:HB3	2.11	0.50
1:K:348:LEU:O	1:K:349:GLU:HB3	2.12	0.50
1:K:334:THR:HG22	1:K:351:ASN:HB2	1.94	0.50
2:B:178:GLU:O	2:B:182:ARG:HG3	2.12	0.49
1:C:658:THR:HG22	1:C:659:SER:O	2.12	0.49
1:E:380:GLU:HG2	1:E:381:PRO:HD2	1.94	0.49
1:E:283:ILE:HB	1:E:386:GLN:CD	2.32	0.49
2:F:43:ARG:HH11	2:F:43:ARG:HG2	1.76	0.49
1:G:162:ILE:O	1:G:164:VAL:N	2.45	0.49
1:G:190:SER:N	1:G:319:GLN:OE1	2.36	0.49
1:G:369:LEU:O	1:G:373:MET:HB2	2.12	0.49
1:G:537:GLU:HG3	1:G:553:ARG:HH21	1.77	0.49
2:H:250:HIS:HA	2:H:254:SER:OG	2.11	0.49
2:H:390:THR:CG2	2:H:419:TYR:OH	2.60	0.49
1:I:207:LYS:O	1:I:211:GLN:HB2	2.12	0.49
1:I:234:ASN:HD22	1:I:236:GLN:HB2	1.74	0.49
1:I:467:ARG:HE	1:I:630:ARG:CG	2.25	0.49
1:K:185:GLN:O	1:K:188:ASN:N	2.45	0.49
1:K:517:LEU:CD2	1:K:517:LEU:H	2.18	0.49
2:L:252:ARG:NH2	2:L:335:GLU:HG3	2.27	0.49
1:A:396:ILE:HD13	1:A:462:ALA:CB	2.42	0.49
1:A:65:LYS:HE2	1:A:134:THR:O	2.12	0.49
1:C:583:PHE:CZ	1:C:590:MET:HE3	2.47	0.49
2:D:109:THR:HG22	2:D:122:PHE:CB	2.42	0.49
1:E:118:ASN:O	1:E:119:GLN:HG3	2.11	0.49
1:E:177:LYS:O	1:E:181:LYS:HG2	2.12	0.49
1:E:288:ARG:HD3	1:E:361:THR:OG1	2.12	0.49
2:F:417:TYR:HA	2:H:184:ILE:CD1	2.40	0.49
2:F:479:ILE:C	2:F:479:ILE:HD12	2.32	0.49
1:G:342:GLN:O	1:G:343:LYS:HB2	2.11	0.49
1:G:415:GLY:C	1:G:440:GLU:HG3	2.32	0.49
1:G:454:THR:HG21	1:G:466:MET:HA	1.94	0.49
1:G:596:TRP:CG	1:G:597:THR:N	2.80	0.49
2:H:189:VAL:HA	2:H:282:ASN:HD22	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:407:ARG:HG2	1:I:407:ARG:HH11	1.77	0.49
2:J:232:LYS:O	2:J:236:ASN:N	2.36	0.49
1:K:146:LEU:HD23	1:K:152:PHE:CG	2.47	0.49
1:K:155:ALA:O	1:K:159:GLU:HG2	2.12	0.49
2:L:432:ARG:HG2	2:L:433:LYS:N	2.27	0.49
2:L:492:ASN:HD22	2:L:494:PHE:HB2	1.77	0.49
1:A:177:LYS:O	1:A:181:LYS:HG2	2.12	0.49
1:C:491:HIS:O	1:C:495:ILE:HG13	2.12	0.49
2:D:382:ASP:OD1	2:D:424:VAL:HG13	2.13	0.49
1:E:69:ALA:HB3	1:E:141:PRO:HA	1.94	0.49
1:G:92:ILE:HB	1:G:112:ILE:CG2	2.42	0.49
1:G:358:HIS:N	1:G:359:PRO:CD	2.75	0.49
1:G:279:HIS:NE2	1:G:380:GLU:N	2.60	0.49
1:G:78:VAL:HA	1:G:370:VAL:HG11	1.94	0.49
1:G:83:ARG:CZ	1:G:83:ARG:HB3	2.42	0.49
2:H:351:THR:HG22	2:H:386:ILE:HG23	1.94	0.49
1:I:634:LEU:N	1:I:634:LEU:CD2	2.75	0.49
1:K:712:ALA:HA	1:K:716:ASN:ND2	2.28	0.49
1:K:670:ILE:HD11	1:K:718:LEU:HD11	1.94	0.49
1:K:71:ARG:O	1:K:75:ALA:CB	2.60	0.49
1:A:179:THR:O	1:A:183:ILE:HG13	2.13	0.49
1:A:444:TYR:O	1:A:445:TYR:CG	2.66	0.49
1:A:552:GLU:CD	1:A:552:GLU:H	2.16	0.49
2:B:337:ALA:HB1	2:B:370:SER:HA	1.92	0.49
2:B:337:ALA:HB3	2:B:373:LYS:HD2	1.94	0.49
1:C:347:PHE:CD1	1:C:347:PHE:C	2.85	0.49
1:G:415:GLY:O	1:G:440:GLU:HG3	2.13	0.49
1:G:455:TRP:CG	1:G:456:ALA:N	2.79	0.49
1:I:283:ILE:CG2	1:I:386:GLN:HG2	2.42	0.49
1:I:463:ILE:HD12	1:I:494:PHE:CE1	2.47	0.49
1:I:534:ARG:HG3	1:I:534:ARG:NH1	2.25	0.49
1:I:664:CYS:HB2	1:I:724:ILE:HD11	1.93	0.49
2:J:66:ALA:HB2	2:J:125:ASP:HA	1.95	0.49
2:D:88:HIS:CD2	2:D:88:HIS:C	2.85	0.49
1:G:537:GLU:HG3	1:G:553:ARG:NH2	2.28	0.49
2:B:417:TYR:HA	2:J:184:ILE:CD1	2.42	0.49
2:J:356:ALA:HB2	2:J:391:LEU:HB2	1.94	0.49
1:K:117:ALA:CB	1:K:121:TYR:HB2	2.40	0.49
1:K:324:ALA:O	1:K:327:VAL:HG12	2.12	0.49
2:L:189:VAL:HA	2:L:282:ASN:HD22	1.77	0.49
1:A:650:MET:SD	2:B:263:ASN:HB2	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ARG:O	1:A:75:ALA:CB	2.61	0.49
2:B:300:PRO:HB3	2:B:509:ARG:HH12	1.77	0.49
1:C:78:VAL:CG1	1:C:79:ILE:N	2.76	0.49
2:D:273:ARG:HD2	2:D:330:TYR:HD1	1.78	0.49
1:E:317:GLY:O	1:E:321:VAL:HG12	2.12	0.49
2:F:492:ASN:ND2	2:F:494:PHE:H	2.05	0.49
1:G:416:ARG:HG3	1:G:439:GLY:O	2.12	0.49
1:G:639:ARG:HB3	1:G:643:GLN:HB3	1.93	0.49
1:G:693:MET:O	1:G:694:LYS:HB2	2.13	0.49
2:H:507:GLN:OE1	2:J:39:LEU:HD23	2.13	0.49
1:I:515:VAL:CG2	1:I:631:GLY:HA3	2.42	0.49
2:J:329:PHE:CE1	2:J:343:GLY:HA3	2.47	0.49
2:J:447:LEU:C	2:J:448:ARG:HG2	2.32	0.49
2:L:227:GLY:O	2:L:231:VAL:HG23	2.13	0.49
2:L:403:GLN:O	2:L:408:VAL:HG22	2.12	0.49
2:B:307:PRO:HG3	2:B:312:THR:O	2.13	0.49
1:C:107:ASP:O	1:C:108:GLU:HG3	2.11	0.49
1:C:411:LEU:HB2	1:C:682:GLN:HG3	1.94	0.49
1:E:265:THR:HB	1:E:341:GLY:H	1.76	0.49
1:E:394:TRP:CE3	1:E:459:ARG:HG3	2.48	0.49
1:E:658:THR:OG1	1:E:702:GLU:HG2	2.13	0.49
2:F:338:LYS:HB3	2:F:361:VAL:HG21	1.93	0.49
2:F:476(C):ASP:C	2:F:477:GLU:H	2.15	0.49
2:H:109:THR:HG22	2:H:122:PHE:HB2	1.93	0.49
1:I:358:HIS:HB2	1:I:369:LEU:HD12	1.94	0.49
1:I:283:ILE:HB	1:I:386:GLN:CD	2.33	0.49
1:I:411:LEU:HB2	1:I:682:GLN:HG3	1.95	0.49
2:J:78:SER:O	2:J:112:GLY:HA2	2.12	0.49
2:L:307:PRO:O	2:L:432:ARG:NH2	2.45	0.49
2:L:273:ARG:HD2	2:L:330:TYR:HD1	1.77	0.49
1:C:179:THR:O	1:C:183:ILE:HG13	2.13	0.49
1:C:283:ILE:HA	1:C:386:GLN:NE2	2.28	0.49
1:C:720:VAL:HG22	1:C:721:ASP:H	1.78	0.49
2:D:108:VAL:O	2:D:122:PHE:HA	2.12	0.49
1:E:354:LEU:C	1:E:354:LEU:HD13	2.33	0.49
1:E:517:LEU:HD21	1:E:632:ALA:HB2	1.93	0.49
1:E:518:PRO:O	1:E:521:ASP:HB2	2.13	0.49
1:G:563:LEU:O	1:G:565:GLY:N	2.46	0.49
1:I:163:PHE:C	1:I:163:PHE:CD1	2.86	0.49
2:J:235:THR:HG22	2:J:237:GLU:HB2	1.93	0.49
2:J:273:ARG:HD2	2:J:330:TYR:CD1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:207:LYS:O	1:K:211:GLN:HB2	2.12	0.49
1:K:275:LEU:HD23	1:K:276:CYS:N	2.28	0.49
1:K:658:THR:CB	1:K:703:LYS:HD3	2.42	0.49
1:A:312:THR:O	1:A:315:ALA:HB3	2.13	0.49
1:A:342:GLN:O	1:A:343:LYS:HB2	2.12	0.49
1:A:467:ARG:CB	1:A:467:ARG:HH11	2.22	0.49
2:B:180:PHE:O	2:B:184:ILE:HG13	2.13	0.49
2:B:193:ILE:HD13	2:B:274:LEU:HD23	1.94	0.49
1:C:615:LYS:HB2	1:C:628:ARG:HB2	1.95	0.49
1:C:63:PHE:N	1:C:63:PHE:CD1	2.81	0.49
1:C:675:VAL:CG1	1:C:707:VAL:HG21	2.42	0.49
1:E:271:GLU:O	1:E:287:GLU:HB2	2.12	0.49
1:E:421:ARG:O	1:E:421:ARG:CD	2.61	0.49
2:B:499:ARG:NH2	2:F:89:ARG:HH11	2.01	0.49
1:G:411:LEU:HD22	1:G:682:GLN:HB2	1.95	0.49
2:H:460:VAL:O	2:H:460:VAL:HG23	2.13	0.49
1:I:206:VAL:HG13	1:I:235:ASP:HB3	1.95	0.49
1:I:517:LEU:N	1:I:564:GLN:HE22	2.09	0.49
2:L:339:ASN:ND2	2:L:367:ASP:OD1	2.45	0.49
2:L:434:ALA:HB3	2:L:460:VAL:HG12	1.95	0.49
1:A:155:ALA:O	1:A:159:GLU:HG2	2.12	0.49
1:A:396:ILE:HD12	1:A:396:ILE:N	2.28	0.49
1:C:117:ALA:C	1:C:119:GLN:N	2.66	0.49
1:C:283:ILE:HG22	1:C:386:GLN:HG2	1.95	0.49
2:D:149:MET:CE	2:D:189:VAL:HG11	2.43	0.49
2:D:325:ASP:HA	2:D:512:ARG:NH1	2.17	0.49
2:D:347:LEU:HD12	2:D:352:VAL:HG21	1.95	0.49
1:E:467:ARG:HE	1:E:630:ARG:HG3	1.77	0.49
1:G:428(L):ALA:HB3	1:G:455:TRP:HD1	1.77	0.49
1:G:482:LEU:N	1:G:483:PRO:HD2	2.27	0.49
1:G:543:VAL:HG11	2:H:117:ARG:HD2	1.94	0.49
2:H:227:GLY:O	2:H:231:VAL:HG23	2.13	0.49
2:H:235:THR:HG22	2:H:237:GLU:HB2	1.94	0.49
2:H:195:MET:SD	2:H:271:VAL:HG21	2.52	0.49
2:J:43:ARG:HH11	2:J:43:ARG:CG	2.26	0.49
2:J:499:ARG:CG	2:J:499:ARG:NH1	2.76	0.49
1:K:117:ALA:C	1:K:119:GLN:N	2.66	0.49
1:K:367:VAL:HG12	1:K:368:ASP:N	2.28	0.49
1:K:626:ARG:NE	1:K:628:ARG:HD2	2.27	0.49
1:A:348:LEU:HD23	1:A:348:LEU:O	2.12	0.48
1:E:455:TRP:CG	1:E:456:ALA:N	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:122:PHE:CD1	2:F:141:ILE:HG23	2.48	0.48
2:F:49:GLY:C	2:F:51:GLY:H	2.15	0.48
1:G:309:ASP:OD1	1:G:312:THR:CG2	2.50	0.48
1:G:523:ARG:HB3	1:G:590:MET:CE	2.39	0.48
1:I:275:LEU:HD23	1:I:276:CYS:H	1.76	0.48
2:J:398:LEU:HD12	2:J:399:PRO:HD2	1.95	0.48
2:B:376:ARG:NH1	2:J:410:LYS:NZ	2.60	0.48
1:K:156:LEU:HD13	1:K:163:PHE:HB2	1.94	0.48
1:K:195:TYR:O	1:K:259:PHE:HA	2.12	0.48
1:C:283:ILE:HB	1:C:386:GLN:CD	2.33	0.48
1:C:517:LEU:CD2	1:C:517:LEU:H	2.17	0.48
1:C:83:ARG:CZ	1:C:83:ARG:HB3	2.43	0.48
1:E:118:ASN:C	1:E:119:GLN:HG3	2.34	0.48
1:E:156:LEU:HD13	1:E:163:PHE:HB2	1.94	0.48
1:E:376:VAL:C	1:E:378:ALA:H	2.15	0.48
1:E:435:VAL:HG22	1:E:436:TYR:H	1.77	0.48
1:E:400:LEU:HD21	1:E:482:LEU:CD1	2.42	0.48
1:E:515:VAL:HB	1:E:631:GLY:C	2.33	0.48
2:F:61:ARG:HB2	2:F:63:LYS:HG3	1.95	0.48
1:G:304:PRO:HD2	1:G:394:TRP:CE2	2.48	0.48
1:G:443:MET:SD	1:G:444:TYR:CE1	3.06	0.48
1:I:123:VAL:HG12	1:I:126:LYS:H	1.79	0.48
1:K:653:LYS:CD	1:K:653:LYS:H	2.12	0.48
1:A:334:THR:CG2	1:A:351:ASN:HB2	2.43	0.48
1:A:358:HIS:N	1:A:359:PRO:CD	2.76	0.48
1:A:515:VAL:CG2	1:A:631:GLY:HA3	2.44	0.48
1:A:626:ARG:C	1:A:627:ILE:HD12	2.33	0.48
2:B:227:GLY:O	2:B:231:VAL:HG23	2.14	0.48
1:C:99:GLN:HB2	1:C:436:TYR:OH	2.13	0.48
2:D:69:ARG:HA	2:D:268:LEU:HD11	1.94	0.48
2:D:317:LYS:HG3	2:D:341:ILE:HD13	1.95	0.48
2:D:492:ASN:HB2	2:D:493:PRO:CD	2.43	0.48
1:E:295:ARG:O	1:E:296:ASN:HB2	2.13	0.48
1:E:400:LEU:HD13	1:E:449:ILE:CD1	2.25	0.48
1:E:596:TRP:CG	1:E:597:THR:N	2.81	0.48
1:E:670:ILE:HD12	1:E:712:ALA:HB1	1.94	0.48
2:F:232:LYS:O	2:F:236:ASN:N	2.42	0.48
1:G:630:ARG:C	1:G:632:ALA:N	2.65	0.48
1:I:455:TRP:CG	1:I:456:ALA:N	2.80	0.48
1:I:625:PHE:HB2	1:I:627:ILE:CD1	2.43	0.48
2:B:417:TYR:HB2	2:J:210:MET:HE2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:469:THR:HG23	2:J:482:HIS:HB3	1.95	0.48
1:K:112:ILE:O	1:K:120:SER:HA	2.12	0.48
1:K:467:ARG:HE	1:K:630:ARG:CG	2.26	0.48
1:A:283:ILE:HD12	1:A:389:VAL:CG2	2.43	0.48
1:A:414:ILE:HD11	1:A:443:MET:N	2.28	0.48
1:A:69:ALA:HB3	1:A:141:PRO:HA	1.96	0.48
1:A:675:VAL:CG1	1:A:707:VAL:HG21	2.43	0.48
1:C:66:ILE:HG22	1:C:137:GLN:HG3	1.95	0.48
1:C:400:LEU:HD11	1:C:482:LEU:CD1	2.44	0.48
1:C:619:ILE:HD11	1:C:626:ARG:HB2	1.95	0.48
1:E:457:PRO:HG2	1:E:458:THR:N	2.20	0.48
1:G:150:SER:O	1:G:153:ALA:N	2.47	0.48
1:G:334:THR:CG2	1:G:351:ASN:HB2	2.44	0.48
1:G:480:HIS:HD2	1:G:482:LEU:H	1.62	0.48
1:I:292:ILE:HD13	1:I:300:VAL:O	2.13	0.48
1:I:316:MET:CE	1:I:337:PHE:CD1	2.95	0.48
2:B:462:VAL:HG21	2:J:169:GLY:HA2	1.95	0.48
1:K:518:PRO:O	1:K:521:ASP:HB2	2.12	0.48
1:K:563:LEU:CD2	1:K:636:VAL:HG22	2.43	0.48
1:K:646:LEU:HD12	2:L:72:LEU:HD21	1.94	0.48
1:A:131:ILE:CG2	1:A:136:ALA:HB2	2.38	0.48
1:A:273:GLN:O	1:A:285:LEU:HD12	2.14	0.48
1:A:467:ARG:NH1	1:A:467:ARG:HB3	2.24	0.48
1:A:528:ALA:HB1	1:A:605:LEU:CD2	2.43	0.48
1:C:77:ARG:NH1	1:C:370:VAL:HG21	2.28	0.48
1:C:504:ILE:CG2	1:C:505:ALA:N	2.77	0.48
2:D:207:SER:HB3	2:D:208:PRO:CD	2.41	0.48
1:E:150:SER:O	1:E:151:LYS:C	2.51	0.48
1:E:146:LEU:HD23	1:E:152:PHE:CG	2.49	0.48
1:E:528:ALA:HB1	1:E:605:LEU:HD22	1.95	0.48
2:F:474:ARG:HD3	2:F:474:ARG:HA	1.63	0.48
2:F:376:ARG:HH11	2:H:410:LYS:HZ2	1.62	0.48
2:H:499:ARG:CG	2:H:499:ARG:NH1	2.77	0.48
1:I:124:ILE:HG23	1:I:152:PHE:HD2	1.77	0.48
1:I:537:GLU:HG3	1:I:553:ARG:HH21	1.78	0.48
2:J:69:ARG:HA	2:J:268:LEU:HD11	1.95	0.48
1:K:405:PRO:CG	1:K:481:ASN:HA	2.44	0.48
2:L:337:ALA:HB1	2:L:370:SER:HA	1.96	0.48
1:A:167:PRO:O	1:A:169:GLY:N	2.47	0.48
2:B:43:ARG:HG2	2:B:43:ARG:NH1	2.28	0.48
1:C:168:LYS:HA	1:C:171:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:ILE:HD12	1:C:389:VAL:CG2	2.44	0.48
1:E:617:GLY:O	1:E:625:PHE:CB	2.50	0.48
2:F:149:MET:CE	2:F:189:VAL:HG11	2.43	0.48
1:G:517:LEU:H	1:G:564:GLN:HE22	1.60	0.48
1:G:517:LEU:HD21	1:G:632:ALA:HB1	1.96	0.48
2:H:501:PHE:N	2:H:501:PHE:CD2	2.78	0.48
2:H:58:GLN:OE1	2:H:63:LYS:HE3	2.13	0.48
1:I:393:GLY:HA3	1:I:455:TRP:CZ3	2.49	0.48
1:I:71:ARG:O	1:I:75:ALA:CB	2.62	0.48
2:J:325:ASP:C	2:J:327:GLY:H	2.17	0.48
2:L:58:GLN:CD	2:L:63:LYS:HE3	2.32	0.48
2:B:309:ASN:HD21	2:B:311:ASN:HB2	1.79	0.48
1:C:308:LEU:HD12	1:C:308:LEU:O	2.13	0.48
1:C:378:ALA:O	1:C:379:GLY:C	2.51	0.48
1:E:93:TYR:HA	1:E:121:TYR:OH	2.14	0.48
2:H:432:ARG:HG2	2:H:433:LYS:N	2.28	0.48
2:H:432:ARG:O	2:H:458:ALA:HA	2.13	0.48
1:I:189:VAL:CG2	1:I:323:LEU:HB2	2.44	0.48
1:I:400:LEU:HD13	1:I:449:ILE:CD1	2.24	0.48
2:J:188:GLY:HA2	2:J:384:PHE:CE2	2.49	0.48
2:J:346:ARG:HH11	2:J:346:ARG:HG3	1.78	0.48
2:J:436:GLY:O	2:J:439:TYR:HB3	2.13	0.48
1:K:270:ILE:HG12	1:K:289:GLU:HG3	1.95	0.48
1:K:411:LEU:HB2	1:K:682:GLN:HG3	1.95	0.48
1:K:417:LEU:HD21	1:K:478:ILE:CD1	2.39	0.48
1:A:78:VAL:CG1	1:A:79:ILE:N	2.77	0.48
1:C:419:ARG:HB2	1:C:476:GLU:HB2	1.95	0.48
1:E:132:ARG:HD3	1:E:159:GLU:OE1	2.14	0.48
1:E:583:PHE:CZ	1:E:590:MET:HE3	2.48	0.48
1:E:95:ASP:OD2	1:E:114:PRO:HA	2.14	0.48
2:F:109:THR:HG22	2:F:122:PHE:HB2	1.95	0.48
2:F:376:ARG:NH1	2:H:410:LYS:NZ	2.62	0.48
2:F:42:ARG:O	2:F:45:ALA:HB3	2.13	0.48
1:G:136:ALA:HB1	1:G:161:VAL:CG1	2.38	0.48
1:G:411:LEU:HG	1:G:412:PRO:O	2.13	0.48
1:G:518:PRO:O	1:G:521:ASP:HB2	2.14	0.48
1:I:517:LEU:HD22	1:I:517:LEU:N	2.22	0.48
1:K:400:LEU:HD21	1:K:482:LEU:CD1	2.44	0.48
1:K:671:VAL:CG2	1:K:691:GLU:HB2	2.44	0.48
2:L:160:ASP:OD1	2:L:198:GLY:HA3	2.14	0.48
2:L:296:ASP:O	2:L:298:ILE:HD12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:GLU:O	1:A:405:PRO:HD3	2.14	0.48
2:B:90:CYS:HB2	2:B:168:GLU:OE2	2.14	0.48
2:B:492:ASN:ND2	2:B:494:PHE:H	2.11	0.48
1:C:390:LYS:HD3	1:C:391:LEU:H	1.75	0.48
1:E:441:ILE:HD12	1:E:478:ILE:HD13	1.95	0.48
2:F:476(A):LEU:C	2:F:476(C):ASP:H	2.16	0.48
1:G:155:ALA:O	1:G:159:GLU:HG2	2.14	0.48
1:G:292:ILE:HG23	1:G:503:PHE:CD2	2.48	0.48
1:G:367:VAL:HG12	1:G:368:ASP:N	2.29	0.48
1:G:553:ARG:NH1	2:H:115:ASN:OD1	2.47	0.48
2:H:193:ILE:HD13	2:H:274:LEU:HD23	1.95	0.48
1:I:164:VAL:HG23	1:I:373:MET:O	2.14	0.48
1:I:64:ASN:H	1:I:137:GLN:HG2	1.79	0.48
2:J:351:THR:HG22	2:J:386:ILE:HG23	1.96	0.48
2:J:91:THR:HG22	2:J:98:GLN:HG2	1.96	0.48
1:K:131:ILE:CG2	1:K:136:ALA:HB2	2.32	0.48
1:K:283:ILE:CG2	1:K:386:GLN:HG2	2.44	0.48
1:A:156:LEU:HD13	1:A:163:PHE:HB2	1.95	0.48
1:A:518:PRO:O	1:A:521:ASP:HB2	2.13	0.48
1:C:473:PHE:O	1:C:615:LYS:NZ	2.33	0.48
1:C:596:TRP:CG	1:C:597:THR:N	2.82	0.48
2:D:178:GLU:HB3	2:D:182:ARG:NH1	2.29	0.48
2:D:348:GLU:O	2:D:350:ARG:HD2	2.14	0.48
2:D:476(C):ASP:HB3	2:D:478:LYS:HG3	1.96	0.48
1:E:339:VAL:HG22	1:E:345:PHE:HB3	1.95	0.48
1:E:683:GLU:HB2	1:E:704:LYS:HG3	1.94	0.48
1:G:627:ILE:N	1:G:627:ILE:HD12	2.29	0.48
2:H:235:THR:HG22	2:H:237:GLU:CB	2.44	0.48
2:H:312:THR:HG22	2:H:313:PRO:O	2.14	0.48
2:H:339:ASN:HD21	2:H:370:SER:HB3	1.79	0.48
1:I:454:THR:HG21	1:I:466:MET:HA	1.95	0.48
1:I:267:PRO:O	1:I:501:THR:HG23	2.14	0.48
2:J:117:ARG:HB3	2:J:280:LEU:HD21	1.94	0.48
1:K:358:HIS:CD2	1:K:362:GLU:OE1	2.67	0.48
1:K:422:PRO:HG3	1:K:473:PHE:CZ	2.49	0.48
1:K:74:ILE:HG23	1:K:75:ALA:N	2.29	0.48
1:A:124:ILE:O	1:A:128:MET:HB2	2.14	0.47
1:A:136:ALA:HB1	1:A:161:VAL:CG1	2.35	0.47
1:A:325:LYS:O	1:A:327:VAL:N	2.46	0.47
1:A:347:PHE:CD1	1:A:347:PHE:O	2.67	0.47
1:A:401:TYR:CD2	1:A:448:MET:HA	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:339:ASN:ND2	2:B:370:SER:HB3	2.29	0.47
1:C:78:VAL:HA	1:C:370:VAL:HG11	1.96	0.47
1:E:376:VAL:C	1:E:378:ALA:N	2.66	0.47
1:E:393:GLY:HA2	1:E:457:PRO:O	2.14	0.47
1:E:634:LEU:N	1:E:634:LEU:CD2	2.76	0.47
1:E:712:ALA:HA	1:E:716:ASN:ND2	2.28	0.47
1:G:446:ASP:OD1	1:G:447:PRO:HD2	2.14	0.47
1:G:670:ILE:HD12	1:G:712:ALA:HB1	1.95	0.47
2:H:339:ASN:ND2	2:H:370:SER:HB3	2.29	0.47
2:H:339:ASN:HB3	2:H:361:VAL:HG12	1.96	0.47
2:H:300:PRO:HA	2:H:509:ARG:NH1	2.28	0.47
1:I:443:MET:HG3	1:I:444:TYR:CE1	2.49	0.47
1:I:457:PRO:CG	1:I:458:THR:H	2.24	0.47
2:J:492:ASN:HB2	2:J:493:PRO:CD	2.43	0.47
1:K:139:VAL:O	1:K:164:VAL:HG12	2.14	0.47
1:K:433:THR:HG22	1:K:434:GLY:N	2.29	0.47
2:L:492:ASN:HD22	2:L:494:PHE:H	1.61	0.47
1:C:162:ILE:O	1:C:164:VAL:N	2.47	0.47
2:D:394:VAL:HG23	2:D:395:PRO:HD2	1.97	0.47
2:D:419:TYR:CE1	2:D:443:SER:HB2	2.48	0.47
2:D:476(C):ASP:C	2:D:477:GLU:H	2.17	0.47
1:E:107:ASP:C	1:E:108:GLU:HG3	2.34	0.47
1:E:653:LYS:CD	1:E:653:LYS:N	2.75	0.47
1:G:289:GLU:OE1	1:G:305:SER:OG	2.31	0.47
1:G:283:ILE:HB	1:G:386:GLN:CD	2.35	0.47
1:G:626:ARG:NE	1:G:628:ARG:HD2	2.28	0.47
2:F:210:MET:HE1	2:H:417:TYR:N	2.29	0.47
1:I:416:ARG:HG3	1:I:439:GLY:O	2.13	0.47
1:I:522:LEU:HD22	1:I:563:LEU:HD13	1.96	0.47
2:J:356:ALA:CB	2:J:391:LEU:HB2	2.44	0.47
1:K:162:ILE:HD13	1:K:377:ALA:O	2.14	0.47
1:K:293:GLN:HB3	1:K:298:LYS:HA	1.96	0.47
1:K:308:LEU:HA	1:K:343:LYS:HE3	1.95	0.47
1:K:292:ILE:HG23	1:K:503:PHE:CD2	2.49	0.47
1:A:163:PHE:C	1:A:163:PHE:CD1	2.87	0.47
1:A:367:VAL:HG12	1:A:368:ASP:N	2.29	0.47
1:A:401:TYR:CE2	1:A:448:MET:HB2	2.49	0.47
2:B:368:ILE:CG1	2:B:408:VAL:HG13	2.43	0.47
1:C:139:VAL:HG11	1:C:156:LEU:HD21	1.96	0.47
1:C:718:LEU:HD23	1:C:718:LEU:H	1.76	0.47
2:D:148:ALA:HB1	2:D:153:ALA:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:492:PRO:HA	1:G:495:ILE:HD12	1.95	0.47
1:G:83:ARG:HH11	1:G:83:ARG:CG	2.27	0.47
1:I:206:VAL:HG13	1:I:235:ASP:CB	2.44	0.47
1:I:517:LEU:H	1:I:517:LEU:CD2	2.20	0.47
2:H:522:LEU:HD23	2:J:151:ASN:HD21	1.79	0.47
2:J:126:PHE:HB2	2:J:160:ASP:OD2	2.13	0.47
1:A:467:ARG:HE	1:A:630:ARG:HG3	1.79	0.47
1:C:67:LEU:HG	1:C:68:ILE:H	1.79	0.47
2:D:138:SER:OG	2:D:139:LYS:N	2.47	0.47
1:E:163:PHE:CD1	1:E:163:PHE:C	2.87	0.47
1:E:65:LYS:HE2	1:E:134:THR:O	2.14	0.47
1:G:283:ILE:HG22	1:G:386:GLN:HG2	1.96	0.47
1:G:317:GLY:O	1:G:321:VAL:HG12	2.14	0.47
1:G:309:ASP:OD2	1:G:343:LYS:HE2	2.14	0.47
1:I:400:LEU:HD11	1:I:482:LEU:CD1	2.43	0.47
1:I:433:THR:HG23	1:I:449:ILE:O	2.14	0.47
2:J:355:VAL:O	2:J:390:THR:HA	2.14	0.47
1:K:358:HIS:HD2	1:K:362:GLU:OE1	1.97	0.47
1:A:484:PHE:O	1:A:487:ALA:HB3	2.14	0.47
2:B:420:GLY:HA3	2:J:184:ILE:CD1	2.37	0.47
2:B:58:GLN:HA	2:B:61:ARG:HH21	1.80	0.47
1:C:309:ASP:OD2	1:C:343:LYS:HE2	2.15	0.47
1:C:401:TYR:CD2	1:C:448:MET:HA	2.50	0.47
1:C:518:PRO:HD2	1:C:521:ASP:OD1	2.15	0.47
2:D:298:ILE:N	2:D:298:ILE:HD12	2.29	0.47
1:E:319:GLN:NE2	1:E:345:PHE:CE1	2.83	0.47
1:G:78:VAL:CG1	1:G:79:ILE:N	2.78	0.47
1:I:178:ILE:CD1	1:I:178:ILE:H	2.08	0.47
2:J:141:ILE:O	2:J:145:MET:HG3	2.14	0.47
1:K:140:HIS:ND1	1:K:141:PRO:N	2.62	0.47
1:K:390:LYS:HD3	1:K:391:LEU:H	1.75	0.47
1:A:146:LEU:HD23	1:A:152:PHE:CD2	2.50	0.47
1:A:285:LEU:N	1:A:285:LEU:HD12	2.29	0.47
1:E:670:ILE:HD11	1:E:718:LEU:HD11	1.96	0.47
2:F:108:VAL:O	2:F:122:PHE:HA	2.14	0.47
1:G:195:TYR:O	1:G:259:PHE:HA	2.15	0.47
1:G:515:VAL:CG2	1:G:631:GLY:HA3	2.45	0.47
1:G:614:LEU:HD22	1:G:627:ILE:HG21	1.95	0.47
2:H:309:ASN:HD21	2:H:311:ASN:HB2	1.80	0.47
1:I:231:ILE:N	1:I:231:ILE:HD12	2.27	0.47
2:J:298:ILE:HG23	2:J:509:ARG:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:LEU:HD11	1:A:482:LEU:CD1	2.45	0.47
2:B:193:ILE:CD1	2:B:274:LEU:HD23	2.45	0.47
2:B:403:GLN:O	2:B:408:VAL:HG22	2.15	0.47
1:C:358:HIS:N	1:C:359:PRO:CD	2.77	0.47
1:C:400:LEU:HD23	1:C:481:ASN:OD1	2.15	0.47
1:E:117:ALA:C	1:E:119:GLN:N	2.68	0.47
1:E:358:HIS:CG	1:E:359:PRO:HD3	2.49	0.47
1:G:140:HIS:ND1	1:G:141:PRO:HD2	2.30	0.47
1:G:720:VAL:HG22	1:G:721:ASP:H	1.80	0.47
2:H:229:ASP:OD1	2:H:229:ASP:N	2.47	0.47
2:H:299:GLU:O	2:H:509:ARG:HA	2.15	0.47
1:I:515:VAL:HG21	1:I:631:GLY:HA3	1.97	0.47
2:J:121:VAL:CG2	2:J:122:PHE:N	2.76	0.47
2:J:261:PHE:CD1	2:J:267:ALA:HA	2.49	0.47
1:K:152:PHE:CE1	1:K:156:LEU:HD11	2.49	0.47
1:K:163:PHE:CD1	1:K:163:PHE:C	2.88	0.47
1:K:275:LEU:HD23	1:K:276:CYS:H	1.80	0.47
1:K:630:ARG:C	1:K:632:ALA:H	2.17	0.47
2:L:492:ASN:HB2	2:L:493:PRO:HD2	1.95	0.47
1:A:289:GLU:OE1	1:A:306:PRO:HD2	2.15	0.47
1:A:617:GLY:O	1:A:625:PHE:CB	2.53	0.47
2:B:484:ALA:O	2:B:488:GLU:OE1	2.33	0.47
2:B:522:LEU:HA	2:F:151:ASN:ND2	2.30	0.47
1:C:658:THR:CB	1:C:703:LYS:HD3	2.40	0.47
1:G:663:LEU:O	1:G:665:PRO:HD3	2.15	0.47
1:I:115:PRO:HG2	1:I:444:TYR:CE2	2.50	0.47
1:I:517:LEU:HB3	1:I:521:ASP:HB3	1.96	0.47
1:I:63:PHE:N	1:I:63:PHE:CD1	2.82	0.47
2:J:58:GLN:CD	2:J:63:LYS:HE3	2.34	0.47
1:K:186:GLU:C	1:K:188:ASN:N	2.68	0.47
1:C:66:ILE:HD13	1:C:88:SER:O	2.14	0.47
1:G:184:ALA:HB1	1:G:189:VAL:HB	1.96	0.47
1:G:551:HIS:HE1	2:L:348:GLU:OE2	1.97	0.47
2:H:307:PRO:HG3	2:H:312:THR:HG22	1.97	0.47
2:H:458:ALA:HB3	2:H:493:PRO:HB3	1.97	0.47
1:I:229:MET:HG3	1:I:229:MET:O	2.15	0.47
1:A:415:GLY:C	1:A:440:GLU:HG3	2.34	0.47
2:B:379:ARG:NH2	2:J:535:ASP:OD2	2.47	0.47
1:C:78:VAL:HG23	1:C:370:VAL:CG1	2.45	0.47
1:C:517:LEU:HD21	1:C:632:ALA:CB	2.45	0.47
2:D:434:ALA:HB3	2:D:460:VAL:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:124:GLN:HE21	2:F:137:HIS:CE1	2.32	0.47
2:F:202:GLY:O	2:F:205:VAL:HG22	2.14	0.47
2:F:432:ARG:HG2	2:F:433:LYS:N	2.30	0.47
1:G:107:ASP:O	1:G:108:GLU:HG3	2.15	0.47
1:G:235:ASP:OD1	1:G:235:ASP:N	2.46	0.47
1:G:71:ARG:O	1:G:75:ALA:CB	2.63	0.47
1:I:518:PRO:O	1:I:521:ASP:HB2	2.15	0.47
1:I:626:ARG:NE	1:I:628:ARG:HD2	2.30	0.47
2:J:476(D):PRO:HA	2:J:479:ILE:HD11	1.97	0.47
1:A:436:TYR:HE1	1:A:439:GLY:CA	2.28	0.47
1:A:658:THR:HG22	1:A:659:SER:O	2.14	0.47
2:B:195:MET:SD	2:B:271:VAL:HG21	2.54	0.47
2:B:355:VAL:O	2:B:390:THR:HA	2.14	0.47
2:D:501:PHE:CE1	2:L:174:ALA:HB2	2.49	0.47
1:E:683:GLU:H	1:E:704:LYS:HG2	1.78	0.47
2:F:390:THR:CG2	2:F:419:TYR:OH	2.63	0.47
1:G:436:TYR:HE1	1:G:439:GLY:CA	2.28	0.47
1:G:63:PHE:CD1	1:G:63:PHE:N	2.83	0.47
2:F:170:VAL:HG11	2:H:460:VAL:HG23	1.96	0.47
2:H:80:GLU:HB2	2:L:517:ARG:NH2	2.30	0.47
2:H:95:MET:HE3	2:H:95:MET:HA	1.97	0.47
1:I:136:ALA:HB1	1:I:161:VAL:CG1	2.34	0.47
1:I:394:TRP:CE3	1:I:459:ARG:HG3	2.50	0.47
1:I:537:GLU:HG3	1:I:553:ARG:NH2	2.30	0.47
1:K:515:VAL:HG21	1:K:631:GLY:HA3	1.97	0.47
1:K:625:PHE:CD1	1:K:627:ILE:HD11	2.49	0.47
1:K:630:ARG:C	1:K:632:ALA:N	2.69	0.47
2:L:390:THR:CG2	2:L:419:TYR:OH	2.63	0.47
2:L:469:THR:HG23	2:L:482:HIS:HB3	1.96	0.47
2:L:479:ILE:HD12	2:L:479:ILE:C	2.33	0.47
2:L:48:LEU:HA	2:L:48:LEU:HD23	1.63	0.47
1:A:117:ALA:CB	1:A:121:TYR:HB2	2.43	0.46
1:A:354:LEU:HD11	1:A:358:HIS:ND1	2.31	0.46
1:A:279:HIS:NE2	1:A:380:GLU:N	2.62	0.46
1:A:583:PHE:CZ	1:A:590:MET:HE3	2.51	0.46
2:B:432:ARG:HG2	2:B:433:LYS:N	2.29	0.46
1:C:396:ILE:HG12	1:C:463:ILE:CD1	2.40	0.46
1:C:292:ILE:HG23	1:C:503:PHE:CD2	2.50	0.46
1:E:292:ILE:H	1:E:292:ILE:CD1	2.07	0.46
2:F:192:GLN:O	2:F:211:THR:HB	2.15	0.46
1:G:625:PHE:CD1	1:G:627:ILE:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:71:ARG:CA	1:G:75:ALA:HB2	2.45	0.46
2:H:196:ILE:HG22	2:H:221:SER:HB2	1.97	0.46
1:I:467:ARG:HH21	1:I:630:ARG:NE	2.14	0.46
2:J:291:PHE:CE1	2:J:348:GLU:HA	2.51	0.46
2:J:309:ASN:HD21	2:J:311:ASN:HB2	1.80	0.46
2:J:382:ASP:HA	2:J:424:VAL:CG1	2.45	0.46
2:J:432:ARG:HG2	2:J:433:LYS:N	2.31	0.46
1:K:283:ILE:HB	1:K:386:GLN:CD	2.36	0.46
1:K:444:TYR:N	1:K:444:TYR:CD1	2.83	0.46
1:K:515:VAL:CG2	1:K:631:GLY:HA3	2.45	0.46
1:A:164:VAL:HG23	1:A:373:MET:O	2.16	0.46
1:A:189:VAL:CG2	1:A:323:LEU:HB2	2.45	0.46
1:A:321:VAL:O	1:A:324:ALA:CB	2.60	0.46
1:C:190:SER:N	1:C:319:GLN:OE1	2.36	0.46
1:C:515:VAL:CG2	1:C:631:GLY:HA3	2.44	0.46
1:C:627:ILE:HD12	1:C:627:ILE:N	2.30	0.46
2:D:229:ASP:O	2:D:233:THR:HG23	2.16	0.46
2:F:336:PHE:O	2:F:373:LYS:NZ	2.40	0.46
1:G:164:VAL:HG23	1:G:377:ALA:CB	2.44	0.46
1:G:419:ARG:HB2	1:G:476:GLU:HB2	1.97	0.46
1:I:285:LEU:HB3	1:I:365:THR:HG21	1.97	0.46
1:I:543:VAL:HG12	1:I:544:SER:N	2.31	0.46
1:I:649:LEU:HD13	2:J:59:HIS:CD2	2.50	0.46
2:J:307:PRO:HG3	2:J:312:THR:HG22	1.95	0.46
2:B:210:MET:HE1	2:J:416:LEU:HG	1.97	0.46
1:K:287:GLU:OE2	1:K:305:SER:N	2.44	0.46
2:L:458:ALA:HB3	2:L:493:PRO:HB3	1.97	0.46
2:L:91:THR:O	2:L:98:GLN:NE2	2.45	0.46
1:A:327:VAL:HG22	1:A:327:VAL:O	2.15	0.46
1:A:517:LEU:HD21	1:A:632:ALA:HB1	1.97	0.46
1:A:670:ILE:CD1	1:A:718:LEU:HD21	2.46	0.46
1:A:675:VAL:HG12	1:A:707:VAL:HG21	1.98	0.46
1:A:411:LEU:HB2	1:A:682:GLN:HG3	1.96	0.46
1:C:146:LEU:HD23	1:C:152:PHE:CG	2.51	0.46
1:C:316:MET:HE3	1:C:337:PHE:HD1	1.79	0.46
1:C:73:GLU:HG3	1:C:74:ILE:H	1.80	0.46
1:C:83:ARG:CG	1:C:83:ARG:HH11	2.26	0.46
2:D:378:VAL:HG13	2:D:388:LEU:CD1	2.45	0.46
1:E:400:LEU:HD11	1:E:482:LEU:CD1	2.45	0.46
1:E:614:LEU:HD22	1:E:627:ILE:HG21	1.96	0.46
1:E:619:ILE:HD11	1:E:626:ARG:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:664:CYS:HB2	1:E:724:ILE:HD11	1.96	0.46
2:F:69:ARG:HA	2:F:268:LEU:HD11	1.97	0.46
1:G:319:GLN:NE2	1:G:345:PHE:CE1	2.83	0.46
1:G:390:LYS:HD3	1:G:390:LYS:C	2.34	0.46
1:G:543:VAL:HG12	1:G:544:SER:N	2.29	0.46
2:H:235:THR:HG22	2:H:235:THR:O	2.15	0.46
2:H:94:ASN:HA	2:H:98:GLN:OE1	2.16	0.46
1:I:316:MET:HE3	1:I:337:PHE:CD1	2.42	0.46
1:I:675:VAL:HG12	1:I:707:VAL:HG21	1.96	0.46
1:I:78:VAL:CG1	1:I:79:ILE:N	2.77	0.46
2:J:239:VAL:HG22	2:J:243:GLU:HB2	1.97	0.46
2:J:346:ARG:NH1	2:J:346:ARG:HG3	2.30	0.46
1:K:541:THR:HG22	1:K:541:THR:O	2.14	0.46
2:L:200:CYS:HB3	2:L:223:MET:HB3	1.96	0.46
2:L:215:PHE:HD2	2:L:259:ALA:HB3	1.81	0.46
2:L:232:LYS:O	2:L:236:ASN:N	2.42	0.46
1:A:528:ALA:CB	1:A:605:LEU:HD22	2.43	0.46
1:A:74:ILE:HG23	1:A:75:ALA:N	2.30	0.46
2:B:149:MET:SD	2:B:186:ALA:HB2	2.56	0.46
2:B:469:THR:CG2	2:B:482:HIS:HB3	2.46	0.46
1:C:547:MET:O	1:C:548:ASP:C	2.52	0.46
1:C:626:ARG:NE	1:C:628:ARG:HD2	2.30	0.46
2:D:119:VAL:HG13	2:D:156:ILE:HD13	1.96	0.46
1:E:348:LEU:HD23	1:E:348:LEU:O	2.16	0.46
1:E:563:LEU:HB3	1:E:564:GLN:H	1.38	0.46
1:E:78:VAL:HA	1:E:370:VAL:HG11	1.98	0.46
1:E:83:ARG:HH11	1:E:83:ARG:CG	2.26	0.46
2:F:252:ARG:NH2	2:F:335:GLU:HG3	2.31	0.46
2:F:339:ASN:HB3	2:F:361:VAL:HG12	1.96	0.46
2:F:314:TYR:CE1	2:F:359:PRO:HG2	2.50	0.46
2:F:382:ASP:HA	2:F:424:VAL:CG1	2.46	0.46
1:G:273:GLN:O	1:G:285:LEU:HD12	2.16	0.46
2:H:108:VAL:O	2:H:122:PHE:HA	2.14	0.46
2:F:460:VAL:HG23	2:H:170:VAL:HG11	1.97	0.46
2:H:458:ALA:O	2:H:493:PRO:HD3	2.15	0.46
2:D:135:GLU:OE1	2:H:89:ARG:NH2	2.48	0.46
1:I:195:TYR:CD2	1:I:208:ILE:HD13	2.51	0.46
1:I:401:TYR:HD2	1:I:448:MET:HA	1.80	0.46
1:I:563:LEU:O	1:I:565:GLY:N	2.48	0.46
2:F:89:ARG:NH2	2:J:135:GLU:OE1	2.48	0.46
1:I:539:ARG:NH2	2:J:326:GLU:OE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:334:THR:CG2	1:K:351:ASN:HB2	2.46	0.46
1:K:401:TYR:CD2	1:K:448:MET:HA	2.49	0.46
1:K:539:ARG:NH2	2:L:326:GLU:OE2	2.49	0.46
2:L:329:PHE:HE1	2:L:343:GLY:HA3	1.77	0.46
1:C:457:PRO:HG2	1:C:458:THR:N	2.18	0.46
1:E:114:PRO:HB2	1:E:115:PRO:HD2	1.97	0.46
1:E:139:VAL:HG11	1:E:156:LEU:HD21	1.98	0.46
1:E:316:MET:O	1:E:320:ALA:HB2	2.15	0.46
1:E:515:VAL:HG21	1:E:631:GLY:HA3	1.97	0.46
1:G:517:LEU:HA	1:G:518:PRO:HD3	1.58	0.46
2:H:138:SER:OG	2:H:139:LYS:N	2.47	0.46
2:H:469:THR:HG23	2:H:482:HIS:HB3	1.96	0.46
1:I:419:ARG:HD2	1:I:601:GLN:OE1	2.15	0.46
1:I:690:ILE:CD1	1:I:699:LEU:HD11	2.46	0.46
1:I:93:TYR:HA	1:I:121:TYR:OH	2.15	0.46
1:K:164:VAL:HG23	1:K:373:MET:O	2.15	0.46
1:K:283:ILE:HD12	1:K:389:VAL:CG2	2.44	0.46
1:K:436:TYR:HE1	1:K:439:GLY:CA	2.28	0.46
2:L:52:GLN:OE1	2:L:52:GLN:O	2.34	0.46
1:A:308:LEU:CD2	1:A:316:MET:SD	2.97	0.46
1:A:541:THR:HG22	1:A:541:THR:O	2.15	0.46
1:A:93:TYR:HD1	1:A:94:SER:O	1.99	0.46
2:B:492:ASN:ND2	2:B:494:PHE:HB2	2.31	0.46
1:C:602:LEU:HD12	1:C:614:LEU:O	2.15	0.46
1:E:140:HIS:ND1	1:E:141:PRO:N	2.64	0.46
1:E:264:VAL:HG13	1:E:340:ASP:HB3	1.97	0.46
1:E:596:TRP:CH2	1:E:600:ASP:O	2.67	0.46
2:F:299:GLU:HB2	2:F:302:LEU:CD1	2.45	0.46
2:F:376:ARG:HH11	2:H:410:LYS:NZ	2.13	0.46
2:F:299:GLU:O	2:F:509:ARG:HA	2.15	0.46
1:G:186:GLU:C	1:G:188:ASN:N	2.68	0.46
1:G:515:VAL:HG21	1:G:631:GLY:HA3	1.96	0.46
1:I:658:THR:HG22	1:I:659:SER:O	2.16	0.46
1:K:518:PRO:O	1:K:521:ASP:N	2.36	0.46
2:L:108:VAL:O	2:L:122:PHE:HA	2.15	0.46
2:L:340:ILE:HG23	2:L:373:LYS:HD3	1.97	0.46
1:A:140:HIS:ND1	1:A:141:PRO:N	2.63	0.46
1:A:414:ILE:HD12	1:A:441:ILE:O	2.15	0.46
1:A:268:ARG:NH2	1:A:497:GLY:O	2.43	0.46
1:A:596:TRP:CG	1:A:597:THR:N	2.83	0.46
1:A:640:THR:OG1	1:A:643:GLN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:GLY:C	2:B:51:GLY:H	2.18	0.46
2:B:423:THR:O	2:B:525:LYS:HE2	2.16	0.46
1:C:530:ALA:HB2	1:C:561:VAL:HG21	1.97	0.46
1:C:68:ILE:CG2	1:C:70:ASN:H	2.29	0.46
1:C:93:TYR:HD1	1:C:94:SER:O	1.98	0.46
1:E:547:MET:O	1:E:548:ASP:C	2.52	0.46
1:G:457:PRO:CG	1:G:458:THR:N	2.78	0.46
1:G:539:ARG:NH2	2:H:326:GLU:OE2	2.48	0.46
2:H:474:ARG:HA	2:H:474:ARG:HD3	1.65	0.46
1:I:363:LEU:HD13	1:I:455:TRP:HB3	1.96	0.46
2:J:50:GLY:HA3	2:J:127:THR:O	2.15	0.46
1:K:528:ALA:CB	1:K:605:LEU:HD22	2.45	0.46
1:A:186:GLU:C	1:A:188:ASN:N	2.69	0.46
1:A:517:LEU:HA	1:A:518:PRO:HD3	1.59	0.46
1:A:577:ASP:HB2	1:A:591:ARG:NH2	2.31	0.46
2:B:235:THR:O	2:B:235:THR:HG22	2.16	0.46
1:C:491:HIS:CE1	1:C:493:LYS:HB2	2.51	0.46
1:C:85:MET:O	1:C:86:GLY:C	2.53	0.46
1:E:150:SER:O	1:E:153:ALA:N	2.48	0.46
1:E:724:ILE:HG22	1:E:725:MET:HG3	1.98	0.46
1:G:93:TYR:HA	1:G:121:TYR:OH	2.15	0.46
1:G:396:ILE:N	1:G:396:ILE:HD12	2.30	0.46
2:H:192:GLN:O	2:H:211:THR:HB	2.16	0.46
1:I:70:ASN:ND2	1:I:145:PHE:CD1	2.84	0.46
1:I:162:ILE:O	1:I:164:VAL:N	2.49	0.46
1:I:661:MET:HG3	1:I:723:VAL:HG13	1.98	0.46
2:J:416:LEU:HB2	2:J:441:VAL:HG22	1.96	0.46
1:K:65:LYS:HA	1:K:88:SER:O	2.16	0.46
1:C:132:ARG:HD3	1:C:159:GLU:OE1	2.15	0.46
1:C:167:PRO:O	1:C:169:GLY:N	2.49	0.46
1:C:415:GLY:C	1:C:440:GLU:HG3	2.36	0.46
1:C:414:ILE:HD12	1:C:441:ILE:O	2.16	0.46
1:C:583:PHE:HZ	1:C:590:MET:HE3	1.80	0.46
1:E:444:TYR:O	1:E:445:TYR:CG	2.69	0.46
1:G:285:LEU:HD12	1:G:285:LEU:N	2.31	0.46
1:G:295:ARG:O	1:G:296:ASN:HB2	2.16	0.46
2:H:476(C):ASP:C	2:H:477:GLU:H	2.19	0.46
1:I:334:THR:CG2	1:I:351:ASN:HB2	2.46	0.46
2:J:227:GLY:O	2:J:231:VAL:HG23	2.16	0.46
2:L:199:PRO:HB3	2:L:222:TYR:CZ	2.51	0.46
2:L:45:ALA:O	2:L:48:LEU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ALA:O	1:A:173:ALA:HB3	2.16	0.46
1:A:658:THR:CB	1:A:703:LYS:HD3	2.46	0.46
1:C:189:VAL:CG2	1:C:323:LEU:HB2	2.45	0.46
1:C:457:PRO:CG	1:C:458:THR:N	2.79	0.46
2:D:232:LYS:O	2:D:236:ASN:N	2.42	0.46
2:F:195:MET:SD	2:F:271:VAL:HG21	2.56	0.46
1:G:92:ILE:CG1	1:G:112:ILE:HD13	2.46	0.46
1:G:156:LEU:HD13	1:G:163:PHE:HB2	1.95	0.46
2:J:124:GLN:HE21	2:J:137:HIS:CE1	2.34	0.46
1:K:229:MET:O	1:K:230:ARG:HB2	2.13	0.46
1:K:690:ILE:CD1	1:K:699:LEU:HD11	2.45	0.46
1:K:713:SER:O	1:K:714:ALA:C	2.55	0.46
2:L:325:ASP:C	2:L:327:GLY:N	2.70	0.46
2:L:474:ARG:HA	2:L:474:ARG:HD3	1.60	0.46
1:A:150:SER:O	1:A:151:LYS:C	2.55	0.45
2:B:43:ARG:HG2	2:B:43:ARG:HH11	1.80	0.45
1:C:112:ILE:O	1:C:120:SER:HA	2.16	0.45
1:C:293:GLN:HB3	1:C:298:LYS:HA	1.97	0.45
1:E:162:ILE:O	1:E:164:VAL:N	2.49	0.45
1:E:304:PRO:HD2	1:E:394:TRP:CE2	2.51	0.45
1:E:347:PHE:CD1	1:E:347:PHE:O	2.69	0.45
2:F:307:PRO:HG3	2:F:312:THR:O	2.16	0.45
2:F:88:HIS:C	2:F:88:HIS:CD2	2.89	0.45
1:G:396:ILE:CG1	1:G:463:ILE:HD13	2.38	0.45
2:H:66:ALA:HB2	2:H:125:ASP:HA	1.98	0.45
2:H:394:VAL:HG23	2:H:395:PRO:HD2	1.98	0.45
2:H:419:TYR:CE1	2:H:443:SER:HB2	2.51	0.45
1:I:334:THR:HG22	1:I:351:ASN:HB2	1.98	0.45
1:K:265:THR:HG21	1:K:342:GLN:NE2	2.31	0.45
1:K:78:VAL:HA	1:K:370:VAL:HG11	1.97	0.45
2:L:295:PRO:O	2:L:513:LYS:HA	2.16	0.45
2:D:476(C):ASP:N	2:D:476(D):PRO:HD3	2.31	0.45
1:E:358:HIS:N	1:E:359:PRO:CD	2.79	0.45
1:E:690:ILE:CD1	1:E:699:LEU:HD11	2.46	0.45
1:E:718:LEU:H	1:E:718:LEU:HD23	1.80	0.45
1:G:365:THR:HG22	1:G:391:LEU:HD22	1.98	0.45
1:G:646:LEU:HD13	2:H:64:LEU:HD13	1.97	0.45
1:I:124:ILE:HG22	1:I:128:MET:CE	2.46	0.45
1:I:190:SER:N	1:I:319:GLN:OE1	2.36	0.45
1:I:68:ILE:HG12	1:I:78:VAL:HG11	1.97	0.45
1:K:517:LEU:HD21	1:K:632:ALA:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:348:GLU:OE2	1:K:551:HIS:HE1	2.00	0.45
1:K:71:ARG:CA	1:K:75:ALA:HB2	2.46	0.45
1:A:395:ALA:C	1:A:396:ILE:HD12	2.37	0.45
2:B:134:SER:H	2:B:137:HIS:HB3	1.81	0.45
2:B:119:VAL:HG13	2:B:156:ILE:HD13	1.98	0.45
2:B:298:ILE:HG23	2:B:509:ARG:HB2	1.98	0.45
2:B:476(C):ASP:C	2:B:477:GLU:H	2.19	0.45
1:C:112:ILE:HD12	1:C:120:SER:O	2.16	0.45
1:C:272:ILE:HG22	1:C:274:VAL:HG13	1.98	0.45
1:C:537:GLU:HG3	1:C:553:ARG:NH2	2.32	0.45
1:E:92:ILE:HG13	1:E:112:ILE:HD13	1.98	0.45
1:E:598:PRO:HD2	2:F:292:PHE:CE1	2.50	0.45
1:G:124:ILE:HG22	1:G:128:MET:CE	2.46	0.45
1:G:497:GLY:O	1:G:499:MET:HG2	2.16	0.45
2:H:337:ALA:HB3	2:H:373:LYS:CD	2.46	0.45
2:H:43:ARG:CG	2:H:43:ARG:HH11	2.30	0.45
1:I:139:VAL:O	1:I:164:VAL:HG12	2.16	0.45
1:I:317:GLY:O	1:I:321:VAL:HG12	2.17	0.45
1:I:353:ARG:HG3	1:I:353:ARG:HH11	1.82	0.45
1:I:484:PHE:HZ	1:I:504:ILE:HD11	1.80	0.45
1:I:411:LEU:HD22	1:I:682:GLN:HG3	1.99	0.45
2:J:522:LEU:HD23	2:L:151:ASN:ND2	2.30	0.45
1:K:136:ALA:HB1	1:K:161:VAL:CG1	2.36	0.45
1:K:265:THR:HB	1:K:341:GLY:N	2.30	0.45
1:A:443:MET:HG3	1:A:444:TYR:CE1	2.52	0.45
2:B:208:PRO:O	2:B:214:ILE:HD11	2.16	0.45
2:B:242:GLU:OE2	2:B:246:GLY:HA3	2.17	0.45
1:C:146:LEU:HD23	1:C:152:PHE:CD2	2.51	0.45
1:C:287:GLU:OE1	1:C:313:ARG:CD	2.64	0.45
1:C:515:VAL:HB	1:C:631:GLY:C	2.36	0.45
2:D:117:ARG:HH21	2:D:280:LEU:HG	1.81	0.45
2:D:390:THR:CG2	2:D:419:TYR:OH	2.65	0.45
1:E:316:MET:CE	1:E:337:PHE:HD1	2.29	0.45
1:E:367:VAL:HG12	1:E:368:ASP:N	2.31	0.45
1:G:189:VAL:CG2	1:G:323:LEU:HB2	2.47	0.45
2:H:149:MET:CE	2:H:186:ALA:HA	2.45	0.45
1:I:396:ILE:HG12	1:I:463:ILE:CD1	2.44	0.45
1:I:517:LEU:H	1:I:564:GLN:HE22	1.65	0.45
1:I:683:GLU:H	1:I:704:LYS:HG2	1.82	0.45
1:I:83:ARG:NH1	1:I:83:ARG:CG	2.79	0.45
2:J:337:ALA:HB1	2:J:370:SER:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:320:ALA:HB1	1:K:335:VAL:HG21	1.98	0.45
1:K:279:HIS:HD2	1:K:380:GLU:O	1.99	0.45
1:K:650:MET:HA	1:K:651:PRO:HD3	1.86	0.45
2:L:273:ARG:HD2	2:L:330:TYR:CD1	2.52	0.45
2:L:460:VAL:O	2:L:460:VAL:HG23	2.16	0.45
1:A:285:LEU:HB3	1:A:365:THR:HG21	1.99	0.45
1:A:348:LEU:O	1:A:349:GLU:HB3	2.16	0.45
1:A:482:LEU:N	1:A:483:PRO:HD2	2.32	0.45
2:B:149:MET:CE	2:B:189:VAL:CG1	2.95	0.45
2:B:126:PHE:HB2	2:B:160:ASP:OD2	2.17	0.45
2:B:474:ARG:HD3	2:B:474:ARG:HA	1.66	0.45
1:C:170:ALA:O	1:C:173:ALA:HB3	2.17	0.45
1:C:455:TRP:C	1:C:455:TRP:CD1	2.87	0.45
1:C:675:VAL:HG12	1:C:707:VAL:HG21	1.98	0.45
2:D:145:MET:HE1	2:D:183:ASN:ND2	2.31	0.45
2:D:291:PHE:CZ	2:D:348:GLU:HA	2.51	0.45
2:D:335:GLU:HA	2:D:338:LYS:HE2	1.98	0.45
2:D:347:LEU:O	2:D:348:GLU:C	2.54	0.45
1:E:128:MET:SD	1:E:131:ILE:HD12	2.56	0.45
1:G:512:PHE:CZ	1:G:515:VAL:HG23	2.51	0.45
1:G:65:LYS:HE2	1:G:134:THR:O	2.16	0.45
1:G:73:GLU:HG3	1:G:74:ILE:H	1.82	0.45
2:H:228:PRO:HB3	2:H:239:VAL:O	2.17	0.45
2:H:299:GLU:HG3	2:H:322:LYS:HB3	1.98	0.45
2:J:228:PRO:HB3	2:J:239:VAL:O	2.17	0.45
2:J:398:LEU:HA	2:J:399:PRO:HD3	1.80	0.45
2:B:189:VAL:HG23	2:J:532:LYS:HE2	1.98	0.45
1:K:308:LEU:HD12	1:K:308:LEU:O	2.16	0.45
2:L:180:PHE:O	2:L:184:ILE:HG13	2.17	0.45
1:A:178:ILE:CD1	1:A:178:ILE:H	2.10	0.45
2:B:492:ASN:HB2	2:B:493:PRO:CD	2.46	0.45
2:D:126:PHE:O	2:D:130:GLY:HA2	2.16	0.45
2:D:410:LYS:NZ	2:L:376:ARG:NH1	2.63	0.45
2:D:61:ARG:HB2	2:D:63:LYS:HG3	1.98	0.45
1:C:646:LEU:HD12	2:D:72:LEU:HD11	1.98	0.45
1:E:516:ASN:CB	1:E:564:GLN:NE2	2.76	0.45
1:E:675:VAL:HG12	1:E:707:VAL:HG21	1.97	0.45
2:F:84:MET:O	2:F:84:MET:HG2	2.15	0.45
1:G:287:GLU:OE1	1:G:287:GLU:N	2.47	0.45
1:G:354:LEU:HD11	1:G:358:HIS:CE1	2.52	0.45
1:G:491:HIS:CE1	1:G:493:LYS:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:514:ARG:HD2	2:H:514:ARG:HA	1.68	0.45
2:H:58:GLN:CD	2:H:63:LYS:HE3	2.37	0.45
1:I:369:LEU:O	1:I:373:MET:HB2	2.16	0.45
2:J:149:MET:CE	2:J:189:VAL:CG1	2.95	0.45
2:J:355:VAL:HB	2:J:390:THR:HG23	1.98	0.45
2:J:460:VAL:CG2	2:J:496:ALA:HB2	2.47	0.45
1:K:504:ILE:CG2	1:K:505:ALA:N	2.80	0.45
1:K:614:LEU:HD22	1:K:627:ILE:HG21	1.96	0.45
1:K:627:ILE:HD12	1:K:627:ILE:N	2.31	0.45
2:L:156:ILE:N	2:L:156:ILE:CD1	2.80	0.45
2:L:390:THR:HG23	2:L:419:TYR:OH	2.17	0.45
1:A:517:LEU:HB3	1:A:521:ASP:HB3	1.98	0.45
1:A:71:ARG:CA	1:A:75:ALA:HB2	2.47	0.45
1:C:625:PHE:CD1	1:C:625:PHE:N	2.85	0.45
2:D:423:THR:O	2:D:525:LYS:HE2	2.17	0.45
1:E:165:GLY:HA2	1:E:331:SER:OG	2.16	0.45
1:E:267:PRO:O	1:E:501:THR:HG23	2.17	0.45
1:E:537:GLU:HG3	1:E:553:ARG:HH21	1.82	0.45
1:E:537:GLU:HG3	1:E:553:ARG:NH2	2.31	0.45
1:E:83:ARG:CZ	1:E:83:ARG:HB3	2.47	0.45
2:F:337:ALA:HB3	2:F:373:LYS:CD	2.43	0.45
2:F:476(C):ASP:O	2:F:478:LYS:N	2.44	0.45
1:G:164:VAL:HG23	1:G:373:MET:O	2.17	0.45
1:G:407:ARG:HH11	1:G:407:ARG:HG2	1.81	0.45
1:G:433:THR:HG21	1:G:435:VAL:HG12	1.94	0.45
1:I:272:ILE:HB	1:I:335:VAL:HG23	1.99	0.45
1:I:302:GLU:OE2	1:I:394:TRP:HZ3	2.00	0.45
1:I:339:VAL:HG22	1:I:345:PHE:HB3	1.99	0.45
1:I:342:GLN:O	1:I:343:LYS:HB2	2.17	0.45
1:I:543:VAL:CG1	2:J:117:ARG:HD2	2.45	0.45
1:I:642:ARG:HH11	2:J:71:ASP:HB3	1.82	0.45
2:J:154:PRO:HG3	2:J:191:PRO:HD2	1.99	0.45
2:J:88:HIS:CD2	2:J:88:HIS:C	2.90	0.45
1:K:376:VAL:HG23	1:K:377:ALA:N	2.31	0.45
2:L:235:THR:HG22	2:L:237:GLU:HB2	1.99	0.45
1:A:491:HIS:CE1	1:A:493:LYS:HB2	2.51	0.45
1:A:653:LYS:N	1:A:653:LYS:CD	2.75	0.45
2:B:66:ALA:HB2	2:B:125:ASP:HA	1.97	0.45
2:B:514:ARG:HD2	2:B:514:ARG:HA	1.72	0.45
2:B:67:ARG:NH1	2:B:67:ARG:HG2	2.31	0.45
1:C:150:SER:O	1:C:151:LYS:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:TYR:HE1	1:C:439:GLY:CA	2.30	0.45
1:C:467:ARG:CB	1:C:467:ARG:HH11	2.28	0.45
1:C:670:ILE:CG1	1:C:718:LEU:HD21	2.42	0.45
2:D:340:ILE:HD13	2:D:374:ALA:HB2	1.99	0.45
1:E:436:TYR:HE1	1:E:439:GLY:CA	2.29	0.45
2:F:121:VAL:HG22	2:F:122:PHE:N	2.31	0.45
2:F:417:TYR:N	2:H:210:MET:HE1	2.32	0.45
2:F:509:ARG:HB3	2:F:509:ARG:HH11	1.81	0.45
1:G:598:PRO:HD2	2:H:292:PHE:CD1	2.52	0.45
2:H:356:ALA:HB2	2:H:391:LEU:HB2	1.97	0.45
2:J:367:ASP:O	2:J:368:ILE:C	2.55	0.45
1:I:642:ARG:NH1	2:J:71:ASP:OD2	2.50	0.45
1:K:214:TYR:HB2	1:K:215:PRO:HA	1.99	0.45
1:K:316:MET:HE3	1:K:337:PHE:HD1	1.82	0.45
1:A:369:LEU:O	1:A:373:MET:HB2	2.17	0.45
2:B:151:ASN:ND2	2:D:522:LEU:HA	2.32	0.45
1:C:342:GLN:O	1:C:343:LYS:HB2	2.15	0.45
1:C:395:ALA:C	1:C:396:ILE:HD12	2.37	0.45
1:C:468:ILE:O	1:C:471:ASP:HB2	2.17	0.45
1:E:272:ILE:HG22	1:E:274:VAL:HG13	1.99	0.45
2:F:180:PHE:O	2:F:183:ASN:HB2	2.17	0.45
1:G:393:GLY:HA3	1:G:455:TRP:CZ3	2.52	0.45
2:H:495:VAL:HG13	2:H:496:ALA:N	2.32	0.45
1:I:414:ILE:HD12	1:I:441:ILE:O	2.17	0.45
1:I:619:ILE:HD12	1:I:625:PHE:C	2.37	0.45
1:I:666:MET:O	1:I:668:GLY:N	2.50	0.45
1:I:720:VAL:HG22	1:I:721:ASP:H	1.82	0.45
2:J:164:ALA:HB2	2:J:176:TYR:HE2	1.82	0.45
2:J:300:PRO:HA	2:J:509:ARG:NH1	2.31	0.45
2:J:484:ALA:O	2:J:488:GLU:OE1	2.35	0.45
1:K:245:SER:C	1:K:247:ASN:N	2.70	0.45
1:K:596:TRP:CH2	1:K:600:ASP:O	2.69	0.45
1:K:83:ARG:HH11	1:K:83:ARG:CG	2.28	0.45
1:A:122:ILE:HA	1:A:146:LEU:CD1	2.45	0.45
1:A:270:ILE:HG12	1:A:289:GLU:HG3	1.98	0.45
1:A:435:VAL:HG22	1:A:436:TYR:H	1.80	0.45
1:A:494:PHE:HD2	1:A:499:MET:HE1	1.82	0.45
1:A:537:GLU:HG3	1:A:553:ARG:HH21	1.82	0.45
1:A:71:ARG:O	1:A:75:ALA:HB2	2.17	0.45
1:A:98:LYS:HG3	1:A:98:LYS:O	2.17	0.45
2:B:83:ASP:HB3	2:B:86:VAL:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:ILE:HD11	1:C:442:SER:C	2.37	0.45
1:C:515:VAL:HG21	1:C:631:GLY:HA3	1.99	0.45
1:C:92:ILE:HD12	1:C:112:ILE:HD13	1.99	0.45
2:D:121:VAL:O	2:D:144:ILE:HD13	2.17	0.45
2:D:235:THR:HG22	2:D:237:GLU:HB2	1.99	0.45
1:E:165:GLY:CA	1:E:331:SER:OG	2.65	0.45
2:F:66:ALA:HB2	2:F:125:ASP:HA	1.98	0.45
1:G:376:VAL:HG23	1:G:377:ALA:N	2.31	0.45
1:G:396:ILE:HD13	1:G:462:ALA:CB	2.47	0.45
1:K:598:PRO:HD2	2:L:292:PHE:CD1	2.51	0.45
2:L:460:VAL:HG21	2:L:496:ALA:CB	2.44	0.45
2:L:476(A):LEU:C	2:L:476(C):ASP:H	2.20	0.45
1:A:347:PHE:C	1:A:347:PHE:CD1	2.90	0.44
1:A:517:LEU:HD21	1:A:632:ALA:HB2	1.98	0.44
2:B:460:VAL:HG23	2:B:460:VAL:O	2.18	0.44
1:C:537:GLU:HG3	1:C:553:ARG:HH21	1.82	0.44
2:D:50:GLY:HA3	2:D:127:THR:O	2.17	0.44
2:D:474:ARG:HD3	2:D:474:ARG:HA	1.63	0.44
2:D:509:ARG:HH11	2:D:509:ARG:HB3	1.82	0.44
1:E:390:LYS:HD3	1:E:391:LEU:H	1.78	0.44
1:E:99:GLN:HB2	1:E:436:TYR:OH	2.16	0.44
1:E:405:PRO:CG	1:E:481:ASN:HA	2.45	0.44
2:F:149:MET:SD	2:F:186:ALA:HB2	2.57	0.44
1:G:124:ILE:O	1:G:128:MET:HB2	2.17	0.44
1:G:283:ILE:CG2	1:G:386:GLN:HG2	2.47	0.44
1:G:347:PHE:CD1	1:G:347:PHE:C	2.90	0.44
2:H:109:THR:HG22	2:H:122:PHE:CB	2.47	0.44
1:I:517:LEU:HA	1:I:518:PRO:HD3	1.57	0.44
1:I:596:TRP:CH2	1:I:600:ASP:O	2.70	0.44
2:J:537:ILE:HG13	2:J:538:PRO:HD2	1.99	0.44
1:K:305:SER:HA	1:K:306:PRO:HD3	1.81	0.44
1:K:627:ILE:HD13	1:K:636:VAL:HB	1.98	0.44
2:H:89:ARG:NH1	2:L:499:ARG:HH21	2.13	0.44
2:L:504:GLU:HG3	2:L:505:VAL:H	1.77	0.44
1:A:288:ARG:HD3	1:A:361:THR:OG1	2.17	0.44
1:A:292:ILE:HG23	1:A:503:PHE:CD2	2.52	0.44
2:B:229:ASP:N	2:B:229:ASP:OD1	2.49	0.44
2:B:329:PHE:HD1	2:B:345:ILE:HG22	1.83	0.44
1:C:456:ALA:CB	1:C:457:PRO:CD	2.94	0.44
2:D:204:ALA:O	2:D:205:VAL:C	2.54	0.44
1:E:518:PRO:O	1:E:519:GLU:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:494:PHE:HA	1:G:499:MET:CE	2.40	0.44
1:G:612:LEU:HD12	1:G:612:LEU:C	2.37	0.44
1:I:229:MET:O	1:I:230:ARG:HB2	2.18	0.44
1:I:627:ILE:N	1:I:627:ILE:HD12	2.33	0.44
1:I:69:ALA:HB3	1:I:141:PRO:HA	1.99	0.44
1:I:704:LYS:H	1:I:704:LYS:HG3	1.58	0.44
1:I:93:TYR:HD1	1:I:94:SER:O	2.00	0.44
2:B:436:GLY:HA2	2:J:173:LEU:HD21	1.99	0.44
2:J:335:GLU:HA	2:J:338:LYS:HE2	1.99	0.44
1:K:118:ASN:HD21	1:K:119:GLN:HE21	1.65	0.44
1:K:443:MET:HG3	1:K:444:TYR:CE1	2.52	0.44
2:B:67:ARG:HH11	2:B:67:ARG:HG2	1.82	0.44
1:C:683:GLU:H	1:C:704:LYS:HG2	1.82	0.44
1:C:661:MET:CE	1:C:726:GLU:HB3	2.46	0.44
2:D:139:LYS:HE2	2:D:139:LYS:HB3	1.74	0.44
2:D:196:ILE:HD13	2:D:214:ILE:HG23	1.99	0.44
1:E:347:PHE:CD1	1:E:347:PHE:C	2.90	0.44
1:E:74:ILE:HG23	1:E:75:ALA:N	2.32	0.44
1:G:150:SER:O	1:G:151:LYS:C	2.56	0.44
1:G:664:CYS:HB2	1:G:724:ILE:HD11	2.00	0.44
2:H:361:VAL:C	2:H:363:ALA:N	2.71	0.44
1:I:256:ASP:N	1:I:256:ASP:OD1	2.50	0.44
1:I:68:ILE:HG12	1:I:78:VAL:CG1	2.47	0.44
1:K:491:HIS:CE1	1:K:493:LYS:HB2	2.52	0.44
1:K:653:LYS:CD	1:K:653:LYS:N	2.78	0.44
1:A:325:LYS:O	1:A:328:GLY:N	2.41	0.44
1:A:405:PRO:CG	1:A:481:ASN:HA	2.47	0.44
1:A:115:PRO:HG2	1:A:444:TYR:CE2	2.52	0.44
1:A:419:ARG:HD2	1:A:601:GLN:OE1	2.17	0.44
1:C:107:ASP:C	1:C:108:GLU:HG3	2.38	0.44
1:C:177:LYS:HB3	1:C:181:LYS:HZ1	1.81	0.44
1:C:271:GLU:O	1:C:287:GLU:HB2	2.18	0.44
1:C:400:LEU:HD13	1:C:449:ILE:CD1	2.25	0.44
1:C:563:LEU:HB3	1:C:564:GLN:H	1.33	0.44
1:C:71:ARG:CA	1:C:75:ALA:HB2	2.48	0.44
2:D:325:ASP:C	2:D:327:GLY:H	2.21	0.44
2:D:447:LEU:O	2:D:448:ARG:HB2	2.16	0.44
1:G:517:LEU:N	1:G:517:LEU:HD22	2.23	0.44
1:I:302:GLU:OE2	1:I:394:TRP:CZ3	2.70	0.44
1:I:77:ARG:HE	1:I:430:ARG:HH22	1.66	0.44
1:I:83:ARG:CZ	1:I:83:ARG:HB3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:69:ARG:HA	2:L:268:LEU:HD11	1.98	0.44
1:A:164:VAL:HG23	1:A:377:ALA:CB	2.48	0.44
2:B:156:ILE:N	2:B:156:ILE:CD1	2.81	0.44
2:B:258:ASP:O	2:B:259:ALA:HB2	2.18	0.44
2:B:297:ARG:NH1	2:B:297:ARG:HG2	2.32	0.44
2:B:368:ILE:HG23	2:B:411:HIS:CG	2.53	0.44
1:C:165:GLY:CA	1:C:331:SER:OG	2.66	0.44
1:C:401:TYR:HD2	1:C:448:MET:HA	1.83	0.44
2:D:425:PRO:HB3	2:D:522:LEU:HB3	2.00	0.44
1:E:264:VAL:HG12	1:E:340:ASP:HB3	2.00	0.44
1:E:414:ILE:HD11	1:E:442:SER:C	2.37	0.44
1:E:457:PRO:CG	1:E:458:THR:N	2.80	0.44
1:E:563:LEU:O	1:E:565:GLY:N	2.50	0.44
1:E:93:TYR:HD1	1:E:94:SER:O	2.01	0.44
2:F:121:VAL:O	2:F:144:ILE:HD13	2.18	0.44
2:F:355:VAL:O	2:F:390:THR:HA	2.16	0.44
1:G:321:VAL:O	1:G:324:ALA:CB	2.60	0.44
1:I:122:ILE:HA	1:I:146:LEU:CD1	2.46	0.44
1:I:388:ASP:O	1:I:390:LYS:N	2.51	0.44
1:K:139:VAL:HG11	1:K:156:LEU:CD2	2.48	0.44
1:K:285:LEU:N	1:K:285:LEU:HD12	2.32	0.44
2:D:410:LYS:HZ2	2:L:376:ARG:HH11	1.65	0.44
1:A:275:LEU:HD23	1:A:276:CYS:H	1.82	0.44
1:C:516:ASN:CB	1:C:564:GLN:NE2	2.76	0.44
1:C:467:ARG:HE	1:C:630:ARG:CG	2.29	0.44
1:E:275:LEU:HD23	1:E:276:CYS:H	1.81	0.44
1:E:273:GLN:O	1:E:285:LEU:HD12	2.18	0.44
1:E:491:HIS:O	1:E:495:ILE:HG13	2.17	0.44
2:F:174:ALA:HB2	2:H:501:PHE:CE1	2.53	0.44
2:F:196:ILE:N	2:F:196:ILE:HD12	2.33	0.44
2:F:401:THR:CG2	2:F:402:SER:N	2.80	0.44
1:G:156:LEU:HD22	1:G:161:VAL:HB	1.99	0.44
1:G:534:ARG:NH1	1:G:534:ARG:HG3	2.33	0.44
1:G:626:ARG:C	1:G:627:ILE:HD12	2.38	0.44
1:G:662:LEU:HD22	1:G:687:LEU:HD12	2.00	0.44
1:G:704:LYS:HG3	1:G:704:LYS:H	1.63	0.44
1:G:99:GLN:O	1:G:100:ALA:O	2.36	0.44
1:I:92:ILE:CG1	1:I:112:ILE:HD13	2.48	0.44
1:I:177:LYS:HE3	1:I:181:LYS:HZ1	1.83	0.44
1:I:354:LEU:HD13	1:I:355:GLN:O	2.17	0.44
1:I:92:ILE:HG13	1:I:112:ILE:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:474:ARG:O	2:J:476:ASP:N	2.47	0.44
2:J:95:MET:HA	2:J:95:MET:HE3	1.99	0.44
1:K:115:PRO:HG2	1:K:444:TYR:CE2	2.52	0.44
1:K:71:ARG:O	1:K:75:ALA:HB2	2.17	0.44
1:A:400:LEU:HD21	1:A:482:LEU:CD1	2.48	0.44
1:A:421:ARG:O	1:A:421:ARG:CD	2.66	0.44
2:B:229:ASP:O	2:B:233:THR:HG23	2.18	0.44
2:B:58:GLN:NE2	2:B:63:LYS:HE3	2.32	0.44
1:C:182:LYS:HA	1:C:185:GLN:HG3	2.00	0.44
1:C:347:PHE:HD1	1:C:347:PHE:O	2.00	0.44
1:C:629:THR:HB	1:C:630:ARG:H	1.71	0.44
2:D:303:ASP:OD1	2:D:508:PRO:HB2	2.18	0.44
1:E:168:LYS:O	1:E:172:GLU:OE1	2.36	0.44
1:E:615:LYS:HB2	1:E:628:ARG:HB2	2.00	0.44
2:F:447:LEU:O	2:F:448:ARG:HB2	2.17	0.44
2:F:501:PHE:CE1	2:H:174:ALA:HB2	2.53	0.44
2:H:378:VAL:HG13	2:H:388:LEU:CD1	2.47	0.44
1:I:393:GLY:HA2	1:I:457:PRO:O	2.17	0.44
1:I:421:ARG:C	1:I:421:ARG:HD3	2.38	0.44
2:J:206:TYR:O	2:J:209:ALA:HB3	2.17	0.44
2:J:95:MET:HE2	2:J:95:MET:HB3	1.89	0.44
1:K:212:ILE:HD12	1:K:260:ILE:CG2	2.47	0.44
1:K:272:ILE:HG22	1:K:274:VAL:HG13	2.00	0.44
2:L:258:ASP:O	2:L:259:ALA:HB2	2.17	0.44
2:L:356:ALA:HB2	2:L:391:LEU:HB2	1.99	0.44
1:A:414:ILE:CD1	1:A:441:ILE:O	2.64	0.44
1:A:441:ILE:HD12	1:A:478:ILE:HD13	1.99	0.44
1:C:186:GLU:OE2	1:C:187:ALA:N	2.51	0.44
2:D:312:THR:HG22	2:D:313:PRO:O	2.17	0.44
2:D:94:ASN:HA	2:D:98:GLN:OE1	2.18	0.44
1:E:539:ARG:NH2	2:F:326:GLU:OE2	2.51	0.44
1:E:640:THR:OG1	1:E:643:GLN:HB2	2.18	0.44
2:F:45:ALA:O	2:F:48:LEU:HB2	2.18	0.44
1:G:653:LYS:N	1:G:653:LYS:CD	2.78	0.44
2:H:374:ALA:HB3	2:H:415:LEU:HD13	1.99	0.44
2:H:440:VAL:O	2:H:444:SER:HB3	2.18	0.44
1:I:156:LEU:HD13	1:I:163:PHE:HB2	1.96	0.44
1:I:209:SER:O	1:I:212:ILE:N	2.51	0.44
1:I:684:GLY:N	1:I:701:ALA:O	2.48	0.44
2:B:184:ILE:CD1	2:J:417:TYR:HA	2.44	0.44
1:K:199:ILE:HD13	1:K:205:ALA:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:388:ASP:O	1:K:390:LYS:N	2.51	0.44
2:L:514:ARG:HD2	2:L:514:ARG:HA	1.67	0.44
1:K:651:PRO:CG	2:L:62:GLY:HA3	2.48	0.44
2:J:498:GLU:HG2	2:L:87:THR:HG23	2.00	0.44
2:B:356:ALA:HB2	2:B:391:LEU:HB2	1.99	0.44
1:C:376:VAL:HG23	1:C:377:ALA:N	2.33	0.44
1:C:455:TRP:CG	1:C:456:ALA:N	2.82	0.44
1:C:518:PRO:O	1:C:521:ASP:HB2	2.17	0.44
1:C:634:LEU:H	1:C:634:LEU:HD23	1.83	0.44
1:E:112:ILE:O	1:E:120:SER:HA	2.18	0.44
1:E:411:LEU:HD22	1:E:682:GLN:CB	2.46	0.44
2:F:366:LEU:HA	2:F:366:LEU:HD23	1.81	0.44
1:G:70:ASN:OD1	1:G:74:ILE:HG21	2.17	0.44
1:I:140:HIS:ND1	1:I:141:PRO:N	2.66	0.44
1:I:150:SER:O	1:I:153:ALA:N	2.51	0.44
1:I:276:CYS:HB2	1:I:277:ASP:H	1.44	0.44
1:I:271:GLU:O	1:I:287:GLU:HB2	2.18	0.44
1:I:71:ARG:NH1	1:I:445:TYR:CG	2.86	0.44
2:J:109:THR:HG22	2:J:122:PHE:CB	2.47	0.44
2:J:374:ALA:HB3	2:J:415:LEU:HD13	1.99	0.44
1:K:334:THR:HG21	1:K:355:GLN:CG	2.47	0.44
1:K:93:TYR:HD1	1:K:94:SER:O	2.01	0.44
3:A:801:BTI:H63	2:B:399:PRO:HD3	2.00	0.43
2:B:205:VAL:HB	2:J:409:ILE:HG23	2.00	0.43
2:B:325:ASP:C	2:B:327:GLY:H	2.20	0.43
2:B:339:ASN:HB3	2:B:361:VAL:HG12	2.00	0.43
1:C:157:GLU:C	1:C:159:GLU:N	2.72	0.43
1:C:552:GLU:H	1:C:552:GLU:CD	2.20	0.43
2:D:479:ILE:C	2:D:479:ILE:HD12	2.39	0.43
1:E:117:ALA:HA	1:E:121:TYR:H	1.82	0.43
1:E:139:VAL:O	1:E:164:VAL:HG12	2.18	0.43
1:E:411:LEU:HB2	1:E:682:GLN:HG3	1.99	0.43
2:F:492:ASN:HB2	2:F:493:PRO:CD	2.46	0.43
1:G:422:PRO:HA	1:G:422(A):PRO:HD3	1.82	0.43
1:G:615:LYS:HB2	1:G:628:ARG:HB2	2.00	0.43
1:G:92:ILE:HG13	1:G:112:ILE:HD13	1.99	0.43
1:I:272:ILE:HG22	1:I:274:VAL:HG13	2.00	0.43
1:I:279:HIS:HD2	1:I:380:GLU:O	2.00	0.43
1:I:446:ASP:OD1	1:I:447:PRO:HD2	2.17	0.43
1:I:598:PRO:HD2	2:J:292:PHE:CD1	2.53	0.43
1:I:71:ARG:O	1:I:75:ALA:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:107:ASP:O	1:K:108:GLU:HG3	2.19	0.43
1:A:150:SER:O	1:A:153:ALA:N	2.51	0.43
1:A:287:GLU:HG3	1:A:308:LEU:HD21	2.00	0.43
1:A:418:THR:O	1:A:437:GLU:HG3	2.18	0.43
1:A:492:PRO:HA	1:A:495:ILE:HD12	2.00	0.43
1:C:179:THR:HG22	1:C:183:ILE:CD1	2.46	0.43
1:C:279:HIS:CD2	1:C:380:GLU:O	2.71	0.43
1:C:283:ILE:CG2	1:C:386:GLN:HG2	2.48	0.43
1:C:482:LEU:N	1:C:483:PRO:HD2	2.32	0.43
1:C:583:PHE:CD1	1:C:583:PHE:N	2.86	0.43
1:E:285:LEU:HD12	1:E:285:LEU:N	2.33	0.43
1:E:467:ARG:HH11	1:E:467:ARG:CB	2.27	0.43
1:E:658:THR:CB	1:E:703:LYS:HD3	2.43	0.43
2:F:134:SER:H	2:F:137:HIS:HB3	1.82	0.43
2:F:372:ARG:NH2	2:H:539:LEU:OXT	2.50	0.43
1:G:167:PRO:C	1:G:169:GLY:H	2.21	0.43
1:G:245:SER:C	1:G:247:ASN:N	2.72	0.43
1:G:258:ILE:HG22	1:G:259:PHE:N	2.33	0.43
1:G:272:ILE:HB	1:G:335:VAL:CG2	2.48	0.43
1:G:532:MET:O	1:G:535:VAL:HB	2.18	0.43
1:G:596:TRP:CH2	1:G:600:ASP:O	2.71	0.43
1:G:682:GLN:OE1	1:G:682:GLN:HA	2.19	0.43
2:H:180:PHE:O	2:H:183:ASN:HB2	2.18	0.43
2:H:460:VAL:CG2	2:H:460:VAL:O	2.66	0.43
1:I:100:ALA:HB3	1:I:103:VAL:HG23	1.99	0.43
1:I:117:ALA:C	1:I:119:GLN:N	2.71	0.43
1:I:92:ILE:HD12	1:I:112:ILE:HD13	1.99	0.43
2:J:514:ARG:HA	2:J:514:ARG:HD2	1.74	0.43
1:K:164:VAL:HG23	1:K:377:ALA:HB2	1.99	0.43
1:K:619:ILE:HD11	1:K:626:ARG:HB2	2.00	0.43
2:L:196:ILE:HD12	2:L:196:ILE:N	2.33	0.43
2:L:298:ILE:HD12	2:L:298:ILE:N	2.33	0.43
1:A:162:ILE:O	1:A:164:VAL:N	2.51	0.43
1:A:93:TYR:HA	1:A:121:TYR:OH	2.17	0.43
2:B:164:ALA:HB2	2:B:176:TYR:HE2	1.83	0.43
2:B:394:VAL:HG23	2:B:395:PRO:HD2	2.00	0.43
2:B:88:HIS:C	2:B:88:HIS:CD2	2.91	0.43
1:C:285:LEU:HD12	1:C:285:LEU:N	2.33	0.43
2:D:460:VAL:CG2	2:D:496:ALA:HB2	2.43	0.43
1:E:414:ILE:CD1	1:E:441:ILE:O	2.66	0.43
2:F:423:THR:O	2:F:525:LYS:HE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:188:ASN:OD1	1:G:188:ASN:O	2.36	0.43
1:G:563:LEU:HD23	1:G:636:VAL:HG22	2.00	0.43
2:H:180:PHE:O	2:H:184:ILE:HG13	2.18	0.43
1:I:245:SER:C	1:I:247:ASN:H	2.20	0.43
1:I:287:GLU:OE2	1:I:305:SER:N	2.45	0.43
1:I:289:GLU:OE1	1:I:306:PRO:HD2	2.18	0.43
1:I:308:LEU:C	1:I:308:LEU:HD12	2.38	0.43
1:I:552:GLU:H	1:I:552:GLU:CD	2.21	0.43
1:K:124:ILE:HG22	1:K:128:MET:CE	2.48	0.43
1:K:675:VAL:HG11	1:K:707:VAL:HG21	1.98	0.43
2:L:196:ILE:HD13	2:L:214:ILE:HG23	1.99	0.43
2:L:351:THR:HG22	2:L:386:ILE:HG23	2.00	0.43
1:A:70:ASN:ND2	1:A:145:PHE:CE1	2.87	0.43
2:B:145:MET:CE	2:B:183:ASN:ND2	2.81	0.43
1:C:273:GLN:HG2	1:C:369:LEU:HD11	2.00	0.43
1:C:327:VAL:HG22	1:C:327:VAL:O	2.18	0.43
1:C:480:HIS:HD2	1:C:482:LEU:H	1.66	0.43
2:D:476(D):PRO:HA	2:D:479:ILE:HD11	2.00	0.43
2:B:80:GLU:HB2	2:D:517:ARG:NH2	2.33	0.43
1:E:285:LEU:HB3	1:E:365:THR:HG21	2.00	0.43
1:E:467:ARG:HD2	1:E:467:ARG:O	2.19	0.43
2:F:258:ASP:O	2:F:259:ALA:HB2	2.17	0.43
1:G:206:VAL:HG13	1:G:235:ASP:CB	2.49	0.43
1:G:229:MET:O	1:G:230:ARG:HB2	2.17	0.43
1:G:256:ASP:OD1	1:G:256:ASP:N	2.52	0.43
1:G:417:LEU:HD21	1:G:478:ILE:CD1	2.46	0.43
1:G:70:ASN:ND2	1:G:145:PHE:CE1	2.86	0.43
1:I:376:VAL:HG23	1:I:377:ALA:N	2.33	0.43
1:K:325:LYS:O	1:K:327:VAL:N	2.52	0.43
1:K:369:LEU:O	1:K:373:MET:HB2	2.17	0.43
2:L:126:PHE:HB2	2:L:160:ASP:OD2	2.18	0.43
1:A:316:MET:HE2	1:A:337:PHE:CD1	2.54	0.43
1:A:99:GLN:O	1:A:100:ALA:O	2.36	0.43
1:C:421:ARG:O	1:C:421:ARG:CD	2.67	0.43
1:C:650:MET:HA	1:C:651:PRO:HD3	1.87	0.43
2:D:145:MET:HE3	2:D:183:ASN:ND2	2.34	0.43
2:D:149:MET:SD	2:D:186:ALA:HB2	2.59	0.43
2:D:202:GLY:HA2	2:D:225:VAL:O	2.18	0.43
2:D:476(A):LEU:C	2:D:476(C):ASP:H	2.20	0.43
2:D:458:ALA:O	2:D:492:ASN:HA	2.19	0.43
1:E:327:VAL:O	1:E:327:VAL:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:VAL:HG23	1:E:377:ALA:CB	2.47	0.43
1:E:421:ARG:HD3	1:E:421:ARG:O	2.19	0.43
1:E:401:TYR:CD2	1:E:448:MET:HA	2.53	0.43
1:E:518:PRO:HD2	1:E:521:ASP:OD1	2.18	0.43
2:F:117:ARG:NH2	2:F:280:LEU:HG	2.33	0.43
1:G:245:SER:C	1:G:247:ASN:H	2.20	0.43
1:G:348:LEU:O	1:G:348:LEU:HD23	2.19	0.43
1:G:393:GLY:HA2	1:G:457:PRO:O	2.19	0.43
1:G:625:PHE:HB2	1:G:627:ILE:CD1	2.48	0.43
1:G:634:LEU:H	1:G:634:LEU:HD23	1.82	0.43
2:H:401:THR:CG2	2:H:402:SER:N	2.80	0.43
1:I:245:SER:C	1:I:247:ASN:N	2.72	0.43
1:I:347:PHE:CD1	1:I:347:PHE:C	2.91	0.43
1:I:396:ILE:HD13	1:I:462:ALA:CB	2.49	0.43
2:J:251:THR:HG21	2:J:260:ALA:CB	2.46	0.43
1:K:354:LEU:HD13	1:K:355:GLN:O	2.17	0.43
1:K:401:TYR:HD2	1:K:448:MET:HA	1.84	0.43
2:L:126:PHE:O	2:L:130:GLY:HA2	2.19	0.43
2:L:200:CYS:O	2:L:223:MET:HA	2.18	0.43
1:A:283:ILE:HG22	1:A:386:GLN:HG2	2.01	0.43
1:A:515:VAL:HB	1:A:631:GLY:C	2.39	0.43
1:C:287:GLU:OE1	1:C:313:ARG:HD2	2.19	0.43
1:C:367:VAL:HG12	1:C:368:ASP:N	2.34	0.43
1:C:617:GLY:O	1:C:625:PHE:CB	2.55	0.43
1:C:517:LEU:HD21	1:C:632:ALA:HB1	2.00	0.43
1:C:693:MET:O	1:C:694:LYS:HB2	2.18	0.43
2:D:74:LEU:HD13	2:D:112:GLY:HA3	2.00	0.43
2:D:210:MET:HE3	2:L:416:LEU:HD23	2.00	0.43
1:E:93:TYR:O	1:E:112:ILE:HG12	2.19	0.43
2:F:531:TRP:CG	2:F:532:LYS:N	2.86	0.43
1:G:287:GLU:OE2	1:G:305:SER:N	2.48	0.43
1:G:325:LYS:O	1:G:327:VAL:N	2.51	0.43
1:G:388:ASP:O	1:G:390:LYS:N	2.52	0.43
1:G:435:VAL:HG22	1:G:436:TYR:N	2.34	0.43
1:G:85:MET:O	1:G:86:GLY:C	2.57	0.43
2:H:367:ASP:O	2:H:368:ILE:C	2.57	0.43
1:I:157:GLU:OE1	1:I:168:LYS:NZ	2.52	0.43
1:I:231:ILE:HG22	1:I:232:ALA:N	2.33	0.43
1:I:515:VAL:HB	1:I:631:GLY:C	2.39	0.43
1:K:675:VAL:HG12	1:K:707:VAL:HG21	1.99	0.43
2:L:235:THR:HG22	2:L:235:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:TYR:HD2	1:A:448:MET:HA	1.84	0.43
1:A:704:LYS:HG3	1:A:704:LYS:H	1.64	0.43
2:B:121:VAL:CG2	2:B:122:PHE:N	2.81	0.43
2:B:339:ASN:HD21	2:B:370:SER:HB3	1.83	0.43
2:D:460:VAL:HG23	2:D:460:VAL:O	2.19	0.43
2:D:492:ASN:ND2	2:D:494:PHE:HB2	2.33	0.43
1:E:162:ILE:HD13	1:E:377:ALA:O	2.19	0.43
2:F:346:ARG:CG	2:F:346:ARG:HH11	2.28	0.43
1:G:271:GLU:O	1:G:287:GLU:HB2	2.18	0.43
1:G:546:ARG:HG2	1:G:546:ARG:H	1.54	0.43
1:G:563:LEU:HB3	1:G:564:GLN:H	1.30	0.43
1:G:68:ILE:CG1	1:G:78:VAL:HG11	2.49	0.43
1:I:411:LEU:HD22	1:I:682:GLN:CG	2.49	0.43
1:I:70:ASN:ND2	1:I:145:PHE:CE1	2.87	0.43
1:I:71:ARG:CA	1:I:75:ALA:HB2	2.48	0.43
2:J:392:ILE:HD12	2:J:428:THR:CG2	2.48	0.43
1:K:354:LEU:HD11	1:K:358:HIS:ND1	2.33	0.43
1:K:517:LEU:HA	1:K:518:PRO:HD3	1.62	0.43
1:K:563:LEU:HB3	1:K:564:GLN:H	1.37	0.43
1:A:308:LEU:HD11	1:A:313:ARG:HD3	2.00	0.43
1:A:164:VAL:HA	1:A:377:ALA:HB1	2.00	0.43
1:A:504:ILE:CG2	1:A:505:ALA:N	2.81	0.43
1:A:563:LEU:HB3	1:A:564:GLN:H	1.25	0.43
2:B:291:PHE:CZ	2:B:348:GLU:HA	2.54	0.43
1:C:110:VAL:HG21	1:C:130:ALA:CB	2.46	0.43
1:C:270:ILE:HG21	1:C:308:LEU:HD21	2.01	0.43
1:C:405:PRO:CG	1:C:481:ASN:HA	2.49	0.43
1:C:605:LEU:CD1	1:C:614:LEU:HD12	2.49	0.43
1:C:690:ILE:CD1	1:C:699:LEU:HD11	2.48	0.43
2:D:196:ILE:HG22	2:D:221:SER:HB2	2.01	0.43
1:E:679:GLN:O	1:E:706:VAL:HG13	2.19	0.43
1:G:292:ILE:N	1:G:292:ILE:HD12	2.11	0.43
1:G:675:VAL:HG11	1:G:707:VAL:HG21	2.00	0.43
2:H:297:ARG:HG2	2:H:297:ARG:HH11	1.83	0.43
1:I:124:ILE:HG22	1:I:128:MET:HE3	2.01	0.43
2:J:498:GLU:HA	2:L:86:VAL:HA	1.99	0.43
1:K:231:ILE:HD12	1:K:231:ILE:N	2.32	0.43
1:K:245:SER:O	1:K:247:ASN:N	2.52	0.43
1:K:354:LEU:HD13	1:K:355:GLN:N	2.34	0.43
1:K:481:ASN:O	1:K:482:LEU:C	2.56	0.43
2:L:155:VAL:C	2:L:156:ILE:HD12	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:356:ALA:CB	2:L:391:LEU:HB2	2.49	0.43
1:A:358:HIS:CG	1:A:359:PRO:HD3	2.54	0.43
2:B:128:VAL:O	2:B:129:LEU:C	2.55	0.43
2:B:531:TRP:CG	2:B:532:LYS:N	2.87	0.43
1:C:670:ILE:HD12	1:C:712:ALA:HB1	2.01	0.43
1:C:74:ILE:HG23	1:C:75:ALA:N	2.33	0.43
2:D:300:PRO:HB3	2:D:509:ARG:HH12	1.83	0.43
2:D:54:ARG:HH11	2:D:54:ARG:HG2	1.82	0.43
1:E:102:HIS:CG	1:E:103:VAL:N	2.87	0.43
1:E:661:MET:HG3	1:E:723:VAL:HG13	2.00	0.43
2:F:325:ASP:C	2:F:327:GLY:H	2.21	0.43
1:G:348:LEU:O	1:G:349:GLU:HB3	2.19	0.43
2:J:196:ILE:HD13	2:J:214:ILE:HG23	2.00	0.43
1:K:443:MET:SD	1:K:444:TYR:CE1	3.11	0.43
1:K:64:ASN:H	1:K:137:GLN:HG2	1.83	0.43
1:K:664:CYS:HB2	1:K:724:ILE:HD11	2.00	0.43
2:L:297:ARG:HG2	2:L:297:ARG:HH11	1.84	0.43
1:A:712:ALA:HA	1:A:716:ASN:ND2	2.34	0.43
2:B:109:THR:HG22	2:B:122:PHE:HB2	2.00	0.43
2:B:183:ASN:OD1	2:B:207:SER:OG	2.26	0.43
2:B:501:PHE:HD2	2:B:501:PHE:N	2.13	0.43
1:C:664:CYS:HB2	1:C:724:ILE:HD11	2.01	0.43
1:E:308:LEU:HD12	1:E:308:LEU:C	2.38	0.43
1:E:316:MET:HG2	1:E:345:PHE:CD2	2.54	0.43
2:F:235:THR:O	2:F:235:THR:HG22	2.18	0.43
2:F:75:ASP:OD1	2:F:272:ARG:NH2	2.48	0.43
2:H:117:ARG:HH21	2:H:280:LEU:HG	1.84	0.43
2:H:303:ASP:OD2	2:H:509:ARG:HD2	2.19	0.43
2:H:434:ALA:HB3	2:H:460:VAL:HG12	2.01	0.43
2:H:468:ALA:O	2:H:472:ILE:HG13	2.18	0.43
2:H:476(D):PRO:HA	2:H:479:ILE:HD11	2.00	0.43
1:I:456:ALA:CB	1:I:457:PRO:CD	2.95	0.43
2:J:222:TYR:C	2:J:222:TYR:CD1	2.93	0.43
1:K:693:MET:O	1:K:694:LYS:HB2	2.19	0.43
1:K:85:MET:O	1:K:86:GLY:C	2.58	0.43
1:A:187:ALA:O	1:A:188:ASN:CG	2.58	0.42
1:A:388:ASP:O	1:A:390:LYS:N	2.52	0.42
1:C:452:LEU:O	1:C:466:MET:CE	2.67	0.42
1:C:71:ARG:O	1:C:75:ALA:CB	2.67	0.42
2:D:460:VAL:HG21	2:D:496:ALA:CB	2.47	0.42
1:E:309:ASP:OD2	1:E:343:LYS:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:543:VAL:CG1	2:F:117:ARG:HD2	2.49	0.42
2:F:206:TYR:O	2:F:209:ALA:HB3	2.18	0.42
2:F:293:ASP:OD2	2:F:294:ASP:N	2.52	0.42
2:F:403:GLN:O	2:F:408:VAL:HG22	2.19	0.42
2:F:58:GLN:HA	2:F:61:ARG:HH21	1.84	0.42
1:G:231:ILE:N	1:G:231:ILE:HD12	2.31	0.42
1:G:212:ILE:HD12	1:G:260:ILE:HG22	2.01	0.42
2:H:392:ILE:HG12	2:H:442:MET:HB3	2.01	0.42
2:H:499:ARG:HD3	2:H:499:ARG:HA	1.88	0.42
1:I:266:GLN:HB3	1:I:500:THR:HG22	2.01	0.42
1:K:319:GLN:NE2	1:K:345:PHE:HE1	2.16	0.42
1:K:454:THR:HG21	1:K:466:MET:HA	2.00	0.42
1:K:459:ARG:O	1:K:463:ILE:HG12	2.19	0.42
1:K:78:VAL:CG1	1:K:79:ILE:N	2.82	0.42
2:L:251:THR:HG21	2:L:260:ALA:CB	2.43	0.42
2:L:340:ILE:CG2	2:L:373:LYS:HD3	2.49	0.42
1:A:317:GLY:O	1:A:321:VAL:HG12	2.19	0.42
2:B:376:ARG:NH1	2:J:410:LYS:HZ2	2.16	0.42
1:C:130:ALA:HA	1:C:133:ALA:CB	2.45	0.42
1:C:319:GLN:NE2	1:C:345:PHE:CE1	2.87	0.42
1:E:176:ASP:OD1	1:E:178:ILE:HD13	2.19	0.42
1:E:421:ARG:HD3	1:E:421:ARG:C	2.39	0.42
1:E:553:ARG:NH1	2:F:115:ASN:OD1	2.52	0.42
1:E:68:ILE:HG12	1:E:78:VAL:HG11	2.01	0.42
2:F:355:VAL:HB	2:F:390:THR:HG23	2.01	0.42
1:G:411:LEU:HB2	1:G:682:GLN:HG3	2.00	0.42
1:G:75:ALA:O	1:G:79:ILE:HG13	2.18	0.42
2:H:50:GLY:HA3	2:H:127:THR:O	2.19	0.42
1:I:118:ASN:HD21	1:I:119:GLN:HE21	1.67	0.42
1:K:191:THR:O	1:K:193:PRO:HD3	2.18	0.42
1:K:396:ILE:HG12	1:K:463:ILE:CD1	2.45	0.42
1:K:625:PHE:N	1:K:625:PHE:CD1	2.87	0.42
1:K:649:LEU:HD13	2:L:59:HIS:CD2	2.54	0.42
2:L:382:ASP:HA	2:L:424:VAL:CG1	2.50	0.42
1:A:353:ARG:HH11	1:A:353:ARG:HG3	1.83	0.42
2:B:303:ASP:OD2	2:B:509:ARG:HD2	2.19	0.42
2:B:52:GLN:OE1	2:B:52:GLN:O	2.37	0.42
1:C:118:ASN:O	1:C:119:GLN:HG3	2.19	0.42
1:C:186:GLU:CD	1:C:186:GLU:N	2.72	0.42
1:C:323:LEU:O	1:C:326:ALA:HB3	2.19	0.42
2:D:252:ARG:HE	2:D:252:ARG:HB2	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:ILE:HG22	1:E:137:GLN:HG3	2.01	0.42
2:F:138:SER:O	2:F:139:LYS:C	2.57	0.42
1:G:191:THR:O	1:G:193:PRO:HD3	2.19	0.42
1:G:354:LEU:C	1:G:354:LEU:HD13	2.40	0.42
1:G:68:ILE:HG12	1:G:78:VAL:CG1	2.50	0.42
2:H:460:VAL:CG2	2:H:496:ALA:HB2	2.46	0.42
1:I:464:GLU:OE2	1:I:464:GLU:HA	2.19	0.42
1:I:628:ARG:HG3	1:I:633:ASP:HA	2.01	0.42
1:I:85:MET:O	1:I:86:GLY:C	2.57	0.42
2:B:533:LYS:HD2	2:J:385:GLU:OE2	2.18	0.42
2:J:479:ILE:C	2:J:479:ILE:HD12	2.37	0.42
2:J:84:MET:SD	2:J:85:PHE:CE1	3.13	0.42
1:K:273:GLN:HG2	1:K:369:LEU:HD11	2.01	0.42
1:K:272:ILE:HB	1:K:335:VAL:CG2	2.49	0.42
1:K:518:PRO:HD2	1:K:521:ASP:OD1	2.20	0.42
1:K:617:GLY:O	1:K:625:PHE:CB	2.52	0.42
1:K:66:ILE:HD13	1:K:88:SER:O	2.19	0.42
2:L:416:LEU:HD13	2:L:441:VAL:HG22	2.01	0.42
1:A:107:ASP:O	1:A:108:GLU:HG3	2.19	0.42
1:A:156:LEU:HD22	1:A:161:VAL:HB	2.02	0.42
1:A:292:ILE:HD13	1:A:300:VAL:O	2.19	0.42
1:A:388:ASP:N	1:A:388:ASP:OD2	2.52	0.42
1:A:625:PHE:CD1	1:A:627:ILE:HD11	2.54	0.42
2:B:234:VAL:CG2	3:I:801:BTI:H83	2.50	0.42
1:C:285:LEU:HB3	1:C:365:THR:HG21	2.02	0.42
1:C:690:ILE:HD12	1:C:699:LEU:HD11	2.01	0.42
2:D:66:ALA:HB2	2:D:125:ASP:HA	2.02	0.42
2:D:200:CYS:O	2:D:223:MET:HA	2.20	0.42
2:D:355:VAL:O	2:D:390:THR:HA	2.19	0.42
1:E:325:LYS:O	1:E:328:GLY:N	2.45	0.42
1:G:467:ARG:HD2	1:G:467:ARG:O	2.19	0.42
1:G:71:ARG:HA	1:G:75:ALA:HB2	2.01	0.42
1:I:130:ALA:HA	1:I:133:ALA:CB	2.43	0.42
1:I:419:ARG:HB2	1:I:476:GLU:HB2	2.00	0.42
1:I:629:THR:H	1:I:632:ALA:HB3	1.84	0.42
2:B:410:LYS:NZ	2:J:376:ARG:HH11	2.17	0.42
2:J:447:LEU:HD23	2:J:447:LEU:HA	1.75	0.42
1:I:651:PRO:CG	2:J:62:GLY:HA3	2.50	0.42
1:K:421:ARG:O	1:K:421:ARG:CD	2.67	0.42
2:L:398:LEU:HD12	2:L:399:PRO:HD2	2.00	0.42
1:A:186:GLU:OE2	1:A:187:ALA:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ILE:HB	1:A:386:GLN:CD	2.40	0.42
1:A:411:LEU:HD22	1:A:682:GLN:CB	2.49	0.42
1:A:583:PHE:CD1	1:A:583:PHE:N	2.88	0.42
1:A:596:TRP:CH2	1:A:600:ASP:O	2.72	0.42
2:B:476(C):ASP:O	2:B:478:LYS:N	2.44	0.42
2:B:48:LEU:HD23	2:B:48:LEU:HA	1.61	0.42
1:C:321:VAL:O	1:C:324:ALA:CB	2.61	0.42
1:C:316:MET:HE2	1:C:337:PHE:HD1	1.84	0.42
1:C:532:MET:O	1:C:535:VAL:HB	2.20	0.42
1:C:563:LEU:O	1:C:565:GLY:N	2.52	0.42
1:C:642:ARG:NH1	2:D:71:ASP:OD2	2.53	0.42
2:D:149:MET:CE	2:D:186:ALA:HA	2.50	0.42
2:D:471:ILE:HG21	2:L:166:ILE:HG13	2.02	0.42
1:E:347:PHE:CZ	1:E:349:GLU:HA	2.54	0.42
1:E:65:LYS:HA	1:E:88:SER:O	2.19	0.42
2:F:347:LEU:O	2:F:348:GLU:C	2.58	0.42
1:G:74:ILE:CD1	1:G:143:TYR:CE2	2.99	0.42
1:G:671:VAL:CG2	1:G:691:GLU:HB2	2.49	0.42
1:G:690:ILE:CD1	1:G:699:LEU:HD11	2.49	0.42
2:H:182:ARG:HH11	2:H:182:ARG:HG3	1.84	0.42
2:H:436:GLY:O	2:H:439:TYR:HB3	2.18	0.42
1:I:214:TYR:HB2	1:I:215:PRO:HA	2.00	0.42
1:I:218:ILE:CD1	1:I:260:ILE:HG12	2.49	0.42
1:I:654:LEU:HA	1:I:654:LEU:HD23	1.89	0.42
1:K:455:TRP:CG	1:K:456:ALA:N	2.85	0.42
2:L:315:ASP:C	2:L:315:ASP:OD1	2.58	0.42
1:A:140:HIS:ND1	1:A:141:PRO:CD	2.82	0.42
1:A:157:GLU:C	1:A:159:GLU:N	2.72	0.42
1:C:325:LYS:O	1:C:327:VAL:N	2.52	0.42
1:C:347:PHE:CZ	1:C:349:GLU:HA	2.55	0.42
2:D:351:THR:HG22	2:D:386:ILE:HG23	2.02	0.42
1:E:283:ILE:HD12	1:E:389:VAL:CG2	2.50	0.42
1:E:627:ILE:N	1:E:627:ILE:HD12	2.34	0.42
1:E:695:MET:SD	2:F:313:PRO:HG3	2.59	0.42
1:G:530:ALA:HB2	1:G:561:VAL:HG21	2.01	0.42
2:H:118:VAL:CG1	2:H:119:VAL:N	2.83	0.42
2:H:48:LEU:HD23	2:H:48:LEU:HA	1.69	0.42
1:I:188:ASN:O	1:I:188:ASN:OD1	2.38	0.42
1:I:380:GLU:HG2	1:I:381:PRO:HD2	2.01	0.42
1:I:414:ILE:HD11	1:I:442:SER:C	2.40	0.42
1:I:422:PRO:HA	1:I:422(A):PRO:HD3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:195:TYR:CD2	1:K:208:ILE:HD13	2.54	0.42
1:K:515:VAL:HB	1:K:631:GLY:C	2.39	0.42
2:L:499:ARG:CG	2:L:499:ARG:NH1	2.80	0.42
2:L:536:ASN:O	2:L:537:ILE:C	2.58	0.42
1:A:274:VAL:HA	1:A:284:TYR:HA	2.02	0.42
1:A:99:GLN:HG3	1:A:100:ALA:H	1.84	0.42
2:B:109:THR:HG22	2:B:122:PHE:HB3	2.01	0.42
2:B:69:ARG:HH12	2:B:160:ASP:CB	2.33	0.42
2:B:180:PHE:O	2:B:183:ASN:HB2	2.19	0.42
1:C:463:ILE:HD12	1:C:494:PHE:CE1	2.54	0.42
2:D:301:SER:HB2	2:D:322:LYS:NZ	2.35	0.42
1:E:276:CYS:HB2	1:E:277:ASP:H	1.41	0.42
1:E:718:LEU:N	1:E:718:LEU:CD2	2.69	0.42
2:F:315:ASP:OD1	2:F:317:LYS:HB2	2.19	0.42
2:F:442:MET:O	2:F:443:SER:C	2.58	0.42
1:G:384:ILE:HB	1:G:388:ASP:HB2	2.01	0.42
1:G:301:GLU:OE2	1:G:397:GLU:OE1	2.37	0.42
1:G:583:PHE:N	1:G:583:PHE:CD1	2.87	0.42
1:I:187:ALA:O	1:I:188:ASN:CG	2.58	0.42
1:I:287:GLU:HG3	1:I:308:LEU:HD21	2.02	0.42
1:I:304:PRO:HD2	1:I:394:TRP:CE2	2.55	0.42
1:I:421:ARG:CD	1:I:421:ARG:O	2.68	0.42
1:I:650:MET:HA	1:I:651:PRO:HD3	1.90	0.42
2:J:193:ILE:CD1	2:J:274:LEU:HD23	2.50	0.42
1:K:146:LEU:HD23	1:K:152:PHE:CD2	2.54	0.42
1:K:390:LYS:C	1:K:390:LYS:HD3	2.39	0.42
2:L:196:ILE:HG22	2:L:221:SER:HB2	2.02	0.42
2:L:355:VAL:O	2:L:390:THR:HA	2.20	0.42
1:A:85:MET:O	1:A:86:GLY:C	2.58	0.42
2:B:285:LYS:HB3	2:B:286:PRO:HD2	2.01	0.42
2:D:141:ILE:O	2:D:145:MET:HG3	2.19	0.42
2:D:299:GLU:HG3	2:D:322:LYS:HB3	2.02	0.42
1:E:279:HIS:CD2	1:E:380:GLU:O	2.71	0.42
1:E:480:HIS:HD2	1:E:482:LEU:HB2	1.82	0.42
1:E:666:MET:HG2	1:E:666:MET:O	2.18	0.42
1:E:85:MET:HB2	1:E:87:ILE:HD11	2.02	0.42
1:G:371:GLU:O	1:G:372:GLN:C	2.58	0.42
1:G:675:VAL:HG12	1:G:707:VAL:HG21	2.01	0.42
1:G:92:ILE:HD12	1:G:112:ILE:CD1	2.50	0.42
1:I:457:PRO:HG2	1:I:458:THR:N	2.27	0.42
1:I:504:ILE:CG2	1:I:505:ALA:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:541:THR:O	1:I:541:THR:HG22	2.20	0.42
1:I:625:PHE:HB2	1:I:627:ILE:HD12	2.02	0.42
1:I:67:LEU:HG	1:I:68:ILE:N	2.32	0.42
2:J:536:ASN:O	2:J:537:ILE:C	2.58	0.42
1:K:157:GLU:C	1:K:159:GLU:N	2.72	0.42
1:K:292:ILE:N	1:K:292:ILE:HD12	2.14	0.42
1:K:446:ASP:HA	1:K:447:PRO:HD2	1.87	0.42
1:K:93:TYR:HA	1:K:121:TYR:OH	2.19	0.42
2:D:539:LEU:OXT	2:L:372:ARG:NH2	2.52	0.42
2:L:524:ASN:O	2:L:525:LYS:C	2.58	0.42
1:A:371:GLU:O	1:A:374:ILE:HG12	2.20	0.42
1:A:302:GLU:OE2	1:A:394:TRP:CZ3	2.73	0.42
1:A:661:MET:HG3	1:A:723:VAL:HG13	2.02	0.42
2:B:319:LEU:CD2	2:B:391:LEU:HD13	2.50	0.42
1:C:140:HIS:ND1	1:C:141:PRO:HD2	2.35	0.42
1:C:266:GLN:HG2	1:C:341:GLY:HA2	2.02	0.42
1:C:354:LEU:HD11	1:C:358:HIS:ND1	2.35	0.42
1:C:583:PHE:CZ	1:C:590:MET:CE	3.02	0.42
2:D:537:ILE:HA	2:D:538:PRO:HD3	1.91	0.42
1:E:358:HIS:CE1	1:E:359:PRO:HD3	2.55	0.42
1:E:515:VAL:HB	1:E:631:GLY:HA3	2.02	0.42
1:E:71:ARG:O	1:E:75:ALA:CB	2.68	0.42
2:F:126:PHE:O	2:F:130:GLY:HA2	2.20	0.42
1:G:186:GLU:N	1:G:186:GLU:CD	2.74	0.42
1:G:279:HIS:NE2	1:G:379:GLY:HA2	2.35	0.42
1:G:455:TRP:C	1:G:455:TRP:CD1	2.87	0.42
1:G:64:ASN:H	1:G:137:GLN:HG2	1.85	0.42
1:G:670:ILE:HD11	1:G:718:LEU:HD11	2.02	0.42
2:H:325:ASP:O	2:H:327:GLY:N	2.53	0.42
2:H:476(C):ASP:N	2:H:476(D):PRO:HD3	2.35	0.42
1:I:235:ASP:N	1:I:235:ASP:OD1	2.47	0.42
1:I:347:PHE:CD1	1:I:347:PHE:O	2.72	0.42
1:I:283:ILE:HD12	1:I:389:VAL:CG2	2.49	0.42
1:I:78:VAL:HA	1:I:370:VAL:HG11	2.02	0.42
2:J:354:VAL:HA	2:J:389:LEU:O	2.20	0.42
1:K:140:HIS:ND1	1:K:141:PRO:CD	2.82	0.42
1:K:665:PRO:HG2	1:K:666:MET:HE2	1.96	0.42
1:A:111:HIS:O	1:A:112:ILE:HG23	2.19	0.42
2:B:50:GLY:HA3	2:B:127:THR:O	2.19	0.42
2:B:367:ASP:O	2:B:368:ILE:C	2.58	0.42
1:C:524:ARG:HA	1:C:590:MET:SD	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:ALA:HB3	1:C:141:PRO:HA	2.01	0.42
2:D:141:ILE:O	2:D:144:ILE:HG13	2.20	0.42
1:E:325:LYS:O	1:E:327:VAL:N	2.53	0.42
1:E:400:LEU:HD23	1:E:400:LEU:HA	1.74	0.42
1:E:85:MET:O	1:E:86:GLY:C	2.58	0.42
1:G:304:PRO:HD2	1:G:394:TRP:CD2	2.55	0.42
1:G:422(A):PRO:O	1:G:422(B):ALA:HB2	2.19	0.42
1:G:504:ILE:CG2	1:G:505:ALA:N	2.82	0.42
1:G:518:PRO:O	1:G:519:GLU:C	2.58	0.42
2:H:222:TYR:HB2	2:H:245:GLY:O	2.20	0.42
1:I:682:GLN:HA	1:I:682:GLN:OE1	2.20	0.42
2:J:205:VAL:O	2:J:208:PRO:HD2	2.20	0.42
2:J:42:ARG:CG	2:J:42:ARG:HH11	2.18	0.42
1:K:140:HIS:CE1	1:K:142:GLY:N	2.84	0.42
1:K:583:PHE:CD1	1:K:583:PHE:N	2.88	0.42
1:K:724:ILE:HG22	1:K:725:MET:HG3	2.01	0.42
1:A:146:LEU:HD23	1:A:152:PHE:CG	2.55	0.41
1:A:165:GLY:CA	1:A:331:SER:OG	2.68	0.41
1:A:279:HIS:HD2	1:A:380:GLU:O	2.03	0.41
2:B:205:VAL:HG23	2:B:206:TYR:N	2.34	0.41
2:B:319:LEU:HD23	2:B:391:LEU:HD13	2.02	0.41
2:B:454:ALA:O	2:B:505:VAL:HA	2.20	0.41
2:D:425:PRO:HB3	2:D:522:LEU:HD13	2.01	0.41
1:E:482:LEU:N	1:E:483:PRO:HD2	2.35	0.41
1:E:515:VAL:HB	1:E:631:GLY:CA	2.50	0.41
1:E:68:ILE:CG2	1:E:70:ASN:H	2.33	0.41
1:E:75:ALA:O	1:E:79:ILE:HG13	2.20	0.41
1:G:78:VAL:HG23	1:G:370:VAL:HG11	2.01	0.41
2:H:202:GLY:O	2:H:205:VAL:HG22	2.20	0.41
2:H:522:LEU:HA	2:J:151:ASN:ND2	2.34	0.41
1:I:140:HIS:CE1	1:I:142:GLY:N	2.88	0.41
1:I:358:HIS:CG	1:I:359:PRO:HD3	2.55	0.41
1:I:518:PRO:HD2	1:I:521:ASP:OD1	2.20	0.41
1:I:663:LEU:O	1:I:665:PRO:HD3	2.20	0.41
1:I:77:ARG:NH1	1:I:370:VAL:CG2	2.80	0.41
1:I:68:ILE:CG1	1:I:78:VAL:HG11	2.50	0.41
1:K:186:GLU:OE2	1:K:187:ALA:N	2.53	0.41
1:K:394:TRP:O	1:K:455:TRP:HA	2.20	0.41
1:K:456:ALA:CB	1:K:457:PRO:HD2	2.34	0.41
1:K:482:LEU:N	1:K:483:PRO:HD2	2.35	0.41
2:L:138:SER:OG	2:L:139:LYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:183:ASN:HD22	2:L:183:ASN:HA	1.67	0.41
2:L:239:VAL:CG2	2:L:243:GLU:HB2	2.50	0.41
1:A:136:ALA:O	1:A:137:GLN:CB	2.69	0.41
1:A:304:PRO:HD2	1:A:394:TRP:CE2	2.56	0.41
1:C:570:VAL:HG22	1:C:581:VAL:HG12	2.02	0.41
1:C:65:LYS:HE2	1:C:134:THR:O	2.19	0.41
1:C:711:ASN:O	1:C:712:ALA:HB2	2.20	0.41
1:E:312:THR:HG21	1:E:343:LYS:HD3	2.01	0.41
1:E:710:ILE:HG22	1:E:711:ASN:N	2.35	0.41
2:F:180:PHE:O	2:F:184:ILE:HG13	2.19	0.41
2:F:462:VAL:HG22	2:H:169:GLY:CA	2.50	0.41
1:G:128:MET:O	1:G:131:ILE:N	2.53	0.41
1:G:167:PRO:C	1:G:169:GLY:N	2.73	0.41
1:G:394:TRP:CE3	1:G:459:ARG:HG3	2.55	0.41
1:G:485:LEU:O	1:G:486:SER:C	2.57	0.41
2:H:83:ASP:HB3	2:H:86:VAL:HG23	2.00	0.41
1:I:150:SER:O	1:I:151:LYS:C	2.58	0.41
1:I:546:ARG:HG2	1:I:546:ARG:H	1.55	0.41
2:J:149:MET:HE1	2:J:189:VAL:HG11	2.00	0.41
1:K:534:ARG:NH1	1:K:534:ARG:HG3	2.35	0.41
1:A:271:GLU:O	1:A:287:GLU:HB2	2.21	0.41
1:A:619:ILE:O	1:A:620:SER:C	2.59	0.41
1:C:140:HIS:ND1	1:C:141:PRO:N	2.68	0.41
1:C:314:ARG:O	1:C:318:GLU:HG3	2.19	0.41
1:C:407:ARG:HH11	1:C:407:ARG:HG2	1.85	0.41
1:C:428(L):ALA:HB3	1:C:455:TRP:CD1	2.49	0.41
1:C:446:ASP:OD1	1:C:447:PRO:HD2	2.19	0.41
1:C:724:ILE:HG22	1:C:725:MET:HG3	2.02	0.41
2:D:138:SER:O	2:D:141:ILE:N	2.53	0.41
2:D:48:LEU:HA	2:D:48:LEU:HD23	1.63	0.41
1:E:268:ARG:NH2	1:E:497:GLY:O	2.45	0.41
1:E:517:LEU:HA	1:E:518:PRO:HD3	1.62	0.41
1:E:490:ASP:OD2	1:E:630:ARG:NH1	2.53	0.41
1:G:195:TYR:CD2	1:G:208:ILE:HD13	2.56	0.41
1:G:234:ASN:O	1:G:237:GLU:HB3	2.19	0.41
1:G:293:GLN:O	1:G:504:ILE:CG2	2.64	0.41
1:G:334:THR:HG21	1:G:355:GLN:CG	2.50	0.41
1:G:695:MET:HG3	2:H:313:PRO:HG3	2.01	0.41
2:H:442:MET:O	2:H:443:SER:C	2.58	0.41
1:I:156:LEU:HD22	1:I:161:VAL:HB	2.02	0.41
1:I:195:TYR:O	1:I:259:PHE:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:270:ILE:HG21	1:I:308:LEU:HD21	2.02	0.41
1:I:325:LYS:O	1:I:327:VAL:N	2.53	0.41
1:I:364:ILE:HG22	1:I:392:THR:O	2.20	0.41
2:J:248:THR:O	2:J:252:ARG:HG2	2.20	0.41
1:K:156:LEU:HD22	1:K:161:VAL:HB	2.03	0.41
1:K:436:TYR:CD1	1:K:436:TYR:C	2.93	0.41
1:K:83:ARG:HB3	1:K:83:ARG:CZ	2.50	0.41
2:L:309:ASN:HD21	2:L:311:ASN:HB2	1.86	0.41
2:D:210:MET:HE1	2:L:416:LEU:HG	2.02	0.41
2:L:432:ARG:O	2:L:459:GLU:N	2.54	0.41
2:L:447:LEU:HD23	2:L:447:LEU:HA	1.78	0.41
1:A:118:ASN:HD21	1:A:119:GLN:HE21	1.68	0.41
1:A:376:VAL:CG2	1:A:377:ALA:N	2.83	0.41
1:A:398:ASN:HB3	1:A:485:LEU:HD13	2.02	0.41
1:A:634:LEU:N	1:A:634:LEU:CD2	2.82	0.41
2:B:248:THR:O	2:B:252:ARG:HG2	2.20	0.41
2:B:401:THR:CG2	2:B:402:SER:N	2.83	0.41
1:C:174:MET:HA	1:C:180:SER:OG	2.20	0.41
1:C:275:LEU:HD23	1:C:276:CYS:H	1.85	0.41
1:C:338:ILE:N	1:C:338:ILE:CD1	2.82	0.41
1:C:358:HIS:CG	1:C:359:PRO:HD3	2.54	0.41
1:C:363:LEU:O	1:C:455:TRP:CE3	2.73	0.41
2:D:206:TYR:O	2:D:209:ALA:HB3	2.20	0.41
1:E:302:GLU:OE2	1:E:394:TRP:CZ3	2.73	0.41
1:E:456:ALA:CB	1:E:457:PRO:HD2	2.35	0.41
1:E:670:ILE:CD1	1:E:718:LEU:HD21	2.50	0.41
1:G:541:THR:O	1:G:541:THR:HG22	2.21	0.41
1:I:90:VAL:HG12	1:I:91:ALA:N	2.35	0.41
2:J:145:MET:HE3	2:J:183:ASN:HD21	1.85	0.41
2:J:229:ASP:N	2:J:229:ASP:OD1	2.52	0.41
1:K:191:THR:O	1:K:193:PRO:CD	2.69	0.41
1:K:295:ARG:O	1:K:296:ASN:HB2	2.20	0.41
2:L:88:HIS:CD2	2:L:88:HIS:C	2.94	0.41
1:A:114:PRO:HB2	1:A:115:PRO:HD2	2.02	0.41
1:A:428(L):ALA:HB3	1:A:455:TRP:CD1	2.44	0.41
2:B:356:ALA:HA	2:B:391:LEU:O	2.19	0.41
2:B:476(C):ASP:N	2:B:476(D):PRO:HD3	2.35	0.41
2:B:509:ARG:HH11	2:B:509:ARG:HB3	1.86	0.41
1:C:357:GLU:CD	1:C:357:GLU:H	2.23	0.41
1:C:396:ILE:HD12	1:C:396:ILE:N	2.36	0.41
2:D:134:SER:H	2:D:137:HIS:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:ASP:O	1:E:108:GLU:CG	2.68	0.41
1:E:563:LEU:CD2	1:E:636:VAL:HG22	2.51	0.41
2:F:417:TYR:N	2:H:210:MET:CE	2.83	0.41
2:F:67:ARG:HG2	2:F:67:ARG:HH11	1.84	0.41
1:G:563:LEU:CD2	1:G:636:VAL:HG22	2.50	0.41
2:H:375:ALA:HA	2:H:415:LEU:HD12	2.03	0.41
2:H:479:ILE:C	2:H:479:ILE:HD12	2.39	0.41
2:J:293:ASP:OD1	2:J:325:ASP:O	2.38	0.41
1:K:274:VAL:HA	1:K:284:TYR:HA	2.02	0.41
1:K:358:HIS:O	1:K:361:THR:N	2.54	0.41
1:K:285:LEU:HB3	1:K:365:THR:HG21	2.02	0.41
1:K:543:VAL:HG12	1:K:544:SER:N	2.35	0.41
2:L:117:ARG:NH2	2:L:280:LEU:HG	2.33	0.41
1:A:140:HIS:CE1	1:A:142:GLY:N	2.85	0.41
1:A:168:LYS:O	1:A:172:GLU:OE1	2.38	0.41
1:A:394:TRP:O	1:A:455:TRP:HA	2.21	0.41
1:C:114:PRO:CB	1:C:115:PRO:HD2	2.50	0.41
1:C:396:ILE:HD13	1:C:462:ALA:CB	2.51	0.41
2:D:90:CYS:HB2	2:D:168:GLU:OE2	2.21	0.41
2:D:182:ARG:NH1	2:D:182:ARG:HG3	2.35	0.41
2:D:244:LEU:HA	2:D:244:LEU:HD12	1.85	0.41
2:D:347:LEU:HD23	2:D:347:LEU:HA	1.84	0.41
2:D:295:PRO:O	2:D:513:LYS:HA	2.20	0.41
1:E:83:ARG:NH1	1:E:83:ARG:CG	2.83	0.41
2:F:182:ARG:NH1	2:F:182:ARG:HG3	2.36	0.41
2:F:347:LEU:HA	2:F:347:LEU:HD23	1.86	0.41
1:G:316:MET:HB3	1:G:337:PHE:CE1	2.55	0.41
2:H:199:PRO:HB3	2:H:222:TYR:CZ	2.56	0.41
1:I:177:LYS:HB3	1:I:181:LYS:HZ1	1.82	0.41
1:I:186:GLU:CD	1:I:186:GLU:N	2.73	0.41
1:I:347:PHE:CZ	1:I:349:GLU:HA	2.56	0.41
1:I:116:PRO:HG3	1:I:444:TYR:CE2	2.55	0.41
1:I:482:LEU:N	1:I:483:PRO:HD2	2.35	0.41
1:I:675:VAL:HG11	1:I:707:VAL:HG21	2.02	0.41
2:J:121:VAL:HG22	2:J:122:PHE:H	1.84	0.41
2:J:312:THR:HG22	2:J:313:PRO:O	2.21	0.41
1:K:114:PRO:HB2	1:K:115:PRO:HD2	2.03	0.41
1:K:164:VAL:HA	1:K:377:ALA:CB	2.51	0.41
1:K:342:GLN:O	1:K:343:LYS:HB2	2.21	0.41
1:K:720:VAL:HG22	1:K:721:ASP:H	1.85	0.41
2:L:192:GLN:O	2:L:211:THR:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:HIS:O	1:A:112:ILE:CG2	2.69	0.41
1:A:112:ILE:O	1:A:120:SER:HA	2.19	0.41
1:A:422:PRO:HA	1:A:422(A):PRO:HD3	1.86	0.41
1:A:610:ALA:HA	1:A:611:PRO:HD3	1.78	0.41
1:A:553:ARG:NH1	2:B:115:ASN:OD1	2.53	0.41
2:B:252:ARG:NH2	2:B:335:GLU:HG3	2.35	0.41
2:B:300:PRO:HB3	2:B:509:ARG:NH1	2.35	0.41
2:B:382:ASP:HA	2:B:424:VAL:CG1	2.51	0.41
2:B:495:VAL:HG13	2:B:496:ALA:N	2.36	0.41
2:B:64:LEU:HA	2:B:64:LEU:HD23	1.83	0.41
2:B:69:ARG:HA	2:B:268:LEU:CD1	2.51	0.41
1:C:139:VAL:O	1:C:164:VAL:HG12	2.20	0.41
1:C:165:GLY:HA2	1:C:331:SER:OG	2.21	0.41
1:C:348:LEU:O	1:C:349:GLU:HB3	2.21	0.41
1:C:421:ARG:O	1:C:421:ARG:HD3	2.21	0.41
1:C:446:ASP:HA	1:C:447:PRO:HD2	1.91	0.41
1:C:458:THR:O	1:C:461:ALA:HB3	2.20	0.41
1:C:537:GLU:HA	1:C:540:ARG:HG3	2.01	0.41
1:C:596:TRP:CH2	1:C:600:ASP:O	2.73	0.41
2:D:300:PRO:O	2:D:303:ASP:HB2	2.20	0.41
1:E:140:HIS:ND1	1:E:141:PRO:CD	2.84	0.41
1:E:273:GLN:HG2	1:E:369:LEU:HD11	2.03	0.41
1:E:455:TRP:CD1	1:E:455:TRP:C	2.91	0.41
1:E:658:THR:HG22	1:E:659:SER:O	2.20	0.41
1:E:71:ARG:NH1	1:E:445:TYR:CG	2.89	0.41
2:F:393:ASP:CG	2:F:432:ARG:HB3	2.41	0.41
1:I:140:HIS:ND1	1:I:141:PRO:CD	2.84	0.41
1:I:422:PRO:HG3	1:I:473:PHE:CZ	2.56	0.41
1:I:74:ILE:HG23	1:I:75:ALA:N	2.35	0.41
2:J:479:ILE:HD12	2:J:480:ALA:H	1.79	0.41
2:B:372:ARG:NH2	2:J:539:LEU:OXT	2.52	0.41
1:K:602:LEU:HD12	1:K:614:LEU:O	2.19	0.41
1:K:627:ILE:HD13	1:K:636:VAL:CG2	2.51	0.41
1:K:77:ARG:HH11	1:K:77:ARG:HG3	1.85	0.41
1:A:266:GLN:H	1:A:266:GLN:HG2	1.49	0.41
1:C:517:LEU:HD11	1:C:632:ALA:HB2	2.02	0.41
2:D:222:TYR:C	2:D:222:TYR:CD1	2.94	0.41
1:E:99:GLN:O	1:E:100:ALA:C	2.59	0.41
1:E:316:MET:HB3	1:E:337:PHE:CE1	2.56	0.41
1:E:64:ASN:H	1:E:137:GLN:HG2	1.85	0.41
2:F:135:GLU:OE1	2:J:89:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:149:MET:CE	2:F:189:VAL:CG1	2.99	0.41
1:G:118:ASN:HD21	1:G:119:GLN:HE21	1.69	0.41
1:G:207:LYS:O	1:G:207:LYS:HD3	2.20	0.41
1:G:390:LYS:HD3	1:G:391:LEU:H	1.77	0.41
2:H:167:GLN:NE2	2:H:167:GLN:N	2.37	0.41
2:H:252:ARG:NH2	2:H:335:GLU:HG3	2.36	0.41
2:H:361:VAL:O	2:H:363:ALA:N	2.53	0.41
1:I:121:TYR:HE2	1:I:445:TYR:OH	2.04	0.41
1:I:124:ILE:CG2	1:I:128:MET:CE	2.99	0.41
1:I:325:LYS:H	1:I:325:LYS:HG3	1.74	0.41
1:I:455:TRP:CD2	1:I:456:ALA:N	2.89	0.41
1:I:70:ASN:OD1	1:I:74:ILE:HG21	2.20	0.41
1:K:339:VAL:HG22	1:K:345:PHE:HB3	2.02	0.41
1:K:416:ARG:HG3	1:K:439:GLY:O	2.21	0.41
1:K:467:ARG:HD2	1:K:467:ARG:O	2.21	0.41
1:K:583:PHE:CZ	1:K:590:MET:HE3	2.56	0.41
1:K:663:LEU:O	1:K:665:PRO:HD3	2.21	0.41
2:L:145:MET:CE	2:L:183:ASN:ND2	2.84	0.41
2:L:303:ASP:OD2	2:L:509:ARG:HD2	2.20	0.41
1:A:191:THR:O	1:A:193:PRO:HD3	2.21	0.41
1:A:316:MET:HE3	1:A:337:PHE:HD1	1.85	0.41
1:A:543:VAL:HG12	1:A:544:SER:N	2.36	0.41
2:B:347:LEU:O	2:B:348:GLU:C	2.58	0.41
2:B:456:PRO:HD3	2:B:506:ILE:O	2.21	0.41
1:C:90:VAL:HG12	1:C:91:ALA:N	2.36	0.41
2:D:205:VAL:HB	2:L:409:ILE:HD13	2.03	0.41
2:D:205:VAL:O	2:D:208:PRO:HD2	2.21	0.41
1:E:396:ILE:CG1	1:E:463:ILE:HD13	2.46	0.41
2:F:173:LEU:HD13	2:H:439:TYR:CD2	2.56	0.41
2:F:392:ILE:HG22	2:F:393:ASP:N	2.35	0.41
1:G:274:VAL:HA	1:G:284:TYR:HA	2.03	0.41
1:G:270:ILE:HG21	1:G:308:LEU:HD21	2.02	0.41
1:G:713:SER:H	1:G:716:ASN:CG	2.24	0.41
2:H:244:LEU:HA	2:H:244:LEU:HD12	1.83	0.41
2:H:476(A):LEU:C	2:H:476(C):ASP:H	2.22	0.41
1:I:157:GLU:C	1:I:159:GLU:N	2.73	0.41
1:I:327:VAL:HG22	1:I:327:VAL:O	2.20	0.41
1:I:467:ARG:HH21	1:I:630:ARG:HE	1.68	0.41
1:I:718:LEU:H	1:I:718:LEU:HD23	1.79	0.41
2:J:347:LEU:HD23	2:J:347:LEU:HA	1.87	0.41
2:B:205:VAL:HB	2:J:409:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:476(C):ASP:C	2:J:477:GLU:H	2.24	0.41
2:J:48:LEU:HA	2:J:48:LEU:HD23	1.71	0.41
2:J:98:GLN:N	2:J:98:GLN:OE1	2.50	0.41
1:K:293:GLN:HA	1:K:299:VAL:HG23	2.02	0.41
1:K:340:ASP:OD1	1:K:344:ASN:HB2	2.21	0.41
1:K:517:LEU:HB3	1:K:521:ASP:HB3	2.03	0.41
1:K:552:GLU:N	1:K:552:GLU:CD	2.73	0.41
1:K:626:ARG:C	1:K:627:ILE:HD12	2.40	0.41
1:K:660:LYS:O	1:K:727:PHE:N	2.51	0.41
2:L:182:ARG:HG3	2:L:182:ARG:HH11	1.86	0.41
2:D:417:TYR:N	2:L:210:MET:HE1	2.36	0.41
2:L:294:ASP:HA	2:L:295:PRO:HD2	1.94	0.41
1:A:384:ILE:HB	1:A:388:ASP:HB2	2.02	0.41
1:A:83:ARG:CG	1:A:83:ARG:NH1	2.80	0.41
2:B:254:SER:O	2:B:255:SER:CB	2.68	0.41
2:B:366:LEU:HA	2:B:366:LEU:HD23	1.87	0.41
1:C:276:CYS:HB2	1:C:277:ASP:H	1.42	0.41
1:C:331:SER:HB3	1:C:332:ALA:H	1.61	0.41
1:C:390:LYS:HD3	1:C:390:LYS:C	2.40	0.41
1:C:461:ALA:O	1:C:464:GLU:HB3	2.21	0.41
2:D:156:ILE:CD1	2:D:156:ILE:N	2.82	0.41
2:D:207:SER:O	2:D:208:PRO:C	2.59	0.41
2:D:250:HIS:HA	2:D:254:SER:OG	2.20	0.41
1:E:270:ILE:HG21	1:E:308:LEU:HD21	2.03	0.41
1:E:485:LEU:O	1:E:486:SER:C	2.59	0.41
1:E:504:ILE:CG2	1:E:505:ALA:H	2.32	0.41
1:E:68:ILE:CG1	1:E:78:VAL:HG11	2.50	0.41
2:F:118:VAL:HG12	2:F:119:VAL:N	2.36	0.41
2:F:273:ARG:HD2	2:F:330:TYR:HD1	1.86	0.41
1:G:340:ASP:OD1	1:G:344:ASN:HB2	2.21	0.41
1:G:658:THR:HG22	1:G:659:SER:O	2.20	0.41
1:G:69:ALA:HB3	1:G:141:PRO:HA	2.02	0.41
1:G:73:GLU:OE1	1:G:451:LYS:NZ	2.51	0.41
1:G:99:GLN:HG3	1:G:100:ALA:H	1.86	0.41
2:F:471:ILE:HG21	2:H:166:ILE:HG13	2.03	0.41
2:H:366:LEU:HA	2:H:366:LEU:HD23	1.79	0.41
1:I:283:ILE:HG22	1:I:386:GLN:CG	2.51	0.41
1:I:334:THR:HG21	1:I:355:GLN:CG	2.51	0.41
1:I:690:ILE:HD12	1:I:699:LEU:HD11	2.02	0.41
2:J:145:MET:CE	2:J:183:ASN:ND2	2.83	0.41
1:K:162:ILE:O	1:K:164:VAL:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:436:TYR:C	1:K:436:TYR:HD1	2.24	0.41
2:L:314:TYR:CE1	2:L:359:PRO:HG2	2.56	0.41
1:A:598:PRO:HD2	2:B:292:PHE:CD1	2.55	0.41
1:A:626:ARG:NE	1:A:628:ARG:HD2	2.36	0.41
1:A:661:MET:CE	1:A:726:GLU:HB3	2.50	0.41
2:B:122:PHE:CD1	2:B:141:ILE:HG23	2.56	0.41
2:B:476(D):PRO:O	2:B:480:ALA:HB2	2.20	0.41
1:C:517:LEU:HB3	1:C:521:ASP:HB3	2.02	0.41
1:C:634:LEU:CD2	1:C:634:LEU:N	2.82	0.41
2:D:120:TYR:CD1	2:D:148:ALA:HA	2.56	0.41
1:E:283:ILE:HG22	1:E:386:GLN:CG	2.49	0.41
1:G:272:ILE:HB	1:G:335:VAL:HG23	2.03	0.41
1:G:353:ARG:HG3	1:G:353:ARG:HH11	1.86	0.41
1:G:378:ALA:O	1:G:379:GLY:O	2.38	0.41
1:G:713:SER:O	1:G:714:ALA:C	2.59	0.41
1:G:543:VAL:CG1	2:H:117:ARG:HD2	2.51	0.41
2:H:346:ARG:HH11	2:H:346:ARG:CG	2.32	0.41
1:I:292:ILE:CD1	1:I:292:ILE:H	2.01	0.41
1:I:99:GLN:HB2	1:I:436:TYR:OH	2.21	0.41
1:I:512:PHE:CZ	1:I:515:VAL:HG23	2.56	0.41
1:I:592:VAL:HG13	1:I:607:VAL:HG22	2.03	0.41
1:I:77:ARG:O	1:I:77:ARG:NH1	2.50	0.41
1:K:288:ARG:HD3	1:K:361:THR:OG1	2.21	0.41
1:K:309:ASP:OD2	1:K:343:LYS:HE2	2.20	0.41
1:K:272:ILE:HB	1:K:335:VAL:HG23	2.03	0.41
2:D:410:LYS:HZ2	2:L:376:ARG:NH1	2.18	0.41
1:A:68:ILE:CG2	1:A:70:ASN:H	2.34	0.40
2:B:205:VAL:O	2:B:208:PRO:HD2	2.21	0.40
2:B:374:ALA:HB3	2:B:415:LEU:HD13	2.03	0.40
1:C:118:ASN:C	1:C:119:GLN:HG3	2.41	0.40
1:C:140:HIS:CE1	1:C:142:GLY:N	2.85	0.40
1:C:164:VAL:HG23	1:C:377:ALA:CB	2.51	0.40
1:C:301:GLU:HG2	1:C:357:GLU:HB3	2.03	0.40
1:C:415:GLY:O	1:C:440:GLU:HG3	2.21	0.40
1:C:525:VAL:O	1:C:526:ALA:C	2.57	0.40
1:C:572:ILE:HG22	1:C:573:ALA:N	2.36	0.40
2:D:336:PHE:O	2:D:337:ALA:C	2.58	0.40
2:D:366:LEU:HD23	2:D:366:LEU:HA	1.97	0.40
2:D:499:ARG:HA	2:D:499:ARG:HD3	1.92	0.40
1:E:157:GLU:C	1:E:159:GLU:N	2.74	0.40
1:E:292:ILE:HD12	1:E:292:ILE:N	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:468:ILE:O	1:E:471:ASP:HB2	2.20	0.40
1:E:583:PHE:CD1	1:E:583:PHE:N	2.88	0.40
1:E:78:VAL:HG23	1:E:370:VAL:HG11	2.02	0.40
2:F:298:ILE:HG23	2:F:509:ARG:HB2	2.03	0.40
2:F:514:ARG:HD2	2:F:514:ARG:HA	1.73	0.40
1:G:118:ASN:C	1:G:119:GLN:HG3	2.41	0.40
1:G:71:ARG:O	1:G:75:ALA:HB2	2.21	0.40
1:G:74:ILE:CG2	1:G:75:ALA:N	2.84	0.40
1:I:497:GLY:O	1:I:499:MET:HG2	2.21	0.40
1:I:517:LEU:HD21	1:I:632:ALA:HB2	2.02	0.40
1:I:630:ARG:O	1:I:632:ALA:N	2.54	0.40
2:J:368:ILE:HG23	2:J:411:HIS:CG	2.56	0.40
1:K:321:VAL:O	1:K:324:ALA:CB	2.61	0.40
1:A:92:ILE:CD1	1:A:112:ILE:HD13	2.49	0.40
1:A:433:THR:CG2	1:A:434:GLY:N	2.83	0.40
1:A:67:LEU:HG	1:A:68:ILE:N	2.35	0.40
2:B:273:ARG:HD2	2:B:330:TYR:CD1	2.57	0.40
1:C:139:VAL:HG11	1:C:156:LEU:CD2	2.51	0.40
2:D:537:ILE:HG13	2:D:538:PRO:HD2	2.03	0.40
1:E:124:ILE:HG22	1:E:128:MET:CE	2.51	0.40
1:E:186:GLU:N	1:E:186:GLU:CD	2.75	0.40
1:E:384:ILE:HB	1:E:388:ASP:HB2	2.04	0.40
2:F:390:THR:HG21	2:F:419:TYR:OH	2.21	0.40
1:G:114:PRO:HB2	1:G:115:PRO:HD2	2.03	0.40
1:G:455:TRP:CD2	1:G:456:ALA:N	2.89	0.40
1:G:405:PRO:CG	1:G:481:ASN:HA	2.51	0.40
1:G:68:ILE:HG12	1:G:78:VAL:HG11	2.03	0.40
2:H:120:TYR:CD1	2:H:148:ALA:HA	2.56	0.40
1:G:597:THR:OG1	2:H:292:PHE:CG	2.74	0.40
2:H:315:ASP:C	2:H:315:ASP:OD1	2.60	0.40
1:I:137:GLN:O	1:I:138:ALA:CB	2.69	0.40
1:I:273:GLN:HG2	1:I:369:LEU:HD11	2.04	0.40
1:I:710:ILE:HG12	1:I:725:MET:HG2	2.02	0.40
2:J:325:ASP:HA	2:J:512:ARG:NH1	2.25	0.40
1:K:139:VAL:HG11	1:K:156:LEU:HD21	2.02	0.40
2:L:195:MET:SD	2:L:271:VAL:HG21	2.61	0.40
1:A:444:TYR:HD1	1:A:444:TYR:H	1.69	0.40
1:A:491:HIS:HA	1:A:492:PRO:HD2	1.92	0.40
2:B:69:ARG:HH12	2:B:160:ASP:CG	2.25	0.40
2:B:294:ASP:HA	2:B:295:PRO:HD2	1.92	0.40
1:C:192:VAL:O	1:C:193:PRO:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:LEU:O	1:C:373:MET:HB2	2.21	0.40
1:C:392:THR:O	1:C:455:TRP:CZ3	2.71	0.40
1:C:666:MET:O	1:C:668:GLY:N	2.54	0.40
1:C:71:ARG:CG	1:C:72:GLY:N	2.85	0.40
2:D:121:VAL:CG2	2:D:122:PHE:N	2.83	0.40
1:E:329:TYR:HE2	1:E:352:THR:HA	1.86	0.40
1:E:78:VAL:CG1	1:E:79:ILE:H	2.33	0.40
1:E:92:ILE:CG1	1:E:112:ILE:HD13	2.50	0.40
1:G:152:PHE:CE1	1:G:156:LEU:HD11	2.56	0.40
1:G:168:LYS:O	1:G:172:GLU:OE1	2.39	0.40
1:G:319:GLN:NE2	1:G:345:PHE:CZ	2.89	0.40
1:G:461:ALA:O	1:G:464:GLU:HB3	2.22	0.40
1:G:610:ALA:HA	1:G:611:PRO:HD3	1.89	0.40
1:G:654:LEU:O	1:G:655:PRO:O	2.38	0.40
1:I:71:ARG:HD3	1:I:445:TYR:CD2	2.56	0.40
2:J:139:LYS:HE2	2:J:139:LYS:HB3	1.85	0.40
1:K:494:PHE:HA	1:K:499:MET:HE1	2.03	0.40
2:D:225:VAL:N	2:L:404:GLU:OE2	2.52	0.40
2:L:413:ALA:O	2:L:416:LEU:HB3	2.21	0.40
2:B:114:ILE:O	2:B:115:ASN:HB2	2.21	0.40
2:B:196:ILE:HG22	2:B:221:SER:HB2	2.02	0.40
1:C:416:ARG:HG3	1:C:439:GLY:O	2.21	0.40
1:C:422:PRO:HA	1:C:422(A):PRO:HD3	1.85	0.40
1:C:435:VAL:HG22	1:C:436:TYR:H	1.87	0.40
1:C:625:PHE:CD1	1:C:627:ILE:HD11	2.56	0.40
2:D:132:SER:HA	2:D:163:GLY:O	2.20	0.40
2:D:298:ILE:CG2	2:D:509:ARG:HB2	2.51	0.40
1:E:456:ALA:CB	1:E:457:PRO:CD	2.94	0.40
1:E:583:PHE:HZ	1:E:590:MET:HE3	1.86	0.40
2:F:78:SER:O	2:F:112:GLY:HA2	2.20	0.40
2:F:476(C):ASP:N	2:F:476(D):PRO:HD3	2.35	0.40
1:G:400:LEU:HD23	1:G:400:LEU:HA	1.68	0.40
1:G:463:ILE:HD12	1:G:494:PHE:CE1	2.56	0.40
1:G:710:ILE:HG22	1:G:711:ASN:N	2.37	0.40
1:G:650:MET:SD	2:H:263:ASN:HB2	2.62	0.40
2:H:329:PHE:CZ	2:H:343:GLY:HA3	2.55	0.40
2:H:476(C):ASP:CG	2:H:478:LYS:HG2	2.42	0.40
1:I:257:ARG:HB2	1:I:257:ARG:HE	1.58	0.40
1:I:68:ILE:CG2	1:I:70:ASN:H	2.34	0.40
1:K:319:GLN:NE2	1:K:345:PHE:CZ	2.89	0.40
1:K:384:ILE:HB	1:K:388:ASP:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:713:SER:O	1:K:714:ALA:O	2.38	0.40
1:K:720:VAL:O	1:K:722:ASP:N	2.54	0.40
2:L:445:LYS:HE3	2:L:503:ASP:OD1	2.22	0.40
2:J:499:ARG:NH2	2:L:89:ARG:HH11	2.04	0.40
1:A:319:GLN:NE2	1:A:345:PHE:CE1	2.89	0.40
1:A:334:THR:HG21	1:A:355:GLN:CG	2.51	0.40
1:A:396:ILE:HG12	1:A:463:ILE:CD1	2.45	0.40
1:A:490:ASP:OD2	1:A:630:ARG:NH1	2.55	0.40
1:A:720:VAL:HG22	1:A:721:ASP:H	1.87	0.40
1:C:534:ARG:NH1	1:C:534:ARG:HG3	2.37	0.40
1:C:677:VAL:CG1	1:C:708:ALA:O	2.69	0.40
2:D:75:ASP:OD2	2:D:115:ASN:N	2.55	0.40
1:E:110:VAL:HG21	1:E:130:ALA:CB	2.46	0.40
1:G:107:ASP:C	1:G:108:GLU:HG3	2.41	0.40
1:G:185:GLN:O	1:G:188:ASN:N	2.49	0.40
1:G:186:GLU:OE2	1:G:187:ALA:N	2.54	0.40
1:G:312:THR:O	1:G:315:ALA:HB3	2.22	0.40
1:G:619:ILE:HD11	1:G:626:ARG:HB2	2.03	0.40
2:H:474:ARG:O	2:H:476:ASP:N	2.51	0.40
1:I:107:ASP:O	1:I:108:GLU:HG3	2.21	0.40
1:K:231:ILE:HG22	1:K:232:ALA:N	2.37	0.40
1:K:77:ARG:NH1	1:K:77:ARG:O	2.53	0.40
2:L:394:VAL:HG23	2:L:395:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	585/681 (86%)	451 (77%)	99 (17%)	35 (6%)	1 12
1	C	585/681 (86%)	456 (78%)	94 (16%)	35 (6%)	1 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	585/681 (86%)	449 (77%)	98 (17%)	38 (6%)	1	10
1	G	638/681 (94%)	502 (79%)	100 (16%)	36 (6%)	2	14
1	I	638/681 (94%)	504 (79%)	94 (15%)	40 (6%)	1	10
1	K	638/681 (94%)	505 (79%)	92 (14%)	41 (6%)	1	10
2	B	504/531 (95%)	444 (88%)	49 (10%)	11 (2%)	6	35
2	D	504/531 (95%)	445 (88%)	47 (9%)	12 (2%)	6	34
2	F	504/531 (95%)	451 (90%)	43 (8%)	10 (2%)	7	38
2	H	504/531 (95%)	451 (90%)	43 (8%)	10 (2%)	7	38
2	J	504/531 (95%)	452 (90%)	43 (8%)	9 (2%)	8	41
2	L	504/531 (95%)	455 (90%)	39 (8%)	10 (2%)	7	38
All	All	6693/7272 (92%)	5565 (83%)	841 (13%)	287 (4%)	2	20

All (287) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	ALA
1	A	137	GLN
1	A	138	ALA
1	A	277	ASP
1	A	331	SER
1	A	389	VAL
2	B	218	LYS
2	B	325	ASP
2	B	476(D)	PRO
1	C	64	ASN
1	C	100	ALA
1	C	137	GLN
1	C	138	ALA
1	C	265	THR
1	C	331	SER
1	C	389	VAL
2	D	218	LYS
2	D	325	ASP
2	D	476(D)	PRO
1	E	64	ASN
1	E	100	ALA
1	E	137	GLN
1	E	138	ALA

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Mol	Chain	Res	Type
1	E	193	PRO
1	E	265	THR
1	E	277	ASP
1	E	331	SER
1	E	389	VAL
1	E	564	GLN
2	F	218	LYS
2	F	325	ASP
2	F	476(D)	PRO
1	G	100	ALA
1	G	137	GLN
1	G	138	ALA
1	G	331	SER
1	G	389	VAL
1	G	409	PHE
1	G	456	ALA
2	H	218	LYS
2	H	325	ASP
2	H	476(D)	PRO
1	I	100	ALA
1	I	137	GLN
1	I	138	ALA
1	I	331	SER
1	I	389	VAL
2	J	218	LYS
2	J	325	ASP
2	J	476(D)	PRO
1	K	100	ALA
1	K	137	GLN
1	K	138	ALA
1	K	277	ASP
1	K	331	SER
1	K	389	VAL
1	K	456	ALA
1	K	564	GLN
2	L	218	LYS
2	L	325	ASP
2	L	476(D)	PRO
1	A	64	ASN
1	A	65	LYS
1	A	72	GLY
1	A	163	PHE

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Mol	Chain	Res	Type
1	A	168	LYS
1	A	265	THR
1	A	326	ALA
1	A	379	GLY
1	A	393	GLY
1	A	596	TRP
2	B	476	ASP
1	C	65	LYS
1	C	162	ILE
1	C	163	PHE
1	C	185	GLN
1	C	277	ASP
1	C	324	ALA
1	C	326	ALA
1	C	379	GLY
1	C	393	GLY
1	C	457	PRO
1	C	564	GLN
1	C	721	ASP
2	D	476	ASP
1	E	65	LYS
1	E	72	GLY
1	E	88	SER
1	E	163	PHE
1	E	168	LYS
1	E	324	ALA
1	E	326	ALA
1	E	379	GLY
1	E	393	GLY
1	E	457	PRO
2	F	476	ASP
1	G	64	ASN
1	G	65	LYS
1	G	163	PHE
1	G	168	LYS
1	G	230	ARG
1	G	265	THR
1	G	277	ASP
1	G	324	ALA
1	G	326	ALA
1	G	379	GLY
1	G	393	GLY

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Mol	Chain	Res	Type
1	G	457	PRO
1	G	564	GLN
1	G	655	PRO
1	G	721	ASP
2	H	476	ASP
1	I	64	ASN
1	I	65	LYS
1	I	162	ILE
1	I	163	PHE
1	I	168	LYS
1	I	185	GLN
1	I	230	ARG
1	I	277	ASP
1	I	324	ALA
1	I	326	ALA
1	I	379	GLY
1	I	393	GLY
1	I	409	PHE
1	I	456	ALA
1	I	457	PRO
1	I	564	GLN
1	I	721	ASP
2	J	476	ASP
1	K	64	ASN
1	K	65	LYS
1	K	163	PHE
1	K	168	LYS
1	K	185	GLN
1	K	230	ARG
1	K	324	ALA
1	K	326	ALA
1	K	379	GLY
1	K	409	PHE
1	K	457	PRO
1	K	596	TRP
1	K	721	ASP
2	L	476	ASP
1	A	112	ILE
1	A	185	GLN
1	A	324	ALA
1	A	457	PRO
1	A	721	ASP

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Mol	Chain	Res	Type
2	B	78	SER
2	B	362	LEU
2	B	393	ASP
2	B	442	MET
1	C	72	GLY
1	C	88	SER
1	C	168	LYS
1	C	630	ARG
1	C	655	PRO
1	E	112	ILE
1	E	162	ILE
1	E	185	GLN
1	E	422(A)	PRO
1	E	519	GLU
1	E	596	TRP
1	E	633	ASP
1	E	655	PRO
1	E	721	ASP
2	F	338	LYS
2	F	393	ASP
1	G	72	GLY
1	G	185	GLN
1	G	630	ARG
2	H	338	LYS
1	I	88	SER
1	I	265	THR
1	I	422(A)	PRO
1	I	655	PRO
2	J	338	LYS
2	J	362	LEU
2	J	393	ASP
1	K	88	SER
1	K	136	ALA
1	K	393	GLY
1	K	422(A)	PRO
1	K	655	PRO
1	K	714	ALA
2	L	393	ASP
2	L	466	LYS
1	A	136	ALA
1	A	193	PRO
1	A	633	ASP

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Mol	Chain	Res	Type
1	C	86	GLY
1	C	94	SER
1	C	112	ILE
1	C	135	GLY
1	C	422(A)	PRO
1	C	456	ALA
1	C	596	TRP
1	C	633	ASP
2	D	78	SER
2	D	393	ASP
1	E	456	ALA
2	F	76	GLU
1	G	112	ILE
1	G	135	GLY
1	G	422(A)	PRO
2	H	393	ASP
2	H	442	MET
2	H	466	LYS
1	I	72	GLY
1	I	97	ASP
1	I	112	ILE
1	I	596	TRP
1	I	609	GLY
1	K	112	ILE
1	K	162	ILE
1	K	200	GLU
1	K	246	LYS
1	K	265	THR
1	K	586	ASP
1	K	630	ARG
1	K	692	ALA
2	L	326	GLU
2	L	368	ILE
1	A	135	GLY
1	A	162	ILE
1	A	266	GLN
1	A	422(A)	PRO
1	A	456	ALA
1	A	630	ARG
1	A	655	PRO
1	A	714	ALA
2	B	77	GLY

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Mol	Chain	Res	Type
2	B	338	LYS
1	C	609	GLY
2	D	76	GLU
1	E	135	GLY
1	E	136	ALA
1	E	190	SER
1	G	88	SER
1	G	136	ALA
1	G	162	ILE
1	G	422(B)	ALA
1	G	586	ASP
2	H	303	ASP
1	I	86	GLY
1	I	633	ASP
1	I	692	ALA
2	J	466	LYS
1	K	71	ARG
1	K	72	GLY
1	K	135	GLY
1	A	123	VAL
1	C	71	ARG
2	F	368	ILE
1	G	94	SER
1	G	97	ASP
1	I	94	SER
1	I	135	GLY
1	I	422(B)	ALA
1	K	123	VAL
1	K	609	GLY
1	A	86	GLY
2	D	50	GLY
2	D	368	ILE
1	E	86	GLY
1	E	123	VAL
1	G	86	GLY
2	D	77	GLY
1	E	447	PRO
2	J	368	ILE
1	K	86	GLY
1	E	609	GLY
2	H	368	ILE
1	I	123	VAL

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Mol	Chain	Res	Type
1	I	127	VAL
1	I	667	PRO
1	A	609	GLY
1	C	123	VAL
2	D	395	PRO
2	D	475	GLY
2	F	154	PRO
2	F	395	PRO
2	L	77	GLY
2	L	537	ILE
2	B	50	GLY
1	E	280	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	474/540 (88%)	417 (88%)	57 (12%)	5 22
1	C	474/540 (88%)	420 (89%)	54 (11%)	5 24
1	E	474/540 (88%)	418 (88%)	56 (12%)	5 23
1	G	520/540 (96%)	461 (89%)	59 (11%)	6 25
1	I	520/540 (96%)	461 (89%)	59 (11%)	6 25
1	K	520/540 (96%)	460 (88%)	60 (12%)	5 24
2	B	415/437 (95%)	392 (94%)	23 (6%)	21 57
2	D	415/437 (95%)	392 (94%)	23 (6%)	21 57
2	F	415/437 (95%)	394 (95%)	21 (5%)	24 60
2	H	415/437 (95%)	390 (94%)	25 (6%)	19 54
2	J	415/437 (95%)	385 (93%)	30 (7%)	14 47
2	L	415/437 (95%)	392 (94%)	23 (6%)	21 57
All	All	5472/5862 (93%)	4982 (91%)	490 (9%)	9 34

All (490) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	PHE
1	A	66	ILE
1	A	67	LEU
1	A	70	ASN
1	A	89	THR
1	A	97	ASP
1	A	99	GLN
1	A	163	PHE
1	A	168	LYS
1	A	182	LYS
1	A	186	GLU
1	A	265	THR
1	A	266	GLN
1	A	275	LEU
1	A	285	LEU
1	A	292	ILE
1	A	344	ASN
1	A	347	PHE
1	A	360	VAL
1	A	375	ARG
1	A	388	ASP
1	A	400	LEU
1	A	416	ARG
1	A	419	ARG
1	A	421	ARG
1	A	436	TYR
1	A	443	MET
1	A	444	TYR
1	A	449	ILE
1	A	455	TRP
1	A	467	ARG
1	A	488	VAL
1	A	517	LEU
1	A	539	ARG
1	A	548	ASP
1	A	553	ARG
1	A	554	ARG
1	A	570	VAL
1	A	571	THR
1	A	577	ASP
1	A	582	SER
1	A	593	THR
1	A	625	PHE

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Mol	Chain	Res	Type
1	A	630	ARG
1	A	634	LEU
1	A	643	GLN
1	A	652	GLU
1	A	653	LYS
1	A	661	MET
1	A	666	MET
1	A	674	ASP
1	A	677	VAL
1	A	683	GLU
1	A	700	ARG
1	A	702	GLU
1	A	711	ASN
1	A	718	LEU
2	B	42	ARG
2	B	43	ARG
2	B	52	GLN
2	B	91	THR
2	B	138	SER
2	B	147	MET
2	B	167	GLN
2	B	224	PHE
2	B	238	GLN
2	B	273	ARG
2	B	288	VAL
2	B	301	SER
2	B	325	ASP
2	B	401	THR
2	B	408	VAL
2	B	448	ARG
2	B	462	VAL
2	B	476	ASP
2	B	476(D)	PRO
2	B	499	ARG
2	B	504	GLU
2	B	509	ARG
2	B	514	ARG
1	C	63	PHE
1	C	66	ILE
1	C	70	ASN
1	C	73	GLU
1	C	89	THR

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Mol	Chain	Res	Type
1	C	97	ASP
1	C	99	GLN
1	C	163	PHE
1	C	168	LYS
1	C	182	LYS
1	C	186	GLU
1	C	275	LEU
1	C	276	CYS
1	C	285	LEU
1	C	292	ILE
1	C	344	ASN
1	C	347	PHE
1	C	360	VAL
1	C	375	ARG
1	C	400	LEU
1	C	416	ARG
1	C	419	ARG
1	C	421	ARG
1	C	436	TYR
1	C	444	TYR
1	C	455	TRP
1	C	467	ARG
1	C	473	PHE
1	C	517	LEU
1	C	520	THR
1	C	539	ARG
1	C	548	ASP
1	C	553	ARG
1	C	554	ARG
1	C	570	VAL
1	C	571	THR
1	C	577	ASP
1	C	582	SER
1	C	593	THR
1	C	625	PHE
1	C	630	ARG
1	C	634	LEU
1	C	643	GLN
1	C	652	GLU
1	C	653	LYS
1	C	661	MET
1	C	666	MET

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Mol	Chain	Res	Type
1	C	674	ASP
1	C	677	VAL
1	C	683	GLU
1	C	700	ARG
1	C	702	GLU
1	C	711	ASN
1	C	718	LEU
2	D	42	ARG
2	D	43	ARG
2	D	52	GLN
2	D	138	SER
2	D	147	MET
2	D	167	GLN
2	D	194	SER
2	D	224	PHE
2	D	273	ARG
2	D	288	VAL
2	D	301	SER
2	D	325	ASP
2	D	401	THR
2	D	408	VAL
2	D	448	ARG
2	D	462	VAL
2	D	476	ASP
2	D	476(D)	PRO
2	D	488	GLU
2	D	493	PRO
2	D	504	GLU
2	D	509	ARG
2	D	514	ARG
1	E	63	PHE
1	E	66	ILE
1	E	70	ASN
1	E	89	THR
1	E	97	ASP
1	E	99	GLN
1	E	163	PHE
1	E	168	LYS
1	E	182	LYS
1	E	186	GLU
1	E	276	CYS
1	E	285	LEU

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Mol	Chain	Res	Type
1	E	292	ILE
1	E	344	ASN
1	E	347	PHE
1	E	360	VAL
1	E	375	ARG
1	E	400	LEU
1	E	416	ARG
1	E	419	ARG
1	E	421	ARG
1	E	435	VAL
1	E	436	TYR
1	E	449	ILE
1	E	455	TRP
1	E	467	ARG
1	E	473	PHE
1	E	488	VAL
1	E	517	LEU
1	E	520	THR
1	E	539	ARG
1	E	548	ASP
1	E	553	ARG
1	E	554	ARG
1	E	570	VAL
1	E	571	THR
1	E	577	ASP
1	E	582	SER
1	E	593	THR
1	E	598	PRO
1	E	625	PHE
1	E	629	THR
1	E	630	ARG
1	E	634	LEU
1	E	643	GLN
1	E	652	GLU
1	E	653	LYS
1	E	661	MET
1	E	666	MET
1	E	674	ASP
1	E	677	VAL
1	E	683	GLU
1	E	700	ARG
1	E	702	GLU

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Mol	Chain	Res	Type
1	E	711	ASN
1	E	718	LEU
2	F	42	ARG
2	F	43	ARG
2	F	52	GLN
2	F	138	SER
2	F	147	MET
2	F	167	GLN
2	F	194	SER
2	F	238	GLN
2	F	273	ARG
2	F	288	VAL
2	F	301	SER
2	F	338	LYS
2	F	401	THR
2	F	408	VAL
2	F	448	ARG
2	F	462	VAL
2	F	476	ASP
2	F	476(D)	PRO
2	F	499	ARG
2	F	509	ARG
2	F	514	ARG
1	G	63	PHE
1	G	66	ILE
1	G	70	ASN
1	G	73	GLU
1	G	89	THR
1	G	97	ASP
1	G	99	GLN
1	G	145	PHE
1	G	163	PHE
1	G	168	LYS
1	G	182	LYS
1	G	186	GLU
1	G	207	LYS
1	G	211	GLN
1	G	230	ARG
1	G	243	GLN
1	G	247	ASN
1	G	256	ASP
1	G	275	LEU

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Mol	Chain	Res	Type
1	G	285	LEU
1	G	292	ILE
1	G	312	THR
1	G	347	PHE
1	G	360	VAL
1	G	375	ARG
1	G	400	LEU
1	G	416	ARG
1	G	419	ARG
1	G	421	ARG
1	G	436	TYR
1	G	455	TRP
1	G	467	ARG
1	G	473	PHE
1	G	488	VAL
1	G	517	LEU
1	G	539	ARG
1	G	542	ARG
1	G	548	ASP
1	G	553	ARG
1	G	554	ARG
1	G	570	VAL
1	G	571	THR
1	G	582	SER
1	G	593	THR
1	G	625	PHE
1	G	629	THR
1	G	630	ARG
1	G	634	LEU
1	G	643	GLN
1	G	652	GLU
1	G	653	LYS
1	G	661	MET
1	G	666	MET
1	G	674	ASP
1	G	683	GLU
1	G	700	ARG
1	G	702	GLU
1	G	711	ASN
1	G	718	LEU
2	H	42	ARG
2	H	43	ARG

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Mol	Chain	Res	Type
2	H	52	GLN
2	H	71	ASP
2	H	119	VAL
2	H	138	SER
2	H	147	MET
2	H	167	GLN
2	H	194	SER
2	H	238	GLN
2	H	273	ARG
2	H	288	VAL
2	H	301	SER
2	H	325	ASP
2	H	390	THR
2	H	401	THR
2	H	408	VAL
2	H	462	VAL
2	H	476	ASP
2	H	476(D)	PRO
2	H	499	ARG
2	H	504	GLU
2	H	509	ARG
2	H	514	ARG
2	H	536	ASN
1	I	63	PHE
1	I	66	ILE
1	I	67	LEU
1	I	70	ASN
1	I	73	GLU
1	I	89	THR
1	I	97	ASP
1	I	99	GLN
1	I	163	PHE
1	I	168	LYS
1	I	182	LYS
1	I	186	GLU
1	I	207	LYS
1	I	230	ARG
1	I	243	GLN
1	I	247	ASN
1	I	256	ASP
1	I	257	ARG
1	I	285	LEU

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Mol	Chain	Res	Type
1	I	292	ILE
1	I	312	THR
1	I	347	PHE
1	I	360	VAL
1	I	375	ARG
1	I	400	LEU
1	I	416	ARG
1	I	419	ARG
1	I	421	ARG
1	I	436	TYR
1	I	444	TYR
1	I	455	TRP
1	I	467	ARG
1	I	488	VAL
1	I	517	LEU
1	I	539	ARG
1	I	548	ASP
1	I	553	ARG
1	I	554	ARG
1	I	570	VAL
1	I	571	THR
1	I	577	ASP
1	I	582	SER
1	I	593	THR
1	I	625	PHE
1	I	629	THR
1	I	630	ARG
1	I	634	LEU
1	I	643	GLN
1	I	652	GLU
1	I	653	LYS
1	I	661	MET
1	I	666	MET
1	I	674	ASP
1	I	677	VAL
1	I	683	GLU
1	I	700	ARG
1	I	702	GLU
1	I	711	ASN
1	I	718	LEU
2	J	42	ARG
2	J	43	ARG

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Mol	Chain	Res	Type
2	J	52	GLN
2	J	71	ASP
2	J	91	THR
2	J	98	GLN
2	J	138	SER
2	J	147	MET
2	J	167	GLN
2	J	194	SER
2	J	273	ARG
2	J	288	VAL
2	J	301	SER
2	J	325	ASP
2	J	354	VAL
2	J	365	CYS
2	J	390	THR
2	J	401	THR
2	J	408	VAL
2	J	448	ARG
2	J	460	VAL
2	J	462	VAL
2	J	476	ASP
2	J	476(D)	PRO
2	J	488	GLU
2	J	493	PRO
2	J	499	ARG
2	J	504	GLU
2	J	509	ARG
2	J	514	ARG
1	K	63	PHE
1	K	66	ILE
1	K	70	ASN
1	K	73	GLU
1	K	89	THR
1	K	97	ASP
1	K	99	GLN
1	K	163	PHE
1	K	168	LYS
1	K	182	LYS
1	K	186	GLU
1	K	211	GLN
1	K	230	ARG
1	K	243	GLN

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Mol	Chain	Res	Type
1	K	247	ASN
1	K	257	ARG
1	K	276	CYS
1	K	285	LEU
1	K	292	ILE
1	K	312	THR
1	K	347	PHE
1	K	360	VAL
1	K	375	ARG
1	K	400	LEU
1	K	416	ARG
1	K	419	ARG
1	K	421	ARG
1	K	436	TYR
1	K	449	ILE
1	K	455	TRP
1	K	467	ARG
1	K	473	PHE
1	K	488	VAL
1	K	517	LEU
1	K	520	THR
1	K	539	ARG
1	K	548	ASP
1	K	553	ARG
1	K	554	ARG
1	K	570	VAL
1	K	571	THR
1	K	577	ASP
1	K	582	SER
1	K	593	THR
1	K	625	PHE
1	K	629	THR
1	K	630	ARG
1	K	634	LEU
1	K	643	GLN
1	K	652	GLU
1	K	653	LYS
1	K	661	MET
1	K	666	MET
1	K	674	ASP
1	K	677	VAL
1	K	683	GLU

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Mol	Chain	Res	Type
1	K	700	ARG
1	K	702	GLU
1	K	711	ASN
1	K	718	LEU
2	L	42	ARG
2	L	43	ARG
2	L	71	ASP
2	L	147	MET
2	L	167	GLN
2	L	194	SER
2	L	238	GLN
2	L	273	ARG
2	L	288	VAL
2	L	301	SER
2	L	365	CYS
2	L	390	THR
2	L	401	THR
2	L	408	VAL
2	L	448	ARG
2	L	462	VAL
2	L	476	ASP
2	L	476(D)	PRO
2	L	488	GLU
2	L	499	ARG
2	L	504	GLU
2	L	509	ARG
2	L	514	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	102	HIS
1	A	119	GLN
1	A	188	ASN
1	A	480	HIS
1	A	550	ASN
1	A	551	HIS
1	A	564	GLN
2	B	52	GLN
2	B	58	GLN
2	B	88	HIS

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Mol	Chain	Res	Type
2	B	100	GLN
2	B	124	GLN
2	B	137	HIS
2	B	151	ASN
2	B	167	GLN
2	B	183	ASN
2	B	309	ASN
2	B	482	HIS
2	B	492	ASN
2	B	536	ASN
1	C	70	ASN
1	C	102	HIS
1	C	119	GLN
1	C	137	GLN
1	C	188	ASN
1	C	351	ASN
1	C	480	HIS
1	C	551	HIS
1	C	564	GLN
1	C	716	ASN
2	D	52	GLN
2	D	58	GLN
2	D	88	HIS
2	D	100	GLN
2	D	151	ASN
2	D	167	GLN
2	D	183	ASN
2	D	309	ASN
2	D	482	HIS
2	D	492	ASN
2	D	536	ASN
1	E	70	ASN
1	E	102	HIS
1	E	119	GLN
1	E	137	GLN
1	E	188	ASN
1	E	351	ASN
1	E	386	GLN
1	E	480	HIS
1	E	551	HIS
1	E	564	GLN
2	F	52	GLN

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Mol	Chain	Res	Type
2	F	58	GLN
2	F	88	HIS
2	F	100	GLN
2	F	151	ASN
2	F	167	GLN
2	F	238	GLN
2	F	309	ASN
2	F	482	HIS
2	F	492	ASN
2	F	536	ASN
1	G	70	ASN
1	G	102	HIS
1	G	119	GLN
1	G	188	ASN
1	G	351	ASN
1	G	386	GLN
1	G	480	HIS
1	G	551	HIS
1	G	564	GLN
2	H	52	GLN
2	H	58	GLN
2	H	88	HIS
2	H	100	GLN
2	H	151	ASN
2	H	167	GLN
2	H	183	ASN
2	H	238	GLN
2	H	309	ASN
2	H	446	HIS
2	H	482	HIS
2	H	492	ASN
2	H	536	ASN
1	I	70	ASN
1	I	102	HIS
1	I	119	GLN
1	I	188	ASN
1	I	386	GLN
1	I	480	HIS
1	I	551	HIS
1	I	564	GLN
1	I	716	ASN
2	J	58	GLN

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Mol	Chain	Res	Type
2	J	88	HIS
2	J	100	GLN
2	J	151	ASN
2	J	167	GLN
2	J	183	ASN
2	J	309	ASN
2	J	482	HIS
2	J	492	ASN
2	J	528	GLN
2	J	536	ASN
1	K	70	ASN
1	K	102	HIS
1	K	119	GLN
1	K	137	GLN
1	K	188	ASN
1	K	342	GLN
1	K	386	GLN
1	K	480	HIS
1	K	551	HIS
1	K	564	GLN
2	L	58	GLN
2	L	88	HIS
2	L	100	GLN
2	L	151	ASN
2	L	167	GLN
2	L	238	GLN
2	L	309	ASN
2	L	482	HIS
2	L	536	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

6 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	BTI	G	801	1	16,16,16	1.85	1 (6%)	21,21,21	2.68	8 (38%)
3	BTI	A	801	1	16,16,16	1.70	1 (6%)	21,21,21	2.41	7 (33%)
3	BTI	C	801	1	16,16,16	1.70	1 (6%)	21,21,21	2.48	7 (33%)
3	BTI	I	801	1	16,16,16	1.75	1 (6%)	21,21,21	2.44	7 (33%)
3	BTI	K	801	1	16,16,16	1.74	1 (6%)	21,21,21	2.43	7 (33%)
3	BTI	E	801	1	16,16,16	1.74	1 (6%)	21,21,21	2.62	8 (38%)

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	BTI	G	801	1	-	4/5/27/27	0/2/2/2
3	BTI	A	801	1	-	2/5/27/27	0/2/2/2
3	BTI	C	801	1	-	0/5/27/27	0/2/2/2
3	BTI	I	801	1	-	2/5/27/27	0/2/2/2
3	BTI	K	801	1	-	3/5/27/27	0/2/2/2
3	BTI	E	801	1	-	1/5/27/27	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	801	BTI	O3-C3	6.71	1.37	1.23
3	I	801	BTI	O3-C3	6.44	1.36	1.23
3	E	801	BTI	O3-C3	6.44	1.36	1.23
3	K	801	BTI	O3-C3	6.38	1.36	1.23
3	C	801	BTI	O3-C3	6.29	1.36	1.23
3	A	801	BTI	O3-C3	6.25	1.36	1.23

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	801	BTI	C4-N2-C3	-5.51	107.49	112.62
3	E	801	BTI	C4-N2-C3	-5.37	107.62	112.62
3	C	801	BTI	C4-N2-C3	-5.32	107.66	112.62
3	I	801	BTI	C4-N2-C3	-5.03	107.93	112.62
3	K	801	BTI	C4-N2-C3	-5.02	107.94	112.62
3	A	801	BTI	C6-C5-C4	4.82	112.84	108.66
3	E	801	BTI	C4-C2-S1	-4.80	100.63	105.20
3	C	801	BTI	N2-C3-N3	4.66	113.13	108.76
3	G	801	BTI	N2-C3-N3	4.61	113.08	108.76
3	E	801	BTI	N2-C3-N3	4.49	112.98	108.76
3	G	801	BTI	C6-C5-N3	-4.48	107.34	113.03
3	G	801	BTI	C5-N3-C3	-4.46	106.64	112.46
3	K	801	BTI	N2-C3-N3	4.32	112.82	108.76
3	I	801	BTI	N2-C3-N3	4.22	112.72	108.76
3	A	801	BTI	C4-N2-C3	-4.19	108.72	112.62
3	E	801	BTI	C6-C5-N3	-4.18	107.72	113.03
3	I	801	BTI	C6-S1-C2	4.13	98.37	89.89
3	A	801	BTI	N2-C3-N3	4.09	112.60	108.76
3	G	801	BTI	C6-S1-C2	3.99	98.09	89.89
3	K	801	BTI	C6-C5-C4	3.97	112.11	108.66
3	C	801	BTI	C6-C5-N3	-3.91	108.06	113.03
3	A	801	BTI	C6-S1-C2	3.91	97.91	89.89
3	C	801	BTI	C6-C5-C4	3.90	112.04	108.66
3	K	801	BTI	C6-C5-N3	-3.90	108.08	113.03
3	I	801	BTI	C6-C5-N3	-3.87	108.11	113.03
3	K	801	BTI	C6-S1-C2	3.75	97.60	89.89
3	A	801	BTI	C6-C5-N3	-3.73	108.29	113.03
3	E	801	BTI	C6-C5-C4	3.72	111.89	108.66
3	I	801	BTI	C5-N3-C3	-3.70	107.64	112.46
3	I	801	BTI	C6-C5-C4	3.68	111.85	108.66
3	G	801	BTI	C6-C5-C4	3.56	111.75	108.66
3	C	801	BTI	C6-S1-C2	3.47	97.02	89.89
3	K	801	BTI	C5-N3-C3	-3.38	108.06	112.46
3	C	801	BTI	C5-N3-C3	-3.18	108.31	112.46
3	A	801	BTI	C5-N3-C3	-3.13	108.39	112.46
3	E	801	BTI	C6-S1-C2	3.07	96.19	89.89
3	E	801	BTI	C5-N3-C3	-3.01	108.53	112.46
3	C	801	BTI	C4-C2-S1	-2.71	102.62	105.20
3	G	801	BTI	C4-C2-S1	-2.68	102.66	105.20
3	K	801	BTI	C4-C2-S1	-2.34	102.97	105.20
3	G	801	BTI	C4-C5-N3	-2.29	100.00	102.43
3	A	801	BTI	C2-C4-C5	2.29	111.59	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	801	BTI	C4-C5-N3	-2.26	100.04	102.43
3	E	801	BTI	C2-C4-N2	-2.15	111.20	113.13

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	801	BTI	S1-C2-C7-C8
3	G	801	BTI	C4-C2-C7-C8
3	A	801	BTI	C11-C10-C9-C8
3	K	801	BTI	C11-C10-C9-C8
3	K	801	BTI	C2-C7-C8-C9
3	A	801	BTI	C2-C7-C8-C9
3	I	801	BTI	C2-C7-C8-C9
3	G	801	BTI	C7-C8-C9-C10
3	I	801	BTI	C11-C10-C9-C8
3	K	801	BTI	C7-C8-C9-C10
3	E	801	BTI	C7-C8-C9-C10
3	G	801	BTI	C2-C7-C8-C9

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	BTI	1	0
3	I	801	BTI	2	0
3	E	801	BTI	1	0

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^{th} 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^2)	Q<0.9
1	A	591/681 (86%)	-0.31	5 (0%)	86 78	17, 65, 113, 128	0
1	C	591/681 (86%)	-0.26	4 (0%)	87 81	17, 65, 113, 128	0
1	E	591/681 (86%)	-0.22	11 (1%)	66 53	17, 66, 113, 128	0
1	G	646/681 (94%)	-0.28	4 (0%)	89 83	15, 67, 112, 128	0
1	I	646/681 (94%)	-0.22	9 (1%)	75 63	16, 67, 112, 127	0
1	K	646/681 (94%)	-0.24	11 (1%)	70 57	16, 68, 112, 128	0
2	B	506/531 (95%)	-0.87	4 (0%)	86 78	10, 26, 57, 101	0
2	D	506/531 (95%)	-0.86	2 (0%)	92 89	11, 26, 58, 101	0
2	F	506/531 (95%)	-0.87	2 (0%)	92 89	12, 27, 58, 100	0
2	H	506/531 (95%)	-0.89	1 (0%)	95 94	10, 26, 58, 101	0
2	J	506/531 (95%)	-0.87	1 (0%)	95 94	11, 26, 58, 100	0
2	L	506/531 (95%)	-0.88	1 (0%)	95 94	11, 26, 57, 100	0
All	All	6747/7272 (92%)	-0.53	55 (0%)	86 78	10, 43, 108, 128	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	329	TYR	3.9
1	E	95	ASP	3.6
2	F	476(A)	LEU	3.5
1	K	159	GLU	3.5
2	D	476(A)	LEU	3.4
1	K	88	SER	3.4
2	H	476(B)	GLY	3.3
1	C	162	ILE	3.3
1	C	286	GLY	3.3
2	B	476(A)	LEU	3.3
2	D	476(B)	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	K	256	ASP	3.2
1	E	152	PHE	3.2
1	I	70	ASN	3.2
1	G	278	SER	3.0
1	A	329	TYR	2.9
2	B	476	ASP	2.8
1	I	88	SER	2.8
2	J	476(A)	LEU	2.7
2	B	476(B)	GLY	2.7
1	K	214	TYR	2.6
1	I	717	SER	2.6
1	A	162	ILE	2.6
1	E	276	CYS	2.6
1	C	152	PHE	2.5
1	I	95	ASP	2.5
1	K	158	ALA	2.5
1	I	135	GLY	2.4
1	A	330	ALA	2.4
1	E	162	ILE	2.4
1	I	384	ILE	2.3
1	E	138	ALA	2.3
1	K	160	GLY	2.3
1	I	708	ALA	2.3
1	G	88	SER	2.3
1	E	64	ASN	2.3
1	E	384	ILE	2.3
1	K	657	ASP	2.3
1	G	96	ALA	2.3
1	K	177	LYS	2.3
1	A	194	GLY	2.2
2	B	475	GLY	2.2
1	G	655	PRO	2.2
1	K	150	SER	2.2
1	E	171	ILE	2.2
1	K	114	PRO	2.1
1	C	329	TYR	2.1
1	E	654	LEU	2.1
1	E	157	GLU	2.1
2	F	476(B)	GLY	2.1
1	I	657	ASP	2.1
2	L	528	GLN	2.0
1	K	656	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	329	TYR	2.0
1	A	181	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BTI	I	801	15/15	0.91	0.23	57,65,68,69	0
3	BTI	K	801	15/15	0.93	0.16	39,50,57,62	0
3	BTI	G	801	15/15	0.94	0.20	43,49,56,60	0
3	BTI	A	801	15/15	0.94	0.16	30,42,56,62	0
3	BTI	E	801	15/15	0.94	0.18	31,39,49,50	0
3	BTI	C	801	15/15	0.95	0.13	30,38,46,47	0

6.5 Other polymers (i)

There are no such residues in this entry.