



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:02 PM GMT

PDB ID : 3QMU  
Title : Bovine glutamate dehydrogenase complexed with epicatechin-3-gallate (ECG)  
Authors : Li, C.; Li, M.; Stanley, C.; Smith, T.J.  
Deposited on : 2011-02-05  
Resolution : 3.62 Å(reported)

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

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

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



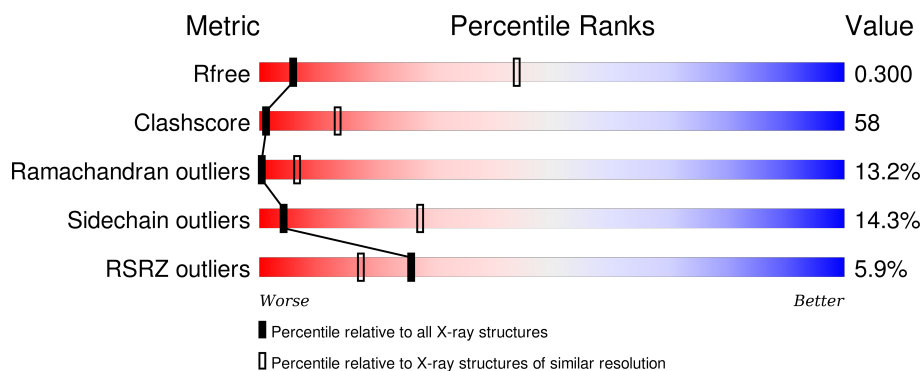
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.62 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1093 (3.80-3.44)
Clashscore	102246	1043 (3.78-3.46)
Ramachandran outliers	100387	1003 (3.78-3.46)
Sidechain outliers	100360	1003 (3.78-3.46)
RSRZ outliers	91569	1100 (3.80-3.44)

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

Mol	Chain	Length	Quality of chain
1	A	501	<div> <div>8%</div> <div>26%</div> <div>55%</div> <div>18%</div> <div>..</div> </div>
1	B	501	<div> <div>7%</div> <div>25%</div> <div>56%</div> <div>17%</div> <div>..</div> </div>
1	C	501	<div> <div>6%</div> <div>27%</div> <div>54%</div> <div>17%</div> <div>..</div> </div>
1	D	501	<div> <div>6%</div> <div>25%</div> <div>56%</div> <div>17%</div> <div>..</div> </div>
1	E	501	<div> <div>8%</div> <div>24%</div> <div>56%</div> <div>18%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	501	
1	G	501	
1	H	501	
1	I	501	
1	J	501	
1	K	501	
1	L	501	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NDP	B	552	-	-	-	X
3	XEG	B	601	-	-	X	-
3	XEG	D	601	-	-	-	X
3	XEG	F	601	-	-	X	-
3	XEG	G	601	-	-	X	-
3	XEG	H	601	-	-	X	-
3	XEG	I	601	-	-	-	X
3	XEG	J	601	-	-	X	-
3	XEG	K	601	-	-	X	-



## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 47520 atoms, of which 0 are hydrogens and 0 are deuteriums.

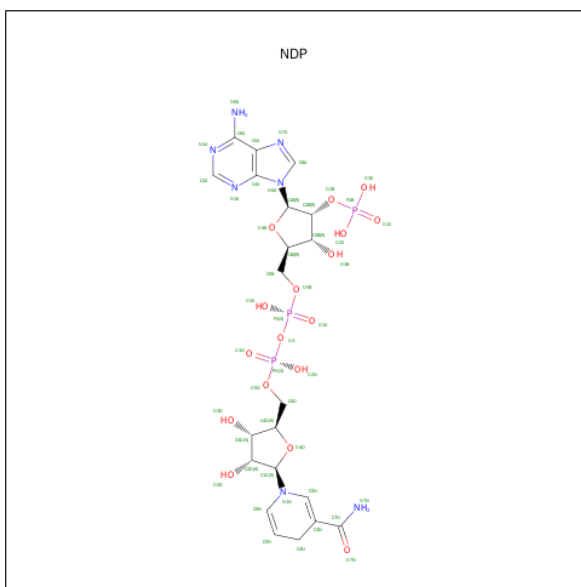
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glutamate dehydrogenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3880	2454	679	728	19			
1	B	496	Total	C	N	O	S	0	0	0
			3880	2454	679	728	19			
1	C	496	Total	C	N	O	S	0	0	0
			3880	2454	679	728	19			
1	D	496	Total	C	N	O	S	0	0	0
			3880	2454	679	728	19			
1	E	496	Total	C	N	O	S	0	0	0
			3880	2454	679	728	19			
1	F	496	Total	C	N	O	S	0	0	0
			3880	2454	679	728	19			
1	G	496	Total	C	N	O	S	0	0	0
			3880	2454	679	728	19			
1	H	496	Total	C	N	O	S	0	0	0
			3880	2454	679	728	19			
1	I	496	Total	C	N	O	S	0	0	0
			3880	2454	679	728	19			
1	J	496	Total	C	N	O	S	0	0	0
			3880	2454	679	728	19			
1	K	496	Total	C	N	O	S	0	0	0
			3880	2454	679	728	19			
1	L	496	Total	C	N	O	S	0	0	0
			3880	2454	679	728	19			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).

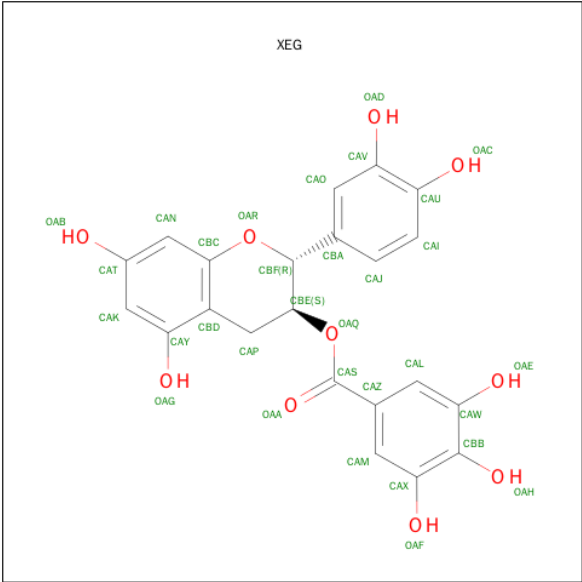




Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	K	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	L	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is (2R,3S)-2-(3,4-DIHYDROXYPHENYL)-5,7-DIHYDROXY-3,4-DIHYDRO-2 H-CHROMEN-3-YL 3,4,5-TRIHYDROXYBENZOATE (three-letter code: XEG) (formula: C<sub>22</sub>H<sub>18</sub>O<sub>10</sub>).





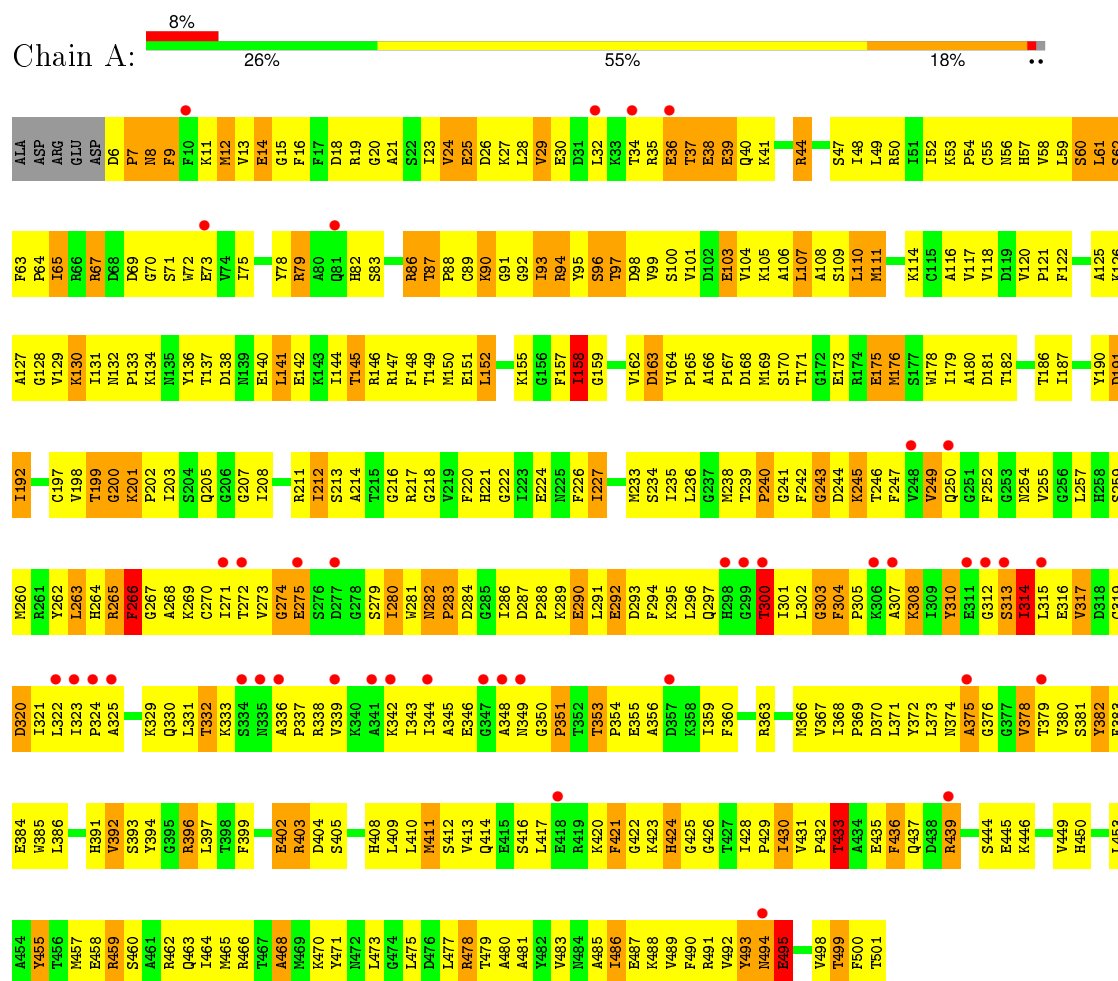
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			32	22	10		
3	B	1	Total	C	O	0	0
			32	22	10		
3	D	1	Total	C	O	0	0
			32	22	10		
3	D	1	Total	C	O	0	0
			32	22	10		
3	E	1	Total	C	O	0	0
			32	22	10		
3	F	1	Total	C	O	0	0
			32	22	10		
3	G	1	Total	C	O	0	0
			32	22	10		
3	H	1	Total	C	O	0	0
			32	22	10		
3	I	1	Total	C	O	0	0
			32	22	10		
3	J	1	Total	C	O	0	0
			32	22	10		
3	K	1	Total	C	O	0	0
			32	22	10		
3	L	1	Total	C	O	0	0
			32	22	10		



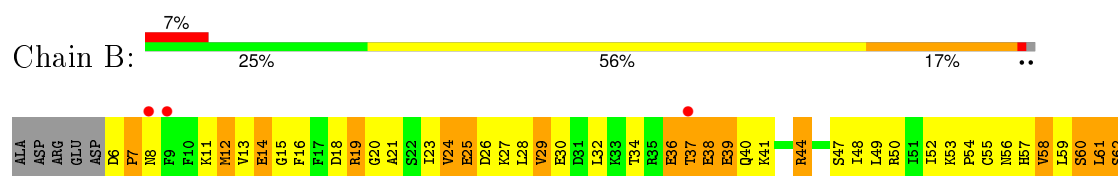
### 3 Residue-property plots

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

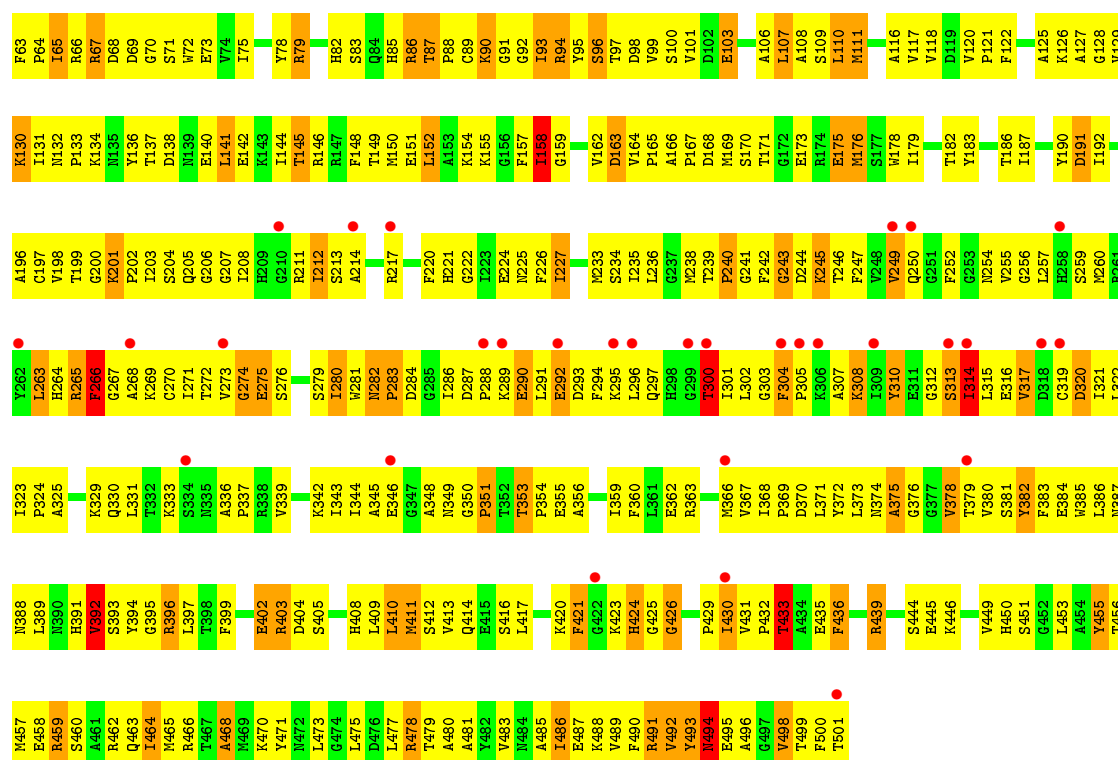
#### • Molecule 1: Glutamate dehydrogenase 1



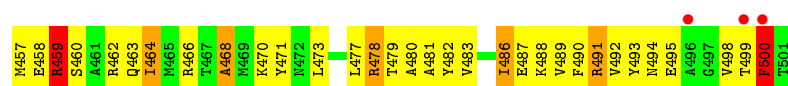
#### • Molecule 1: Glutamate dehydrogenase 1



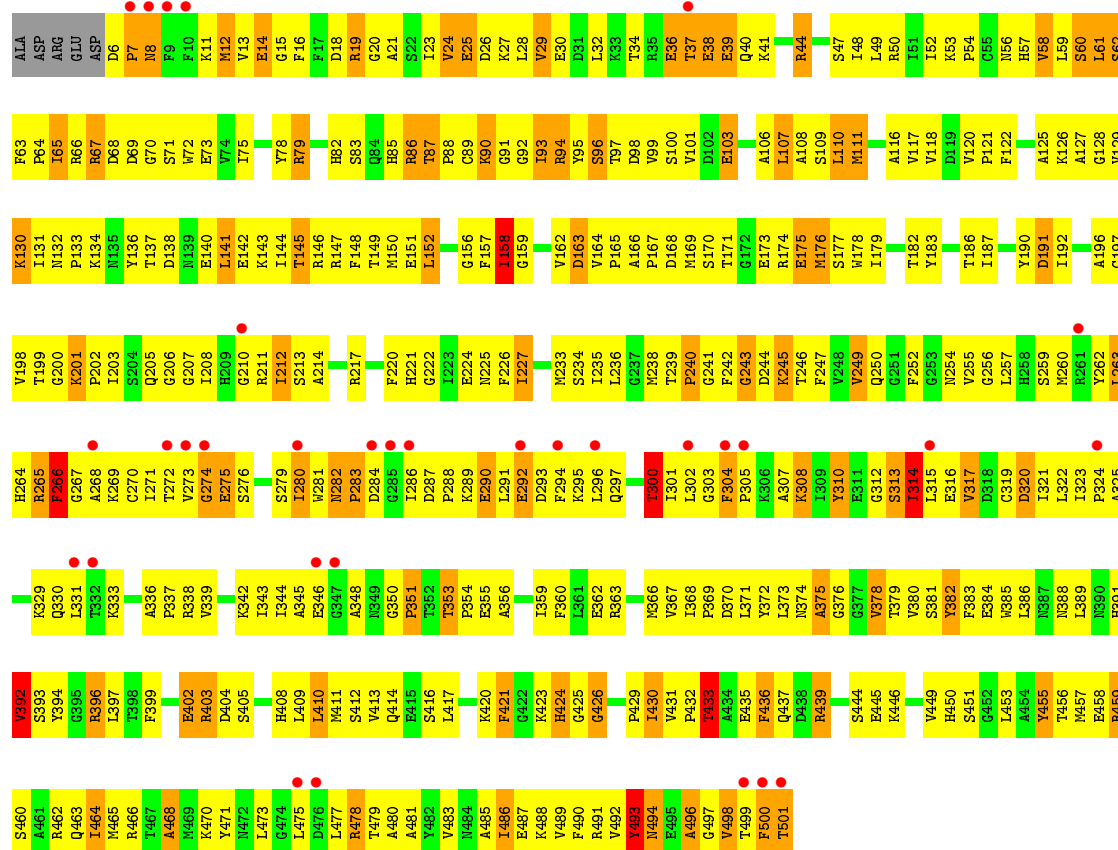




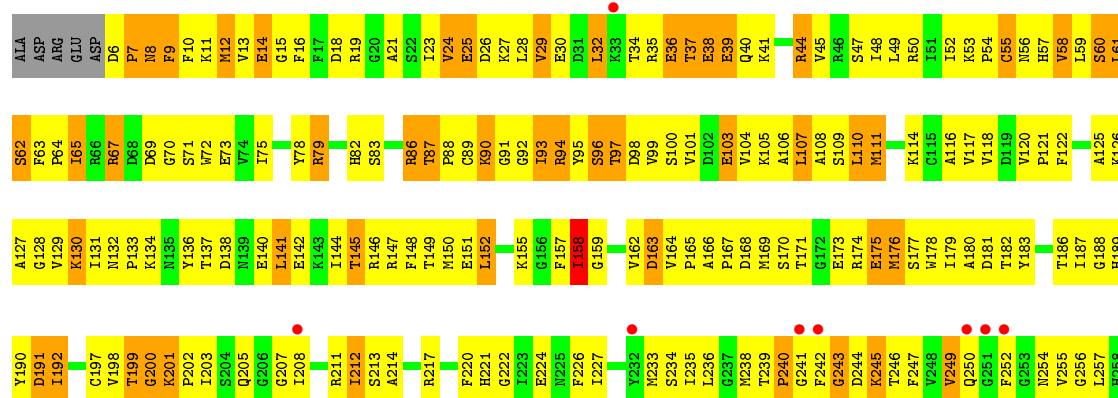




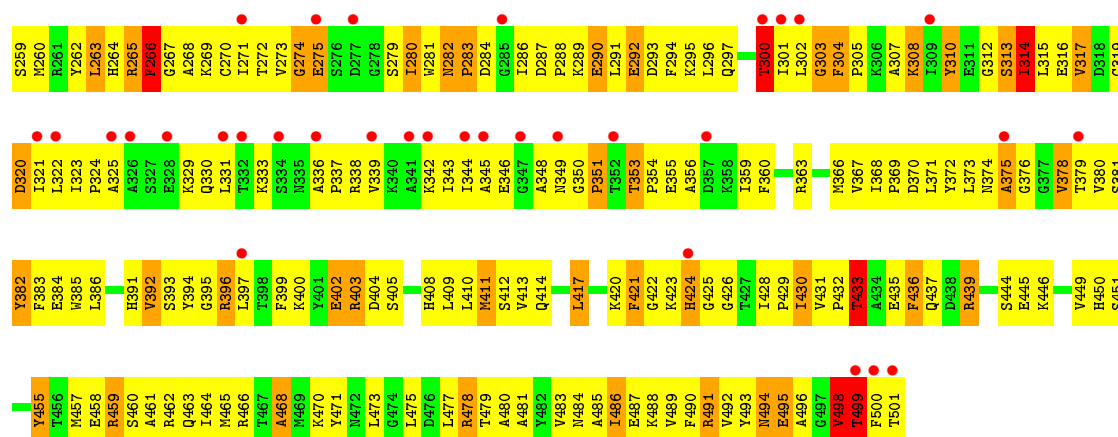
● Molecule 1: Glutamate dehydrogenase 1



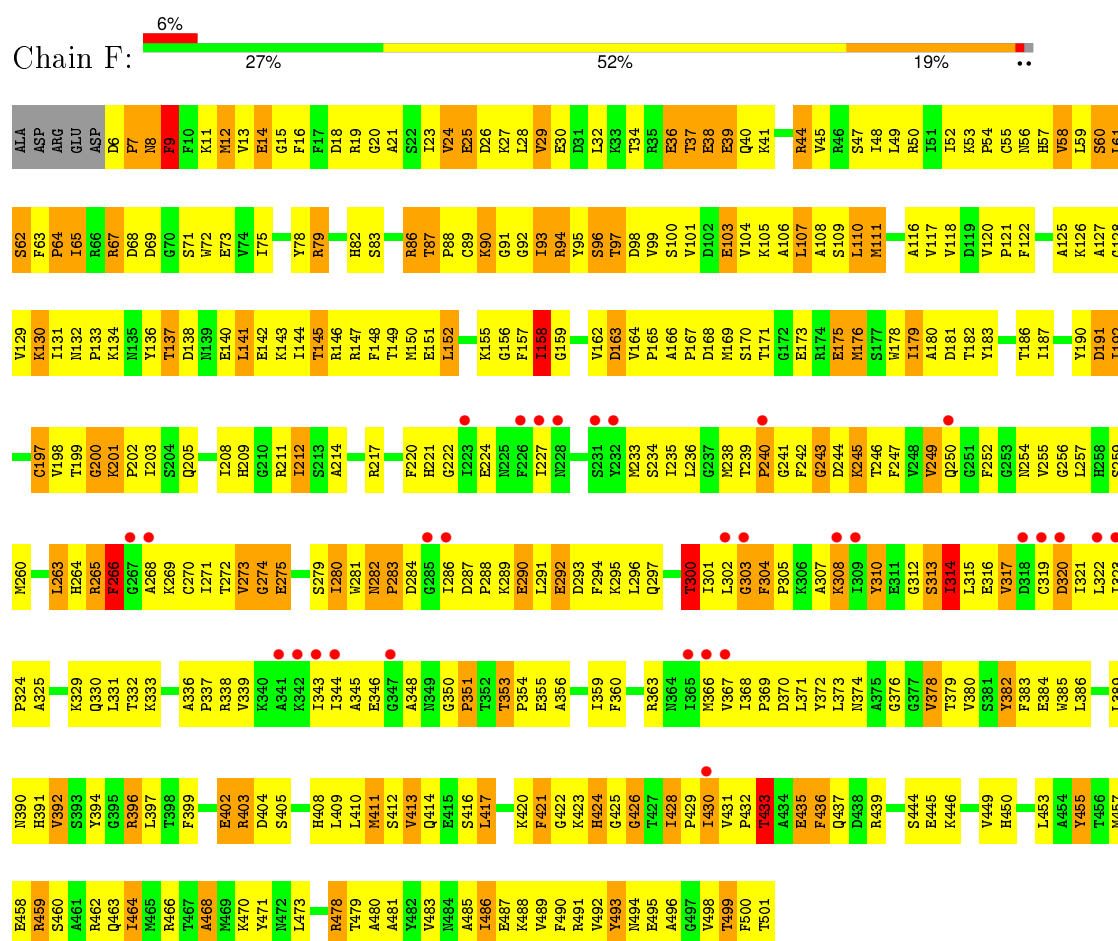
● Molecule 1: Glutamate dehydrogenase 1



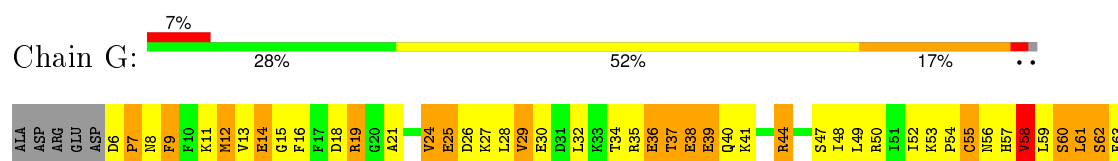




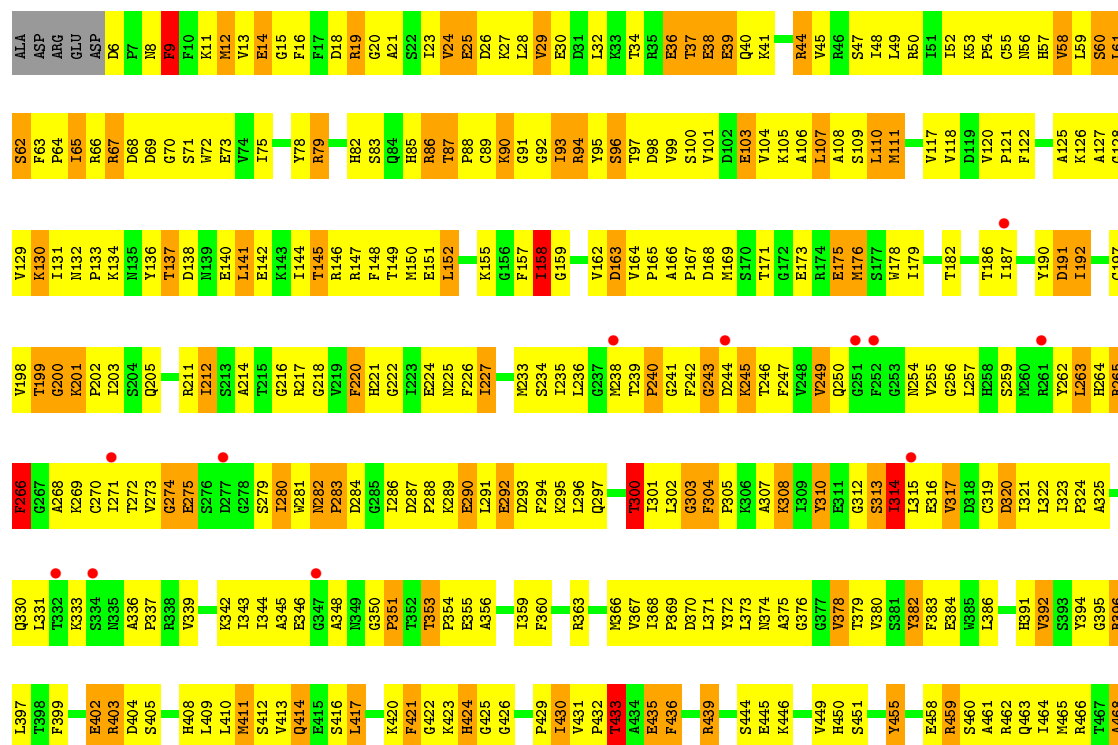
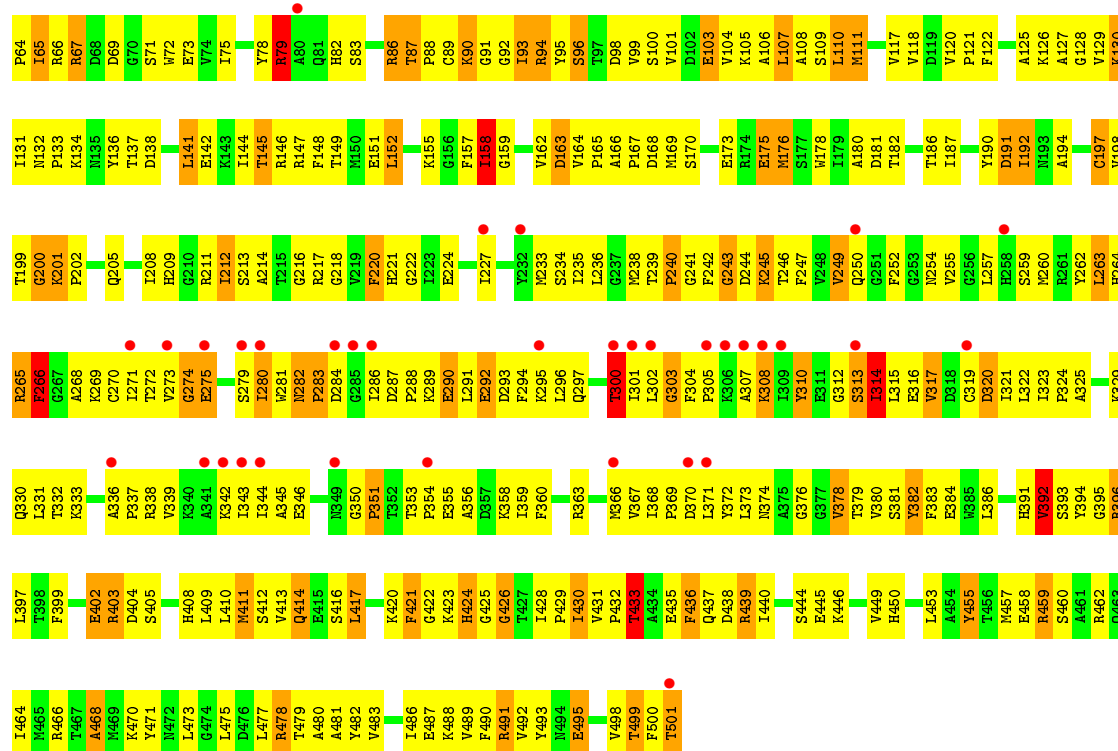
### • Molecule 1: Glutamate dehydrogenase 1



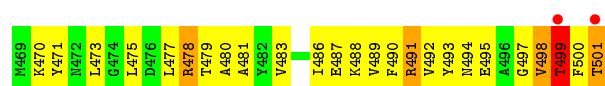
### • Molecule 1: Glutamate dehydrogenase 1



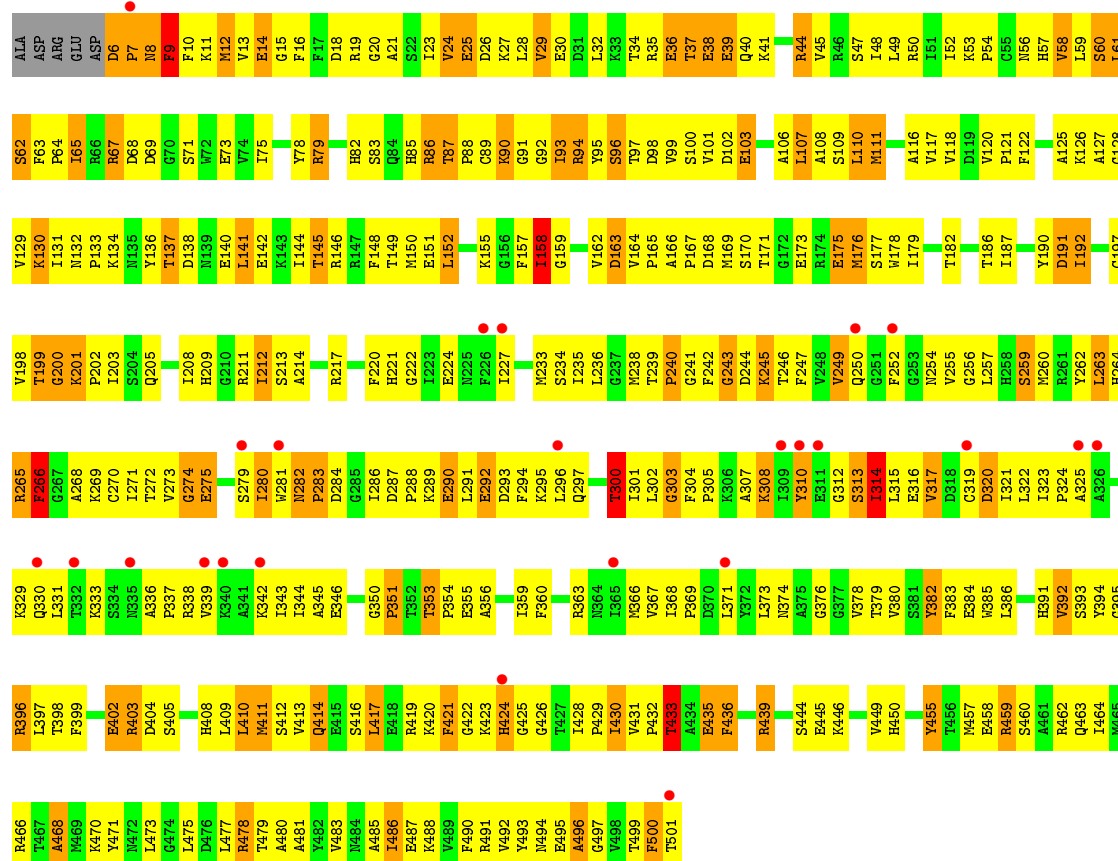




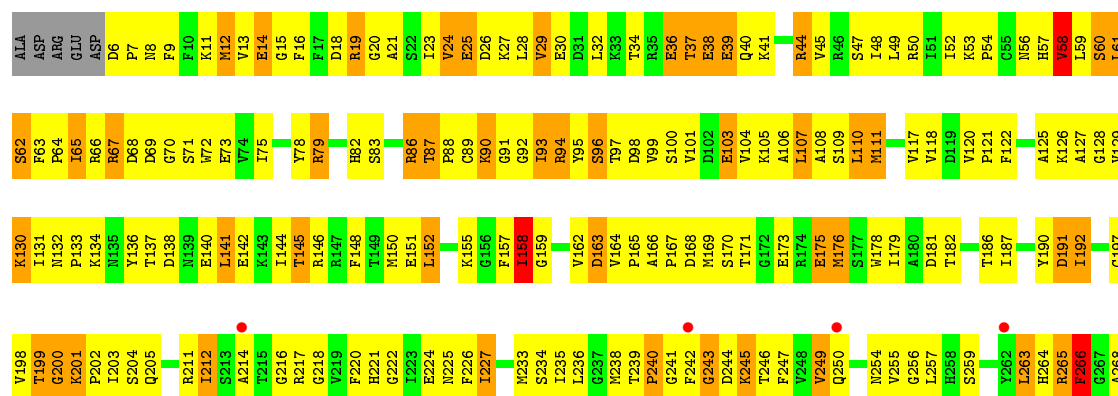




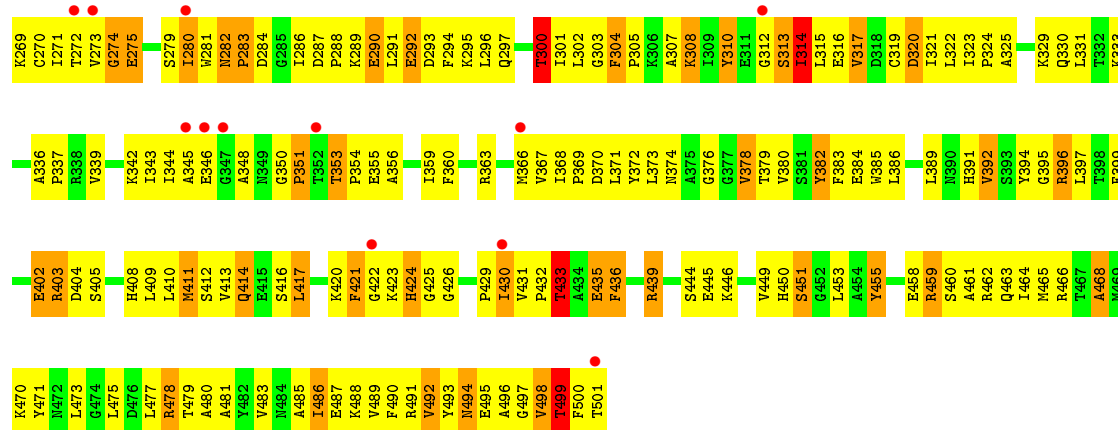
• Molecule 1: Glutamate dehydrogenase 1



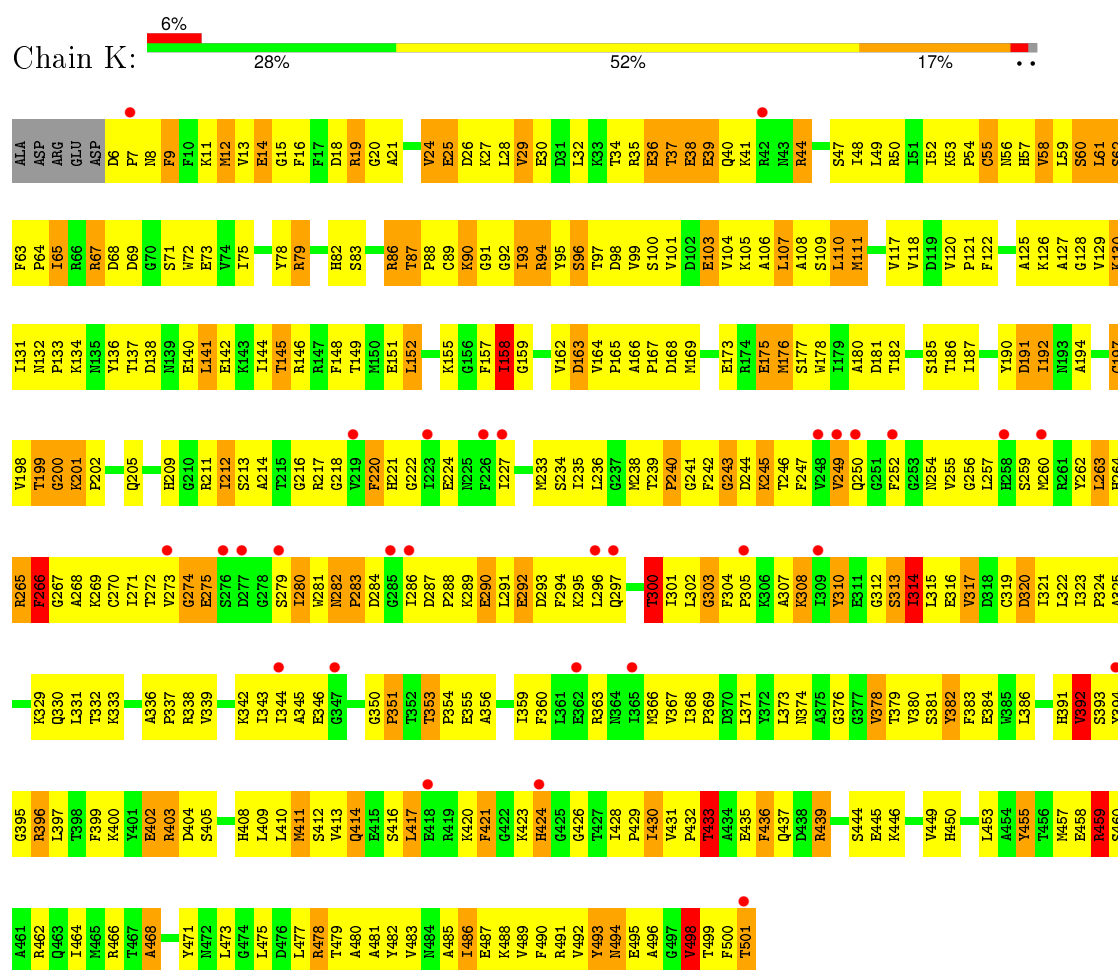
• Molecule 1: Glutamate dehydrogenase 1



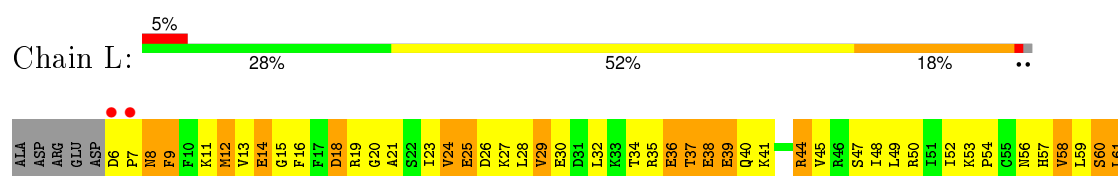




• Molecule 1: Glutamate dehydrogenase 1



• Molecule 1: Glutamate dehydrogenase 1









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.12Å 433.18Å 95.17Å 90.00° 118.74° 90.00°	Depositor
Resolution (Å)	49.71 – 3.62 49.71 – 3.62	Depositor EDS
% Data completeness (in resolution range)	95.0 (49.71-3.62) 95.0 (49.71-3.62)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_353)	Depositor
R, $R_{free}$	0.257 , 0.302 0.252 , 0.300	Depositor DCC
$R_{free}$ test set	3755 reflections (5.46%)	DCC
Wilson B-factor (Å <sup>2</sup> )	101.1	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 112.7	EDS
Estimated twinning fraction	0.036 for -h-l,k,h 0.036 for l,k,-h-l 0.038 for h,-k,-h-l 0.036 for -h-l,-k,l 0.428 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 75039 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	47520	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

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

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

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	0.53	0/3963	0.64	0/5351
1	B	0.53	0/3963	0.67	0/5351
1	C	0.54	1/3963 (0.0%)	0.66	1/5351 (0.0%)
1	D	0.54	0/3963	0.66	0/5351
1	E	0.53	0/3963	0.64	0/5351
1	F	0.55	1/3963 (0.0%)	0.79	3/5351 (0.1%)
1	G	0.53	1/3963 (0.0%)	0.63	1/5351 (0.0%)
1	H	0.54	0/3963	0.63	0/5351
1	I	0.50	0/3963	0.63	0/5351
1	J	0.53	0/3963	0.63	0/5351
1	K	0.53	1/3963 (0.0%)	0.65	2/5351 (0.0%)
1	L	0.51	0/3963	0.63	0/5351
All	All	0.53	4/47556 (0.0%)	0.66	7/64212 (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	D	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	197	CYS	CB-SG	-8.22	1.68	1.82
1	G	197	CYS	CB-SG	-7.69	1.69	1.82
1	F	197	CYS	CB-SG	-5.43	1.73	1.81
1	C	89	CYS	CB-SG	-5.40	1.73	1.81

All (7) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	459	ARG	NE-CZ-NH1	-22.15	109.22	120.30
1	F	459	ARG	NE-CZ-NH2	21.93	131.27	120.30
1	F	459	ARG	CD-NE-CZ	11.59	139.82	123.60
1	K	459	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	C	459	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	G	392	VAL	CB-CA-C	-5.30	101.33	111.40
1	K	392	VAL	CB-CA-C	-5.13	101.66	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	8	ASN	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3880	0	3848	497	2
1	B	3880	0	3848	502	2
1	C	3880	0	3848	490	0
1	D	3880	0	3848	483	1
1	E	3880	0	3848	505	1
1	F	3880	0	3848	476	0
1	G	3880	0	3848	460	0
1	H	3880	0	3848	479	0
1	I	3880	0	3848	464	0
1	J	3880	0	3848	483	0
1	K	3880	0	3848	456	0
1	L	3880	0	3848	460	0
2	A	48	0	26	8	0
2	B	48	0	26	2	0
2	C	48	0	26	5	0
2	D	48	0	26	2	0
2	E	48	0	26	5	0
2	F	48	0	26	5	0
2	G	48	0	26	4	0
2	H	48	0	26	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	48	0	26	5	0
2	J	48	0	26	2	0
2	K	48	0	26	5	0
2	L	48	0	26	7	0
3	A	32	0	18	8	0
3	B	32	0	18	10	0
3	D	64	0	35	13	0
3	E	32	0	18	8	0
3	F	32	0	18	10	0
3	G	32	0	18	10	0
3	H	32	0	18	14	0
3	I	32	0	18	7	0
3	J	32	0	18	12	0
3	K	32	0	18	9	0
3	L	32	0	18	6	0
All	All	47520	0	46703	5482	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 58.

All (5482) 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:371:LEU:HD23	1:E:481:ALA:HB1	1.26	1.15
1:D:24:VAL:HG13	1:D:483:VAL:HG13	1.26	1.13
1:I:408:HIS:HB3	1:K:436:PHE:CD2	1.82	1.13
1:G:436:PHE:CD2	1:L:408:HIS:HB3	1.85	1.12
1:F:99:VAL:HG11	1:F:128:GLY:HA3	1.34	1.10
1:I:436:PHE:CD2	1:J:408:HIS:HB3	1.85	1.10
1:A:371:LEU:HD23	1:A:481:ALA:HB1	1.20	1.09
1:L:111:MET:HE2	2:L:552:NDP:H72N	1.16	1.09
1:H:24:VAL:HG13	1:H:483:VAL:HG13	1.34	1.08
1:B:24:VAL:HG13	1:B:483:VAL:HG13	1.33	1.07
1:H:408:HIS:HB3	1:L:436:PHE:CD2	1.88	1.07
1:E:99:VAL:HG11	1:E:128:GLY:HA3	1.35	1.07
1:E:487:GLU:HG2	1:E:491:ARG:HH22	1.20	1.06
1:C:99:VAL:HG11	1:C:128:GLY:HA3	1.33	1.05
1:A:94:ARG:HG3	1:A:169:MET:HB2	1.37	1.05
1:H:79:ARG:HG2	1:H:127:ALA:HB2	1.39	1.04
1:J:24:VAL:HG13	1:J:483:VAL:HG13	1.33	1.04
1:D:367:VAL:O	1:D:477:LEU:HD23	1.58	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:408:HIS:HB3	1:E:436:PHE:CD2	1.94	1.02
1:E:94:ARG:HG3	1:E:169:MET:HB2	1.37	1.02
1:A:99:VAL:HG11	1:A:128:GLY:HA3	1.38	1.01
1:B:367:VAL:O	1:B:477:LEU:HD23	1.60	1.01
1:L:111:MET:CE	2:L:552:NDP:H72N	1.73	1.01
1:I:94:ARG:HG3	1:I:169:MET:HB2	1.44	1.00
1:A:501:THR:HG23	1:D:147:ARG:HD3	1.43	1.00
1:G:94:ARG:HG3	1:G:169:MET:HB2	1.43	0.99
1:L:94:ARG:HG3	1:L:169:MET:HB2	1.42	0.99
1:A:371:LEU:HD23	1:A:481:ALA:CB	1.92	0.99
1:A:111:MET:HE2	2:A:552:NDP:H72N	1.24	0.99
1:C:436:PHE:CD2	1:D:408:HIS:HB3	1.96	0.99
1:B:94:ARG:HG3	1:B:169:MET:HB2	1.42	0.99
1:D:99:VAL:HG11	1:D:128:GLY:HA3	1.42	0.99
1:B:99:VAL:HG11	1:B:128:GLY:HA3	1.41	0.99
1:B:408:HIS:HB3	1:F:436:PHE:CD2	1.97	0.99
1:J:94:ARG:HG3	1:J:169:MET:HB2	1.45	0.99
1:B:78:TYR:CE2	1:B:101:VAL:HG22	1.96	0.99
1:I:111:MET:HE2	2:I:552:NDP:H72N	1.25	0.99
1:J:79:ARG:HG2	1:J:127:ALA:HB2	1.42	0.99
1:D:78:TYR:CE2	1:D:101:VAL:HG22	1.97	0.98
1:A:487:GLU:HG2	1:A:491:ARG:HH22	1.27	0.98
1:H:99:VAL:HG11	1:H:128:GLY:HA3	1.45	0.98
1:G:66:ARG:HH11	1:J:500:PHE:HZ	0.98	0.98
1:D:94:ARG:HG3	1:D:169:MET:HB2	1.42	0.98
1:D:336:ALA:HB3	1:D:337:PRO:HD3	1.46	0.98
1:I:6:ASP:HB2	1:I:353:THR:HB	1.44	0.98
1:A:436:PHE:CD2	1:F:408:HIS:HB3	1.99	0.98
1:H:336:ALA:HB3	1:H:337:PRO:HD3	1.46	0.98
1:J:336:ALA:HB3	1:J:337:PRO:HD3	1.45	0.98
1:K:94:ARG:HG3	1:K:169:MET:HB2	1.41	0.98
1:G:79:ARG:HG2	1:G:127:ALA:HB2	1.43	0.98
1:C:94:ARG:HG3	1:C:169:MET:HB2	1.46	0.97
1:A:78:TYR:CE2	1:A:101:VAL:HG22	2.00	0.97
1:G:99:VAL:HG11	1:G:128:GLY:HA3	1.45	0.97
1:K:79:ARG:HG2	1:K:127:ALA:HB2	1.46	0.97
1:B:72:TRP:HE1	1:E:498:VAL:HG11	1.24	0.97
1:E:79:ARG:HG2	1:E:127:ALA:HB2	1.45	0.97
1:H:94:ARG:HG3	1:H:169:MET:HB2	1.46	0.96
1:K:78:TYR:CE2	1:K:101:VAL:HG22	2.00	0.96
1:B:91:GLY:HA3	1:B:125:ALA:O	1.65	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:336:ALA:HB3	1:F:337:PRO:HD3	1.47	0.96
1:A:336:ALA:HB3	1:A:337:PRO:HD3	1.47	0.96
1:G:336:ALA:HB3	1:G:337:PRO:HD3	1.47	0.96
1:H:408:HIS:HB3	1:L:436:PHE:HD2	1.28	0.96
1:B:336:ALA:HB3	1:B:337:PRO:HD3	1.46	0.96
1:A:91:GLY:HA3	1:A:125:ALA:O	1.65	0.96
1:K:99:VAL:HG11	1:K:128:GLY:HA3	1.45	0.96
1:I:336:ALA:HB3	1:I:337:PRO:HD3	1.47	0.96
3:G:601:XEG:HAL	1:L:209:HIS:HE1	1.30	0.96
1:E:371:LEU:HD23	1:E:481:ALA:CB	1.96	0.96
1:I:491:ARG:HD2	3:I:601:XEG:OAB	1.64	0.96
1:D:436:PHE:CD2	1:E:408:HIS:HB3	2.01	0.95
1:L:65:ILE:HD11	1:L:75:ILE:HD11	1.48	0.95
1:B:118:VAL:HG23	1:B:120:VAL:HG23	1.45	0.95
1:J:99:VAL:HG11	1:J:128:GLY:HA3	1.46	0.95
1:A:408:HIS:HB3	1:B:436:PHE:CD2	2.00	0.95
1:A:117:VAL:HG21	1:A:371:LEU:HG	1.46	0.95
1:G:66:ARG:NH1	1:J:500:PHE:HZ	1.63	0.95
1:I:436:PHE:HD2	1:J:408:HIS:HB3	1.25	0.95
1:C:408:HIS:HB3	1:E:436:PHE:HD2	1.32	0.95
3:A:601:XEG:HAL	1:F:209:HIS:HE1	1.29	0.95
1:K:91:GLY:HA3	1:K:125:ALA:O	1.67	0.95
1:K:118:VAL:HG23	1:K:120:VAL:HG23	1.48	0.95
1:G:78:TYR:CE2	1:G:101:VAL:HG22	2.01	0.95
1:D:91:GLY:HA3	1:D:125:ALA:O	1.66	0.94
1:K:24:VAL:HG13	1:K:483:VAL:HG13	1.48	0.94
1:A:79:ARG:HG2	1:A:127:ALA:HB2	1.49	0.94
1:I:99:VAL:HG11	1:I:128:GLY:HA3	1.49	0.94
1:F:94:ARG:HG3	1:F:169:MET:HB2	1.47	0.94
1:E:78:TYR:CE2	1:E:101:VAL:HG22	2.02	0.94
1:D:487:GLU:O	1:D:491:ARG:HG3	1.66	0.94
1:D:65:ILE:HD11	1:D:75:ILE:HD11	1.49	0.94
1:G:24:VAL:HG13	1:G:483:VAL:HG13	1.50	0.94
1:B:371:LEU:HD23	1:B:481:ALA:HB1	1.48	0.94
1:B:408:HIS:HB3	1:F:436:PHE:HD2	1.32	0.94
1:D:79:ARG:HG2	1:D:127:ALA:HB2	1.49	0.94
1:A:250:GLN:HB3	1:A:324:PRO:HA	1.49	0.94
1:G:118:VAL:HG23	1:G:120:VAL:HG23	1.49	0.94
1:K:336:ALA:HB3	1:K:337:PRO:HD3	1.48	0.94
1:H:371:LEU:HD23	1:H:481:ALA:HB1	1.47	0.94
1:I:371:LEU:HD23	1:I:481:ALA:HB1	1.47	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:91:GLY:HA3	1:G:125:ALA:O	1.67	0.94
1:J:78:TYR:CE2	1:J:101:VAL:HG22	2.03	0.93
1:E:336:ALA:HB3	1:E:337:PRO:HD3	1.48	0.93
1:A:28:LEU:HD12	1:A:28:LEU:H	1.33	0.93
1:H:78:TYR:CE2	1:H:101:VAL:HG22	2.02	0.93
1:I:408:HIS:HB3	1:K:436:PHE:HD2	1.17	0.93
1:I:209:HIS:HE1	3:K:601:XEG:HAL	1.28	0.93
1:I:65:ILE:HD11	1:I:75:ILE:HD11	1.48	0.93
1:L:336:ALA:HB3	1:L:337:PRO:HD3	1.47	0.93
1:F:250:GLN:HB3	1:F:324:PRO:HA	1.50	0.93
1:I:250:GLN:HB3	1:I:324:PRO:HA	1.51	0.93
1:D:250:GLN:HB3	1:D:324:PRO:HA	1.51	0.92
1:E:117:VAL:HG21	1:E:371:LEU:HG	1.49	0.92
1:I:91:GLY:HA3	1:I:125:ALA:O	1.69	0.92
1:K:250:GLN:HB3	1:K:324:PRO:HA	1.50	0.92
1:L:371:LEU:HD23	1:L:481:ALA:HB1	1.50	0.92
1:C:336:ALA:HB3	1:C:337:PRO:HD3	1.48	0.92
1:E:152:LEU:HD12	1:E:157:PHE:HB2	1.51	0.92
1:J:371:LEU:HD23	1:J:481:ALA:HB1	1.51	0.92
1:K:28:LEU:HD12	1:K:28:LEU:H	1.35	0.92
1:C:250:GLN:HB3	1:C:324:PRO:HA	1.51	0.92
1:J:250:GLN:HB3	1:J:324:PRO:HA	1.52	0.92
1:A:111:MET:CE	2:A:552:NDP:H72N	1.83	0.92
1:C:436:PHE:HD2	1:D:408:HIS:HB3	1.31	0.92
1:I:12:MET:H	1:I:14:GLU:HG2	1.34	0.91
1:G:28:LEU:H	1:G:28:LEU:HD12	1.35	0.91
1:E:250:GLN:HB3	1:E:324:PRO:HA	1.50	0.91
1:B:65:ILE:HD11	1:B:75:ILE:HD11	1.52	0.91
1:E:111:MET:HE2	2:E:552:NDP:H72N	1.34	0.91
1:G:436:PHE:HD2	1:L:408:HIS:HB3	1.23	0.91
1:D:436:PHE:HD1	1:D:436:PHE:O	1.53	0.91
1:D:436:PHE:HD2	1:E:408:HIS:HB3	1.33	0.91
1:I:118:VAL:HG23	1:I:120:VAL:HG23	1.50	0.91
1:G:382:TYR:CE2	1:G:386:LEU:HD11	2.06	0.91
1:B:250:GLN:HB3	1:B:324:PRO:HA	1.52	0.91
1:F:78:TYR:CE2	1:F:101:VAL:HG22	2.05	0.91
1:F:79:ARG:HG2	1:F:127:ALA:HB2	1.53	0.91
1:C:28:LEU:H	1:C:28:LEU:HD12	1.35	0.91
1:A:346:GLU:OE1	1:A:478:ARG:NH2	2.02	0.91
1:E:28:LEU:HD12	1:E:28:LEU:H	1.33	0.91
1:G:250:GLN:HB3	1:G:324:PRO:HA	1.50	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:382:TYR:CE2	1:K:386:LEU:HD11	2.05	0.91
1:H:250:GLN:HB3	1:H:324:PRO:HA	1.50	0.91
1:E:91:GLY:HA3	1:E:125:ALA:O	1.70	0.90
1:I:111:MET:CE	2:I:552:NDP:H72N	1.84	0.90
1:D:371:LEU:HD23	1:D:481:ALA:HB1	1.51	0.90
1:A:16:PHE:HE2	1:A:354:PRO:HG3	1.35	0.90
1:L:99:VAL:HG11	1:L:128:GLY:HA3	1.51	0.90
1:K:12:MET:H	1:K:14:GLU:HG2	1.36	0.90
1:C:78:TYR:CE2	1:C:101:VAL:HG22	2.05	0.90
1:B:12:MET:H	1:B:14:GLU:HG2	1.35	0.90
1:A:436:PHE:HD2	1:F:408:HIS:HB3	1.36	0.90
1:C:91:GLY:HA3	1:C:125:ALA:O	1.70	0.90
1:E:498:VAL:HG23	1:E:500:PHE:HE2	1.37	0.90
1:L:12:MET:H	1:L:14:GLU:HG2	1.35	0.90
1:L:250:GLN:HB3	1:L:324:PRO:HA	1.52	0.90
1:E:16:PHE:HE2	1:E:354:PRO:HG3	1.36	0.90
1:G:152:LEU:HD12	1:G:157:PHE:HB2	1.54	0.89
1:L:118:VAL:HG23	1:L:120:VAL:HG23	1.54	0.89
1:K:371:LEU:HD23	1:K:481:ALA:HB1	1.53	0.89
1:D:12:MET:H	1:D:14:GLU:HG2	1.36	0.89
1:H:12:MET:H	1:H:14:GLU:HG2	1.38	0.89
1:A:24:VAL:HG13	1:A:483:VAL:HG13	1.54	0.89
1:A:152:LEU:HD12	1:A:157:PHE:HB2	1.52	0.89
1:F:28:LEU:H	1:F:28:LEU:HD12	1.35	0.89
1:L:78:TYR:CE2	1:L:101:VAL:HG22	2.08	0.89
1:A:383:PHE:CE2	1:F:397:LEU:HD11	2.06	0.89
1:E:65:ILE:HD11	1:E:75:ILE:HD11	1.55	0.89
1:I:28:LEU:H	1:I:28:LEU:HD12	1.38	0.89
1:A:65:ILE:HD11	1:A:75:ILE:HD11	1.55	0.89
1:B:79:ARG:HG2	1:B:127:ALA:HB2	1.52	0.89
1:K:152:LEU:HD12	1:K:157:PHE:HB2	1.55	0.89
1:C:397:LEU:HD11	1:E:383:PHE:CE2	2.07	0.88
1:L:491:ARG:HD3	3:L:601:XEG:OAB	1.73	0.88
1:F:12:MET:H	1:F:14:GLU:HG2	1.38	0.88
1:B:490:PHE:CE2	1:B:494:ASN:HB2	2.08	0.88
1:H:489:VAL:O	1:H:492:VAL:HG22	1.71	0.88
1:G:12:MET:H	1:G:14:GLU:HG2	1.38	0.88
1:C:12:MET:H	1:C:14:GLU:HG2	1.39	0.88
1:A:56:ASN:O	1:A:57:HIS:HD2	1.55	0.88
1:E:24:VAL:HG13	1:E:483:VAL:HG13	1.55	0.88
1:D:118:VAL:HG23	1:D:120:VAL:HG23	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:436:PHE:HD1	1:E:436:PHE:O	1.54	0.88
1:E:12:MET:H	1:E:14:GLU:HG2	1.37	0.88
1:I:79:ARG:HG2	1:I:127:ALA:HB2	1.53	0.88
1:B:382:TYR:CE2	1:B:386:LEU:HD11	2.09	0.88
1:D:394:TYR:HB2	1:D:445:GLU:HG3	1.53	0.88
1:C:382:TYR:CE2	1:C:386:LEU:HD11	2.08	0.88
1:A:12:MET:H	1:A:14:GLU:HG2	1.38	0.88
1:C:436:PHE:O	1:C:436:PHE:HD1	1.55	0.88
1:F:265:ARG:O	1:F:266:PHE:HB2	1.74	0.87
1:A:436:PHE:HD1	1:A:436:PHE:O	1.56	0.87
1:F:111:MET:CE	2:F:552:NDP:H72N	1.88	0.87
1:B:436:PHE:O	1:B:436:PHE:HD1	1.56	0.87
1:E:56:ASN:O	1:E:57:HIS:HD2	1.57	0.87
1:K:487:GLU:O	1:K:491:ARG:HG3	1.75	0.87
1:J:12:MET:H	1:J:14:GLU:HG2	1.37	0.87
1:E:346:GLU:OE1	1:E:478:ARG:NH2	2.08	0.87
1:H:265:ARG:O	1:H:266:PHE:HB2	1.73	0.87
1:E:382:TYR:CE2	1:E:386:LEU:HD11	2.09	0.87
1:F:91:GLY:HA3	1:F:125:ALA:O	1.73	0.87
1:C:56:ASN:O	1:C:57:HIS:HD2	1.58	0.87
1:B:28:LEU:HD12	1:B:28:LEU:H	1.40	0.86
1:G:498:VAL:HG22	1:L:142:GLU:OE2	1.74	0.86
1:E:265:ARG:O	1:E:266:PHE:HB2	1.76	0.86
1:G:371:LEU:HD23	1:G:481:ALA:HB1	1.55	0.86
1:C:265:ARG:O	1:C:266:PHE:HB2	1.73	0.86
1:F:382:TYR:CE2	1:F:386:LEU:HD11	2.10	0.86
1:E:118:VAL:HG23	1:E:120:VAL:HG23	1.57	0.86
1:A:367:VAL:O	1:A:477:LEU:HD23	1.75	0.86
1:A:265:ARG:O	1:A:266:PHE:HB2	1.76	0.86
1:I:209:HIS:CE1	3:K:601:XEG:HAL	2.11	0.86
1:J:265:ARG:O	1:J:266:PHE:HB2	1.74	0.86
1:H:152:LEU:HD12	1:H:157:PHE:HB2	1.58	0.86
1:H:16:PHE:HE2	1:H:354:PRO:HG3	1.41	0.86
1:J:28:LEU:HD12	1:J:28:LEU:H	1.40	0.86
1:K:414:GLN:OE1	1:K:429:PRO:HD2	1.76	0.86
1:I:78:TYR:CE2	1:I:101:VAL:HG22	2.11	0.86
1:D:473:LEU:HD22	1:D:480:ALA:HB2	1.58	0.85
1:J:436:PHE:O	1:J:436:PHE:HD1	1.58	0.85
1:K:436:PHE:O	1:K:436:PHE:HD1	1.59	0.85
1:F:436:PHE:O	1:F:436:PHE:HD1	1.58	0.85
1:L:28:LEU:H	1:L:28:LEU:HD12	1.38	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:LEU:HD12	1:D:28:LEU:H	1.41	0.85
1:H:28:LEU:HD12	1:H:28:LEU:H	1.41	0.85
1:A:408:HIS:HB3	1:B:436:PHE:HD2	1.33	0.85
1:J:56:ASN:O	1:J:57:HIS:HD2	1.59	0.85
1:L:91:GLY:HA3	1:L:125:ALA:O	1.75	0.85
1:D:382:TYR:CE2	1:D:386:LEU:HD11	2.12	0.85
1:F:118:VAL:HG23	1:F:120:VAL:HG23	1.58	0.85
1:J:91:GLY:HA3	1:J:125:ALA:O	1.77	0.85
1:C:118:VAL:HG23	1:C:120:VAL:HG23	1.59	0.84
1:J:118:VAL:HG23	1:J:120:VAL:HG23	1.58	0.84
1:G:164:VAL:HG13	1:G:198:VAL:HA	1.58	0.84
1:F:288:PRO:HA	1:F:291:LEU:HB2	1.60	0.84
1:L:164:VAL:HG13	1:L:198:VAL:HA	1.60	0.84
1:B:214:ALA:HB1	1:B:380:VAL:HG21	1.59	0.84
1:H:91:GLY:HA3	1:H:125:ALA:O	1.78	0.84
1:A:199:THR:HG22	1:A:384:GLU:HG2	1.59	0.84
1:G:265:ARG:O	1:G:266:PHE:HB2	1.78	0.84
1:B:473:LEU:HD22	1:B:480:ALA:HB2	1.59	0.84
1:G:288:PRO:HA	1:G:291:LEU:HB2	1.58	0.84
1:C:209:HIS:HE1	3:E:601:XEG:HAL	1.43	0.84
1:E:487:GLU:HG2	1:E:491:ARG:NH2	1.92	0.84
1:F:65:ILE:HD11	1:F:75:ILE:HD11	1.59	0.84
1:K:56:ASN:O	1:K:57:HIS:HD2	1.60	0.84
1:B:349:ASN:HB2	2:B:552:NDP:O2D	1.77	0.84
1:G:408:HIS:HB3	1:H:436:PHE:CD2	2.12	0.84
1:C:164:VAL:HG13	1:C:198:VAL:HA	1.59	0.83
1:H:67:ARG:HD3	1:H:73:GLU:OE2	1.78	0.83
1:I:265:ARG:O	1:I:266:PHE:HB2	1.77	0.83
1:L:79:ARG:HG2	1:L:127:ALA:HB2	1.59	0.83
1:D:24:VAL:CG1	1:D:483:VAL:HG13	2.07	0.83
1:C:288:PRO:HA	1:C:291:LEU:HB2	1.60	0.83
1:K:265:ARG:O	1:K:266:PHE:HB2	1.76	0.83
1:J:436:PHE:CD2	1:K:408:HIS:HB3	2.13	0.83
1:H:436:PHE:O	1:H:436:PHE:HD1	1.61	0.83
1:E:164:VAL:HG13	1:E:198:VAL:HA	1.59	0.83
1:K:111:MET:CE	2:K:552:NDP:H72N	1.92	0.83
1:L:288:PRO:HA	1:L:291:LEU:HB2	1.60	0.83
1:B:394:TYR:HB2	1:B:445:GLU:HG3	1.61	0.83
1:L:87:THR:HB	1:L:88:PRO:HD3	1.60	0.83
1:H:118:VAL:HG23	1:H:120:VAL:HG23	1.61	0.83
1:K:288:PRO:HA	1:K:291:LEU:HB2	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:288:PRO:HA	1:E:291:LEU:HB2	1.60	0.83
1:D:164:VAL:HG13	1:D:198:VAL:HA	1.60	0.83
1:E:199:THR:HG22	1:E:384:GLU:HG2	1.60	0.83
1:F:56:ASN:O	1:F:57:HIS:HD2	1.59	0.83
1:A:118:VAL:HG23	1:A:120:VAL:HG23	1.61	0.83
1:D:96:SER:O	1:D:99:VAL:HG23	1.78	0.83
1:K:65:ILE:HD11	1:K:75:ILE:HD11	1.59	0.83
1:K:164:VAL:HG13	1:K:198:VAL:HA	1.59	0.82
1:J:67:ARG:HD3	1:J:73:GLU:OE2	1.79	0.82
1:I:164:VAL:HG13	1:I:198:VAL:HA	1.60	0.82
1:C:255:VAL:HG13	1:C:325:ALA:HB1	1.61	0.82
3:G:601:XEG:HAL	1:L:209:HIS:CE1	2.15	0.82
1:K:87:THR:HB	1:K:88:PRO:HD3	1.61	0.82
1:C:45:VAL:HG13	1:C:490:PHE:HE1	1.44	0.82
1:G:52:ILE:HG12	1:G:493:TYR:HE2	1.45	0.82
1:A:288:PRO:HA	1:A:291:LEU:HB2	1.60	0.82
1:C:152:LEU:HD12	1:C:157:PHE:HB2	1.62	0.82
1:A:366:MET:HB2	1:A:475:LEU:HD13	1.59	0.82
1:J:288:PRO:HA	1:J:291:LEU:HB2	1.61	0.82
1:C:79:ARG:HG2	1:C:127:ALA:HB2	1.59	0.82
1:G:56:ASN:O	1:G:57:HIS:HD2	1.60	0.82
1:A:382:TYR:CE2	1:A:386:LEU:HD11	2.15	0.82
1:G:52:ILE:HG12	1:G:493:TYR:CE2	2.15	0.82
1:G:408:HIS:HB3	1:H:436:PHE:HD2	1.44	0.82
1:F:473:LEU:HD22	1:F:480:ALA:HB2	1.62	0.82
1:K:16:PHE:HE2	1:K:354:PRO:HG3	1.43	0.82
1:G:459:ARG:NH2	3:G:601:XEG:OAH	2.13	0.81
1:G:87:THR:HB	1:G:88:PRO:HD3	1.63	0.81
1:F:287:ASP:O	1:F:291:LEU:HD13	1.81	0.81
1:G:287:ASP:O	1:G:291:LEU:HD13	1.79	0.81
1:K:287:ASP:O	1:K:291:LEU:HD13	1.80	0.81
1:D:214:ALA:HB1	1:D:380:VAL:HG21	1.60	0.81
1:G:436:PHE:HD1	1:G:436:PHE:O	1.62	0.81
1:I:87:THR:HB	1:I:88:PRO:HD3	1.60	0.81
1:I:288:PRO:HA	1:I:291:LEU:HB2	1.60	0.81
1:J:152:LEU:HD12	1:J:157:PHE:HB2	1.62	0.81
1:B:164:VAL:HG13	1:B:198:VAL:HA	1.63	0.81
1:H:288:PRO:HA	1:H:291:LEU:HB2	1.60	0.81
1:D:321:ILE:HG12	1:D:343:ILE:HB	1.63	0.81
1:H:214:ALA:HB1	1:H:380:VAL:HG21	1.61	0.81
1:A:164:VAL:HG13	1:A:198:VAL:HA	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:164:VAL:HG13	1:F:198:VAL:HA	1.63	0.81
1:D:226:PHE:CE2	1:D:465:MET:HE2	2.15	0.81
1:H:65:ILE:HD11	1:H:75:ILE:HD11	1.62	0.81
1:H:56:ASN:O	1:H:57:HIS:HD2	1.64	0.81
1:A:287:ASP:O	1:A:291:LEU:HD13	1.81	0.81
1:L:321:ILE:HG12	1:L:343:ILE:HB	1.63	0.81
1:F:152:LEU:HD12	1:F:157:PHE:HB2	1.62	0.81
1:D:152:LEU:HD12	1:D:157:PHE:HB2	1.61	0.81
1:F:255:VAL:HG13	1:F:325:ALA:HB1	1.62	0.81
1:B:321:ILE:HG12	1:B:343:ILE:HB	1.63	0.81
1:D:479:THR:O	1:D:483:VAL:HG23	1.81	0.80
1:K:199:THR:HG22	1:K:384:GLU:HG2	1.62	0.80
1:D:265:ARG:O	1:D:266:PHE:HB2	1.82	0.80
1:G:414:GLN:OE1	1:G:429:PRO:HD2	1.82	0.80
1:J:287:ASP:O	1:J:291:LEU:HD13	1.82	0.80
1:L:473:LEU:HD22	1:L:480:ALA:HB2	1.63	0.80
1:J:16:PHE:HE2	1:J:354:PRO:HG3	1.44	0.80
1:C:87:THR:HB	1:C:88:PRO:HD3	1.64	0.80
1:K:255:VAL:HG13	1:K:325:ALA:HB1	1.63	0.80
1:D:67:ARG:HD3	1:D:73:GLU:OE2	1.82	0.80
1:L:111:MET:HE2	2:L:552:NDP:N7N	1.94	0.80
1:J:24:VAL:HB	1:J:28:LEU:HD11	1.64	0.80
3:A:601:XEG:HAL	1:F:209:HIS:CE1	2.16	0.80
1:H:321:ILE:HG12	1:H:343:ILE:HB	1.63	0.80
1:E:111:MET:CE	2:E:552:NDP:H72N	1.95	0.80
1:C:87:THR:HB	1:C:88:PRO:CD	2.12	0.80
1:L:287:ASP:O	1:L:291:LEU:HD13	1.80	0.80
1:D:56:ASN:O	1:D:57:HIS:HD2	1.63	0.80
1:E:287:ASP:O	1:E:291:LEU:HD13	1.82	0.80
1:J:321:ILE:HG12	1:J:343:ILE:HB	1.64	0.80
1:B:265:ARG:O	1:B:266:PHE:HB2	1.80	0.80
1:I:56:ASN:O	1:I:57:HIS:HD2	1.63	0.80
1:E:366:MET:HB2	1:E:475:LEU:HD13	1.62	0.80
1:A:321:ILE:HG12	1:A:343:ILE:HB	1.64	0.80
1:G:255:VAL:HG13	1:G:325:ALA:HB1	1.63	0.80
1:L:436:PHE:HD1	1:L:436:PHE:O	1.64	0.80
1:B:96:SER:O	1:B:99:VAL:HG23	1.80	0.80
1:C:287:ASP:O	1:C:291:LEU:HD13	1.81	0.80
1:B:152:LEU:HD12	1:B:157:PHE:HB2	1.63	0.80
1:G:16:PHE:HE2	1:G:354:PRO:HG3	1.45	0.80
1:L:56:ASN:O	1:L:57:HIS:HD2	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:6:ASP:N	1:L:353:THR:HG1	1.80	0.79
1:I:287:ASP:O	1:I:291:LEU:HD13	1.80	0.79
1:H:488:LYS:HZ3	3:H:601:XEG:CAK	1.95	0.79
1:A:111:MET:HE2	2:A:552:NDP:N7N	1.98	0.79
1:C:201:LYS:O	1:C:211:ARG:NH1	2.14	0.79
1:J:488:LYS:HA	1:J:491:ARG:HG3	1.62	0.79
1:G:96:SER:O	1:G:99:VAL:HG23	1.82	0.79
1:H:287:ASP:O	1:H:291:LEU:HD13	1.82	0.79
1:A:16:PHE:CE2	1:A:354:PRO:HG3	2.17	0.79
1:L:265:ARG:O	1:L:266:PHE:HB2	1.79	0.79
1:C:65:ILE:HD11	1:C:75:ILE:HD11	1.64	0.79
1:A:498:VAL:HG11	1:D:66:ARG:HD2	1.64	0.79
1:D:281:TRP:CD1	1:D:283:PRO:HD3	2.18	0.79
1:F:321:ILE:HG12	1:F:343:ILE:HB	1.64	0.79
1:K:321:ILE:HG12	1:K:343:ILE:HB	1.63	0.79
1:I:152:LEU:HD12	1:I:157:PHE:HB2	1.63	0.79
1:K:93:ILE:HG22	1:K:127:ALA:HB3	1.64	0.79
1:D:288:PRO:HA	1:D:291:LEU:HB2	1.65	0.79
1:B:67:ARG:HD3	1:B:73:GLU:OE2	1.81	0.79
1:H:281:TRP:CD1	1:H:283:PRO:HD3	2.18	0.79
1:E:255:VAL:HG13	1:E:325:ALA:HB1	1.64	0.79
1:K:96:SER:O	1:K:99:VAL:HG23	1.82	0.79
1:J:65:ILE:HD11	1:J:75:ILE:HD11	1.64	0.79
1:J:382:TYR:CE2	1:J:386:LEU:HD11	2.16	0.79
1:H:492:VAL:HG23	1:H:493:TYR:N	1.98	0.78
1:H:488:LYS:NZ	3:H:601:XEG:CAK	2.46	0.78
1:E:396:ARG:HG3	1:E:396:ARG:HH11	1.48	0.78
1:B:479:THR:O	1:B:483:VAL:HG23	1.83	0.78
1:C:111:MET:CE	2:C:552:NDP:H72N	1.96	0.78
1:C:473:LEU:HD22	1:C:480:ALA:HB2	1.63	0.78
1:J:281:TRP:CD1	1:J:283:PRO:HD3	2.18	0.78
1:H:24:VAL:HB	1:H:28:LEU:HD11	1.63	0.78
1:K:67:ARG:HD3	1:K:73:GLU:OE2	1.84	0.78
1:C:321:ILE:HG12	1:C:343:ILE:HB	1.64	0.78
1:G:321:ILE:HG12	1:G:343:ILE:HB	1.64	0.78
1:J:255:VAL:HG13	1:J:325:ALA:HB1	1.65	0.78
1:J:272:THR:HG22	1:J:281:TRP:HA	1.65	0.78
1:B:455:TYR:HE1	1:B:459:ARG:HD3	1.48	0.78
1:D:436:PHE:CD1	1:D:436:PHE:O	2.37	0.78
1:A:96:SER:O	1:A:99:VAL:HG23	1.84	0.78
1:F:201:LYS:O	1:F:211:ARG:NH1	2.15	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:321:ILE:HG12	1:I:343:ILE:HB	1.64	0.78
1:J:413:VAL:HG12	1:J:429:PRO:HG3	1.66	0.78
1:G:199:THR:HG22	1:G:384:GLU:HG2	1.65	0.78
1:G:214:ALA:HB1	1:G:380:VAL:HG21	1.66	0.78
1:A:87:THR:HB	1:A:88:PRO:HD3	1.65	0.78
1:I:473:LEU:HD22	1:I:480:ALA:HB2	1.66	0.78
1:L:24:VAL:HB	1:L:28:LEU:HD11	1.65	0.78
1:D:212:ILE:H	1:D:212:ILE:HD13	1.47	0.78
1:F:67:ARG:HD3	1:F:73:GLU:OE2	1.83	0.78
1:I:436:PHE:O	1:I:436:PHE:HD1	1.65	0.78
1:E:87:THR:HB	1:E:88:PRO:HD3	1.64	0.78
1:C:96:SER:O	1:C:99:VAL:HG23	1.83	0.78
1:B:371:LEU:HD23	1:B:481:ALA:CB	2.14	0.78
1:E:93:ILE:HG22	1:E:127:ALA:HB3	1.65	0.78
1:E:24:VAL:HB	1:E:28:LEU:HD11	1.66	0.78
1:E:16:PHE:CE2	1:E:354:PRO:HG3	2.18	0.78
1:E:281:TRP:CD1	1:E:283:PRO:HD3	2.19	0.78
1:E:494:ASN:O	1:E:495:GLU:HG2	1.84	0.77
1:C:45:VAL:HG13	1:C:490:PHE:CE1	2.18	0.77
1:H:272:THR:HG22	1:H:281:TRP:HA	1.66	0.77
1:G:65:ILE:HD11	1:G:75:ILE:HD11	1.65	0.77
1:E:436:PHE:CD1	1:E:436:PHE:O	2.37	0.77
1:H:164:VAL:HG13	1:H:198:VAL:HA	1.66	0.77
1:C:67:ARG:HD3	1:C:73:GLU:OE2	1.84	0.77
1:L:152:LEU:HD12	1:L:157:PHE:HB2	1.65	0.77
1:A:369:PRO:HG3	1:A:478:ARG:N	1.99	0.77
1:I:24:VAL:HB	1:I:28:LEU:HD11	1.67	0.77
1:C:382:TYR:HE2	1:C:386:LEU:HD21	1.49	0.77
1:E:367:VAL:O	1:E:477:LEU:HD23	1.85	0.77
1:J:87:THR:HB	1:J:88:PRO:HD3	1.67	0.77
1:B:281:TRP:CD1	1:B:283:PRO:HD3	2.18	0.77
1:J:214:ALA:HB1	1:J:380:VAL:HG21	1.67	0.77
1:D:87:THR:HB	1:D:88:PRO:HD3	1.66	0.77
1:H:24:VAL:CG1	1:H:483:VAL:HG13	2.14	0.77
1:A:165:PRO:HD2	1:A:197:CYS:O	1.85	0.77
1:K:281:TRP:CD1	1:K:283:PRO:HD3	2.20	0.77
1:L:255:VAL:HG13	1:L:325:ALA:HB1	1.66	0.77
1:G:24:VAL:HB	1:G:28:LEU:HD11	1.65	0.77
1:H:96:SER:O	1:H:99:VAL:HG23	1.85	0.77
1:G:111:MET:CE	2:G:552:NDP:H72N	1.97	0.77
1:A:281:TRP:CD1	1:A:283:PRO:HD3	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:96:SER:O	1:E:99:VAL:HG23	1.84	0.77
1:A:255:VAL:HG13	1:A:325:ALA:HB1	1.64	0.77
1:C:24:VAL:HB	1:C:28:LEU:HD11	1.67	0.77
1:H:87:THR:HB	1:H:88:PRO:HD3	1.67	0.77
1:B:287:ASP:O	1:B:291:LEU:HD13	1.85	0.77
1:B:288:PRO:HA	1:B:291:LEU:HB2	1.66	0.77
1:A:67:ARG:HD3	1:A:73:GLU:OE2	1.84	0.77
1:B:255:VAL:HG13	1:B:325:ALA:HB1	1.66	0.77
1:A:455:TYR:HE1	1:A:459:ARG:HD3	1.50	0.77
1:H:394:TYR:HB2	1:H:445:GLU:HG3	1.67	0.77
1:E:245:LYS:HG2	1:E:320:ASP:OD1	1.85	0.77
1:B:24:VAL:CG1	1:B:483:VAL:HG13	2.12	0.76
1:E:498:VAL:HG23	1:E:500:PHE:CE2	2.20	0.76
1:A:24:VAL:HB	1:A:28:LEU:HD11	1.66	0.76
1:I:371:LEU:HD23	1:I:481:ALA:CB	2.15	0.76
1:L:272:THR:HG22	1:L:281:TRP:HA	1.67	0.76
1:F:7:PRO:HG3	1:F:353:THR:HG21	1.66	0.76
1:L:420:LYS:NZ	1:L:420:LYS:O	2.18	0.76
1:E:321:ILE:HG12	1:E:343:ILE:HB	1.64	0.76
1:L:96:SER:O	1:L:99:VAL:HG23	1.86	0.76
1:E:455:TYR:HE1	1:E:459:ARG:HD3	1.50	0.76
1:F:87:THR:HB	1:F:88:PRO:CD	2.15	0.76
1:C:99:VAL:CG1	1:C:128:GLY:HA3	2.15	0.76
1:G:394:TYR:HB2	1:G:445:GLU:HG3	1.67	0.76
1:F:87:THR:HB	1:F:88:PRO:HD3	1.66	0.76
1:H:492:VAL:HG23	1:H:493:TYR:H	1.49	0.76
1:L:281:TRP:CD1	1:L:283:PRO:HD3	2.21	0.76
1:A:147:ARG:HD2	1:D:501:THR:HG22	1.66	0.76
1:I:255:VAL:HG13	1:I:325:ALA:HB1	1.67	0.76
1:G:473:LEU:HD22	1:G:480:ALA:HB2	1.67	0.76
1:A:245:LYS:HG2	1:A:320:ASP:OD1	1.84	0.76
1:H:255:VAL:HG13	1:H:325:ALA:HB1	1.66	0.76
1:I:272:THR:HG22	1:I:281:TRP:HA	1.68	0.76
1:G:245:LYS:HG2	1:G:320:ASP:OD1	1.86	0.76
1:B:212:ILE:HD13	1:B:212:ILE:H	1.49	0.76
1:G:281:TRP:CD1	1:G:283:PRO:HD3	2.21	0.76
1:A:396:ARG:HG3	1:A:396:ARG:HH11	1.51	0.76
1:I:396:ARG:HG3	1:I:396:ARG:HH11	1.50	0.76
1:B:24:VAL:HB	1:B:28:LEU:HD11	1.67	0.76
1:I:86:ARG:HG2	1:I:121:PRO:C	2.05	0.76
1:I:87:THR:HB	1:I:88:PRO:CD	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:367:VAL:O	1:J:477:LEU:HD23	1.86	0.76
1:B:56:ASN:O	1:B:57:HIS:HD2	1.68	0.76
1:K:24:VAL:HB	1:K:28:LEU:HD11	1.66	0.76
1:H:367:VAL:O	1:H:477:LEU:HD23	1.85	0.76
1:D:287:ASP:O	1:D:291:LEU:HD13	1.86	0.76
1:I:281:TRP:CD1	1:I:283:PRO:HD3	2.21	0.76
1:C:281:TRP:CD1	1:C:283:PRO:HD3	2.20	0.76
1:F:214:ALA:HB1	1:F:380:VAL:HG21	1.65	0.76
1:D:455:TYR:HE1	1:D:459:ARG:HD3	1.50	0.76
1:I:432:PRO:HA	1:J:412:SER:HB3	1.67	0.75
1:F:96:SER:O	1:F:99:VAL:HG23	1.85	0.75
1:I:209:HIS:HE1	3:K:601:XEG:CAL	1.99	0.75
1:K:272:THR:HG22	1:K:281:TRP:HA	1.66	0.75
1:B:87:THR:HB	1:B:88:PRO:HD3	1.66	0.75
1:F:45:VAL:HG13	1:F:490:PHE:HE1	1.49	0.75
1:C:214:ALA:HB1	1:C:380:VAL:HG21	1.67	0.75
1:A:6:ASP:N	1:A:355:GLU:HG3	2.02	0.75
1:I:96:SER:O	1:I:99:VAL:HG23	1.86	0.75
1:H:412:SER:HB3	1:L:432:PRO:HA	1.67	0.75
1:E:414:GLN:OE1	1:E:429:PRO:HD2	1.86	0.75
1:G:93:ILE:HG22	1:G:127:ALA:HB3	1.67	0.75
1:G:6:ASP:HA	1:G:355:GLU:HG3	1.68	0.75
1:L:249:VAL:HG13	1:L:273:VAL:HG13	1.68	0.75
1:D:421:PHE:CE1	1:D:423:LYS:HG3	2.21	0.75
1:A:369:PRO:HD3	1:A:477:LEU:HB2	1.69	0.75
1:E:90:LYS:HB2	1:E:122:PHE:CD1	2.22	0.75
1:J:24:VAL:CG1	1:J:483:VAL:HG13	2.14	0.75
1:E:165:PRO:HD2	1:E:197:CYS:O	1.85	0.75
1:B:93:ILE:HG22	1:B:127:ALA:HB3	1.66	0.75
1:L:87:THR:HB	1:L:88:PRO:CD	2.16	0.75
1:J:249:VAL:HG13	1:J:273:VAL:HG13	1.68	0.75
1:B:366:MET:HB2	1:B:475:LEU:HD13	1.67	0.75
1:K:249:VAL:HG13	1:K:273:VAL:HG13	1.69	0.75
1:H:8:ASN:HB3	1:H:9:PHE:CE2	2.21	0.75
1:B:27:LYS:HD2	1:B:471:TYR:OH	1.86	0.75
1:J:164:VAL:HG13	1:J:198:VAL:HA	1.67	0.75
1:J:96:SER:O	1:J:99:VAL:HG23	1.87	0.75
1:L:336:ALA:HB1	1:L:359:ILE:HG21	1.69	0.75
1:I:24:VAL:HG13	1:I:483:VAL:HG13	1.67	0.75
1:F:281:TRP:CD1	1:F:283:PRO:HD3	2.20	0.75
1:D:371:LEU:HD23	1:D:481:ALA:CB	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:ARG:HD3	1:E:73:GLU:OE2	1.87	0.75
1:D:255:VAL:HG13	1:D:325:ALA:HB1	1.67	0.75
1:K:245:LYS:HG2	1:K:320:ASP:OD1	1.87	0.75
1:L:245:LYS:HG2	1:L:320:ASP:OD1	1.87	0.75
1:L:396:ARG:HG3	1:L:396:ARG:HH11	1.51	0.75
1:K:473:LEU:HD22	1:K:480:ALA:HB2	1.69	0.75
1:H:382:TYR:CE2	1:H:386:LEU:HD11	2.22	0.75
1:G:165:PRO:HD2	1:G:197:CYS:O	1.87	0.75
1:C:6:ASP:N	1:C:353:THR:HG1	1.84	0.75
1:B:272:THR:HG22	1:B:281:TRP:HA	1.68	0.75
1:L:455:TYR:HE1	1:L:459:ARG:HD3	1.50	0.75
1:D:36:GLU:HB3	1:D:40:GLN:HG2	1.69	0.74
1:C:272:THR:HG22	1:C:281:TRP:HA	1.69	0.74
1:B:36:GLU:HB3	1:B:40:GLN:HG2	1.69	0.74
1:A:336:ALA:HB1	1:A:359:ILE:HG21	1.69	0.74
1:A:93:ILE:HG22	1:A:127:ALA:HB3	1.69	0.74
1:A:397:LEU:HD11	1:B:383:PHE:CE2	2.22	0.74
1:K:214:ALA:HB1	1:K:380:VAL:HG21	1.69	0.74
1:H:413:VAL:HG12	1:H:429:PRO:HG3	1.68	0.74
1:L:403:ARG:O	1:L:403:ARG:HG2	1.86	0.74
1:E:286:ILE:HB	1:E:291:LEU:HD21	1.69	0.74
1:L:371:LEU:HD23	1:L:481:ALA:CB	2.17	0.74
1:D:498:VAL:HG23	1:D:499:THR:H	1.52	0.74
1:I:416:SER:HB3	1:K:428:ILE:O	1.87	0.74
1:E:249:VAL:HG13	1:E:273:VAL:HG13	1.70	0.74
1:I:67:ARG:HD3	1:I:73:GLU:OE2	1.87	0.74
1:K:165:PRO:HD2	1:K:197:CYS:O	1.88	0.74
1:C:165:PRO:HD2	1:C:197:CYS:O	1.88	0.74
1:A:382:TYR:HE2	1:A:386:LEU:HD21	1.52	0.74
1:A:346:GLU:CD	1:A:478:ARG:HH22	1.89	0.74
1:H:249:VAL:HG13	1:H:273:VAL:HG13	1.69	0.74
1:F:99:VAL:CG1	1:F:128:GLY:HA3	2.15	0.74
1:G:421:PHE:CE1	1:G:423:LYS:HG3	2.23	0.74
1:F:245:LYS:HG2	1:F:320:ASP:OD1	1.88	0.74
1:G:356:ALA:HB1	1:G:360:PHE:CE2	2.23	0.74
1:D:24:VAL:HB	1:D:28:LEU:HD11	1.68	0.74
1:A:436:PHE:O	1:A:436:PHE:CD1	2.39	0.74
1:G:67:ARG:HD3	1:G:73:GLU:OE2	1.86	0.74
1:J:455:TYR:HE1	1:J:459:ARG:HD3	1.53	0.74
1:F:272:THR:HG22	1:F:281:TRP:HA	1.69	0.74
1:B:421:PHE:CE1	1:B:423:LYS:HG3	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:421:PHE:CE1	1:K:423:LYS:HG3	2.22	0.74
1:J:394:TYR:HB2	1:J:445:GLU:HG3	1.69	0.74
1:G:397:LEU:HD11	1:H:383:PHE:CE2	2.23	0.74
1:E:152:LEU:HD12	1:E:157:PHE:CB	2.17	0.74
1:L:214:ALA:HB1	1:L:380:VAL:HG21	1.70	0.74
1:D:272:THR:HG22	1:D:281:TRP:HA	1.69	0.74
1:H:473:LEU:HD22	1:H:480:ALA:HB2	1.69	0.73
1:J:336:ALA:HB1	1:J:359:ILE:HG21	1.69	0.73
1:H:87:THR:HB	1:H:88:PRO:CD	2.18	0.73
1:I:286:ILE:HB	1:I:291:LEU:HD21	1.70	0.73
1:I:36:GLU:HB3	1:I:40:GLN:HG2	1.70	0.73
1:I:199:THR:HG22	1:I:384:GLU:HG2	1.70	0.73
1:K:356:ALA:HB1	1:K:360:PHE:CE2	2.23	0.73
1:E:212:ILE:HD13	1:E:212:ILE:H	1.53	0.73
1:I:86:ARG:NH1	1:I:492:VAL:HG21	2.03	0.73
1:F:382:TYR:HE2	1:F:386:LEU:HD21	1.52	0.73
1:L:199:THR:HG22	1:L:384:GLU:HG2	1.71	0.73
1:E:36:GLU:HB3	1:E:40:GLN:HG2	1.70	0.73
1:H:245:LYS:HG2	1:H:320:ASP:OD1	1.88	0.73
1:J:90:LYS:HB2	1:J:122:PHE:CD1	2.23	0.73
1:A:152:LEU:HD12	1:A:157:PHE:CB	2.17	0.73
1:A:386:LEU:HD21	1:F:391:HIS:O	1.88	0.73
1:G:272:THR:HG22	1:G:281:TRP:HA	1.67	0.73
1:I:356:ALA:HB1	1:I:360:PHE:CE2	2.24	0.73
1:I:336:ALA:HB1	1:I:359:ILE:HG21	1.68	0.73
1:E:272:THR:HG22	1:E:281:TRP:HA	1.70	0.73
1:A:212:ILE:HD13	1:A:212:ILE:H	1.52	0.73
1:C:245:LYS:HG2	1:C:320:ASP:OD1	1.88	0.73
1:B:226:PHE:CE2	1:B:465:MET:HE2	2.23	0.73
1:E:356:ALA:HB1	1:E:360:PHE:HE2	1.53	0.73
1:J:87:THR:HB	1:J:88:PRO:CD	2.18	0.73
1:G:356:ALA:HB1	1:G:360:PHE:HE2	1.54	0.73
1:C:36:GLU:HB3	1:C:40:GLN:HG2	1.69	0.73
1:I:403:ARG:O	1:I:403:ARG:HG2	1.88	0.73
1:C:436:PHE:CD1	1:C:436:PHE:O	2.41	0.73
1:A:249:VAL:HG13	1:A:273:VAL:HG13	1.71	0.73
1:H:345:ALA:HB1	1:H:373:LEU:CD2	2.19	0.73
1:A:286:ILE:HB	1:A:291:LEU:HD21	1.70	0.73
1:L:86:ARG:HG2	1:L:121:PRO:C	2.08	0.73
1:A:136:TYR:HB2	1:A:141:LEU:HD23	1.70	0.73
1:H:90:LYS:HB2	1:H:122:PHE:CD1	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:THR:HG22	1:A:281:TRP:HA	1.70	0.73
1:D:27:LYS:HD2	1:D:471:TYR:OH	1.88	0.73
1:D:336:ALA:HB1	1:D:359:ILE:HG21	1.71	0.73
1:F:36:GLU:HB3	1:F:40:GLN:HG2	1.70	0.73
1:A:36:GLU:HB3	1:A:40:GLN:HG2	1.69	0.73
1:J:436:PHE:HD2	1:K:408:HIS:HB3	1.49	0.73
1:A:414:GLN:OE1	1:A:429:PRO:HD2	1.88	0.73
1:B:436:PHE:O	1:B:436:PHE:CD1	2.40	0.73
1:H:336:ALA:HB1	1:H:359:ILE:HG21	1.70	0.73
1:K:371:LEU:HD23	1:K:481:ALA:CB	2.19	0.73
1:A:90:LYS:HB2	1:A:122:PHE:CD1	2.24	0.73
1:F:286:ILE:HB	1:F:291:LEU:HD21	1.70	0.73
1:C:286:ILE:HB	1:C:291:LEU:HD21	1.70	0.73
1:D:366:MET:HB2	1:D:475:LEU:HD13	1.71	0.73
1:G:396:ARG:HH11	1:G:396:ARG:HG3	1.53	0.73
1:C:391:HIS:O	1:E:386:LEU:HD21	1.88	0.72
1:A:413:VAL:HG12	1:A:429:PRO:HG3	1.70	0.72
1:G:87:THR:HB	1:G:88:PRO:CD	2.19	0.72
1:J:414:GLN:OE1	1:J:429:PRO:HD2	1.89	0.72
1:E:336:ALA:HB1	1:E:359:ILE:HG21	1.70	0.72
1:C:371:LEU:HD23	1:C:481:ALA:HB1	1.70	0.72
1:F:345:ALA:HB1	1:F:373:LEU:CD2	2.19	0.72
1:C:345:ALA:HB1	1:C:373:LEU:CD2	2.18	0.72
1:J:421:PHE:CE1	1:J:423:LYS:HG3	2.24	0.72
1:C:455:TYR:HE1	1:C:459:ARG:HD3	1.54	0.72
1:K:479:THR:O	1:K:483:VAL:HG23	1.89	0.72
1:A:323:ILE:HG22	1:A:345:ALA:HB3	1.71	0.72
1:L:212:ILE:H	1:L:212:ILE:HD13	1.54	0.72
1:B:136:TYR:HB2	1:B:141:LEU:HD23	1.70	0.72
1:H:421:PHE:CE1	1:H:423:LYS:HG3	2.25	0.72
1:D:356:ALA:HB1	1:D:360:PHE:CE2	2.24	0.72
1:E:52:ILE:HG12	1:E:493:TYR:HE2	1.54	0.72
1:D:93:ILE:HG22	1:D:127:ALA:HB3	1.70	0.72
1:F:24:VAL:HB	1:F:28:LEU:HD11	1.69	0.72
1:I:249:VAL:HG13	1:I:273:VAL:HG13	1.69	0.72
1:J:36:GLU:HB3	1:J:40:GLN:HG2	1.71	0.72
1:I:455:TYR:HE1	1:I:459:ARG:HD3	1.55	0.72
1:J:383:PHE:CE2	1:K:397:LEU:HD11	2.25	0.72
1:A:402:GLU:C	1:A:404:ASP:H	1.93	0.72
1:E:214:ALA:HB1	1:E:380:VAL:HG21	1.72	0.72
1:K:436:PHE:CD1	1:K:436:PHE:O	2.43	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ASN:OD1	1:A:134:LYS:HG2	1.90	0.72
1:I:420:LYS:O	1:I:420:LYS:NZ	2.19	0.72
1:B:369:PRO:HD3	1:B:477:LEU:HB2	1.71	0.72
1:I:9:PHE:HB3	1:I:329:LYS:NZ	2.04	0.72
1:B:356:ALA:HB1	1:B:360:PHE:CE2	2.25	0.72
1:G:212:ILE:H	1:G:212:ILE:HD13	1.53	0.72
1:H:371:LEU:HD23	1:H:481:ALA:CB	2.20	0.72
1:E:356:ALA:HB1	1:E:360:PHE:CE2	2.25	0.72
1:A:421:PHE:CE1	1:A:423:LYS:HG3	2.25	0.72
1:I:245:LYS:HG2	1:I:320:ASP:OD1	1.89	0.72
1:G:36:GLU:HB3	1:G:40:GLN:HG2	1.72	0.72
1:A:201:LYS:HB3	1:A:205:GLN:HB2	1.72	0.72
1:G:371:LEU:HD23	1:G:481:ALA:CB	2.19	0.72
1:I:165:PRO:HD2	1:I:197:CYS:O	1.90	0.72
1:B:488:LYS:HZ2	3:B:601:XEG:CAK	2.03	0.72
1:G:286:ILE:HB	1:G:291:LEU:HD21	1.72	0.72
1:A:356:ALA:HB1	1:A:360:PHE:CE2	2.24	0.72
1:B:90:LYS:HB2	1:B:122:PHE:CD1	2.24	0.72
1:H:488:LYS:NZ	3:H:601:XEG:HAK	2.04	0.72
1:J:436:PHE:CD1	1:J:436:PHE:O	2.43	0.72
1:I:409:LEU:HD23	1:K:409:LEU:HD23	1.71	0.72
1:B:336:ALA:HB1	1:B:359:ILE:HG21	1.71	0.72
1:J:479:THR:O	1:J:483:VAL:HG23	1.90	0.71
1:D:323:ILE:HG22	1:D:345:ALA:HB3	1.72	0.71
1:F:323:ILE:HG22	1:F:345:ALA:HB3	1.72	0.71
1:H:136:TYR:HB2	1:H:141:LEU:HD23	1.72	0.71
1:E:369:PRO:HG3	1:E:478:ARG:N	2.05	0.71
1:G:428:ILE:O	1:L:416:SER:HB3	1.89	0.71
1:K:459:ARG:NH2	3:K:601:XEG:OAH	2.23	0.71
1:F:45:VAL:HG13	1:F:490:PHE:CE1	2.24	0.71
1:B:488:LYS:O	1:B:491:ARG:HB2	1.90	0.71
1:K:286:ILE:HB	1:K:291:LEU:HD21	1.72	0.71
1:G:249:VAL:HG13	1:G:273:VAL:HG13	1.70	0.71
1:L:36:GLU:HB3	1:L:40:GLN:HG2	1.70	0.71
1:H:40:GLN:NE2	1:H:44:ARG:HB2	2.06	0.71
1:F:429:PRO:O	1:F:431:VAL:N	2.23	0.71
1:F:336:ALA:HB1	1:F:359:ILE:HG21	1.72	0.71
1:C:336:ALA:HB1	1:C:359:ILE:HG21	1.72	0.71
1:H:391:HIS:O	1:H:392:VAL:HG13	1.91	0.71
1:J:245:LYS:HG2	1:J:320:ASP:OD1	1.89	0.71
1:F:90:LYS:HB2	1:F:122:PHE:CD1	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:165:PRO:HD2	1:L:197:CYS:O	1.90	0.71
1:B:286:ILE:HB	1:B:291:LEU:HD21	1.72	0.71
1:K:356:ALA:HB1	1:K:360:PHE:HE2	1.53	0.71
1:H:36:GLU:HB3	1:H:40:GLN:HG2	1.70	0.71
1:L:345:ALA:HB1	1:L:373:LEU:CD2	2.21	0.71
1:L:356:ALA:HB1	1:L:360:PHE:CE2	2.25	0.71
1:D:490:PHE:CE2	1:D:494:ASN:HB2	2.25	0.71
1:I:214:ALA:HB1	1:I:380:VAL:HG21	1.72	0.71
1:A:356:ALA:HB1	1:A:360:PHE:HE2	1.53	0.71
1:B:414:GLN:OE1	1:B:429:PRO:HD2	1.90	0.71
1:C:356:ALA:HB1	1:C:360:PHE:CE2	2.25	0.71
1:D:24:VAL:HG13	1:D:483:VAL:CG1	2.14	0.71
1:E:201:LYS:HB3	1:E:205:GLN:HB2	1.73	0.71
1:F:165:PRO:HD2	1:F:197:CYS:O	1.91	0.71
1:H:455:TYR:HE1	1:H:459:ARG:HD3	1.55	0.71
1:I:323:ILE:HG22	1:I:345:ALA:HB3	1.72	0.71
1:K:500:PHE:C	1:L:501:THR:HB	2.10	0.71
1:H:412:SER:CB	1:L:432:PRO:HA	2.21	0.71
1:I:356:ALA:HB1	1:I:360:PHE:HE2	1.55	0.71
1:B:413:VAL:HG12	1:B:429:PRO:HG3	1.72	0.71
1:K:212:ILE:H	1:K:212:ILE:HD13	1.54	0.71
1:K:36:GLU:HB3	1:K:40:GLN:HG2	1.72	0.71
1:D:414:GLN:OE1	1:D:429:PRO:HD2	1.91	0.71
1:G:336:ALA:HB1	1:G:359:ILE:HG21	1.72	0.71
1:D:234:SER:C	1:D:236:LEU:H	1.94	0.71
1:K:396:ARG:HG3	1:K:396:ARG:HH11	1.55	0.71
1:D:27:LYS:HB2	1:D:471:TYR:OH	1.91	0.70
1:A:116:ALA:HA	3:A:601:XEG:OAC	1.91	0.70
1:K:87:THR:HB	1:K:88:PRO:CD	2.21	0.70
1:L:286:ILE:HB	1:L:291:LEU:HD21	1.70	0.70
1:I:345:ALA:HB1	1:I:373:LEU:CD2	2.21	0.70
1:H:497:GLY:O	1:H:499:THR:N	2.24	0.70
1:E:382:TYR:HD2	1:E:382:TYR:O	1.73	0.70
1:B:86:ARG:HG2	1:B:121:PRO:C	2.12	0.70
1:J:286:ILE:HB	1:J:291:LEU:HD21	1.74	0.70
1:L:323:ILE:HG22	1:L:345:ALA:HB3	1.72	0.70
1:A:394:TYR:HB2	1:A:445:GLU:HG3	1.72	0.70
1:D:249:VAL:HG13	1:D:273:VAL:HG13	1.72	0.70
1:E:40:GLN:NE2	1:E:44:ARG:HB2	2.06	0.70
1:G:403:ARG:HG2	1:G:403:ARG:O	1.90	0.70
1:H:436:PHE:CD1	1:H:436:PHE:O	2.44	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:PHE:CE2	1:E:397:LEU:HD11	2.25	0.70
1:D:286:ILE:HB	1:D:291:LEU:HD21	1.74	0.70
1:J:40:GLN:NE2	1:J:44:ARG:HB2	2.06	0.70
1:J:345:ALA:HB1	1:J:373:LEU:CD2	2.21	0.70
1:B:323:ILE:HG22	1:B:345:ALA:HB3	1.74	0.70
1:D:245:LYS:HG2	1:D:320:ASP:OD1	1.90	0.70
1:K:429:PRO:O	1:K:431:VAL:N	2.25	0.70
1:A:397:LEU:HD11	1:B:383:PHE:CZ	2.26	0.70
1:G:479:THR:O	1:G:483:VAL:HG23	1.92	0.70
1:H:247:PHE:HA	1:H:321:ILE:O	1.92	0.70
1:H:250:GLN:NE2	2:H:552:NDP:H2A	2.06	0.70
1:A:87:THR:HB	1:A:88:PRO:CD	2.22	0.70
1:E:136:TYR:HB2	1:E:141:LEU:HD23	1.71	0.70
1:K:403:ARG:HG2	1:K:403:ARG:O	1.91	0.70
1:L:255:VAL:HG12	2:L:552:NDP:O2N	1.91	0.70
1:E:413:VAL:HG12	1:E:429:PRO:HG3	1.71	0.70
1:K:336:ALA:HB1	1:K:359:ILE:HG21	1.74	0.70
1:L:24:VAL:HG13	1:L:483:VAL:HG13	1.71	0.70
1:I:432:PRO:HA	1:J:412:SER:CB	2.21	0.70
1:C:259:SER:O	1:C:263:LEU:HB2	1.90	0.70
1:B:403:ARG:HG2	1:B:403:ARG:O	1.91	0.70
1:B:27:LYS:HB2	1:B:471:TYR:OH	1.92	0.70
1:B:165:PRO:HD2	1:B:197:CYS:O	1.91	0.70
1:D:165:PRO:HD2	1:D:197:CYS:O	1.92	0.70
1:F:356:ALA:HB1	1:F:360:PHE:CE2	2.26	0.70
1:E:421:PHE:CE1	1:E:423:LYS:HG3	2.25	0.70
1:A:403:ARG:O	1:A:403:ARG:HG2	1.91	0.70
1:H:212:ILE:HD13	1:H:212:ILE:H	1.57	0.70
1:E:369:PRO:HD3	1:E:477:LEU:HB2	1.72	0.70
1:J:473:LEU:HD22	1:J:480:ALA:HB2	1.74	0.70
1:F:436:PHE:O	1:F:436:PHE:CD1	2.44	0.70
1:F:111:MET:HE2	2:F:552:NDP:H72N	1.55	0.70
1:L:356:ALA:HB1	1:L:360:PHE:HE2	1.56	0.70
1:K:40:GLN:NE2	1:K:44:ARG:HB2	2.07	0.70
1:H:403:ARG:HG2	1:H:403:ARG:O	1.91	0.70
1:D:383:PHE:CZ	1:E:397:LEU:HD11	2.27	0.70
1:E:91:GLY:O	1:E:165:PRO:HA	1.92	0.70
1:D:488:LYS:NZ	3:D:502:XEG:CAK	2.54	0.70
1:J:356:ALA:HB1	1:J:360:PHE:CE2	2.27	0.70
1:D:87:THR:HB	1:D:88:PRO:CD	2.21	0.70
1:H:323:ILE:HG22	1:H:345:ALA:HB3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:323:ILE:HG22	1:E:345:ALA:HB3	1.72	0.70
1:I:421:PHE:CE1	1:I:423:LYS:HG3	2.26	0.70
1:G:429:PRO:O	1:G:431:VAL:N	2.25	0.69
1:B:40:GLN:NE2	1:B:44:ARG:HB2	2.06	0.69
1:H:86:ARG:HG2	1:H:121:PRO:C	2.12	0.69
1:L:247:PHE:HA	1:L:321:ILE:O	1.92	0.69
1:B:245:LYS:HG2	1:B:320:ASP:OD1	1.91	0.69
1:A:429:PRO:O	1:A:431:VAL:N	2.25	0.69
1:B:87:THR:HB	1:B:88:PRO:CD	2.22	0.69
1:K:16:PHE:CE2	1:K:354:PRO:HG3	2.27	0.69
1:B:247:PHE:HA	1:B:321:ILE:O	1.92	0.69
1:J:489:VAL:O	1:J:492:VAL:HG23	1.92	0.69
1:I:40:GLN:NE2	1:I:44:ARG:HB2	2.07	0.69
1:D:420:LYS:O	1:D:420:LYS:NZ	2.25	0.69
1:H:479:THR:O	1:H:483:VAL:HG23	1.92	0.69
1:K:146:ARG:HG2	1:K:182:THR:OG1	1.92	0.69
1:E:458:GLU:O	1:E:460:SER:N	2.25	0.69
1:D:247:PHE:HA	1:D:321:ILE:O	1.92	0.69
1:F:259:SER:O	1:F:263:LEU:HB2	1.92	0.69
1:C:421:PHE:CE1	1:C:423:LYS:HG3	2.28	0.69
1:A:214:ALA:HB1	1:A:380:VAL:HG21	1.74	0.69
1:B:72:TRP:NE1	1:E:498:VAL:HG11	2.04	0.69
1:G:455:TYR:O	1:G:455:TYR:HD1	1.75	0.69
1:A:473:LEU:HD22	1:A:480:ALA:HB2	1.75	0.69
1:C:90:LYS:HB2	1:C:122:PHE:CD1	2.28	0.69
1:G:247:PHE:HA	1:G:321:ILE:O	1.92	0.69
1:K:111:MET:HE2	2:K:552:NDP:H72N	1.55	0.69
1:F:421:PHE:CE1	1:F:423:LYS:HG3	2.27	0.69
1:C:9:PHE:HB3	1:C:329:LYS:NZ	2.07	0.69
1:C:8:ASN:HB3	1:C:9:PHE:CD1	2.27	0.69
1:K:52:ILE:HG12	1:K:493:TYR:CE2	2.27	0.69
1:F:212:ILE:H	1:F:212:ILE:HD13	1.58	0.69
1:I:413:VAL:HG12	1:I:429:PRO:HG3	1.75	0.69
1:L:9:PHE:HB3	1:L:329:LYS:NZ	2.07	0.69
1:A:345:ALA:HB1	1:A:373:LEU:CD2	2.23	0.69
1:E:345:ALA:HB1	1:E:373:LEU:CD2	2.22	0.69
1:E:394:TYR:HB2	1:E:445:GLU:HG3	1.73	0.69
1:D:136:TYR:HB2	1:D:141:LEU:HD23	1.72	0.69
1:K:323:ILE:HG22	1:K:345:ALA:HB3	1.74	0.69
1:G:397:LEU:HD11	1:H:383:PHE:CZ	2.27	0.69
1:F:479:THR:O	1:F:483:VAL:HG23	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:SER:C	1:B:236:LEU:H	1.94	0.69
1:D:356:ALA:HB1	1:D:360:PHE:HE2	1.55	0.69
1:H:409:LEU:HD12	1:L:436:PHE:CE2	2.27	0.69
1:J:165:PRO:HD2	1:J:197:CYS:O	1.91	0.69
1:K:394:TYR:HB2	1:K:445:GLU:HG3	1.75	0.69
1:E:479:THR:O	1:E:483:VAL:HG23	1.92	0.69
1:C:86:ARG:HG2	1:C:121:PRO:C	2.12	0.69
1:F:247:PHE:HA	1:F:321:ILE:O	1.93	0.69
1:I:247:PHE:HA	1:I:321:ILE:O	1.92	0.69
1:H:414:GLN:OE1	1:H:429:PRO:HD2	1.92	0.69
1:F:136:TYR:HB2	1:F:141:LEU:HD23	1.74	0.69
1:L:67:ARG:HD3	1:L:73:GLU:OE2	1.90	0.69
1:K:136:TYR:HB2	1:K:141:LEU:HD23	1.75	0.69
1:A:391:HIS:O	1:A:392:VAL:HG13	1.91	0.69
1:D:120:VAL:HG13	1:D:382:TYR:CD1	2.28	0.69
1:D:90:LYS:HB2	1:D:122:PHE:CD1	2.27	0.69
1:I:7:PRO:HG2	1:I:11:LYS:HD3	1.74	0.69
1:A:91:GLY:O	1:A:165:PRO:HA	1.92	0.69
1:F:86:ARG:HG2	1:F:121:PRO:C	2.14	0.69
1:B:249:VAL:HG13	1:B:273:VAL:HG13	1.73	0.69
1:C:323:ILE:HG22	1:C:345:ALA:HB3	1.74	0.69
1:K:345:ALA:HB1	1:K:373:LEU:CD2	2.23	0.69
1:J:136:TYR:HB2	1:J:141:LEU:HD23	1.73	0.69
1:B:208:ILE:HB	1:B:384:GLU:HA	1.75	0.69
1:C:52:ILE:HD13	1:C:489:VAL:HG12	1.75	0.69
1:L:421:PHE:CE1	1:L:423:LYS:HG3	2.28	0.69
1:J:429:PRO:O	1:J:431:VAL:N	2.26	0.69
1:B:52:ILE:HD13	1:B:489:VAL:HG12	1.74	0.69
1:H:286:ILE:HB	1:H:291:LEU:HD21	1.73	0.69
1:J:234:SER:C	1:J:236:LEU:H	1.95	0.69
1:E:473:LEU:HD22	1:E:480:ALA:HB2	1.75	0.69
1:G:152:LEU:HD12	1:G:157:PHE:CB	2.22	0.69
1:C:247:PHE:HA	1:C:321:ILE:O	1.92	0.69
1:C:249:VAL:HG13	1:C:273:VAL:HG13	1.73	0.69
1:C:40:GLN:NE2	1:C:44:ARG:HB2	2.08	0.69
1:I:90:LYS:HB2	1:I:122:PHE:CD1	2.28	0.69
1:A:99:VAL:CG1	1:A:128:GLY:HA3	2.21	0.68
1:F:491:ARG:HD2	3:F:601:XEG:HAN	1.75	0.68
1:H:199:THR:HG22	1:H:384:GLU:HG2	1.75	0.68
1:E:90:LYS:HG3	1:E:122:PHE:CE1	2.27	0.68
1:B:120:VAL:HG13	1:B:382:TYR:CD1	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:247:PHE:HA	1:J:321:ILE:O	1.92	0.68
1:G:304:PHE:CD1	1:G:305:PRO:HD2	2.29	0.68
1:K:304:PHE:CD1	1:K:305:PRO:HD2	2.29	0.68
1:F:249:VAL:HG13	1:F:273:VAL:HG13	1.73	0.68
1:F:356:ALA:HB1	1:F:360:PHE:HE2	1.57	0.68
1:I:212:ILE:H	1:I:212:ILE:HD13	1.57	0.68
1:E:403:ARG:HG2	1:E:403:ARG:O	1.92	0.68
1:D:86:ARG:HG2	1:D:121:PRO:C	2.14	0.68
1:G:40:GLN:NE2	1:G:44:ARG:HB2	2.07	0.68
1:D:402:GLU:C	1:D:404:ASP:H	1.97	0.68
1:J:212:ILE:HD13	1:J:212:ILE:H	1.55	0.68
1:A:382:TYR:HD2	1:A:382:TYR:O	1.76	0.68
1:C:356:ALA:HB1	1:C:360:PHE:HE2	1.56	0.68
1:E:132:ASN:OD1	1:E:134:LYS:HG2	1.94	0.68
1:E:227:ILE:HD13	1:E:233:MET:SD	2.33	0.68
1:K:90:LYS:HB2	1:K:122:PHE:CD1	2.29	0.68
1:G:345:ALA:HB1	1:G:373:LEU:CD2	2.23	0.68
1:H:356:ALA:HB1	1:H:360:PHE:CE2	2.28	0.68
1:F:304:PHE:CD1	1:F:305:PRO:HD2	2.29	0.68
1:L:479:THR:O	1:L:483:VAL:HG23	1.94	0.68
1:C:209:HIS:CE1	3:E:601:XEG:HAL	2.26	0.68
1:A:40:GLN:NE2	1:A:44:ARG:HB2	2.07	0.68
1:L:40:GLN:NE2	1:L:44:ARG:HB2	2.08	0.68
1:E:304:PHE:CD1	1:E:305:PRO:HD2	2.29	0.68
1:D:40:GLN:NE2	1:D:44:ARG:HB2	2.08	0.68
1:D:369:PRO:HD3	1:D:477:LEU:HB2	1.76	0.68
1:B:356:ALA:HB1	1:B:360:PHE:HE2	1.57	0.68
1:H:304:PHE:CD1	1:H:305:PRO:HD2	2.29	0.68
1:G:16:PHE:CE2	1:G:354:PRO:HG3	2.28	0.68
1:J:323:ILE:HG22	1:J:345:ALA:HB3	1.76	0.68
1:H:293:ASP:O	1:H:297:GLN:HB3	1.93	0.68
1:G:436:PHE:O	1:G:436:PHE:CD1	2.45	0.68
1:J:371:LEU:HD23	1:J:481:ALA:CB	2.23	0.68
1:J:356:ALA:HB1	1:J:360:PHE:HE2	1.58	0.68
1:J:383:PHE:CZ	1:K:397:LEU:HD11	2.29	0.68
1:E:87:THR:HB	1:E:88:PRO:CD	2.22	0.68
1:G:90:LYS:HB2	1:G:122:PHE:CD1	2.29	0.68
1:K:247:PHE:HA	1:K:321:ILE:O	1.93	0.68
1:L:366:MET:HB2	1:L:475:LEU:HD13	1.76	0.68
1:F:40:GLN:NE2	1:F:44:ARG:HB2	2.08	0.68
1:I:259:SER:O	1:I:263:LEU:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:6:ASP:N	1:K:332:THR:HB	2.08	0.68
1:C:200:GLY:HA2	1:C:211:ARG:HD2	1.77	0.68
1:C:212:ILE:HD13	1:C:212:ILE:H	1.59	0.68
1:D:403:ARG:HG2	1:D:403:ARG:O	1.92	0.68
1:H:234:SER:C	1:H:236:LEU:H	1.96	0.67
1:K:221:HIS:HA	1:K:224:GLU:HB3	1.76	0.67
1:G:221:HIS:HA	1:G:224:GLU:HB3	1.75	0.67
1:B:333:LYS:HB2	1:B:355:GLU:HB3	1.76	0.67
1:J:366:MET:HB2	1:J:475:LEU:HD13	1.74	0.67
1:I:304:PHE:CD1	1:I:305:PRO:HD2	2.29	0.67
1:C:136:TYR:HB2	1:C:141:LEU:HD23	1.75	0.67
1:G:132:ASN:OD1	1:G:134:LYS:HG2	1.94	0.67
1:A:304:PHE:CD1	1:A:305:PRO:HD2	2.29	0.67
1:D:90:LYS:HG3	1:D:122:PHE:CE1	2.29	0.67
1:A:479:THR:O	1:A:483:VAL:HG23	1.95	0.67
1:C:91:GLY:O	1:C:165:PRO:HA	1.93	0.67
1:D:270:CYS:O	1:D:286:ILE:HG12	1.94	0.67
1:L:259:SER:O	1:L:263:LEU:HB2	1.95	0.67
1:B:391:HIS:O	1:B:392:VAL:HG13	1.95	0.67
1:A:6:ASP:HA	1:A:332:THR:HB	1.77	0.67
1:G:227:ILE:HD13	1:G:233:MET:SD	2.35	0.67
1:L:234:SER:C	1:L:236:LEU:H	1.98	0.67
1:H:458:GLU:O	1:H:460:SER:N	2.27	0.67
1:E:247:PHE:HA	1:E:321:ILE:O	1.94	0.67
1:H:90:LYS:HG3	1:H:122:PHE:CE1	2.29	0.67
1:J:403:ARG:HG2	1:J:403:ARG:O	1.93	0.67
1:D:413:VAL:HG12	1:D:429:PRO:HG3	1.76	0.67
1:G:455:TYR:HE1	1:G:459:ARG:HD3	1.58	0.67
1:H:366:MET:HB2	1:H:475:LEU:HD13	1.75	0.67
1:A:90:LYS:HG3	1:A:122:PHE:CE1	2.30	0.67
1:A:141:LEU:HD22	1:A:144:ILE:HD12	1.77	0.67
1:I:436:PHE:CE2	1:J:409:LEU:HD12	2.30	0.67
1:C:304:PHE:CD1	1:C:305:PRO:HD2	2.29	0.67
1:L:304:PHE:CD1	1:L:305:PRO:HD2	2.29	0.67
1:B:270:CYS:O	1:B:286:ILE:HG12	1.95	0.67
1:K:259:SER:O	1:K:263:LEU:HB2	1.95	0.67
1:I:177:SER:OG	1:K:496:ALA:HA	1.93	0.67
1:G:409:LEU:HD23	1:L:409:LEU:HD23	1.75	0.67
1:A:458:GLU:O	1:A:460:SER:N	2.28	0.67
1:L:6:ASP:C	1:L:8:ASN:H	1.98	0.67
1:F:200:GLY:HA2	1:F:211:ARG:HD2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:234:SER:C	1:I:236:LEU:H	1.97	0.67
1:H:8:ASN:HB3	1:H:9:PHE:CZ	2.30	0.67
1:L:458:GLU:O	1:L:460:SER:N	2.28	0.67
1:F:396:ARG:HH11	1:F:396:ARG:HG3	1.60	0.67
1:A:199:THR:HG22	1:A:384:GLU:CG	2.25	0.67
1:C:479:THR:O	1:C:483:VAL:HG23	1.94	0.67
1:G:136:TYR:HB2	1:G:141:LEU:HD23	1.75	0.67
1:F:414:GLN:OE1	1:F:429:PRO:HD2	1.94	0.67
1:I:366:MET:HB2	1:I:475:LEU:HD13	1.77	0.67
1:C:429:PRO:O	1:C:431:VAL:N	2.28	0.66
1:B:99:VAL:CG1	1:B:128:GLY:HA3	2.22	0.66
1:J:90:LYS:HG3	1:J:122:PHE:CE1	2.30	0.66
1:J:304:PHE:CD1	1:J:305:PRO:HD2	2.29	0.66
1:C:93:ILE:HG22	1:C:127:ALA:HB3	1.78	0.66
1:D:304:PHE:CD1	1:D:305:PRO:HD2	2.30	0.66
1:G:323:ILE:HG22	1:G:345:ALA:HB3	1.75	0.66
1:B:217:ARG:CD	1:B:450:HIS:CD2	2.78	0.66
1:G:259:SER:O	1:G:263:LEU:HB2	1.95	0.66
1:C:396:ARG:HG3	1:C:396:ARG:HH11	1.59	0.66
1:J:86:ARG:HG2	1:J:121:PRO:C	2.14	0.66
1:L:496:ALA:O	1:L:497:GLY:O	2.13	0.66
1:H:356:ALA:HB1	1:H:360:PHE:HE2	1.59	0.66
1:A:227:ILE:HD13	1:A:233:MET:SD	2.35	0.66
1:D:208:ILE:CG2	1:D:384:GLU:HB2	2.25	0.66
1:B:402:GLU:C	1:B:404:ASP:H	1.98	0.66
1:G:6:ASP:OD2	1:G:332:THR:HB	1.94	0.66
1:K:491:ARG:HD3	3:K:601:XEG:OAB	1.95	0.66
1:J:142:GLU:HB2	1:J:178:TRP:CZ2	2.30	0.66
1:B:304:PHE:CD1	1:B:305:PRO:HD2	2.30	0.66
1:I:496:ALA:HB1	1:J:181:ASP:OD2	1.94	0.66
1:K:132:ASN:OD1	1:K:134:LYS:HG2	1.95	0.66
1:G:413:VAL:HG21	1:L:413:VAL:HG21	1.76	0.66
1:E:382:TYR:HE2	1:E:386:LEU:HD21	1.60	0.66
1:A:86:ARG:HG2	1:A:121:PRO:C	2.15	0.66
1:A:402:GLU:O	1:A:404:ASP:N	2.26	0.66
1:C:458:GLU:O	1:C:460:SER:N	2.28	0.66
1:B:146:ARG:HG2	1:B:182:THR:OG1	1.94	0.66
1:G:146:ARG:HG2	1:G:182:THR:OG1	1.95	0.66
1:E:346:GLU:CD	1:E:478:ARG:HH22	1.97	0.66
1:D:458:GLU:O	1:D:460:SER:N	2.28	0.66
1:H:429:PRO:O	1:H:431:VAL:N	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:498:VAL:HG23	1:H:500:PHE:CE2	2.30	0.66
1:J:391:HIS:O	1:J:392:VAL:HG13	1.95	0.66
1:L:136:TYR:HB2	1:L:141:LEU:HD23	1.78	0.66
1:D:132:ASN:OD1	1:D:134:LYS:HG2	1.96	0.66
1:D:146:ARG:HG2	1:D:182:THR:OG1	1.96	0.66
1:L:436:PHE:CD1	1:L:436:PHE:O	2.48	0.66
1:A:247:PHE:HA	1:A:321:ILE:O	1.95	0.66
1:E:90:LYS:HB2	1:E:122:PHE:HD1	1.61	0.66
1:E:111:MET:HE2	2:E:552:NDP:N7N	2.07	0.66
1:B:488:LYS:NZ	3:B:601:XEG:CAK	2.59	0.66
1:F:234:SER:C	1:F:236:LEU:H	1.99	0.66
1:J:488:LYS:NZ	3:J:601:XEG:CAK	2.58	0.66
1:D:208:ILE:HB	1:D:384:GLU:HA	1.78	0.66
1:I:16:PHE:HE2	1:I:354:PRO:HG3	1.60	0.66
1:K:333:LYS:HB2	1:K:355:GLU:HB3	1.78	0.66
1:C:488:LYS:O	1:C:491:ARG:HB3	1.95	0.66
1:G:413:VAL:HG12	1:G:429:PRO:HG3	1.78	0.66
1:E:86:ARG:HG2	1:E:121:PRO:C	2.16	0.66
1:E:199:THR:HG22	1:E:384:GLU:CG	2.26	0.66
1:J:270:CYS:O	1:J:286:ILE:HG12	1.96	0.66
1:C:110:LEU:HD23	1:C:111:MET:N	2.10	0.66
1:I:458:GLU:O	1:I:460:SER:N	2.29	0.66
1:F:146:ARG:HG2	1:F:182:THR:OG1	1.96	0.66
1:J:396:ARG:HH11	1:J:396:ARG:HG3	1.61	0.66
1:C:270:CYS:O	1:C:286:ILE:HG12	1.95	0.66
1:D:499:THR:C	1:D:500:PHE:HD2	1.99	0.66
1:L:48:ILE:O	1:L:52:ILE:HG13	1.96	0.66
1:E:402:GLU:C	1:E:404:ASP:H	1.98	0.66
1:B:208:ILE:CG2	1:B:384:GLU:HB2	2.26	0.66
1:I:414:GLN:OE1	1:I:429:PRO:HD2	1.96	0.65
1:C:414:GLN:OE1	1:C:430:ILE:HG12	1.95	0.65
1:A:333:LYS:HB2	1:A:355:GLU:HB3	1.78	0.65
1:G:455:TYR:C	1:G:455:TYR:HD1	1.99	0.65
1:K:455:TYR:HE1	1:K:459:ARG:HD3	1.61	0.65
1:I:152:LEU:HD12	1:I:157:PHE:CB	2.25	0.65
1:A:259:SER:O	1:A:263:LEU:HB2	1.97	0.65
1:D:91:GLY:O	1:D:165:PRO:HA	1.96	0.65
1:C:111:MET:HE2	2:C:552:NDP:H72N	1.62	0.65
1:K:227:ILE:HD13	1:K:233:MET:SD	2.36	0.65
1:C:455:TYR:HD1	1:C:455:TYR:C	1.99	0.65
1:F:396:ARG:O	1:F:396:ARG:HG3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:199:THR:HG22	1:J:384:GLU:HG2	1.77	0.65
1:F:458:GLU:O	1:F:460:SER:N	2.29	0.65
1:F:52:ILE:HD13	1:F:489:VAL:HG12	1.79	0.65
1:L:414:GLN:OE1	1:L:429:PRO:HD2	1.97	0.65
1:B:333:LYS:HD2	1:B:355:GLU:OE1	1.97	0.65
1:K:382:TYR:HE2	1:K:386:LEU:HD21	1.62	0.65
1:G:383:PHE:CE2	1:L:397:LEU:HD11	2.30	0.65
1:K:152:LEU:HD12	1:K:157:PHE:CB	2.25	0.65
1:L:152:LEU:HD12	1:L:157:PHE:CB	2.26	0.65
1:D:396:ARG:HH11	1:D:396:ARG:HG3	1.60	0.65
1:C:403:ARG:O	1:C:403:ARG:HG2	1.97	0.65
1:J:333:LYS:HB2	1:J:355:GLU:HB3	1.78	0.65
1:C:333:LYS:HB2	1:C:355:GLU:HB3	1.79	0.65
1:I:479:THR:O	1:I:483:VAL:HG23	1.94	0.65
1:E:56:ASN:O	1:E:57:HIS:CD2	2.46	0.65
1:I:396:ARG:HG3	1:I:396:ARG:O	1.95	0.65
1:J:293:ASP:O	1:J:297:GLN:HB3	1.94	0.65
1:L:108:ALA:HB2	1:L:126:LYS:N	2.11	0.65
1:G:487:GLU:HG2	1:G:491:ARG:HH22	1.61	0.65
1:G:402:GLU:C	1:G:404:ASP:H	2.00	0.65
1:E:99:VAL:CG1	1:E:128:GLY:HA3	2.18	0.65
1:F:173:GLU:HB2	1:F:202:PRO:HD3	1.79	0.65
1:B:490:PHE:HE2	1:B:494:ASN:HB2	1.60	0.65
1:C:108:ALA:HB2	1:C:126:LYS:N	2.12	0.65
1:E:429:PRO:O	1:E:431:VAL:N	2.29	0.65
1:I:255:VAL:HG12	2:I:552:NDP:O2N	1.97	0.65
1:D:333:LYS:HB2	1:D:355:GLU:HB3	1.78	0.65
1:G:333:LYS:HB2	1:G:355:GLU:HB3	1.79	0.65
1:E:333:LYS:HB2	1:E:355:GLU:HB3	1.78	0.65
1:A:383:PHE:CZ	1:F:397:LEU:HD11	2.32	0.65
1:F:420:LYS:NZ	1:F:420:LYS:O	2.25	0.65
1:C:8:ASN:HB3	1:C:9:PHE:CE1	2.32	0.65
1:I:227:ILE:HD13	1:I:233:MET:SD	2.36	0.65
1:H:396:ARG:O	1:H:396:ARG:HG3	1.97	0.65
1:D:409:LEU:HD23	1:E:409:LEU:HD23	1.78	0.65
1:C:165:PRO:O	1:C:198:VAL:HG23	1.97	0.65
1:B:150:MET:HG3	1:E:501:THR:OG1	1.96	0.65
1:L:413:VAL:HG12	1:L:429:PRO:HG3	1.78	0.65
1:A:501:THR:CG2	1:D:147:ARG:HD3	2.25	0.65
1:A:150:MET:HG3	1:D:501:THR:HG23	1.79	0.65
1:C:455:TYR:CD1	1:C:455:TYR:C	2.70	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:ALA:HB1	1:D:373:LEU:CD2	2.27	0.65
1:F:414:GLN:OE1	1:F:430:ILE:HG12	1.95	0.65
1:I:9:PHE:HB3	1:I:329:LYS:HZ3	1.60	0.65
1:D:488:LYS:HZ2	3:D:502:XEG:CAK	2.09	0.65
1:H:270:CYS:O	1:H:286:ILE:HG12	1.96	0.65
1:F:270:CYS:O	1:F:286:ILE:HG12	1.96	0.65
1:F:108:ALA:HB2	1:F:126:LYS:N	2.12	0.65
1:B:90:LYS:HG3	1:B:122:PHE:CE1	2.32	0.65
1:F:91:GLY:O	1:F:165:PRO:HA	1.97	0.65
1:J:436:PHE:CE2	1:K:409:LEU:HD12	2.32	0.64
1:G:409:LEU:HD12	1:H:436:PHE:CE2	2.32	0.64
1:K:270:CYS:O	1:K:286:ILE:HG12	1.97	0.64
1:B:132:ASN:OD1	1:B:134:LYS:HG2	1.95	0.64
1:E:259:SER:O	1:E:263:LEU:HB2	1.97	0.64
1:H:333:LYS:HB2	1:H:355:GLU:HB3	1.79	0.64
1:E:141:LEU:HD22	1:E:144:ILE:HD12	1.78	0.64
1:D:374:ASN:C	1:D:376:GLY:H	2.00	0.64
1:B:420:LYS:O	1:B:420:LYS:NZ	2.26	0.64
1:C:414:GLN:OE1	1:C:429:PRO:HD2	1.96	0.64
1:L:8:ASN:O	1:L:329:LYS:HD2	1.97	0.64
1:L:396:ARG:O	1:L:396:ARG:HG3	1.97	0.64
1:F:455:TYR:HD1	1:F:455:TYR:C	2.00	0.64
1:K:234:SER:C	1:K:236:LEU:H	1.99	0.64
1:A:366:MET:HA	1:A:475:LEU:HB3	1.80	0.64
1:A:414:GLN:OE1	1:A:430:ILE:HG12	1.97	0.64
1:E:61:LEU:HD11	1:E:151:GLU:HB3	1.79	0.64
1:E:116:ALA:HA	3:E:601:XEG:OAC	1.97	0.64
1:F:56:ASN:O	1:F:57:HIS:CD2	2.48	0.64
1:D:152:LEU:HD12	1:D:157:PHE:CB	2.27	0.64
1:K:238:MET:O	1:K:240:PRO:HD3	1.98	0.64
1:C:493:TYR:O	1:C:495:GLU:N	2.29	0.64
1:B:333:LYS:HA	1:B:336:ALA:HB2	1.80	0.64
1:G:173:GLU:HB2	1:G:202:PRO:HD3	1.80	0.64
1:K:455:TYR:O	1:K:455:TYR:HD1	1.81	0.64
1:C:234:SER:C	1:C:236:LEU:H	1.99	0.64
1:D:61:LEU:HD11	1:D:151:GLU:HB3	1.79	0.64
1:G:111:MET:HE2	2:G:552:NDP:H72N	1.62	0.64
1:H:374:ASN:C	1:H:376:GLY:H	2.01	0.64
1:L:227:ILE:HD13	1:L:233:MET:SD	2.38	0.64
1:I:413:VAL:HG21	1:K:413:VAL:HG21	1.77	0.64
1:A:409:LEU:HD23	1:B:409:LEU:HD23	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:LYS:HB3	1:B:205:GLN:HB2	1.80	0.64
1:B:489:VAL:O	1:B:492:VAL:HG23	1.98	0.64
1:J:238:MET:O	1:J:240:PRO:HD3	1.98	0.64
1:C:250:GLN:NE2	2:C:552:NDP:H2A	2.13	0.64
1:G:270:CYS:O	1:G:286:ILE:HG12	1.98	0.64
1:L:270:CYS:O	1:L:286:ILE:HG12	1.97	0.64
1:A:323:ILE:CG2	1:A:345:ALA:HB3	2.27	0.64
1:D:323:ILE:CG2	1:D:345:ALA:HB3	2.27	0.64
1:H:396:ARG:HH11	1:H:396:ARG:HG3	1.62	0.64
1:D:217:ARG:CD	1:D:450:HIS:CD2	2.80	0.64
1:C:413:VAL:HG21	1:E:413:VAL:HG21	1.80	0.64
1:A:56:ASN:O	1:A:57:HIS:CD2	2.45	0.64
1:G:234:SER:C	1:G:236:LEU:H	2.00	0.64
1:C:499:THR:HG22	1:F:65:ILE:HG23	1.79	0.64
1:I:270:CYS:O	1:I:286:ILE:HG12	1.98	0.64
1:L:93:ILE:HG22	1:L:127:ALA:HB3	1.79	0.64
1:H:238:MET:O	1:H:240:PRO:HD3	1.98	0.64
1:B:149:THR:HB	1:B:182:THR:HG21	1.80	0.64
1:D:227:ILE:HD13	1:D:233:MET:SD	2.38	0.64
1:L:221:HIS:HA	1:L:224:GLU:HB3	1.80	0.64
1:D:333:LYS:HD2	1:D:355:GLU:OE1	1.97	0.64
1:B:487:GLU:O	1:B:491:ARG:HG3	1.98	0.64
1:L:323:ILE:CG2	1:L:345:ALA:HB3	2.28	0.64
1:J:458:GLU:O	1:J:460:SER:N	2.31	0.64
1:D:293:ASP:O	1:D:297:GLN:HB3	1.98	0.64
1:J:108:ALA:HB2	1:J:126:LYS:N	2.13	0.64
1:I:221:HIS:HA	1:I:224:GLU:HB3	1.80	0.64
1:I:136:TYR:HB2	1:I:141:LEU:HD23	1.78	0.64
1:A:420:LYS:NZ	1:A:420:LYS:O	2.28	0.64
1:E:414:GLN:OE1	1:E:430:ILE:HG12	1.98	0.64
1:D:99:VAL:CG1	1:D:128:GLY:HA3	2.24	0.64
1:B:61:LEU:HD11	1:B:151:GLU:HB3	1.79	0.64
1:I:495:GLU:O	1:I:496:ALA:HB2	1.98	0.64
1:K:402:GLU:C	1:K:404:ASP:H	1.99	0.64
1:E:270:CYS:O	1:E:286:ILE:HG12	1.98	0.64
1:H:412:SER:N	1:L:433:THR:HG22	2.12	0.64
1:K:108:ALA:HB2	1:K:126:LYS:N	2.13	0.64
1:K:86:ARG:HG2	1:K:121:PRO:C	2.17	0.64
1:A:61:LEU:HD11	1:A:151:GLU:HB3	1.80	0.64
1:F:371:LEU:HD23	1:F:481:ALA:HB1	1.79	0.64
1:H:27:LYS:HD2	1:H:471:TYR:OH	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:333:LYS:HD2	1:F:355:GLU:OE1	1.98	0.63
1:B:48:ILE:O	1:B:52:ILE:HG13	1.98	0.63
1:K:337:PRO:HB3	1:K:363:ARG:HD2	1.80	0.63
1:D:494:ASN:C	1:D:494:ASN:HD22	2.02	0.63
1:I:132:ASN:OD1	1:I:134:LYS:HG2	1.97	0.63
1:J:146:ARG:HG2	1:J:182:THR:OG1	1.98	0.63
1:K:413:VAL:HG12	1:K:429:PRO:HG3	1.80	0.63
1:A:369:PRO:HD3	1:A:477:LEU:CB	2.28	0.63
1:J:93:ILE:HG22	1:J:127:ALA:HB3	1.80	0.63
1:I:7:PRO:HD2	1:I:11:LYS:HB3	1.81	0.63
1:K:6:ASP:HB2	1:K:353:THR:HG21	1.80	0.63
1:C:333:LYS:HD2	1:C:355:GLU:OE1	1.98	0.63
1:L:201:LYS:HB3	1:L:205:GLN:HB2	1.80	0.63
1:I:108:ALA:HB2	1:I:126:LYS:N	2.12	0.63
1:L:90:LYS:HB2	1:L:122:PHE:CD1	2.33	0.63
1:B:91:GLY:O	1:B:165:PRO:HA	1.97	0.63
1:L:9:PHE:HB3	1:L:329:LYS:HZ3	1.63	0.63
1:E:148:PHE:CZ	1:E:152:LEU:HD21	2.33	0.63
1:F:323:ILE:CG2	1:F:345:ALA:HB3	2.28	0.63
1:F:455:TYR:CD1	1:F:455:TYR:C	2.72	0.63
1:E:391:HIS:O	1:E:392:VAL:HG13	1.98	0.63
1:L:300:THR:HG23	1:L:301:ILE:H	1.63	0.63
1:G:61:LEU:HD11	1:G:151:GLU:HB3	1.81	0.63
1:J:382:TYR:HE2	1:J:386:LEU:HD21	1.64	0.63
1:C:34:THR:HG22	1:C:36:GLU:H	1.63	0.63
1:I:391:HIS:O	1:I:392:VAL:HG13	1.99	0.63
1:H:402:GLU:C	1:H:404:ASP:H	2.01	0.63
1:E:293:ASP:O	1:E:297:GLN:HB3	1.99	0.63
1:B:24:VAL:HG13	1:B:483:VAL:CG1	2.19	0.63
1:J:333:LYS:HD2	1:J:355:GLU:OE1	1.98	0.63
1:H:165:PRO:HD2	1:H:197:CYS:O	1.98	0.63
1:I:323:ILE:CG2	1:I:345:ALA:HB3	2.28	0.63
1:I:300:THR:HG23	1:I:301:ILE:H	1.64	0.63
1:A:270:CYS:O	1:A:286:ILE:HG12	1.98	0.63
1:J:333:LYS:HA	1:J:336:ALA:HB2	1.81	0.63
1:F:337:PRO:HB3	1:F:363:ARG:HD2	1.81	0.63
1:F:201:LYS:HD3	1:F:384:GLU:OE1	1.98	0.63
1:G:498:VAL:HG11	1:J:66:ARG:NH1	2.13	0.63
1:F:90:LYS:HG3	1:F:122:PHE:CE1	2.34	0.63
1:G:238:MET:O	1:G:240:PRO:HD3	1.99	0.63
1:B:366:MET:HA	1:B:475:LEU:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:146:ARG:HG2	1:H:182:THR:OG1	1.99	0.63
1:B:58:VAL:HG13	1:E:60:SER:HB2	1.81	0.63
1:F:333:LYS:HB2	1:F:355:GLU:HB3	1.78	0.63
1:K:201:LYS:HB3	1:K:205:GLN:HB2	1.80	0.63
1:C:337:PRO:HB3	1:C:363:ARG:HD2	1.81	0.63
1:B:345:ALA:HB1	1:B:373:LEU:CD2	2.29	0.63
1:F:455:TYR:HD1	1:F:455:TYR:O	1.82	0.63
1:L:402:GLU:C	1:L:404:ASP:H	2.01	0.63
1:D:337:PRO:HB3	1:D:363:ARG:HD2	1.81	0.63
1:B:92:GLY:HA2	1:B:166:ALA:O	1.98	0.63
1:G:337:PRO:HB3	1:G:363:ARG:HD2	1.81	0.63
1:A:92:GLY:HA2	1:A:166:ALA:O	1.98	0.63
1:F:24:VAL:HG13	1:F:483:VAL:HG13	1.81	0.63
1:D:321:ILE:CG1	1:D:343:ILE:HB	2.29	0.63
1:D:238:MET:O	1:D:240:PRO:HD3	1.99	0.63
1:C:9:PHE:HA	1:C:329:LYS:HD3	1.81	0.63
1:B:108:ALA:HB2	1:B:126:LYS:N	2.13	0.63
1:B:259:SER:O	1:B:263:LEU:HB2	1.99	0.63
1:B:374:ASN:C	1:B:376:GLY:H	2.00	0.63
1:F:110:LEU:HD23	1:F:111:MET:N	2.13	0.63
1:J:250:GLN:NE2	2:J:552:NDP:H2A	2.14	0.63
1:L:166:ALA:HA	1:L:176:MET:HE2	1.81	0.63
1:B:321:ILE:CG1	1:B:343:ILE:HB	2.29	0.63
1:A:34:THR:HG22	1:A:36:GLU:H	1.63	0.63
1:D:52:ILE:HD13	1:D:489:VAL:HG12	1.79	0.63
1:J:141:LEU:O	1:J:145:THR:HG23	1.99	0.63
1:C:132:ASN:OD1	1:C:134:LYS:HG2	1.99	0.63
1:D:158:ILE:HG23	1:D:158:ILE:O	1.98	0.63
1:D:100:SER:HB3	1:D:103:GLU:HB2	1.80	0.62
1:H:99:VAL:CG1	1:H:128:GLY:HA3	2.27	0.62
1:H:333:LYS:HD2	1:H:355:GLU:OE1	1.99	0.62
1:L:391:HIS:O	1:L:392:VAL:HG13	1.99	0.62
1:E:337:PRO:HB3	1:E:363:ARG:HD2	1.79	0.62
1:H:455:TYR:HD1	1:H:455:TYR:C	2.02	0.62
1:H:414:GLN:OE1	1:H:430:ILE:HG12	1.99	0.62
1:C:52:ILE:HD13	1:C:489:VAL:CG1	2.29	0.62
1:B:293:ASP:O	1:B:297:GLN:HB3	1.98	0.62
1:I:436:PHE:CD1	1:I:436:PHE:O	2.49	0.62
1:I:382:TYR:CE2	1:I:386:LEU:HD11	2.34	0.62
1:C:146:ARG:HG2	1:C:182:THR:OG1	1.98	0.62
1:I:201:LYS:O	1:I:211:ARG:NH1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:TYR:C	1:A:455:TYR:HD1	2.03	0.62
1:L:238:MET:O	1:L:240:PRO:HD3	1.99	0.62
1:E:323:ILE:CG2	1:E:345:ALA:HB3	2.28	0.62
1:C:420:LYS:O	1:C:420:LYS:NZ	2.26	0.62
1:A:234:SER:C	1:A:236:LEU:H	2.03	0.62
1:C:402:GLU:C	1:C:404:ASP:H	2.01	0.62
1:H:333:LYS:HA	1:H:336:ALA:HB2	1.81	0.62
1:K:173:GLU:HB2	1:K:202:PRO:HD3	1.80	0.62
1:E:455:TYR:HD1	1:E:455:TYR:C	2.03	0.62
1:D:366:MET:HA	1:D:475:LEU:HB3	1.80	0.62
1:F:59:LEU:HB2	1:F:157:PHE:CE2	2.35	0.62
1:H:413:VAL:HG12	1:H:414:GLN:N	2.14	0.62
1:I:141:LEU:HD22	1:I:144:ILE:HD12	1.82	0.62
1:A:107:LEU:HD22	1:A:126:LYS:HD3	1.80	0.62
1:L:132:ASN:OD1	1:L:134:LYS:HG2	1.99	0.62
1:G:455:TYR:CD1	1:G:455:TYR:C	2.70	0.62
1:D:92:GLY:HA2	1:D:166:ALA:O	1.98	0.62
1:H:300:THR:HG23	1:H:301:ILE:H	1.65	0.62
1:A:16:PHE:HE2	1:A:354:PRO:CG	2.08	0.62
1:B:396:ARG:HG3	1:B:396:ARG:HH11	1.64	0.62
1:D:149:THR:HB	1:D:182:THR:HG21	1.80	0.62
1:B:501:THR:HG21	1:E:147:ARG:HD2	1.80	0.62
1:I:48:ILE:O	1:I:52:ILE:HG13	1.99	0.62
1:F:293:ASP:O	1:F:297:GLN:HB3	1.99	0.62
1:D:333:LYS:HA	1:D:336:ALA:HB2	1.80	0.62
1:F:86:ARG:NH1	1:F:492:VAL:HG11	2.14	0.62
1:I:34:THR:HG22	1:I:36:GLU:H	1.64	0.62
1:B:429:PRO:O	1:B:431:VAL:N	2.33	0.62
1:A:499:THR:O	1:A:499:THR:HG22	1.99	0.62
1:F:52:ILE:HD13	1:F:489:VAL:CG1	2.29	0.62
1:F:9:PHE:HB3	1:F:329:LYS:NZ	2.13	0.62
1:G:293:ASP:O	1:G:297:GLN:HB3	2.00	0.62
1:F:403:ARG:HG2	1:F:403:ARG:O	1.99	0.62
1:A:337:PRO:HB3	1:A:363:ARG:HD2	1.80	0.62
1:K:333:LYS:HA	1:K:336:ALA:HB2	1.81	0.62
1:I:238:MET:O	1:I:240:PRO:HD3	2.00	0.62
1:L:321:ILE:CG1	1:L:343:ILE:HB	2.29	0.62
1:C:455:TYR:O	1:C:455:TYR:HD1	1.82	0.62
1:B:323:ILE:CG2	1:B:345:ALA:HB3	2.29	0.62
1:E:99:VAL:HG11	1:E:128:GLY:CA	2.22	0.62
1:C:409:LEU:HD23	1:E:409:LEU:HD23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:333:LYS:HB2	1:I:355:GLU:HB3	1.82	0.62
1:E:92:GLY:HA2	1:E:166:ALA:O	1.98	0.62
1:K:199:THR:HG22	1:K:384:GLU:CG	2.29	0.62
1:G:382:TYR:HE2	1:G:386:LEU:HD21	1.64	0.62
1:K:455:TYR:HD1	1:K:455:TYR:C	2.03	0.62
1:J:455:TYR:HD1	1:J:455:TYR:C	2.03	0.62
1:F:34:THR:HG22	1:F:36:GLU:H	1.63	0.62
1:H:34:THR:HG22	1:H:36:GLU:H	1.65	0.62
1:J:396:ARG:O	1:J:396:ARG:HG3	2.00	0.62
1:E:106:ALA:O	1:E:109:SER:HB3	1.99	0.62
1:K:9:PHE:HB3	1:K:329:LYS:HZ3	1.65	0.62
1:C:99:VAL:HG11	1:C:128:GLY:CA	2.21	0.62
1:D:429:PRO:O	1:D:431:VAL:N	2.32	0.62
1:G:333:LYS:HA	1:G:336:ALA:HB2	1.82	0.62
1:J:99:VAL:CG1	1:J:128:GLY:HA3	2.27	0.62
1:L:333:LYS:HD2	1:L:355:GLU:OE1	1.99	0.62
1:L:16:PHE:HE2	1:L:354:PRO:HG3	1.64	0.62
1:L:445:GLU:O	1:L:449:VAL:HG23	2.00	0.62
1:A:293:ASP:O	1:A:297:GLN:HB3	2.00	0.62
1:E:234:SER:C	1:E:236:LEU:H	2.02	0.62
1:A:159:GLY:O	1:A:162:VAL:HG12	2.00	0.62
1:I:428:ILE:O	1:J:416:SER:HB3	1.99	0.62
1:E:493:TYR:O	1:E:495:GLU:N	2.32	0.62
1:H:336:ALA:CB	1:H:337:PRO:HD3	2.27	0.62
1:G:99:VAL:CG1	1:G:128:GLY:HA3	2.25	0.62
1:B:337:PRO:HB3	1:B:363:ARG:HD2	1.82	0.62
1:D:201:LYS:HB3	1:D:205:GLN:HB2	1.80	0.62
1:L:6:ASP:O	1:L:8:ASN:N	2.32	0.62
1:F:208:ILE:HG22	1:F:211:ARG:HB2	1.81	0.62
1:C:201:LYS:HD3	1:C:384:GLU:OE1	2.00	0.62
1:A:48:ILE:O	1:A:52:ILE:HG13	2.00	0.62
1:G:498:VAL:HG21	1:G:500:PHE:CZ	2.34	0.62
1:L:242:PHE:O	1:L:244:ASP:N	2.33	0.62
1:B:94:ARG:HG3	1:B:169:MET:CB	2.26	0.62
1:G:445:GLU:O	1:G:449:VAL:HG23	2.00	0.62
1:F:93:ILE:HG22	1:F:127:ALA:HB3	1.80	0.62
1:G:366:MET:HB2	1:G:475:LEU:HD13	1.81	0.62
1:B:8:ASN:HD22	1:B:329:LYS:HD2	1.64	0.62
1:B:196:ALA:CB	1:B:389:LEU:CD2	2.78	0.62
1:G:409:LEU:O	1:G:411:MET:N	2.31	0.61
1:B:34:THR:HG22	1:B:36:GLU:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:GLU:O	1:B:460:SER:N	2.33	0.61
1:L:382:TYR:CE2	1:L:386:LEU:HD11	2.35	0.61
1:C:499:THR:CG2	1:F:147:ARG:HE	2.13	0.61
1:D:273:VAL:O	1:D:314:ILE:HD12	2.00	0.61
1:L:34:THR:HG22	1:L:36:GLU:H	1.64	0.61
1:K:9:PHE:HB3	1:K:329:LYS:NZ	2.14	0.61
1:I:416:SER:CB	1:K:429:PRO:HA	2.30	0.61
1:F:300:THR:HG23	1:F:301:ILE:H	1.65	0.61
1:I:321:ILE:CG1	1:I:343:ILE:HB	2.30	0.61
1:E:34:THR:HG22	1:E:36:GLU:H	1.64	0.61
1:A:38:GLU:HG2	1:A:39:GLU:H	1.65	0.61
1:C:177:SER:OG	1:E:496:ALA:HA	2.00	0.61
1:F:402:GLU:C	1:F:404:ASP:H	2.03	0.61
1:G:333:LYS:HD2	1:G:355:GLU:OE1	2.00	0.61
1:I:100:SER:HB3	1:I:103:GLU:HB2	1.82	0.61
1:K:321:ILE:CG1	1:K:343:ILE:HB	2.31	0.61
1:F:148:PHE:CZ	1:F:152:LEU:HD21	2.35	0.61
1:J:34:THR:HG22	1:J:36:GLU:H	1.65	0.61
1:D:242:PHE:O	1:D:244:ASP:N	2.33	0.61
1:F:227:ILE:HD13	1:F:233:MET:SD	2.41	0.61
1:C:92:GLY:HA2	1:C:166:ALA:O	2.00	0.61
1:C:152:LEU:HD12	1:C:157:PHE:CB	2.29	0.61
1:D:300:THR:HG23	1:D:301:ILE:H	1.65	0.61
1:H:142:GLU:HB2	1:H:178:TRP:CZ2	2.36	0.61
1:D:259:SER:O	1:D:263:LEU:HB2	2.01	0.61
1:D:379:THR:O	1:D:382:TYR:HB3	2.00	0.61
1:G:201:LYS:HB3	1:G:205:GLN:HB2	1.81	0.61
1:C:116:ALA:O	1:C:488:LYS:HD2	2.00	0.61
1:L:91:GLY:O	1:L:165:PRO:HA	2.00	0.61
1:B:273:VAL:O	1:B:314:ILE:HD12	2.00	0.61
1:A:279:SER:HB2	1:A:310:TYR:O	2.00	0.61
1:E:38:GLU:HG2	1:E:39:GLU:H	1.65	0.61
1:C:293:ASP:O	1:C:297:GLN:HB3	1.99	0.61
1:B:242:PHE:O	1:B:244:ASP:N	2.33	0.61
1:J:300:THR:HG23	1:J:301:ILE:H	1.65	0.61
1:G:60:SER:HB2	1:J:58:VAL:HG13	1.83	0.61
1:G:429:PRO:HA	1:L:416:SER:CB	2.31	0.61
1:A:94:ARG:HG3	1:A:169:MET:CB	2.23	0.61
1:A:173:GLU:HB2	1:A:202:PRO:HD3	1.81	0.61
1:K:455:TYR:CD1	1:K:455:TYR:C	2.73	0.61
1:C:173:GLU:HB2	1:C:202:PRO:HD3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:ILE:HG22	1:C:211:ARG:HB2	1.80	0.61
1:D:108:ALA:HB2	1:D:126:LYS:N	2.14	0.61
1:I:394:TYR:HB2	1:I:445:GLU:HG3	1.83	0.61
1:J:409:LEU:O	1:J:411:MET:N	2.32	0.61
1:E:414:GLN:HB2	1:E:429:PRO:CG	2.30	0.61
1:A:111:MET:CE	2:A:552:NDP:N7N	2.60	0.61
1:B:99:VAL:HB	1:B:130:LYS:HB3	1.83	0.61
1:K:91:GLY:O	1:K:165:PRO:HA	1.99	0.61
1:I:201:LYS:HB3	1:I:205:GLN:HB2	1.82	0.61
1:E:279:SER:HB2	1:E:310:TYR:O	2.00	0.61
1:I:333:LYS:HD2	1:I:355:GLU:OE1	1.99	0.61
1:B:379:THR:O	1:B:382:TYR:HB3	2.01	0.61
1:K:333:LYS:HD2	1:K:355:GLU:OE1	2.00	0.61
1:L:333:LYS:HB2	1:L:355:GLU:HB3	1.83	0.61
1:J:56:ASN:O	1:J:57:HIS:CD2	2.48	0.61
1:B:152:LEU:HD12	1:B:157:PHE:CB	2.30	0.61
1:H:107:LEU:HD22	1:H:126:LYS:HD3	1.82	0.61
1:G:58:VAL:HG13	1:J:60:SER:HB2	1.82	0.61
1:C:242:PHE:O	1:C:244:ASP:N	2.34	0.61
1:E:321:ILE:CG1	1:E:343:ILE:HB	2.31	0.61
1:D:225:ASN:OD1	1:D:458:GLU:HG3	2.01	0.61
1:C:397:LEU:HD11	1:E:383:PHE:CD2	2.36	0.61
1:L:337:PRO:HB3	1:L:363:ARG:HD2	1.83	0.61
1:H:48:ILE:O	1:H:52:ILE:HG13	2.01	0.61
1:C:300:THR:HG23	1:C:301:ILE:H	1.65	0.61
1:H:455:TYR:CD1	1:H:455:TYR:C	2.74	0.61
1:J:455:TYR:C	1:J:455:TYR:CD1	2.74	0.61
1:L:274:GLY:CA	1:L:279:SER:HA	2.31	0.61
1:K:34:THR:HG22	1:K:36:GLU:H	1.64	0.61
1:F:48:ILE:O	1:F:52:ILE:HG13	2.00	0.61
1:F:242:PHE:O	1:F:244:ASP:N	2.33	0.61
1:C:333:LYS:HA	1:C:336:ALA:HB2	1.83	0.61
1:E:24:VAL:O	1:E:27:LYS:N	2.34	0.61
1:L:200:GLY:HA2	1:L:211:ARG:CD	2.31	0.61
1:G:247:PHE:CZ	1:G:270:CYS:HB2	2.36	0.61
1:C:59:LEU:HB2	1:C:157:PHE:CE2	2.36	0.61
1:H:274:GLY:CA	1:H:279:SER:HA	2.31	0.61
1:I:274:GLY:CA	1:I:279:SER:HA	2.30	0.61
1:L:38:GLU:HG2	1:L:39:GLU:H	1.66	0.61
1:K:323:ILE:CG2	1:K:345:ALA:HB3	2.30	0.61
1:E:107:LEU:HD22	1:E:126:LYS:HD3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:242:PHE:C	1:E:244:ASP:H	2.04	0.61
1:J:27:LYS:HD2	1:J:471:TYR:OH	2.01	0.60
1:D:436:PHE:HD1	1:D:436:PHE:C	2.04	0.60
1:A:413:VAL:HG21	1:F:413:VAL:HG21	1.83	0.60
1:H:247:PHE:CZ	1:H:270:CYS:HB2	2.36	0.60
1:H:321:ILE:CG1	1:H:343:ILE:HB	2.31	0.60
1:C:202:PRO:HG2	1:C:205:GLN:CG	2.31	0.60
1:J:148:PHE:CZ	1:J:152:LEU:HD21	2.36	0.60
1:E:402:GLU:O	1:E:404:ASP:N	2.30	0.60
1:F:132:ASN:OD1	1:F:134:LYS:HG2	2.00	0.60
1:L:293:ASP:O	1:L:297:GLN:HB3	2.00	0.60
1:I:293:ASP:O	1:I:297:GLN:HB3	2.00	0.60
1:D:16:PHE:HE2	1:D:354:PRO:HG3	1.66	0.60
1:D:34:THR:HG22	1:D:36:GLU:H	1.66	0.60
1:F:200:GLY:HA2	1:F:211:ARG:CD	2.31	0.60
1:F:391:HIS:O	1:F:392:VAL:HG13	2.02	0.60
1:D:455:TYR:C	1:D:455:TYR:HD1	2.04	0.60
1:H:323:ILE:CG2	1:H:345:ALA:HB3	2.30	0.60
1:L:394:TYR:HB2	1:L:445:GLU:HG3	1.82	0.60
1:H:61:LEU:HD11	1:H:151:GLU:HB3	1.83	0.60
1:I:242:PHE:O	1:I:244:ASP:N	2.34	0.60
1:J:132:ASN:OD1	1:J:134:LYS:HG2	2.00	0.60
1:K:242:PHE:C	1:K:244:ASP:H	2.05	0.60
1:E:300:THR:HG23	1:E:301:ILE:H	1.65	0.60
1:C:397:LEU:HD11	1:E:383:PHE:CZ	2.36	0.60
1:H:382:TYR:HE2	1:H:386:LEU:HD21	1.65	0.60
1:I:25:GLU:O	1:I:29:VAL:HG23	2.01	0.60
1:K:274:GLY:CA	1:K:279:SER:HA	2.32	0.60
1:C:242:PHE:C	1:C:244:ASP:H	2.05	0.60
1:F:242:PHE:C	1:F:244:ASP:H	2.04	0.60
1:E:242:PHE:O	1:E:244:ASP:N	2.35	0.60
1:B:300:THR:HG23	1:B:301:ILE:H	1.65	0.60
1:J:227:ILE:HD13	1:J:233:MET:SD	2.41	0.60
1:L:106:ALA:O	1:L:109:SER:HB3	2.01	0.60
1:C:323:ILE:CG2	1:C:345:ALA:HB3	2.30	0.60
1:G:323:ILE:CG2	1:G:345:ALA:HB3	2.31	0.60
1:B:501:THR:HG21	1:E:147:ARG:CD	2.30	0.60
1:A:242:PHE:O	1:A:244:ASP:N	2.35	0.60
1:C:190:TYR:O	1:C:191:ASP:HB2	2.01	0.60
1:A:409:LEU:HD23	1:F:409:LEU:HD23	1.82	0.60
1:I:111:MET:HE2	2:I:552:NDP:N7N	2.08	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:333:LYS:HA	1:E:336:ALA:HB2	1.82	0.60
1:H:8:ASN:HB3	1:H:9:PHE:CD2	2.37	0.60
1:G:242:PHE:C	1:G:244:ASP:H	2.05	0.60
1:J:402:GLU:C	1:J:404:ASP:H	2.05	0.60
1:K:414:GLN:HB2	1:K:429:PRO:CG	2.32	0.60
1:A:501:THR:HG23	1:D:147:ARG:CD	2.25	0.60
1:J:497:GLY:HA3	1:K:146:ARG:NH2	2.16	0.60
1:I:120:VAL:HG13	1:I:382:TYR:CD1	2.36	0.60
1:A:333:LYS:HA	1:A:336:ALA:HB2	1.82	0.60
1:J:247:PHE:CZ	1:J:270:CYS:HB2	2.37	0.60
1:H:201:LYS:HB3	1:H:205:GLN:HB2	1.84	0.60
1:K:56:ASN:O	1:K:57:HIS:CD2	2.49	0.60
1:J:274:GLY:CA	1:J:279:SER:HA	2.31	0.60
1:C:274:GLY:CA	1:C:279:SER:HA	2.31	0.60
1:H:245:LYS:HE2	1:H:245:LYS:H	1.67	0.60
1:I:242:PHE:C	1:I:244:ASP:H	2.05	0.60
1:A:346:GLU:CD	1:A:478:ARG:NH2	2.52	0.60
1:B:90:LYS:HB2	1:B:122:PHE:HD1	1.66	0.60
1:E:333:LYS:HD2	1:E:355:GLU:OE1	2.01	0.60
1:B:238:MET:O	1:B:240:PRO:HD3	2.00	0.60
1:B:455:TYR:C	1:B:455:TYR:HD1	2.05	0.60
1:G:274:GLY:CA	1:G:279:SER:HA	2.31	0.60
1:L:141:LEU:HD22	1:L:144:ILE:HD12	1.84	0.60
1:I:106:ALA:O	1:I:109:SER:HB3	2.01	0.60
1:I:402:GLU:C	1:I:404:ASP:H	2.04	0.60
1:K:61:LEU:HD11	1:K:151:GLU:HB3	1.83	0.60
1:F:333:LYS:HA	1:F:336:ALA:HB2	1.83	0.60
3:A:601:XEG:CAL	1:F:209:HIS:HE1	2.08	0.60
1:I:93:ILE:HG22	1:I:127:ALA:HB3	1.84	0.60
1:A:56:ASN:C	1:A:57:HIS:HD2	2.05	0.60
1:L:92:GLY:HA2	1:L:166:ALA:O	2.02	0.60
1:K:300:THR:HG23	1:K:301:ILE:H	1.67	0.60
1:C:9:PHE:HB3	1:C:329:LYS:HZ2	1.66	0.60
1:D:242:PHE:C	1:D:244:ASP:H	2.04	0.60
1:E:374:ASN:C	1:E:376:GLY:H	2.05	0.60
1:B:227:ILE:HD13	1:B:233:MET:SD	2.41	0.60
1:E:382:TYR:C	1:E:382:TYR:CD2	2.73	0.60
1:E:48:ILE:O	1:E:52:ILE:HG13	2.02	0.60
1:I:382:TYR:HE2	1:I:386:LEU:HD21	1.67	0.60
1:C:394:TYR:HB2	1:C:445:GLU:HG3	1.84	0.60
1:E:56:ASN:C	1:E:57:HIS:HD2	2.05	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:ILE:HG23	1:B:366:MET:HE3	1.84	0.60
1:C:129:VAL:O	1:C:131:ILE:N	2.35	0.60
1:B:118:VAL:CG2	1:B:120:VAL:HG23	2.28	0.60
1:H:148:PHE:CZ	1:H:152:LEU:HD21	2.37	0.60
1:J:152:LEU:HD12	1:J:157:PHE:CB	2.32	0.60
1:D:274:GLY:CA	1:D:279:SER:HA	2.31	0.60
1:F:274:GLY:CA	1:F:279:SER:HA	2.32	0.60
1:A:106:ALA:O	1:A:109:SER:HB3	2.02	0.60
1:H:382:TYR:HD2	1:H:382:TYR:O	1.84	0.59
1:C:200:GLY:HA2	1:C:211:ARG:CD	2.32	0.59
1:G:321:ILE:CG1	1:G:343:ILE:HB	2.32	0.59
1:F:152:LEU:HD12	1:F:157:PHE:CB	2.29	0.59
1:G:34:THR:HG22	1:G:36:GLU:H	1.65	0.59
1:A:108:ALA:HB2	1:A:126:LYS:N	2.17	0.59
1:E:149:THR:HB	1:E:182:THR:HG21	1.84	0.59
1:K:293:ASP:O	1:K:297:GLN:HB3	2.00	0.59
1:G:458:GLU:O	1:G:460:SER:N	2.35	0.59
1:E:173:GLU:HB2	1:E:202:PRO:HD3	1.84	0.59
1:G:91:GLY:O	1:G:165:PRO:HA	2.01	0.59
1:E:6:ASP:N	1:E:355:GLU:HG3	2.17	0.59
1:J:344:ILE:HB	1:J:367:VAL:HG12	1.85	0.59
1:H:56:ASN:O	1:H:57:HIS:CD2	2.52	0.59
3:J:601:XEG:HAL	1:K:209:HIS:HE1	1.66	0.59
1:I:245:LYS:HE2	1:I:245:LYS:H	1.67	0.59
1:K:242:PHE:O	1:K:244:ASP:N	2.35	0.59
1:H:227:ILE:HD13	1:H:233:MET:SD	2.42	0.59
1:F:99:VAL:HG11	1:F:128:GLY:CA	2.21	0.59
1:A:300:THR:HG23	1:A:301:ILE:H	1.66	0.59
1:D:436:PHE:CD1	1:D:436:PHE:C	2.75	0.59
1:I:337:PRO:HB3	1:I:363:ARG:HD2	1.83	0.59
1:I:91:GLY:O	1:I:165:PRO:HA	2.02	0.59
1:K:247:PHE:CZ	1:K:270:CYS:HB2	2.36	0.59
1:G:56:ASN:O	1:G:57:HIS:CD2	2.50	0.59
1:H:487:GLU:O	1:H:491:ARG:HG2	2.02	0.59
1:H:413:VAL:CG1	1:H:429:PRO:HG3	2.32	0.59
1:I:38:GLU:HG2	1:I:39:GLU:H	1.67	0.59
1:H:58:VAL:HG13	1:K:60:SER:HB2	1.84	0.59
1:G:414:GLN:HB2	1:G:429:PRO:CG	2.33	0.59
1:J:201:LYS:HB3	1:J:205:GLN:HB2	1.84	0.59
1:A:333:LYS:HD2	1:A:355:GLU:OE1	2.02	0.59
1:G:166:ALA:HA	1:G:176:MET:HE2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:16:PHE:HE2	1:E:354:PRO:CG	2.11	0.59
1:C:321:ILE:CG1	1:C:343:ILE:HB	2.32	0.59
1:L:173:GLU:HB2	1:L:202:PRO:HD3	1.84	0.59
1:C:38:GLU:HG2	1:C:39:GLU:H	1.67	0.59
1:C:48:ILE:O	1:C:52:ILE:HG13	2.01	0.59
1:B:95:TYR:HB3	1:B:133:PRO:HG3	1.84	0.59
1:D:159:GLY:O	1:D:162:VAL:HG12	2.02	0.59
1:B:190:TYR:O	1:B:191:ASP:HB2	2.02	0.59
1:E:420:LYS:NZ	1:E:420:LYS:O	2.30	0.59
1:I:414:GLN:OE1	1:I:430:ILE:HG12	2.03	0.59
1:E:94:ARG:HG3	1:E:169:MET:CB	2.23	0.59
1:B:117:VAL:HG21	1:B:371:LEU:HG	1.85	0.59
1:B:409:LEU:HD12	1:F:436:PHE:CE2	2.38	0.59
1:C:149:THR:HB	1:C:182:THR:HG21	1.83	0.59
1:I:455:TYR:HD1	1:I:455:TYR:C	2.05	0.59
1:E:455:TYR:C	1:E:455:TYR:CD1	2.74	0.59
1:C:238:MET:O	1:C:240:PRO:HD3	2.02	0.59
1:B:148:PHE:CZ	1:B:152:LEU:HD21	2.38	0.59
1:E:273:VAL:O	1:E:314:ILE:HD12	2.03	0.59
1:A:273:VAL:O	1:A:314:ILE:HD12	2.03	0.59
1:L:455:TYR:C	1:L:455:TYR:HD1	2.06	0.59
1:L:16:PHE:CE1	1:L:478:ARG:HD3	2.38	0.59
1:I:445:GLU:O	1:I:449:VAL:HG23	2.02	0.59
1:B:246:THR:HG22	1:B:269:LYS:O	2.02	0.59
1:F:129:VAL:O	1:F:131:ILE:N	2.36	0.59
1:E:369:PRO:HD3	1:E:477:LEU:CB	2.33	0.59
1:J:413:VAL:HG12	1:J:414:GLN:N	2.17	0.59
1:I:16:PHE:CE1	1:I:478:ARG:HD3	2.38	0.59
1:I:492:VAL:HG23	1:J:204:SER:O	2.01	0.59
1:I:397:LEU:HD11	1:K:383:PHE:CE2	2.37	0.59
1:G:24:VAL:O	1:G:27:LYS:N	2.35	0.59
1:H:344:ILE:HB	1:H:367:VAL:HG12	1.85	0.59
1:I:173:GLU:HB2	1:I:202:PRO:HD3	1.84	0.59
1:A:382:TYR:C	1:A:382:TYR:CD2	2.76	0.59
1:A:455:TYR:C	1:A:455:TYR:CD1	2.74	0.59
1:H:282:ASN:C	1:H:284:ASP:H	2.06	0.59
1:J:282:ASN:C	1:J:284:ASP:H	2.06	0.59
1:A:147:ARG:CD	1:D:501:THR:HG22	2.30	0.59
1:D:48:ILE:O	1:D:52:ILE:HG13	2.02	0.59
1:J:141:LEU:HD22	1:J:144:ILE:HD12	1.85	0.59
1:G:242:PHE:O	1:G:244:ASP:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:THR:OG1	1:B:187:ILE:N	2.35	0.59
1:B:369:PRO:HD3	1:B:477:LEU:CB	2.33	0.59
1:D:99:VAL:HB	1:D:130:LYS:HB3	1.85	0.59
1:B:436:PHE:C	1:B:436:PHE:HD1	2.05	0.59
1:A:24:VAL:O	1:A:27:LYS:N	2.34	0.59
1:C:217:ARG:CZ	1:C:450:HIS:HD2	2.16	0.59
1:J:488:LYS:NZ	3:J:601:XEG:HAK	2.18	0.59
1:H:281:TRP:HD1	1:H:283:PRO:HD3	1.68	0.59
1:B:274:GLY:CA	1:B:279:SER:HA	2.32	0.59
1:C:282:ASN:C	1:C:284:ASP:H	2.06	0.59
1:B:242:PHE:C	1:B:244:ASP:H	2.05	0.59
1:E:146:ARG:HG2	1:E:182:THR:OG1	2.03	0.59
1:B:206:GLY:O	1:B:388:ASN:ND2	2.27	0.59
1:I:199:THR:HG22	1:I:384:GLU:CG	2.31	0.59
1:B:494:ASN:HD22	1:B:494:ASN:C	2.06	0.59
1:F:238:MET:O	1:F:240:PRO:HD3	2.02	0.59
1:A:455:TYR:O	1:A:455:TYR:HD1	1.86	0.59
1:D:366:MET:HB2	1:D:475:LEU:HD22	1.85	0.59
1:H:487:GLU:HG2	1:H:491:ARG:HH21	1.68	0.59
1:C:273:VAL:O	1:C:314:ILE:HD12	2.03	0.59
1:F:141:LEU:HD22	1:F:144:ILE:HD12	1.84	0.59
1:K:257:LEU:HD11	1:K:292:GLU:OE2	2.02	0.59
1:A:499:THR:HG23	1:F:146:ARG:NH1	2.18	0.59
1:C:227:ILE:HD13	1:C:233:MET:SD	2.42	0.59
1:L:333:LYS:HA	1:L:336:ALA:HB2	1.85	0.59
1:A:90:LYS:HB2	1:A:122:PHE:HD1	1.66	0.59
1:H:152:LEU:HD12	1:H:157:PHE:CB	2.30	0.59
1:J:273:VAL:O	1:J:314:ILE:HD12	2.02	0.59
1:D:455:TYR:C	1:D:455:TYR:CD1	2.76	0.59
1:G:181:ASP:OD1	1:H:501:THR:HG22	2.02	0.59
1:L:242:PHE:C	1:L:244:ASP:H	2.05	0.59
1:K:458:GLU:O	1:K:460:SER:N	2.35	0.59
1:K:24:VAL:O	1:K:27:LYS:N	2.35	0.59
1:G:86:ARG:HG2	1:G:121:PRO:C	2.22	0.59
1:F:490:PHE:O	1:F:491:ARG:C	2.42	0.59
1:L:495:GLU:O	1:L:496:ALA:HB2	2.02	0.59
1:D:343:ILE:HG23	1:D:366:MET:HE3	1.84	0.59
1:E:274:GLY:CA	1:E:279:SER:HA	2.33	0.59
1:F:7:PRO:HD3	1:F:332:THR:CG2	2.33	0.59
1:J:323:ILE:CG2	1:J:345:ALA:HB3	2.32	0.59
1:C:396:ARG:O	1:C:396:ARG:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:ALA:HB2	1:E:126:LYS:N	2.17	0.59
1:G:9:PHE:HB3	1:G:329:LYS:NZ	2.18	0.59
1:B:100:SER:HB3	1:B:103:GLU:HB2	1.84	0.58
1:L:99:VAL:CG1	1:L:128:GLY:HA3	2.29	0.58
1:I:56:ASN:O	1:I:57:HIS:CD2	2.52	0.58
1:H:273:VAL:O	1:H:314:ILE:HD12	2.03	0.58
1:H:142:GLU:OE2	1:L:500:PHE:HZ	1.85	0.58
1:D:106:ALA:O	1:D:109:SER:HB3	2.03	0.58
1:F:61:LEU:HD11	1:F:151:GLU:HB3	1.85	0.58
1:G:501:THR:O	1:J:150:MET:HG3	2.02	0.58
1:A:321:ILE:CG1	1:A:343:ILE:HB	2.32	0.58
1:B:436:PHE:C	1:B:436:PHE:CD1	2.77	0.58
1:E:202:PRO:HG2	1:E:205:GLN:CG	2.33	0.58
1:G:92:GLY:HA2	1:G:166:ALA:O	2.03	0.58
1:I:200:GLY:HA2	1:I:211:ARG:CD	2.34	0.58
1:F:343:ILE:HG23	1:F:366:MET:HE3	1.85	0.58
1:K:264:HIS:O	1:K:266:PHE:N	2.36	0.58
1:A:149:THR:HB	1:A:182:THR:HG21	1.85	0.58
1:F:273:VAL:O	1:F:314:ILE:HD12	2.02	0.58
1:F:38:GLU:HG2	1:F:39:GLU:H	1.67	0.58
1:G:41:LYS:HA	1:G:44:ARG:HB3	1.86	0.58
1:B:142:GLU:OE2	1:F:500:PHE:CE2	2.55	0.58
1:J:242:PHE:O	1:J:244:ASP:N	2.36	0.58
1:E:436:PHE:CD1	1:E:436:PHE:C	2.76	0.58
1:J:337:PRO:HB3	1:J:363:ARG:HD2	1.85	0.58
1:K:165:PRO:O	1:K:198:VAL:HG23	2.02	0.58
1:F:120:VAL:HG13	1:F:382:TYR:CD1	2.39	0.58
1:L:200:GLY:HA2	1:L:211:ARG:HD2	1.85	0.58
1:K:111:MET:HE3	2:K:552:NDP:H72N	1.67	0.58
1:L:148:PHE:CZ	1:L:152:LEU:HD21	2.38	0.58
1:A:245:LYS:HE2	1:A:245:LYS:H	1.69	0.58
1:G:273:VAL:O	1:G:314:ILE:HD12	2.04	0.58
1:J:107:LEU:HD22	1:J:126:LYS:HD3	1.85	0.58
1:B:196:ALA:CB	1:B:389:LEU:HD21	2.32	0.58
1:D:496:ALA:HA	1:E:177:SER:OG	2.03	0.58
1:H:132:ASN:OD1	1:H:134:LYS:HG2	2.02	0.58
1:H:242:PHE:O	1:H:244:ASP:N	2.36	0.58
1:D:246:THR:HG22	1:D:269:LYS:O	2.03	0.58
1:K:409:LEU:O	1:K:411:MET:N	2.34	0.58
1:K:414:GLN:OE1	1:K:430:ILE:HG12	2.04	0.58
1:I:92:GLY:HA2	1:I:166:ALA:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:343:ILE:HG23	1:K:366:MET:HE3	1.85	0.58
1:L:245:LYS:HE2	1:L:245:LYS:H	1.66	0.58
1:B:141:LEU:O	1:B:145:THR:HG23	2.03	0.58
1:F:257:LEU:HD11	1:F:292:GLU:OE2	2.03	0.58
1:K:186:THR:OG1	1:K:187:ILE:N	2.36	0.58
1:H:93:ILE:HG22	1:H:127:ALA:HB3	1.86	0.58
1:J:167:PRO:HD3	1:J:176:MET:SD	2.44	0.58
1:B:336:ALA:CB	1:B:337:PRO:HD3	2.26	0.58
1:G:395:GLY:O	1:G:397:LEU:N	2.36	0.58
1:A:148:PHE:CZ	1:A:152:LEU:HD21	2.37	0.58
1:A:383:PHE:CD2	1:F:397:LEU:HD11	2.38	0.58
1:C:90:LYS:HG3	1:C:122:PHE:CE1	2.39	0.58
1:G:498:VAL:HG11	1:J:66:ARG:HH11	1.68	0.58
1:J:281:TRP:HD1	1:J:283:PRO:HD3	1.67	0.58
1:C:257:LEU:HD11	1:C:292:GLU:OE2	2.03	0.58
1:L:16:PHE:CD1	1:L:478:ARG:HD3	2.39	0.58
1:A:242:PHE:C	1:A:244:ASP:H	2.04	0.58
1:D:196:ALA:CB	1:D:389:LEU:CD2	2.81	0.58
1:J:61:LEU:HD11	1:J:151:GLU:HB3	1.84	0.58
1:G:108:ALA:HB2	1:G:126:LYS:N	2.18	0.58
1:H:259:SER:O	1:H:263:LEU:HB2	2.03	0.58
1:D:24:VAL:O	1:D:25:GLU:C	2.42	0.58
1:A:118:VAL:HG11	1:A:375:ALA:CB	2.34	0.58
1:F:413:VAL:HG12	1:F:429:PRO:HG3	1.86	0.58
1:B:382:TYR:C	1:B:382:TYR:CD2	2.76	0.58
1:G:343:ILE:HG23	1:G:366:MET:HE3	1.86	0.58
1:D:282:ASN:C	1:D:284:ASP:H	2.06	0.58
1:J:245:LYS:H	1:J:245:LYS:HE2	1.68	0.58
1:E:141:LEU:O	1:E:145:THR:HG23	2.02	0.58
1:I:90:LYS:HG3	1:I:122:PHE:CE1	2.38	0.58
1:E:142:GLU:HB2	1:E:178:TRP:CZ2	2.39	0.58
1:A:60:SER:HB2	1:D:58:VAL:HG13	1.85	0.58
1:D:382:TYR:CD2	1:D:382:TYR:C	2.76	0.58
1:I:16:PHE:CD1	1:I:478:ARG:HD3	2.39	0.58
1:A:25:GLU:O	1:A:29:VAL:HG23	2.04	0.58
1:C:217:ARG:CZ	1:C:450:HIS:CD2	2.86	0.58
1:J:13:VAL:O	1:J:14:GLU:C	2.41	0.58
1:L:282:ASN:C	1:L:284:ASP:H	2.07	0.58
1:G:38:GLU:HG2	1:G:39:GLU:H	1.69	0.58
1:C:346:GLU:CD	1:C:351:PRO:HD2	2.24	0.58
1:E:247:PHE:CZ	1:E:270:CYS:HB2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:457:MET:O	1:D:460:SER:HB2	2.04	0.58
1:J:414:GLN:OE1	1:J:430:ILE:HG12	2.04	0.58
1:D:369:PRO:HD3	1:D:477:LEU:CB	2.34	0.58
1:C:201:LYS:HB3	1:C:205:GLN:HB2	1.86	0.58
1:C:209:HIS:HE1	3:E:601:XEG:CAL	2.15	0.58
1:B:455:TYR:CE1	1:B:459:ARG:HD3	2.36	0.58
1:F:279:SER:HB2	1:F:310:TYR:O	2.04	0.58
1:H:413:VAL:HG12	1:H:429:PRO:CG	2.34	0.58
1:J:374:ASN:C	1:J:376:GLY:H	2.05	0.58
1:C:61:LEU:HD11	1:C:151:GLU:HB3	1.84	0.58
1:D:391:HIS:O	1:D:392:VAL:HG13	2.04	0.58
1:J:413:VAL:CG1	1:J:429:PRO:HG3	2.33	0.58
1:G:414:GLN:OE1	1:G:430:ILE:HG12	2.03	0.58
1:D:117:VAL:HG21	1:D:371:LEU:HG	1.86	0.58
1:D:121:PRO:HD2	1:D:382:TYR:CE1	2.39	0.58
1:I:336:ALA:CB	1:I:337:PRO:HD3	2.29	0.58
1:L:395:GLY:O	1:L:397:LEU:N	2.37	0.58
1:H:167:PRO:HD3	1:H:176:MET:SD	2.43	0.58
1:B:282:ASN:C	1:B:284:ASP:H	2.07	0.58
1:I:282:ASN:C	1:I:284:ASP:H	2.06	0.58
1:C:245:LYS:H	1:C:245:LYS:HE2	1.69	0.58
1:F:345:ALA:HB1	1:F:373:LEU:HD21	1.86	0.58
1:K:48:ILE:O	1:K:52:ILE:HG13	2.04	0.58
1:H:110:LEU:HD23	1:H:111:MET:N	2.19	0.58
1:D:90:LYS:HB2	1:D:122:PHE:HD1	1.69	0.58
1:H:337:PRO:HB3	1:H:363:ARG:HD2	1.84	0.58
1:I:455:TYR:CD1	1:I:455:TYR:C	2.77	0.58
1:B:498:VAL:HG11	1:E:72:TRP:HZ2	1.68	0.58
1:K:59:LEU:HB2	1:K:157:PHE:CE2	2.39	0.58
1:F:321:ILE:CG1	1:F:343:ILE:HB	2.31	0.58
1:G:247:PHE:CE1	1:G:270:CYS:HB2	2.39	0.58
1:L:247:PHE:CZ	1:L:270:CYS:HB2	2.39	0.58
1:H:150:MET:HG3	1:K:501:THR:OG1	2.04	0.58
1:K:217:ARG:CZ	1:K:450:HIS:CD2	2.87	0.57
1:G:90:LYS:HG3	1:G:122:PHE:CE1	2.39	0.57
1:L:12:MET:N	1:L:14:GLU:HG2	2.15	0.57
1:I:468:ALA:CB	1:I:480:ALA:HB1	2.33	0.57
3:B:601:XEG:CAL	3:B:601:XEG:HAPA	2.34	0.57
1:I:247:PHE:CZ	1:I:270:CYS:HB2	2.38	0.57
1:D:148:PHE:CZ	1:D:152:LEU:HD21	2.39	0.57
1:K:500:PHE:HB3	1:L:500:PHE:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:186:THR:OG1	1:G:187:ILE:N	2.32	0.57
1:G:391:HIS:O	1:G:392:VAL:HG13	2.04	0.57
1:J:259:SER:O	1:J:263:LEU:HB2	2.04	0.57
1:G:488:LYS:O	1:G:492:VAL:HG23	2.02	0.57
1:K:217:ARG:CZ	1:K:450:HIS:HD2	2.17	0.57
1:J:321:ILE:CG1	1:J:343:ILE:HB	2.31	0.57
1:L:199:THR:HG22	1:L:384:GLU:CG	2.33	0.57
1:G:300:THR:HG23	1:G:301:ILE:H	1.67	0.57
1:B:281:TRP:HD1	1:B:283:PRO:HD3	1.67	0.57
1:B:279:SER:HB2	1:B:310:TYR:O	2.04	0.57
1:F:346:GLU:CD	1:F:351:PRO:HD2	2.25	0.57
1:G:344:ILE:HB	1:G:367:VAL:HG12	1.86	0.57
1:E:436:PHE:HD1	1:E:436:PHE:C	2.06	0.57
1:B:369:PRO:HG3	1:B:478:ARG:N	2.20	0.57
1:D:94:ARG:HG3	1:D:169:MET:CB	2.26	0.57
1:I:333:LYS:HA	1:I:336:ALA:HB2	1.86	0.57
1:F:201:LYS:HB3	1:F:205:GLN:HB2	1.87	0.57
1:L:382:TYR:HE2	1:L:386:LEU:HD21	1.67	0.57
1:J:56:ASN:C	1:J:57:HIS:HD2	2.07	0.57
1:H:141:LEU:HD22	1:H:144:ILE:HD12	1.85	0.57
1:A:499:THR:HA	1:F:146:ARG:NH1	2.20	0.57
1:D:190:TYR:O	1:D:191:ASP:HB2	2.03	0.57
1:H:60:SER:HB2	1:K:58:VAL:HG13	1.85	0.57
1:F:190:TYR:O	1:F:191:ASP:HB2	2.04	0.57
1:A:247:PHE:CZ	1:A:270:CYS:HB2	2.39	0.57
1:B:225:ASN:OD1	1:B:458:GLU:HG3	2.03	0.57
1:B:96:SER:C	1:B:98:ASP:H	2.08	0.57
1:J:91:GLY:O	1:J:165:PRO:HA	2.05	0.57
1:J:497:GLY:O	1:J:499:THR:N	2.36	0.57
1:C:146:ARG:CZ	1:E:500:PHE:HB2	2.35	0.57
1:A:141:LEU:O	1:A:145:THR:HG23	2.05	0.57
1:H:92:GLY:HA2	1:H:166:ALA:O	2.04	0.57
1:L:264:HIS:O	1:L:266:PHE:N	2.37	0.57
1:D:226:PHE:CZ	1:D:465:MET:HE2	2.40	0.57
1:I:280:ILE:HG22	1:I:281:TRP:H	1.70	0.57
1:F:245:LYS:HE2	1:F:245:LYS:H	1.69	0.57
1:K:41:LYS:HA	1:K:44:ARG:HB3	1.85	0.57
1:D:95:TYR:HB3	1:D:133:PRO:HG3	1.86	0.57
1:H:242:PHE:C	1:H:244:ASP:H	2.07	0.57
1:E:186:THR:OG1	1:E:187:ILE:N	2.38	0.57
1:D:129:VAL:O	1:D:131:ILE:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:374:ASN:C	1:G:376:GLY:H	2.06	0.57
1:I:186:THR:OG1	1:I:187:ILE:N	2.36	0.57
1:D:488:LYS:O	1:D:491:ARG:HB2	2.04	0.57
1:F:202:PRO:HG2	1:F:205:GLN:CG	2.34	0.57
1:C:56:ASN:C	1:C:57:HIS:HD2	2.07	0.57
1:J:455:TYR:HD1	1:J:455:TYR:O	1.88	0.57
1:K:282:ASN:C	1:K:284:ASP:H	2.08	0.57
1:G:282:ASN:C	1:G:284:ASP:H	2.07	0.57
1:L:455:TYR:C	1:L:455:TYR:CD1	2.77	0.57
1:H:38:GLU:HG2	1:H:39:GLU:H	1.69	0.57
1:H:108:ALA:HB2	1:H:126:LYS:N	2.19	0.57
1:G:9:PHE:HB3	1:G:329:LYS:HZ3	1.68	0.57
1:B:159:GLY:O	1:B:162:VAL:HG12	2.04	0.57
1:E:129:VAL:O	1:E:131:ILE:N	2.37	0.57
1:B:38:GLU:HG2	1:B:39:GLU:H	1.69	0.57
1:C:391:HIS:O	1:C:392:VAL:HG13	2.04	0.57
1:B:165:PRO:O	1:B:198:VAL:HG23	2.04	0.57
1:G:59:LEU:HB2	1:G:157:PHE:CE2	2.38	0.57
1:D:281:TRP:HD1	1:D:283:PRO:HD3	1.66	0.57
1:I:148:PHE:CZ	1:I:152:LEU:HD21	2.39	0.57
1:B:455:TYR:C	1:B:455:TYR:CD1	2.77	0.57
1:C:279:SER:HB2	1:C:310:TYR:O	2.03	0.57
1:K:374:ASN:C	1:K:376:GLY:H	2.07	0.57
1:E:118:VAL:HG11	1:E:375:ALA:CB	2.34	0.57
1:E:455:TYR:O	1:E:455:TYR:HD1	1.87	0.57
1:F:247:PHE:CZ	1:F:270:CYS:HB2	2.40	0.57
1:C:264:HIS:O	1:C:266:PHE:N	2.37	0.57
1:K:273:VAL:O	1:K:314:ILE:HD12	2.04	0.57
1:L:280:ILE:HG22	1:L:281:TRP:H	1.70	0.57
1:A:221:HIS:HA	1:A:224:GLU:HB3	1.86	0.57
1:H:129:VAL:O	1:H:131:ILE:N	2.38	0.57
1:L:186:THR:OG1	1:L:187:ILE:N	2.37	0.57
1:E:118:VAL:HG11	1:E:375:ALA:HB1	1.86	0.57
1:H:416:SER:HB3	1:L:428:ILE:O	2.05	0.57
1:G:413:VAL:HG11	1:L:413:VAL:HG22	1.85	0.57
1:L:94:ARG:HG3	1:L:169:MET:CB	2.28	0.57
1:B:382:TYR:HD2	1:B:382:TYR:C	2.08	0.57
1:K:176:MET:HG3	1:K:198:VAL:CG2	2.35	0.57
1:K:445:GLU:O	1:K:449:VAL:HG23	2.04	0.57
3:D:502:XEG:HAPA	3:D:502:XEG:CAL	2.34	0.57
1:E:458:GLU:C	1:E:460:SER:N	2.58	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:PRO:HG2	1:C:205:GLN:HG3	1.86	0.57
1:A:59:LEU:HB2	1:A:157:PHE:CE2	2.39	0.57
1:F:445:GLU:O	1:F:449:VAL:HG23	2.04	0.57
1:L:167:PRO:HD3	1:L:176:MET:HG2	1.87	0.57
1:A:274:GLY:CA	1:A:279:SER:HA	2.34	0.57
1:I:281:TRP:HD1	1:I:283:PRO:HD3	1.70	0.57
1:E:366:MET:HA	1:E:475:LEU:HB3	1.87	0.57
1:J:413:VAL:HG12	1:J:429:PRO:CG	2.34	0.57
1:F:100:SER:HB3	1:F:103:GLU:HB2	1.86	0.57
1:F:99:VAL:HB	1:F:130:LYS:HB3	1.87	0.57
1:I:16:PHE:CE2	1:I:354:PRO:HG3	2.40	0.57
1:G:100:SER:HB3	1:G:103:GLU:HB2	1.87	0.57
1:K:92:GLY:HA2	1:K:166:ALA:O	2.04	0.57
3:F:601:XEG:HAPA	3:F:601:XEG:CAL	2.34	0.57
1:C:56:ASN:O	1:C:57:HIS:CD2	2.48	0.57
1:C:343:ILE:HG23	1:C:366:MET:HE3	1.87	0.57
1:B:226:PHE:CZ	1:B:465:MET:HE2	2.40	0.57
1:I:239:THR:O	1:I:241:GLY:N	2.38	0.57
1:D:322:LEU:HD22	1:D:323:ILE:N	2.20	0.57
1:D:489:VAL:O	1:D:492:VAL:HG12	2.05	0.57
1:K:38:GLU:HG2	1:K:39:GLU:H	1.70	0.57
1:K:141:LEU:HD22	1:K:144:ILE:HD12	1.87	0.57
1:C:186:THR:OG1	1:C:187:ILE:N	2.38	0.57
1:I:419:ARG:HD2	1:K:428:ILE:HD11	1.87	0.57
1:D:414:GLN:OE1	1:D:430:ILE:HG12	2.05	0.57
1:I:99:VAL:CG1	1:I:128:GLY:HA3	2.29	0.57
1:I:166:ALA:HA	1:I:176:MET:HE2	1.87	0.57
1:F:167:PRO:HD3	1:F:176:MET:SD	2.44	0.57
1:K:247:PHE:CE1	1:K:270:CYS:HB2	2.40	0.57
1:J:488:LYS:HZ2	3:J:601:XEG:CAK	2.16	0.57
1:A:281:TRP:HD1	1:A:283:PRO:HD3	1.69	0.57
3:D:601:XEG:HAPA	3:D:601:XEG:CAL	2.34	0.57
1:F:8:ASN:CG	1:F:9:PHE:H	2.07	0.57
1:L:159:GLY:O	1:L:162:VAL:HG12	2.05	0.57
1:A:129:VAL:O	1:A:131:ILE:N	2.38	0.57
1:I:433:THR:HG22	1:J:412:SER:N	2.20	0.56
1:J:436:PHE:CD1	1:J:436:PHE:C	2.79	0.56
1:J:436:PHE:HD1	1:J:436:PHE:C	2.07	0.56
1:H:468:ALA:CB	1:H:480:ALA:HB1	2.35	0.56
1:A:432:PRO:HA	1:F:412:SER:HB3	1.87	0.56
1:J:176:MET:HG3	1:J:198:VAL:CG2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:255:VAL:HG12	2:F:552:NDP:O2N	2.05	0.56
1:L:201:LYS:O	1:L:211:ARG:NH1	2.34	0.56
1:I:264:HIS:O	1:I:266:PHE:N	2.38	0.56
1:D:56:ASN:O	1:D:57:HIS:CD2	2.52	0.56
1:J:52:ILE:HD13	1:J:489:VAL:CG1	2.35	0.56
1:H:279:SER:HB2	1:H:310:TYR:O	2.05	0.56
1:J:279:SER:HB2	1:J:310:TYR:O	2.05	0.56
1:E:41:LYS:HA	1:E:44:ARG:HB3	1.87	0.56
1:B:24:VAL:O	1:B:25:GLU:C	2.42	0.56
1:D:96:SER:C	1:D:98:ASP:H	2.07	0.56
1:A:6:ASP:CA	1:A:332:THR:HB	2.35	0.56
1:K:167:PRO:HD3	1:K:176:MET:HG2	1.86	0.56
1:K:382:TYR:HD2	1:K:382:TYR:O	1.88	0.56
1:C:446:LYS:HG3	1:C:450:HIS:CE1	2.40	0.56
1:F:264:HIS:O	1:F:266:PHE:N	2.38	0.56
1:J:12:MET:N	1:J:14:GLU:HG2	2.16	0.56
1:J:382:TYR:CD2	1:J:382:TYR:C	2.79	0.56
1:G:264:HIS:O	1:G:266:PHE:N	2.38	0.56
1:A:41:LYS:HA	1:A:44:ARG:HB3	1.87	0.56
1:J:38:GLU:HG2	1:J:39:GLU:H	1.69	0.56
1:B:217:ARG:NE	1:B:450:HIS:HD2	2.03	0.56
1:I:141:LEU:O	1:I:145:THR:HG23	2.05	0.56
1:J:129:VAL:O	1:J:131:ILE:N	2.38	0.56
1:D:38:GLU:HG2	1:D:39:GLU:H	1.69	0.56
1:A:367:VAL:C	1:A:477:LEU:HD23	2.26	0.56
1:E:99:VAL:HB	1:E:130:LYS:HB3	1.88	0.56
1:C:413:VAL:HG12	1:C:429:PRO:HG3	1.88	0.56
1:A:436:PHE:HD1	1:A:436:PHE:C	2.07	0.56
1:K:201:LYS:O	1:K:211:ARG:NH1	2.36	0.56
1:D:166:ALA:HA	1:D:176:MET:HE2	1.88	0.56
1:K:24:VAL:CG1	1:K:483:VAL:HG13	2.30	0.56
1:H:264:HIS:O	1:H:266:PHE:N	2.38	0.56
1:H:247:PHE:CE1	1:H:270:CYS:HB2	2.41	0.56
1:C:24:VAL:HG13	1:C:483:VAL:HG13	1.87	0.56
1:L:100:SER:HB3	1:L:103:GLU:HB2	1.87	0.56
1:B:12:MET:N	1:B:14:GLU:HG2	2.15	0.56
1:F:468:ALA:CB	1:F:480:ALA:HB1	2.36	0.56
1:L:25:GLU:O	1:L:29:VAL:HG23	2.05	0.56
1:K:56:ASN:C	1:K:57:HIS:HD2	2.08	0.56
1:G:48:ILE:O	1:G:52:ILE:HG13	2.05	0.56
1:C:148:PHE:CZ	1:C:152:LEU:HD21	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:488:LYS:HZ3	3:H:601:XEG:HAK	1.63	0.56
1:I:59:LEU:HB2	1:I:157:PHE:CE2	2.40	0.56
1:E:396:ARG:CG	1:E:396:ARG:HH11	2.18	0.56
1:C:141:LEU:HD22	1:C:144:ILE:HD12	1.86	0.56
1:B:196:ALA:HB2	1:B:389:LEU:HD23	1.88	0.56
1:K:47:SER:O	1:K:50:ARG:N	2.38	0.56
1:K:344:ILE:HB	1:K:367:VAL:HG12	1.87	0.56
1:B:158:ILE:O	1:B:158:ILE:HG23	2.05	0.56
1:G:246:THR:HG22	1:G:269:LYS:O	2.05	0.56
1:D:221:HIS:HA	1:D:224:GLU:HB3	1.87	0.56
1:A:186:THR:OG1	1:A:187:ILE:N	2.39	0.56
1:K:158:ILE:HG23	1:K:158:ILE:O	2.05	0.56
1:I:413:VAL:HG22	1:K:413:VAL:HG11	1.88	0.56
1:B:36:GLU:CB	1:B:40:GLN:HG2	2.35	0.56
1:L:99:VAL:HB	1:L:130:LYS:HB3	1.87	0.56
1:F:282:ASN:C	1:F:284:ASP:H	2.07	0.56
1:K:245:LYS:HE2	1:K:245:LYS:H	1.70	0.56
1:L:36:GLU:CB	1:L:40:GLN:HG2	2.36	0.56
1:F:498:VAL:O	1:F:500:PHE:CE2	2.59	0.56
1:G:257:LEU:HD11	1:G:292:GLU:OE2	2.05	0.56
1:A:257:LEU:HD11	1:A:292:GLU:OE2	2.05	0.56
1:E:69:ASP:OD2	1:E:71:SER:HB2	2.06	0.56
1:F:69:ASP:OD2	1:F:71:SER:HB2	2.05	0.56
1:K:246:THR:HG22	1:K:269:LYS:O	2.05	0.56
1:E:343:ILE:HG23	1:E:366:MET:HE3	1.87	0.56
1:J:468:ALA:CB	1:J:480:ALA:HB1	2.35	0.56
1:D:382:TYR:HD2	1:D:382:TYR:C	2.08	0.56
1:C:436:PHE:HD1	1:C:436:PHE:C	2.08	0.56
1:I:9:PHE:HA	1:I:329:LYS:HD3	1.88	0.56
1:G:217:ARG:CZ	1:G:450:HIS:HD2	2.18	0.56
1:G:176:MET:HG3	1:G:198:VAL:CG2	2.36	0.56
1:C:468:ALA:CB	1:C:480:ALA:HB1	2.35	0.56
1:B:142:GLU:HB2	1:B:178:TRP:CZ2	2.40	0.56
1:I:346:GLU:OE1	1:I:478:ARG:NH2	2.38	0.56
1:G:99:VAL:HB	1:G:130:LYS:HB3	1.88	0.56
3:I:601:XEG:CAL	3:I:601:XEG:HAPA	2.35	0.56
1:K:337:PRO:HA	1:K:363:ARG:HH21	1.70	0.56
1:L:9:PHE:HA	1:L:329:LYS:HD3	1.87	0.56
1:I:167:PRO:HD3	1:I:176:MET:HG2	1.88	0.56
1:C:167:PRO:HD3	1:C:176:MET:SD	2.45	0.56
1:B:493:TYR:O	1:B:494:ASN:C	2.44	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:MET:N	1:E:14:GLU:HG2	2.16	0.56
1:H:16:PHE:CE2	1:H:354:PRO:HG3	2.32	0.56
1:B:366:MET:HB2	1:B:475:LEU:HD22	1.86	0.56
1:E:281:TRP:HD1	1:E:283:PRO:HD3	1.69	0.56
1:G:420:LYS:O	1:G:420:LYS:NZ	2.29	0.56
1:A:36:GLU:CB	1:A:40:GLN:HG2	2.36	0.56
1:C:345:ALA:HB1	1:C:373:LEU:HD21	1.86	0.56
1:B:322:LEU:HD22	1:B:323:ILE:N	2.20	0.56
1:C:23:ILE:HG22	1:C:471:TYR:CD1	2.40	0.56
1:D:458:GLU:C	1:D:460:SER:N	2.59	0.56
1:D:468:ALA:CB	1:D:480:ALA:HB1	2.36	0.56
1:A:118:VAL:HG11	1:A:375:ALA:HB1	1.86	0.56
1:D:121:PRO:O	1:D:122:PHE:HD2	1.89	0.56
1:I:12:MET:N	1:I:14:GLU:HG2	2.14	0.56
1:B:167:PRO:HD3	1:B:176:MET:SD	2.46	0.56
1:B:173:GLU:HB2	1:B:202:PRO:HD3	1.88	0.56
1:E:336:ALA:CB	1:E:337:PRO:HD3	2.30	0.56
3:K:601:XEG:CAL	3:K:601:XEG:HAPA	2.35	0.56
1:C:255:VAL:HG12	2:C:552:NDP:O2N	2.06	0.56
1:C:166:ALA:HA	1:C:176:MET:HE2	1.88	0.56
1:J:264:HIS:O	1:J:266:PHE:N	2.37	0.56
1:D:497:GLY:HA3	1:E:146:ARG:HH21	1.70	0.56
1:J:289:LYS:O	1:J:290:GLU:HB2	2.06	0.56
1:B:16:PHE:HE2	1:B:354:PRO:HG3	1.69	0.56
1:C:500:PHE:N	1:C:500:PHE:CD1	2.72	0.56
1:D:36:GLU:CB	1:D:40:GLN:HG2	2.35	0.56
1:C:436:PHE:CE2	1:D:409:LEU:HD12	2.41	0.56
1:J:167:PRO:HD3	1:J:176:MET:CG	2.35	0.56
1:K:94:ARG:HG3	1:K:169:MET:CB	2.27	0.56
1:A:458:GLU:C	1:A:460:SER:N	2.59	0.56
1:I:200:GLY:HA2	1:I:211:ARG:HD2	1.86	0.56
1:F:24:VAL:O	1:F:25:GLU:C	2.43	0.56
1:K:148:PHE:CZ	1:K:152:LEU:HD21	2.40	0.56
1:F:12:MET:HG3	1:F:13:VAL:H	1.71	0.56
1:A:12:MET:N	1:A:14:GLU:HG2	2.16	0.56
1:D:264:HIS:O	1:D:266:PHE:N	2.38	0.56
1:D:279:SER:HB2	1:D:310:TYR:O	2.05	0.56
1:H:239:THR:O	1:H:241:GLY:N	2.37	0.56
1:F:221:HIS:HA	1:F:224:GLU:HB3	1.87	0.56
1:H:289:LYS:O	1:H:290:GLU:HB2	2.06	0.56
1:L:110:LEU:HD23	1:L:111:MET:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:436:PHE:HD1	1:F:436:PHE:C	2.09	0.56
1:J:173:GLU:HB2	1:J:202:PRO:HD3	1.88	0.56
3:G:601:XEG:CAL	3:G:601:XEG:HAPA	2.36	0.56
1:G:201:LYS:O	1:G:211:ARG:NH1	2.36	0.56
1:H:167:PRO:HD3	1:H:176:MET:CG	2.36	0.56
1:B:247:PHE:CZ	1:B:270:CYS:HB2	2.41	0.56
1:J:48:ILE:O	1:J:52:ILE:HG13	2.06	0.56
1:E:245:LYS:H	1:E:245:LYS:HE2	1.71	0.56
1:I:274:GLY:HA3	1:I:279:SER:HA	1.87	0.56
1:C:36:GLU:CB	1:C:40:GLN:HG2	2.35	0.56
1:H:36:GLU:CB	1:H:40:GLN:HG2	2.36	0.56
1:K:396:ARG:HG3	1:K:396:ARG:O	2.06	0.56
1:F:9:PHE:HA	1:F:329:LYS:HD3	1.87	0.56
1:L:346:GLU:OE1	1:L:478:ARG:NH2	2.39	0.56
1:C:129:VAL:O	1:C:129:VAL:HG12	2.06	0.56
1:K:346:GLU:CD	1:K:351:PRO:HD2	2.27	0.56
1:I:99:VAL:HB	1:I:130:LYS:HB3	1.88	0.56
1:J:247:PHE:CE1	1:J:270:CYS:HB2	2.40	0.56
1:E:25:GLU:O	1:E:29:VAL:HG23	2.05	0.56
1:I:24:VAL:O	1:I:27:LYS:N	2.39	0.56
1:A:455:TYR:CE1	1:A:459:ARG:HD3	2.37	0.56
1:H:280:ILE:HG22	1:H:281:TRP:H	1.70	0.56
1:A:282:ASN:C	1:A:284:ASP:H	2.09	0.56
1:L:281:TRP:HD1	1:L:283:PRO:HD3	1.70	0.56
1:D:141:LEU:O	1:D:145:THR:HG23	2.06	0.56
1:E:238:MET:O	1:E:240:PRO:HD3	2.05	0.56
1:E:264:HIS:O	1:E:266:PHE:N	2.38	0.55
1:J:433:THR:HG22	1:K:412:SER:CA	2.36	0.55
1:H:409:LEU:O	1:H:411:MET:N	2.35	0.55
1:H:436:PHE:CD1	1:H:436:PHE:C	2.80	0.55
1:H:436:PHE:C	1:H:436:PHE:HD1	2.09	0.55
1:B:478:ARG:O	1:B:481:ALA:N	2.39	0.55
1:I:110:LEU:HD23	1:I:111:MET:N	2.21	0.55
1:B:201:LYS:HD3	1:B:201:LYS:H	1.70	0.55
1:G:199:THR:HG22	1:G:384:GLU:CG	2.35	0.55
1:A:464:ILE:O	1:A:468:ALA:HB3	2.06	0.55
1:L:120:VAL:HG13	1:L:382:TYR:CD1	2.41	0.55
1:J:7:PRO:CB	1:J:329:LYS:HD2	2.36	0.55
1:F:446:LYS:HG3	1:F:450:HIS:CE1	2.41	0.55
1:E:282:ASN:C	1:E:284:ASP:H	2.10	0.55
1:L:279:SER:HB2	1:L:310:TYR:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:281:TRP:HD1	1:G:283:PRO:HD3	1.70	0.55
1:D:455:TYR:O	1:D:455:TYR:HD1	1.90	0.55
1:B:141:LEU:HD22	1:B:144:ILE:HD12	1.88	0.55
1:B:221:HIS:HA	1:B:224:GLU:HB3	1.87	0.55
1:G:499:THR:HG23	1:L:181:ASP:OD1	2.06	0.55
1:J:221:HIS:HA	1:J:224:GLU:HB3	1.87	0.55
1:G:96:SER:C	1:G:98:ASP:H	2.10	0.55
1:A:142:GLU:HB2	1:A:178:TRP:CZ2	2.42	0.55
1:D:165:PRO:O	1:D:198:VAL:HG23	2.06	0.55
1:K:25:GLU:O	1:K:29:VAL:HG23	2.06	0.55
1:G:346:GLU:OE1	1:G:478:ARG:NH2	2.39	0.55
1:L:491:ARG:HD3	3:L:601:XEG:HOAB	1.71	0.55
1:A:56:ASN:C	1:A:57:HIS:CD2	2.80	0.55
1:C:87:THR:CB	1:C:88:PRO:CD	2.83	0.55
1:D:247:PHE:CZ	1:D:270:CYS:HB2	2.42	0.55
1:G:110:LEU:HD23	1:G:111:MET:N	2.20	0.55
1:A:280:ILE:HG22	1:A:281:TRP:H	1.71	0.55
1:C:274:GLY:HA3	1:C:279:SER:HA	1.88	0.55
1:F:36:GLU:CB	1:F:40:GLN:HG2	2.36	0.55
1:B:413:VAL:HG12	1:B:414:GLN:N	2.21	0.55
1:G:417:LEU:HD21	1:L:417:LEU:HD21	1.88	0.55
1:E:221:HIS:HA	1:E:224:GLU:HB3	1.88	0.55
1:J:24:VAL:O	1:J:27:LYS:N	2.39	0.55
1:J:24:VAL:O	1:J:25:GLU:C	2.44	0.55
1:J:90:LYS:HB2	1:J:122:PHE:HD1	1.69	0.55
1:H:382:TYR:C	1:H:382:TYR:CD2	2.77	0.55
1:F:165:PRO:O	1:F:198:VAL:HG23	2.06	0.55
1:A:445:GLU:O	1:A:449:VAL:HG23	2.06	0.55
1:H:214:ALA:CB	1:H:380:VAL:HG21	2.34	0.55
1:K:274:GLY:HA3	1:K:279:SER:HA	1.89	0.55
1:F:280:ILE:HG22	1:F:281:TRP:H	1.71	0.55
1:L:396:ARG:CG	1:L:396:ARG:HH11	2.18	0.55
1:H:147:ARG:HD2	1:K:501:THR:HG21	1.88	0.55
1:A:238:MET:O	1:A:240:PRO:HD3	2.05	0.55
1:D:196:ALA:CB	1:D:389:LEU:HD21	2.36	0.55
1:J:257:LEU:HD11	1:J:292:GLU:OE2	2.07	0.55
1:A:246:THR:HG22	1:A:269:LYS:O	2.06	0.55
1:I:159:GLY:O	1:I:162:VAL:HG12	2.05	0.55
1:B:289:LYS:O	1:B:290:GLU:HB2	2.07	0.55
1:L:429:PRO:O	1:L:431:VAL:N	2.40	0.55
1:B:41:LYS:HA	1:B:44:ARG:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:PHE:CD1	1:C:436:PHE:C	2.80	0.55
1:A:202:PRO:HG2	1:A:205:GLN:CG	2.35	0.55
1:D:198:VAL:O	1:D:201:LYS:HE3	2.06	0.55
1:G:25:GLU:O	1:G:29:VAL:HG23	2.07	0.55
1:H:52:ILE:HD13	1:H:489:VAL:CG1	2.35	0.55
1:F:217:ARG:CZ	1:F:450:HIS:CD2	2.89	0.55
1:F:394:TYR:HB2	1:F:445:GLU:HG3	1.87	0.55
1:K:395:GLY:O	1:K:397:LEU:N	2.40	0.55
1:H:176:MET:HG3	1:H:198:VAL:CG2	2.36	0.55
3:H:601:XEG:HAPA	3:H:601:XEG:CAL	2.36	0.55
1:I:41:LYS:HA	1:I:44:ARG:HB3	1.89	0.55
1:C:41:LYS:HA	1:C:44:ARG:HB3	1.87	0.55
1:I:257:LEU:HD11	1:I:292:GLU:OE2	2.06	0.55
1:A:420:LYS:HG2	1:A:420:LYS:O	2.06	0.55
1:J:242:PHE:C	1:J:244:ASP:H	2.07	0.55
1:C:221:HIS:HA	1:C:224:GLU:HB3	1.87	0.55
1:H:24:VAL:O	1:H:27:LYS:N	2.39	0.55
1:B:457:MET:O	1:B:460:SER:HB2	2.07	0.55
1:F:176:MET:HG3	1:F:198:VAL:CG2	2.36	0.55
1:K:13:VAL:O	1:K:14:GLU:C	2.45	0.55
1:G:13:VAL:O	1:G:14:GLU:C	2.45	0.55
1:G:56:ASN:C	1:G:57:HIS:HD2	2.09	0.55
1:D:455:TYR:CE1	1:D:459:ARG:HD3	2.38	0.55
1:L:239:THR:O	1:L:241:GLY:N	2.39	0.55
1:D:234:SER:O	1:D:236:LEU:N	2.39	0.55
1:F:149:THR:HB	1:F:182:THR:HG21	1.87	0.55
1:A:100:SER:HB3	1:A:103:GLU:HB2	1.88	0.55
1:A:69:ASP:OD2	1:A:71:SER:HB2	2.06	0.55
1:D:41:LYS:HA	1:D:44:ARG:HB3	1.88	0.55
1:J:167:PRO:HD3	1:J:176:MET:HG2	1.89	0.55
1:I:85:HIS:HD2	1:I:492:VAL:HG11	1.72	0.55
3:G:601:XEG:CAL	1:L:209:HIS:HE1	2.10	0.55
1:B:383:PHE:HA	1:B:386:LEU:HD12	1.88	0.55
1:B:488:LYS:HA	1:B:491:ARG:HG3	1.88	0.55
1:J:280:ILE:HG22	1:J:281:TRP:H	1.70	0.55
1:J:41:LYS:HA	1:J:44:ARG:HB3	1.89	0.55
1:I:107:LEU:HD22	1:I:126:LYS:HD3	1.88	0.55
1:D:289:LYS:O	1:D:290:GLU:HB2	2.07	0.55
1:D:257:LEU:HD11	1:D:292:GLU:OE2	2.07	0.55
1:J:217:ARG:NE	1:J:450:HIS:HD2	2.05	0.55
1:A:99:VAL:HB	1:A:130:LYS:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6:ASP:HA	1:G:355:GLU:CG	2.36	0.55
1:B:315:LEU:O	1:B:339:VAL:HG12	2.07	0.55
1:F:92:GLY:HA2	1:F:166:ALA:O	2.06	0.55
1:G:500:PHE:HB2	1:I:501:THR:OG1	2.07	0.55
1:L:24:VAL:O	1:L:27:LYS:N	2.40	0.55
1:L:468:ALA:CB	1:L:480:ALA:HB1	2.37	0.55
1:L:59:LEU:HB2	1:L:157:PHE:CE2	2.41	0.55
1:K:280:ILE:HG22	1:K:281:TRP:H	1.72	0.55
1:L:273:VAL:O	1:L:314:ILE:HD12	2.07	0.55
1:I:273:VAL:O	1:I:314:ILE:HD12	2.07	0.55
1:L:455:TYR:CE1	1:L:459:ARG:HD3	2.36	0.55
1:D:245:LYS:HE2	1:D:245:LYS:H	1.70	0.55
1:B:245:LYS:H	1:B:245:LYS:HE2	1.71	0.55
1:G:491:ARG:O	1:G:495:GLU:HB2	2.07	0.55
1:C:493:TYR:C	1:C:495:GLU:H	2.10	0.55
1:D:446:LYS:HG3	1:D:450:HIS:CE1	2.42	0.55
1:L:257:LEU:HD11	1:L:292:GLU:OE2	2.07	0.55
1:B:106:ALA:O	1:B:109:SER:HB3	2.06	0.55
1:F:493:TYR:O	1:F:494:ASN:C	2.44	0.55
1:A:494:ASN:O	1:A:495:GLU:HB2	2.06	0.55
1:I:158:ILE:HG23	1:I:158:ILE:O	2.07	0.55
1:E:382:TYR:C	1:E:382:TYR:HD2	2.08	0.55
1:B:176:MET:HG3	1:B:198:VAL:CG2	2.37	0.55
1:K:99:VAL:CG1	1:K:128:GLY:HA3	2.26	0.55
1:K:468:ALA:CB	1:K:480:ALA:HB1	2.37	0.55
1:F:382:TYR:CD2	1:F:382:TYR:C	2.80	0.55
1:F:217:ARG:CZ	1:F:450:HIS:HD2	2.19	0.55
1:J:382:TYR:O	1:J:382:TYR:HD2	1.90	0.55
1:B:61:LEU:O	1:B:62:SER:HB2	2.07	0.55
1:J:488:LYS:O	1:J:491:ARG:HB2	2.07	0.55
1:G:274:GLY:HA3	1:G:279:SER:HA	1.89	0.55
1:E:38:GLU:CG	1:E:39:GLU:N	2.70	0.55
1:K:402:GLU:O	1:K:404:ASP:N	2.40	0.55
1:I:58:VAL:HG13	1:L:60:SER:HB2	1.87	0.55
1:L:477:LEU:H	1:L:477:LEU:HD22	1.71	0.55
1:L:250:GLN:NE2	2:L:552:NDP:H2A	2.21	0.55
1:H:25:GLU:O	1:H:29:VAL:HG23	2.07	0.55
1:H:337:PRO:HA	1:H:363:ARG:HH21	1.72	0.55
1:B:198:VAL:O	1:B:201:LYS:HE3	2.07	0.55
1:A:336:ALA:CB	1:A:337:PRO:HD3	2.29	0.55
1:G:382:TYR:C	1:G:382:TYR:CD2	2.79	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:165:PRO:O	1:G:198:VAL:HG23	2.06	0.55
1:C:247:PHE:CZ	1:C:270:CYS:HB2	2.41	0.55
1:C:499:THR:HG22	1:F:65:ILE:CG2	2.35	0.55
1:D:274:GLY:HA3	1:D:279:SER:HA	1.89	0.55
1:E:281:TRP:O	1:E:282:ASN:HB2	2.06	0.55
1:A:281:TRP:O	1:A:282:ASN:HB2	2.07	0.55
1:J:239:THR:O	1:J:241:GLY:N	2.39	0.55
1:G:141:LEU:HD22	1:G:144:ILE:HD12	1.89	0.55
1:C:458:GLU:C	1:C:460:SER:N	2.60	0.55
1:G:107:LEU:HD22	1:G:126:LYS:HD3	1.89	0.55
1:I:129:VAL:O	1:I:131:ILE:N	2.40	0.55
1:G:47:SER:O	1:G:50:ARG:N	2.38	0.55
1:E:346:GLU:CD	1:E:351:PRO:HD2	2.27	0.55
1:J:433:THR:HG22	1:K:412:SER:HA	1.89	0.55
1:D:383:PHE:HA	1:D:386:LEU:HD12	1.88	0.55
1:A:255:VAL:HG12	2:A:552:NDP:O2N	2.06	0.55
1:B:337:PRO:HA	1:B:363:ARG:HH21	1.72	0.55
1:G:217:ARG:CZ	1:G:450:HIS:CD2	2.90	0.55
1:G:382:TYR:O	1:G:382:TYR:HD2	1.90	0.55
1:C:24:VAL:O	1:C:25:GLU:C	2.45	0.55
1:D:445:GLU:O	1:D:449:VAL:HG23	2.06	0.55
1:D:56:ASN:C	1:D:57:HIS:HD2	2.09	0.55
3:J:601:XEG:CAL	3:J:601:XEG:HAPA	2.37	0.55
1:B:280:ILE:HG22	1:B:281:TRP:H	1.72	0.55
1:G:412:SER:CA	1:H:433:THR:HG22	2.37	0.55
3:D:601:XEG:CAZ	3:D:601:XEG:CAP	2.85	0.55
1:J:36:GLU:CB	1:J:40:GLN:HG2	2.37	0.55
1:I:458:GLU:C	1:I:460:SER:N	2.61	0.55
1:I:60:SER:HB2	1:L:58:VAL:HG13	1.88	0.55
1:E:159:GLY:O	1:E:162:VAL:HG12	2.07	0.55
1:A:291:LEU:HD12	1:A:304:PHE:CZ	2.42	0.54
1:F:436:PHE:CD1	1:F:436:PHE:C	2.81	0.54
1:K:120:VAL:HG13	1:K:382:TYR:CD1	2.42	0.54
1:D:201:LYS:H	1:D:201:LYS:HD3	1.71	0.54
1:G:120:VAL:HG13	1:G:382:TYR:CD1	2.41	0.54
1:G:167:PRO:HD3	1:G:176:MET:SD	2.47	0.54
1:E:458:GLU:C	1:E:460:SER:H	2.11	0.54
1:E:468:ALA:CB	1:E:480:ALA:HB1	2.37	0.54
1:F:301:ILE:O	1:F:302:LEU:HG	2.08	0.54
1:E:56:ASN:C	1:E:57:HIS:CD2	2.80	0.54
1:K:291:LEU:HD12	1:K:304:PHE:CZ	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:HIS:O	1:B:266:PHE:N	2.39	0.54
1:F:41:LYS:HA	1:F:44:ARG:HB3	1.88	0.54
1:B:446:LYS:HG3	1:B:450:HIS:CE1	2.42	0.54
1:C:107:LEU:HD22	1:C:126:LYS:HD3	1.88	0.54
1:K:175:GLU:O	1:K:178:TRP:HB2	2.07	0.54
1:E:301:ILE:O	1:E:302:LEU:HG	2.07	0.54
1:J:121:PRO:O	1:J:122:PHE:HD2	1.91	0.54
1:H:100:SER:HB3	1:H:103:GLU:HB2	1.89	0.54
1:K:167:PRO:HD3	1:K:176:MET:SD	2.48	0.54
1:D:173:GLU:HB2	1:D:202:PRO:HD3	1.88	0.54
1:C:337:PRO:HA	1:C:363:ARG:HH21	1.72	0.54
1:C:120:VAL:HG13	1:C:382:TYR:CD1	2.42	0.54
3:E:601:XEG:CAZ	3:E:601:XEG:CAP	2.86	0.54
1:H:56:ASN:C	1:H:57:HIS:HD2	2.10	0.54
1:H:455:TYR:O	1:H:455:TYR:HD1	1.90	0.54
1:B:274:GLY:HA3	1:B:279:SER:HA	1.90	0.54
1:K:281:TRP:HD1	1:K:283:PRO:HD3	1.69	0.54
1:F:6:ASP:N	1:F:332:THR:HB	2.22	0.54
1:G:245:LYS:H	1:G:245:LYS:HE2	1.70	0.54
1:H:257:LEU:HD11	1:H:292:GLU:OE2	2.07	0.54
1:E:246:THR:HG22	1:E:269:LYS:O	2.07	0.54
1:D:25:GLU:O	1:D:29:VAL:HG23	2.08	0.54
1:H:24:VAL:O	1:H:25:GLU:C	2.45	0.54
1:B:468:ALA:CB	1:B:480:ALA:HB1	2.37	0.54
1:C:99:VAL:HB	1:C:130:LYS:HB3	1.88	0.54
1:G:148:PHE:CZ	1:G:152:LEU:HD21	2.42	0.54
1:B:499:THR:HG21	1:E:65:ILE:CG2	2.38	0.54
1:I:291:LEU:HD12	1:I:304:PHE:CZ	2.42	0.54
1:A:498:VAL:HG22	1:A:500:PHE:H	1.71	0.54
1:E:274:GLY:HA3	1:E:279:SER:HA	1.89	0.54
1:I:279:SER:HB2	1:I:310:TYR:O	2.05	0.54
1:B:56:ASN:O	1:B:57:HIS:CD2	2.57	0.54
1:D:142:GLU:HB2	1:D:178:TRP:CZ2	2.42	0.54
1:L:246:THR:HG22	1:L:269:LYS:O	2.07	0.54
1:D:369:PRO:HG3	1:D:478:ARG:N	2.23	0.54
1:B:412:SER:N	1:F:433:THR:HG22	2.22	0.54
1:A:491:ARG:CZ	1:A:491:ARG:HB2	2.38	0.54
1:A:165:PRO:O	1:A:198:VAL:HG23	2.08	0.54
1:F:25:GLU:O	1:F:29:VAL:HG23	2.07	0.54
1:F:90:LYS:HB2	1:F:122:PHE:HD1	1.73	0.54
1:D:315:LEU:O	1:D:339:VAL:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:107:LEU:HD22	1:F:126:LYS:HD3	1.89	0.54
1:J:190:TYR:O	1:J:191:ASP:HB2	2.07	0.54
1:C:69:ASP:OD2	1:C:71:SER:HB2	2.08	0.54
1:G:413:VAL:HG12	1:G:414:GLN:N	2.23	0.54
1:A:264:HIS:O	1:A:266:PHE:N	2.40	0.54
1:A:414:GLN:HB2	1:A:429:PRO:CG	2.38	0.54
1:H:94:ARG:HG3	1:H:169:MET:CB	2.30	0.54
3:G:601:XEG:CAZ	3:G:601:XEG:CAP	2.84	0.54
1:B:121:PRO:O	1:B:122:PHE:HD2	1.91	0.54
1:F:24:VAL:O	1:F:27:LYS:N	2.40	0.54
1:I:56:ASN:C	1:I:57:HIS:HD2	2.11	0.54
1:H:274:GLY:HA3	1:H:279:SER:HA	1.89	0.54
1:L:274:GLY:HA3	1:L:279:SER:HA	1.88	0.54
1:A:38:GLU:CG	1:A:39:GLU:N	2.70	0.54
1:B:414:GLN:OE1	1:B:430:ILE:HG12	2.08	0.54
1:L:97:THR:OG1	1:L:132:ASN:HB2	2.07	0.54
1:K:391:HIS:O	1:K:392:VAL:HG13	2.06	0.54
1:E:291:LEU:HD12	1:E:304:PHE:CZ	2.43	0.54
1:A:436:PHE:CE2	1:F:409:LEU:HD12	2.41	0.54
1:G:99:VAL:HG11	1:G:128:GLY:CA	2.31	0.54
1:K:382:TYR:CD2	1:K:382:TYR:C	2.78	0.54
1:F:202:PRO:HG2	1:F:205:GLN:HG3	1.90	0.54
1:E:464:ILE:O	1:E:468:ALA:HB3	2.07	0.54
1:H:492:VAL:CG2	1:H:493:TYR:H	2.17	0.54
1:K:110:LEU:HD23	1:K:111:MET:N	2.23	0.54
1:B:455:TYR:O	1:B:455:TYR:HD1	1.90	0.54
1:B:323:ILE:HG22	1:B:345:ALA:O	2.08	0.54
1:F:129:VAL:HG12	1:F:129:VAL:O	2.07	0.54
1:G:252:PHE:HE2	1:G:260:MET:SD	2.31	0.54
1:H:186:THR:OG1	1:H:187:ILE:N	2.41	0.54
1:I:246:THR:HG22	1:I:269:LYS:O	2.08	0.54
1:D:336:ALA:CB	1:D:337:PRO:HD3	2.26	0.54
1:J:337:PRO:HA	1:J:363:ARG:HH21	1.72	0.54
1:K:96:SER:C	1:K:98:ASP:H	2.11	0.54
1:C:167:PRO:HD3	1:C:176:MET:HG2	1.89	0.54
1:H:166:ALA:HA	1:H:176:MET:HE2	1.90	0.54
1:C:499:THR:HG23	1:F:147:ARG:HE	1.72	0.54
1:I:247:PHE:CE1	1:I:270:CYS:HB2	2.42	0.54
1:K:321:ILE:HD11	1:K:343:ILE:HD12	1.90	0.54
1:F:274:GLY:HA3	1:F:279:SER:HA	1.89	0.54
1:J:322:LEU:HD22	1:J:323:ILE:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:THR:O	1:B:241:GLY:N	2.41	0.54
1:G:322:LEU:HD22	1:G:323:ILE:N	2.23	0.54
1:H:458:GLU:C	1:H:460:SER:H	2.10	0.54
1:H:221:HIS:HA	1:H:224:GLU:HB3	1.88	0.54
1:F:186:THR:OG1	1:F:187:ILE:N	2.39	0.54
1:E:247:PHE:CE1	1:E:270:CYS:HB2	2.42	0.54
1:A:307:ALA:O	1:A:308:LYS:HB2	2.08	0.54
1:D:337:PRO:HA	1:D:363:ARG:HH21	1.72	0.54
1:I:337:PRO:HA	1:I:363:ARG:HH21	1.73	0.54
1:D:488:LYS:NZ	3:D:502:XEG:HAK	2.22	0.54
1:G:24:VAL:O	1:G:25:GLU:C	2.47	0.54
1:H:369:PRO:HD3	1:H:477:LEU:HB2	1.89	0.54
1:E:7:PRO:HD3	1:E:355:GLU:HG3	1.89	0.54
1:E:59:LEU:HB2	1:E:157:PHE:CE2	2.43	0.54
3:L:601:XEG:CAL	3:L:601:XEG:HAPA	2.37	0.54
1:D:214:ALA:CB	1:D:380:VAL:HG21	2.36	0.54
1:D:291:LEU:HD12	1:D:304:PHE:CZ	2.43	0.54
1:D:500:PHE:CD2	1:D:500:PHE:N	2.75	0.54
1:K:315:LEU:O	1:K:339:VAL:HG12	2.07	0.54
1:E:36:GLU:CB	1:E:40:GLN:HG2	2.36	0.54
1:A:322:LEU:HD22	1:A:323:ILE:N	2.23	0.54
1:F:246:THR:HG22	1:F:269:LYS:O	2.08	0.54
1:E:47:SER:O	1:E:50:ARG:N	2.39	0.54
1:J:110:LEU:HD23	1:J:111:MET:N	2.22	0.54
1:J:186:THR:OG1	1:J:187:ILE:N	2.40	0.54
1:L:414:GLN:OE1	1:L:430:ILE:HG12	2.06	0.54
1:L:436:PHE:HD1	1:L:436:PHE:C	2.11	0.54
1:B:25:GLU:O	1:B:29:VAL:HG23	2.08	0.54
1:D:413:VAL:HG12	1:D:414:GLN:N	2.22	0.54
1:E:414:GLN:HB2	1:E:429:PRO:HG2	1.89	0.54
1:A:337:PRO:HA	1:A:363:ARG:HH21	1.73	0.54
1:D:167:PRO:HD3	1:D:176:MET:HG2	1.89	0.54
1:G:468:ALA:CB	1:G:480:ALA:HB1	2.38	0.54
1:B:13:VAL:O	1:B:14:GLU:C	2.46	0.54
1:C:167:PRO:HD3	1:C:176:MET:CG	2.37	0.54
1:H:13:VAL:O	1:H:14:GLU:C	2.45	0.54
1:C:301:ILE:O	1:C:302:LEU:HG	2.08	0.54
1:L:167:PRO:HD3	1:L:176:MET:CG	2.38	0.54
3:E:601:XEG:HAPA	3:E:601:XEG:CAL	2.38	0.54
1:K:366:MET:HB2	1:K:475:LEU:HD13	1.90	0.54
1:B:234:SER:C	1:B:236:LEU:N	2.62	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:ILE:HG22	1:D:281:TRP:H	1.72	0.54
1:K:279:SER:HB2	1:K:310:TYR:O	2.07	0.54
1:G:280:ILE:HG22	1:G:281:TRP:H	1.72	0.54
1:C:280:ILE:HG22	1:C:281:TRP:H	1.72	0.54
1:D:239:THR:O	1:D:241:GLY:N	2.41	0.54
1:L:457:MET:O	1:L:460:SER:HB2	2.08	0.54
1:J:460:SER:O	1:J:461:ALA:C	2.46	0.54
1:I:97:THR:OG1	1:I:132:ASN:HB2	2.07	0.54
1:J:217:ARG:NE	1:J:450:HIS:CD2	2.76	0.54
1:D:53:LYS:N	1:D:54:PRO:CD	2.70	0.54
1:A:346:GLU:CD	1:A:351:PRO:HD2	2.27	0.54
1:C:392:VAL:HG11	1:E:386:LEU:HD13	1.90	0.54
1:A:436:PHE:C	1:A:436:PHE:CD1	2.78	0.54
1:B:121:PRO:HD2	1:B:382:TYR:CE1	2.43	0.54
3:A:601:XEG:HAPA	3:A:601:XEG:CAL	2.38	0.54
1:K:382:TYR:HD2	1:K:382:TYR:C	2.11	0.54
1:K:346:GLU:OE1	1:K:478:ARG:NH2	2.41	0.54
1:H:321:ILE:HD11	1:H:343:ILE:HD12	1.90	0.54
1:J:291:LEU:HD12	1:J:304:PHE:CZ	2.43	0.54
1:F:491:ARG:HD2	3:F:601:XEG:CAN	2.38	0.54
1:D:52:ILE:HD13	1:D:489:VAL:CG1	2.37	0.54
1:I:322:LEU:HD22	1:I:323:ILE:N	2.23	0.54
1:E:322:LEU:HD22	1:E:323:ILE:N	2.23	0.54
1:D:141:LEU:HD22	1:D:144:ILE:HD12	1.90	0.54
1:H:458:GLU:C	1:H:460:SER:N	2.60	0.54
1:I:417:LEU:HD21	1:K:417:LEU:HD21	1.90	0.54
1:J:106:ALA:O	1:J:109:SER:HB3	2.08	0.54
1:D:186:THR:OG1	1:D:187:ILE:N	2.37	0.54
1:H:409:LEU:CD1	1:L:436:PHE:CE2	2.91	0.53
1:F:337:PRO:HA	1:F:363:ARG:HH21	1.71	0.53
1:G:337:PRO:HA	1:G:363:ARG:HH21	1.72	0.53
1:E:114:LYS:NZ	1:E:349:ASN:HD21	2.06	0.53
1:C:24:VAL:O	1:C:27:LYS:N	2.41	0.53
1:G:12:MET:HG3	1:G:13:VAL:H	1.73	0.53
1:B:291:LEU:HD12	1:B:304:PHE:CZ	2.43	0.53
1:F:7:PRO:HD3	1:F:332:THR:HG22	1.90	0.53
1:G:281:TRP:O	1:G:282:ASN:HB2	2.08	0.53
1:G:315:LEU:O	1:G:339:VAL:HG12	2.07	0.53
1:L:339:VAL:HG21	1:L:360:PHE:HE1	1.73	0.53
1:D:234:SER:C	1:D:236:LEU:N	2.62	0.53
1:E:445:GLU:O	1:E:449:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:457:MET:O	1:I:460:SER:HB2	2.08	0.53
1:L:346:GLU:CD	1:L:351:PRO:HD2	2.28	0.53
1:B:129:VAL:O	1:B:131:ILE:N	2.41	0.53
1:C:289:LYS:O	1:C:290:GLU:HB2	2.07	0.53
1:L:61:LEU:HD11	1:L:151:GLU:HB3	1.89	0.53
1:B:257:LEU:HD11	1:B:292:GLU:OE2	2.08	0.53
1:I:413:VAL:CG2	1:K:413:VAL:HG21	2.38	0.53
1:I:429:PRO:O	1:I:431:VAL:N	2.41	0.53
1:A:301:ILE:O	1:A:302:LEU:HG	2.07	0.53
1:K:149:THR:HB	1:K:182:THR:HG21	1.90	0.53
1:B:202:PRO:HG2	1:B:205:GLN:CG	2.38	0.53
1:F:336:ALA:CB	1:F:337:PRO:HD3	2.29	0.53
1:G:455:TYR:HE2	1:L:399:PHE:HB2	1.72	0.53
3:A:601:XEG:CAP	3:A:601:XEG:CAZ	2.86	0.53
1:H:90:LYS:HB2	1:H:122:PHE:HD1	1.69	0.53
1:L:247:PHE:CE1	1:L:270:CYS:HB2	2.43	0.53
1:F:56:ASN:C	1:F:57:HIS:HD2	2.11	0.53
1:A:500:PHE:HE2	1:D:66:ARG:HH11	1.55	0.53
1:E:245:LYS:HB3	1:E:320:ASP:CB	2.38	0.53
1:A:245:LYS:HB3	1:A:320:ASP:CB	2.38	0.53
1:A:396:ARG:NH2	1:B:456:THR:HG23	2.23	0.53
1:C:281:TRP:HD1	1:C:283:PRO:HD3	1.70	0.53
1:I:38:GLU:CG	1:I:39:GLU:N	2.72	0.53
1:B:136:TYR:HB2	1:B:141:LEU:CD2	2.38	0.53
1:L:38:GLU:CG	1:L:39:GLU:N	2.71	0.53
1:L:41:LYS:HA	1:L:44:ARG:HB3	1.89	0.53
1:D:47:SER:O	1:D:50:ARG:N	2.41	0.53
1:I:383:PHE:CE2	1:J:397:LEU:HD11	2.42	0.53
1:L:289:LYS:O	1:L:290:GLU:HB2	2.08	0.53
1:G:436:PHE:C	1:G:436:PHE:CD1	2.81	0.53
1:A:247:PHE:CE1	1:A:270:CYS:HB2	2.43	0.53
1:J:202:PRO:HG2	1:J:205:GLN:CG	2.39	0.53
1:K:167:PRO:HD3	1:K:176:MET:CG	2.37	0.53
3:D:502:XEG:CAP	3:D:502:XEG:CAZ	2.86	0.53
1:H:343:ILE:HG23	1:H:366:MET:HE3	1.90	0.53
1:E:7:PRO:O	1:E:8:ASN:HB3	2.09	0.53
1:D:13:VAL:O	1:D:14:GLU:C	2.46	0.53
1:H:91:GLY:O	1:H:165:PRO:HA	2.07	0.53
1:L:291:LEU:HD12	1:L:304:PHE:CZ	2.43	0.53
1:H:487:GLU:CG	1:H:491:ARG:HH21	2.20	0.53
1:J:274:GLY:HA3	1:J:279:SER:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:279:SER:HB2	1:G:310:TYR:O	2.07	0.53
1:H:41:LYS:HA	1:H:44:ARG:HB3	1.90	0.53
1:G:149:THR:HB	1:G:182:THR:HG21	1.89	0.53
1:L:301:ILE:O	1:L:302:LEU:HG	2.09	0.53
1:F:9:PHE:HB3	1:F:329:LYS:HZ3	1.73	0.53
1:H:106:ALA:O	1:H:109:SER:HB3	2.09	0.53
1:E:289:LYS:O	1:E:290:GLU:HB2	2.08	0.53
1:E:100:SER:HB3	1:E:103:GLU:HB2	1.89	0.53
1:L:129:VAL:O	1:L:131:ILE:N	2.42	0.53
1:D:458:GLU:C	1:D:460:SER:H	2.11	0.53
1:A:409:LEU:O	1:A:411:MET:N	2.36	0.53
1:G:6:ASP:CG	1:G:6:ASP:O	2.47	0.53
1:K:90:LYS:HG3	1:K:122:PHE:CE1	2.44	0.53
1:K:12:MET:HG3	1:K:13:VAL:H	1.73	0.53
1:D:12:MET:N	1:D:14:GLU:HG2	2.16	0.53
3:F:601:XEG:CAP	3:F:601:XEG:CAZ	2.85	0.53
1:A:386:LEU:HD13	1:F:392:VAL:HG11	1.90	0.53
1:F:247:PHE:CE1	1:F:270:CYS:HB2	2.43	0.53
1:C:56:ASN:C	1:C:57:HIS:CD2	2.82	0.53
1:G:291:LEU:HD12	1:G:304:PHE:CZ	2.43	0.53
1:B:445:GLU:O	1:B:449:VAL:HG23	2.08	0.53
1:H:459:ARG:NH2	3:H:601:XEG:OAH	2.42	0.53
1:F:245:LYS:HB3	1:F:320:ASP:CB	2.39	0.53
1:H:322:LEU:HD22	1:H:323:ILE:N	2.22	0.53
1:L:300:THR:O	1:L:301:ILE:HG23	2.08	0.53
1:F:289:LYS:O	1:F:290:GLU:HB2	2.08	0.53
1:I:432:PRO:HA	1:J:412:SER:OG	2.08	0.53
1:J:94:ARG:HG3	1:J:169:MET:CB	2.29	0.53
1:J:336:ALA:CB	1:J:337:PRO:HD3	2.26	0.53
1:J:96:SER:C	1:J:98:ASP:H	2.10	0.53
1:J:477:LEU:HD22	1:J:477:LEU:H	1.73	0.53
1:G:307:ALA:O	1:G:308:LYS:HB2	2.09	0.53
1:C:371:LEU:HD23	1:C:481:ALA:CB	2.39	0.53
1:D:323:ILE:HG22	1:D:345:ALA:O	2.09	0.53
1:L:458:GLU:C	1:L:460:SER:H	2.12	0.53
1:L:458:GLU:C	1:L:460:SER:N	2.60	0.53
1:F:344:ILE:HB	1:F:367:VAL:HG12	1.91	0.53
1:L:158:ILE:HG23	1:L:158:ILE:O	2.08	0.53
1:I:409:LEU:HD12	1:K:436:PHE:CE2	2.43	0.53
1:C:412:SER:HB3	1:E:432:PRO:HA	1.90	0.53
1:I:382:TYR:C	1:I:382:TYR:CD2	2.82	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ALA:CB	1:A:480:ALA:HB1	2.38	0.53
1:H:300:THR:O	1:H:301:ILE:HG23	2.09	0.53
1:K:12:MET:N	1:K:14:GLU:HG2	2.16	0.53
1:C:291:LEU:HD12	1:C:304:PHE:CZ	2.44	0.53
1:H:217:ARG:NE	1:H:450:HIS:HD2	2.07	0.53
1:E:239:THR:O	1:E:241:GLY:N	2.41	0.53
1:B:212:ILE:H	1:B:212:ILE:CD1	2.14	0.53
1:G:36:GLU:CB	1:G:40:GLN:HG2	2.37	0.53
1:G:491:ARG:HB2	1:G:491:ARG:NH1	2.23	0.53
1:A:374:ASN:C	1:A:376:GLY:H	2.09	0.53
1:K:436:PHE:C	1:K:436:PHE:HD1	2.12	0.53
1:B:99:VAL:HG11	1:B:128:GLY:CA	2.28	0.53
1:J:99:VAL:HB	1:J:130:LYS:HB3	1.91	0.53
1:H:478:ARG:O	1:H:481:ALA:N	2.41	0.53
1:L:337:PRO:HA	1:L:363:ARG:HH21	1.73	0.53
1:C:208:ILE:CG2	1:C:211:ARG:HB2	2.38	0.53
1:H:205:GLN:OE1	1:L:496:ALA:HB2	2.08	0.53
1:B:234:SER:O	1:B:236:LEU:N	2.41	0.53
1:G:111:MET:HE3	2:G:552:NDP:H72N	1.72	0.53
1:E:280:ILE:HG22	1:E:281:TRP:H	1.73	0.53
1:H:245:LYS:HB3	1:H:320:ASP:CB	2.39	0.53
1:F:38:GLU:C	1:F:40:GLN:H	2.12	0.53
1:I:300:THR:O	1:I:301:ILE:HG23	2.09	0.53
1:C:16:PHE:CE1	1:C:478:ARG:HD3	2.43	0.53
1:C:246:THR:HG22	1:C:269:LYS:O	2.08	0.53
1:G:436:PHE:HD1	1:G:436:PHE:C	2.10	0.53
1:H:412:SER:CA	1:L:433:THR:HG22	2.38	0.53
1:L:436:PHE:CD1	1:L:436:PHE:C	2.82	0.53
1:J:19:ARG:NE	1:J:479:THR:HG21	2.24	0.53
1:H:96:SER:C	1:H:98:ASP:H	2.11	0.53
1:G:459:ARG:CZ	3:G:601:XEG:OAH	2.56	0.53
1:I:395:GLY:O	1:I:397:LEU:N	2.41	0.53
1:H:379:THR:O	1:H:382:TYR:HB3	2.08	0.53
1:C:25:GLU:O	1:C:29:VAL:HG23	2.08	0.53
1:F:87:THR:CB	1:F:88:PRO:CD	2.86	0.53
1:L:24:VAL:O	1:L:25:GLU:C	2.46	0.53
1:H:167:PRO:HD3	1:H:176:MET:HG2	1.91	0.53
1:L:286:ILE:O	1:L:286:ILE:HG13	2.09	0.53
1:H:488:LYS:O	1:H:491:ARG:HG3	2.09	0.53
1:C:245:LYS:HB3	1:C:320:ASP:CB	2.38	0.53
1:C:38:GLU:CG	1:C:39:GLU:N	2.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:38:GLU:C	1:J:40:GLN:H	2.12	0.53
1:D:85:HIS:CD2	1:D:492:VAL:HG11	2.44	0.53
1:E:95:TYR:HB3	1:E:133:PRO:HG3	1.90	0.53
1:J:460:SER:O	1:J:463:GLN:N	2.42	0.53
1:F:116:ALA:O	1:F:488:LYS:HD2	2.08	0.53
1:I:436:PHE:HD1	1:I:436:PHE:C	2.12	0.53
1:G:436:PHE:CE2	1:L:409:LEU:HD12	2.44	0.53
1:B:458:GLU:C	1:B:460:SER:N	2.61	0.53
1:C:100:SER:HB3	1:C:103:GLU:HB2	1.91	0.53
1:J:25:GLU:O	1:J:29:VAL:HG23	2.08	0.53
1:B:344:ILE:HB	1:B:367:VAL:HG12	1.90	0.53
1:A:372:TYR:CD2	1:A:464:ILE:HD11	2.44	0.53
1:J:321:ILE:HD11	1:J:343:ILE:HD12	1.90	0.53
1:E:455:TYR:CE1	1:E:459:ARG:HD3	2.37	0.53
1:J:379:THR:O	1:J:382:TYR:HB3	2.09	0.53
1:G:245:LYS:HB3	1:G:320:ASP:CB	2.39	0.53
1:F:281:TRP:O	1:F:282:ASN:HB2	2.09	0.53
1:D:500:PHE:HD2	1:D:500:PHE:N	2.07	0.53
1:H:38:GLU:C	1:H:40:GLN:H	2.12	0.53
1:K:322:LEU:HD22	1:K:323:ILE:N	2.23	0.53
1:H:312:GLY:O	1:H:313:SER:C	2.47	0.53
1:J:458:GLU:C	1:J:460:SER:N	2.62	0.53
1:I:301:ILE:O	1:I:302:LEU:HG	2.08	0.53
1:B:301:ILE:O	1:B:302:LEU:HG	2.09	0.53
1:G:428:ILE:HD11	1:L:419:ARG:HD2	1.91	0.53
1:I:13:VAL:O	1:I:14:GLU:C	2.47	0.53
1:I:455:TYR:HD1	1:I:455:TYR:O	1.93	0.53
1:G:214:ALA:CB	1:G:380:VAL:HG21	2.37	0.53
1:L:6:ASP:C	1:L:8:ASN:N	2.63	0.53
1:H:301:ILE:O	1:H:302:LEU:HG	2.09	0.53
3:B:601:XEG:CAZ	3:B:601:XEG:CAP	2.87	0.53
1:F:307:ALA:O	1:F:308:LYS:HB2	2.08	0.53
1:F:121:PRO:HD2	1:F:382:TYR:CE1	2.44	0.53
1:B:421:PHE:HE1	1:B:423:LYS:O	1.92	0.53
1:C:322:LEU:HD22	1:C:323:ILE:N	2.24	0.53
1:I:90:LYS:HB2	1:I:122:PHE:HD1	1.70	0.53
1:L:141:LEU:O	1:L:145:THR:HG23	2.09	0.53
1:C:97:THR:OG1	1:C:132:ASN:HB2	2.09	0.53
1:K:458:GLU:C	1:K:460:SER:N	2.61	0.53
1:B:142:GLU:OE2	1:F:500:PHE:CZ	2.62	0.53
1:D:196:ALA:HB2	1:D:389:LEU:HD23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:ILE:O	1:F:158:ILE:HG23	2.09	0.53
1:K:252:PHE:HE2	1:K:260:MET:SD	2.32	0.53
1:H:397:LEU:HD11	1:L:383:PHE:CE2	2.44	0.53
1:C:344:ILE:HB	1:C:367:VAL:HG12	1.90	0.53
1:B:203:ILE:N	1:B:203:ILE:HD12	2.24	0.53
1:E:366:MET:HG3	1:E:477:LEU:HD21	1.91	0.52
1:F:96:SER:C	1:F:98:ASP:H	2.12	0.52
1:H:473:LEU:HD23	1:H:479:THR:OG1	2.10	0.52
1:B:24:VAL:O	1:B:27:LYS:N	2.43	0.52
1:I:346:GLU:CD	1:I:351:PRO:HD2	2.29	0.52
1:B:167:PRO:HD3	1:B:176:MET:HG2	1.91	0.52
3:K:601:XEG:CAZ	3:K:601:XEG:CAP	2.85	0.52
1:F:208:ILE:CG2	1:F:211:ARG:HB2	2.40	0.52
1:C:247:PHE:CE1	1:C:270:CYS:HB2	2.44	0.52
1:K:56:ASN:C	1:K:57:HIS:CD2	2.82	0.52
1:K:307:ALA:O	1:K:308:LYS:HB2	2.09	0.52
1:L:455:TYR:HD1	1:L:455:TYR:O	1.92	0.52
1:G:339:VAL:HG21	1:G:360:PHE:HE1	1.74	0.52
1:I:36:GLU:CB	1:I:40:GLN:HG2	2.36	0.52
1:J:38:GLU:CG	1:J:39:GLU:N	2.72	0.52
1:I:345:ALA:HB1	1:I:373:LEU:HD21	1.91	0.52
1:F:315:LEU:O	1:F:339:VAL:HG12	2.10	0.52
1:D:374:ASN:C	1:D:376:GLY:N	2.62	0.52
1:H:374:ASN:C	1:H:376:GLY:N	2.62	0.52
1:L:16:PHE:CE2	1:L:354:PRO:HG3	2.43	0.52
1:J:217:ARG:CD	1:J:450:HIS:CD2	2.92	0.52
1:B:53:LYS:N	1:B:54:PRO:CD	2.72	0.52
1:E:165:PRO:O	1:E:198:VAL:HG23	2.08	0.52
1:B:52:ILE:HD13	1:B:489:VAL:CG1	2.37	0.52
1:E:337:PRO:HA	1:E:363:ARG:HH21	1.73	0.52
1:A:24:VAL:O	1:A:25:GLU:C	2.48	0.52
1:L:13:VAL:O	1:L:14:GLU:C	2.47	0.52
1:C:12:MET:HG3	1:C:13:VAL:H	1.73	0.52
1:K:281:TRP:O	1:K:282:ASN:HB2	2.08	0.52
1:D:421:PHE:HE1	1:D:423:LYS:O	1.92	0.52
1:F:281:TRP:HD1	1:F:283:PRO:HD3	1.70	0.52
1:F:38:GLU:CG	1:F:39:GLU:N	2.72	0.52
1:F:222:GLY:HA3	1:F:373:LEU:CD1	2.40	0.52
1:J:301:ILE:O	1:J:302:LEU:HG	2.09	0.52
1:E:420:LYS:O	1:E:420:LYS:HG2	2.08	0.52
1:C:23:ILE:HG22	1:C:471:TYR:HD1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:289:LYS:O	1:I:290:GLU:HB2	2.09	0.52
1:G:239:THR:O	1:G:241:GLY:N	2.43	0.52
1:E:300:THR:O	1:E:301:ILE:HG23	2.09	0.52
1:A:343:ILE:HG23	1:A:366:MET:HE3	1.91	0.52
1:D:344:ILE:HB	1:D:367:VAL:HG12	1.91	0.52
1:B:337:PRO:HG3	1:B:359:ILE:HD12	1.91	0.52
1:I:202:PRO:HG2	1:I:205:GLN:CG	2.38	0.52
1:J:307:ALA:O	1:J:308:LYS:HB2	2.10	0.52
1:I:307:ALA:O	1:I:308:LYS:HB2	2.08	0.52
1:L:307:ALA:O	1:L:308:LYS:HB2	2.08	0.52
1:D:281:TRP:O	1:D:282:ASN:HB2	2.10	0.52
1:K:36:GLU:CB	1:K:40:GLN:HG2	2.37	0.52
1:D:38:GLU:C	1:D:40:GLN:H	2.13	0.52
1:I:411:MET:HA	1:I:414:GLN:HB3	1.92	0.52
1:A:167:PRO:HD3	1:A:176:MET:HG2	1.92	0.52
1:E:110:LEU:HD23	1:E:111:MET:N	2.23	0.52
1:E:396:ARG:NH1	1:E:396:ARG:HG3	2.22	0.52
1:I:339:VAL:HG21	1:I:360:PHE:HE1	1.74	0.52
1:L:38:GLU:C	1:L:40:GLN:H	2.13	0.52
1:K:488:LYS:O	1:K:492:VAL:HG23	2.09	0.52
1:G:402:GLU:O	1:G:404:ASP:N	2.36	0.52
1:B:196:ALA:CB	1:B:389:LEU:HD23	2.40	0.52
1:F:97:THR:OG1	1:F:132:ASN:HB2	2.09	0.52
1:C:23:ILE:CG2	1:C:471:TYR:HD1	2.22	0.52
1:A:47:SER:O	1:A:50:ARG:N	2.39	0.52
1:K:414:GLN:HB2	1:K:429:PRO:HG2	1.91	0.52
1:G:413:VAL:HG21	1:L:413:VAL:CG2	2.39	0.52
1:A:300:THR:O	1:A:301:ILE:HG23	2.10	0.52
1:C:391:HIS:O	1:E:386:LEU:CD2	2.57	0.52
1:C:433:THR:HG22	1:D:412:SER:N	2.24	0.52
1:I:94:ARG:HG3	1:I:169:MET:CB	2.30	0.52
1:A:167:PRO:HD3	1:A:176:MET:SD	2.50	0.52
1:F:166:ALA:HA	1:F:176:MET:HE2	1.91	0.52
1:L:96:SER:C	1:L:98:ASP:H	2.12	0.52
1:K:300:THR:O	1:K:301:ILE:HG23	2.10	0.52
1:J:281:TRP:O	1:J:282:ASN:HB2	2.09	0.52
1:B:281:TRP:O	1:B:282:ASN:HB2	2.10	0.52
1:H:217:ARG:NE	1:H:450:HIS:CD2	2.77	0.52
1:B:56:ASN:C	1:B:57:HIS:HD2	2.13	0.52
1:G:412:SER:HA	1:H:433:THR:HG22	1.89	0.52
1:C:222:GLY:HA3	1:C:373:LEU:CD1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:402:GLU:O	1:D:404:ASP:N	2.40	0.52
1:G:458:GLU:C	1:G:460:SER:N	2.61	0.52
1:H:69:ASP:OD2	1:H:71:SER:HB2	2.09	0.52
1:K:106:ALA:O	1:K:109:SER:HB3	2.10	0.52
1:E:257:LEU:HD11	1:E:292:GLU:OE2	2.09	0.52
1:K:413:VAL:HG12	1:K:414:GLN:N	2.23	0.52
1:K:432:PRO:O	1:K:433:THR:O	2.27	0.52
1:H:412:SER:OG	1:L:432:PRO:HA	2.09	0.52
1:B:38:GLU:CG	1:B:39:GLU:N	2.73	0.52
1:A:96:SER:C	1:A:98:ASP:H	2.13	0.52
1:J:86:ARG:HG2	1:J:121:PRO:CA	2.40	0.52
1:B:330:GLN:O	1:B:331:LEU:HD12	2.10	0.52
1:D:167:PRO:HD3	1:D:176:MET:CG	2.40	0.52
1:H:291:LEU:HD12	1:H:304:PHE:CZ	2.44	0.52
1:H:307:ALA:O	1:H:308:LYS:HB2	2.09	0.52
1:E:7:PRO:HD3	1:E:355:GLU:CG	2.39	0.52
1:J:339:VAL:HG21	1:J:360:PHE:HE1	1.74	0.52
1:F:167:PRO:HD3	1:F:176:MET:HG2	1.91	0.52
1:B:498:VAL:HG23	1:B:499:THR:N	2.24	0.52
1:D:321:ILE:HD11	1:D:343:ILE:HD12	1.92	0.52
1:C:323:ILE:HG22	1:C:345:ALA:O	2.09	0.52
1:H:38:GLU:CG	1:H:39:GLU:N	2.72	0.52
1:L:345:ALA:HB1	1:L:373:LEU:HD21	1.91	0.52
1:B:374:ASN:C	1:B:376:GLY:N	2.63	0.52
1:B:203:ILE:H	1:B:203:ILE:HD12	1.75	0.52
1:J:69:ASP:OD2	1:J:71:SER:HB2	2.10	0.52
1:G:106:ALA:O	1:G:109:SER:HB3	2.10	0.52
1:C:158:ILE:HG23	1:C:158:ILE:O	2.10	0.52
1:F:63:PHE:N	1:F:63:PHE:CD2	2.78	0.52
1:I:436:PHE:CD1	1:I:436:PHE:C	2.83	0.52
1:E:52:ILE:HD13	1:E:489:VAL:CG1	2.40	0.52
1:I:85:HIS:CD2	1:I:492:VAL:HG11	2.44	0.52
1:K:100:SER:HB3	1:K:103:GLU:HB2	1.91	0.52
1:B:86:ARG:HG2	1:B:121:PRO:CA	2.40	0.52
1:K:383:PHE:HA	1:K:386:LEU:HD12	1.92	0.52
1:K:478:ARG:O	1:K:481:ALA:N	2.42	0.52
1:A:24:VAL:CG1	1:A:483:VAL:HG13	2.34	0.52
1:J:234:SER:C	1:J:236:LEU:N	2.63	0.52
1:E:24:VAL:O	1:E:25:GLU:C	2.47	0.52
1:F:300:THR:O	1:F:301:ILE:HG23	2.09	0.52
1:F:321:ILE:HD11	1:F:343:ILE:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:THR:O	1:C:301:ILE:HG23	2.10	0.52
1:G:300:THR:O	1:G:301:ILE:HG23	2.10	0.52
1:I:286:ILE:HG13	1:I:286:ILE:O	2.09	0.52
1:B:321:ILE:HD11	1:B:343:ILE:HD12	1.91	0.52
1:L:281:TRP:O	1:L:282:ASN:HB2	2.09	0.52
1:F:322:LEU:HD22	1:F:323:ILE:N	2.24	0.52
1:L:322:LEU:HD22	1:L:323:ILE:N	2.24	0.52
1:L:107:LEU:HD22	1:L:126:LYS:HD3	1.92	0.52
1:L:90:LYS:HG3	1:L:122:PHE:CE1	2.44	0.52
1:F:69:ASP:OD2	1:F:71:SER:CB	2.57	0.52
1:A:239:THR:O	1:A:241:GLY:N	2.42	0.52
1:D:203:ILE:N	1:D:203:ILE:HD12	2.24	0.52
1:F:374:ASN:C	1:F:376:GLY:H	2.12	0.52
1:H:190:TYR:O	1:H:191:ASP:HB2	2.09	0.52
1:E:344:ILE:HB	1:E:367:VAL:HG12	1.92	0.52
1:E:413:VAL:HG12	1:E:414:GLN:N	2.24	0.52
1:K:99:VAL:HB	1:K:130:LYS:HB3	1.92	0.52
1:J:100:SER:HB3	1:J:103:GLU:HB2	1.92	0.52
1:K:166:ALA:HA	1:K:176:MET:HE2	1.91	0.52
1:D:167:PRO:HD3	1:D:176:MET:SD	2.49	0.52
1:G:382:TYR:CE2	1:G:386:LEU:CD1	2.89	0.52
1:G:167:PRO:HD3	1:G:176:MET:HG2	1.92	0.52
1:F:167:PRO:HD3	1:F:176:MET:CG	2.40	0.52
1:F:382:TYR:O	1:F:382:TYR:HD2	1.92	0.52
1:L:202:PRO:HG2	1:L:205:GLN:CG	2.40	0.52
1:I:234:SER:O	1:I:236:LEU:N	2.43	0.52
1:D:286:ILE:O	1:D:286:ILE:HG13	2.10	0.52
1:A:274:GLY:HA3	1:A:279:SER:HA	1.91	0.52
1:A:312:GLY:O	1:A:313:SER:C	2.48	0.52
1:H:136:TYR:HB2	1:H:141:LEU:CD2	2.40	0.52
1:L:312:GLY:O	1:L:313:SER:C	2.48	0.52
1:F:141:LEU:O	1:F:145:THR:HG23	2.10	0.52
1:C:458:GLU:C	1:C:460:SER:H	2.13	0.52
1:I:242:PHE:N	1:I:242:PHE:CD1	2.78	0.52
1:D:69:ASP:OD2	1:D:71:SER:HB2	2.10	0.52
1:D:24:VAL:O	1:D:27:LYS:N	2.43	0.52
1:G:94:ARG:HG3	1:G:169:MET:CB	2.29	0.52
1:A:110:LEU:HD23	1:A:111:MET:N	2.25	0.52
1:A:114:LYS:NZ	1:A:349:ASN:HD21	2.08	0.52
1:B:416:SER:HB3	1:F:428:ILE:O	2.10	0.52
1:J:92:GLY:HA2	1:J:166:ALA:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:330:GLN:O	1:K:331:LEU:HD12	2.10	0.52
1:J:234:SER:O	1:J:236:LEU:N	2.42	0.52
1:L:99:VAL:HA	1:L:103:GLU:OE1	2.10	0.52
1:A:13:VAL:O	1:A:14:GLU:C	2.47	0.52
1:C:307:ALA:O	1:C:308:LYS:HB2	2.10	0.52
1:D:301:ILE:O	1:D:302:LEU:HG	2.09	0.52
1:F:323:ILE:HG22	1:F:345:ALA:O	2.10	0.52
1:D:492:VAL:HG13	1:D:493:TYR:N	2.24	0.52
1:H:315:LEU:O	1:H:339:VAL:HG12	2.10	0.52
1:I:458:GLU:C	1:I:460:SER:H	2.13	0.52
1:F:16:PHE:CE1	1:F:478:ARG:HD3	2.45	0.52
1:K:289:LYS:O	1:K:290:GLU:HB2	2.10	0.52
1:J:63:PHE:N	1:J:63:PHE:CD2	2.78	0.52
1:G:202:PRO:HG2	1:G:205:GLN:CG	2.40	0.52
1:H:446:LYS:HG3	1:H:450:HIS:CE1	2.46	0.52
1:K:245:LYS:HB3	1:K:320:ASP:CB	2.40	0.52
1:E:446:LYS:HG3	1:E:450:HIS:CE1	2.45	0.52
1:C:38:GLU:C	1:C:40:GLN:H	2.12	0.52
1:D:97:THR:OG1	1:D:132:ASN:HB2	2.10	0.52
1:E:190:TYR:O	1:E:191:ASP:HB2	2.10	0.52
1:A:289:LYS:O	1:A:290:GLU:HB2	2.08	0.52
1:F:106:ALA:O	1:F:109:SER:HB3	2.10	0.52
1:L:432:PRO:O	1:L:433:THR:O	2.28	0.51
1:B:38:GLU:C	1:B:40:GLN:H	2.13	0.51
1:J:86:ARG:O	1:J:87:THR:O	2.28	0.51
1:H:99:VAL:HB	1:H:130:LYS:HB3	1.91	0.51
1:G:382:TYR:C	1:G:382:TYR:HD2	2.12	0.51
1:F:291:LEU:HD12	1:F:304:PHE:CZ	2.45	0.51
1:B:307:ALA:O	1:B:308:LYS:HB2	2.10	0.51
1:G:38:GLU:CG	1:G:39:GLU:N	2.73	0.51
1:A:315:LEU:O	1:A:339:VAL:HG12	2.10	0.51
1:D:217:ARG:NE	1:D:450:HIS:HD2	2.08	0.51
1:G:289:LYS:O	1:G:290:GLU:HB2	2.09	0.51
1:D:346:GLU:CD	1:D:351:PRO:HD2	2.30	0.51
1:D:28:LEU:CD1	1:D:28:LEU:H	2.20	0.51
1:B:412:SER:HB3	1:F:432:PRO:HA	1.92	0.51
1:C:6:ASP:HB2	1:C:353:THR:HB	1.91	0.51
1:B:12:MET:HG2	1:B:14:GLU:OE2	2.10	0.51
1:L:382:TYR:CD2	1:L:382:TYR:C	2.84	0.51
1:C:399:PHE:HB2	1:E:455:TYR:HE2	1.75	0.51
1:F:264:HIS:CE1	1:F:287:ASP:OD1	2.62	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:56:ASN:C	1:J:57:HIS:CD2	2.83	0.51
1:L:304:PHE:HD2	1:L:307:ALA:HB2	1.75	0.51
1:B:247:PHE:CE1	1:B:270:CYS:HB2	2.44	0.51
1:K:312:GLY:O	1:K:313:SER:C	2.48	0.51
1:K:339:VAL:HG21	1:K:360:PHE:HE1	1.76	0.51
1:E:315:LEU:O	1:E:339:VAL:HG12	2.11	0.51
1:E:136:TYR:HB2	1:E:141:LEU:CD2	2.40	0.51
1:K:222:GLY:HA3	1:K:373:LEU:CD1	2.41	0.51
1:I:82:HIS:HD2	1:I:83:SER:HB2	1.75	0.51
1:A:99:VAL:HG11	1:A:128:GLY:CA	2.26	0.51
1:F:382:TYR:HD2	1:F:382:TYR:C	2.14	0.51
1:L:167:PRO:HD3	1:L:176:MET:SD	2.49	0.51
1:G:301:ILE:O	1:G:302:LEU:HG	2.11	0.51
1:G:56:ASN:C	1:G:57:HIS:CD2	2.83	0.51
1:D:247:PHE:CE1	1:D:270:CYS:HB2	2.44	0.51
1:D:307:ALA:O	1:D:308:LYS:HB2	2.09	0.51
1:H:217:ARG:CD	1:H:450:HIS:CD2	2.94	0.51
1:I:312:GLY:O	1:I:313:SER:C	2.48	0.51
1:J:245:LYS:HB3	1:J:320:ASP:CB	2.40	0.51
1:H:460:SER:O	1:H:461:ALA:C	2.48	0.51
1:F:242:PHE:N	1:F:242:PHE:CD1	2.79	0.51
1:I:69:ASP:OD2	1:I:71:SER:HB2	2.11	0.51
1:A:226:PHE:CE2	1:A:465:MET:HE2	2.45	0.51
1:E:307:ALA:O	1:E:308:LYS:HB2	2.09	0.51
1:L:411:MET:HA	1:L:414:GLN:HB3	1.93	0.51
1:C:432:PRO:HA	1:D:412:SER:HB3	1.92	0.51
1:D:337:PRO:HG3	1:D:359:ILE:HD12	1.91	0.51
1:B:382:TYR:HE2	1:B:386:LEU:HD21	1.75	0.51
1:K:201:LYS:HD3	1:K:384:GLU:OE1	2.10	0.51
1:K:28:LEU:H	1:K:28:LEU:CD1	2.13	0.51
1:J:343:ILE:HG23	1:J:366:MET:HE3	1.92	0.51
1:J:312:GLY:O	1:J:313:SER:C	2.47	0.51
1:L:86:ARG:HG2	1:L:121:PRO:CA	2.39	0.51
1:F:13:VAL:O	1:F:14:GLU:C	2.48	0.51
1:C:12:MET:N	1:C:14:GLU:HG2	2.18	0.51
1:C:86:ARG:NH1	1:C:492:VAL:HG11	2.25	0.51
1:L:56:ASN:C	1:L:57:HIS:HD2	2.14	0.51
1:I:281:TRP:O	1:I:282:ASN:HB2	2.10	0.51
1:H:175:GLU:HA	1:H:178:TRP:CE3	2.45	0.51
1:H:147:ARG:CD	1:K:501:THR:HG21	2.40	0.51
1:D:245:LYS:HB3	1:D:320:ASP:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:ALA:CB	1:D:389:LEU:HD23	2.41	0.51
1:D:38:GLU:CG	1:D:39:GLU:N	2.73	0.51
1:J:436:PHE:CE2	1:K:409:LEU:CD1	2.94	0.51
1:G:429:PRO:HA	1:L:416:SER:HB2	1.92	0.51
1:E:90:LYS:HG3	1:E:122:PHE:CD1	2.46	0.51
1:J:473:LEU:HD23	1:J:479:THR:OG1	2.10	0.51
1:B:412:SER:CB	1:F:432:PRO:HA	2.41	0.51
1:K:107:LEU:HD22	1:K:126:LYS:HD3	1.93	0.51
1:H:477:LEU:H	1:H:477:LEU:HD22	1.75	0.51
1:I:176:MET:HG3	1:I:198:VAL:CG2	2.41	0.51
1:C:13:VAL:O	1:C:14:GLU:C	2.47	0.51
1:C:382:TYR:C	1:C:382:TYR:CD2	2.81	0.51
1:L:165:PRO:O	1:L:198:VAL:HG23	2.10	0.51
1:I:396:ARG:NH1	1:I:396:ARG:CG	2.74	0.51
1:E:312:GLY:O	1:E:313:SER:C	2.49	0.51
1:I:245:LYS:HB3	1:I:320:ASP:CB	2.41	0.51
1:A:208:ILE:CG2	1:A:211:ARG:HB2	2.41	0.51
1:I:495:GLU:O	1:I:496:ALA:CB	2.58	0.51
1:J:458:GLU:C	1:J:460:SER:H	2.13	0.51
1:A:82:HIS:ND1	1:A:109:SER:HA	2.26	0.51
1:H:97:THR:OG1	1:H:132:ASN:HB2	2.10	0.51
1:J:61:LEU:O	1:J:62:SER:HB2	2.11	0.51
1:I:344:ILE:HB	1:I:367:VAL:HG12	1.92	0.51
1:B:23:ILE:HG22	1:B:471:TYR:HD1	1.75	0.51
1:C:96:SER:C	1:C:98:ASP:H	2.13	0.51
1:C:432:PRO:O	1:C:433:THR:O	2.28	0.51
1:I:86:ARG:HG2	1:I:121:PRO:CA	2.40	0.51
1:E:167:PRO:HD3	1:E:176:MET:HG2	1.92	0.51
1:C:336:ALA:CB	1:C:337:PRO:HD3	2.29	0.51
1:C:304:PHE:HD2	1:C:307:ALA:HB2	1.76	0.51
1:G:321:ILE:HD11	1:G:343:ILE:HD12	1.93	0.51
1:K:286:ILE:O	1:K:286:ILE:HG13	2.11	0.51
1:J:488:LYS:HZ3	3:J:601:XEG:CAK	2.22	0.51
1:A:396:ARG:HG3	1:A:396:ARG:O	2.11	0.51
1:D:493:TYR:O	1:D:494:ASN:C	2.48	0.51
1:F:458:GLU:C	1:F:460:SER:N	2.62	0.51
1:E:162:VAL:O	1:E:163:ASP:HB2	2.10	0.51
1:I:61:LEU:HD11	1:I:151:GLU:HB3	1.91	0.51
1:L:252:PHE:HE2	1:L:260:MET:SD	2.34	0.51
1:A:58:VAL:HG13	1:D:60:SER:HB2	1.91	0.51
1:K:202:PRO:HG2	1:K:205:GLN:CG	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:346:GLU:CD	1:G:351:PRO:HD2	2.30	0.51
1:H:286:ILE:HG13	1:H:286:ILE:O	2.11	0.51
1:C:264:HIS:CE1	1:C:287:ASP:OD1	2.63	0.51
1:K:301:ILE:O	1:K:302:LEU:HG	2.10	0.51
1:F:239:THR:O	1:F:241:GLY:N	2.44	0.51
1:G:38:GLU:C	1:G:40:GLN:H	2.14	0.51
1:L:315:LEU:O	1:L:339:VAL:HG12	2.10	0.51
1:K:38:GLU:C	1:K:40:GLN:H	2.14	0.51
1:H:234:SER:C	1:H:236:LEU:N	2.64	0.51
1:H:225:ASN:OD1	1:H:458:GLU:HG3	2.11	0.51
1:B:97:THR:OG1	1:B:132:ASN:HB2	2.11	0.51
1:J:300:THR:O	1:J:301:ILE:HG23	2.10	0.51
1:D:110:LEU:HD23	1:D:111:MET:N	2.26	0.51
1:D:118:VAL:HG11	1:D:375:ALA:HB1	1.93	0.51
1:C:409:LEU:HD12	1:E:436:PHE:CE2	2.46	0.51
1:E:413:VAL:HG12	1:E:429:PRO:CG	2.41	0.51
1:A:487:GLU:CG	1:A:491:ARG:HH22	2.11	0.51
1:I:118:VAL:CG2	1:I:120:VAL:HG23	2.33	0.51
1:A:176:MET:HG2	1:A:200:GLY:HA3	1.93	0.51
1:D:202:PRO:HG2	1:D:205:GLN:CG	2.40	0.51
1:K:24:VAL:O	1:K:25:GLU:C	2.49	0.51
1:K:336:ALA:CB	1:K:337:PRO:HD3	2.30	0.51
1:H:117:VAL:HG21	1:H:371:LEU:HG	1.92	0.51
1:I:24:VAL:O	1:I:25:GLU:C	2.48	0.51
1:E:13:VAL:O	1:E:14:GLU:C	2.48	0.51
1:C:321:ILE:HD11	1:C:343:ILE:HD12	1.91	0.51
1:C:281:TRP:O	1:C:282:ASN:HB2	2.10	0.51
1:C:339:VAL:HG21	1:C:360:PHE:HE1	1.76	0.51
1:D:402:GLU:C	1:D:404:ASP:N	2.64	0.51
1:H:234:SER:O	1:H:236:LEU:N	2.43	0.51
1:H:108:ALA:HB2	1:H:126:LYS:HB2	1.92	0.51
1:D:82:HIS:ND1	1:D:109:SER:HA	2.25	0.51
1:G:374:ASN:C	1:G:376:GLY:N	2.64	0.51
1:K:69:ASP:OD2	1:K:71:SER:HB2	2.11	0.51
1:I:433:THR:HG21	1:J:411:MET:HB3	1.93	0.51
1:G:414:GLN:HB2	1:G:429:PRO:HG2	1.92	0.51
1:L:111:MET:CE	2:L:552:NDP:N7N	2.58	0.51
1:G:147:ARG:HH21	1:J:499:THR:HG22	1.75	0.51
1:L:12:MET:HG3	1:L:13:VAL:H	1.75	0.51
1:C:382:TYR:HD2	1:C:382:TYR:O	1.94	0.51
1:I:304:PHE:HD2	1:I:307:ALA:HB2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:GLN:O	1:D:331:LEU:HD12	2.10	0.51
1:A:339:VAL:HG21	1:A:360:PHE:HE1	1.76	0.51
1:C:185:SER:HB2	1:E:501:THR:HG22	1.92	0.51
1:J:217:ARG:CZ	1:J:450:HIS:HD2	2.24	0.51
1:B:82:HIS:ND1	1:B:109:SER:HA	2.25	0.51
1:J:246:THR:HG22	1:J:269:LYS:O	2.10	0.51
1:I:416:SER:HB2	1:K:429:PRO:HA	1.92	0.51
1:A:413:VAL:HG12	1:A:414:GLN:N	2.26	0.51
1:I:6:ASP:OD1	1:I:12:MET:HB3	2.11	0.51
1:G:336:ALA:CB	1:G:337:PRO:HD3	2.29	0.51
1:A:167:PRO:HD3	1:A:176:MET:CG	2.40	0.51
1:K:382:TYR:CE2	1:K:386:LEU:CD1	2.88	0.51
1:D:176:MET:HG3	1:D:198:VAL:CG2	2.41	0.51
1:A:386:LEU:CD2	1:F:391:HIS:O	2.56	0.51
1:J:175:GLU:HA	1:J:178:TRP:CE3	2.46	0.51
1:B:211:ARG:HA	1:B:380:VAL:HG11	1.93	0.51
1:H:281:TRP:O	1:H:282:ASN:HB2	2.10	0.51
1:L:245:LYS:HB3	1:L:320:ASP:CB	2.40	0.51
1:G:312:GLY:O	1:G:313:SER:C	2.48	0.51
1:A:38:GLU:HG2	1:A:39:GLU:N	2.27	0.51
1:D:312:GLY:O	1:D:313:SER:C	2.49	0.51
1:L:323:ILE:HG22	1:L:345:ALA:O	2.11	0.51
1:K:458:GLU:C	1:K:460:SER:H	2.14	0.51
1:C:106:ALA:O	1:C:109:SER:HB3	2.11	0.51
1:E:252:PHE:HE2	1:E:260:MET:SD	2.34	0.51
1:B:60:SER:HB2	1:E:58:VAL:HG13	1.93	0.51
1:G:69:ASP:OD2	1:G:71:SER:HB2	2.10	0.51
1:I:436:PHE:CE2	1:J:409:LEU:CD1	2.94	0.50
1:G:409:LEU:HD23	1:H:409:LEU:HD23	1.93	0.50
1:A:286:ILE:O	1:A:286:ILE:HG13	2.12	0.50
1:B:372:TYR:CE2	1:B:460:SER:HB3	2.46	0.50
1:A:349:ASN:HB2	2:A:552:NDP:O2D	2.11	0.50
1:B:312:GLY:O	1:B:313:SER:C	2.49	0.50
1:A:201:LYS:H	1:A:201:LYS:HD3	1.77	0.50
1:H:382:TYR:C	1:H:382:TYR:HD2	2.14	0.50
1:J:286:ILE:O	1:J:286:ILE:HG13	2.11	0.50
1:I:473:LEU:HD23	1:I:479:THR:OG1	2.12	0.50
1:F:304:PHE:HD2	1:F:307:ALA:HB2	1.76	0.50
1:B:204:SER:HB2	1:F:492:VAL:HG22	1.93	0.50
1:L:208:ILE:HG22	1:L:211:ARG:HB2	1.93	0.50
1:E:217:ARG:HG2	1:E:262:TYR:CD1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:141:LEU:O	1:H:145:THR:HG23	2.11	0.50
1:J:136:TYR:HB2	1:J:141:LEU:CD2	2.41	0.50
1:D:396:ARG:O	1:D:396:ARG:HG3	2.10	0.50
1:A:162:VAL:O	1:A:163:ASP:HB2	2.10	0.50
1:I:446:LYS:HG3	1:I:450:HIS:CE1	2.46	0.50
1:F:498:VAL:HG13	1:F:500:PHE:HE2	1.76	0.50
1:L:374:ASN:C	1:L:376:GLY:H	2.14	0.50
1:G:175:GLU:O	1:G:178:TRP:HB2	2.11	0.50
1:K:129:VAL:O	1:K:131:ILE:N	2.44	0.50
1:J:433:THR:HG22	1:K:412:SER:N	2.26	0.50
1:A:344:ILE:HB	1:A:367:VAL:HG12	1.92	0.50
1:C:416:SER:HB3	1:E:428:ILE:O	2.11	0.50
3:I:601:XEG:CAZ	3:I:601:XEG:CAP	2.88	0.50
1:I:167:PRO:HD3	1:I:176:MET:CG	2.40	0.50
1:L:118:VAL:HG23	1:L:118:VAL:O	2.12	0.50
3:L:601:XEG:CAZ	3:L:601:XEG:CAP	2.88	0.50
1:C:445:GLU:O	1:C:449:VAL:HG23	2.11	0.50
1:F:56:ASN:C	1:F:57:HIS:CD2	2.84	0.50
3:H:601:XEG:CAP	3:H:601:XEG:CAZ	2.89	0.50
1:G:396:ARG:CG	1:G:396:ARG:HH11	2.22	0.50
1:E:402:GLU:C	1:E:404:ASP:N	2.65	0.50
1:G:175:GLU:HA	1:G:178:TRP:CE3	2.46	0.50
1:A:104:VAL:HG23	1:A:105:LYS:N	2.26	0.50
1:B:110:LEU:HD23	1:B:111:MET:N	2.26	0.50
1:D:409:LEU:O	1:D:411:MET:N	2.40	0.50
1:A:414:GLN:HB2	1:A:429:PRO:HG2	1.94	0.50
1:E:167:PRO:HD3	1:E:176:MET:CG	2.41	0.50
1:G:117:VAL:HG21	1:G:371:LEU:HG	1.93	0.50
1:A:23:ILE:HG22	1:A:471:TYR:HD1	1.76	0.50
1:B:214:ALA:CB	1:B:380:VAL:HG21	2.34	0.50
1:G:304:PHE:HD2	1:G:307:ALA:HB2	1.76	0.50
1:I:38:GLU:C	1:I:40:GLN:H	2.13	0.50
1:I:315:LEU:O	1:I:339:VAL:HG12	2.10	0.50
1:K:38:GLU:CG	1:K:39:GLU:N	2.74	0.50
1:J:446:LYS:HG3	1:J:450:HIS:CE1	2.46	0.50
1:I:477:LEU:HD22	1:I:477:LEU:H	1.75	0.50
1:H:246:THR:HG22	1:H:269:LYS:O	2.12	0.50
1:L:69:ASP:OD2	1:L:71:SER:HB2	2.11	0.50
1:D:432:PRO:O	1:D:433:THR:O	2.29	0.50
1:B:412:SER:OG	1:F:432:PRO:HA	2.12	0.50
1:E:198:VAL:O	1:E:201:LYS:HE3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:LEU:HD23	1:C:479:THR:OG1	2.12	0.50
1:C:176:MET:HG3	1:C:198:VAL:CG2	2.41	0.50
1:F:473:LEU:HD23	1:F:479:THR:OG1	2.12	0.50
1:B:116:ALA:O	1:B:488:LYS:HD2	2.11	0.50
1:D:226:PHE:CD2	1:D:465:MET:HE2	2.47	0.50
1:D:56:ASN:C	1:D:57:HIS:CD2	2.85	0.50
1:J:38:GLU:O	1:J:40:GLN:N	2.45	0.50
1:E:208:ILE:CG2	1:E:211:ARG:HB2	2.41	0.50
1:G:458:GLU:C	1:G:460:SER:H	2.15	0.50
1:C:69:ASP:OD2	1:C:71:SER:CB	2.60	0.50
1:B:344:ILE:O	1:B:367:VAL:HA	2.11	0.50
1:I:12:MET:HG3	1:I:13:VAL:H	1.77	0.50
1:I:86:ARG:HH12	1:I:492:VAL:HG21	1.72	0.50
1:B:166:ALA:HA	1:B:176:MET:HE2	1.93	0.50
1:B:286:ILE:HG13	1:B:286:ILE:O	2.10	0.50
1:H:274:GLY:HA2	1:H:279:SER:HA	1.93	0.50
1:I:396:ARG:CG	1:I:396:ARG:HH11	2.16	0.50
1:C:315:LEU:O	1:C:339:VAL:HG12	2.12	0.50
1:H:339:VAL:HG21	1:H:360:PHE:HE1	1.75	0.50
1:F:498:VAL:O	1:F:500:PHE:HE2	1.94	0.50
1:K:374:ASN:C	1:K:376:GLY:N	2.64	0.50
1:D:203:ILE:H	1:D:203:ILE:HD12	1.75	0.50
1:A:252:PHE:HE2	1:A:260:MET:SD	2.34	0.50
1:E:304:PHE:HD2	1:E:307:ALA:HB2	1.77	0.50
1:G:409:LEU:CD1	1:H:436:PHE:CE2	2.94	0.50
1:A:366:MET:HG3	1:A:477:LEU:HD21	1.93	0.50
1:E:96:SER:O	1:E:130:LYS:HA	2.11	0.50
1:E:382:TYR:CE2	1:E:386:LEU:CD1	2.90	0.50
1:J:499:THR:C	1:J:500:PHE:HD2	2.15	0.50
1:I:12:MET:H	1:I:14:GLU:CG	2.17	0.50
1:G:212:ILE:H	1:G:212:ILE:CD1	2.18	0.50
1:H:330:GLN:O	1:H:331:LEU:HD12	2.12	0.50
1:I:234:SER:C	1:I:236:LEU:N	2.64	0.50
1:L:234:SER:C	1:L:236:LEU:N	2.64	0.50
1:D:61:LEU:O	1:D:62:SER:HB2	2.11	0.50
1:H:488:LYS:HZ2	3:H:601:XEG:CAK	2.21	0.50
1:J:273:VAL:HB	1:J:280:ILE:HD11	1.94	0.50
1:H:38:GLU:O	1:H:40:GLN:N	2.44	0.50
1:K:141:LEU:O	1:K:145:THR:HG23	2.11	0.50
1:A:61:LEU:O	1:A:62:SER:HB2	2.12	0.50
1:E:82:HIS:CD2	1:E:82:HIS:C	2.85	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:82:HIS:HD2	1:L:83:SER:HB2	1.77	0.50
1:G:55:CYS:HB3	1:G:82:HIS:HA	1.94	0.50
1:I:142:GLU:HB2	1:I:178:TRP:CZ2	2.46	0.50
1:B:458:GLU:C	1:B:460:SER:H	2.15	0.50
1:E:96:SER:C	1:E:98:ASP:H	2.13	0.50
1:D:414:GLN:HB2	1:D:429:PRO:CG	2.42	0.50
1:B:167:PRO:HD3	1:B:176:MET:CG	2.42	0.50
1:J:496:ALA:HA	1:K:177:SER:OG	2.11	0.50
1:K:121:PRO:CD	1:K:382:TYR:CE1	2.95	0.50
1:A:458:GLU:C	1:A:460:SER:H	2.14	0.50
1:D:12:MET:HG2	1:D:14:GLU:OE2	2.11	0.50
1:C:87:THR:CB	1:C:88:PRO:HD3	2.39	0.50
1:D:226:PHE:CD2	1:D:465:MET:CE	2.94	0.50
1:A:396:ARG:CG	1:A:396:ARG:HH11	2.21	0.50
1:E:38:GLU:HG2	1:E:39:GLU:N	2.27	0.50
1:F:38:GLU:HG2	1:F:39:GLU:N	2.27	0.50
1:G:72:TRP:HB3	1:J:47:SER:HB3	1.92	0.50
1:C:421:PHE:HE1	1:C:423:LYS:O	1.95	0.50
1:F:421:PHE:HE1	1:F:423:LYS:O	1.94	0.50
1:J:108:ALA:HB2	1:J:126:LYS:HB2	1.93	0.50
1:F:23:ILE:HG22	1:F:471:TYR:CD1	2.46	0.50
1:C:96:SER:O	1:C:130:LYS:HA	2.11	0.50
1:A:198:VAL:O	1:A:201:LYS:HE3	2.12	0.50
1:H:350:GLY:N	1:H:351:PRO:HD3	2.27	0.50
1:J:304:PHE:HD2	1:J:307:ALA:HB2	1.77	0.50
1:G:12:MET:N	1:G:14:GLU:HG2	2.18	0.50
1:C:499:THR:HG21	1:F:64:PRO:O	2.12	0.50
1:B:304:PHE:HD2	1:B:307:ALA:HB2	1.77	0.50
1:A:38:GLU:C	1:A:40:GLN:H	2.15	0.50
1:A:132:ASN:OD1	1:A:134:LYS:CG	2.58	0.50
1:F:312:GLY:O	1:F:313:SER:C	2.49	0.50
1:K:492:VAL:O	1:K:493:TYR:C	2.50	0.50
1:G:345:ALA:HB1	1:G:373:LEU:HD21	1.93	0.50
1:E:374:ASN:C	1:E:376:GLY:N	2.66	0.50
1:J:374:ASN:C	1:J:376:GLY:N	2.65	0.50
1:K:175:GLU:HA	1:K:178:TRP:CE3	2.46	0.50
1:L:53:LYS:HB3	1:L:54:PRO:HD3	1.92	0.50
1:G:190:TYR:O	1:G:191:ASP:HB2	2.10	0.50
1:H:411:MET:HB3	1:L:433:THR:HG21	1.93	0.50
1:K:78:TYR:CD2	1:K:101:VAL:HG22	2.46	0.50
1:I:455:TYR:CE1	1:I:459:ARG:HD3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:488:LYS:HZ3	3:D:502:XEG:CAK	2.22	0.50
1:C:382:TYR:C	1:C:382:TYR:HD2	2.15	0.50
1:J:274:GLY:HA2	1:J:279:SER:HA	1.93	0.50
1:A:146:ARG:HG2	1:A:182:THR:OG1	2.12	0.50
1:H:8:ASN:C	1:H:9:PHE:CD2	2.84	0.50
1:E:38:GLU:C	1:E:40:GLN:H	2.15	0.50
1:C:312:GLY:O	1:C:313:SER:C	2.49	0.50
1:B:222:GLY:HA3	1:B:373:LEU:CD1	2.42	0.50
1:G:95:TYR:HB3	1:G:133:PRO:HG3	1.93	0.50
1:C:242:PHE:CD1	1:C:242:PHE:N	2.79	0.50
1:H:61:LEU:O	1:H:62:SER:HB2	2.12	0.50
1:A:493:TYR:O	1:A:495:GLU:N	2.45	0.50
1:L:20:GLY:O	1:L:21:ALA:C	2.49	0.50
1:D:372:TYR:CE2	1:D:460:SER:HB3	2.47	0.49
1:B:372:TYR:CD2	1:B:464:ILE:HD11	2.47	0.49
1:D:478:ARG:O	1:D:481:ALA:N	2.42	0.49
1:F:432:PRO:O	1:F:433:THR:O	2.30	0.49
1:B:78:TYR:CD2	1:B:101:VAL:HG22	2.46	0.49
1:K:446:LYS:HG3	1:K:450:HIS:CE1	2.47	0.49
1:H:12:MET:HG2	1:H:14:GLU:OE2	2.11	0.49
1:F:12:MET:N	1:F:14:GLU:HG2	2.17	0.49
1:H:202:PRO:HG2	1:H:205:GLN:CG	2.42	0.49
1:J:455:TYR:CE1	1:J:459:ARG:HD3	2.41	0.49
1:G:412:SER:N	1:H:433:THR:HG22	2.27	0.49
1:E:339:VAL:HG21	1:E:360:PHE:HE1	1.76	0.49
1:C:38:GLU:HG2	1:C:39:GLU:N	2.27	0.49
1:D:208:ILE:HG22	1:D:384:GLU:HB2	1.93	0.49
1:L:367:VAL:O	1:L:477:LEU:HD23	2.12	0.49
1:D:276:SER:HB2	2:D:552:NDP:O2B	2.12	0.49
1:A:9:PHE:HB3	1:A:329:LYS:HZ3	1.77	0.49
1:K:190:TYR:O	1:K:191:ASP:HB2	2.12	0.49
1:C:374:ASN:C	1:C:376:GLY:H	2.16	0.49
1:K:239:THR:O	1:K:241:GLY:N	2.44	0.49
1:H:63:PHE:CD2	1:H:63:PHE:N	2.80	0.49
1:I:432:PRO:O	1:I:433:THR:O	2.30	0.49
1:K:198:VAL:O	1:K:201:LYS:HE3	2.12	0.49
1:K:27:LYS:HD2	1:K:471:TYR:OH	2.12	0.49
1:H:120:VAL:HG13	1:H:382:TYR:CD1	2.48	0.49
1:G:330:GLN:O	1:G:331:LEU:HD12	2.13	0.49
1:A:90:LYS:HG3	1:A:122:PHE:CD1	2.46	0.49
1:A:86:ARG:O	1:A:87:THR:O	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:86:ARG:NH1	1:H:492:VAL:HG11	2.26	0.49
1:H:86:ARG:O	1:H:87:THR:O	2.29	0.49
1:F:234:SER:C	1:F:236:LEU:N	2.66	0.49
1:A:455:TYR:HE2	1:F:399:PHE:HB2	1.77	0.49
1:H:176:MET:HE3	1:H:179:ILE:HD12	1.94	0.49
1:G:57:HIS:ND1	1:J:155:LYS:HE2	2.27	0.49
1:A:281:TRP:O	1:A:282:ASN:CB	2.60	0.49
1:C:420:LYS:O	1:C:421:PHE:HB2	2.13	0.49
1:K:345:ALA:HB1	1:K:373:LEU:HD21	1.92	0.49
1:L:421:PHE:HE1	1:L:423:LYS:O	1.95	0.49
1:H:460:SER:O	1:H:463:GLN:N	2.44	0.49
1:G:242:PHE:N	1:G:242:PHE:CD1	2.80	0.49
1:K:82:HIS:HD2	1:K:83:SER:HB2	1.77	0.49
1:A:304:PHE:HD2	1:A:307:ALA:HB2	1.77	0.49
1:B:121:PRO:CD	1:B:382:TYR:CE1	2.95	0.49
1:K:201:LYS:HD3	1:K:201:LYS:H	1.77	0.49
1:I:65:ILE:HD11	1:I:75:ILE:CD1	2.33	0.49
1:A:393:SER:OG	3:B:601:XEG:CAM	2.60	0.49
1:L:142:GLU:HB2	1:L:178:TRP:CZ2	2.47	0.49
1:L:234:SER:O	1:L:236:LEU:N	2.45	0.49
3:J:601:XEG:CAZ	3:J:601:XEG:CAP	2.90	0.49
1:D:322:LEU:HD22	1:D:323:ILE:H	1.77	0.49
1:K:95:TYR:HB3	1:K:133:PRO:HG3	1.94	0.49
1:F:458:GLU:C	1:F:460:SER:H	2.16	0.49
1:J:346:GLU:CD	1:J:351:PRO:HD2	2.31	0.49
1:G:129:VAL:O	1:G:131:ILE:N	2.44	0.49
1:D:344:ILE:O	1:D:367:VAL:HA	2.11	0.49
1:D:382:TYR:HE2	1:D:386:LEU:HD21	1.77	0.49
1:B:409:LEU:O	1:B:411:MET:N	2.43	0.49
1:I:12:MET:HG2	1:I:14:GLU:OE2	2.12	0.49
1:G:383:PHE:HA	1:G:386:LEU:HD12	1.95	0.49
1:H:86:ARG:HG2	1:H:121:PRO:CA	2.41	0.49
1:J:265:ARG:O	1:J:266:PHE:CB	2.52	0.49
1:K:304:PHE:HD2	1:K:307:ALA:HB2	1.76	0.49
1:L:321:ILE:HD11	1:L:343:ILE:HD12	1.95	0.49
1:J:493:TYR:O	1:J:494:ASN:C	2.50	0.49
1:F:38:GLU:O	1:F:40:GLN:N	2.45	0.49
1:H:420:LYS:NZ	1:H:420:LYS:O	2.34	0.49
1:J:323:ILE:HG22	1:J:345:ALA:O	2.13	0.49
1:B:346:GLU:CD	1:B:351:PRO:HD2	2.32	0.49
1:H:191:ASP:O	1:H:192:ILE:C	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:252:PHE:HE2	1:I:260:MET:SD	2.34	0.49
1:I:63:PHE:N	1:I:63:PHE:CD2	2.80	0.49
1:A:264:HIS:CE1	1:A:287:ASP:OD1	2.66	0.49
1:A:413:VAL:HG12	1:A:429:PRO:CG	2.40	0.49
1:I:350:GLY:N	1:I:351:PRO:HD3	2.27	0.49
1:E:176:MET:HE3	1:E:179:ILE:HD12	1.94	0.49
1:G:371:LEU:HD22	1:G:482:TYR:CD2	2.48	0.49
1:H:346:GLU:CD	1:H:351:PRO:HD2	2.33	0.49
1:G:167:PRO:HD3	1:G:176:MET:CG	2.43	0.49
1:E:372:TYR:CD2	1:E:464:ILE:HD11	2.47	0.49
1:J:382:TYR:C	1:J:382:TYR:HD2	2.16	0.49
1:G:286:ILE:HG13	1:G:286:ILE:O	2.12	0.49
1:G:274:GLY:HA2	1:G:279:SER:HA	1.95	0.49
1:J:421:PHE:HE1	1:J:423:LYS:O	1.95	0.49
1:C:455:TYR:CE1	1:C:459:ARG:HD3	2.42	0.49
1:H:242:PHE:CD1	1:H:242:PHE:N	2.80	0.49
1:H:82:HIS:HD2	1:H:83:SER:HB2	1.78	0.49
1:J:501:THR:HG22	1:K:181:ASP:OD1	2.12	0.49
1:J:53:LYS:HB3	1:J:54:PRO:HD3	1.94	0.49
1:E:203:ILE:N	1:E:203:ILE:HD12	2.27	0.49
1:C:58:VAL:HG13	1:F:60:SER:HB2	1.95	0.49
1:E:9:PHE:HB3	1:E:329:LYS:HZ3	1.78	0.49
1:B:47:SER:O	1:B:50:ARG:N	2.44	0.49
1:I:149:THR:HB	1:I:182:THR:HG21	1.94	0.49
1:D:23:ILE:HG22	1:D:471:TYR:HD1	1.77	0.49
1:C:432:PRO:HA	1:D:412:SER:CB	2.43	0.49
1:J:121:PRO:O	1:J:122:PHE:CD2	2.65	0.49
1:E:176:MET:HG2	1:E:200:GLY:HA3	1.94	0.49
1:G:6:ASP:CG	1:G:332:THR:HB	2.32	0.49
1:L:65:ILE:HD11	1:L:75:ILE:CD1	2.34	0.49
1:I:96:SER:C	1:I:98:ASP:H	2.15	0.49
1:I:202:PRO:HG2	1:I:205:GLN:HG3	1.95	0.49
1:B:396:ARG:HG3	1:B:396:ARG:O	2.11	0.49
1:J:12:MET:HG2	1:J:14:GLU:OE2	2.12	0.49
1:G:16:PHE:N	1:G:16:PHE:CD2	2.81	0.49
1:J:282:ASN:O	1:J:284:ASP:N	2.45	0.49
1:L:212:ILE:H	1:L:212:ILE:CD1	2.18	0.49
1:L:222:GLY:HA3	1:L:373:LEU:CD1	2.42	0.49
1:K:500:PHE:O	1:L:501:THR:HB	2.12	0.49
1:I:421:PHE:HE1	1:I:423:LYS:O	1.94	0.49
1:C:453:LEU:CD2	1:C:453:LEU:C	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:217:ARG:CZ	1:I:450:HIS:HD2	2.25	0.49
1:K:242:PHE:CD1	1:K:242:PHE:N	2.79	0.49
1:C:350:GLY:N	1:C:351:PRO:HD3	2.27	0.49
1:F:350:GLY:N	1:F:351:PRO:HD3	2.27	0.49
1:G:159:GLY:O	1:G:162:VAL:HG12	2.12	0.49
1:E:104:VAL:HG23	1:E:105:LYS:N	2.28	0.49
1:A:446:LYS:HG3	1:A:450:HIS:CE1	2.48	0.49
1:E:286:ILE:O	1:E:286:ILE:HG13	2.11	0.49
1:D:38:GLU:O	1:D:40:GLN:N	2.45	0.49
1:B:38:GLU:O	1:B:40:GLN:N	2.46	0.49
1:D:78:TYR:CD2	1:D:101:VAL:HG22	2.44	0.49
1:B:176:MET:HE3	1:B:179:ILE:HD12	1.94	0.49
1:K:99:VAL:HG11	1:K:128:GLY:CA	2.32	0.49
1:A:16:PHE:CD2	1:A:16:PHE:N	2.80	0.49
1:C:199:THR:HG22	1:C:384:GLU:HG2	1.93	0.49
1:A:95:TYR:HB3	1:A:133:PRO:HG3	1.93	0.49
1:A:136:TYR:HB2	1:A:141:LEU:CD2	2.41	0.49
1:L:202:PRO:HG2	1:L:205:GLN:HG3	1.94	0.49
1:I:343:ILE:HG23	1:I:366:MET:HE3	1.95	0.49
1:K:16:PHE:N	1:K:16:PHE:CD2	2.79	0.49
1:J:59:LEU:HB2	1:J:157:PHE:CE2	2.48	0.49
1:F:7:PRO:HB3	1:F:353:THR:HB	1.94	0.49
1:C:239:THR:O	1:C:241:GLY:N	2.44	0.49
1:L:217:ARG:CZ	1:L:450:HIS:HD2	2.25	0.49
1:H:421:PHE:HE1	1:H:423:LYS:O	1.96	0.49
1:C:453:LEU:O	1:C:453:LEU:HD23	2.13	0.49
1:C:20:GLY:O	1:C:21:ALA:C	2.51	0.49
1:C:63:PHE:CD2	1:C:63:PHE:N	2.80	0.49
1:G:158:ILE:HG23	1:G:158:ILE:O	2.12	0.49
1:G:432:PRO:O	1:G:433:THR:O	2.30	0.49
1:A:321:ILE:HD11	1:A:343:ILE:HD12	1.95	0.49
1:C:397:LEU:CD1	1:E:383:PHE:CE2	2.91	0.49
1:D:121:PRO:CD	1:D:382:TYR:CE1	2.95	0.49
1:A:409:LEU:HD12	1:B:436:PHE:CE2	2.48	0.49
1:B:202:PRO:HG2	1:B:205:GLN:HG3	1.95	0.49
1:J:315:LEU:O	1:J:339:VAL:HG12	2.12	0.49
1:H:275:GLU:O	2:H:552:NDP:H2A	2.13	0.49
1:L:12:MET:HG2	1:L:14:GLU:OE2	2.13	0.49
1:L:198:VAL:O	1:L:201:LYS:HE3	2.13	0.49
1:H:201:LYS:H	1:H:201:LYS:HD3	1.76	0.49
1:I:265:ARG:O	1:I:266:PHE:CB	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:56:ASN:C	1:H:57:HIS:CD2	2.85	0.49
1:I:56:ASN:C	1:I:57:HIS:CD2	2.86	0.49
1:D:274:GLY:HA2	1:D:279:SER:HA	1.95	0.49
1:E:281:TRP:O	1:E:282:ASN:CB	2.60	0.49
1:E:345:ALA:HB1	1:E:373:LEU:HD21	1.95	0.49
1:K:136:TYR:HB2	1:K:141:LEU:CD2	2.42	0.49
1:G:141:LEU:O	1:G:145:THR:HG23	2.13	0.49
1:B:300:THR:O	1:B:301:ILE:HG23	2.12	0.49
1:A:295:LYS:HG3	1:A:296:LEU:HD22	1.95	0.49
1:G:66:ARG:NH1	1:J:500:PHE:CZ	2.52	0.49
1:A:176:MET:HE3	1:A:179:ILE:HD12	1.94	0.49
1:G:27:LYS:HD2	1:G:471:TYR:OH	2.12	0.49
1:J:344:ILE:O	1:J:367:VAL:HA	2.13	0.49
1:J:369:PRO:HD3	1:J:477:LEU:HB2	1.94	0.49
1:H:250:GLN:NE2	2:H:552:NDP:C2A	2.74	0.49
1:L:86:ARG:NH1	1:L:492:VAL:HG21	2.28	0.49
1:H:52:ILE:HD13	1:H:489:VAL:HG12	1.95	0.49
1:C:286:ILE:O	1:C:286:ILE:HG13	2.13	0.49
1:K:255:VAL:HG12	2:K:552:NDP:O2N	2.13	0.49
1:L:56:ASN:O	1:L:57:HIS:CD2	2.55	0.49
1:B:273:VAL:HB	1:B:280:ILE:HD11	1.95	0.49
1:D:339:VAL:HG21	1:D:360:PHE:HE1	1.77	0.49
1:A:402:GLU:C	1:A:404:ASP:N	2.60	0.49
1:E:140:GLU:O	1:E:144:ILE:HG13	2.13	0.49
1:G:501:THR:C	1:J:150:MET:HG3	2.33	0.49
1:C:16:PHE:HE2	1:C:354:PRO:HG3	1.77	0.49
1:E:295:LYS:HG3	1:E:296:LEU:HD22	1.95	0.49
1:I:53:LYS:HB3	1:I:54:PRO:HD3	1.95	0.49
1:E:367:VAL:C	1:E:477:LEU:HD23	2.33	0.49
1:D:372:TYR:CD2	1:D:464:ILE:HD11	2.48	0.49
1:J:409:LEU:HD23	1:K:409:LEU:HD23	1.94	0.49
1:A:369:PRO:HG3	1:A:478:ARG:CA	2.43	0.49
1:C:390:ASN:O	1:C:392:VAL:HG22	2.13	0.49
1:A:485:ALA:O	1:A:486:ILE:C	2.51	0.49
1:A:491:ARG:NH1	1:A:491:ARG:HB2	2.28	0.49
1:H:96:SER:O	1:H:130:LYS:HA	2.12	0.49
1:I:118:VAL:HG23	1:I:118:VAL:O	2.13	0.49
1:E:202:PRO:HG2	1:E:205:GLN:HG3	1.95	0.49
1:I:99:VAL:HA	1:I:103:GLU:OE1	2.12	0.49
1:G:446:LYS:HG3	1:G:450:HIS:CE1	2.48	0.49
1:H:87:THR:CB	1:H:88:PRO:CD	2.89	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:12:MET:HG3	1:J:13:VAL:H	1.77	0.49
1:C:238:MET:HE1	1:C:343:ILE:HD11	1.94	0.49
1:H:59:LEU:HB2	1:H:157:PHE:CE2	2.48	0.49
1:L:87:THR:CB	1:L:88:PRO:CD	2.89	0.49
1:D:300:THR:O	1:D:301:ILE:HG23	2.13	0.49
1:A:498:VAL:C	1:A:500:PHE:H	2.16	0.49
1:H:273:VAL:HB	1:H:280:ILE:HD11	1.94	0.49
1:F:273:VAL:HB	1:F:280:ILE:HD11	1.95	0.49
1:B:208:ILE:HG22	1:B:384:GLU:HB2	1.93	0.49
1:I:45:VAL:HG13	1:I:490:PHE:HE1	1.77	0.49
1:G:63:PHE:CD2	1:G:63:PHE:N	2.80	0.49
1:I:412:SER:OG	1:K:432:PRO:HA	2.13	0.48
1:G:147:ARG:HH21	1:J:499:THR:CG2	2.26	0.48
1:I:7:PRO:CG	1:I:11:LYS:HD3	2.40	0.48
1:B:93:ILE:CG2	1:B:127:ALA:HB3	2.41	0.48
1:A:6:ASP:OD1	1:A:332:THR:HG21	2.13	0.48
1:J:96:SER:O	1:J:130:LYS:HA	2.13	0.48
1:G:121:PRO:CD	1:G:382:TYR:CE1	2.96	0.48
1:G:52:ILE:HD13	1:G:489:VAL:CG1	2.43	0.48
1:A:500:PHE:HE2	1:D:66:ARG:HD3	1.77	0.48
1:C:38:GLU:O	1:C:40:GLN:N	2.46	0.48
1:H:323:ILE:HG22	1:H:345:ALA:O	2.13	0.48
1:I:323:ILE:HG22	1:I:345:ALA:O	2.13	0.48
1:K:52:ILE:HD13	1:K:489:VAL:CG1	2.43	0.48
1:G:222:GLY:HA3	1:G:373:LEU:CD1	2.42	0.48
1:A:499:THR:HA	1:F:146:ARG:CZ	2.42	0.48
1:J:242:PHE:CD1	1:J:242:PHE:N	2.81	0.48
1:L:344:ILE:HB	1:L:367:VAL:HG12	1.94	0.48
1:I:190:TYR:O	1:I:191:ASP:HB2	2.12	0.48
1:L:63:PHE:N	1:L:63:PHE:CD2	2.81	0.48
1:B:367:VAL:C	1:B:477:LEU:HD23	2.33	0.48
1:D:96:SER:O	1:D:130:LYS:HA	2.13	0.48
1:J:176:MET:HG2	1:J:200:GLY:HA3	1.95	0.48
1:K:350:GLY:N	1:K:351:PRO:HD3	2.28	0.48
1:H:304:PHE:HD2	1:H:307:ALA:HB2	1.77	0.48
1:H:12:MET:HG3	1:H:13:VAL:H	1.77	0.48
1:F:286:ILE:O	1:F:286:ILE:HG13	2.14	0.48
1:D:421:PHE:CZ	1:D:423:LYS:HG3	2.48	0.48
1:K:421:PHE:HE1	1:K:423:LYS:O	1.96	0.48
1:L:446:LYS:HG3	1:L:450:HIS:CE1	2.48	0.48
1:D:222:GLY:HA3	1:D:373:LEU:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:225:ASN:OD1	1:J:458:GLU:HG3	2.13	0.48
1:B:107:LEU:HD22	1:B:126:LYS:HD3	1.94	0.48
1:C:428:ILE:O	1:D:416:SER:HB3	2.14	0.48
1:E:346:GLU:CD	1:E:478:ARG:NH2	2.60	0.48
1:H:19:ARG:NE	1:H:479:THR:HG21	2.29	0.48
1:J:23:ILE:HG22	1:J:471:TYR:HD1	1.78	0.48
1:J:201:LYS:H	1:J:201:LYS:HD3	1.77	0.48
1:B:382:TYR:HD2	1:B:382:TYR:O	1.96	0.48
1:A:382:TYR:C	1:A:382:TYR:HD2	2.12	0.48
1:H:198:VAL:O	1:H:201:LYS:HE3	2.13	0.48
1:J:16:PHE:CE2	1:J:354:PRO:HG3	2.35	0.48
1:G:421:PHE:HE1	1:G:423:LYS:O	1.96	0.48
1:I:38:GLU:HG2	1:I:39:GLU:N	2.29	0.48
1:B:322:LEU:HD22	1:B:323:ILE:H	1.77	0.48
1:C:9:PHE:HB3	1:C:329:LYS:HZ3	1.77	0.48
1:K:132:ASN:OD1	1:K:134:LYS:CG	2.61	0.48
1:E:82:HIS:ND1	1:E:109:SER:HA	2.28	0.48
1:L:242:PHE:CD1	1:L:242:PHE:N	2.77	0.48
1:E:242:PHE:N	1:E:242:PHE:CD1	2.81	0.48
1:C:191:ASP:O	1:C:192:ILE:C	2.51	0.48
1:C:82:HIS:ND1	1:C:109:SER:HA	2.28	0.48
1:K:63:PHE:CD2	1:K:63:PHE:N	2.81	0.48
1:K:436:PHE:CD1	1:K:436:PHE:C	2.82	0.48
1:H:23:ILE:HG22	1:H:471:TYR:HD1	1.78	0.48
1:D:118:VAL:CG2	1:D:120:VAL:HG23	2.36	0.48
1:D:96:SER:C	1:D:98:ASP:N	2.67	0.48
1:B:378:VAL:HG12	1:B:379:THR:N	2.29	0.48
1:G:24:VAL:CG1	1:G:483:VAL:HG13	2.30	0.48
1:E:336:ALA:HB3	1:E:337:PRO:CD	2.34	0.48
1:I:208:ILE:HG22	1:I:211:ARG:HB2	1.96	0.48
1:E:28:LEU:H	1:E:28:LEU:CD1	2.12	0.48
1:B:12:MET:HG3	1:B:13:VAL:H	1.77	0.48
1:L:45:VAL:HG13	1:L:490:PHE:HE1	1.77	0.48
1:A:383:PHE:CE2	1:F:397:LEU:CD1	2.90	0.48
1:E:12:MET:HG3	1:E:13:VAL:H	1.77	0.48
1:J:118:VAL:HG23	1:J:118:VAL:O	2.14	0.48
1:I:321:ILE:HD11	1:I:343:ILE:HD12	1.95	0.48
1:L:38:GLU:HG2	1:L:39:GLU:N	2.28	0.48
1:J:222:GLY:HA3	1:J:373:LEU:CD1	2.43	0.48
1:B:245:LYS:HB3	1:B:320:ASP:CB	2.43	0.48
1:K:234:SER:C	1:K:236:LEU:N	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:82:HIS:C	1:H:82:HIS:CD2	2.87	0.48
1:F:82:HIS:C	1:F:82:HIS:CD2	2.86	0.48
1:D:350:GLY:N	1:D:351:PRO:HD3	2.28	0.48
1:J:350:GLY:N	1:J:351:PRO:HD3	2.28	0.48
1:C:68:ASP:OD2	1:C:140:GLU:HG3	2.14	0.48
1:G:432:PRO:HA	1:L:412:SER:HB3	1.94	0.48
1:H:412:SER:N	1:L:433:THR:CG2	2.76	0.48
1:D:477:LEU:H	1:D:477:LEU:HD22	1.78	0.48
1:B:96:SER:O	1:B:130:LYS:HA	2.13	0.48
1:H:366:MET:HG3	1:H:477:LEU:HD21	1.96	0.48
1:G:176:MET:HG3	1:G:198:VAL:HG22	1.95	0.48
1:L:117:VAL:HG12	1:L:118:VAL:HG13	1.96	0.48
1:F:382:TYR:O	1:F:385:TRP:HB3	2.13	0.48
1:B:214:ALA:HB1	1:B:380:VAL:CG2	2.39	0.48
1:K:281:TRP:O	1:K:282:ASN:CB	2.61	0.48
1:G:281:TRP:O	1:G:282:ASN:CB	2.61	0.48
1:F:339:VAL:HG21	1:F:360:PHE:HE1	1.77	0.48
1:J:191:ASP:O	1:J:192:ILE:C	2.51	0.48
1:J:82:HIS:C	1:J:82:HIS:CD2	2.87	0.48
1:F:23:ILE:HG22	1:F:471:TYR:HD1	1.78	0.48
1:K:159:GLY:O	1:K:162:VAL:HG12	2.14	0.48
1:G:432:PRO:HA	1:L:412:SER:CB	2.43	0.48
1:G:413:VAL:HG11	1:L:413:VAL:CG2	2.43	0.48
1:E:201:LYS:H	1:E:201:LYS:HD3	1.79	0.48
1:A:330:GLN:O	1:A:331:LEU:HD12	2.13	0.48
1:A:473:LEU:HD23	1:A:479:THR:OG1	2.13	0.48
1:E:61:LEU:O	1:E:62:SER:HB2	2.13	0.48
1:E:473:LEU:HD23	1:E:479:THR:OG1	2.13	0.48
1:E:16:PHE:N	1:E:16:PHE:CD2	2.82	0.48
1:F:490:PHE:C	1:F:490:PHE:CD2	2.86	0.48
1:B:499:THR:HG22	1:B:499:THR:O	2.14	0.48
1:B:486:ILE:O	1:B:487:GLU:C	2.51	0.48
1:A:12:MET:HG3	1:A:13:VAL:H	1.78	0.48
1:J:175:GLU:O	1:J:178:TRP:HB2	2.12	0.48
1:L:473:LEU:HD23	1:L:479:THR:OG1	2.13	0.48
1:L:343:ILE:HG23	1:L:366:MET:HE3	1.95	0.48
1:J:52:ILE:HD13	1:J:489:VAL:HG11	1.96	0.48
1:D:273:VAL:HB	1:D:280:ILE:HD11	1.96	0.48
1:C:274:GLY:HA2	1:C:279:SER:HA	1.96	0.48
1:A:217:ARG:HG2	1:A:262:TYR:CD1	2.48	0.48
1:B:402:GLU:O	1:B:404:ASP:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:PHE:CD1	1:D:242:PHE:N	2.82	0.48
1:G:490:PHE:C	1:G:490:PHE:CD2	2.87	0.48
1:F:96:SER:O	1:F:130:LYS:HA	2.14	0.48
1:C:411:MET:HA	1:C:414:GLN:HB3	1.96	0.48
1:A:96:SER:O	1:A:130:LYS:HA	2.14	0.48
1:B:339:VAL:HG21	1:B:360:PHE:HE1	1.77	0.48
1:G:166:ALA:CA	1:G:176:MET:HE2	2.43	0.48
1:A:372:TYR:CE2	1:A:460:SER:HB3	2.48	0.48
1:H:78:TYR:CD2	1:H:101:VAL:HG22	2.48	0.48
1:I:167:PRO:HD3	1:I:176:MET:SD	2.54	0.48
1:J:370:ASP:OD1	1:J:371:LEU:N	2.45	0.48
1:J:331:LEU:O	1:J:353:THR:HG23	2.14	0.48
1:C:176:MET:HG2	1:C:200:GLY:HA3	1.95	0.48
1:A:121:PRO:O	1:A:122:PHE:HD2	1.95	0.48
1:B:491:ARG:O	1:B:495:GLU:HG3	2.14	0.48
1:C:234:SER:C	1:C:236:LEU:N	2.65	0.48
1:F:87:THR:CB	1:F:88:PRO:HD3	2.42	0.48
1:J:211:ARG:HA	1:J:380:VAL:HG11	1.96	0.48
1:D:87:THR:CB	1:D:88:PRO:CD	2.91	0.48
1:A:345:ALA:HB1	1:A:373:LEU:HD21	1.96	0.48
1:E:214:ALA:CB	1:E:380:VAL:HG21	2.43	0.48
1:B:432:PRO:O	1:B:433:THR:O	2.31	0.48
1:D:241:GLY:C	1:D:243:GLY:H	2.17	0.48
1:L:421:PHE:O	1:L:423:LYS:N	2.47	0.48
1:L:95:TYR:HB3	1:L:133:PRO:HG3	1.94	0.48
1:B:89:CYS:H	1:B:163:ASP:HA	1.78	0.48
1:C:295:LYS:HG3	1:C:296:LEU:HD22	1.96	0.48
1:F:20:GLY:O	1:F:21:ALA:C	2.51	0.48
1:B:18:ASP:HA	1:B:21:ALA:CB	2.43	0.48
1:A:190:TYR:O	1:A:191:ASP:HB2	2.13	0.48
1:E:321:ILE:HD11	1:E:343:ILE:HD12	1.96	0.48
1:E:86:ARG:HG2	1:E:121:PRO:CA	2.44	0.48
1:D:488:LYS:HA	1:D:491:ARG:HD3	1.96	0.48
1:C:111:MET:HE3	2:C:552:NDP:H72N	1.77	0.48
1:J:330:GLN:O	1:J:331:LEU:HD12	2.14	0.48
1:F:201:LYS:HD3	1:F:201:LYS:H	1.78	0.48
1:B:498:VAL:HG23	1:B:500:PHE:CD2	2.48	0.48
1:H:211:ARG:HA	1:H:380:VAL:HG11	1.95	0.48
1:H:455:TYR:CE1	1:H:459:ARG:HD3	2.44	0.48
1:K:274:GLY:HA2	1:K:279:SER:HA	1.96	0.48
1:B:350:GLY:N	1:B:351:PRO:HD3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:82:HIS:HD2	1:E:83:SER:HB2	1.78	0.48
1:G:432:PRO:HA	1:L:412:SER:OG	2.13	0.48
1:E:86:ARG:NH1	1:E:492:VAL:HG21	2.28	0.48
1:A:114:LYS:HZ2	2:A:552:NDP:C7N	2.26	0.48
1:A:432:PRO:HA	1:F:412:SER:CB	2.44	0.48
1:B:408:HIS:HE1	1:F:435:GLU:OE1	1.97	0.48
1:E:166:ALA:HA	1:E:176:MET:HE2	1.95	0.48
1:I:214:ALA:CB	1:I:380:VAL:HG21	2.44	0.48
1:C:201:LYS:HD3	1:C:201:LYS:H	1.79	0.48
1:B:488:LYS:NZ	3:B:601:XEG:HAK	2.29	0.48
1:L:464:ILE:O	1:L:468:ALA:HB3	2.13	0.48
1:K:264:HIS:CE1	1:K:287:ASP:OD1	2.66	0.48
1:K:490:PHE:C	1:K:490:PHE:CD2	2.87	0.48
1:B:162:VAL:O	1:B:163:ASP:HB2	2.14	0.48
1:F:493:TYR:HD1	1:F:493:TYR:HA	1.52	0.48
1:K:142:GLU:HB2	1:K:178:TRP:CZ2	2.49	0.48
1:F:82:HIS:HD2	1:F:83:SER:HB2	1.77	0.48
1:C:55:CYS:HB3	1:C:82:HIS:HA	1.95	0.48
1:I:149:THR:O	1:I:150:MET:C	2.52	0.48
1:C:156:GLY:O	1:F:155:LYS:HE3	2.14	0.48
1:L:413:VAL:HG12	1:L:414:GLN:N	2.29	0.48
1:L:431:VAL:HA	1:L:432:PRO:HD2	1.72	0.48
1:E:383:PHE:HA	1:E:386:LEU:HD12	1.96	0.48
1:J:468:ALA:HB1	1:J:480:ALA:HB1	1.96	0.48
1:D:86:ARG:HG2	1:D:121:PRO:CA	2.43	0.48
1:D:378:VAL:HG12	1:D:379:THR:N	2.28	0.48
1:A:428:ILE:O	1:F:416:SER:HB3	2.13	0.48
1:I:117:VAL:HG12	1:I:118:VAL:HG13	1.95	0.48
1:A:171:THR:HA	1:A:175:GLU:OE2	2.14	0.48
1:K:117:VAL:HG21	1:K:371:LEU:HG	1.95	0.48
1:K:473:LEU:HD23	1:K:479:THR:OG1	2.14	0.48
1:I:201:LYS:HD3	1:I:384:GLU:OE1	2.14	0.48
1:C:336:ALA:HB3	1:C:337:PRO:CD	2.34	0.48
1:J:236:LEU:HD12	1:J:238:MET:HE2	1.96	0.48
1:A:86:ARG:NH1	1:A:492:VAL:HG21	2.29	0.48
1:I:500:PHE:O	1:I:501:THR:O	2.31	0.48
1:L:201:LYS:HD3	1:L:384:GLU:OE1	2.14	0.48
1:H:155:LYS:HE2	1:K:57:HIS:ND1	2.28	0.48
1:D:211:ARG:HA	1:D:380:VAL:HG11	1.94	0.48
1:J:487:GLU:O	1:J:491:ARG:HG2	2.14	0.48
1:J:488:LYS:CA	1:J:491:ARG:HG3	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:459:ARG:NH2	3:J:601:XEG:OAH	2.47	0.48
1:D:271:ILE:HD11	1:D:283:PRO:HG3	1.95	0.48
1:I:274:GLY:HA2	1:I:279:SER:HA	1.95	0.48
1:C:273:VAL:HB	1:C:280:ILE:HD11	1.95	0.48
1:A:242:PHE:CD1	1:A:242:PHE:N	2.80	0.48
1:C:82:HIS:HD2	1:C:83:SER:HB2	1.79	0.48
1:L:190:TYR:O	1:L:191:ASP:HB2	2.13	0.48
1:C:180:ALA:O	1:C:181:ASP:C	2.52	0.48
1:E:348:ALA:HB3	1:E:351:PRO:HG3	1.95	0.47
1:J:432:PRO:O	1:J:433:THR:O	2.32	0.47
1:A:350:GLY:N	1:A:351:PRO:HD3	2.29	0.47
1:E:491:ARG:O	1:E:495:GLU:HG3	2.14	0.47
1:J:464:ILE:O	1:J:468:ALA:HB3	2.14	0.47
1:J:176:MET:HE3	1:J:179:ILE:HD12	1.96	0.47
1:G:117:VAL:HG12	1:G:118:VAL:HG13	1.95	0.47
1:G:201:LYS:HD3	1:G:384:GLU:OE1	2.14	0.47
1:J:478:ARG:O	1:J:481:ALA:N	2.44	0.47
1:J:255:VAL:HG12	2:J:552:NDP:O2N	2.14	0.47
1:C:86:ARG:HG2	1:C:121:PRO:CA	2.44	0.47
1:B:276:SER:HB2	2:B:552:NDP:O2B	2.14	0.47
1:J:274:GLY:HA3	1:J:314:ILE:CD1	2.44	0.47
1:L:281:TRP:O	1:L:282:ASN:CB	2.62	0.47
1:H:222:GLY:HA3	1:H:373:LEU:CD1	2.44	0.47
1:H:345:ALA:HB1	1:H:373:LEU:HD21	1.95	0.47
1:G:38:GLU:HG2	1:G:39:GLU:N	2.29	0.47
1:D:242:PHE:C	1:D:244:ASP:N	2.68	0.47
1:F:242:PHE:C	1:F:244:ASP:N	2.68	0.47
1:A:242:PHE:C	1:A:244:ASP:N	2.68	0.47
1:B:69:ASP:OD2	1:B:71:SER:HB2	2.14	0.47
1:K:104:VAL:HG23	1:K:105:LYS:N	2.29	0.47
1:E:90:LYS:HE2	1:E:381:SER:HB3	1.95	0.47
1:I:121:PRO:HD3	1:I:382:TYR:CE1	2.48	0.47
1:I:382:TYR:HD2	1:I:382:TYR:C	2.18	0.47
1:K:214:ALA:CB	1:K:380:VAL:HG21	2.41	0.47
1:I:399:PHE:HB2	1:K:455:TYR:HE2	1.79	0.47
1:L:6:ASP:N	1:L:355:GLU:CG	2.77	0.47
1:I:165:PRO:O	1:I:198:VAL:HG23	2.13	0.47
1:I:211:ARG:O	1:I:211:ARG:HG2	2.14	0.47
1:B:393:SER:OG	3:F:601:XEG:CAM	2.62	0.47
1:A:65:ILE:HD11	1:A:75:ILE:CD1	2.37	0.47
1:H:201:LYS:HA	1:H:202:PRO:HD2	1.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:273:VAL:HB	1:L:280:ILE:HD11	1.96	0.47
1:D:107:LEU:HD22	1:D:126:LYS:HD3	1.95	0.47
1:K:295:LYS:HG3	1:K:296:LEU:HD22	1.97	0.47
1:J:18:ASP:HA	1:J:21:ALA:CB	2.44	0.47
1:F:68:ASP:OD2	1:F:140:GLU:HG3	2.13	0.47
1:I:20:GLY:O	1:I:21:ALA:C	2.53	0.47
1:C:175:GLU:HA	1:C:178:TRP:CE3	2.49	0.47
1:E:294:PHE:CE1	1:E:304:PHE:HD1	2.32	0.47
1:I:432:PRO:CA	1:J:412:SER:HB3	2.41	0.47
1:J:166:ALA:HA	1:J:176:MET:HE2	1.96	0.47
1:J:90:LYS:HG3	1:J:122:PHE:CD1	2.48	0.47
1:I:99:VAL:HG11	1:I:128:GLY:CA	2.35	0.47
1:G:350:GLY:N	1:G:351:PRO:HD3	2.29	0.47
1:G:478:ARG:O	1:G:481:ALA:N	2.44	0.47
1:H:344:ILE:O	1:H:367:VAL:HA	2.13	0.47
1:G:201:LYS:H	1:G:201:LYS:HD3	1.79	0.47
1:E:330:GLN:O	1:E:331:LEU:HD12	2.12	0.47
1:C:6:ASP:HB2	1:C:353:THR:CG2	2.44	0.47
1:F:211:ARG:O	1:F:211:ARG:HG2	2.14	0.47
1:H:176:MET:HG2	1:H:200:GLY:HA3	1.95	0.47
1:K:273:VAL:HB	1:K:280:ILE:HD11	1.95	0.47
1:I:38:GLU:O	1:I:40:GLN:N	2.47	0.47
1:B:413:VAL:CG1	1:B:429:PRO:HG3	2.43	0.47
1:I:95:TYR:HB3	1:I:133:PRO:HG3	1.96	0.47
1:F:402:GLU:O	1:F:404:ASP:N	2.47	0.47
1:E:369:PRO:HG3	1:E:478:ARG:CA	2.44	0.47
1:D:38:GLU:HG2	1:D:39:GLU:N	2.29	0.47
1:D:19:ARG:NE	1:D:479:THR:HG21	2.30	0.47
1:D:468:ALA:HB1	1:D:480:ALA:HB1	1.96	0.47
1:E:498:VAL:O	1:E:500:PHE:CD2	2.67	0.47
1:B:87:THR:CB	1:B:88:PRO:CD	2.92	0.47
1:K:118:VAL:CG2	1:K:120:VAL:HG23	2.34	0.47
1:H:366:MET:HA	1:H:475:LEU:HB3	1.97	0.47
1:F:176:MET:HG3	1:F:198:VAL:HG22	1.97	0.47
1:C:490:PHE:C	1:C:490:PHE:CD2	2.87	0.47
1:C:198:VAL:O	1:C:201:LYS:HE3	2.14	0.47
1:D:12:MET:HG3	1:D:13:VAL:H	1.79	0.47
1:L:264:HIS:CE1	1:L:287:ASP:OD1	2.67	0.47
1:D:304:PHE:HD2	1:D:307:ALA:HB2	1.78	0.47
1:J:281:TRP:O	1:J:282:ASN:CB	2.62	0.47
1:H:241:GLY:C	1:H:243:GLY:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:38:GLU:HG2	1:J:39:GLU:N	2.30	0.47
1:A:421:PHE:HE1	1:A:423:LYS:O	1.97	0.47
1:E:421:PHE:HE1	1:E:423:LYS:O	1.97	0.47
1:L:350:GLY:N	1:L:351:PRO:HD3	2.29	0.47
1:D:108:ALA:HB2	1:D:126:LYS:HB2	1.96	0.47
1:K:242:PHE:C	1:K:244:ASP:N	2.68	0.47
1:F:61:LEU:HA	1:F:61:LEU:HD13	1.69	0.47
1:H:72:TRP:HB3	1:K:47:SER:HB3	1.97	0.47
1:J:295:LYS:HG3	1:J:296:LEU:HD22	1.97	0.47
1:D:18:ASP:HA	1:D:21:ALA:CB	2.44	0.47
1:F:175:GLU:HA	1:F:178:TRP:CE3	2.50	0.47
1:J:162:VAL:O	1:J:163:ASP:HB2	2.14	0.47
1:B:6:ASP:N	1:B:7:PRO:HD2	2.29	0.47
1:E:63:PHE:CD2	1:E:63:PHE:N	2.82	0.47
1:A:63:PHE:N	1:A:63:PHE:CD2	2.83	0.47
1:I:433:THR:HG22	1:J:412:SER:CA	2.45	0.47
1:A:117:VAL:HG12	1:A:118:VAL:HG13	1.96	0.47
1:D:90:LYS:HG3	1:D:122:PHE:CD1	2.49	0.47
1:A:110:LEU:HD21	1:A:349:ASN:OD1	2.14	0.47
1:F:431:VAL:HA	1:F:432:PRO:HD2	1.71	0.47
1:E:93:ILE:CG2	1:E:127:ALA:HB3	2.41	0.47
1:E:167:PRO:HD3	1:E:176:MET:SD	2.54	0.47
1:J:496:ALA:HB2	1:K:205:GLN:OE1	2.15	0.47
1:K:12:MET:HG2	1:K:14:GLU:OE2	2.15	0.47
1:H:90:LYS:HG3	1:H:122:PHE:CD1	2.49	0.47
1:C:294:PHE:CE1	1:C:304:PHE:HD1	2.33	0.47
1:H:173:GLU:HB2	1:H:202:PRO:HD3	1.95	0.47
1:E:273:VAL:HB	1:E:280:ILE:HD11	1.97	0.47
1:C:141:LEU:O	1:C:145:THR:HG23	2.15	0.47
1:L:256:GLY:HA2	1:L:259:SER:OG	2.15	0.47
1:J:402:GLU:O	1:J:404:ASP:N	2.44	0.47
1:D:460:SER:O	1:D:463:GLN:N	2.48	0.47
1:I:413:VAL:HG11	1:J:413:VAL:HG22	1.97	0.47
1:C:99:VAL:HA	1:C:103:GLU:OE1	2.14	0.47
1:C:413:VAL:HG22	1:E:413:VAL:HG11	1.96	0.47
1:I:86:ARG:HH12	1:I:492:VAL:CG2	2.28	0.47
1:G:464:ILE:O	1:G:468:ALA:HB3	2.15	0.47
1:G:117:VAL:HG12	1:G:118:VAL:N	2.29	0.47
1:J:288:PRO:HA	1:J:291:LEU:HD22	1.97	0.47
1:C:490:PHE:O	1:C:491:ARG:C	2.53	0.47
1:F:121:PRO:CD	1:F:382:TYR:CE1	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:234:SER:C	1:G:236:LEU:N	2.68	0.47
1:G:273:VAL:HB	1:G:280:ILE:HD11	1.96	0.47
1:J:47:SER:O	1:J:50:ARG:N	2.44	0.47
1:J:345:ALA:HB1	1:J:373:LEU:HD21	1.96	0.47
1:B:241:GLY:C	1:B:243:GLY:H	2.17	0.47
1:F:420:LYS:O	1:F:421:PHE:HB2	2.13	0.47
1:B:154:LYS:NZ	1:E:501:THR:HG21	2.30	0.47
1:B:132:ASN:OD1	1:B:134:LYS:CG	2.61	0.47
1:I:242:PHE:C	1:I:244:ASP:N	2.68	0.47
1:A:9:PHE:HA	1:A:329:LYS:NZ	2.28	0.47
1:E:490:PHE:CD2	1:E:490:PHE:C	2.88	0.47
1:A:18:ASP:HA	1:A:21:ALA:HB3	1.97	0.47
1:A:294:PHE:CE1	1:A:304:PHE:HD1	2.32	0.47
1:E:121:PRO:O	1:E:122:PHE:HD2	1.97	0.47
1:D:382:TYR:HD2	1:D:382:TYR:O	1.98	0.47
1:B:409:LEU:CD1	1:F:436:PHE:CE2	2.98	0.47
1:F:411:MET:HA	1:F:414:GLN:HB3	1.96	0.47
1:F:429:PRO:C	1:F:431:VAL:N	2.68	0.47
1:J:198:VAL:O	1:J:201:LYS:HE3	2.14	0.47
1:I:7:PRO:O	1:I:8:ASN:HB2	2.15	0.47
1:A:7:PRO:HD3	1:A:355:GLU:HG3	1.96	0.47
3:D:502:XEG:CAM	1:E:393:SER:OG	2.63	0.47
1:G:28:LEU:CD1	1:G:28:LEU:H	2.13	0.47
1:A:250:GLN:HG2	1:A:330:GLN:HE21	1.79	0.47
1:G:86:ARG:O	1:G:87:THR:O	2.32	0.47
1:G:87:THR:CB	1:G:88:PRO:CD	2.91	0.47
1:G:202:PRO:HG2	1:G:205:GLN:HG3	1.97	0.47
1:L:370:ASP:OD1	1:L:371:LEU:N	2.48	0.47
1:G:59:LEU:HD12	1:G:59:LEU:HA	1.64	0.47
1:A:86:ARG:HG2	1:A:121:PRO:CA	2.44	0.47
1:H:52:ILE:HD13	1:H:489:VAL:HG11	1.97	0.47
1:J:7:PRO:HB2	1:J:329:LYS:HD2	1.96	0.47
1:I:264:HIS:CE1	1:I:287:ASP:OD1	2.67	0.47
1:L:238:MET:HE1	1:L:343:ILE:HD11	1.96	0.47
1:K:15:GLY:O	1:K:16:PHE:C	2.53	0.47
1:J:52:ILE:HD13	1:J:489:VAL:HG12	1.96	0.47
1:I:281:TRP:O	1:I:282:ASN:CB	2.62	0.47
1:I:282:ASN:O	1:I:284:ASP:N	2.47	0.47
1:G:396:ARG:HG3	1:G:396:ARG:O	2.13	0.47
1:I:241:GLY:C	1:I:243:GLY:H	2.18	0.47
1:H:47:SER:O	1:H:50:ARG:N	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:GLY:HA3	1:E:373:LEU:CD1	2.44	0.47
1:G:323:ILE:HG22	1:G:345:ALA:O	2.15	0.47
1:F:396:ARG:CG	1:F:396:ARG:HH11	2.28	0.47
1:G:141:LEU:HD22	1:G:141:LEU:HA	1.76	0.47
1:B:402:GLU:C	1:B:404:ASP:N	2.66	0.47
1:F:498:VAL:O	1:F:499:THR:OG1	2.29	0.47
1:D:175:GLU:HA	1:D:178:TRP:CE3	2.49	0.47
1:G:82:HIS:HD2	1:G:83:SER:HB2	1.80	0.47
1:I:171:THR:HA	1:I:175:GLU:OE2	2.15	0.47
1:C:142:GLU:HB2	1:C:178:TRP:CZ2	2.49	0.47
1:L:116:ALA:O	1:L:488:LYS:HD2	2.13	0.47
1:G:89:CYS:H	1:G:163:ASP:HA	1.79	0.47
1:F:295:LYS:HG3	1:F:296:LEU:HD22	1.95	0.47
1:C:89:CYS:H	1:C:163:ASP:HA	1.80	0.47
1:A:203:ILE:N	1:A:203:ILE:HD12	2.30	0.47
1:G:429:PRO:C	1:G:431:VAL:N	2.68	0.47
1:H:468:ALA:HB1	1:H:480:ALA:HB1	1.97	0.47
1:J:87:THR:CB	1:J:88:PRO:CD	2.90	0.47
1:E:111:MET:CE	2:E:552:NDP:N7N	2.69	0.47
3:B:601:XEG:CAZ	3:B:601:XEG:HAPA	2.45	0.47
1:L:28:LEU:H	1:L:28:LEU:CD1	2.16	0.47
1:J:120:VAL:HG13	1:J:382:TYR:CD1	2.49	0.47
1:B:281:TRP:O	1:B:282:ASN:CB	2.63	0.47
1:A:273:VAL:HB	1:A:280:ILE:HD11	1.97	0.47
1:C:281:TRP:O	1:C:282:ASN:CB	2.63	0.47
1:C:282:ASN:O	1:C:284:ASP:N	2.46	0.47
1:E:213:SER:HB2	1:E:262:TYR:CE2	2.50	0.47
1:L:38:GLU:O	1:L:40:GLN:N	2.48	0.47
1:B:413:VAL:HG12	1:B:429:PRO:CG	2.43	0.47
1:H:175:GLU:O	1:H:178:TRP:HB2	2.15	0.47
1:K:396:ARG:CG	1:K:396:ARG:HH11	2.24	0.47
1:I:217:ARG:CZ	1:I:450:HIS:CD2	2.98	0.47
1:A:129:VAL:HG12	1:A:129:VAL:O	2.15	0.47
1:I:383:PHE:CD2	1:I:383:PHE:N	2.83	0.47
1:C:82:HIS:C	1:C:82:HIS:CD2	2.88	0.47
1:K:420:LYS:HG2	1:K:420:LYS:O	2.15	0.47
1:E:264:HIS:CE1	1:E:287:ASP:OD1	2.68	0.47
1:B:38:GLU:HG2	1:B:39:GLU:N	2.29	0.47
1:E:485:ALA:O	1:E:486:ILE:C	2.52	0.47
1:C:413:VAL:CG2	1:E:413:VAL:HG11	2.45	0.47
1:A:489:VAL:O	1:A:492:VAL:HB	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LYS:HA	1:A:14:GLU:HG3	1.97	0.47
1:C:234:SER:O	1:C:236:LEU:N	2.48	0.47
1:L:211:ARG:HG2	1:L:211:ARG:O	2.15	0.47
1:C:59:LEU:HD12	1:C:59:LEU:HA	1.59	0.47
1:D:59:LEU:HA	1:D:59:LEU:HD12	1.68	0.47
1:E:396:ARG:NH1	1:E:396:ARG:CG	2.75	0.47
1:B:56:ASN:C	1:B:57:HIS:CD2	2.88	0.47
1:G:396:ARG:NH1	1:G:396:ARG:HG3	2.26	0.47
3:D:601:XEG:CAZ	3:D:601:XEG:HAPA	2.44	0.47
1:I:256:GLY:HA2	1:I:259:SER:OG	2.15	0.47
1:B:217:ARG:HD3	1:B:450:HIS:CD2	2.50	0.47
1:K:234:SER:O	1:K:236:LEU:N	2.48	0.47
1:H:95:TYR:HB3	1:H:133:PRO:HG3	1.97	0.47
1:L:69:ASP:OD2	1:L:71:SER:CB	2.63	0.47
1:K:82:HIS:CD2	1:K:82:HIS:C	2.88	0.47
1:K:89:CYS:H	1:K:163:ASP:HA	1.80	0.47
1:G:104:VAL:HG23	1:G:105:LYS:N	2.30	0.47
1:H:203:ILE:HD12	1:H:203:ILE:H	1.80	0.47
1:J:158:ILE:O	1:J:158:ILE:HG23	2.15	0.47
1:D:473:LEU:H	1:D:473:LEU:HD12	1.79	0.47
1:D:473:LEU:HD23	1:D:479:THR:OG1	2.15	0.47
1:B:372:TYR:HE2	1:B:460:SER:HB3	1.79	0.47
1:D:121:PRO:O	1:D:122:PHE:CD2	2.68	0.47
1:G:336:ALA:HB3	1:G:337:PRO:CD	2.33	0.47
3:G:601:XEG:CAM	1:L:393:SER:OG	2.63	0.47
1:I:459:ARG:NH2	3:I:601:XEG:OAH	2.49	0.47
1:L:336:ALA:CB	1:L:337:PRO:HD3	2.29	0.47
1:F:250:GLN:NE2	2:F:552:NDP:H2A	2.30	0.47
1:F:264:HIS:HE1	1:F:287:ASP:OD1	1.98	0.47
1:J:7:PRO:O	1:J:8:ASN:OD1	2.32	0.47
1:I:273:VAL:HB	1:I:280:ILE:HD11	1.96	0.47
1:H:8:ASN:C	1:H:9:PHE:CG	2.88	0.47
1:J:36:GLU:O	1:J:37:THR:C	2.54	0.47
1:H:38:GLU:HG2	1:H:39:GLU:N	2.30	0.47
1:L:402:GLU:C	1:L:404:ASP:N	2.69	0.47
1:E:242:PHE:C	1:E:244:ASP:N	2.67	0.47
1:J:256:GLY:HA2	1:J:259:SER:OG	2.14	0.47
1:J:82:HIS:HD2	1:J:83:SER:HB2	1.80	0.47
1:H:158:ILE:O	1:H:158:ILE:HG23	2.15	0.47
1:D:473:LEU:HD22	1:D:480:ALA:CB	2.40	0.46
1:B:468:ALA:HB1	1:B:480:ALA:HB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:8:ASN:O	1:I:9:PHE:C	2.53	0.46
1:E:166:ALA:HB1	1:E:167:PRO:HD2	1.96	0.46
1:K:99:VAL:HA	1:K:103:GLU:OE1	2.14	0.46
1:A:464:ILE:O	1:A:468:ALA:CB	2.63	0.46
1:G:61:LEU:O	1:G:62:SER:HB2	2.15	0.46
1:H:12:MET:N	1:H:14:GLU:HG2	2.17	0.46
1:K:111:MET:HE2	2:K:552:NDP:N7N	2.28	0.46
1:B:59:LEU:HA	1:B:59:LEU:HD12	1.65	0.46
1:L:59:LEU:HA	1:L:59:LEU:HD12	1.70	0.46
1:I:396:ARG:HG3	1:I:396:ARG:NH1	2.25	0.46
1:G:38:GLU:O	1:G:40:GLN:N	2.49	0.46
1:K:396:ARG:HG3	1:K:396:ARG:NH1	2.27	0.46
1:A:61:LEU:O	1:A:62:SER:CB	2.63	0.46
1:B:8:ASN:ND2	1:B:329:LYS:HD2	2.30	0.46
1:A:82:HIS:HD2	1:A:83:SER:HB2	1.80	0.46
1:E:180:ALA:O	1:E:181:ASP:C	2.54	0.46
1:D:82:HIS:CD2	1:D:82:HIS:C	2.89	0.46
1:F:171:THR:HA	1:F:175:GLU:OE2	2.15	0.46
1:A:18:ASP:HA	1:A:21:ALA:CB	2.45	0.46
1:H:203:ILE:HD12	1:H:203:ILE:N	2.30	0.46
1:K:464:ILE:O	1:K:468:ALA:HB3	2.14	0.46
1:H:378:VAL:HG12	1:H:379:THR:N	2.30	0.46
1:L:8:ASN:O	1:L:329:LYS:CD	2.62	0.46
1:C:337:PRO:HG3	1:C:359:ILE:HD12	1.98	0.46
1:F:176:MET:HE3	1:F:179:ILE:HD12	1.97	0.46
1:F:28:LEU:HD23	1:F:490:PHE:CG	2.50	0.46
1:D:288:PRO:HA	1:D:291:LEU:HD22	1.96	0.46
1:B:265:ARG:O	1:B:266:PHE:CB	2.58	0.46
1:J:490:PHE:CE2	1:J:494:ASN:HB2	2.50	0.46
1:H:281:TRP:O	1:H:282:ASN:CB	2.63	0.46
1:J:214:ALA:CB	1:J:380:VAL:HG21	2.39	0.46
1:H:420:LYS:O	1:H:421:PHE:HB2	2.16	0.46
1:H:141:LEU:HD22	1:H:141:LEU:HA	1.76	0.46
1:D:490:PHE:CD2	1:D:490:PHE:C	2.89	0.46
1:G:132:ASN:OD1	1:G:134:LYS:CG	2.62	0.46
1:B:242:PHE:N	1:B:242:PHE:CD1	2.81	0.46
1:G:242:PHE:C	1:G:244:ASP:N	2.68	0.46
1:C:61:LEU:O	1:C:62:SER:HB2	2.15	0.46
1:H:162:VAL:O	1:H:163:ASP:HB2	2.14	0.46
1:G:295:LYS:HG3	1:G:296:LEU:HD22	1.96	0.46
1:E:478:ARG:O	1:E:481:ALA:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:412:SER:HB3	1:K:432:PRO:HA	1.97	0.46
1:F:99:VAL:HA	1:F:103:GLU:OE1	2.15	0.46
1:D:367:VAL:C	1:D:477:LEU:HD23	2.32	0.46
1:B:477:LEU:HD22	1:B:477:LEU:H	1.80	0.46
1:A:202:PRO:HG2	1:A:205:GLN:HG3	1.97	0.46
1:G:473:LEU:HD23	1:G:479:THR:OG1	2.15	0.46
1:B:493:TYR:O	1:B:495:GLU:N	2.48	0.46
1:F:378:VAL:HG12	1:F:379:THR:N	2.29	0.46
1:F:383:PHE:HD1	1:F:449:VAL:HG13	1.79	0.46
1:J:383:PHE:HA	1:J:386:LEU:HD12	1.97	0.46
1:L:493:TYR:O	1:L:494:ASN:C	2.54	0.46
1:I:294:PHE:CE1	1:I:304:PHE:HD1	2.33	0.46
3:J:601:XEG:HAJ	3:J:601:XEG:HBE	1.75	0.46
1:I:36:GLU:O	1:I:37:THR:C	2.54	0.46
1:L:36:GLU:O	1:L:37:THR:C	2.54	0.46
1:J:241:GLY:C	1:J:243:GLY:H	2.19	0.46
1:K:323:ILE:HG22	1:K:345:ALA:O	2.13	0.46
1:F:95:TYR:HB3	1:F:133:PRO:HG3	1.98	0.46
1:J:97:THR:OG1	1:J:132:ASN:HB2	2.15	0.46
1:B:171:THR:HA	1:B:175:GLU:OE2	2.14	0.46
1:F:499:THR:C	1:F:500:PHE:CD2	2.88	0.46
1:J:61:LEU:O	1:J:62:SER:CB	2.61	0.46
1:F:82:HIS:ND1	1:F:109:SER:HA	2.31	0.46
1:I:69:ASP:OD2	1:I:71:SER:CB	2.64	0.46
1:D:206:GLY:O	1:D:388:ASN:ND2	2.29	0.46
1:H:20:GLY:O	1:H:21:ALA:C	2.53	0.46
1:D:378:VAL:O	1:D:381:SER:HB2	2.15	0.46
1:A:337:PRO:HG3	1:A:359:ILE:HD12	1.98	0.46
3:I:601:XEG:CAZ	3:I:601:XEG:HAPA	2.46	0.46
1:F:111:MET:HE3	2:F:552:NDP:H72N	1.75	0.46
1:E:372:TYR:CE2	1:E:460:SER:HB3	2.51	0.46
1:C:93:ILE:HD11	1:C:179:ILE:HD11	1.97	0.46
1:A:90:LYS:HE2	1:A:381:SER:HB3	1.96	0.46
1:E:11:LYS:HA	1:E:14:GLU:HG3	1.97	0.46
1:H:211:ARG:O	1:H:211:ARG:HG2	2.14	0.46
1:J:15:GLY:O	1:J:16:PHE:C	2.53	0.46
1:L:282:ASN:O	1:L:284:ASP:N	2.47	0.46
1:F:281:TRP:O	1:F:282:ASN:CB	2.63	0.46
1:B:421:PHE:CZ	1:B:423:LYS:HG3	2.49	0.46
1:F:141:LEU:HD22	1:F:141:LEU:HA	1.75	0.46
1:C:457:MET:O	1:C:460:SER:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:402:GLU:C	1:K:404:ASP:N	2.68	0.46
1:L:275:GLU:OE2	1:L:301:ILE:HG13	2.15	0.46
1:H:256:GLY:HA2	1:H:259:SER:OG	2.15	0.46
1:L:369:PRO:HD3	1:L:477:LEU:HB2	1.97	0.46
1:D:171:THR:HA	1:D:175:GLU:OE2	2.15	0.46
1:C:16:PHE:CD2	1:C:16:PHE:N	2.81	0.46
1:K:241:GLY:C	1:K:243:GLY:H	2.19	0.46
1:E:226:PHE:CE2	1:E:465:MET:HE2	2.51	0.46
1:L:89:CYS:H	1:L:163:ASP:HA	1.80	0.46
1:B:295:LYS:HG3	1:B:296:LEU:HD22	1.98	0.46
1:F:453:LEU:CD2	1:F:453:LEU:C	2.84	0.46
1:D:372:TYR:HE2	1:D:460:SER:HB3	1.81	0.46
1:H:337:PRO:HG3	1:H:359:ILE:HD12	1.97	0.46
1:F:93:ILE:HD11	1:F:179:ILE:HD11	1.97	0.46
1:A:383:PHE:HA	1:A:386:LEU:HD12	1.96	0.46
1:I:464:ILE:O	1:I:468:ALA:HB3	2.16	0.46
1:F:11:LYS:HA	1:F:14:GLU:HG3	1.98	0.46
1:H:121:PRO:O	1:H:122:PHE:HD2	1.98	0.46
1:F:117:VAL:HG12	1:F:118:VAL:CG1	2.46	0.46
1:H:271:ILE:HD11	1:H:283:PRO:HG3	1.98	0.46
1:H:274:GLY:HA3	1:H:314:ILE:CD1	2.44	0.46
1:K:38:GLU:O	1:K:40:GLN:N	2.49	0.46
1:C:453:LEU:HD23	1:C:453:LEU:C	2.35	0.46
1:E:149:THR:O	1:E:150:MET:C	2.54	0.46
1:D:162:VAL:O	1:D:163:ASP:HB2	2.15	0.46
1:F:191:ASP:O	1:F:192:ILE:C	2.54	0.46
1:C:316:GLU:O	1:C:317:VAL:C	2.54	0.46
1:L:149:THR:HB	1:L:182:THR:HG21	1.98	0.46
1:B:473:LEU:H	1:B:473:LEU:HD12	1.81	0.46
1:B:96:SER:C	1:B:98:ASP:N	2.69	0.46
1:K:86:ARG:HG2	1:K:121:PRO:CA	2.46	0.46
3:D:502:XEG:CAZ	3:D:502:XEG:HAPA	2.45	0.46
1:L:337:PRO:HG3	1:L:359:ILE:HD12	1.98	0.46
1:K:250:GLN:HG2	1:K:330:GLN:HE21	1.81	0.46
1:F:176:MET:HG2	1:F:200:GLY:HA3	1.97	0.46
1:E:460:SER:O	1:E:463:GLN:N	2.49	0.46
1:C:378:VAL:HG12	1:C:379:THR:N	2.31	0.46
1:E:241:GLY:C	1:E:243:GLY:H	2.19	0.46
1:L:274:GLY:HA2	1:L:279:SER:HA	1.95	0.46
1:A:396:ARG:NH1	1:A:396:ARG:HG3	2.24	0.46
1:L:322:LEU:HD22	1:L:323:ILE:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:322:LEU:HD22	1:I:323:ILE:H	1.80	0.46
1:G:490:PHE:O	1:G:492:VAL:N	2.49	0.46
1:B:82:HIS:C	1:B:82:HIS:CD2	2.89	0.46
1:F:344:ILE:O	1:F:367:VAL:HA	2.15	0.46
1:A:374:ASN:C	1:A:376:GLY:N	2.69	0.46
1:I:368:ILE:HA	1:I:369:PRO:HD3	1.76	0.46
1:F:316:GLU:O	1:F:317:VAL:C	2.54	0.46
1:I:11:LYS:HA	1:I:14:GLU:HG3	1.97	0.46
1:K:202:PRO:HG2	1:K:205:GLN:HG3	1.98	0.46
1:K:336:ALA:HB3	1:K:337:PRO:CD	2.34	0.46
1:E:110:LEU:HD21	1:E:349:ASN:OD1	2.16	0.46
1:G:264:HIS:CE1	1:G:287:ASP:OD1	2.68	0.46
1:H:65:ILE:HD11	1:H:75:ILE:CD1	2.42	0.46
1:B:274:GLY:HA2	1:B:279:SER:HA	1.96	0.46
1:B:226:PHE:CD2	1:B:465:MET:CE	2.98	0.46
1:A:69:ASP:OD2	1:A:71:SER:CB	2.64	0.46
1:K:69:ASP:OD2	1:K:71:SER:CB	2.64	0.46
1:J:20:GLY:O	1:J:21:ALA:C	2.53	0.46
1:E:350:GLY:N	1:E:351:PRO:HD3	2.31	0.46
1:B:94:ARG:CZ	1:B:169:MET:HG3	2.45	0.46
1:H:99:VAL:HA	1:H:103:GLU:OE1	2.16	0.46
1:J:337:PRO:HG3	1:J:359:ILE:HD12	1.97	0.46
1:C:146:ARG:NH1	1:E:500:PHE:HB2	2.30	0.46
1:A:7:PRO:HD3	1:A:355:GLU:CG	2.45	0.46
1:E:250:GLN:HG2	1:E:330:GLN:HE21	1.80	0.46
1:K:6:ASP:HB2	1:K:353:THR:CG2	2.45	0.46
1:H:255:VAL:HG12	2:H:552:NDP:O2N	2.15	0.46
1:L:56:ASN:C	1:L:57:HIS:CD2	2.88	0.46
1:E:396:ARG:O	1:E:396:ARG:HG3	2.15	0.46
1:J:271:ILE:HD11	1:J:283:PRO:HG3	1.98	0.46
1:F:7:PRO:HG3	1:F:353:THR:CG2	2.41	0.46
1:A:212:ILE:HG12	1:A:213:SER:H	1.80	0.46
1:F:36:GLU:O	1:F:37:THR:C	2.54	0.46
1:I:222:GLY:HA3	1:I:373:LEU:CD1	2.45	0.46
1:A:208:ILE:HG22	1:A:211:ARG:HB2	1.98	0.46
1:E:132:ASN:HA	1:E:133:PRO:HD3	1.79	0.46
1:D:132:ASN:HA	1:D:133:PRO:HD3	1.80	0.46
1:G:47:SER:HB3	1:J:72:TRP:HB3	1.97	0.46
1:F:55:CYS:HB3	1:F:82:HIS:HA	1.98	0.46
1:J:53:LYS:N	1:J:54:PRO:CD	2.78	0.46
1:J:89:CYS:H	1:J:163:ASP:HA	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:149:THR:O	1:L:150:MET:C	2.54	0.46
1:L:316:GLU:O	1:L:317:VAL:C	2.54	0.46
1:H:295:LYS:HG3	1:H:296:LEU:HD22	1.97	0.46
1:G:316:GLU:O	1:G:317:VAL:C	2.54	0.46
1:J:417:LEU:HD12	1:J:417:LEU:HA	1.81	0.46
1:I:412:SER:CB	1:K:432:PRO:HA	2.45	0.46
1:A:368:ILE:HA	1:A:369:PRO:HD3	1.72	0.46
1:B:473:LEU:HD23	1:B:479:THR:OG1	2.16	0.46
1:C:433:THR:HG22	1:D:412:SER:CA	2.46	0.46
1:I:250:GLN:HG2	1:I:330:GLN:HE21	1.81	0.46
1:J:93:ILE:HD11	1:J:179:ILE:HD11	1.98	0.46
1:K:90:LYS:HB2	1:K:122:PHE:HD1	1.78	0.46
1:I:96:SER:O	1:I:130:LYS:HA	2.16	0.46
1:D:486:ILE:O	1:D:487:GLU:C	2.52	0.46
1:A:460:SER:O	1:A:463:GLN:N	2.49	0.46
1:K:486:ILE:O	1:K:487:GLU:C	2.54	0.46
1:I:93:ILE:HD11	1:I:179:ILE:HD11	1.98	0.46
1:C:250:GLN:HG2	1:C:330:GLN:HE21	1.81	0.46
1:H:331:LEU:O	1:H:353:THR:HG23	2.14	0.46
1:L:12:MET:H	1:L:14:GLU:CG	2.18	0.46
1:L:117:VAL:HG12	1:L:118:VAL:N	2.31	0.46
3:F:601:XEG:HAPA	3:F:601:XEG:CAZ	2.44	0.46
1:F:294:PHE:CE1	1:F:304:PHE:HD1	2.33	0.46
1:G:294:PHE:CE1	1:G:304:PHE:HD1	2.34	0.46
1:J:59:LEU:HD12	1:J:59:LEU:HA	1.67	0.46
1:F:152:LEU:HD13	1:F:152:LEU:HA	1.60	0.46
3:J:601:XEG:CAM	1:K:393:SER:OG	2.63	0.46
1:J:271:ILE:HG23	1:J:272:THR:N	2.31	0.46
1:B:271:ILE:HG23	1:B:272:THR:N	2.31	0.46
1:F:241:GLY:C	1:F:243:GLY:H	2.19	0.46
1:K:313:SER:HB2	1:K:315:LEU:CD2	2.46	0.46
1:D:136:TYR:HB2	1:D:141:LEU:CD2	2.41	0.46
1:H:132:ASN:HA	1:H:133:PRO:HD3	1.83	0.46
1:G:417:LEU:CD2	1:L:417:LEU:HD21	2.45	0.46
1:G:69:ASP:OD2	1:G:71:SER:CB	2.64	0.46
1:E:45:VAL:HG13	1:E:490:PHE:HE1	1.80	0.46
1:H:18:ASP:HA	1:H:21:ALA:CB	2.45	0.46
1:I:374:ASN:C	1:I:376:GLY:H	2.19	0.46
1:I:116:ALA:O	1:I:488:LYS:HD2	2.15	0.46
1:D:399:PHE:HE1	1:D:444:SER:HA	1.81	0.46
1:I:47:SER:O	1:I:50:ARG:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:399:PHE:HE1	1:E:444:SER:HA	1.81	0.46
1:L:330:GLN:O	1:L:331:LEU:HD12	2.16	0.46
1:H:79:ARG:HG2	1:H:127:ALA:CB	2.28	0.46
1:C:409:LEU:HD23	1:D:409:LEU:HD23	1.98	0.46
1:B:369:PRO:CD	1:B:477:LEU:HB2	2.43	0.46
1:J:336:ALA:HB3	1:J:337:PRO:CD	2.32	0.46
1:E:176:MET:HG3	1:E:198:VAL:CG2	2.46	0.46
1:A:166:ALA:HB1	1:A:167:PRO:HD2	1.98	0.46
1:G:455:TYR:CE1	1:G:459:ARG:HD3	2.46	0.46
1:A:116:ALA:O	1:A:488:LYS:HD2	2.16	0.46
1:G:470:LYS:HE3	1:G:470:LYS:HB2	1.72	0.46
1:G:121:PRO:O	1:G:122:PHE:HD2	1.99	0.46
1:H:118:VAL:O	1:H:118:VAL:HG23	2.14	0.46
1:C:473:LEU:H	1:C:473:LEU:HD12	1.81	0.46
1:C:211:ARG:O	1:C:211:ARG:HG2	2.16	0.46
1:I:468:ALA:HB1	1:I:480:ALA:HB1	1.96	0.46
1:B:490:PHE:O	1:B:491:ARG:C	2.55	0.46
1:J:8:ASN:O	1:J:11:LYS:O	2.33	0.46
1:L:171:THR:HA	1:L:175:GLU:OE2	2.16	0.46
1:F:117:VAL:HG12	1:F:118:VAL:HG13	1.97	0.46
1:E:116:ALA:O	1:E:488:LYS:HD2	2.15	0.46
1:D:281:TRP:O	1:D:282:ASN:CB	2.63	0.46
1:B:271:ILE:HG23	1:B:272:THR:HG23	1.98	0.46
1:H:322:LEU:HD22	1:H:323:ILE:H	1.80	0.46
1:L:217:ARG:CZ	1:L:450:HIS:CD2	2.99	0.46
1:K:501:THR:HA	1:L:501:THR:HG21	1.97	0.46
1:G:457:MET:O	1:G:460:SER:HB2	2.16	0.46
1:F:16:PHE:N	1:F:16:PHE:CD2	2.80	0.46
1:I:146:ARG:HG2	1:I:182:THR:OG1	2.16	0.46
1:J:159:GLY:O	1:J:162:VAL:HG12	2.16	0.46
1:C:159:GLY:O	1:C:162:VAL:HG12	2.16	0.46
1:I:316:GLU:O	1:I:317:VAL:C	2.54	0.46
1:D:451:SER:OG	1:E:400:LYS:HB3	2.16	0.46
1:A:470:LYS:HE3	1:A:470:LYS:HB2	1.77	0.46
1:B:176:MET:HG3	1:B:198:VAL:HG22	1.98	0.45
1:B:87:THR:CB	1:B:88:PRO:HD3	2.44	0.45
1:F:330:GLN:O	1:F:331:LEU:HD12	2.16	0.45
1:I:176:MET:HE3	1:I:179:ILE:HD12	1.97	0.45
1:E:464:ILE:O	1:E:468:ALA:CB	2.65	0.45
1:K:59:LEU:HD12	1:K:59:LEU:HA	1.60	0.45
1:C:11:LYS:HA	1:C:14:GLU:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:236:LEU:HD12	1:L:238:MET:HE2	1.97	0.45
1:B:59:LEU:CD2	1:B:61:LEU:HD22	2.46	0.45
1:G:15:GLY:O	1:G:16:PHE:C	2.54	0.45
1:B:271:ILE:HD11	1:B:283:PRO:HG3	1.97	0.45
1:H:217:ARG:CZ	1:H:450:HIS:HD2	2.29	0.45
1:F:274:GLY:HA2	1:F:279:SER:HA	1.97	0.45
1:B:414:GLN:HB2	1:B:429:PRO:CG	2.46	0.45
1:B:108:ALA:HB2	1:B:126:LYS:HB2	1.98	0.45
1:B:348:ALA:HB3	1:B:351:PRO:HG3	1.97	0.45
1:K:457:MET:O	1:K:460:SER:HB2	2.16	0.45
1:J:242:PHE:C	1:J:244:ASP:N	2.70	0.45
1:B:15:GLY:O	1:B:16:PHE:C	2.55	0.45
1:J:395:GLY:O	1:J:397:LEU:N	2.50	0.45
1:H:82:HIS:ND1	1:H:109:SER:HA	2.31	0.45
1:G:241:GLY:C	1:G:243:GLY:H	2.19	0.45
1:F:23:ILE:CG2	1:F:471:TYR:HD1	2.29	0.45
1:C:498:VAL:HG11	1:F:72:TRP:HZ2	1.81	0.45
1:K:316:GLU:O	1:K:317:VAL:C	2.54	0.45
1:K:429:PRO:C	1:K:431:VAL:N	2.69	0.45
1:A:348:ALA:HB3	1:A:351:PRO:HG3	1.96	0.45
1:E:176:MET:HG3	1:E:198:VAL:HG22	1.98	0.45
1:J:96:SER:C	1:J:98:ASP:N	2.70	0.45
1:K:86:ARG:O	1:K:87:THR:O	2.35	0.45
1:H:294:PHE:CE1	1:H:304:PHE:HD1	2.34	0.45
1:A:385:TRP:HZ3	1:F:391:HIS:HB3	1.80	0.45
1:G:11:LYS:HA	1:G:14:GLU:HG3	1.98	0.45
1:F:86:ARG:HG2	1:F:121:PRO:CA	2.46	0.45
1:H:15:GLY:O	1:H:16:PHE:C	2.54	0.45
1:C:241:GLY:C	1:C:243:GLY:H	2.20	0.45
1:G:402:GLU:C	1:G:404:ASP:N	2.67	0.45
1:G:367:VAL:O	1:G:477:LEU:HD23	2.16	0.45
1:F:374:ASN:C	1:F:376:GLY:N	2.69	0.45
1:F:15:GLY:O	1:F:16:PHE:C	2.54	0.45
1:F:16:PHE:HE2	1:F:354:PRO:HG3	1.80	0.45
1:D:348:ALA:HB3	1:D:351:PRO:HG3	1.97	0.45
1:I:344:ILE:O	1:I:367:VAL:HA	2.17	0.45
1:F:162:VAL:O	1:F:163:ASP:HB2	2.16	0.45
1:K:378:VAL:HG12	1:K:379:THR:N	2.31	0.45
1:L:295:LYS:HG3	1:L:296:LEU:HD22	1.98	0.45
1:C:155:LYS:HE3	1:F:156:GLY:O	2.15	0.45
1:H:53:LYS:HB3	1:H:54:PRO:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:464:ILE:O	1:D:468:ALA:HB3	2.16	0.45
1:G:411:MET:HA	1:G:414:GLN:HB3	1.99	0.45
1:J:166:ALA:C	1:J:176:MET:HE1	2.37	0.45
1:B:72:TRP:HZ2	1:E:498:VAL:HG21	1.81	0.45
1:A:176:MET:HG3	1:A:198:VAL:CG2	2.47	0.45
1:K:117:VAL:HG12	1:K:118:VAL:HG13	1.97	0.45
1:K:449:VAL:O	1:K:450:HIS:C	2.55	0.45
1:H:288:PRO:HA	1:H:291:LEU:HD22	1.97	0.45
1:K:11:LYS:HA	1:K:14:GLU:HG3	1.97	0.45
1:L:45:VAL:HG13	1:L:490:PHE:CE1	2.51	0.45
1:C:379:THR:O	1:C:382:TYR:HB3	2.16	0.45
1:F:86:ARG:HH11	1:F:492:VAL:HG11	1.81	0.45
1:J:378:VAL:HG12	1:J:379:THR:N	2.30	0.45
1:I:236:LEU:HD12	1:I:238:MET:HE2	1.97	0.45
1:D:294:PHE:CE1	1:D:304:PHE:HD1	2.34	0.45
1:B:294:PHE:CE1	1:B:304:PHE:HD1	2.34	0.45
1:J:271:ILE:HG23	1:J:272:THR:HG23	1.98	0.45
1:A:271:ILE:HD11	1:A:283:PRO:HG3	1.98	0.45
1:A:38:GLU:O	1:A:40:GLN:N	2.49	0.45
1:G:396:ARG:CG	1:G:396:ARG:NH1	2.79	0.45
1:J:420:LYS:O	1:J:421:PHE:HB2	2.16	0.45
1:E:322:LEU:HD22	1:E:323:ILE:H	1.81	0.45
1:I:132:ASN:HA	1:I:133:PRO:HD3	1.76	0.45
1:E:69:ASP:OD2	1:E:71:SER:CB	2.63	0.45
1:I:162:VAL:O	1:I:163:ASP:HB2	2.17	0.45
1:C:15:GLY:O	1:C:16:PHE:C	2.55	0.45
1:C:344:ILE:O	1:C:367:VAL:HA	2.17	0.45
1:C:162:VAL:O	1:C:163:ASP:HB2	2.16	0.45
1:H:68:ASP:OD2	1:H:140:GLU:HG3	2.16	0.45
1:H:412:SER:HB3	1:L:432:PRO:CA	2.40	0.45
1:H:412:SER:HA	1:L:433:THR:HG22	1.98	0.45
1:E:86:ARG:O	1:E:87:THR:O	2.35	0.45
1:B:93:ILE:HD11	1:B:179:ILE:HD11	1.97	0.45
1:J:99:VAL:HA	1:J:103:GLU:OE1	2.16	0.45
1:G:78:TYR:CD2	1:G:101:VAL:HG22	2.46	0.45
1:D:93:ILE:HD11	1:D:179:ILE:HD11	1.98	0.45
1:G:121:PRO:O	1:G:122:PHE:CD2	2.70	0.45
1:E:337:PRO:HG3	1:E:359:ILE:HD12	1.97	0.45
1:L:11:LYS:HA	1:L:14:GLU:HG3	1.98	0.45
3:F:601:XEG:HBE	3:F:601:XEG:HAJ	1.76	0.45
1:E:65:ILE:HD11	1:E:75:ILE:CD1	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:GLU:O	1:A:144:ILE:HG13	2.17	0.45
1:B:490:PHE:C	1:B:490:PHE:CD2	2.89	0.45
1:F:383:PHE:HA	1:F:386:LEU:HD12	1.98	0.45
1:G:234:SER:O	1:G:236:LEU:N	2.50	0.45
1:B:288:PRO:HA	1:B:291:LEU:HD22	1.98	0.45
1:H:271:ILE:HG23	1:H:272:THR:N	2.31	0.45
1:J:211:ARG:HG2	1:J:211:ARG:O	2.15	0.45
1:G:313:SER:HB2	1:G:315:LEU:CD2	2.47	0.45
1:E:217:ARG:CZ	1:E:450:HIS:HD2	2.30	0.45
1:C:36:GLU:O	1:C:37:THR:C	2.54	0.45
1:A:322:LEU:HD22	1:A:323:ILE:H	1.81	0.45
1:D:85:HIS:HD2	1:D:492:VAL:HG11	1.80	0.45
1:E:132:ASN:OD1	1:E:134:LYS:CG	2.62	0.45
1:D:132:ASN:OD1	1:D:134:LYS:CG	2.63	0.45
1:H:61:LEU:O	1:H:62:SER:CB	2.63	0.45
1:B:142:GLU:OE2	1:F:500:PHE:CD2	2.70	0.45
1:H:242:PHE:C	1:H:244:ASP:N	2.70	0.45
1:E:89:CYS:H	1:E:163:ASP:HA	1.81	0.45
1:H:53:LYS:N	1:H:54:PRO:CD	2.79	0.45
1:I:295:LYS:HG3	1:I:296:LEU:HD22	1.98	0.45
1:I:413:VAL:HG12	1:I:414:GLN:N	2.30	0.45
1:K:409:LEU:C	1:K:411:MET:H	2.18	0.45
1:H:409:LEU:CD1	1:L:436:PHE:CZ	3.00	0.45
1:A:117:VAL:HG12	1:A:118:VAL:CG1	2.47	0.45
1:A:477:LEU:HD22	1:A:477:LEU:H	1.80	0.45
1:B:382:TYR:O	1:B:385:TRP:HB3	2.16	0.45
1:H:370:ASP:OD1	1:H:371:LEU:N	2.48	0.45
1:L:336:ALA:HB3	1:L:337:PRO:CD	2.33	0.45
1:L:208:ILE:CG2	1:L:211:ARG:HB2	2.47	0.45
1:L:294:PHE:CE1	1:L:304:PHE:HD1	2.34	0.45
1:G:209:HIS:HE1	3:H:601:XEG:HAL	1.82	0.45
1:H:282:ASN:O	1:H:284:ASP:N	2.45	0.45
1:H:8:ASN:HB3	1:H:9:PHE:CE1	2.51	0.45
1:E:38:GLU:O	1:E:40:GLN:N	2.49	0.45
1:A:222:GLY:HA3	1:A:373:LEU:CD1	2.47	0.45
1:K:38:GLU:HG2	1:K:39:GLU:N	2.31	0.45
1:G:344:ILE:O	1:G:367:VAL:HA	2.16	0.45
1:J:433:THR:HG23	1:K:412:SER:OG	2.17	0.45
1:D:409:LEU:HD23	1:E:409:LEU:CD2	2.46	0.45
1:I:250:GLN:NE2	2:I:552:NDP:H2A	2.31	0.45
1:G:99:VAL:HA	1:G:103:GLU:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:87:THR:CB	1:K:88:PRO:CD	2.93	0.45
1:I:198:VAL:O	1:I:201:LYS:HE3	2.17	0.45
1:E:468:ALA:HB1	1:E:480:ALA:HB1	1.99	0.45
1:C:383:PHE:HA	1:C:386:LEU:HD12	1.98	0.45
1:L:468:ALA:HB1	1:L:480:ALA:HB1	1.99	0.45
1:L:493:TYR:O	1:L:495:GLU:N	2.49	0.45
1:D:303:GLY:O	1:D:304:PHE:HB2	2.17	0.45
1:D:59:LEU:CD2	1:D:61:LEU:HD22	2.46	0.45
1:K:220:PHE:O	1:K:222:GLY:N	2.50	0.45
1:C:396:ARG:HG3	1:C:396:ARG:NH1	2.29	0.45
1:A:82:HIS:CD2	1:A:82:HIS:C	2.88	0.45
1:I:367:VAL:O	1:I:477:LEU:HD23	2.17	0.45
1:B:316:GLU:O	1:B:317:VAL:C	2.55	0.45
1:K:53:LYS:N	1:K:54:PRO:CD	2.80	0.45
1:A:344:ILE:O	1:A:367:VAL:HA	2.16	0.45
1:D:413:VAL:HG12	1:D:429:PRO:CG	2.45	0.45
1:E:432:PRO:O	1:E:433:THR:O	2.34	0.45
1:A:429:PRO:C	1:A:431:VAL:N	2.68	0.45
1:I:337:PRO:HG3	1:I:359:ILE:HD12	1.98	0.45
1:F:337:PRO:HG3	1:F:359:ILE:HD12	1.97	0.45
1:K:176:MET:HG3	1:K:198:VAL:HG22	1.98	0.45
1:D:176:MET:HE3	1:D:179:ILE:HD12	1.97	0.45
1:K:337:PRO:HG3	1:K:359:ILE:HD12	1.99	0.45
1:H:303:GLY:O	1:H:304:PHE:HB2	2.17	0.45
1:G:211:ARG:HG2	1:G:211:ARG:O	2.17	0.45
1:C:28:LEU:CD1	1:C:28:LEU:H	2.13	0.45
1:C:176:MET:HE3	1:C:179:ILE:HD12	1.99	0.45
1:G:12:MET:HG2	1:G:14:GLU:OE2	2.17	0.45
1:L:176:MET:HG3	1:L:198:VAL:CG2	2.46	0.45
1:L:288:PRO:HA	1:L:291:LEU:HD22	1.98	0.45
1:D:211:ARG:O	1:D:214:ALA:HB3	2.17	0.45
1:L:152:LEU:HA	1:L:152:LEU:HD13	1.68	0.45
1:I:313:SER:HB2	1:I:315:LEU:CD2	2.47	0.45
1:A:213:SER:HB2	1:A:262:TYR:CE2	2.52	0.45
1:F:372:TYR:CZ	1:F:457:MET:HE2	2.52	0.45
1:B:399:PHE:HB2	1:F:455:TYR:HE2	1.82	0.45
1:A:241:GLY:C	1:A:243:GLY:H	2.20	0.45
1:F:142:GLU:HB2	1:F:178:TRP:CZ2	2.51	0.45
1:J:316:GLU:O	1:J:317:VAL:C	2.55	0.45
1:D:68:ASP:OD2	1:D:140:GLU:HG3	2.17	0.45
1:E:470:LYS:HB2	1:E:470:LYS:HE3	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:416:SER:HB3	1:K:429:PRO:HA	1.99	0.45
1:A:78:TYR:CD2	1:A:101:VAL:HG22	2.50	0.45
1:B:72:TRP:CZ2	1:E:498:VAL:HG21	2.51	0.45
1:D:485:ALA:O	1:D:486:ILE:C	2.55	0.45
1:I:199:THR:HA	1:I:384:GLU:OE1	2.16	0.45
1:F:234:SER:O	1:F:236:LEU:N	2.49	0.45
1:G:288:PRO:HA	1:G:291:LEU:HD22	1.99	0.45
1:D:366:MET:CB	1:D:475:LEU:HD13	2.46	0.45
1:J:16:PHE:CD2	1:J:16:PHE:N	2.85	0.45
1:G:271:ILE:HG23	1:G:272:THR:N	2.32	0.45
1:L:241:GLY:C	1:L:243:GLY:H	2.20	0.45
1:H:432:PRO:O	1:H:433:THR:O	2.35	0.45
1:E:212:ILE:H	1:E:212:ILE:CD1	2.16	0.45
1:A:214:ALA:CB	1:A:380:VAL:HG21	2.44	0.45
1:K:322:LEU:HD22	1:K:323:ILE:H	1.81	0.45
1:B:399:PHE:HE1	1:B:444:SER:HA	1.81	0.45
1:K:61:LEU:O	1:K:62:SER:HB2	2.17	0.45
1:I:53:LYS:N	1:I:54:PRO:CD	2.79	0.45
1:A:316:GLU:O	1:A:317:VAL:C	2.55	0.45
1:F:104:VAL:HG23	1:F:105:LYS:N	2.31	0.45
1:E:303:GLY:O	1:E:304:PHE:HB2	2.17	0.45
1:G:431:VAL:HA	1:G:432:PRO:HD2	1.73	0.45
1:G:429:PRO:HA	1:L:416:SER:HB3	1.97	0.45
1:A:370:ASP:OD1	1:A:371:LEU:N	2.47	0.45
1:L:250:GLN:HG2	1:L:330:GLN:HE21	1.82	0.45
1:H:464:ILE:O	1:H:468:ALA:HB3	2.17	0.45
1:E:52:ILE:CG1	1:E:493:TYR:HE2	2.26	0.45
1:J:165:PRO:O	1:J:198:VAL:HG23	2.16	0.45
1:A:166:ALA:HA	1:A:176:MET:HE2	1.99	0.45
1:F:198:VAL:O	1:F:201:LYS:HE3	2.16	0.45
1:E:23:ILE:HG22	1:E:471:TYR:HD1	1.82	0.45
1:F:303:GLY:O	1:F:304:PHE:HB2	2.17	0.45
1:F:444:SER:OG	1:F:446:LYS:N	2.50	0.45
1:K:288:PRO:HA	1:K:291:LEU:HD22	1.99	0.45
1:A:149:THR:O	1:A:150:MET:C	2.55	0.45
1:G:274:GLY:HA3	1:G:314:ILE:CD1	2.47	0.45
1:L:396:ARG:CG	1:L:396:ARG:NH1	2.76	0.45
1:J:421:PHE:CZ	1:J:423:LYS:HG3	2.52	0.45
1:K:36:GLU:O	1:K:37:THR:C	2.55	0.45
1:D:149:THR:O	1:D:150:MET:C	2.55	0.45
1:A:89:CYS:H	1:A:163:ASP:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:PHE:CD2	1:B:16:PHE:N	2.85	0.45
1:D:69:ASP:OD2	1:D:71:SER:CB	2.65	0.45
1:G:142:GLU:HB2	1:G:178:TRP:CZ2	2.52	0.45
1:I:45:VAL:HG13	1:I:490:PHE:CE1	2.51	0.45
1:H:159:GLY:O	1:H:162:VAL:HG12	2.17	0.45
1:E:18:ASP:HA	1:E:21:ALA:HB3	1.97	0.45
1:A:117:VAL:HG12	1:A:118:VAL:N	2.32	0.45
1:I:330:GLN:O	1:I:331:LEU:HD12	2.17	0.45
1:I:117:VAL:HG21	1:I:371:LEU:HG	1.99	0.45
1:G:96:SER:C	1:G:98:ASP:N	2.70	0.45
1:G:86:ARG:HG2	1:G:121:PRO:CA	2.47	0.45
1:J:303:GLY:O	1:J:304:PHE:HB2	2.17	0.45
1:C:468:ALA:HB1	1:C:480:ALA:HB1	1.99	0.45
1:C:444:SER:OG	1:C:446:LYS:N	2.50	0.45
1:C:264:HIS:HE1	1:C:287:ASP:OD1	1.99	0.45
1:C:303:GLY:O	1:C:304:PHE:HB2	2.17	0.45
1:F:117:VAL:HG12	1:F:118:VAL:N	2.32	0.45
1:I:288:PRO:HA	1:I:291:LEU:HD22	1.99	0.45
1:H:271:ILE:HG23	1:H:272:THR:HG23	1.99	0.45
1:K:315:LEU:N	1:K:315:LEU:HD22	2.32	0.45
1:I:315:LEU:HD22	1:I:315:LEU:N	2.32	0.45
1:F:256:GLY:HA2	1:F:259:SER:OG	2.17	0.45
1:B:149:THR:O	1:B:150:MET:C	2.55	0.45
1:E:234:SER:C	1:E:236:LEU:N	2.69	0.45
1:L:242:PHE:C	1:L:244:ASP:N	2.68	0.45
1:D:82:HIS:HD2	1:D:83:SER:HB2	1.81	0.45
1:E:171:THR:HA	1:E:175:GLU:OE2	2.16	0.45
1:B:82:HIS:HD2	1:B:83:SER:HB2	1.81	0.45
1:I:485:ALA:O	1:I:486:ILE:C	2.56	0.45
1:H:417:LEU:HA	1:H:417:LEU:HD12	1.83	0.45
1:D:382:TYR:O	1:D:385:TRP:HB3	2.18	0.44
1:E:429:PRO:C	1:E:431:VAL:N	2.70	0.44
1:J:202:PRO:HG2	1:J:205:GLN:HG3	1.97	0.44
1:E:93:ILE:HD11	1:E:179:ILE:HD11	1.99	0.44
1:A:176:MET:HG3	1:A:198:VAL:HG22	1.98	0.44
1:B:90:LYS:HG3	1:B:122:PHE:CD1	2.52	0.44
1:K:211:ARG:HA	1:K:380:VAL:HG11	1.98	0.44
1:G:386:LEU:HD13	1:L:392:VAL:HG11	1.99	0.44
3:K:601:XEG:CAZ	3:K:601:XEG:HAPA	2.47	0.44
1:G:61:LEU:HD13	1:G:61:LEU:HA	1.68	0.44
1:L:382:TYR:C	1:L:382:TYR:HD2	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:THR:O	1:B:500:PHE:CD2	2.70	0.44
1:F:288:PRO:HA	1:F:291:LEU:HD22	1.98	0.44
1:H:205:GLN:CD	1:L:496:ALA:HB2	2.38	0.44
1:K:294:PHE:CE1	1:K:304:PHE:HD1	2.34	0.44
1:C:152:LEU:HA	1:C:152:LEU:HD13	1.59	0.44
1:B:236:LEU:HD12	1:B:238:MET:HE2	1.98	0.44
1:D:456:THR:HG23	1:E:396:ARG:NH2	2.31	0.44
1:K:35:ARG:C	1:K:37:THR:H	2.21	0.44
1:K:396:ARG:CG	1:K:396:ARG:NH1	2.80	0.44
1:G:136:TYR:HB2	1:G:141:LEU:CD2	2.44	0.44
1:G:491:ARG:CZ	1:G:491:ARG:HB2	2.47	0.44
1:C:242:PHE:C	1:C:244:ASP:N	2.68	0.44
1:D:89:CYS:H	1:D:163:ASP:HA	1.83	0.44
1:G:477:LEU:H	1:G:477:LEU:HD22	1.82	0.44
1:H:89:CYS:H	1:H:163:ASP:HA	1.81	0.44
1:C:417:LEU:HD21	1:E:417:LEU:HD21	1.99	0.44
1:F:486:ILE:O	1:F:487:GLU:C	2.56	0.44
1:I:203:ILE:HG22	1:I:203:ILE:O	2.17	0.44
1:L:203:ILE:HG22	1:L:203:ILE:O	2.17	0.44
1:E:489:VAL:O	1:E:492:VAL:HB	2.17	0.44
1:J:176:MET:HG3	1:J:198:VAL:HG21	1.99	0.44
1:E:78:TYR:CD2	1:E:101:VAL:HG22	2.51	0.44
1:A:15:GLY:O	1:A:16:PHE:C	2.55	0.44
1:D:265:ARG:O	1:D:266:PHE:CB	2.58	0.44
1:D:59:LEU:HB2	1:D:157:PHE:CE2	2.52	0.44
1:B:303:GLY:O	1:B:304:PHE:HB2	2.17	0.44
1:B:366:MET:CB	1:B:475:LEU:HD13	2.44	0.44
1:B:61:LEU:O	1:B:62:SER:CB	2.65	0.44
1:K:399:PHE:HE1	1:K:444:SER:HA	1.82	0.44
1:C:271:ILE:HG23	1:C:272:THR:N	2.33	0.44
1:H:431:VAL:HA	1:H:432:PRO:HD2	1.75	0.44
1:L:315:LEU:HD22	1:L:315:LEU:N	2.32	0.44
1:I:421:PHE:CE1	1:I:425:GLY:N	2.85	0.44
1:H:402:GLU:O	1:H:404:ASP:N	2.45	0.44
1:E:236:LEU:HD12	1:E:238:MET:HE2	1.98	0.44
1:D:16:PHE:CD2	1:D:16:PHE:N	2.86	0.44
1:E:175:GLU:O	1:E:178:TRP:HB2	2.17	0.44
1:C:16:PHE:CE2	1:C:354:PRO:HG3	2.52	0.44
1:D:203:ILE:HA	1:D:207:GLY:H	1.82	0.44
1:F:18:ASP:HA	1:F:21:ALA:CB	2.48	0.44
1:B:6:ASP:N	1:B:7:PRO:CD	2.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:LYS:HB3	1:C:54:PRO:HD3	1.99	0.44
1:C:60:SER:HB2	1:F:58:VAL:HG13	1.98	0.44
1:D:295:LYS:HG3	1:D:296:LEU:HD22	1.98	0.44
1:A:490:PHE:C	1:A:490:PHE:CD2	2.91	0.44
1:B:477:LEU:O	1:B:478:ARG:C	2.55	0.44
1:H:96:SER:C	1:H:98:ASP:N	2.70	0.44
1:I:6:ASP:O	1:I:8:ASN:N	2.50	0.44
1:I:87:THR:CB	1:I:88:PRO:CD	2.89	0.44
1:I:9:PHE:HB3	1:I:329:LYS:HZ2	1.80	0.44
1:E:202:PRO:HG2	1:E:205:GLN:HG2	1.99	0.44
1:A:93:ILE:HD11	1:A:179:ILE:HD11	2.00	0.44
1:D:116:ALA:O	1:D:488:LYS:HD2	2.17	0.44
1:G:117:VAL:HG12	1:G:118:VAL:CG1	2.48	0.44
1:A:158:ILE:HG23	1:A:158:ILE:O	2.18	0.44
1:J:171:THR:HA	1:J:175:GLU:OE2	2.17	0.44
1:F:86:ARG:O	1:F:87:THR:O	2.35	0.44
1:L:211:ARG:HA	1:L:380:VAL:HG11	2.00	0.44
1:D:271:ILE:CD1	1:D:283:PRO:HG3	2.48	0.44
1:D:274:GLY:HA3	1:D:314:ILE:CD1	2.47	0.44
1:K:271:ILE:HG23	1:K:272:THR:N	2.32	0.44
1:L:271:ILE:HG23	1:L:272:THR:N	2.33	0.44
1:I:271:ILE:HD11	1:I:283:PRO:HG3	1.98	0.44
1:A:36:GLU:O	1:A:37:THR:C	2.56	0.44
1:G:36:GLU:O	1:G:37:THR:C	2.55	0.44
1:H:36:GLU:O	1:H:37:THR:C	2.54	0.44
1:C:421:PHE:CZ	1:C:423:LYS:HG3	2.53	0.44
1:L:18:ASP:HA	1:L:21:ALA:CB	2.48	0.44
1:L:18:ASP:HA	1:L:21:ALA:HB3	2.00	0.44
1:C:18:ASP:HA	1:C:21:ALA:HB3	2.00	0.44
1:L:68:ASP:OD2	1:L:140:GLU:HG3	2.18	0.44
1:D:316:GLU:O	1:D:317:VAL:C	2.55	0.44
1:E:477:LEU:HD22	1:E:477:LEU:H	1.82	0.44
1:H:473:LEU:H	1:H:473:LEU:HD12	1.81	0.44
1:K:93:ILE:CG2	1:K:127:ALA:HB3	2.40	0.44
1:D:166:ALA:HB1	1:D:167:PRO:HD2	1.99	0.44
1:L:9:PHE:HB3	1:L:329:LYS:HZ2	1.83	0.44
1:F:464:ILE:O	1:F:468:ALA:HB3	2.17	0.44
1:H:52:ILE:HG12	1:H:493:TYR:HE2	1.83	0.44
1:F:385:TRP:CZ2	1:F:389:LEU:HD11	2.52	0.44
1:I:303:GLY:O	1:I:304:PHE:HB2	2.17	0.44
1:L:303:GLY:O	1:L:304:PHE:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:399:PHE:HB2	1:H:455:TYR:HE2	1.82	0.44
1:E:271:ILE:HD11	1:E:283:PRO:HG3	2.00	0.44
1:E:274:GLY:HA3	1:E:314:ILE:CD1	2.48	0.44
1:D:492:VAL:CG1	1:D:493:TYR:N	2.80	0.44
1:K:212:ILE:CD1	1:K:212:ILE:H	2.20	0.44
1:F:313:SER:HB2	1:F:315:LEU:CD2	2.48	0.44
1:F:421:PHE:CZ	1:F:423:LYS:HG3	2.52	0.44
1:F:421:PHE:CE1	1:F:425:GLY:N	2.86	0.44
1:F:370:ASP:OD1	1:F:371:LEU:N	2.50	0.44
1:K:9:PHE:HA	1:K:329:LYS:HD3	1.98	0.44
1:L:374:ASN:C	1:L:376:GLY:N	2.71	0.44
1:I:175:GLU:HA	1:I:178:TRP:CE3	2.52	0.44
1:C:18:ASP:HA	1:C:21:ALA:CB	2.47	0.44
1:F:137:THR:HG23	1:F:140:GLU:CD	2.37	0.44
1:E:53:LYS:N	1:E:54:PRO:CD	2.81	0.44
1:E:288:PRO:HA	1:E:291:LEU:HD22	1.99	0.44
1:H:416:SER:OG	1:L:431:VAL:HG13	2.18	0.44
1:E:486:ILE:O	1:E:487:GLU:C	2.56	0.44
1:E:52:ILE:HD13	1:E:489:VAL:HG12	1.99	0.44
3:G:601:XEG:CAZ	3:G:601:XEG:HAPA	2.47	0.44
1:B:382:TYR:CE2	1:B:386:LEU:CD1	2.92	0.44
1:F:250:GLN:HG2	1:F:330:GLN:HE21	1.82	0.44
1:C:28:LEU:HD23	1:C:490:PHE:CG	2.53	0.44
1:C:201:LYS:HA	1:C:202:PRO:HD2	1.80	0.44
1:B:499:THR:HG21	1:E:65:ILE:HG23	2.00	0.44
1:B:498:VAL:CG1	1:E:72:TRP:HZ2	2.30	0.44
1:F:12:MET:HG2	1:F:14:GLU:OE2	2.17	0.44
1:H:492:VAL:CG2	1:H:493:TYR:N	2.68	0.44
1:F:90:LYS:HG3	1:F:122:PHE:CD1	2.52	0.44
1:H:214:ALA:HB1	1:H:380:VAL:CG2	2.40	0.44
1:B:152:LEU:HA	1:B:152:LEU:HD13	1.54	0.44
1:A:396:ARG:NH1	1:A:396:ARG:CG	2.78	0.44
1:D:141:LEU:HA	1:D:141:LEU:HD22	1.66	0.44
1:H:69:ASP:OD2	1:H:71:SER:CB	2.66	0.44
1:B:18:ASP:HA	1:B:21:ALA:HB3	1.98	0.44
1:K:18:ASP:HA	1:K:21:ALA:HB3	2.00	0.44
1:E:344:ILE:O	1:E:367:VAL:HA	2.16	0.44
1:I:409:LEU:CD2	1:K:409:LEU:HD23	2.42	0.44
1:A:303:GLY:O	1:A:304:PHE:HB2	2.17	0.44
1:D:117:VAL:HG12	1:D:118:VAL:HG13	2.00	0.44
1:C:432:PRO:HA	1:D:412:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:VAL:HG11	1:F:413:VAL:CG2	2.48	0.44
1:I:16:PHE:N	1:I:16:PHE:CD2	2.85	0.44
1:I:6:ASP:N	1:I:354:PRO:HD2	2.32	0.44
1:B:66:ARG:HD2	1:E:500:PHE:HZ	1.83	0.44
3:A:601:XEG:HAPA	3:A:601:XEG:CAZ	2.47	0.44
1:H:275:GLU:OE2	1:H:301:ILE:HG13	2.16	0.44
1:L:96:SER:O	1:L:130:LYS:HA	2.17	0.44
1:L:117:VAL:HG12	1:L:118:VAL:CG1	2.48	0.44
1:A:52:ILE:HD13	1:A:489:VAL:CG1	2.47	0.44
1:G:155:LYS:HE2	1:J:57:HIS:ND1	2.33	0.44
1:G:236:LEU:HD12	1:G:238:MET:HE2	1.98	0.44
1:D:271:ILE:HG23	1:D:272:THR:N	2.32	0.44
1:E:274:GLY:HA2	1:E:279:SER:HA	1.98	0.44
1:A:180:ALA:O	1:A:181:ASP:C	2.56	0.44
1:B:212:ILE:HG12	1:B:213:SER:H	1.82	0.44
1:G:315:LEU:N	1:G:315:LEU:HD22	2.32	0.44
1:E:36:GLU:O	1:E:37:THR:C	2.55	0.44
1:J:245:LYS:HE3	1:J:245:LYS:HB2	1.87	0.44
1:C:313:SER:HB2	1:C:315:LEU:CD2	2.47	0.44
1:I:108:ALA:HB2	1:I:126:LYS:HB2	2.00	0.44
1:C:95:TYR:HB3	1:C:133:PRO:HG3	1.99	0.44
1:A:236:LEU:HD22	1:A:342:LYS:HD2	1.99	0.44
1:E:234:SER:O	1:E:236:LEU:N	2.51	0.44
1:I:18:ASP:HA	1:I:21:ALA:CB	2.47	0.44
1:C:171:THR:HA	1:C:175:GLU:OE2	2.18	0.44
1:H:316:GLU:O	1:H:317:VAL:C	2.55	0.44
1:G:18:ASP:HA	1:G:21:ALA:HB3	1.99	0.44
1:E:316:GLU:O	1:E:317:VAL:C	2.56	0.44
1:A:53:LYS:N	1:A:54:PRO:CD	2.81	0.44
1:E:117:VAL:HG12	1:E:118:VAL:HG13	1.99	0.44
1:D:470:LYS:C	1:D:471:TYR:HD2	2.21	0.44
1:D:473:LEU:N	1:D:473:LEU:HD12	2.33	0.44
1:I:413:VAL:CG2	1:K:413:VAL:HG11	2.47	0.44
1:I:436:PHE:CZ	1:J:409:LEU:CD1	3.01	0.44
1:L:409:LEU:O	1:L:411:MET:N	2.45	0.44
1:C:413:VAL:HG12	1:C:414:GLN:N	2.33	0.44
1:A:7:PRO:HB2	1:A:8:ASN:H	1.66	0.44
1:B:85:HIS:CD2	1:B:492:VAL:HG21	2.52	0.44
1:K:121:PRO:HD2	1:K:382:TYR:CE1	2.53	0.44
1:H:477:LEU:O	1:H:478:ARG:C	2.55	0.44
1:J:294:PHE:CE1	1:J:304:PHE:HD1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:349:ASN:HB2	2:E:552:NDP:O2D	2.18	0.44
1:G:250:GLN:HG2	1:G:330:GLN:HE21	1.81	0.44
1:L:490:PHE:CD2	1:L:490:PHE:C	2.91	0.44
1:H:52:ILE:HG12	1:H:493:TYR:CE2	2.52	0.44
1:F:382:TYR:CE2	1:F:386:LEU:CD1	2.93	0.44
1:L:199:THR:HA	1:L:384:GLU:OE1	2.17	0.44
1:B:59:LEU:HB2	1:B:157:PHE:CE2	2.53	0.44
1:H:314:ILE:HG12	1:H:314:ILE:H	1.48	0.44
1:A:274:GLY:HA3	1:A:314:ILE:CD1	2.48	0.44
1:L:271:ILE:HD11	1:L:283:PRO:HG3	1.99	0.44
1:C:274:GLY:HA3	1:C:314:ILE:CD1	2.48	0.44
1:B:423:LYS:O	1:B:424:HIS:C	2.56	0.44
1:H:322:LEU:HD13	1:H:322:LEU:C	2.38	0.44
1:F:38:GLU:C	1:F:40:GLN:N	2.71	0.44
1:D:331:LEU:O	1:D:353:THR:HG23	2.17	0.44
1:A:315:LEU:N	1:A:315:LEU:HD22	2.32	0.44
1:C:421:PHE:CE1	1:C:425:GLY:N	2.85	0.44
1:L:16:PHE:CD2	1:L:16:PHE:N	2.86	0.44
1:F:402:GLU:C	1:F:404:ASP:N	2.71	0.44
1:E:142:GLU:HA	1:E:178:TRP:CZ3	2.53	0.44
1:I:369:PRO:HD3	1:I:477:LEU:HB2	2.00	0.44
1:E:203:ILE:H	1:E:203:ILE:HD12	1.83	0.44
1:K:378:VAL:O	1:K:381:SER:HB2	2.17	0.44
1:I:68:ASP:OD2	1:I:140:GLU:HG3	2.18	0.44
1:J:104:VAL:HG23	1:J:105:LYS:N	2.32	0.44
1:C:470:LYS:HE3	1:C:470:LYS:HB2	1.75	0.44
1:A:265:ARG:O	1:A:266:PHE:CB	2.55	0.44
1:H:470:LYS:HB2	1:H:470:LYS:HE3	1.80	0.44
1:C:391:HIS:HB3	1:E:385:TRP:HZ3	1.82	0.44
1:A:413:VAL:CG1	1:A:429:PRO:HG3	2.43	0.44
1:I:117:VAL:HG12	1:I:118:VAL:N	2.32	0.44
1:B:498:VAL:HG23	1:B:500:PHE:HD2	1.83	0.44
1:C:117:VAL:HG12	1:C:118:VAL:CG1	2.48	0.44
1:A:12:MET:HG2	1:A:14:GLU:OE2	2.18	0.44
1:C:275:GLU:OE2	1:C:301:ILE:HG13	2.18	0.44
1:I:152:LEU:HD13	1:I:152:LEU:HA	1.64	0.44
1:B:282:ASN:O	1:B:284:ASP:N	2.48	0.44
1:B:274:GLY:HA3	1:B:314:ILE:CD1	2.47	0.44
1:D:313:SER:HB2	1:D:315:LEU:CD2	2.48	0.44
1:L:313:SER:HB2	1:L:315:LEU:CD2	2.48	0.44
1:G:180:ALA:O	1:G:181:ASP:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:499:THR:HA	1:H:501:THR:HG23	1.99	0.44
1:G:134:LYS:HG2	1:G:134:LYS:H	1.64	0.44
1:K:132:ASN:HA	1:K:133:PRO:HD3	1.80	0.44
1:E:256:GLY:HA2	1:E:259:SER:OG	2.18	0.44
1:J:18:ASP:HA	1:J:21:ALA:HB3	2.00	0.44
1:F:159:GLY:O	1:F:162:VAL:HG12	2.18	0.44
1:I:486:ILE:O	1:I:487:GLU:C	2.56	0.44
1:F:53:LYS:HB3	1:F:54:PRO:HD3	1.99	0.44
1:A:399:PHE:HE1	1:A:444:SER:HA	1.82	0.44
1:B:470:LYS:C	1:B:471:TYR:HD2	2.21	0.44
1:C:395:GLY:O	1:C:397:LEU:N	2.50	0.44
1:E:32:LEU:HD21	1:E:494:ASN:HD21	1.81	0.44
1:A:433:THR:HG22	1:F:412:SER:N	2.33	0.44
1:B:409:LEU:HD23	1:F:409:LEU:HD23	1.99	0.44
1:A:486:ILE:O	1:A:487:GLU:C	2.55	0.44
1:K:217:ARG:HG2	1:K:262:TYR:CD1	2.53	0.44
1:F:468:ALA:HB1	1:F:480:ALA:HB1	2.00	0.44
1:A:382:TYR:HE2	1:A:386:LEU:CD2	2.26	0.44
1:F:121:PRO:O	1:F:122:PHE:HD2	2.01	0.44
3:E:601:XEG:CAZ	3:E:601:XEG:HAPA	2.47	0.44
1:D:366:MET:CG	1:D:475:LEU:HD22	2.48	0.44
1:E:314:ILE:H	1:E:314:ILE:HG12	1.49	0.44
1:L:274:GLY:HA3	1:L:314:ILE:CD1	2.48	0.44
1:H:373:LEU:HD12	1:H:373:LEU:HA	1.79	0.44
1:H:47:SER:HB3	1:K:72:TRP:HB3	2.00	0.44
1:J:322:LEU:HD22	1:J:323:ILE:H	1.81	0.44
1:G:322:LEU:HD22	1:G:323:ILE:H	1.81	0.44
1:A:61:LEU:HD13	1:A:61:LEU:HA	1.73	0.44
1:J:256:GLY:O	1:J:257:LEU:C	2.56	0.44
1:E:129:VAL:O	1:E:129:VAL:HG12	2.18	0.44
1:F:18:ASP:HA	1:F:21:ALA:HB3	2.00	0.44
1:F:453:LEU:HD23	1:F:453:LEU:O	2.17	0.44
1:A:478:ARG:O	1:A:481:ALA:N	2.48	0.43
1:B:460:SER:O	1:B:463:GLN:N	2.51	0.43
1:D:86:ARG:HG2	1:D:121:PRO:HA	2.00	0.43
1:C:414:GLN:HB2	1:C:429:PRO:HG2	2.00	0.43
1:B:331:LEU:O	1:B:353:THR:HG23	2.18	0.43
1:J:399:PHE:HE1	1:J:444:SER:HA	1.83	0.43
1:B:386:LEU:O	1:B:387:ASN:C	2.56	0.43
1:G:198:VAL:O	1:G:201:LYS:HE3	2.18	0.43
1:I:211:ARG:HA	1:I:380:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:313:SER:HB2	1:J:315:LEU:CD2	2.48	0.43
1:H:11:LYS:HA	1:H:14:GLU:HG3	1.99	0.43
3:L:601:XEG:CAZ	3:L:601:XEG:HAPA	2.47	0.43
1:F:275:GLU:OE2	1:F:301:ILE:HG13	2.17	0.43
1:K:303:GLY:O	1:K:304:PHE:HB2	2.18	0.43
1:F:271:ILE:HG23	1:F:272:THR:N	2.33	0.43
1:F:245:LYS:HB2	1:F:245:LYS:HE3	1.87	0.43
1:A:313:SER:HB2	1:A:315:LEU:CD2	2.48	0.43
1:H:38:GLU:C	1:H:40:GLN:N	2.71	0.43
1:H:38:GLU:CD	1:H:39:GLU:N	2.71	0.43
1:J:322:LEU:HD13	1:J:322:LEU:C	2.37	0.43
1:B:373:LEU:HA	1:B:373:LEU:HD12	1.70	0.43
1:I:275:GLU:OE2	1:I:301:ILE:HG13	2.16	0.43
1:E:55:CYS:HB3	1:E:82:HIS:HA	2.00	0.43
1:L:82:HIS:C	1:L:82:HIS:CD2	2.91	0.43
1:J:221:HIS:H	1:J:221:HIS:HD1	1.65	0.43
1:L:344:ILE:O	1:L:367:VAL:HA	2.18	0.43
1:I:61:LEU:O	1:I:62:SER:HB2	2.18	0.43
1:G:191:ASP:O	1:G:192:ILE:C	2.55	0.43
1:K:191:ASP:O	1:K:192:ILE:C	2.56	0.43
1:C:374:ASN:C	1:C:376:GLY:N	2.71	0.43
1:C:47:SER:O	1:C:50:ARG:N	2.49	0.43
1:C:252:PHE:HE2	1:C:260:MET:SD	2.41	0.43
1:F:417:LEU:HA	1:F:417:LEU:HD12	1.74	0.43
1:D:19:ARG:CZ	1:D:479:THR:HG21	2.48	0.43
1:F:96:SER:C	1:F:98:ASP:N	2.71	0.43
1:A:288:PRO:HA	1:A:291:LEU:HD22	2.00	0.43
1:J:19:ARG:CD	1:J:479:THR:HG21	2.47	0.43
1:D:436:PHE:CE2	1:E:409:LEU:HD12	2.52	0.43
1:A:96:SER:C	1:A:98:ASP:N	2.71	0.43
1:I:120:VAL:HG13	1:I:121:PRO:HD2	2.00	0.43
1:I:86:ARG:O	1:I:87:THR:O	2.35	0.43
1:A:93:ILE:CG2	1:A:127:ALA:HB3	2.43	0.43
1:J:11:LYS:HA	1:J:14:GLU:HG3	2.00	0.43
1:H:16:PHE:CD2	1:H:16:PHE:N	2.84	0.43
3:E:601:XEG:HAJ	3:E:601:XEG:HBE	1.81	0.43
1:C:271:ILE:HD11	1:C:283:PRO:HG3	2.00	0.43
1:C:345:ALA:HB1	1:C:373:LEU:HD22	1.98	0.43
1:D:322:LEU:C	1:D:322:LEU:HD13	2.39	0.43
1:E:421:PHE:CZ	1:E:423:LYS:HG3	2.53	0.43
1:D:217:ARG:HD3	1:D:450:HIS:CD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:LEU:O	1:C:62:SER:CB	2.66	0.43
1:J:82:HIS:ND1	1:J:109:SER:HA	2.33	0.43
1:H:399:PHE:HE1	1:H:444:SER:HA	1.84	0.43
1:E:370:ASP:OD1	1:E:371:LEU:N	2.51	0.43
1:I:435:GLU:OE1	1:J:408:HIS:HE1	2.01	0.43
1:D:410:LEU:O	1:D:411:MET:HG2	2.19	0.43
1:A:436:PHE:CE2	1:F:409:LEU:CD1	3.01	0.43
1:G:455:TYR:CE2	1:L:399:PHE:HB2	2.53	0.43
1:B:86:ARG:HG2	1:B:121:PRO:HA	1.99	0.43
1:D:79:ARG:HG2	1:D:127:ALA:CB	2.36	0.43
1:G:121:PRO:HD2	1:G:382:TYR:CE1	2.54	0.43
1:A:457:MET:O	1:A:460:SER:HB2	2.17	0.43
1:E:61:LEU:O	1:E:62:SER:CB	2.66	0.43
1:F:238:MET:HE1	1:F:343:ILE:HD11	2.00	0.43
1:H:166:ALA:CA	1:H:176:MET:HE2	2.48	0.43
1:G:275:GLU:OE2	1:G:301:ILE:HG13	2.18	0.43
1:K:65:ILE:HD11	1:K:75:ILE:CD1	2.40	0.43
1:D:291:LEU:CD1	1:D:291:LEU:N	2.82	0.43
1:J:490:PHE:O	1:J:491:ARG:C	2.56	0.43
1:D:271:ILE:HG23	1:D:272:THR:HG23	2.00	0.43
1:J:314:ILE:H	1:J:314:ILE:HG12	1.48	0.43
1:I:82:HIS:C	1:I:82:HIS:CD2	2.91	0.43
1:D:18:ASP:HA	1:D:21:ALA:HB3	1.99	0.43
1:K:216:GLY:C	1:K:218:GLY:N	2.71	0.43
1:D:8:ASN:CG	1:D:329:LYS:HD2	2.38	0.43
1:H:104:VAL:HG23	1:H:105:LYS:N	2.33	0.43
1:B:28:LEU:H	1:B:28:LEU:CD1	2.18	0.43
1:J:19:ARG:HD2	1:J:479:THR:CG2	2.48	0.43
1:D:383:PHE:N	1:D:383:PHE:CD2	2.86	0.43
1:D:409:LEU:C	1:D:411:MET:H	2.20	0.43
1:A:413:VAL:HG11	1:F:413:VAL:HG22	2.01	0.43
1:F:413:VAL:HG12	1:F:414:GLN:N	2.33	0.43
1:E:93:ILE:HA	1:E:127:ALA:O	2.19	0.43
1:G:337:PRO:HG3	1:G:359:ILE:HD12	1.99	0.43
1:G:217:ARG:HG2	1:G:262:TYR:CD1	2.53	0.43
1:J:238:MET:HE1	1:J:343:ILE:HD11	1.99	0.43
1:J:291:LEU:N	1:J:291:LEU:CD1	2.82	0.43
1:L:121:PRO:CD	1:L:382:TYR:CE1	3.01	0.43
1:C:121:PRO:HD2	1:C:382:TYR:CE1	2.53	0.43
1:C:383:PHE:CE2	1:D:397:LEU:HD11	2.54	0.43
1:C:86:ARG:O	1:C:87:THR:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:ARG:O	1:C:266:PHE:CB	2.52	0.43
1:I:271:ILE:HG23	1:I:272:THR:N	2.33	0.43
1:I:38:GLU:C	1:I:40:GLN:N	2.71	0.43
1:H:313:SER:HB2	1:H:315:LEU:CD2	2.48	0.43
1:C:460:SER:O	1:C:463:GLN:N	2.51	0.43
1:L:383:PHE:N	1:L:383:PHE:CD2	2.83	0.43
1:J:69:ASP:OD2	1:J:71:SER:CB	2.66	0.43
1:B:20:GLY:O	1:B:21:ALA:C	2.57	0.43
1:A:191:ASP:O	1:A:192:ILE:C	2.56	0.43
1:F:47:SER:O	1:F:50:ARG:N	2.50	0.43
1:G:437:GLN:OE1	1:G:437:GLN:HA	2.17	0.43
1:I:382:TYR:O	1:I:382:TYR:HD2	2.01	0.43
1:B:313:SER:HB2	1:B:315:LEU:CD2	2.48	0.43
1:G:176:MET:HG2	1:G:200:GLY:HA3	2.01	0.43
1:I:176:MET:HG2	1:I:200:GLY:HA3	2.01	0.43
1:C:383:PHE:HD1	1:C:449:VAL:HG13	1.83	0.43
1:J:12:MET:H	1:J:14:GLU:CG	2.20	0.43
1:J:383:PHE:CD2	1:J:383:PHE:N	2.87	0.43
1:D:59:LEU:HD23	1:D:61:LEU:CD2	2.48	0.43
1:B:366:MET:HB2	1:B:475:LEU:CD1	2.44	0.43
1:G:255:VAL:HG12	2:G:552:NDP:O2N	2.19	0.43
1:G:399:PHE:HE1	1:G:444:SER:HA	1.83	0.43
1:I:59:LEU:HD12	1:I:59:LEU:HA	1.64	0.43
1:A:274:GLY:HA2	1:A:279:SER:HA	1.99	0.43
1:F:274:GLY:HA3	1:F:314:ILE:CD1	2.48	0.43
1:A:323:ILE:HG22	1:A:345:ALA:O	2.18	0.43
1:H:421:PHE:CZ	1:H:423:LYS:HG3	2.52	0.43
1:A:412:SER:HA	1:B:433:THR:HG22	2.00	0.43
1:C:141:LEU:HA	1:C:141:LEU:HD22	1.72	0.43
1:B:256:GLY:HA2	1:B:259:SER:OG	2.18	0.43
1:B:370:ASP:O	1:B:374:ASN:OD1	2.37	0.43
1:B:242:PHE:C	1:B:244:ASP:N	2.68	0.43
1:H:132:ASN:OD1	1:H:134:LYS:CG	2.66	0.43
1:G:191:ASP:HB3	1:G:194:ALA:HB2	2.01	0.43
1:F:89:CYS:H	1:F:163:ASP:HA	1.83	0.43
1:E:18:ASP:HA	1:E:21:ALA:CB	2.47	0.43
1:E:417:LEU:HA	1:E:417:LEU:HD12	1.79	0.43
1:F:53:LYS:N	1:F:54:PRO:CD	2.81	0.43
1:J:226:PHE:CE2	1:J:465:MET:HE2	2.53	0.43
1:D:38:GLU:C	1:D:40:GLN:N	2.72	0.43
1:B:470:LYS:HE3	1:B:470:LYS:HB2	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:THR:O	1:B:483:VAL:CG2	2.61	0.43
1:E:96:SER:C	1:E:98:ASP:N	2.72	0.43
1:D:414:GLN:HB2	1:D:429:PRO:HG2	2.01	0.43
1:E:409:LEU:O	1:E:411:MET:N	2.41	0.43
1:B:368:ILE:HA	1:B:369:PRO:HD3	1.79	0.43
1:D:94:ARG:CZ	1:D:169:MET:HG3	2.48	0.43
1:B:118:VAL:HG11	1:B:375:ALA:HB1	2.01	0.43
1:H:383:PHE:HA	1:H:386:LEU:HD12	2.01	0.43
1:H:346:GLU:OE1	1:H:478:ARG:NH2	2.51	0.43
1:E:8:ASN:HD21	1:E:10:PHE:HB2	1.82	0.43
1:I:176:MET:HG3	1:I:198:VAL:HG22	2.00	0.43
1:L:121:PRO:HD3	1:L:382:TYR:CE1	2.54	0.43
1:A:152:LEU:HD13	1:A:152:LEU:HA	1.57	0.43
1:F:491:ARG:CD	3:F:601:XEG:HAN	2.46	0.43
1:D:152:LEU:HD13	1:D:152:LEU:HA	1.53	0.43
1:J:271:ILE:CD1	1:J:283:PRO:HG3	2.49	0.43
1:G:420:LYS:O	1:G:420:LYS:HG2	2.19	0.43
1:E:212:ILE:HG12	1:E:213:SER:H	1.83	0.43
1:C:370:ASP:OD1	1:C:371:LEU:N	2.51	0.43
1:E:211:ARG:HA	1:E:380:VAL:HG11	1.99	0.43
1:L:423:LYS:O	1:L:424:HIS:C	2.56	0.43
1:C:212:ILE:CD1	1:C:212:ILE:H	2.23	0.43
1:F:396:ARG:HG3	1:F:396:ARG:NH1	2.30	0.43
1:I:89:CYS:H	1:I:163:ASP:HA	1.83	0.43
1:J:217:ARG:CZ	1:J:450:HIS:CD2	3.01	0.43
1:E:117:VAL:HG12	1:E:118:VAL:CG1	2.48	0.43
1:F:429:PRO:C	1:F:431:VAL:H	2.21	0.43
1:J:86:ARG:HG2	1:J:121:PRO:HA	1.99	0.43
1:G:90:LYS:HB2	1:G:122:PHE:HD1	1.77	0.43
1:A:468:ALA:HB1	1:A:480:ALA:HB1	2.00	0.43
1:K:12:MET:HG3	1:K:13:VAL:HG12	2.01	0.43
1:D:11:LYS:HA	1:D:14:GLU:HG3	2.01	0.43
1:A:394:TYR:CZ	1:F:397:LEU:CD2	3.02	0.43
1:A:87:THR:CB	1:A:88:PRO:CD	2.95	0.43
1:F:383:PHE:N	1:F:383:PHE:CD2	2.87	0.43
1:J:385:TRP:CZ2	1:J:389:LEU:HD11	2.53	0.43
1:D:498:VAL:HG23	1:D:499:THR:N	2.29	0.43
1:I:339:VAL:HG21	1:I:360:PHE:CE1	2.54	0.43
1:E:313:SER:HB2	1:E:315:LEU:CD2	2.47	0.43
1:E:315:LEU:HD22	1:E:315:LEU:N	2.32	0.43
1:C:322:LEU:HD22	1:C:323:ILE:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:38:GLU:C	1:J:40:GLN:N	2.71	0.43
1:L:339:VAL:HG21	1:L:360:PHE:CE1	2.52	0.43
1:I:423:LYS:O	1:I:424:HIS:C	2.56	0.43
1:H:396:ARG:HH11	1:H:396:ARG:CG	2.29	0.43
1:B:132:ASN:HA	1:B:133:PRO:HD3	1.78	0.43
1:J:275:GLU:OE2	1:J:301:ILE:HG13	2.18	0.43
1:I:137:THR:HG23	1:I:140:GLU:CD	2.38	0.43
1:D:479:THR:O	1:D:483:VAL:CG2	2.58	0.43
1:I:433:THR:CG2	1:J:412:SER:N	2.82	0.43
1:E:395:GLY:O	1:E:397:LEU:N	2.52	0.43
1:D:99:VAL:HG11	1:D:128:GLY:CA	2.29	0.43
1:F:412:SER:O	1:F:416:SER:HB2	2.18	0.43
1:I:6:ASP:N	1:I:7:PRO:HD3	2.33	0.43
1:K:371:LEU:HD22	1:K:482:TYR:CD2	2.54	0.43
1:A:16:PHE:HD2	1:A:16:PHE:N	2.16	0.43
1:L:378:VAL:HG12	1:L:379:THR:N	2.34	0.43
1:B:499:THR:C	1:B:500:PHE:HD2	2.21	0.43
1:E:12:MET:HG2	1:E:14:GLU:OE2	2.18	0.43
1:C:117:VAL:HG12	1:C:118:VAL:N	2.34	0.43
1:C:382:TYR:O	1:C:385:TRP:HB3	2.19	0.43
1:C:236:LEU:HD12	1:C:238:MET:HE2	2.01	0.43
1:L:214:ALA:CB	1:L:380:VAL:HG21	2.42	0.43
1:K:264:HIS:HE1	1:K:287:ASP:OD1	2.02	0.43
1:B:287:ASP:HA	1:B:288:PRO:HD2	1.86	0.43
1:J:492:VAL:O	1:J:493:TYR:C	2.57	0.43
1:B:271:ILE:CD1	1:B:283:PRO:HG3	2.49	0.43
1:K:274:GLY:HA3	1:K:314:ILE:CD1	2.48	0.43
1:L:38:GLU:C	1:L:40:GLN:N	2.72	0.43
1:H:236:LEU:HD12	1:H:238:MET:HE2	2.01	0.43
1:H:374:ASN:O	1:H:376:GLY:N	2.52	0.43
1:H:402:GLU:C	1:H:404:ASP:N	2.70	0.43
1:C:132:ASN:HA	1:C:133:PRO:HD3	1.84	0.43
1:C:402:GLU:O	1:C:404:ASP:N	2.48	0.43
1:L:15:GLY:O	1:L:16:PHE:C	2.57	0.43
1:I:217:ARG:HG2	1:I:262:TYR:CD1	2.54	0.43
1:I:449:VAL:O	1:I:450:HIS:C	2.57	0.43
1:C:61:LEU:HA	1:C:61:LEU:HD13	1.70	0.43
1:F:16:PHE:N	1:F:16:PHE:HD2	2.17	0.43
1:F:82:HIS:O	1:F:82:HIS:CD2	2.72	0.43
1:I:490:PHE:C	1:I:490:PHE:CD2	2.92	0.43
1:B:183:TYR:CD2	1:B:183:TYR:C	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:429:PRO:C	1:G:431:VAL:H	2.22	0.43
1:A:117:VAL:HG21	1:A:371:LEU:CG	2.33	0.43
1:H:470:LYS:C	1:H:471:TYR:HD2	2.23	0.43
1:D:368:ILE:HA	1:D:369:PRO:HD3	1.78	0.43
1:D:429:PRO:C	1:D:431:VAL:N	2.72	0.43
1:A:111:MET:HE3	2:A:552:NDP:H72N	1.76	0.43
1:B:378:VAL:O	1:B:381:SER:HB2	2.19	0.43
1:D:202:PRO:HG2	1:D:205:GLN:HG3	2.00	0.43
1:K:455:TYR:CE1	1:K:459:ARG:HD3	2.48	0.43
1:I:208:ILE:CG2	1:I:211:ARG:HB2	2.49	0.43
1:E:157:PHE:O	1:E:158:ILE:HB	2.19	0.43
1:J:339:VAL:HG21	1:J:360:PHE:CE1	2.54	0.43
1:C:12:MET:HG2	1:C:14:GLU:OE2	2.19	0.43
1:L:166:ALA:CA	1:L:176:MET:HE2	2.46	0.43
1:H:176:MET:HG3	1:H:198:VAL:HG22	2.00	0.43
1:K:275:GLU:OE2	1:K:301:ILE:HG13	2.18	0.43
1:K:16:PHE:HD2	1:K:16:PHE:N	2.16	0.43
1:E:271:ILE:HG23	1:E:272:THR:N	2.34	0.43
1:I:314:ILE:H	1:I:314:ILE:HG12	1.47	0.43
1:D:423:LYS:O	1:D:424:HIS:C	2.57	0.43
1:A:97:THR:OG1	1:A:132:ASN:HB2	2.19	0.43
1:G:35:ARG:C	1:G:37:THR:H	2.21	0.43
1:D:373:LEU:HD12	1:D:373:LEU:HA	1.71	0.43
1:H:44:ARG:HG3	1:H:45:VAL:N	2.33	0.43
1:K:38:GLU:C	1:K:40:GLN:N	2.73	0.43
1:E:345:ALA:HB1	1:E:373:LEU:HD22	2.00	0.43
1:F:143:LYS:O	1:F:144:ILE:C	2.56	0.43
1:L:421:PHE:CE1	1:L:425:GLY:N	2.86	0.43
1:G:373:LEU:HA	1:G:373:LEU:HD12	1.76	0.43
1:D:256:GLY:HA2	1:D:259:SER:OG	2.18	0.43
1:F:61:LEU:O	1:F:62:SER:HB2	2.19	0.43
1:G:82:HIS:CD2	1:G:82:HIS:C	2.92	0.43
1:E:191:ASP:O	1:E:192:ILE:C	2.57	0.43
1:F:175:GLU:O	1:F:178:TRP:HB2	2.19	0.43
1:L:23:ILE:HG22	1:L:471:TYR:HD1	1.83	0.43
1:B:252:PHE:HE2	1:B:260:MET:SD	2.41	0.43
1:G:378:VAL:HG12	1:G:379:THR:N	2.33	0.43
1:B:68:ASP:OD2	1:B:140:GLU:HG3	2.18	0.43
1:F:470:LYS:HB2	1:F:470:LYS:HE3	1.75	0.43
1:J:429:PRO:C	1:J:431:VAL:N	2.68	0.43
1:A:275:GLU:OE2	1:A:301:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:HIS:HE1	1:A:287:ASP:OD1	2.01	0.43
1:H:473:LEU:N	1:H:473:LEU:HD12	2.34	0.43
1:C:431:VAL:HA	1:C:432:PRO:HD2	1.70	0.43
1:K:96:SER:C	1:K:98:ASP:N	2.72	0.43
1:K:477:LEU:HD22	1:K:477:LEU:H	1.84	0.43
1:L:336:ALA:CB	1:L:359:ILE:HG21	2.46	0.43
1:L:96:SER:C	1:L:98:ASP:N	2.72	0.43
1:C:176:MET:SD	1:C:176:MET:N	2.92	0.43
1:A:86:ARG:HG2	1:A:121:PRO:HA	2.01	0.43
1:C:287:ASP:HA	1:C:288:PRO:HD2	1.84	0.43
1:J:455:TYR:HE2	1:K:399:PHE:HB2	1.83	0.43
1:A:314:ILE:H	1:A:314:ILE:HG12	1.48	0.43
1:D:421:PHE:O	1:D:423:LYS:N	2.51	0.43
1:H:423:LYS:O	1:H:424:HIS:C	2.57	0.43
1:A:211:ARG:HA	1:A:380:VAL:HG11	2.01	0.43
1:F:9:PHE:HB3	1:F:329:LYS:HZ2	1.82	0.43
1:L:82:HIS:ND1	1:L:109:SER:HA	2.34	0.43
1:B:53:LYS:HB3	1:B:54:PRO:HD3	2.01	0.43
1:K:191:ASP:HB3	1:K:194:ALA:HB2	2.00	0.43
1:K:18:ASP:HA	1:K:21:ALA:CB	2.49	0.43
1:C:104:VAL:HG23	1:C:105:LYS:N	2.33	0.43
1:C:486:ILE:O	1:C:487:GLU:C	2.58	0.43
1:L:486:ILE:O	1:L:487:GLU:C	2.56	0.43
1:J:203:ILE:HD12	1:J:203:ILE:N	2.33	0.43
1:E:275:GLU:OE2	1:E:301:ILE:HG13	2.19	0.42
1:K:429:PRO:C	1:K:431:VAL:H	2.23	0.42
1:B:38:GLU:C	1:B:40:GLN:N	2.72	0.42
1:B:19:ARG:NE	1:B:479:THR:HG21	2.34	0.42
1:D:99:VAL:HA	1:D:103:GLU:OE1	2.19	0.42
1:I:117:VAL:HG12	1:I:118:VAL:CG1	2.49	0.42
1:G:208:ILE:HG22	1:G:211:ARG:HB2	1.99	0.42
1:G:211:ARG:HA	1:G:380:VAL:HG11	2.00	0.42
1:B:11:LYS:HA	1:B:14:GLU:HG3	2.00	0.42
1:B:485:ALA:O	1:B:486:ILE:C	2.58	0.42
1:C:382:TYR:CE2	1:C:386:LEU:CD1	2.92	0.42
1:J:12:MET:HG3	1:J:13:VAL:HG12	2.01	0.42
1:H:202:PRO:HG2	1:H:205:GLN:HG3	2.01	0.42
1:E:245:LYS:HE3	1:E:245:LYS:HB2	1.84	0.42
1:B:421:PHE:CE1	1:B:425:GLY:N	2.87	0.42
1:K:421:PHE:CZ	1:K:423:LYS:HG3	2.53	0.42
1:H:220:PHE:O	1:H:222:GLY:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:PHE:CZ	1:A:423:LYS:HG3	2.53	0.42
1:L:38:GLU:CD	1:L:39:GLU:N	2.73	0.42
1:B:322:LEU:HD13	1:B:322:LEU:C	2.39	0.42
1:C:423:LYS:O	1:C:424:HIS:C	2.57	0.42
1:F:421:PHE:O	1:F:423:LYS:N	2.50	0.42
1:F:423:LYS:O	1:F:424:HIS:C	2.57	0.42
1:K:52:ILE:HD13	1:K:489:VAL:HG12	2.01	0.42
1:L:108:ALA:HB2	1:L:126:LYS:HB2	2.00	0.42
1:C:134:LYS:HG2	1:C:134:LYS:H	1.68	0.42
1:E:236:LEU:HD22	1:E:342:LYS:HD2	2.01	0.42
1:K:344:ILE:O	1:K:367:VAL:HA	2.19	0.42
1:C:500:PHE:N	1:C:500:PHE:HD1	2.17	0.42
1:G:417:LEU:HA	1:G:417:LEU:HD12	1.84	0.42
1:E:45:VAL:HG13	1:E:490:PHE:CE1	2.54	0.42
1:L:137:THR:HG23	1:L:140:GLU:CD	2.40	0.42
1:G:18:ASP:HA	1:G:21:ALA:CB	2.49	0.42
1:F:180:ALA:O	1:F:181:ASP:C	2.56	0.42
1:G:338:ARG:HB3	1:G:338:ARG:CZ	2.49	0.42
1:L:470:LYS:HE3	1:L:470:LYS:HB2	1.76	0.42
1:E:338:ARG:CZ	1:E:338:ARG:HB3	2.48	0.42
1:J:429:PRO:C	1:J:431:VAL:H	2.22	0.42
1:J:435:GLU:OE1	1:K:408:HIS:HE1	2.02	0.42
1:B:36:GLU:O	1:B:37:THR:C	2.57	0.42
1:E:52:ILE:HD13	1:E:489:VAL:HG11	2.01	0.42
1:C:414:GLN:HB2	1:C:429:PRO:CG	2.49	0.42
1:C:413:VAL:CG2	1:E:413:VAL:HG21	2.49	0.42
1:A:431:VAL:HA	1:A:432:PRO:HD2	1.73	0.42
1:B:412:SER:CA	1:F:433:THR:HG22	2.48	0.42
1:A:336:ALA:CB	1:A:359:ILE:HG21	2.46	0.42
1:L:399:PHE:HE1	1:L:444:SER:HA	1.84	0.42
1:I:100:SER:OG	1:I:102:ASP:N	2.52	0.42
1:A:27:LYS:HD2	1:A:471:TYR:OH	2.19	0.42
1:A:157:PHE:O	1:A:158:ILE:HB	2.19	0.42
1:B:487:GLU:O	1:B:491:ARG:CG	2.66	0.42
1:B:488:LYS:HB3	3:B:601:XEG:OAD	2.19	0.42
1:L:93:ILE:HD11	1:L:179:ILE:HD11	2.01	0.42
1:L:287:ASP:HA	1:L:288:PRO:HD2	1.84	0.42
3:H:601:XEG:CAZ	3:H:601:XEG:HAPA	2.48	0.42
1:H:271:ILE:CD1	1:H:283:PRO:HG3	2.49	0.42
1:G:271:ILE:HD11	1:G:283:PRO:HG3	2.01	0.42
1:I:420:LYS:O	1:I:420:LYS:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:171:THR:HA	1:H:175:GLU:OE2	2.19	0.42
1:K:236:LEU:HD12	1:K:238:MET:HE2	2.01	0.42
1:J:132:ASN:OD1	1:J:134:LYS:CG	2.64	0.42
1:B:175:GLU:HA	1:B:178:TRP:CE3	2.54	0.42
1:H:221:HIS:H	1:H:221:HIS:HD1	1.67	0.42
1:I:18:ASP:HA	1:I:21:ALA:HB3	2.00	0.42
1:D:70:GLY:O	1:D:72:TRP:CZ3	2.72	0.42
1:D:252:PHE:HE2	1:D:260:MET:SD	2.42	0.42
1:J:372:TYR:CD1	1:J:372:TYR:C	2.92	0.42
1:C:338:ARG:CZ	1:C:338:ARG:HB3	2.49	0.42
1:D:36:GLU:O	1:D:37:THR:C	2.57	0.42
1:G:408:HIS:HE1	1:H:435:GLU:OE1	2.02	0.42
1:D:413:VAL:CG1	1:D:429:PRO:HG3	2.47	0.42
1:H:6:ASP:N	1:H:355:GLU:HG3	2.33	0.42
1:J:477:LEU:N	1:J:477:LEU:HD22	2.34	0.42
1:C:6:ASP:HB2	1:C:353:THR:CB	2.49	0.42
1:B:65:ILE:HD11	1:B:75:ILE:CD1	2.35	0.42
1:L:379:THR:O	1:L:382:TYR:HB3	2.18	0.42
1:G:236:LEU:HD22	1:G:342:LYS:HD2	2.01	0.42
1:D:214:ALA:HB1	1:D:380:VAL:CG2	2.40	0.42
1:D:264:HIS:CE1	1:D:287:ASP:OD1	2.73	0.42
3:J:601:XEG:CAZ	3:J:601:XEG:HAPA	2.49	0.42
1:E:271:ILE:HG23	1:E:272:THR:HG23	2.01	0.42
1:K:273:VAL:HB	1:K:280:ILE:CD1	2.49	0.42
1:C:273:VAL:HB	1:C:280:ILE:CD1	2.50	0.42
1:I:35:ARG:C	1:I:37:THR:H	2.23	0.42
1:C:38:GLU:C	1:C:40:GLN:N	2.71	0.42
1:F:322:LEU:HD22	1:F:323:ILE:H	1.83	0.42
1:J:423:LYS:O	1:J:424:HIS:C	2.57	0.42
1:A:373:LEU:HA	1:A:373:LEU:HD12	1.82	0.42
1:D:236:LEU:HD12	1:D:238:MET:HE2	2.01	0.42
1:F:315:LEU:N	1:F:315:LEU:HD22	2.34	0.42
1:H:313:SER:O	1:H:315:LEU:N	2.51	0.42
1:D:210:GLY:CA	1:D:446:LYS:HZ3	2.32	0.42
1:K:180:ALA:O	1:K:181:ASP:C	2.57	0.42
1:C:368:ILE:HA	1:C:369:PRO:HD3	1.75	0.42
1:I:494:ASN:ND2	1:I:494:ASN:O	2.52	0.42
1:B:464:ILE:O	1:B:468:ALA:HB3	2.18	0.42
1:E:382:TYR:HE2	1:E:386:LEU:CD2	2.31	0.42
1:J:470:LYS:C	1:J:471:TYR:HD2	2.23	0.42
1:F:414:GLN:HB2	1:F:429:PRO:CG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ASP:N	1:A:7:PRO:HD3	2.34	0.42
1:B:121:PRO:O	1:B:122:PHE:CD2	2.71	0.42
1:F:203:ILE:HD12	1:F:203:ILE:N	2.34	0.42
1:D:176:MET:HG3	1:D:198:VAL:HG22	2.02	0.42
1:G:19:ARG:NE	1:G:479:THR:HG21	2.34	0.42
1:I:399:PHE:HE1	1:I:444:SER:HA	1.85	0.42
1:J:366:MET:HG3	1:J:477:LEU:HD21	2.01	0.42
1:C:464:ILE:O	1:C:468:ALA:HB3	2.18	0.42
1:A:386:LEU:CD2	1:F:392:VAL:HG13	2.50	0.42
1:A:95:TYR:OH	1:A:145:THR:HG22	2.19	0.42
1:G:12:MET:HG3	1:G:13:VAL:HG12	2.01	0.42
1:F:236:LEU:HD12	1:F:238:MET:HE2	2.01	0.42
1:F:287:ASP:HA	1:F:288:PRO:HD2	1.84	0.42
1:J:382:TYR:CE2	1:J:386:LEU:CD1	2.96	0.42
1:B:264:HIS:CE1	1:B:287:ASP:OD1	2.73	0.42
1:I:155:LYS:HE2	1:L:57:HIS:ND1	2.34	0.42
1:K:314:ILE:HG12	1:K:314:ILE:H	1.48	0.42
1:I:274:GLY:HA3	1:I:314:ILE:CD1	2.49	0.42
1:G:271:ILE:HG23	1:G:272:THR:HG23	2.01	0.42
1:G:412:SER:OG	1:H:433:THR:HG23	2.18	0.42
1:J:445:GLU:O	1:J:449:VAL:HG23	2.20	0.42
1:I:38:GLU:CD	1:I:39:GLU:N	2.73	0.42
1:K:313:SER:O	1:K:315:LEU:N	2.50	0.42
1:E:38:GLU:OE2	1:E:40:GLN:N	2.52	0.42
1:A:38:GLU:CD	1:A:39:GLU:N	2.73	0.42
1:E:323:ILE:HG22	1:E:345:ALA:O	2.20	0.42
1:C:52:ILE:CD1	1:C:489:VAL:HG12	2.47	0.42
1:K:368:ILE:HA	1:K:369:PRO:HD3	1.73	0.42
1:G:368:ILE:HA	1:G:369:PRO:HD3	1.73	0.42
1:H:412:SER:HB3	1:L:431:VAL:O	2.20	0.42
1:C:130:LYS:O	1:C:130:LYS:HG3	2.18	0.42
1:C:412:SER:CB	1:E:432:PRO:HA	2.50	0.42
1:I:379:THR:O	1:I:382:TYR:HB3	2.19	0.42
3:I:601:XEG:HBE	3:I:601:XEG:HAJ	1.74	0.42
1:K:117:VAL:HG12	1:K:118:VAL:N	2.34	0.42
1:E:336:ALA:CB	1:E:359:ILE:HG21	2.47	0.42
1:B:490:PHE:HE2	1:B:494:ASN:CB	2.31	0.42
3:B:601:XEG:HAJ	3:B:601:XEG:HBE	1.76	0.42
1:G:498:VAL:HG21	1:G:500:PHE:CE2	2.54	0.42
1:F:399:PHE:HE1	1:F:444:SER:HA	1.84	0.42
1:B:211:ARG:O	1:B:214:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:264:HIS:HE1	1:L:287:ASP:OD1	2.02	0.42
1:D:475:LEU:HA	1:D:475:LEU:HD23	1.79	0.42
1:L:217:ARG:HG2	1:L:262:TYR:CD1	2.54	0.42
1:E:208:ILE:HG22	1:E:211:ARG:HB2	2.00	0.42
1:K:220:PHE:C	1:K:222:GLY:N	2.72	0.42
1:H:315:LEU:N	1:H:315:LEU:HD22	2.34	0.42
1:J:95:TYR:HB3	1:J:133:PRO:HG3	2.01	0.42
1:K:453:LEU:O	1:K:457:MET:HB2	2.20	0.42
1:H:216:GLY:C	1:H:218:GLY:N	2.73	0.42
1:H:226:PHE:CE2	1:H:465:MET:HE2	2.54	0.42
1:E:477:LEU:O	1:E:478:ARG:C	2.58	0.42
1:L:412:SER:O	1:L:416:SER:HB2	2.20	0.42
1:A:477:LEU:O	1:A:478:ARG:C	2.57	0.42
1:C:412:SER:N	1:E:433:THR:HG22	2.35	0.42
1:B:315:LEU:HG	1:B:331:LEU:HD11	2.01	0.42
1:A:142:GLU:HA	1:A:178:TRP:CZ3	2.54	0.42
1:A:175:GLU:HA	1:A:178:TRP:CE3	2.54	0.42
1:J:130:LYS:HG3	1:J:130:LYS:O	2.19	0.42
1:K:200:GLY:HA2	1:K:211:ARG:CD	2.50	0.42
1:L:99:VAL:HG11	1:L:128:GLY:CA	2.35	0.42
1:C:288:PRO:HA	1:C:291:LEU:HD22	1.99	0.42
1:D:288:PRO:CA	1:D:291:LEU:HD22	2.50	0.42
1:I:57:HIS:ND1	1:L:155:LYS:HE2	2.34	0.42
1:J:486:ILE:O	1:J:487:GLU:C	2.58	0.42
1:H:282:ASN:C	1:H:284:ASP:N	2.73	0.42
1:J:38:GLU:CD	1:J:39:GLU:N	2.72	0.42
1:I:243:GLY:C	1:I:245:LYS:H	2.23	0.42
1:C:256:GLY:HA2	1:C:259:SER:OG	2.19	0.42
1:C:256:GLY:O	1:C:257:LEU:C	2.58	0.42
1:K:494:ASN:O	1:K:496:ALA:N	2.40	0.42
1:L:136:TYR:HB2	1:L:141:LEU:CD2	2.47	0.42
1:F:8:ASN:O	1:F:329:LYS:HD2	2.20	0.42
1:B:275:GLU:OE2	1:B:301:ILE:HG13	2.20	0.42
1:J:61:LEU:HA	1:J:61:LEU:HD13	1.78	0.42
1:D:20:GLY:O	1:D:21:ALA:C	2.57	0.42
1:D:6:ASP:HA	1:D:7:PRO:HD2	1.77	0.42
1:K:498:VAL:HB	1:K:499:THR:H	1.35	0.42
1:A:378:VAL:HG12	1:A:379:THR:N	2.35	0.42
1:G:53:LYS:N	1:G:54:PRO:CD	2.82	0.42
1:K:68:ASP:OD2	1:K:140:GLU:HG3	2.19	0.42
1:E:368:ILE:HA	1:E:369:PRO:HD3	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:470:LYS:HE3	1:D:470:LYS:HB2	1.76	0.42
1:K:411:MET:HA	1:K:414:GLN:HB3	2.02	0.42
1:B:473:LEU:N	1:B:473:LEU:HD12	2.35	0.42
1:J:19:ARG:HD2	1:J:479:THR:HG21	2.02	0.42
1:D:414:GLN:HB2	1:D:429:PRO:HD2	2.01	0.42
1:A:409:LEU:CD2	1:B:409:LEU:HD23	2.48	0.42
1:I:455:TYR:HE2	1:J:399:PHE:HB2	1.85	0.42
1:D:166:ALA:CA	1:D:176:MET:HE2	2.50	0.42
1:H:368:ILE:HA	1:H:369:PRO:HD3	1.75	0.42
1:A:121:PRO:O	1:A:122:PHE:CD2	2.73	0.42
1:H:86:ARG:HG2	1:H:121:PRO:HA	2.00	0.42
1:C:203:ILE:HG21	1:C:209:HIS:NE2	2.35	0.42
1:I:288:PRO:N	1:I:291:LEU:HD22	2.35	0.42
1:F:426:GLY:HA3	1:I:308:LYS:NZ	2.35	0.42
1:D:282:ASN:O	1:D:284:ASP:N	2.47	0.42
1:E:38:GLU:CD	1:E:39:GLU:N	2.73	0.42
1:H:396:ARG:NH1	1:H:396:ARG:HG3	2.33	0.42
1:L:61:LEU:HA	1:L:61:LEU:HD13	1.67	0.42
1:J:348:ALA:HB3	1:J:351:PRO:HG3	2.00	0.42
1:H:18:ASP:HA	1:H:21:ALA:HB3	2.02	0.42
1:A:216:GLY:C	1:A:218:GLY:N	2.72	0.42
1:I:470:LYS:HB2	1:I:470:LYS:HE3	1.78	0.42
1:F:338:ARG:CZ	1:F:338:ARG:HB3	2.50	0.42
1:E:481:ALA:O	1:E:484:ASN:N	2.52	0.42
1:I:413:VAL:CG1	1:I:429:PRO:HG3	2.48	0.42
1:E:87:THR:CB	1:E:88:PRO:CD	2.94	0.42
1:A:432:PRO:O	1:A:433:THR:O	2.37	0.42
1:A:205:GLN:OE1	1:B:496:ALA:HB2	2.20	0.42
1:B:86:ARG:O	1:B:87:THR:O	2.38	0.42
1:H:117:VAL:HG12	1:H:118:VAL:HG13	2.01	0.42
1:K:491:ARG:O	1:K:495:GLU:HG2	2.20	0.42
1:I:264:HIS:HE1	1:I:287:ASP:OD1	2.03	0.42
1:K:227:ILE:HD11	1:K:343:ILE:CD1	2.49	0.42
1:L:87:THR:CB	1:L:88:PRO:HD3	2.41	0.42
1:B:236:LEU:HD21	1:B:342:LYS:HB3	2.02	0.42
1:J:273:VAL:HB	1:J:280:ILE:CD1	2.50	0.42
1:A:181:ASP:O	1:A:182:THR:C	2.58	0.42
1:G:273:VAL:HB	1:G:280:ILE:CD1	2.50	0.42
1:B:57:HIS:ND1	1:E:155:LYS:HE2	2.35	0.42
1:F:271:ILE:HD11	1:F:283:PRO:HG3	2.01	0.42
1:K:423:LYS:O	1:K:424:HIS:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:LYS:HE3	1:C:245:LYS:HB2	1.87	0.42
1:J:45:VAL:O	1:J:47:SER:N	2.53	0.42
1:E:97:THR:OG1	1:E:132:ASN:HB2	2.20	0.42
1:B:217:ARG:NE	1:B:450:HIS:CD2	2.85	0.42
1:K:134:LYS:H	1:K:134:LYS:HG2	1.64	0.42
1:A:499:THR:O	1:A:499:THR:CG2	2.67	0.42
1:F:457:MET:O	1:F:460:SER:HB2	2.20	0.42
1:C:108:ALA:HB2	1:C:126:LYS:HB2	2.02	0.42
1:A:234:SER:O	1:A:236:LEU:N	2.51	0.42
1:A:236:LEU:HD12	1:A:238:MET:HE2	2.02	0.42
1:B:55:CYS:HB3	1:B:82:HIS:HA	2.02	0.42
1:B:203:ILE:HA	1:B:207:GLY:H	1.85	0.42
1:B:69:ASP:OD2	1:B:71:SER:CB	2.68	0.42
1:J:216:GLY:C	1:J:218:GLY:N	2.72	0.42
1:B:63:PHE:N	1:B:63:PHE:CD2	2.88	0.42
1:H:372:TYR:C	1:H:372:TYR:CD1	2.93	0.42
1:H:409:LEU:C	1:H:411:MET:H	2.21	0.42
1:E:86:ARG:HG2	1:E:121:PRO:HA	2.02	0.42
1:B:411:MET:HB3	1:F:433:THR:HG21	2.01	0.42
1:G:201:LYS:HA	1:G:202:PRO:HD2	1.77	0.42
1:L:6:ASP:N	1:L:355:GLU:HG3	2.35	0.42
1:J:287:ASP:HA	1:J:288:PRO:HD2	1.86	0.42
1:C:330:GLN:O	1:C:331:LEU:HD12	2.18	0.42
1:C:6:ASP:HB2	1:C:353:THR:HG21	2.00	0.42
1:F:166:ALA:HB1	1:F:167:PRO:HD2	2.02	0.42
1:B:12:MET:HG3	1:B:13:VAL:HG12	2.01	0.42
1:C:199:THR:HG22	1:C:384:GLU:CG	2.49	0.42
1:A:382:TYR:CE2	1:A:386:LEU:CD1	2.94	0.42
1:B:498:VAL:CG2	1:B:500:PHE:CD2	3.03	0.42
1:A:393:SER:OG	3:B:601:XEG:CAX	2.68	0.42
1:B:488:LYS:CA	1:B:491:ARG:HG3	2.49	0.42
1:C:117:VAL:HG12	1:C:118:VAL:HG13	2.01	0.42
1:L:175:GLU:HA	1:L:178:TRP:CE3	2.55	0.42
1:J:117:VAL:HG12	1:J:118:VAL:N	2.34	0.42
1:G:303:GLY:O	1:G:304:PHE:HB2	2.18	0.42
1:L:236:LEU:HD22	1:L:342:LYS:HD2	2.02	0.42
1:B:238:MET:HE1	1:B:343:ILE:HD11	2.02	0.42
1:H:491:ARG:HD2	3:H:601:XEG:OAB	2.20	0.42
1:J:65:ILE:HD11	1:J:75:ILE:CD1	2.45	0.42
1:J:282:ASN:C	1:J:284:ASP:N	2.73	0.42
1:K:271:ILE:HG23	1:K:272:THR:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:423:LYS:O	1:G:424:HIS:C	2.58	0.42
1:A:212:ILE:CD1	1:A:212:ILE:H	2.15	0.42
1:A:421:PHE:O	1:A:423:LYS:N	2.52	0.42
1:H:45:VAL:O	1:H:47:SER:N	2.53	0.42
1:D:494:ASN:ND2	1:D:494:ASN:C	2.73	0.42
1:A:412:SER:CA	1:B:433:THR:HG22	2.50	0.42
1:C:315:LEU:HD22	1:C:315:LEU:N	2.34	0.42
1:I:421:PHE:CZ	1:I:423:LYS:HG3	2.54	0.42
1:K:97:THR:OG1	1:K:132:ASN:HB2	2.20	0.42
1:A:234:SER:C	1:A:236:LEU:N	2.69	0.42
1:F:368:ILE:HA	1:F:369:PRO:HD3	1.76	0.42
1:A:338:ARG:CZ	1:A:338:ARG:HB3	2.49	0.42
1:K:338:ARG:HB3	1:K:338:ARG:CZ	2.49	0.42
1:A:366:MET:CG	1:A:477:LEU:HD21	2.49	0.42
1:H:24:VAL:HG13	1:H:483:VAL:CG1	2.26	0.42
1:C:96:SER:C	1:C:98:ASP:N	2.73	0.42
1:B:409:LEU:C	1:B:411:MET:H	2.22	0.42
1:G:96:SER:O	1:G:130:LYS:HA	2.20	0.42
1:B:70:GLY:O	1:B:72:TRP:CZ3	2.72	0.42
1:A:202:PRO:HG2	1:A:205:GLN:HG2	2.01	0.42
1:K:468:ALA:HB1	1:K:480:ALA:HB1	2.01	0.42
1:K:19:ARG:NE	1:K:479:THR:HG21	2.34	0.42
1:D:65:ILE:HD11	1:D:75:ILE:CD1	2.34	0.42
1:H:117:VAL:HG12	1:H:118:VAL:N	2.35	0.42
1:A:28:LEU:H	1:A:28:LEU:CD1	2.11	0.42
1:J:288:PRO:N	1:J:291:LEU:HD22	2.35	0.42
1:J:477:LEU:O	1:J:478:ARG:C	2.58	0.42
1:E:457:MET:O	1:E:460:SER:HB2	2.19	0.42
1:L:382:TYR:O	1:L:382:TYR:HD2	2.03	0.42
1:L:86:ARG:HG2	1:L:121:PRO:HA	2.01	0.42
1:F:491:ARG:HD2	3:F:601:XEG:OAB	2.19	0.42
1:J:485:ALA:O	1:J:488:LYS:N	2.53	0.42
1:A:271:ILE:HG23	1:A:272:THR:HG23	2.02	0.42
1:L:396:ARG:HG3	1:L:396:ARG:NH1	2.26	0.42
1:F:243:GLY:C	1:F:245:LYS:H	2.23	0.42
1:H:345:ALA:HB1	1:H:373:LEU:HD22	2.00	0.42
1:A:38:GLU:OE2	1:A:40:GLN:N	2.53	0.42
1:A:421:PHE:CE1	1:A:425:GLY:N	2.88	0.42
1:G:38:GLU:C	1:G:40:GLN:N	2.73	0.42
1:I:373:LEU:HA	1:I:373:LEU:HD12	1.72	0.42
1:E:423:LYS:O	1:E:424:HIS:C	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:PHE:CD1	1:C:421:PHE:O	2.72	0.42
1:K:256:GLY:HA2	1:K:259:SER:OG	2.20	0.42
1:L:402:GLU:O	1:L:404:ASP:N	2.51	0.42
1:F:132:ASN:HA	1:F:133:PRO:HD3	1.84	0.42
1:J:70:GLY:O	1:J:72:TRP:CZ3	2.73	0.42
1:K:55:CYS:HB3	1:K:82:HIS:HA	2.00	0.42
1:J:473:LEU:H	1:J:473:LEU:HD12	1.85	0.41
1:D:378:VAL:CG1	1:D:379:THR:N	2.83	0.41
1:B:339:VAL:HG23	1:B:339:VAL:O	2.20	0.41
1:G:212:ILE:HG12	1:G:213:SER:H	1.84	0.41
1:I:393:SER:OG	3:K:601:XEG:CAM	2.68	0.41
1:J:315:LEU:N	1:J:315:LEU:HD22	2.35	0.41
1:J:250:GLN:HG2	1:J:330:GLN:HE21	1.85	0.41
1:A:75:ILE:CD1	1:A:144:ILE:HG23	2.51	0.41
1:F:294:PHE:O	1:F:300:THR:O	2.38	0.41
1:G:16:PHE:N	1:G:16:PHE:HD2	2.18	0.41
1:H:490:PHE:C	1:H:490:PHE:CD2	2.94	0.41
1:K:339:VAL:HG21	1:K:360:PHE:CE1	2.55	0.41
1:F:373:LEU:HD12	1:F:373:LEU:HA	1.75	0.41
1:J:421:PHE:O	1:J:423:LYS:N	2.51	0.41
1:A:345:ALA:HB1	1:A:373:LEU:HD22	2.01	0.41
1:L:373:LEU:HA	1:L:373:LEU:HD12	1.74	0.41
1:K:212:ILE:HG12	1:K:213:SER:H	1.85	0.41
1:I:421:PHE:O	1:I:423:LYS:N	2.49	0.41
1:F:396:ARG:CG	1:F:396:ARG:NH1	2.83	0.41
1:F:149:THR:O	1:F:150:MET:C	2.58	0.41
1:I:175:GLU:O	1:I:178:TRP:HB2	2.20	0.41
1:L:191:ASP:O	1:L:192:ILE:C	2.58	0.41
1:A:53:LYS:HB3	1:A:54:PRO:HD3	2.02	0.41
1:G:378:VAL:O	1:G:381:SER:HB2	2.20	0.41
1:A:70:GLY:O	1:A:72:TRP:CZ3	2.73	0.41
1:E:188:GLY:O	1:E:189:HIS:C	2.58	0.41
1:E:378:VAL:HG12	1:E:379:THR:N	2.35	0.41
1:J:68:ASP:OD2	1:J:140:GLU:HG3	2.20	0.41
1:E:264:HIS:HE1	1:E:287:ASP:OD1	2.03	0.41
1:I:410:LEU:O	1:I:411:MET:HG2	2.20	0.41
1:I:413:VAL:HG12	1:I:429:PRO:CG	2.45	0.41
1:I:431:VAL:HG13	1:J:416:SER:OG	2.20	0.41
1:A:301:ILE:HD12	1:A:301:ILE:O	2.21	0.41
1:J:166:ALA:HB1	1:J:167:PRO:HD2	2.02	0.41
1:I:15:GLY:O	1:I:16:PHE:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:THR:HA	1:A:384:GLU:OE1	2.20	0.41
3:A:601:XEG:HAJ	3:A:601:XEG:HBE	1.82	0.41
1:K:167:PRO:HD2	1:K:199:THR:O	2.20	0.41
1:I:397:LEU:CD2	1:K:394:TYR:CZ	3.04	0.41
1:H:264:HIS:CE1	1:H:287:ASP:OD1	2.73	0.41
1:H:348:ALA:HB3	1:H:351:PRO:HG3	2.01	0.41
1:A:372:TYR:HE2	1:A:460:SER:HB3	1.85	0.41
1:B:494:ASN:ND2	1:B:494:ASN:C	2.73	0.41
1:C:121:PRO:CD	1:C:382:TYR:CE1	3.02	0.41
1:L:176:MET:N	1:L:176:MET:SD	2.92	0.41
1:H:165:PRO:O	1:H:198:VAL:HG23	2.21	0.41
1:H:57:HIS:ND1	1:K:155:LYS:HE2	2.35	0.41
1:D:213:SER:HB2	1:D:262:TYR:CE2	2.55	0.41
1:H:445:GLU:O	1:H:446:LYS:C	2.58	0.41
1:D:425:GLY:O	1:D:426:GLY:C	2.57	0.41
1:D:498:VAL:HG23	1:D:500:PHE:CE2	2.53	0.41
1:H:421:PHE:O	1:H:423:LYS:N	2.51	0.41
1:L:35:ARG:O	1:L:37:THR:HG22	2.20	0.41
1:C:339:VAL:HG21	1:C:360:PHE:CE1	2.55	0.41
1:I:322:LEU:C	1:I:322:LEU:HD13	2.40	0.41
1:F:421:PHE:CD1	1:F:421:PHE:O	2.73	0.41
1:L:421:PHE:CZ	1:L:423:LYS:HG3	2.55	0.41
1:C:136:TYR:HB2	1:C:141:LEU:CD2	2.47	0.41
1:J:396:ARG:HG3	1:J:396:ARG:NH1	2.33	0.41
1:K:236:LEU:HD22	1:K:342:LYS:HD2	2.01	0.41
1:B:350:GLY:N	1:B:370:ASP:OD2	2.51	0.41
1:L:477:LEU:HD22	1:L:477:LEU:N	2.34	0.41
1:H:395:GLY:O	1:H:397:LEU:N	2.54	0.41
1:F:16:PHE:CE2	1:F:354:PRO:HG3	2.55	0.41
1:G:431:VAL:HG13	1:G:431:VAL:O	2.20	0.41
1:B:19:ARG:CZ	1:B:479:THR:HG21	2.51	0.41
1:G:94:ARG:CZ	1:G:169:MET:HG3	2.50	0.41
1:J:176:MET:HG3	1:J:198:VAL:HG22	2.02	0.41
1:B:166:ALA:HB1	1:B:167:PRO:HD2	2.03	0.41
1:B:90:LYS:HE3	1:B:90:LYS:HB3	1.91	0.41
1:K:176:MET:HG3	1:K:198:VAL:HG21	2.02	0.41
1:K:211:ARG:O	1:K:211:ARG:HG2	2.19	0.41
1:K:121:PRO:O	1:K:122:PHE:HD2	2.03	0.41
1:I:176:MET:N	1:I:176:MET:SD	2.92	0.41
1:I:201:LYS:HA	1:I:202:PRO:HD2	1.78	0.41
1:E:59:LEU:HD12	1:E:59:LEU:HA	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:288:PRO:CA	1:J:291:LEU:HD22	2.49	0.41
1:H:121:PRO:O	1:H:122:PHE:CD2	2.73	0.41
1:H:85:HIS:HB2	1:H:492:VAL:HG21	2.02	0.41
1:B:395:GLY:O	1:B:397:LEU:N	2.53	0.41
1:D:212:ILE:HG12	1:D:213:SER:H	1.85	0.41
1:G:421:PHE:CZ	1:G:423:LYS:HG3	2.54	0.41
1:E:217:ARG:CZ	1:E:450:HIS:CD2	3.03	0.41
1:D:315:LEU:HD22	1:D:315:LEU:N	2.34	0.41
1:I:90:LYS:HG3	1:I:122:PHE:CD1	2.54	0.41
1:J:134:LYS:H	1:J:134:LYS:HG2	1.64	0.41
1:C:16:PHE:N	1:C:16:PHE:HD2	2.18	0.41
1:L:485:ALA:O	1:L:486:ILE:C	2.57	0.41
1:A:155:LYS:HE3	1:D:156:GLY:O	2.21	0.41
1:L:216:GLY:C	1:L:218:GLY:N	2.73	0.41
1:H:66:ARG:HG2	1:H:66:ARG:H	1.62	0.41
1:D:183:TYR:CD2	1:D:183:TYR:C	2.93	0.41
1:F:437:GLN:OE1	1:F:437:GLN:HA	2.20	0.41
1:I:433:THR:HG22	1:J:412:SER:HA	2.02	0.41
1:I:336:ALA:HB3	1:I:337:PRO:CD	2.33	0.41
1:I:353:THR:OG1	1:I:355:GLU:HB2	2.20	0.41
1:B:383:PHE:N	1:B:383:PHE:CD2	2.87	0.41
1:K:121:PRO:HD3	1:K:382:TYR:CE1	2.55	0.41
1:H:291:LEU:N	1:H:291:LEU:CD1	2.83	0.41
1:K:485:ALA:O	1:K:486:ILE:C	2.58	0.41
1:C:45:VAL:HG22	1:C:490:PHE:CZ	2.55	0.41
3:L:601:XEG:HBE	3:L:601:XEG:HAJ	1.75	0.41
1:F:379:THR:O	1:F:382:TYR:HB3	2.19	0.41
1:J:117:VAL:HG12	1:J:118:VAL:HG13	2.01	0.41
1:D:275:GLU:OE2	1:D:301:ILE:HG13	2.20	0.41
1:B:291:LEU:N	1:B:291:LEU:CD1	2.83	0.41
1:H:273:VAL:HB	1:H:280:ILE:CD1	2.50	0.41
1:F:273:VAL:HB	1:F:280:ILE:CD1	2.50	0.41
1:F:282:ASN:O	1:F:284:ASP:N	2.47	0.41
1:C:322:LEU:C	1:C:322:LEU:HD13	2.41	0.41
1:L:212:ILE:HG12	1:L:213:SER:H	1.84	0.41
1:B:429:PRO:C	1:B:431:VAL:N	2.72	0.41
1:H:142:GLU:OE2	1:L:500:PHE:CZ	2.71	0.41
1:F:136:TYR:HB2	1:F:141:LEU:CD2	2.45	0.41
1:L:90:LYS:HB2	1:L:122:PHE:HD1	1.80	0.41
1:C:174:ARG:O	1:C:177:SER:HB3	2.20	0.41
1:J:227:ILE:O	1:J:227:ILE:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:175:GLU:HA	1:E:178:TRP:CE3	2.54	0.41
1:H:70:GLY:O	1:H:72:TRP:CZ3	2.73	0.41
1:H:55:CYS:HB3	1:H:82:HIS:HA	2.03	0.41
1:D:433:THR:HG22	1:E:412:SER:HA	2.01	0.41
1:C:137:THR:HG23	1:C:140:GLU:CD	2.41	0.41
1:F:453:LEU:HD23	1:F:453:LEU:C	2.40	0.41
1:J:414:GLN:HB2	1:J:429:PRO:HG2	2.02	0.41
1:C:429:PRO:C	1:C:431:VAL:N	2.70	0.41
1:I:88:PRO:HG3	1:I:385:TRP:CZ2	2.56	0.41
1:G:6:ASP:O	1:G:7:PRO:C	2.59	0.41
1:B:315:LEU:HD22	1:B:315:LEU:N	2.35	0.41
1:F:203:ILE:H	1:F:203:ILE:HD12	1.84	0.41
1:A:121:PRO:CD	1:A:382:TYR:CE1	3.03	0.41
1:E:70:GLY:O	1:E:72:TRP:CZ3	2.73	0.41
1:C:399:PHE:HE1	1:C:444:SER:HA	1.84	0.41
1:G:287:ASP:HA	1:G:288:PRO:HD2	1.87	0.41
1:C:203:ILE:HD12	1:C:203:ILE:N	2.36	0.41
1:K:287:ASP:HA	1:K:288:PRO:HD2	1.87	0.41
1:L:288:PRO:N	1:L:291:LEU:HD22	2.35	0.41
3:H:601:XEG:HAJ	3:H:601:XEG:HBE	1.73	0.41
1:A:35:ARG:C	1:A:37:THR:H	2.24	0.41
1:B:431:VAL:HA	1:B:432:PRO:HD2	1.71	0.41
1:K:141:LEU:HA	1:K:141:LEU:HD22	1.74	0.41
1:G:220:PHE:O	1:G:222:GLY:N	2.53	0.41
1:D:15:GLY:O	1:D:16:PHE:C	2.58	0.41
1:G:82:HIS:ND1	1:G:109:SER:HA	2.35	0.41
1:E:9:PHE:HA	1:E:329:LYS:NZ	2.35	0.41
1:I:23:ILE:HG22	1:I:471:TYR:HD1	1.84	0.41
1:J:498:VAL:HG12	1:J:498:VAL:O	2.21	0.41
1:G:409:LEU:C	1:G:411:MET:N	2.74	0.41
1:C:392:VAL:CG1	1:E:386:LEU:CD1	2.98	0.41
1:E:86:ARG:HH12	1:E:492:VAL:CG2	2.33	0.41
1:J:471:TYR:O	1:J:473:LEU:HD12	2.21	0.41
1:C:433:THR:HG22	1:D:412:SER:HA	2.03	0.41
1:A:409:LEU:C	1:A:411:MET:H	2.21	0.41
1:J:499:THR:O	1:J:500:PHE:HD2	2.03	0.41
1:B:118:VAL:O	1:B:118:VAL:HG23	2.20	0.41
1:K:477:LEU:O	1:K:478:ARG:C	2.58	0.41
1:D:93:ILE:CG2	1:D:127:ALA:HB3	2.44	0.41
1:G:470:LYS:C	1:G:471:TYR:HD2	2.24	0.41
1:K:331:LEU:O	1:K:353:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:GLY:O	1:E:16:PHE:C	2.59	0.41
1:L:120:VAL:HG13	1:L:121:PRO:HD2	2.02	0.41
1:C:90:LYS:HB2	1:C:122:PHE:HD1	1.77	0.41
1:H:152:LEU:HD13	1:H:152:LEU:HA	1.61	0.41
1:G:227:ILE:HD11	1:G:343:ILE:CD1	2.50	0.41
1:D:87:THR:CB	1:D:88:PRO:HD3	2.44	0.41
1:H:445:GLU:O	1:H:449:VAL:HG23	2.20	0.41
1:L:314:ILE:HG12	1:L:314:ILE:H	1.47	0.41
1:I:35:ARG:O	1:I:37:THR:HG22	2.20	0.41
1:E:339:VAL:HG21	1:E:360:PHE:CE1	2.55	0.41
1:A:134:LYS:HG2	1:A:134:LYS:H	1.57	0.41
1:A:339:VAL:HG23	1:A:339:VAL:O	2.21	0.41
1:L:322:LEU:C	1:L:322:LEU:HD13	2.41	0.41
1:E:322:LEU:C	1:E:322:LEU:HD13	2.41	0.41
1:A:211:ARG:O	1:A:211:ARG:HG2	2.19	0.41
1:C:143:LYS:O	1:C:144:ILE:C	2.58	0.41
1:L:460:SER:O	1:L:463:GLN:N	2.53	0.41
1:A:227:ILE:CG2	1:A:227:ILE:O	2.68	0.41
1:H:61:LEU:HD13	1:H:61:LEU:HA	1.77	0.41
1:J:402:GLU:C	1:J:404:ASP:N	2.72	0.41
1:E:181:ASP:O	1:E:182:THR:C	2.59	0.41
1:F:61:LEU:O	1:F:62:SER:CB	2.69	0.41
1:H:256:GLY:O	1:H:257:LEU:C	2.59	0.41
1:I:417:LEU:HD21	1:K:417:LEU:CD2	2.49	0.41
1:F:252:PHE:HE2	1:F:260:MET:SD	2.44	0.41
1:L:188:GLY:O	1:L:189:HIS:C	2.58	0.41
1:A:366:MET:HB2	1:A:475:LEU:CD1	2.40	0.41
1:B:29:VAL:O	1:B:41:LYS:HD3	2.21	0.41
1:E:491:ARG:CZ	1:E:491:ARG:HB2	2.50	0.41
1:C:436:PHE:CE2	1:D:409:LEU:CD1	3.03	0.41
1:B:412:SER:O	1:B:416:SER:HB2	2.20	0.41
1:F:414:GLN:HB2	1:F:429:PRO:HG2	2.03	0.41
1:J:90:LYS:CB	1:J:122:PHE:CD1	3.01	0.41
1:D:336:ALA:CB	1:D:337:PRO:CD	2.97	0.41
1:K:108:ALA:HB1	1:K:125:ALA:HA	2.03	0.41
1:G:449:VAL:O	1:G:450:HIS:C	2.58	0.41
1:C:78:TYR:CD2	1:C:101:VAL:HG22	2.54	0.41
1:C:118:VAL:O	1:C:118:VAL:HG23	2.21	0.41
1:C:445:GLU:O	1:C:446:LYS:C	2.59	0.41
1:C:203:ILE:H	1:C:203:ILE:HD12	1.86	0.41
1:I:238:MET:HE1	1:I:343:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:294:PHE:O	1:K:300:THR:O	2.39	0.41
1:A:412:SER:O	1:A:416:SER:HB2	2.21	0.41
1:E:421:PHE:O	1:E:423:LYS:N	2.51	0.41
1:K:490:PHE:O	1:K:492:VAL:N	2.54	0.41
1:I:460:SER:O	1:I:463:GLN:N	2.53	0.41
1:L:132:ASN:HA	1:L:133:PRO:HD3	1.76	0.41
1:B:8:ASN:HD22	1:B:329:LYS:CD	2.31	0.41
1:L:53:LYS:N	1:L:54:PRO:CD	2.83	0.41
1:J:501:THR:HB	1:K:185:SER:HB2	2.03	0.41
1:F:485:ALA:O	1:F:486:ILE:C	2.59	0.41
1:D:174:ARG:O	1:D:177:SER:HB3	2.20	0.41
1:C:372:TYR:CD1	1:C:372:TYR:C	2.93	0.41
1:K:437:GLN:HA	1:K:437:GLN:OE1	2.20	0.41
1:D:63:PHE:N	1:D:63:PHE:CD2	2.89	0.41
1:I:338:ARG:HB3	1:I:338:ARG:CZ	2.51	0.41
1:I:414:GLN:HB2	1:I:429:PRO:CG	2.51	0.41
1:J:414:GLN:HB2	1:J:429:PRO:CG	2.50	0.41
1:J:432:PRO:HA	1:K:412:SER:HB3	2.02	0.41
1:A:294:PHE:O	1:A:300:THR:O	2.39	0.41
1:E:121:PRO:CD	1:E:382:TYR:CE1	3.03	0.41
1:C:412:SER:O	1:C:416:SER:HB2	2.21	0.41
1:B:410:LEU:O	1:B:411:MET:HG2	2.21	0.41
1:I:8:ASN:O	1:I:10:PHE:N	2.54	0.41
1:C:94:ARG:HG3	1:C:169:MET:CB	2.34	0.41
1:A:167:PRO:HD2	1:A:199:THR:O	2.20	0.41
1:H:366:MET:HB2	1:H:475:LEU:HD22	2.02	0.41
1:E:331:LEU:O	1:E:353:THR:HG23	2.21	0.41
1:J:236:LEU:HD22	1:J:342:LYS:HD2	2.03	0.41
1:J:315:LEU:HG	1:J:331:LEU:HD11	2.03	0.41
1:E:460:SER:O	1:E:461:ALA:C	2.59	0.41
1:H:250:GLN:HG2	1:H:330:GLN:HE21	1.85	0.41
1:C:176:MET:HG3	1:C:198:VAL:HG22	2.01	0.41
1:C:90:LYS:HE2	1:C:381:SER:HB3	2.02	0.41
1:B:155:LYS:HE2	1:E:57:HIS:ND1	2.36	0.41
1:L:201:LYS:HD3	1:L:201:LYS:H	1.86	0.41
1:L:288:PRO:CA	1:L:291:LEU:HD22	2.51	0.41
1:B:475:LEU:HA	1:B:475:LEU:HD23	1.80	0.41
1:B:273:VAL:HB	1:B:280:ILE:CD1	2.51	0.41
1:A:271:ILE:HG23	1:A:272:THR:N	2.34	0.41
1:L:243:GLY:C	1:L:245:LYS:H	2.24	0.41
1:H:414:GLN:HB2	1:H:429:PRO:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:GLY:O	1:B:426:GLY:C	2.58	0.41
1:E:35:ARG:C	1:E:37:THR:H	2.24	0.41
1:D:339:VAL:O	1:D:339:VAL:HG23	2.20	0.41
1:A:423:LYS:O	1:A:424:HIS:C	2.58	0.41
1:G:35:ARG:O	1:G:37:THR:HG22	2.21	0.41
1:I:212:ILE:HG12	1:I:213:SER:H	1.86	0.41
1:L:180:ALA:O	1:L:181:ASP:C	2.58	0.41
1:L:417:LEU:HD12	1:L:417:LEU:HA	1.83	0.41
1:H:137:THR:HG23	1:H:140:GLU:CD	2.41	0.41
1:G:216:GLY:C	1:G:218:GLY:N	2.72	0.41
1:E:174:ARG:HB3	1:E:174:ARG:HE	1.64	0.41
1:E:294:PHE:O	1:E:300:THR:O	2.39	0.41
1:D:38:GLU:CD	1:D:39:GLU:N	2.74	0.41
1:K:412:SER:O	1:K:416:SER:HB2	2.21	0.41
1:I:412:SER:O	1:I:416:SER:HB2	2.21	0.41
1:H:412:SER:O	1:H:416:SER:HB2	2.21	0.41
1:E:121:PRO:O	1:E:122:PHE:CD2	2.74	0.41
1:J:28:LEU:H	1:J:28:LEU:CD1	2.18	0.41
1:D:118:VAL:HG11	1:D:375:ALA:CB	2.51	0.41
1:C:429:PRO:C	1:C:431:VAL:H	2.25	0.41
1:C:431:VAL:HG13	1:C:431:VAL:O	2.21	0.41
1:D:411:MET:HA	1:D:414:GLN:HB3	2.02	0.41
1:E:409:LEU:C	1:E:411:MET:H	2.23	0.41
1:A:433:THR:HG22	1:F:412:SER:CA	2.51	0.41
1:E:498:VAL:O	1:E:499:THR:C	2.59	0.41
1:B:205:GLN:HE22	1:F:496:ALA:HB2	1.86	0.41
1:F:336:ALA:HB3	1:F:337:PRO:CD	2.34	0.41
1:B:86:ARG:HH12	1:B:492:VAL:HG13	1.85	0.41
1:L:390:ASN:O	1:L:392:VAL:HG22	2.21	0.41
1:H:288:PRO:CA	1:H:291:LEU:HD22	2.51	0.41
1:H:382:TYR:CE2	1:H:386:LEU:CD1	3.00	0.41
1:H:477:LEU:N	1:H:477:LEU:HD22	2.36	0.41
1:E:353:THR:OG1	1:E:355:GLU:HB2	2.20	0.41
1:I:166:ALA:CA	1:I:176:MET:HE2	2.49	0.41
1:I:201:LYS:HD3	1:I:201:LYS:H	1.86	0.41
1:J:368:ILE:HA	1:J:369:PRO:HD3	1.76	0.41
1:E:24:VAL:CG1	1:E:483:VAL:HG13	2.37	0.41
1:C:166:ALA:CA	1:C:176:MET:HE2	2.48	0.41
1:G:152:LEU:HA	1:G:152:LEU:HD13	1.61	0.41
1:F:390:ASN:O	1:F:392:VAL:HG22	2.21	0.41
1:C:400:LYS:HB2	1:E:455:TYR:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:500:PHE:HE2	1:J:142:GLU:OE2	2.04	0.41
1:B:397:LEU:HD11	1:F:383:PHE:CE2	2.56	0.41
1:J:382:TYR:O	1:J:385:TRP:HB3	2.21	0.41
1:G:238:MET:HE1	1:G:343:ILE:HD11	2.03	0.41
1:G:288:PRO:N	1:G:291:LEU:HD22	2.36	0.41
1:G:294:PHE:O	1:G:300:THR:O	2.39	0.41
1:B:236:LEU:HD22	1:B:342:LYS:HD2	2.02	0.41
1:H:488:LYS:HZ2	3:H:601:XEG:HAK	1.84	0.41
1:H:490:PHE:O	1:H:491:ARG:C	2.59	0.41
1:J:490:PHE:C	1:J:490:PHE:CD2	2.94	0.41
3:J:601:XEG:HAL	1:K:209:HIS:CE1	2.51	0.41
1:E:282:ASN:O	1:E:284:ASP:N	2.51	0.41
1:H:217:ARG:HG2	1:H:262:TYR:CD1	2.56	0.41
1:C:282:ASN:C	1:C:284:ASP:N	2.73	0.41
1:D:421:PHE:CE1	1:D:425:GLY:N	2.89	0.41
1:E:38:GLU:C	1:E:40:GLN:N	2.74	0.41
1:J:38:GLU:OE2	1:J:40:GLN:N	2.54	0.41
1:E:211:ARG:HG2	1:E:211:ARG:O	2.19	0.41
1:H:38:GLU:OE2	1:H:40:GLN:N	2.53	0.41
1:L:35:ARG:C	1:L:37:THR:H	2.23	0.41
1:D:236:LEU:HD22	1:D:342:LYS:HD2	2.02	0.41
1:D:236:LEU:HD21	1:D:342:LYS:HB3	2.03	0.41
1:C:421:PHE:O	1:C:423:LYS:N	2.50	0.41
1:J:212:ILE:H	1:J:212:ILE:CD1	2.19	0.41
1:F:460:SER:O	1:F:463:GLN:N	2.54	0.41
1:D:396:ARG:HH11	1:D:396:ARG:CG	2.28	0.41
1:F:371:LEU:HD23	1:F:481:ALA:CB	2.47	0.41
1:F:498:VAL:HG22	1:F:498:VAL:O	2.20	0.41
1:C:348:ALA:HB3	1:C:351:PRO:HG3	2.03	0.41
1:E:9:PHE:HB3	1:E:329:LYS:NZ	2.34	0.41
1:E:203:ILE:HA	1:E:207:GLY:H	1.86	0.41
1:K:20:GLY:O	1:K:21:ALA:C	2.59	0.41
1:G:438:ASP:O	1:G:440:ILE:N	2.53	0.41
1:C:437:GLN:HA	1:C:437:GLN:OE1	2.19	0.41
1:G:372:TYR:C	1:G:372:TYR:CD1	2.94	0.41
1:I:431:VAL:O	1:J:412:SER:HB3	2.21	0.41
1:K:431:VAL:HA	1:K:432:PRO:HD2	1.72	0.41
1:J:90:LYS:HA	1:J:164:VAL:O	2.21	0.41
1:I:121:PRO:CD	1:I:382:TYR:CE1	3.03	0.41
1:K:94:ARG:CZ	1:K:169:MET:HG3	2.51	0.41
1:G:6:ASP:CA	1:G:355:GLU:HG3	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ILE:HA	1:A:127:ALA:O	2.21	0.41
1:A:175:GLU:O	1:A:178:TRP:HB2	2.20	0.41
1:A:178:TRP:O	1:A:179:ILE:C	2.58	0.41
1:C:331:LEU:O	1:C:353:THR:HG23	2.21	0.41
1:C:473:LEU:N	1:C:473:LEU:HD12	2.35	0.41
1:E:372:TYR:CD1	1:E:372:TYR:C	2.94	0.41
1:K:12:MET:H	1:K:14:GLU:CG	2.21	0.41
1:G:59:LEU:CD2	1:G:61:LEU:HD22	2.50	0.41
1:C:382:TYR:HE2	1:C:386:LEU:CD2	2.27	0.41
1:C:444:SER:OG	1:C:446:LYS:HB3	2.21	0.41
1:G:291:LEU:CD1	1:G:291:LEU:N	2.85	0.41
1:I:236:LEU:HD22	1:I:342:LYS:HD2	2.02	0.41
1:D:61:LEU:O	1:D:62:SER:CB	2.69	0.41
1:B:59:LEU:HD23	1:B:61:LEU:CD2	2.51	0.41
1:B:59:LEU:HD23	1:B:61:LEU:HD22	2.03	0.41
1:J:274:GLY:HA3	1:J:314:ILE:HD13	2.03	0.41
1:F:243:GLY:C	1:F:245:LYS:HE2	2.41	0.41
1:C:243:GLY:C	1:C:245:LYS:H	2.24	0.41
1:J:421:PHE:CE1	1:J:425:GLY:N	2.88	0.41
1:C:459:ARG:NH2	3:D:601:XEG:OAH	2.54	0.41
1:D:393:SER:OG	3:D:601:XEG:CAM	2.69	0.41
1:J:44:ARG:HG3	1:J:45:VAL:N	2.36	0.41
1:D:243:GLY:C	1:D:245:LYS:HE2	2.41	0.41
1:J:141:LEU:HD22	1:J:141:LEU:HA	1.73	0.41
1:C:396:ARG:CG	1:C:396:ARG:NH1	2.82	0.41
1:L:301:ILE:HD12	1:L:301:ILE:O	2.21	0.41
1:J:132:ASN:HA	1:J:133:PRO:HD3	1.82	0.41
1:I:82:HIS:ND1	1:I:109:SER:HA	2.35	0.41
1:L:47:SER:O	1:L:50:ARG:N	2.49	0.41
1:E:437:GLN:HA	1:E:437:GLN:OE1	2.19	0.41
1:G:358:LYS:HA	1:G:358:LYS:HD2	1.97	0.41
1:D:29:VAL:O	1:D:41:LYS:HD3	2.20	0.40
1:B:38:GLU:CD	1:B:39:GLU:N	2.75	0.40
1:E:411:MET:HA	1:E:414:GLN:HB3	2.03	0.40
1:C:416:SER:CB	1:E:429:PRO:HA	2.51	0.40
1:A:114:LYS:HZ1	1:A:349:ASN:HD21	1.69	0.40
1:A:429:PRO:C	1:A:431:VAL:H	2.23	0.40
1:J:201:LYS:HA	1:J:202:PRO:HD2	1.72	0.40
1:J:79:ARG:HG2	1:J:127:ALA:CB	2.31	0.40
1:B:353:THR:OG1	1:B:355:GLU:HB2	2.21	0.40
3:G:601:XEG:HAJ	3:G:601:XEG:HBE	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:203:ILE:HG21	1:F:209:HIS:NE2	2.35	0.40
1:K:383:PHE:N	1:K:383:PHE:CD2	2.89	0.40
1:E:158:ILE:O	1:E:158:ILE:HG23	2.21	0.40
1:E:59:LEU:CD2	1:E:61:LEU:HD22	2.51	0.40
1:F:199:THR:HG22	1:F:384:GLU:HG2	2.02	0.40
1:C:166:ALA:HB1	1:C:167:PRO:HD2	2.01	0.40
1:H:90:LYS:CB	1:H:122:PHE:CD1	3.00	0.40
1:C:294:PHE:O	1:C:300:THR:O	2.38	0.40
1:J:117:VAL:HG12	1:J:118:VAL:CG1	2.51	0.40
1:D:61:LEU:HA	1:D:61:LEU:HD13	1.79	0.40
1:G:393:SER:OG	3:H:601:XEG:CAM	2.69	0.40
1:I:271:ILE:HG23	1:I:272:THR:HG23	2.03	0.40
1:B:226:PHE:CD2	1:B:465:MET:HE2	2.56	0.40
1:C:371:LEU:HD22	1:C:482:TYR:CD2	2.56	0.40
1:F:322:LEU:HD13	1:F:322:LEU:C	2.42	0.40
1:A:322:LEU:HD13	1:A:322:LEU:C	2.41	0.40
1:I:256:GLY:O	1:I:257:LEU:C	2.59	0.40
1:G:132:ASN:HA	1:G:133:PRO:HD3	1.81	0.40
1:D:210:GLY:HA2	1:D:446:LYS:HZ3	1.85	0.40
1:H:149:THR:HB	1:H:182:THR:HG21	2.03	0.40
1:L:61:LEU:O	1:L:62:SER:HB2	2.21	0.40
1:D:276:SER:HB3	2:D:552:NDP:O1X	2.20	0.40
1:K:409:LEU:C	1:K:411:MET:N	2.74	0.40
1:H:411:MET:C	1:L:433:THR:HG22	2.42	0.40
1:L:255:VAL:CG1	2:L:552:NDP:O2N	2.67	0.40
1:D:477:LEU:O	1:D:478:ARG:C	2.59	0.40
1:E:413:VAL:CG1	1:E:429:PRO:HG3	2.46	0.40
1:I:478:ARG:O	1:I:481:ALA:N	2.54	0.40
1:C:149:THR:O	1:C:150:MET:C	2.60	0.40
1:E:167:PRO:HD2	1:E:199:THR:O	2.21	0.40
1:B:336:ALA:CB	1:B:337:PRO:CD	2.98	0.40
1:B:378:VAL:CG1	1:B:379:THR:N	2.84	0.40
1:G:468:ALA:HB1	1:G:480:ALA:HB1	2.02	0.40
1:G:370:ASP:OD1	1:G:371:LEU:N	2.54	0.40
1:I:398:THR:O	1:I:399:PHE:C	2.59	0.40
1:J:236:LEU:HD21	1:J:342:LYS:HB3	2.03	0.40
1:F:176:MET:HG3	1:F:198:VAL:HG21	2.03	0.40
1:A:386:LEU:CD1	1:F:392:VAL:CG1	2.99	0.40
1:H:86:ARG:NH1	1:H:492:VAL:CG1	2.84	0.40
1:C:90:LYS:HG3	1:C:122:PHE:CD1	2.56	0.40
1:C:288:PRO:N	1:C:291:LEU:HD22	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:288:PRO:N	1:K:291:LEU:HD22	2.36	0.40
1:D:59:LEU:HD23	1:D:61:LEU:HD22	2.03	0.40
1:B:61:LEU:HA	1:B:61:LEU:HD13	1.78	0.40
1:E:243:GLY:C	1:E:245:LYS:HE2	2.42	0.40
1:H:414:GLN:HB2	1:H:429:PRO:CG	2.51	0.40
1:F:38:GLU:CD	1:F:39:GLU:N	2.75	0.40
1:A:38:GLU:C	1:A:40:GLN:N	2.74	0.40
1:L:213:SER:HB2	1:L:262:TYR:CE2	2.56	0.40
1:H:212:ILE:CD1	1:H:212:ILE:H	2.20	0.40
1:B:217:ARG:HD2	1:B:450:HIS:CD2	2.56	0.40
1:A:227:ILE:O	1:A:227:ILE:HG22	2.20	0.40
1:D:370:ASP:O	1:D:374:ASN:OD1	2.40	0.40
1:B:58:VAL:CG1	1:E:60:SER:HB2	2.51	0.40
1:F:348:ALA:HB3	1:F:351:PRO:HG3	2.02	0.40
1:F:158:ILE:O	1:F:183:TYR:HE1	2.03	0.40
1:A:9:PHE:HA	1:A:329:LYS:HZ3	1.85	0.40
1:C:175:GLU:O	1:C:178:TRP:HB2	2.20	0.40
1:A:203:ILE:HA	1:A:207:GLY:H	1.86	0.40
1:I:203:ILE:N	1:I:203:ILE:HD12	2.36	0.40
1:C:406:ASN:HD22	1:C:406:ASN:HA	1.73	0.40
1:D:477:LEU:N	1:D:477:LEU:HD22	2.37	0.40
1:B:99:VAL:HA	1:B:103:GLU:OE1	2.21	0.40
1:B:99:VAL:HG23	1:B:130:LYS:HA	2.04	0.40
1:A:353:THR:OG1	1:A:355:GLU:HB2	2.20	0.40
1:I:491:ARG:HD2	3:I:601:XEG:HOAB	1.75	0.40
1:K:164:VAL:HG13	1:K:198:VAL:CA	2.42	0.40
1:K:117:VAL:HG12	1:K:118:VAL:CG1	2.50	0.40
1:K:473:LEU:HD12	1:K:473:LEU:H	1.86	0.40
1:G:88:PRO:HG2	1:G:122:PHE:CE2	2.56	0.40
1:G:394:TYR:CZ	1:L:397:LEU:CD2	3.04	0.40
1:C:45:VAL:HG22	1:C:490:PHE:HZ	1.87	0.40
1:H:301:ILE:O	1:H:301:ILE:HD12	2.22	0.40
1:L:130:LYS:HG3	1:L:130:LYS:O	2.22	0.40
1:C:202:PRO:HG2	1:C:205:GLN:HG2	2.04	0.40
1:E:16:PHE:HD2	1:E:16:PHE:N	2.19	0.40
1:D:12:MET:HG3	1:D:13:VAL:HG12	2.02	0.40
1:B:396:ARG:NE	3:F:601:XEG:OAF	2.47	0.40
1:G:287:ASP:C	1:G:291:LEU:HD13	2.40	0.40
1:I:288:PRO:CA	1:I:291:LEU:HD22	2.51	0.40
1:K:288:PRO:CA	1:K:291:LEU:HD22	2.51	0.40
1:C:35:ARG:C	1:C:37:THR:H	2.23	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:313:SER:O	1:L:315:LEU:N	2.51	0.40
1:E:141:LEU:HD22	1:E:141:LEU:HA	1.72	0.40
1:E:227:ILE:CG2	1:E:227:ILE:O	2.69	0.40
1:H:339:VAL:HG21	1:H:360:PHE:CE1	2.55	0.40
1:H:236:LEU:HD21	1:H:342:LYS:HB3	2.04	0.40
1:K:256:GLY:O	1:K:257:LEU:C	2.59	0.40
1:C:453:LEU:O	1:C:457:MET:HB2	2.22	0.40
1:J:396:ARG:CG	1:J:396:ARG:NH1	2.84	0.40
1:A:236:LEU:HD21	1:A:342:LYS:HB3	2.04	0.40
1:J:129:VAL:HG12	1:J:129:VAL:O	2.21	0.40
1:A:9:PHE:HB3	1:A:329:LYS:NZ	2.35	0.40
1:I:191:ASP:O	1:I:192:ILE:C	2.59	0.40
1:J:316:GLU:HB2	1:J:317:VAL:H	1.71	0.40
1:I:203:ILE:O	1:I:203:ILE:CG2	2.69	0.40
1:E:117:VAL:HG12	1:E:118:VAL:N	2.35	0.40
1:E:301:ILE:O	1:E:301:ILE:HD12	2.21	0.40
1:J:431:VAL:HA	1:J:432:PRO:HD2	1.75	0.40
1:C:392:VAL:HG13	1:E:386:LEU:CD2	2.52	0.40
1:G:6:ASP:N	1:G:7:PRO:HD3	2.36	0.40
1:K:176:MET:HG2	1:K:200:GLY:HA3	2.02	0.40
1:G:213:SER:HB2	1:G:262:TYR:CE2	2.57	0.40
1:G:167:PRO:HD2	1:G:199:THR:O	2.21	0.40
1:K:6:ASP:OD1	1:K:7:PRO:N	2.55	0.40
1:F:166:ALA:CA	1:F:176:MET:HE2	2.50	0.40
1:E:27:LYS:HD2	1:E:471:TYR:OH	2.21	0.40
1:C:121:PRO:O	1:C:122:PHE:HD2	2.05	0.40
1:C:383:PHE:N	1:C:383:PHE:CD2	2.86	0.40
1:C:444:SER:O	1:C:445:GLU:C	2.58	0.40
1:I:500:PHE:HB3	1:I:501:THR:H	1.75	0.40
1:C:301:ILE:O	1:C:301:ILE:HD12	2.22	0.40
1:F:445:GLU:O	1:F:446:LYS:C	2.59	0.40
1:L:167:PRO:HD2	1:L:199:THR:O	2.22	0.40
1:L:201:LYS:HA	1:L:202:PRO:HD2	1.78	0.40
1:L:291:LEU:CD1	1:L:291:LEU:N	2.85	0.40
1:F:59:LEU:HD12	1:F:59:LEU:HA	1.57	0.40
1:K:271:ILE:HD11	1:K:283:PRO:HG3	2.02	0.40
1:L:271:ILE:CD1	1:L:283:PRO:HG3	2.52	0.40
1:I:273:VAL:HB	1:I:280:ILE:CD1	2.51	0.40
1:G:421:PHE:CE1	1:G:425:GLY:N	2.90	0.40
1:G:420:LYS:O	1:G:421:PHE:HB2	2.21	0.40
1:H:243:GLY:C	1:H:245:LYS:HE2	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:GLU:CD	1:C:39:GLU:N	2.75	0.40
1:H:421:PHE:CE1	1:H:425:GLY:N	2.89	0.40
1:D:315:LEU:HG	1:D:331:LEU:HD11	2.02	0.40
1:J:243:GLY:C	1:J:245:LYS:H	2.25	0.40
1:E:421:PHE:CE1	1:E:425:GLY:N	2.89	0.40
1:C:8:ASN:C	1:C:9:PHE:CG	2.94	0.40
1:G:220:PHE:C	1:G:222:GLY:N	2.74	0.40
1:G:322:LEU:C	1:G:322:LEU:HD13	2.41	0.40
1:H:236:LEU:HD22	1:H:342:LYS:HD2	2.03	0.40
1:F:221:HIS:HB2	1:F:457:MET:HG2	2.02	0.40
1:D:217:ARG:NE	1:D:450:HIS:CD2	2.89	0.40
1:C:242:PHE:N	1:C:242:PHE:HD1	2.20	0.40
1:I:402:GLU:C	1:I:404:ASP:N	2.72	0.40
1:G:129:VAL:O	1:G:129:VAL:HG12	2.21	0.40
1:J:451:SER:OG	1:K:400:LYS:HB3	2.22	0.40
1:C:477:LEU:H	1:C:477:LEU:HD22	1.86	0.40
1:L:183:TYR:C	1:L:183:TYR:CD2	2.95	0.40
1:D:338:ARG:CZ	1:D:338:ARG:HB3	2.52	0.40
1:C:358:LYS:HA	1:C:358:LYS:HD2	1.98	0.40
1:I:414:GLN:HB2	1:I:429:PRO:HG2	2.04	0.40
1:K:413:VAL:HG12	1:K:429:PRO:CG	2.50	0.40
1:H:409:LEU:C	1:H:411:MET:N	2.75	0.40
1:F:409:LEU:O	1:F:411:MET:N	2.49	0.40
1:H:99:VAL:HG11	1:H:128:GLY:CA	2.32	0.40
1:A:201:LYS:HA	1:A:202:PRO:HD2	1.76	0.40
1:K:211:ARG:O	1:K:214:ALA:HB3	2.22	0.40
1:L:490:PHE:C	1:L:492:VAL:H	2.25	0.40
1:A:141:LEU:HA	1:A:141:LEU:HD22	1.73	0.40
1:F:291:LEU:N	1:F:291:LEU:CD1	2.85	0.40
1:G:288:PRO:CA	1:G:291:LEU:HD22	2.51	0.40
1:K:291:LEU:N	1:K:291:LEU:CD1	2.85	0.40
1:D:294:PHE:O	1:D:300:THR:O	2.40	0.40
1:D:282:ASN:C	1:D:284:ASP:N	2.73	0.40
1:A:271:ILE:CD1	1:A:283:PRO:HG3	2.52	0.40
1:L:271:ILE:HG23	1:L:272:THR:HG23	2.03	0.40
1:I:271:ILE:CD1	1:I:283:PRO:HG3	2.51	0.40
1:H:8:ASN:ND2	1:H:9:PHE:CZ	2.88	0.40
1:F:282:ASN:C	1:F:284:ASP:N	2.74	0.40
1:G:412:SER:O	1:G:416:SER:HB2	2.21	0.40
1:G:425:GLY:O	1:G:426:GLY:C	2.60	0.40
1:B:243:GLY:C	1:B:245:LYS:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:LYS:O	1:D:144:ILE:C	2.59	0.40
1:C:493:TYR:HA	1:C:493:TYR:HD1	1.59	0.40
1:H:227:ILE:O	1:H:227:ILE:HG22	2.20	0.40
1:D:433:THR:HG22	1:E:412:SER:CA	2.52	0.40
1:A:20:GLY:O	1:A:21:ALA:C	2.59	0.40
1:J:203:ILE:HD12	1:J:203:ILE:H	1.86	0.40
1:E:183:TYR:CD2	1:E:183:TYR:C	2.95	0.40
1:A:437:GLN:OE1	1:A:437:GLN:HA	2.22	0.40
1:G:453:LEU:CD2	1:G:453:LEU:C	2.89	0.40
1:B:453:LEU:CD2	1:B:453:LEU:C	2.90	0.40
1:D:437:GLN:OE1	1:D:437:GLN:HA	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:362:GLU:O	1:E:38:GLU:OE2[1_556]	2.11	0.09
1:A:38:GLU:OE2	1:B:362:GLU:O[1_455]	2.12	0.08
1:A:36:GLU:OE2	1:B:362:GLU:O[1_455]	2.17	0.03

## 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	494/501 (99%)	313 (63%)	113 (23%)	68 (14%)	0	6
1	B	494/501 (99%)	322 (65%)	104 (21%)	68 (14%)	0	6
1	C	494/501 (99%)	321 (65%)	107 (22%)	66 (13%)	0	6
1	D	494/501 (99%)	318 (64%)	112 (23%)	64 (13%)	0	7
1	E	494/501 (99%)	313 (63%)	113 (23%)	68 (14%)	0	6
1	F	494/501 (99%)	319 (65%)	111 (22%)	64 (13%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	494/501 (99%)	325 (66%)	106 (22%)	63 (13%)	0	7
1	H	494/501 (99%)	322 (65%)	106 (22%)	66 (13%)	0	6
1	I	494/501 (99%)	321 (65%)	108 (22%)	65 (13%)	0	6
1	J	494/501 (99%)	321 (65%)	110 (22%)	63 (13%)	0	7
1	K	494/501 (99%)	324 (66%)	108 (22%)	62 (13%)	0	7
1	L	494/501 (99%)	320 (65%)	111 (22%)	63 (13%)	0	7
All	All	5928/6012 (99%)	3839 (65%)	1309 (22%)	780 (13%)	0	6

All (780) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	PRO
1	A	12	MET
1	A	30	GLU
1	A	62	SER
1	A	87	THR
1	A	130	LYS
1	A	266	PHE
1	A	282	ASN
1	A	290	GLU
1	A	317	VAL
1	A	319	CYS
1	A	421	PHE
1	A	424	HIS
1	A	433	THR
1	A	468	ALA
1	A	494	ASN
1	A	495	GLU
1	B	12	MET
1	B	30	GLU
1	B	39	GLU
1	B	62	SER
1	B	87	THR
1	B	130	LYS
1	B	168	ASP
1	B	191	ASP
1	B	266	PHE
1	B	282	ASN
1	B	290	GLU
1	B	317	VAL

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Mol	Chain	Res	Type
1	B	319	CYS
1	B	421	PHE
1	B	424	HIS
1	B	433	THR
1	B	468	ALA
1	C	7	PRO
1	C	12	MET
1	C	30	GLU
1	C	62	SER
1	C	87	THR
1	C	130	LYS
1	C	191	ASP
1	C	266	PHE
1	C	282	ASN
1	C	290	GLU
1	C	317	VAL
1	C	319	CYS
1	C	421	PHE
1	C	424	HIS
1	C	433	THR
1	C	468	ALA
1	C	494	ASN
1	C	500	PHE
1	D	12	MET
1	D	30	GLU
1	D	39	GLU
1	D	62	SER
1	D	67	ARG
1	D	87	THR
1	D	130	LYS
1	D	168	ASP
1	D	191	ASP
1	D	266	PHE
1	D	282	ASN
1	D	290	GLU
1	D	317	VAL
1	D	319	CYS
1	D	421	PHE
1	D	424	HIS
1	D	433	THR
1	D	468	ALA
1	D	496	ALA

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Mol	Chain	Res	Type
1	E	12	MET
1	E	30	GLU
1	E	62	SER
1	E	87	THR
1	E	130	LYS
1	E	191	ASP
1	E	266	PHE
1	E	282	ASN
1	E	290	GLU
1	E	317	VAL
1	E	319	CYS
1	E	403	ARG
1	E	421	PHE
1	E	424	HIS
1	E	433	THR
1	E	468	ALA
1	E	494	ASN
1	E	495	GLU
1	F	8	ASN
1	F	12	MET
1	F	30	GLU
1	F	62	SER
1	F	87	THR
1	F	130	LYS
1	F	168	ASP
1	F	191	ASP
1	F	266	PHE
1	F	282	ASN
1	F	290	GLU
1	F	317	VAL
1	F	319	CYS
1	F	421	PHE
1	F	424	HIS
1	F	430	ILE
1	F	433	THR
1	F	468	ALA
1	G	12	MET
1	G	30	GLU
1	G	39	GLU
1	G	62	SER
1	G	87	THR
1	G	130	LYS

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Mol	Chain	Res	Type
1	G	191	ASP
1	G	266	PHE
1	G	282	ASN
1	G	290	GLU
1	G	317	VAL
1	G	319	CYS
1	G	396	ARG
1	G	410	LEU
1	G	421	PHE
1	G	424	HIS
1	G	433	THR
1	G	468	ALA
1	H	12	MET
1	H	30	GLU
1	H	39	GLU
1	H	62	SER
1	H	87	THR
1	H	130	LYS
1	H	168	ASP
1	H	191	ASP
1	H	266	PHE
1	H	282	ASN
1	H	290	GLU
1	H	317	VAL
1	H	319	CYS
1	H	410	LEU
1	H	421	PHE
1	H	424	HIS
1	H	433	THR
1	H	468	ALA
1	H	498	VAL
1	I	9	PHE
1	I	12	MET
1	I	30	GLU
1	I	62	SER
1	I	87	THR
1	I	130	LYS
1	I	266	PHE
1	I	282	ASN
1	I	290	GLU
1	I	317	VAL
1	I	319	CYS

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Mol	Chain	Res	Type
1	I	421	PHE
1	I	424	HIS
1	I	433	THR
1	I	468	ALA
1	I	496	ALA
1	I	500	PHE
1	J	12	MET
1	J	30	GLU
1	J	39	GLU
1	J	62	SER
1	J	87	THR
1	J	130	LYS
1	J	168	ASP
1	J	191	ASP
1	J	266	PHE
1	J	282	ASN
1	J	290	GLU
1	J	317	VAL
1	J	319	CYS
1	J	396	ARG
1	J	410	LEU
1	J	421	PHE
1	J	424	HIS
1	J	433	THR
1	J	468	ALA
1	J	498	VAL
1	K	12	MET
1	K	30	GLU
1	K	39	GLU
1	K	62	SER
1	K	87	THR
1	K	130	LYS
1	K	191	ASP
1	K	266	PHE
1	K	282	ASN
1	K	290	GLU
1	K	317	VAL
1	K	319	CYS
1	K	410	LEU
1	K	421	PHE
1	K	424	HIS
1	K	433	THR

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Mol	Chain	Res	Type
1	K	468	ALA
1	K	494	ASN
1	L	12	MET
1	L	30	GLU
1	L	62	SER
1	L	87	THR
1	L	130	LYS
1	L	266	PHE
1	L	282	ASN
1	L	290	GLU
1	L	317	VAL
1	L	319	CYS
1	L	421	PHE
1	L	424	HIS
1	L	433	THR
1	L	468	ALA
1	L	496	ALA
1	L	497	GLY
1	A	25	GLU
1	A	39	GLU
1	A	67	ARG
1	A	163	ASP
1	A	168	ASP
1	A	191	ASP
1	A	240	PRO
1	A	243	GLY
1	A	254	ASN
1	A	265	ARG
1	A	274	GLY
1	A	300	THR
1	A	313	SER
1	A	314	ILE
1	A	351	PRO
1	A	396	ARG
1	A	403	ARG
1	A	410	LEU
1	A	426	GLY
1	A	430	ILE
1	A	459	ARG
1	A	466	ARG
1	A	493	TYR
1	B	25	GLU

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Mol	Chain	Res	Type
1	B	37	THR
1	B	67	ARG
1	B	163	ASP
1	B	235	ILE
1	B	240	PRO
1	B	243	GLY
1	B	265	ARG
1	B	274	GLY
1	B	300	THR
1	B	313	SER
1	B	314	ILE
1	B	351	PRO
1	B	396	ARG
1	B	410	LEU
1	B	426	GLY
1	B	430	ILE
1	B	466	ARG
1	B	493	TYR
1	B	498	VAL
1	C	9	PHE
1	C	25	GLU
1	C	37	THR
1	C	39	GLU
1	C	67	ARG
1	C	163	ASP
1	C	168	ASP
1	C	235	ILE
1	C	240	PRO
1	C	243	GLY
1	C	254	ASN
1	C	265	ARG
1	C	274	GLY
1	C	300	THR
1	C	314	ILE
1	C	351	PRO
1	C	396	ARG
1	C	410	LEU
1	C	426	GLY
1	C	430	ILE
1	C	459	ARG
1	C	466	ARG
1	C	491	ARG

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Mol	Chain	Res	Type
1	D	25	GLU
1	D	37	THR
1	D	103	GLU
1	D	235	ILE
1	D	240	PRO
1	D	243	GLY
1	D	265	ARG
1	D	274	GLY
1	D	300	THR
1	D	313	SER
1	D	314	ILE
1	D	396	ARG
1	D	410	LEU
1	D	426	GLY
1	D	430	ILE
1	D	459	ARG
1	D	466	ARG
1	E	8	ASN
1	E	25	GLU
1	E	39	GLU
1	E	67	ARG
1	E	163	ASP
1	E	168	ASP
1	E	235	ILE
1	E	240	PRO
1	E	243	GLY
1	E	254	ASN
1	E	265	ARG
1	E	274	GLY
1	E	300	THR
1	E	313	SER
1	E	314	ILE
1	E	351	PRO
1	E	375	ALA
1	E	396	ARG
1	E	410	LEU
1	E	426	GLY
1	E	430	ILE
1	E	459	ARG
1	E	466	ARG
1	E	499	THR
1	F	9	PHE

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Mol	Chain	Res	Type
1	F	25	GLU
1	F	37	THR
1	F	39	GLU
1	F	67	ARG
1	F	163	ASP
1	F	240	PRO
1	F	243	GLY
1	F	254	ASN
1	F	265	ARG
1	F	274	GLY
1	F	300	THR
1	F	314	ILE
1	F	351	PRO
1	F	396	ARG
1	F	403	ARG
1	F	410	LEU
1	F	426	GLY
1	F	459	ARG
1	F	466	ARG
1	G	25	GLU
1	G	67	ARG
1	G	168	ASP
1	G	220	PHE
1	G	235	ILE
1	G	240	PRO
1	G	243	GLY
1	G	254	ASN
1	G	265	ARG
1	G	274	GLY
1	G	300	THR
1	G	314	ILE
1	G	351	PRO
1	G	403	ARG
1	G	426	GLY
1	G	430	ILE
1	G	466	ARG
1	G	491	ARG
1	H	9	PHE
1	H	25	GLU
1	H	37	THR
1	H	67	ARG
1	H	163	ASP

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Mol	Chain	Res	Type
1	H	235	ILE
1	H	240	PRO
1	H	243	GLY
1	H	265	ARG
1	H	274	GLY
1	H	300	THR
1	H	313	SER
1	H	314	ILE
1	H	351	PRO
1	H	396	ARG
1	H	426	GLY
1	H	430	ILE
1	H	466	ARG
1	H	499	THR
1	I	25	GLU
1	I	37	THR
1	I	39	GLU
1	I	67	ARG
1	I	163	ASP
1	I	168	ASP
1	I	191	ASP
1	I	235	ILE
1	I	240	PRO
1	I	243	GLY
1	I	254	ASN
1	I	265	ARG
1	I	274	GLY
1	I	300	THR
1	I	314	ILE
1	I	351	PRO
1	I	396	ARG
1	I	410	LEU
1	I	426	GLY
1	I	430	ILE
1	I	459	ARG
1	I	466	ARG
1	J	25	GLU
1	J	37	THR
1	J	67	ARG
1	J	158	ILE
1	J	163	ASP
1	J	235	ILE

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Mol	Chain	Res	Type
1	J	240	PRO
1	J	243	GLY
1	J	265	ARG
1	J	274	GLY
1	J	300	THR
1	J	313	SER
1	J	314	ILE
1	J	351	PRO
1	J	403	ARG
1	J	426	GLY
1	J	430	ILE
1	J	466	ARG
1	K	25	GLU
1	K	67	ARG
1	K	168	ASP
1	K	220	PHE
1	K	235	ILE
1	K	240	PRO
1	K	243	GLY
1	K	254	ASN
1	K	265	ARG
1	K	274	GLY
1	K	300	THR
1	K	314	ILE
1	K	351	PRO
1	K	396	ARG
1	K	403	ARG
1	K	426	GLY
1	K	430	ILE
1	K	459	ARG
1	K	466	ARG
1	K	493	TYR
1	L	25	GLU
1	L	37	THR
1	L	39	GLU
1	L	67	ARG
1	L	158	ILE
1	L	168	ASP
1	L	191	ASP
1	L	235	ILE
1	L	240	PRO
1	L	243	GLY

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Mol	Chain	Res	Type
1	L	254	ASN
1	L	265	ARG
1	L	274	GLY
1	L	300	THR
1	L	313	SER
1	L	314	ILE
1	L	351	PRO
1	L	396	ARG
1	L	410	LEU
1	L	426	GLY
1	L	430	ILE
1	L	459	ARG
1	L	466	ARG
1	A	32	LEU
1	A	37	THR
1	A	38	GLU
1	A	235	ILE
1	A	268	ALA
1	A	308	LYS
1	A	375	ALA
1	A	439	ARG
1	A	478	ARG
1	A	499	THR
1	B	32	LEU
1	B	38	GLU
1	B	103	GLU
1	B	254	ASN
1	B	268	ALA
1	B	308	LYS
1	B	375	ALA
1	B	403	ARG
1	B	459	ARG
1	B	478	ARG
1	C	32	LEU
1	C	38	GLU
1	C	103	GLU
1	C	158	ILE
1	C	308	LYS
1	C	313	SER
1	C	403	ARG
1	D	32	LEU
1	D	38	GLU

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Mol	Chain	Res	Type
1	D	163	ASP
1	D	254	ASN
1	D	268	ALA
1	D	308	LYS
1	D	351	PRO
1	D	375	ALA
1	D	403	ARG
1	D	478	ARG
1	D	493	TYR
1	E	7	PRO
1	E	32	LEU
1	E	37	THR
1	E	38	GLU
1	E	268	ALA
1	E	308	LYS
1	E	478	ARG
1	F	32	LEU
1	F	38	GLU
1	F	103	GLU
1	F	235	ILE
1	F	308	LYS
1	F	313	SER
1	G	8	ASN
1	G	32	LEU
1	G	37	THR
1	G	38	GLU
1	G	44	ARG
1	G	158	ILE
1	G	163	ASP
1	G	308	LYS
1	G	313	SER
1	G	439	ARG
1	G	459	ARG
1	G	478	ARG
1	H	32	LEU
1	H	38	GLU
1	H	103	GLU
1	H	220	PHE
1	H	254	ASN
1	H	268	ALA
1	H	308	LYS
1	H	403	ARG

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Mol	Chain	Res	Type
1	H	459	ARG
1	I	32	LEU
1	I	38	GLU
1	I	103	GLU
1	I	220	PHE
1	I	268	ALA
1	I	308	LYS
1	I	313	SER
1	I	403	ARG
1	I	439	ARG
1	J	32	LEU
1	J	38	GLU
1	J	103	GLU
1	J	220	PHE
1	J	254	ASN
1	J	268	ALA
1	J	308	LYS
1	J	439	ARG
1	J	459	ARG
1	J	499	THR
1	K	32	LEU
1	K	37	THR
1	K	38	GLU
1	K	163	ASP
1	K	268	ALA
1	K	308	LYS
1	K	313	SER
1	K	478	ARG
1	K	498	VAL
1	L	32	LEU
1	L	38	GLU
1	L	103	GLU
1	L	163	ASP
1	L	220	PHE
1	L	268	ALA
1	L	308	LYS
1	L	403	ARG
1	L	499	THR
1	A	8	ASN
1	A	44	ARG
1	A	64	PRO
1	A	103	GLU

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Mol	Chain	Res	Type
1	A	158	ILE
1	A	220	PHE
1	A	411	MET
1	B	7	PRO
1	B	44	ARG
1	B	220	PHE
1	B	439	ARG
1	C	44	ARG
1	C	268	ALA
1	C	411	MET
1	D	44	ARG
1	D	158	ILE
1	D	220	PHE
1	D	439	ARG
1	D	498	VAL
1	E	44	ARG
1	E	103	GLU
1	E	220	PHE
1	E	411	MET
1	E	439	ARG
1	F	44	ARG
1	F	158	ILE
1	F	220	PHE
1	F	268	ALA
1	F	411	MET
1	G	64	PRO
1	G	268	ALA
1	H	44	ARG
1	H	158	ILE
1	H	411	MET
1	H	414	GLN
1	H	478	ARG
1	I	44	ARG
1	I	411	MET
1	I	478	ARG
1	J	44	ARG
1	J	411	MET
1	J	414	GLN
1	J	478	ARG
1	K	44	ARG
1	K	64	PRO
1	K	103	GLU

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Mol	Chain	Res	Type
1	K	158	ILE
1	K	414	GLN
1	K	439	ARG
1	L	44	ARG
1	L	439	ARG
1	L	478	ARG
1	A	275	GLU
1	B	64	PRO
1	B	158	ILE
1	B	275	GLU
1	B	491	ARG
1	B	494	ASN
1	C	64	PRO
1	C	220	PHE
1	C	275	GLU
1	C	478	ARG
1	D	64	PRO
1	D	275	GLU
1	E	64	PRO
1	E	275	GLU
1	E	486	ILE
1	F	7	PRO
1	F	275	GLU
1	F	486	ILE
1	G	103	GLU
1	G	275	GLU
1	G	411	MET
1	G	414	GLN
1	H	275	GLU
1	H	375	ALA
1	H	439	ARG
1	H	451	SER
1	I	7	PRO
1	I	64	PRO
1	I	275	GLU
1	I	414	GLN
1	I	497	GLY
1	J	64	PRO
1	J	275	GLU
1	J	451	SER
1	K	275	GLU
1	L	275	GLU

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Mol	Chain	Res	Type
1	L	411	MET
1	A	200	GLY
1	A	332	THR
1	B	200	GLY
1	B	392	VAL
1	B	411	MET
1	B	451	SER
1	C	58	VAL
1	C	486	ILE
1	D	200	GLY
1	D	486	ILE
1	E	158	ILE
1	E	451	SER
1	F	64	PRO
1	F	478	ARG
1	G	7	PRO
1	G	79	ARG
1	H	64	PRO
1	H	227	ILE
1	I	8	ASN
1	I	158	ILE
1	J	486	ILE
1	K	411	MET
1	L	7	PRO
1	L	64	PRO
1	A	486	ILE
1	B	29	VAL
1	B	486	ILE
1	C	29	VAL
1	C	179	ILE
1	C	464	ILE
1	D	29	VAL
1	E	200	GLY
1	F	29	VAL
1	F	464	ILE
1	G	200	GLY
1	H	29	VAL
1	J	29	VAL
1	J	58	VAL
1	K	58	VAL
1	K	200	GLY
1	L	58	VAL

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Mol	Chain	Res	Type
1	B	58	VAL
1	B	227	ILE
1	B	267	GLY
1	B	464	ILE
1	D	392	VAL
1	D	464	ILE
1	G	29	VAL
1	H	58	VAL
1	H	283	PRO
1	I	29	VAL
1	I	58	VAL
1	I	200	GLY
1	I	283	PRO
1	I	486	ILE
1	J	200	GLY
1	J	227	ILE
1	J	283	PRO
1	K	29	VAL
1	L	29	VAL
1	L	200	GLY
1	L	283	PRO
1	L	486	ILE
1	A	283	PRO
1	C	200	GLY
1	C	283	PRO
1	C	422	GLY
1	D	227	ILE
1	D	267	GLY
1	E	283	PRO
1	E	498	VAL
1	F	58	VAL
1	F	283	PRO
1	F	422	GLY
1	G	58	VAL
1	G	283	PRO
1	G	303	GLY
1	H	200	GLY
1	H	422	GLY
1	H	486	ILE
1	I	422	GLY
1	K	283	PRO
1	K	303	GLY

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Mol	Chain	Res	Type
1	K	486	ILE
1	L	422	GLY
1	A	29	VAL
1	A	267	GLY
1	A	303	GLY
1	B	304	PHE
1	C	303	GLY
1	C	304	PHE
1	D	58	VAL
1	D	283	PRO
1	D	304	PHE
1	E	29	VAL
1	E	58	VAL
1	E	304	PHE
1	F	179	ILE
1	F	303	GLY
1	F	304	PHE
1	G	486	ILE
1	H	304	PHE
1	J	304	PHE
1	J	422	GLY
1	K	267	GLY
1	A	227	ILE
1	A	304	PHE
1	A	422	GLY
1	B	283	PRO
1	C	273	VAL
1	E	267	GLY
1	E	303	GLY
1	E	422	GLY
1	F	200	GLY
1	F	273	VAL
1	G	422	GLY
1	H	303	GLY
1	I	303	GLY
1	L	303	GLY
1	L	304	PHE

### 5.3.2 Protein sidechains ⓘ

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



resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	416/420 (99%)	357 (86%)	59 (14%)	4	28
1	B	416/420 (99%)	360 (86%)	56 (14%)	5	30
1	C	416/420 (99%)	358 (86%)	58 (14%)	4	28
1	D	416/420 (99%)	356 (86%)	60 (14%)	4	27
1	E	416/420 (99%)	356 (86%)	60 (14%)	4	27
1	F	416/420 (99%)	355 (85%)	61 (15%)	4	26
1	G	416/420 (99%)	357 (86%)	59 (14%)	4	28
1	H	416/420 (99%)	357 (86%)	59 (14%)	4	28
1	I	416/420 (99%)	357 (86%)	59 (14%)	4	28
1	J	416/420 (99%)	354 (85%)	62 (15%)	4	25
1	K	416/420 (99%)	358 (86%)	58 (14%)	4	28
1	L	416/420 (99%)	354 (85%)	62 (15%)	4	25
All	All	4992/5040 (99%)	4279 (86%)	713 (14%)	4	27

All (713) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	PHE
1	A	14	GLU
1	A	19	ARG
1	A	24	VAL
1	A	26	ASP
1	A	36	GLU
1	A	49	LEU
1	A	55	CYS
1	A	60	SER
1	A	61	LEU
1	A	65	ILE
1	A	79	ARG
1	A	86	ARG
1	A	90	LYS
1	A	93	ILE
1	A	94	ARG
1	A	96	SER
1	A	97	THR

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Mol	Chain	Res	Type
1	A	107	LEU
1	A	110	LEU
1	A	111	MET
1	A	137	THR
1	A	138	ASP
1	A	141	LEU
1	A	145	THR
1	A	152	LEU
1	A	158	ILE
1	A	170	SER
1	A	175	GLU
1	A	176	MET
1	A	192	ILE
1	A	199	THR
1	A	201	LYS
1	A	212	ILE
1	A	245	LYS
1	A	249	VAL
1	A	263	LEU
1	A	266	PHE
1	A	280	ILE
1	A	292	GLU
1	A	300	THR
1	A	310	TYR
1	A	314	ILE
1	A	320	ASP
1	A	353	THR
1	A	378	VAL
1	A	382	TYR
1	A	392	VAL
1	A	402	GLU
1	A	405	SER
1	A	417	LEU
1	A	433	THR
1	A	435	GLU
1	A	436	PHE
1	A	439	ARG
1	A	453	LEU
1	A	455	TYR
1	A	462	ARG
1	A	495	GLU
1	B	14	GLU

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Mol	Chain	Res	Type
1	B	19	ARG
1	B	24	VAL
1	B	26	ASP
1	B	36	GLU
1	B	49	LEU
1	B	60	SER
1	B	61	LEU
1	B	65	ILE
1	B	79	ARG
1	B	86	ARG
1	B	90	LYS
1	B	93	ILE
1	B	94	ARG
1	B	96	SER
1	B	107	LEU
1	B	110	LEU
1	B	111	MET
1	B	137	THR
1	B	138	ASP
1	B	141	LEU
1	B	145	THR
1	B	152	LEU
1	B	158	ILE
1	B	170	SER
1	B	175	GLU
1	B	176	MET
1	B	192	ILE
1	B	199	THR
1	B	201	LYS
1	B	212	ILE
1	B	245	LYS
1	B	249	VAL
1	B	263	LEU
1	B	266	PHE
1	B	280	ILE
1	B	292	GLU
1	B	300	THR
1	B	310	TYR
1	B	314	ILE
1	B	320	ASP
1	B	353	THR
1	B	378	VAL

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Mol	Chain	Res	Type
1	B	382	TYR
1	B	392	VAL
1	B	402	GLU
1	B	405	SER
1	B	417	LEU
1	B	433	THR
1	B	435	GLU
1	B	436	PHE
1	B	439	ARG
1	B	455	TYR
1	B	462	ARG
1	B	492	VAL
1	B	494	ASN
1	C	9	PHE
1	C	14	GLU
1	C	19	ARG
1	C	24	VAL
1	C	26	ASP
1	C	36	GLU
1	C	49	LEU
1	C	60	SER
1	C	61	LEU
1	C	65	ILE
1	C	79	ARG
1	C	86	ARG
1	C	90	LYS
1	C	93	ILE
1	C	94	ARG
1	C	96	SER
1	C	97	THR
1	C	107	LEU
1	C	110	LEU
1	C	111	MET
1	C	137	THR
1	C	138	ASP
1	C	141	LEU
1	C	145	THR
1	C	152	LEU
1	C	158	ILE
1	C	170	SER
1	C	175	GLU
1	C	176	MET

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Mol	Chain	Res	Type
1	C	192	ILE
1	C	201	LYS
1	C	212	ILE
1	C	245	LYS
1	C	249	VAL
1	C	263	LEU
1	C	266	PHE
1	C	280	ILE
1	C	292	GLU
1	C	300	THR
1	C	310	TYR
1	C	314	ILE
1	C	320	ASP
1	C	353	THR
1	C	378	VAL
1	C	382	TYR
1	C	392	VAL
1	C	402	GLU
1	C	405	SER
1	C	413	VAL
1	C	417	LEU
1	C	428	ILE
1	C	433	THR
1	C	435	GLU
1	C	436	PHE
1	C	439	ARG
1	C	455	TYR
1	C	462	ARG
1	C	500	PHE
1	D	7	PRO
1	D	14	GLU
1	D	19	ARG
1	D	24	VAL
1	D	26	ASP
1	D	36	GLU
1	D	49	LEU
1	D	60	SER
1	D	61	LEU
1	D	65	ILE
1	D	79	ARG
1	D	86	ARG
1	D	90	LYS

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Mol	Chain	Res	Type
1	D	93	ILE
1	D	94	ARG
1	D	96	SER
1	D	107	LEU
1	D	110	LEU
1	D	111	MET
1	D	137	THR
1	D	138	ASP
1	D	141	LEU
1	D	145	THR
1	D	152	LEU
1	D	158	ILE
1	D	170	SER
1	D	175	GLU
1	D	176	MET
1	D	192	ILE
1	D	199	THR
1	D	201	LYS
1	D	212	ILE
1	D	245	LYS
1	D	249	VAL
1	D	263	LEU
1	D	266	PHE
1	D	280	ILE
1	D	292	GLU
1	D	300	THR
1	D	310	TYR
1	D	314	ILE
1	D	320	ASP
1	D	353	THR
1	D	378	VAL
1	D	382	TYR
1	D	392	VAL
1	D	402	GLU
1	D	405	SER
1	D	417	LEU
1	D	433	THR
1	D	435	GLU
1	D	436	PHE
1	D	439	ARG
1	D	453	LEU
1	D	455	TYR

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Mol	Chain	Res	Type
1	D	462	ARG
1	D	493	TYR
1	D	494	ASN
1	D	500	PHE
1	D	501	THR
1	E	9	PHE
1	E	14	GLU
1	E	19	ARG
1	E	24	VAL
1	E	26	ASP
1	E	36	GLU
1	E	49	LEU
1	E	55	CYS
1	E	60	SER
1	E	61	LEU
1	E	65	ILE
1	E	79	ARG
1	E	86	ARG
1	E	90	LYS
1	E	93	ILE
1	E	94	ARG
1	E	96	SER
1	E	97	THR
1	E	107	LEU
1	E	110	LEU
1	E	111	MET
1	E	137	THR
1	E	138	ASP
1	E	141	LEU
1	E	145	THR
1	E	152	LEU
1	E	158	ILE
1	E	170	SER
1	E	175	GLU
1	E	176	MET
1	E	192	ILE
1	E	199	THR
1	E	201	LYS
1	E	212	ILE
1	E	245	LYS
1	E	249	VAL
1	E	263	LEU

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Mol	Chain	Res	Type
1	E	266	PHE
1	E	280	ILE
1	E	292	GLU
1	E	300	THR
1	E	310	TYR
1	E	314	ILE
1	E	320	ASP
1	E	353	THR
1	E	378	VAL
1	E	382	TYR
1	E	392	VAL
1	E	402	GLU
1	E	405	SER
1	E	417	LEU
1	E	433	THR
1	E	435	GLU
1	E	436	PHE
1	E	439	ARG
1	E	455	TYR
1	E	462	ARG
1	E	491	ARG
1	E	498	VAL
1	E	499	THR
1	F	9	PHE
1	F	14	GLU
1	F	19	ARG
1	F	24	VAL
1	F	26	ASP
1	F	36	GLU
1	F	49	LEU
1	F	60	SER
1	F	61	LEU
1	F	65	ILE
1	F	79	ARG
1	F	86	ARG
1	F	90	LYS
1	F	93	ILE
1	F	94	ARG
1	F	96	SER
1	F	97	THR
1	F	107	LEU
1	F	110	LEU

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Mol	Chain	Res	Type
1	F	111	MET
1	F	137	THR
1	F	138	ASP
1	F	141	LEU
1	F	145	THR
1	F	152	LEU
1	F	158	ILE
1	F	170	SER
1	F	175	GLU
1	F	176	MET
1	F	192	ILE
1	F	201	LYS
1	F	212	ILE
1	F	245	LYS
1	F	249	VAL
1	F	263	LEU
1	F	266	PHE
1	F	280	ILE
1	F	292	GLU
1	F	300	THR
1	F	310	TYR
1	F	314	ILE
1	F	320	ASP
1	F	353	THR
1	F	378	VAL
1	F	382	TYR
1	F	392	VAL
1	F	402	GLU
1	F	405	SER
1	F	413	VAL
1	F	417	LEU
1	F	428	ILE
1	F	433	THR
1	F	435	GLU
1	F	436	PHE
1	F	439	ARG
1	F	455	TYR
1	F	462	ARG
1	F	493	TYR
1	F	495	GLU
1	F	499	THR
1	F	501	THR

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Mol	Chain	Res	Type
1	G	9	PHE
1	G	14	GLU
1	G	19	ARG
1	G	24	VAL
1	G	26	ASP
1	G	36	GLU
1	G	49	LEU
1	G	55	CYS
1	G	58	VAL
1	G	60	SER
1	G	61	LEU
1	G	65	ILE
1	G	79	ARG
1	G	86	ARG
1	G	90	LYS
1	G	93	ILE
1	G	94	ARG
1	G	96	SER
1	G	107	LEU
1	G	110	LEU
1	G	111	MET
1	G	137	THR
1	G	138	ASP
1	G	141	LEU
1	G	145	THR
1	G	152	LEU
1	G	158	ILE
1	G	170	SER
1	G	175	GLU
1	G	176	MET
1	G	192	ILE
1	G	201	LYS
1	G	212	ILE
1	G	245	LYS
1	G	249	VAL
1	G	263	LEU
1	G	266	PHE
1	G	280	ILE
1	G	292	GLU
1	G	300	THR
1	G	310	TYR
1	G	314	ILE

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Mol	Chain	Res	Type
1	G	320	ASP
1	G	353	THR
1	G	378	VAL
1	G	382	TYR
1	G	392	VAL
1	G	402	GLU
1	G	405	SER
1	G	417	LEU
1	G	433	THR
1	G	435	GLU
1	G	436	PHE
1	G	439	ARG
1	G	455	TYR
1	G	462	ARG
1	G	495	GLU
1	G	499	THR
1	G	501	THR
1	H	9	PHE
1	H	14	GLU
1	H	19	ARG
1	H	24	VAL
1	H	26	ASP
1	H	36	GLU
1	H	49	LEU
1	H	60	SER
1	H	61	LEU
1	H	65	ILE
1	H	79	ARG
1	H	86	ARG
1	H	90	LYS
1	H	93	ILE
1	H	94	ARG
1	H	96	SER
1	H	107	LEU
1	H	110	LEU
1	H	111	MET
1	H	137	THR
1	H	138	ASP
1	H	141	LEU
1	H	145	THR
1	H	152	LEU
1	H	158	ILE

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Mol	Chain	Res	Type
1	H	175	GLU
1	H	176	MET
1	H	192	ILE
1	H	199	THR
1	H	201	LYS
1	H	212	ILE
1	H	245	LYS
1	H	249	VAL
1	H	263	LEU
1	H	266	PHE
1	H	280	ILE
1	H	292	GLU
1	H	300	THR
1	H	310	TYR
1	H	314	ILE
1	H	320	ASP
1	H	353	THR
1	H	378	VAL
1	H	382	TYR
1	H	392	VAL
1	H	402	GLU
1	H	405	SER
1	H	417	LEU
1	H	433	THR
1	H	435	GLU
1	H	436	PHE
1	H	439	ARG
1	H	455	TYR
1	H	462	ARG
1	H	491	ARG
1	H	494	ASN
1	H	495	GLU
1	H	499	THR
1	H	501	THR
1	I	6	ASP
1	I	9	PHE
1	I	14	GLU
1	I	19	ARG
1	I	24	VAL
1	I	26	ASP
1	I	36	GLU
1	I	49	LEU

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Mol	Chain	Res	Type
1	I	60	SER
1	I	61	LEU
1	I	65	ILE
1	I	79	ARG
1	I	86	ARG
1	I	90	LYS
1	I	93	ILE
1	I	94	ARG
1	I	96	SER
1	I	107	LEU
1	I	110	LEU
1	I	111	MET
1	I	137	THR
1	I	138	ASP
1	I	141	LEU
1	I	145	THR
1	I	152	LEU
1	I	158	ILE
1	I	170	SER
1	I	175	GLU
1	I	176	MET
1	I	192	ILE
1	I	199	THR
1	I	201	LYS
1	I	212	ILE
1	I	245	LYS
1	I	249	VAL
1	I	259	SER
1	I	263	LEU
1	I	266	PHE
1	I	280	ILE
1	I	292	GLU
1	I	300	THR
1	I	310	TYR
1	I	314	ILE
1	I	320	ASP
1	I	353	THR
1	I	378	VAL
1	I	382	TYR
1	I	392	VAL
1	I	402	GLU
1	I	405	SER

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Mol	Chain	Res	Type
1	I	417	LEU
1	I	433	THR
1	I	435	GLU
1	I	436	PHE
1	I	439	ARG
1	I	455	TYR
1	I	462	ARG
1	I	493	TYR
1	I	499	THR
1	J	6	ASP
1	J	9	PHE
1	J	14	GLU
1	J	19	ARG
1	J	24	VAL
1	J	26	ASP
1	J	36	GLU
1	J	49	LEU
1	J	58	VAL
1	J	60	SER
1	J	61	LEU
1	J	65	ILE
1	J	79	ARG
1	J	86	ARG
1	J	90	LYS
1	J	93	ILE
1	J	94	ARG
1	J	96	SER
1	J	107	LEU
1	J	110	LEU
1	J	111	MET
1	J	137	THR
1	J	138	ASP
1	J	141	LEU
1	J	145	THR
1	J	152	LEU
1	J	158	ILE
1	J	170	SER
1	J	175	GLU
1	J	176	MET
1	J	192	ILE
1	J	199	THR
1	J	201	LYS

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Mol	Chain	Res	Type
1	J	212	ILE
1	J	245	LYS
1	J	249	VAL
1	J	263	LEU
1	J	266	PHE
1	J	280	ILE
1	J	292	GLU
1	J	300	THR
1	J	310	TYR
1	J	314	ILE
1	J	320	ASP
1	J	353	THR
1	J	378	VAL
1	J	382	TYR
1	J	392	VAL
1	J	402	GLU
1	J	405	SER
1	J	417	LEU
1	J	433	THR
1	J	435	GLU
1	J	436	PHE
1	J	439	ARG
1	J	453	LEU
1	J	455	TYR
1	J	462	ARG
1	J	492	VAL
1	J	494	ASN
1	J	495	GLU
1	J	499	THR
1	K	8	ASN
1	K	9	PHE
1	K	14	GLU
1	K	19	ARG
1	K	24	VAL
1	K	26	ASP
1	K	36	GLU
1	K	49	LEU
1	K	55	CYS
1	K	60	SER
1	K	61	LEU
1	K	65	ILE
1	K	79	ARG

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Mol	Chain	Res	Type
1	K	86	ARG
1	K	90	LYS
1	K	93	ILE
1	K	94	ARG
1	K	96	SER
1	K	107	LEU
1	K	110	LEU
1	K	111	MET
1	K	137	THR
1	K	138	ASP
1	K	141	LEU
1	K	145	THR
1	K	152	LEU
1	K	158	ILE
1	K	175	GLU
1	K	176	MET
1	K	192	ILE
1	K	199	THR
1	K	201	LYS
1	K	212	ILE
1	K	245	LYS
1	K	249	VAL
1	K	263	LEU
1	K	266	PHE
1	K	280	ILE
1	K	292	GLU
1	K	300	THR
1	K	310	TYR
1	K	314	ILE
1	K	320	ASP
1	K	353	THR
1	K	378	VAL
1	K	382	TYR
1	K	392	VAL
1	K	402	GLU
1	K	405	SER
1	K	417	LEU
1	K	433	THR
1	K	435	GLU
1	K	436	PHE
1	K	439	ARG
1	K	455	TYR

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Mol	Chain	Res	Type
1	K	462	ARG
1	K	498	VAL
1	K	501	THR
1	L	8	ASN
1	L	9	PHE
1	L	14	GLU
1	L	18	ASP
1	L	19	ARG
1	L	24	VAL
1	L	26	ASP
1	L	36	GLU
1	L	49	LEU
1	L	60	SER
1	L	61	LEU
1	L	65	ILE
1	L	79	ARG
1	L	86	ARG
1	L	90	LYS
1	L	93	ILE
1	L	94	ARG
1	L	96	SER
1	L	107	LEU
1	L	110	LEU
1	L	111	MET
1	L	137	THR
1	L	138	ASP
1	L	141	LEU
1	L	145	THR
1	L	152	LEU
1	L	158	ILE
1	L	170	SER
1	L	175	GLU
1	L	176	MET
1	L	192	ILE
1	L	199	THR
1	L	201	LYS
1	L	212	ILE
1	L	245	LYS
1	L	249	VAL
1	L	263	LEU
1	L	266	PHE
1	L	280	ILE

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Mol	Chain	Res	Type
1	L	292	GLU
1	L	300	THR
1	L	310	TYR
1	L	314	ILE
1	L	320	ASP
1	L	353	THR
1	L	378	VAL
1	L	382	TYR
1	L	392	VAL
1	L	402	GLU
1	L	405	SER
1	L	417	LEU
1	L	433	THR
1	L	435	GLU
1	L	436	PHE
1	L	439	ARG
1	L	455	TYR
1	L	462	ARG
1	L	495	GLU
1	L	498	VAL
1	L	499	THR
1	L	500	PHE
1	L	501	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	HIS
1	A	139	ASN
1	A	254	ASN
1	A	264	HIS
1	A	297	GLN
1	A	330	GLN
1	A	406	ASN
1	A	424	HIS
1	B	8	ASN
1	B	139	ASN
1	B	205	GLN
1	B	254	ASN
1	B	264	HIS
1	B	297	GLN
1	B	330	GLN

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Mol	Chain	Res	Type
1	B	406	ASN
1	B	450	HIS
1	B	494	ASN
1	C	82	HIS
1	C	209	HIS
1	C	250	GLN
1	C	254	ASN
1	C	264	HIS
1	C	297	GLN
1	C	330	GLN
1	C	388	ASN
1	C	406	ASN
1	D	85	HIS
1	D	139	ASN
1	D	254	ASN
1	D	264	HIS
1	D	297	GLN
1	D	330	GLN
1	D	406	ASN
1	D	424	HIS
1	D	450	HIS
1	D	494	ASN
1	E	82	HIS
1	E	254	ASN
1	E	264	HIS
1	E	297	GLN
1	E	330	GLN
1	E	406	ASN
1	E	424	HIS
1	F	82	HIS
1	F	205	GLN
1	F	209	HIS
1	F	250	GLN
1	F	254	ASN
1	F	264	HIS
1	F	297	GLN
1	F	330	GLN
1	F	406	ASN
1	F	424	HIS
1	G	82	HIS
1	G	84	GLN
1	G	254	ASN

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Mol	Chain	Res	Type
1	G	264	HIS
1	G	297	GLN
1	G	330	GLN
1	G	406	ASN
1	G	408	HIS
1	H	82	HIS
1	H	84	GLN
1	H	250	GLN
1	H	254	ASN
1	H	264	HIS
1	H	297	GLN
1	H	330	GLN
1	H	406	ASN
1	H	494	ASN
1	I	56	ASN
1	I	82	HIS
1	I	85	HIS
1	I	209	HIS
1	I	250	GLN
1	I	254	ASN
1	I	264	HIS
1	I	297	GLN
1	I	330	GLN
1	I	406	ASN
1	I	494	ASN
1	J	82	HIS
1	J	84	GLN
1	J	250	GLN
1	J	254	ASN
1	J	264	HIS
1	J	297	GLN
1	J	330	GLN
1	J	406	ASN
1	J	424	HIS
1	J	494	ASN
1	K	82	HIS
1	K	84	GLN
1	K	209	HIS
1	K	254	ASN
1	K	264	HIS
1	K	297	GLN
1	K	330	GLN

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Mol	Chain	Res	Type
1	K	406	ASN
1	K	408	HIS
1	K	494	ASN
1	L	8	ASN
1	L	82	HIS
1	L	209	HIS
1	L	250	GLN
1	L	254	ASN
1	L	264	HIS
1	L	297	GLN
1	L	330	GLN
1	L	406	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

24 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
2	NDP	A	552	-	42,52,52	1.63	4 (9%)	55,80,80	2.04	5 (9%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	XEG	A	601	-	35,35,35	1.31	4 (11%)	52,52,52	1.20	3 (5%)
2	NDP	B	552	-	42,52,52	1.61	5 (11%)	55,80,80	2.09	4 (7%)
3	XEG	B	601	-	35,35,35	1.27	3 (8%)	52,52,52	1.33	4 (7%)
2	NDP	C	552	-	42,52,52	1.59	4 (9%)	55,80,80	1.99	4 (7%)
3	XEG	D	502	-	35,35,35	1.25	2 (5%)	52,52,52	1.39	6 (11%)
2	NDP	D	552	-	42,52,52	1.59	5 (11%)	55,80,80	2.09	4 (7%)
3	XEG	D	601	-	35,35,35	1.42	4 (11%)	52,52,52	1.37	9 (17%)
2	NDP	E	552	-	42,52,52	1.61	5 (11%)	55,80,80	2.03	5 (9%)
3	XEG	E	601	-	35,35,35	1.31	3 (8%)	52,52,52	1.20	4 (7%)
2	NDP	F	552	-	42,52,52	1.58	4 (9%)	55,80,80	1.98	4 (7%)
3	XEG	F	601	-	35,35,35	1.36	5 (14%)	52,52,52	1.35	7 (13%)
2	NDP	G	552	-	42,52,52	1.61	4 (9%)	55,80,80	2.02	4 (7%)
3	XEG	G	601	-	35,35,35	1.42	4 (11%)	52,52,52	1.27	4 (7%)
2	NDP	H	552	-	42,52,52	1.54	4 (9%)	55,80,80	1.90	4 (7%)
3	XEG	H	601	-	35,35,35	1.27	3 (8%)	52,52,52	1.45	7 (13%)
2	NDP	I	552	-	42,52,52	1.62	5 (11%)	55,80,80	2.03	4 (7%)
3	XEG	I	601	-	35,35,35	1.46	6 (17%)	52,52,52	1.35	6 (11%)
2	NDP	J	552	-	42,52,52	1.53	4 (9%)	55,80,80	1.93	3 (5%)
3	XEG	J	601	-	35,35,35	1.26	3 (8%)	52,52,52	1.47	9 (17%)
2	NDP	K	552	-	42,52,52	1.60	4 (9%)	55,80,80	2.01	3 (5%)
3	XEG	K	601	-	35,35,35	1.42	4 (11%)	52,52,52	1.20	3 (5%)
2	NDP	L	552	-	42,52,52	1.61	5 (11%)	55,80,80	2.05	3 (5%)
3	XEG	L	601	-	35,35,35	1.49	7 (20%)	52,52,52	1.33	7 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDP	A	552	-	-	0/30/77/77	0/5/5/5
3	XEG	A	601	-	-	2/12/24/24	0/4/4/4
2	NDP	B	552	-	-	0/30/77/77	0/5/5/5
3	XEG	B	601	-	-	2/12/24/24	0/4/4/4
2	NDP	C	552	-	-	0/30/77/77	0/5/5/5
3	XEG	D	502	-	-	2/12/24/24	0/4/4/4
2	NDP	D	552	-	-	0/30/77/77	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	XEG	D	601	-	-	2/12/24/24	0/4/4/4
2	NDP	E	552	-	-	0/30/77/77	0/5/5/5
3	XEG	E	601	-	-	2/12/24/24	0/4/4/4
2	NDP	F	552	-	-	0/30/77/77	0/5/5/5
3	XEG	F	601	-	-	2/12/24/24	0/4/4/4
2	NDP	G	552	-	-	0/30/77/77	0/5/5/5
3	XEG	G	601	-	-	2/12/24/24	0/4/4/4
2	NDP	H	552	-	-	0/30/77/77	0/5/5/5
3	XEG	H	601	-	-	2/12/24/24	0/4/4/4
2	NDP	I	552	-	-	0/30/77/77	0/5/5/5
3	XEG	I	601	-	-	2/12/24/24	0/4/4/4
2	NDP	J	552	-	-	0/30/77/77	0/5/5/5
3	XEG	J	601	-	-	2/12/24/24	0/4/4/4
2	NDP	K	552	-	-	0/30/77/77	0/5/5/5
3	XEG	K	601	-	-	2/12/24/24	0/4/4/4
2	NDP	L	552	-	-	0/30/77/77	0/5/5/5
3	XEG	L	601	-	-	2/12/24/24	0/4/4/4

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	601	XEG	OAR-CBF	-4.32	1.37	1.45
3	J	601	XEG	OAR-CBF	-4.31	1.37	1.45
3	L	601	XEG	OAR-CBF	-3.71	1.38	1.45
3	I	601	XEG	OAR-CBF	-3.70	1.38	1.45
3	D	502	XEG	OAR-CBF	-3.58	1.38	1.45
3	B	601	XEG	OAR-CBF	-3.56	1.39	1.45
3	A	601	XEG	OAR-CBF	-3.51	1.39	1.45
3	K	601	XEG	OAR-CBF	-3.50	1.39	1.45
3	E	601	XEG	OAR-CBF	-3.42	1.39	1.45
3	G	601	XEG	OAQ-CAS	-3.39	1.27	1.34
3	G	601	XEG	OAR-CBF	-3.33	1.39	1.45
3	D	601	XEG	OAR-CBF	-3.19	1.39	1.45
3	E	601	XEG	OAQ-CAS	-3.18	1.28	1.34
3	K	601	XEG	OAQ-CAS	-3.17	1.28	1.34
3	F	601	XEG	OAR-CBF	-3.16	1.39	1.45
3	F	601	XEG	OAQ-CAS	-3.16	1.28	1.34
3	D	502	XEG	OAQ-CAS	-3.14	1.28	1.34
3	D	601	XEG	OAQ-CAS	-3.11	1.28	1.34
3	B	601	XEG	OAQ-CAS	-3.07	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	XEG	OAQ-CAS	-2.99	1.28	1.34
3	I	601	XEG	OAQ-CAS	-2.76	1.28	1.34
3	H	601	XEG	OAQ-CAS	-2.76	1.28	1.34
3	L	601	XEG	OAQ-CAS	-2.70	1.29	1.34
3	J	601	XEG	OAQ-CAS	-2.56	1.29	1.34
2	E	552	NDP	C2N-C3N	2.00	1.39	1.34
3	B	601	XEG	CAK-CAT	2.01	1.42	1.39
3	L	601	XEG	CAN-CAT	2.01	1.42	1.39
2	H	552	NDP	C2A-N1A	2.02	1.37	1.33
3	H	601	XEG	CAK-CAT	2.04	1.42	1.39
3	F	601	XEG	CAK-CAY	2.07	1.41	1.38
2	B	552	NDP	C2N-C3N	2.08	1.39	1.34
2	D	552	NDP	C2N-C3N	2.09	1.39	1.34
3	A	601	XEG	CBC-CBD	2.10	1.42	1.40
3	I	601	XEG	CAK-CAY	2.14	1.41	1.38
3	I	601	XEG	CAN-CBC	2.15	1.42	1.38
2	C	552	NDP	C2A-N1A	2.15	1.38	1.33
3	J	601	XEG	CAK-CAT	2.16	1.42	1.39
2	F	552	NDP	C2A-N1A	2.16	1.38	1.33
2	I	552	NDP	C2N-C3N	2.17	1.40	1.34
2	L	552	NDP	C2N-C3N	2.19	1.40	1.34
3	L	601	XEG	CAK-CAY	2.23	1.42	1.38
2	L	552	NDP	C2A-N1A	2.24	1.38	1.33
2	I	552	NDP	C2A-N1A	2.25	1.38	1.33
3	L	601	XEG	CAN-CBC	2.26	1.43	1.38
2	D	552	NDP	C2A-N1A	2.27	1.38	1.33
2	J	552	NDP	C2A-N1A	2.30	1.38	1.33
2	G	552	NDP	C2A-N1A	2.37	1.38	1.33
2	B	552	NDP	C2A-N1A	2.39	1.38	1.33
2	K	552	NDP	C2A-N1A	2.46	1.38	1.33
2	E	552	NDP	C2A-N1A	2.59	1.38	1.33
2	A	552	NDP	C2A-N1A	2.62	1.38	1.33
3	E	601	XEG	CAK-CAT	2.82	1.43	1.39
3	I	601	XEG	CBC-CBD	2.86	1.43	1.40
3	L	601	XEG	CAK-CAT	2.87	1.43	1.39
3	A	601	XEG	CAK-CAT	2.90	1.43	1.39
3	L	601	XEG	CBC-CBD	2.92	1.44	1.40
3	F	601	XEG	CBC-CBD	2.92	1.44	1.40
3	G	601	XEG	CBC-CBD	2.99	1.44	1.40
3	I	601	XEG	CAK-CAT	3.08	1.44	1.39
3	K	601	XEG	CBC-CBD	3.10	1.44	1.40
3	F	601	XEG	CAK-CAT	3.14	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	601	XEG	CAK-CAT	3.15	1.44	1.39
3	D	601	XEG	CAK-CAT	3.22	1.44	1.39
2	H	552	NDP	C2A-N3A	3.23	1.37	1.32
3	K	601	XEG	CAK-CAT	3.25	1.44	1.39
2	F	552	NDP	C6N-C5N	3.28	1.39	1.33
2	J	552	NDP	C2A-N3A	3.30	1.38	1.32
2	L	552	NDP	C2A-N3A	3.31	1.38	1.32
3	D	601	XEG	CBC-CBD	3.33	1.44	1.40
2	J	552	NDP	C6N-C5N	3.38	1.39	1.33
2	C	552	NDP	C6N-C5N	3.40	1.39	1.33
2	K	552	NDP	C2A-N3A	3.42	1.38	1.32
2	D	552	NDP	C2A-N3A	3.45	1.38	1.32
2	C	552	NDP	C2A-N3A	3.45	1.38	1.32
2	G	552	NDP	C2A-N3A	3.46	1.38	1.32
2	H	552	NDP	C6N-C5N	3.46	1.40	1.33
2	K	552	NDP	C6N-C5N	3.47	1.40	1.33
2	B	552	NDP	C2A-N3A	3.47	1.38	1.32
2	I	552	NDP	C2A-N3A	3.49	1.38	1.32
2	G	552	NDP	C6N-C5N	3.50	1.40	1.33
2	E	552	NDP	C6N-C5N	3.50	1.40	1.33
2	I	552	NDP	C6N-C5N	3.51	1.40	1.33
2	F	552	NDP	C2A-N3A	3.52	1.38	1.32
2	A	552	NDP	C6N-C5N	3.55	1.40	1.33
2	L	552	NDP	C6N-C5N	3.59	1.40	1.33
2	B	552	NDP	C6N-C5N	3.68	1.40	1.33
2	E	552	NDP	C2A-N3A	3.73	1.38	1.32
2	D	552	NDP	C6N-C5N	3.75	1.40	1.33
2	A	552	NDP	C2A-N3A	3.75	1.38	1.32
2	J	552	NDP	O7N-C7N	6.74	1.41	1.24
2	H	552	NDP	O7N-C7N	6.79	1.41	1.24
2	L	552	NDP	O7N-C7N	7.07	1.42	1.24
2	D	552	NDP	O7N-C7N	7.07	1.42	1.24
2	I	552	NDP	O7N-C7N	7.08	1.42	1.24
2	C	552	NDP	O7N-C7N	7.08	1.42	1.24
2	F	552	NDP	O7N-C7N	7.08	1.42	1.24
2	K	552	NDP	O7N-C7N	7.13	1.42	1.24
2	E	552	NDP	O7N-C7N	7.13	1.42	1.24
2	A	552	NDP	O7N-C7N	7.19	1.42	1.24
2	G	552	NDP	O7N-C7N	7.22	1.42	1.24
2	B	552	NDP	O7N-C7N	7.25	1.42	1.24

All (116) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	552	NDP	N3A-C2A-N1A	-12.63	119.22	128.89
2	D	552	NDP	N3A-C2A-N1A	-12.55	119.29	128.89
2	L	552	NDP	N3A-C2A-N1A	-12.19	119.56	128.89
2	I	552	NDP	N3A-C2A-N1A	-11.95	119.74	128.89
2	A	552	NDP	N3A-C2A-N1A	-11.71	119.92	128.89
2	E	552	NDP	N3A-C2A-N1A	-11.70	119.94	128.89
2	F	552	NDP	N3A-C2A-N1A	-11.60	120.01	128.89
2	G	552	NDP	N3A-C2A-N1A	-11.52	120.07	128.89
2	C	552	NDP	N3A-C2A-N1A	-11.48	120.10	128.89
2	K	552	NDP	N3A-C2A-N1A	-11.46	120.12	128.89
2	J	552	NDP	N3A-C2A-N1A	-11.10	120.40	128.89
2	H	552	NDP	N3A-C2A-N1A	-10.73	120.68	128.89
2	K	552	NDP	PN-O3-PA	-6.23	115.25	132.73
2	G	552	NDP	PN-O3-PA	-6.17	115.40	132.73
2	A	552	NDP	PN-O3-PA	-6.06	115.71	132.73
2	E	552	NDP	PN-O3-PA	-5.89	116.18	132.73
2	H	552	NDP	PN-O3-PA	-5.89	116.19	132.73
2	J	552	NDP	PN-O3-PA	-5.73	116.65	132.73
2	C	552	NDP	PN-O3-PA	-5.71	116.70	132.73
2	F	552	NDP	PN-O3-PA	-5.61	116.96	132.73
2	L	552	NDP	PN-O3-PA	-5.59	117.04	132.73
2	D	552	NDP	PN-O3-PA	-5.59	117.04	132.73
2	B	552	NDP	PN-O3-PA	-5.54	117.16	132.73
2	I	552	NDP	PN-O3-PA	-5.54	117.18	132.73
3	B	601	XEG	CAN-CBC-CBD	-2.70	118.45	122.18
3	D	502	XEG	CAN-CBC-CBD	-2.60	118.58	122.18
3	H	601	XEG	CAZ-CAL-CAW	-2.53	118.06	120.03
3	J	601	XEG	CAZ-CAL-CAW	-2.40	118.16	120.03
2	C	552	NDP	C4A-C5A-N7A	-2.39	107.28	109.48
3	D	502	XEG	CAZ-CAL-CAW	-2.37	118.17	120.03
3	L	601	XEG	CAN-CBC-CBD	-2.24	119.07	122.18
3	D	601	XEG	CAL-CAW-CBB	-2.21	119.06	120.42
3	D	601	XEG	CAN-CBC-CBD	-2.18	119.16	122.18
2	F	552	NDP	C4A-C5A-N7A	-2.10	107.55	109.48
3	J	601	XEG	CAL-CAW-CBB	-2.05	119.16	120.42
2	I	552	NDP	C4A-C5A-N7A	-2.04	107.60	109.48
2	A	552	NDP	C4A-C5A-N7A	-2.03	107.61	109.48
2	G	552	NDP	C4A-C5A-N7A	-2.02	107.62	109.48
3	F	601	XEG	CAN-CBC-CBD	-2.01	119.40	122.18
2	E	552	NDP	C1D-N1N-C2N	-2.00	117.42	120.91
2	A	552	NDP	O2B-C2B-C1B	2.00	117.82	110.02
3	J	601	XEG	CAY-CBD-CBC	2.01	120.57	117.30
3	D	601	XEG	OAR-CBC-CAN	2.01	119.90	116.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	601	XEG	OAR-CBC-CAN	2.04	119.94	116.37
2	D	552	NDP	O2B-C2B-C1B	2.05	118.01	110.02
2	E	552	NDP	O2B-C2B-C1B	2.05	118.02	110.02
3	E	601	XEG	OAR-CBF-CBE	2.06	114.66	108.55
3	L	601	XEG	OAG-CAY-CBD	2.06	122.61	117.83
2	H	552	NDP	O2B-C2B-C1B	2.06	118.05	110.02
3	F	601	XEG	CAY-CBD-CBC	2.07	120.67	117.30
3	I	601	XEG	CAY-CBD-CBC	2.08	120.68	117.30
3	I	601	XEG	OAG-CAY-CBD	2.08	122.65	117.83
3	L	601	XEG	CAY-CBD-CBC	2.11	120.72	117.30
3	F	601	XEG	CAX-CBB-CAW	2.11	120.70	119.55
3	G	601	XEG	OAG-CAY-CBD	2.11	122.73	117.83
2	B	552	NDP	O2B-C2B-C1B	2.12	118.29	110.02
3	J	601	XEG	OAR-CBC-CAN	2.15	120.13	116.37
3	A	601	XEG	OAR-CBC-CAN	2.16	120.15	116.37
3	D	601	XEG	OAF-CAX-CBB	2.16	123.53	117.91
3	D	601	XEG	CAY-CBD-CBC	2.17	120.82	117.30
3	H	601	XEG	OAR-CBC-CAN	2.18	120.19	116.37
3	E	601	XEG	OAR-CBC-CAN	2.20	120.23	116.37
3	D	601	XEG	CAX-CBB-CAW	2.24	120.78	119.55
3	H	601	XEG	CAX-CBB-CAW	2.30	120.81	119.55
3	I	601	XEG	OAR-CBC-CAN	2.33	120.46	116.37
3	L	601	XEG	OAR-CBF-CBE	2.34	115.49	108.55
3	J	601	XEG	CAX-CBB-CAW	2.34	120.83	119.55
3	G	601	XEG	OAR-CBF-CBE	2.35	115.53	108.55
2	I	552	NDP	O4D-C1D-N1N	2.38	113.09	108.07
3	J	601	XEG	OAR-CBF-CBE	2.40	115.69	108.55
3	L	601	XEG	OAR-CBC-CAN	2.41	120.59	116.37
3	K	601	XEG	OAR-CBF-CBE	2.44	115.78	108.55
2	B	552	NDP	O4D-C1D-N1N	2.44	113.21	108.07
2	L	552	NDP	O4D-C1D-N1N	2.46	113.27	108.07
2	F	552	NDP	O4D-C1D-N1N	2.48	113.30	108.07
3	D	601	XEG	OAR-CBF-CBE	2.48	115.92	108.55
3	I	601	XEG	OAR-CBF-CBE	2.49	115.94	108.55
3	F	601	XEG	OAR-CBF-CBE	2.50	115.97	108.55
2	J	552	NDP	O4D-C1D-N1N	2.53	113.41	108.07
2	E	552	NDP	O4D-C1D-N1N	2.53	113.41	108.07
3	H	601	XEG	OAR-CBF-CBE	2.53	116.06	108.55
2	H	552	NDP	O4D-C1D-N1N	2.58	113.53	108.07
2	A	552	NDP	O4D-C1D-N1N	2.64	113.65	108.07
2	C	552	NDP	O4D-C1D-N1N	2.70	113.77	108.07
3	D	502	XEG	CAM-CAZ-CAL	2.73	122.89	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	552	NDP	O4D-C1D-N1N	2.74	113.86	108.07
3	B	601	XEG	OAR-CBC-CAN	2.76	121.20	116.37
2	G	552	NDP	O4D-C1D-N1N	2.79	113.96	108.07
3	D	502	XEG	OAR-CBC-CAN	2.83	121.33	116.37
2	K	552	NDP	O4D-C1D-N1N	2.90	114.20	108.07
3	E	601	XEG	CBE-OAQ-CAS	3.15	122.92	117.43
3	A	601	XEG	CBE-OAQ-CAS	3.19	122.98	117.43
3	H	601	XEG	CAM-CAZ-CAL	3.29	123.56	119.64
3	J	601	XEG	CAM-CAZ-CAL	3.34	123.62	119.64
3	K	601	XEG	OAQ-CAS-CAZ	3.45	117.81	111.90
3	D	502	XEG	CBE-OAQ-CAS	3.58	123.66	117.43
3	H	601	XEG	OAQ-CAS-CAZ	3.59	118.07	111.90
3	G	601	XEG	OAQ-CAS-CAZ	3.61	118.09	111.90
3	D	601	XEG	OAQ-CAS-CAZ	3.62	118.12	111.90
3	F	601	XEG	OAQ-CAS-CAZ	3.65	118.16	111.90
3	B	601	XEG	CBE-OAQ-CAS	3.72	123.90	117.43
3	J	601	XEG	OAQ-CAS-CAZ	3.73	118.30	111.90
3	G	601	XEG	CBE-OAQ-CAS	3.76	123.97	117.43
3	D	502	XEG	OAQ-CAS-CAZ	3.76	118.36	111.90
3	E	601	XEG	OAQ-CAS-CAZ	3.80	118.43	111.90
3	I	601	XEG	OAQ-CAS-CAZ	3.86	118.53	111.90
3	L	601	XEG	CBE-OAQ-CAS	3.92	124.26	117.43
3	K	601	XEG	CBE-OAQ-CAS	3.93	124.28	117.43
3	B	601	XEG	OAQ-CAS-CAZ	3.94	118.67	111.90
3	L	601	XEG	OAQ-CAS-CAZ	3.95	118.68	111.90
3	I	601	XEG	CBE-OAQ-CAS	3.97	124.35	117.43
3	A	601	XEG	OAQ-CAS-CAZ	3.99	118.75	111.90
3	D	601	XEG	CBE-OAQ-CAS	4.07	124.51	117.43
3	F	601	XEG	CBE-OAQ-CAS	4.17	124.69	117.43
3	H	601	XEG	CBE-OAQ-CAS	4.18	124.70	117.43
3	J	601	XEG	CBE-OAQ-CAS	4.19	124.73	117.43

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	601	XEG	CBE-OAQ-CAS-OAA
3	D	502	XEG	CBE-OAQ-CAS-OAA
3	I	601	XEG	CBE-OAQ-CAS-OAA
3	F	601	XEG	CBE-OAQ-CAS-OAA
3	A	601	XEG	CBE-OAQ-CAS-OAA
3	D	601	XEG	CBE-OAQ-CAS-OAA

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Mol	Chain	Res	Type	Atoms
3	B	601	XEG	CBE-OAQ-CAS-OAA
3	E	601	XEG	CBE-OAQ-CAS-OAA
3	K	601	XEG	CBE-OAQ-CAS-OAA
3	G	601	XEG	CBE-OAQ-CAS-OAA
3	H	601	XEG	CBE-OAQ-CAS-OAA
3	D	502	XEG	CBE-OAQ-CAS-CAZ
3	J	601	XEG	CBE-OAQ-CAS-OAA
3	B	601	XEG	CBE-OAQ-CAS-CAZ
3	E	601	XEG	CBE-OAQ-CAS-CAZ
3	A	601	XEG	CBE-OAQ-CAS-CAZ
3	L	601	XEG	CBE-OAQ-CAS-CAZ
3	H	601	XEG	CBE-OAQ-CAS-CAZ
3	I	601	XEG	CBE-OAQ-CAS-CAZ
3	J	601	XEG	CBE-OAQ-CAS-CAZ
3	G	601	XEG	CBE-OAQ-CAS-CAZ
3	K	601	XEG	CBE-OAQ-CAS-CAZ
3	F	601	XEG	CBE-OAQ-CAS-CAZ
3	D	601	XEG	CBE-OAQ-CAS-CAZ

There are no ring outliers.

24 monomers are involved in 161 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	552	NDP	8	0
3	A	601	XEG	8	0
2	B	552	NDP	2	0
3	B	601	XEG	10	0
2	C	552	NDP	5	0
3	D	502	XEG	8	0
2	D	552	NDP	2	0
3	D	601	XEG	5	0
2	E	552	NDP	5	0
3	E	601	XEG	8	0
2	F	552	NDP	5	0
3	F	601	XEG	10	0
2	G	552	NDP	4	0
3	G	601	XEG	10	0
2	H	552	NDP	4	0
3	H	601	XEG	14	0
2	I	552	NDP	5	0
3	I	601	XEG	7	0
2	J	552	NDP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	601	XEG	12	0
2	K	552	NDP	5	0
3	K	601	XEG	9	0
2	L	552	NDP	7	0
3	L	601	XEG	6	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	496/501 (99%)	0.25	41 (8%)	14	10	63, 122, 279, 367	0
1	B	496/501 (99%)	0.21	34 (6%)	20	13	63, 121, 276, 367	0
1	C	496/501 (99%)	0.25	32 (6%)	22	15	62, 121, 277, 365	0
1	D	496/501 (99%)	0.25	32 (6%)	22	15	61, 122, 276, 369	0
1	E	496/501 (99%)	0.37	41 (8%)	14	10	64, 122, 279, 366	0
1	F	496/501 (99%)	0.23	30 (6%)	25	17	62, 121, 278, 365	0
1	G	496/501 (99%)	0.28	35 (7%)	19	13	61, 120, 278, 368	0
1	H	496/501 (99%)	0.07	14 (2%)	56	42	60, 120, 276, 365	0
1	I	496/501 (99%)	0.09	24 (4%)	34	23	59, 121, 278, 365	0
1	J	496/501 (99%)	0.10	16 (3%)	51	37	61, 120, 276, 364	0
1	K	496/501 (99%)	0.23	30 (6%)	25	17	62, 122, 279, 368	0
1	L	496/501 (99%)	0.13	23 (4%)	36	25	60, 121, 278, 366	0
All	All	5952/6012 (99%)	0.21	352 (5%)	26	17	59, 121, 278, 369	0

All (352) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	285	GLY	13.7
1	E	501	THR	9.7
1	G	308	LYS	9.5
1	F	342	LYS	9.4
1	K	285	GLY	9.1
1	A	347	GLY	9.0
1	C	227	ILE	8.2
1	D	10	PHE	8.0
1	F	227	ILE	7.4
1	D	305	PRO	7.1
1	D	9	PHE	7.1

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Mol	Chain	Res	Type	RSRZ
1	D	37	THR	7.0
1	C	322	LEU	6.9
1	C	226	PHE	6.7
1	C	342	LYS	6.7
1	F	319	CYS	6.6
1	C	285	GLY	6.4
1	A	298	HIS	6.3
1	G	306	LYS	6.3
1	D	501	THR	6.2
1	G	309	ILE	6.2
1	E	252	PHE	6.1
1	F	285	GLY	6.0
1	D	272	THR	6.0
1	K	249	VAL	5.9
1	F	226	PHE	5.9
1	E	322	LEU	5.7
1	G	305	PRO	5.6
1	K	347	GLY	5.6
1	B	305	PRO	5.6
1	C	499	THR	5.5
1	A	315	LEU	5.5
1	D	296	LEU	5.5
1	B	334	SER	5.5
1	F	365	ILE	5.4
1	G	307	ALA	5.4
1	C	344	ILE	5.4
1	F	344	ILE	5.3
1	C	267	GLY	5.3
1	E	250	GLN	5.3
1	A	300	THR	5.3
1	L	312	GLY	5.2
1	D	304	PHE	5.1
1	E	349	ASN	5.0
1	D	273	VAL	5.0
1	J	242	PHE	4.9
1	E	341	ALA	4.9
1	E	352	THR	4.9
1	A	322	LEU	4.9
1	G	342	LYS	4.8
1	K	286	ILE	4.7
1	A	334	SER	4.7
1	G	284	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
1	I	319	CYS	4.6
1	I	279	SER	4.6
1	C	365	ILE	4.6
1	E	275	GLU	4.6
1	G	501	THR	4.6
1	L	314	ILE	4.6
1	A	324	PRO	4.6
1	H	251	GLY	4.5
1	B	296	LEU	4.5
1	G	349	ASN	4.5
1	E	357	ASP	4.5
1	B	346	GLU	4.4
1	I	250	GLN	4.4
1	C	321	ILE	4.3
1	E	339	VAL	4.3
1	F	232	TYR	4.3
1	K	227	ILE	4.2
1	B	304	PHE	4.2
1	K	297	GLN	4.2
1	F	318	ASP	4.2
1	E	277	ASP	4.1
1	I	296	LEU	4.1
1	F	343	ILE	4.1
1	C	268	ALA	4.1
1	C	241	GLY	4.1
1	E	285	GLY	4.1
1	B	295	LYS	4.1
1	K	248	VAL	4.1
1	K	252	PHE	4.1
1	B	9	PHE	4.1
1	E	424	HIS	4.0
1	F	367	VAL	4.0
1	A	336	ALA	4.0
1	B	37	THR	4.0
1	B	210	GLY	4.0
1	J	272	THR	4.0
1	H	347	GLY	4.0
1	G	301	ILE	4.0
1	A	311	GLU	3.9
1	B	262	TYR	3.9
1	L	311	GLU	3.9
1	E	345	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	348	ALA	3.9
1	H	315	LEU	3.9
1	G	344	ILE	3.8
1	E	241	GLY	3.8
1	B	318	ASP	3.8
1	F	308	LYS	3.8
1	F	366	MET	3.8
1	D	274	GLY	3.8
1	J	501	THR	3.7
1	E	251	GLY	3.7
1	I	340	LYS	3.7
1	K	250	GLN	3.7
1	C	228	ASN	3.7
1	F	341	ALA	3.7
1	H	252	PHE	3.7
1	A	10	PHE	3.7
1	F	322	LEU	3.7
1	K	226	PHE	3.6
1	G	313	SER	3.6
1	L	305	PRO	3.6
1	I	326	ALA	3.6
1	F	240	PRO	3.6
1	D	347	GLY	3.6
1	L	334	SER	3.5
1	I	501	THR	3.5
1	H	501	THR	3.5
1	A	299	GLY	3.5
1	K	42	ARG	3.5
1	E	347	GLY	3.5
1	E	499	THR	3.5
1	D	8	ASN	3.5
1	F	268	ALA	3.5
1	I	311	GLU	3.4
1	A	275	GLU	3.4
1	I	332	THR	3.4
1	K	344	ILE	3.4
1	K	501	THR	3.4
1	A	357	ASP	3.4
1	C	367	VAL	3.4
1	E	344	ILE	3.4
1	C	223	ILE	3.4
1	C	345	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	321	ILE	3.3
1	D	332	THR	3.3
1	G	227	ILE	3.3
1	B	273	VAL	3.3
1	G	280	ILE	3.3
1	F	320	ASP	3.3
1	I	424	HIS	3.3
1	L	313	SER	3.3
1	B	8	ASN	3.3
1	E	336	ALA	3.2
1	K	365	ILE	3.2
1	L	279	SER	3.2
1	E	326	ALA	3.2
1	G	275	GLU	3.2
1	L	371	LEU	3.2
1	B	289	LYS	3.2
1	G	286	ILE	3.2
1	E	325	ALA	3.2
1	J	262	TYR	3.2
1	C	240	PRO	3.2
1	L	227	ILE	3.2
1	I	342	LYS	3.2
1	B	249	VAL	3.1
1	F	228	ASN	3.1
1	A	335	ASN	3.1
1	E	232	TYR	3.1
1	D	294	PHE	3.1
1	K	424	HIS	3.1
1	F	223	ILE	3.1
1	E	309	ILE	3.1
1	L	365	ILE	3.1
1	L	501	THR	3.1
1	C	252	PHE	3.0
1	A	342	LYS	3.0
1	F	231	SER	3.0
1	G	232	TYR	3.0
1	A	271	ILE	3.0
1	I	309	ILE	3.0
1	F	309	ILE	3.0
1	L	332	THR	3.0
1	A	250	GLN	3.0
1	B	258	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	250	GLN	3.0
1	B	214	ALA	3.0
1	J	280	ILE	3.0
1	G	370	ASP	2.9
1	G	300	THR	2.9
1	D	261	ARG	2.9
1	A	248	VAL	2.9
1	G	354	PRO	2.9
1	C	347	GLY	2.9
1	I	330	GLN	2.9
1	E	242	PHE	2.9
1	H	499	THR	2.9
1	J	250	GLN	2.9
1	B	366	MET	2.9
1	A	323	ILE	2.9
1	I	365	ILE	2.9
1	D	210	GLY	2.8
1	E	300	THR	2.8
1	A	349	ASN	2.8
1	E	328	GLU	2.8
1	E	33	LYS	2.8
1	G	366	MET	2.8
1	J	352	THR	2.8
1	A	32	LEU	2.8
1	I	335	ASN	2.8
1	F	302	LEU	2.8
1	H	332	THR	2.8
1	I	227	ILE	2.8
1	K	362	GLU	2.7
1	D	475	LEU	2.7
1	B	292	GLU	2.7
1	E	397	LEU	2.7
1	B	306	LYS	2.7
1	K	296	LEU	2.7
1	B	313	SER	2.7
1	K	305	PRO	2.7
1	B	268	ALA	2.7
1	G	371	LEU	2.7
1	L	278	GLY	2.7
1	I	371	LEU	2.7
1	K	258	HIS	2.7
1	B	422	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	500	PHE	2.7
1	A	81	GLN	2.7
1	B	319	CYS	2.6
1	D	499	THR	2.6
1	E	302	LEU	2.6
1	F	286	ILE	2.6
1	A	73	GLU	2.6
1	H	334	SER	2.6
1	D	331	LEU	2.6
1	K	418	GLU	2.6
1	L	7	PRO	2.6
1	A	277	ASP	2.6
1	I	252	PHE	2.6
1	G	279	SER	2.6
1	A	439	ARG	2.5
1	L	6	ASP	2.5
1	B	288	PRO	2.5
1	H	271	ILE	2.5
1	B	299	GLY	2.5
1	C	341	ALA	2.5
1	A	375	ALA	2.5
1	E	332	THR	2.5
1	G	273	VAL	2.5
1	D	500	PHE	2.5
1	G	341	ALA	2.5
1	J	347	GLY	2.5
1	A	325	ALA	2.5
1	J	214	ALA	2.5
1	G	295	LYS	2.5
1	D	302	LEU	2.4
1	F	250	GLN	2.4
1	J	346	GLU	2.4
1	K	7	PRO	2.4
1	B	430	ILE	2.4
1	G	343	ILE	2.4
1	J	366	MET	2.4
1	D	292	GLU	2.4
1	C	371	LEU	2.4
1	C	349	ASN	2.4
1	A	36	GLU	2.4
1	A	312	GLY	2.4
1	B	501	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	347	GLY	2.4
1	L	295	LYS	2.4
1	D	268	ALA	2.4
1	K	309	ILE	2.4
1	E	379	THR	2.4
1	K	394	TYR	2.3
1	K	277	ASP	2.3
1	D	7	PRO	2.3
1	I	7	PRO	2.3
1	I	226	PHE	2.3
1	D	315	LEU	2.3
1	B	300	THR	2.3
1	E	342	LYS	2.3
1	I	310	TYR	2.3
1	B	217	ARG	2.3
1	I	325	ALA	2.3
1	D	285	GLY	2.3
1	L	130	LYS	2.3
1	A	344	ILE	2.3
1	C	343	ILE	2.3
1	C	496	ALA	2.3
1	J	273	VAL	2.3
1	A	307	ALA	2.3
1	C	247	PHE	2.3
1	E	500	PHE	2.3
1	A	339	VAL	2.3
1	D	286	ILE	2.3
1	C	250	GLN	2.2
1	K	279	SER	2.2
1	B	379	THR	2.2
1	K	219	VAL	2.2
1	D	324	PRO	2.2
1	C	124	GLY	2.2
1	A	379	THR	2.2
1	A	313	SER	2.2
1	G	80	ALA	2.2
1	G	302	LEU	2.2
1	B	250	GLN	2.2
1	L	352	THR	2.2
1	L	309	ILE	2.2
1	J	430	ILE	2.2
1	L	271	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	34	THR	2.2
1	H	277	ASP	2.2
1	K	276	SER	2.2
1	E	271	ILE	2.2
1	E	331	LEU	2.2
1	A	306	LYS	2.2
1	J	312	GLY	2.2
1	L	357	ASP	2.2
1	C	270	CYS	2.1
1	A	494	ASN	2.1
1	D	346	GLU	2.1
1	L	289	LYS	2.1
1	H	244	ASP	2.1
1	F	303	GLY	2.1
1	E	375	ALA	2.1
1	B	314	ILE	2.1
1	D	284	ASP	2.1
1	D	476	ASP	2.1
1	K	273	VAL	2.1
1	F	267	GLY	2.1
1	J	345	ALA	2.1
1	L	484	ASN	2.1
1	D	280	ILE	2.1
1	A	34	THR	2.1
1	B	309	ILE	2.1
1	C	286	ILE	2.1
1	I	281	TRP	2.1
1	C	126	LYS	2.1
1	F	323	ILE	2.1
1	F	430	ILE	2.1
1	G	336	ALA	2.1
1	K	223	ILE	2.1
1	E	301	ILE	2.1
1	K	260	MET	2.1
1	A	418	GLU	2.1
1	J	422	GLY	2.0
1	A	341	ALA	2.0
1	H	187	ILE	2.0
1	H	238	MET	2.0
1	H	261	ARG	2.0
1	G	258	HIS	2.0
1	G	271	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	272	THR	2.0
1	E	208	ILE	2.0
1	E	334	SER	2.0
1	I	339	VAL	2.0
1	G	319	CYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	XEG	D	601	32/32	0.51	0.56	2.88	100,132,151,156	0
3	XEG	I	601	32/32	0.79	0.55	2.44	96,132,147,159	0
3	XEG	L	601	32/32	0.63	0.40	1.84	92,132,145,155	0
3	XEG	H	601	32/32	0.76	0.36	1.47	97,130,150,154	0
3	XEG	K	601	32/32	0.79	0.29	0.94	102,130,147,149	0
2	NDP	B	552	48/48	0.61	0.42	0.92	140,186,224,364	0
3	XEG	J	601	32/32	0.84	0.27	0.70	96,130,150,156	0
3	XEG	A	601	32/32	0.78	0.29	0.68	99,134,143,145	0
3	XEG	G	601	32/32	0.85	0.28	0.55	100,132,145,147	0
2	NDP	F	552	48/48	0.81	0.34	0.22	136,176,207,282	0
3	XEG	E	601	32/32	0.79	0.23	0.15	103,133,146,148	0
3	XEG	D	502	32/32	0.86	0.24	-0.10	89,132,147,152	0
3	XEG	B	601	32/32	0.86	0.22	-0.15	90,132,147,149	0
2	NDP	D	552	48/48	0.74	0.30	-0.16	140,184,224,364	0
2	NDP	I	552	48/48	0.79	0.28	-0.18	139,178,205,364	0
3	XEG	F	601	32/32	0.75	0.27	-0.18	101,132,147,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NDP	C	552	48/48	0.81	0.32	-0.35	139,176,207,305	0
2	NDP	G	552	48/48	0.78	0.26	-0.41	134,178,204,311	0
2	NDP	L	552	48/48	0.82	0.22	-0.48	137,179,207,364	0
2	NDP	J	552	48/48	0.78	0.25	-0.51	123,184,207,309	0
2	NDP	H	552	48/48	0.75	0.25	-0.55	131,184,207,312	0
2	NDP	E	552	48/48	0.71	0.30	-0.65	139,181,209,278	0
2	NDP	K	552	48/48	0.79	0.26	-0.65	137,179,205,315	0
2	NDP	A	552	48/48	0.76	0.24	-0.68	138,182,210,364	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.