



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:18 AM GMT

PDB ID : 3E1K  
Title : Crystal structure of Kluyveromyces lactis Gal80p in complex with the acidic activation domain of Gal4p  
Authors : Thoden, J.B.; Holden, H.M.  
Deposited on : 2008-08-04  
Resolution : 3.00 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

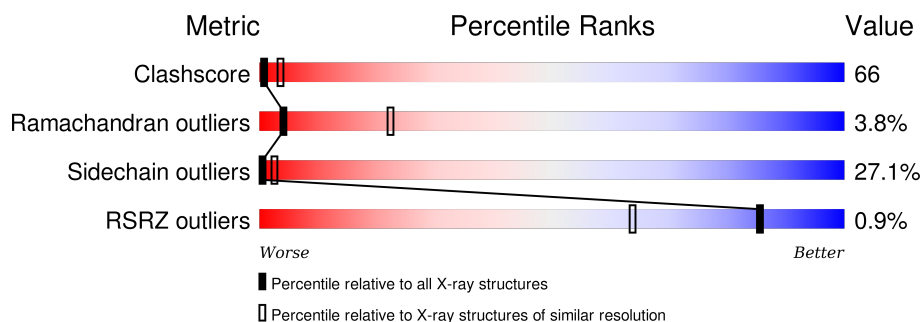
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	465	
1	C	465	
1	E	465	
1	G	465	
1	I	465	
1	K	465	
1	M	465	

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Mol	Chain	Length	Quality of chain
1	O	465	
2	B	22	
2	D	22	
2	F	22	
2	H	22	
2	J	22	
2	L	22	
2	N	22	
2	P	22	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 26057 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 Galactose/lactose metabolism regulatory protein GAL80.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3153	2024	527	593	9			
1	C	393	Total	C	N	O	S	0	0	0
			3136	2013	525	589	9			
1	E	393	Total	C	N	O	S	0	0	0
			3136	2013	525	589	9			
1	G	393	Total	C	N	O	S	0	0	0
			3136	2013	525	589	9			
1	I	393	Total	C	N	O	S	0	0	0
			3136	2013	525	589	9			
1	K	393	Total	C	N	O	S	0	0	0
			3136	2013	525	589	9			
1	M	393	Total	C	N	O	S	0	0	0
			3136	2013	525	589	9			
1	O	393	Total	C	N	O	S	0	0	0
			3136	2013	525	589	9			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	458	LEU	-	EXPRESSION TAG	UNP Q06433
A	459	GLU	-	EXPRESSION TAG	UNP Q06433
A	460	HIS	-	EXPRESSION TAG	UNP Q06433
A	461	HIS	-	EXPRESSION TAG	UNP Q06433
A	462	HIS	-	EXPRESSION TAG	UNP Q06433
A	463	HIS	-	EXPRESSION TAG	UNP Q06433
A	464	HIS	-	EXPRESSION TAG	UNP Q06433
A	465	HIS	-	EXPRESSION TAG	UNP Q06433
C	458	LEU	-	EXPRESSION TAG	UNP Q06433
C	459	GLU	-	EXPRESSION TAG	UNP Q06433
C	460	HIS	-	EXPRESSION TAG	UNP Q06433
C	461	HIS	-	EXPRESSION TAG	UNP Q06433
C	462	HIS	-	EXPRESSION TAG	UNP Q06433

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Chain	Residue	Modelled	Actual	Comment	Reference
C	463	HIS	-	EXPRESSION TAG	UNP Q06433
C	464	HIS	-	EXPRESSION TAG	UNP Q06433
C	465	HIS	-	EXPRESSION TAG	UNP Q06433
E	458	LEU	-	EXPRESSION TAG	UNP Q06433
E	459	GLU	-	EXPRESSION TAG	UNP Q06433
E	460	HIS	-	EXPRESSION TAG	UNP Q06433
E	461	HIS	-	EXPRESSION TAG	UNP Q06433
E	462	HIS	-	EXPRESSION TAG	UNP Q06433
E	463	HIS	-	EXPRESSION TAG	UNP Q06433
E	464	HIS	-	EXPRESSION TAG	UNP Q06433
E	465	HIS	-	EXPRESSION TAG	UNP Q06433
G	458	LEU	-	EXPRESSION TAG	UNP Q06433
G	459	GLU	-	EXPRESSION TAG	UNP Q06433
G	460	HIS	-	EXPRESSION TAG	UNP Q06433
G	461	HIS	-	EXPRESSION TAG	UNP Q06433
G	462	HIS	-	EXPRESSION TAG	UNP Q06433
G	463	HIS	-	EXPRESSION TAG	UNP Q06433
G	464	HIS	-	EXPRESSION TAG	UNP Q06433
G	465	HIS	-	EXPRESSION TAG	UNP Q06433
I	458	LEU	-	EXPRESSION TAG	UNP Q06433
I	459	GLU	-	EXPRESSION TAG	UNP Q06433
I	460	HIS	-	EXPRESSION TAG	UNP Q06433
I	461	HIS	-	EXPRESSION TAG	UNP Q06433
I	462	HIS	-	EXPRESSION TAG	UNP Q06433
I	463	HIS	-	EXPRESSION TAG	UNP Q06433
I	464	HIS	-	EXPRESSION TAG	UNP Q06433
I	465	HIS	-	EXPRESSION TAG	UNP Q06433
K	458	LEU	-	EXPRESSION TAG	UNP Q06433
K	459	GLU	-	EXPRESSION TAG	UNP Q06433
K	460	HIS	-	EXPRESSION TAG	UNP Q06433
K	461	HIS	-	EXPRESSION TAG	UNP Q06433
K	462	HIS	-	EXPRESSION TAG	UNP Q06433
K	463	HIS	-	EXPRESSION TAG	UNP Q06433
K	464	HIS	-	EXPRESSION TAG	UNP Q06433
K	465	HIS	-	EXPRESSION TAG	UNP Q06433
M	458	LEU	-	EXPRESSION TAG	UNP Q06433
M	459	GLU	-	EXPRESSION TAG	UNP Q06433
M	460	HIS	-	EXPRESSION TAG	UNP Q06433
M	461	HIS	-	EXPRESSION TAG	UNP Q06433
M	462	HIS	-	EXPRESSION TAG	UNP Q06433
M	463	HIS	-	EXPRESSION TAG	UNP Q06433
M	464	HIS	-	EXPRESSION TAG	UNP Q06433

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Chain	Residue	Modelled	Actual	Comment	Reference
M	465	HIS	-	EXPRESSION TAG	UNP Q06433
O	458	LEU	-	EXPRESSION TAG	UNP Q06433
O	459	GLU	-	EXPRESSION TAG	UNP Q06433
O	460	HIS	-	EXPRESSION TAG	UNP Q06433
O	461	HIS	-	EXPRESSION TAG	UNP Q06433
O	462	HIS	-	EXPRESSION TAG	UNP Q06433
O	463	HIS	-	EXPRESSION TAG	UNP Q06433
O	464	HIS	-	EXPRESSION TAG	UNP Q06433
O	465	HIS	-	EXPRESSION TAG	UNP Q06433

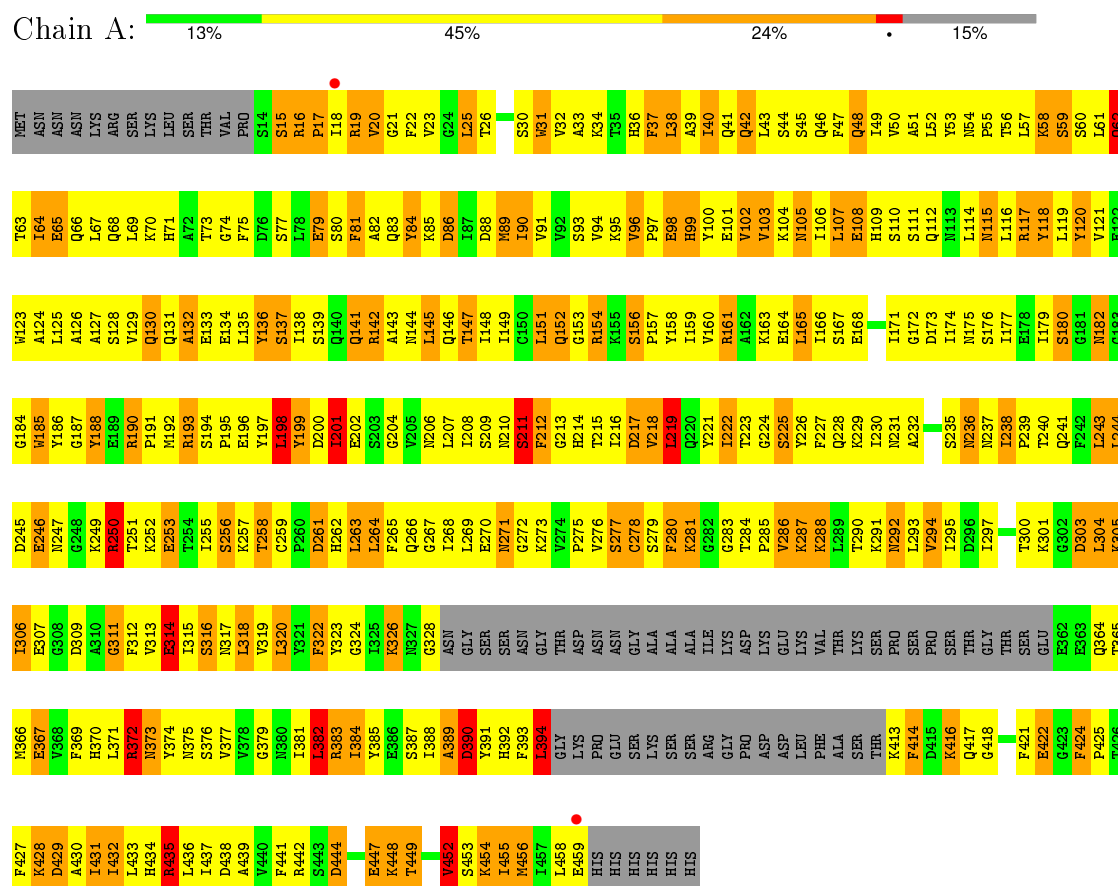
- Molecule 2 is a protein called Lactose regulatory protein LAC9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	14	Total	C	N	O	S	0	0	0
			119	77	16	25	1			
2	D	14	Total	C	N	O	S	0	0	0
			119	77	16	25	1			
2	F	14	Total	C	N	O	S	0	0	0
			119	77	16	25	1			
2	H	14	Total	C	N	O	S	0	0	0
			119	77	16	25	1			
2	J	14	Total	C	N	O	S	0	0	0
			119	77	16	25	1			
2	L	14	Total	C	N	O	S	0	0	0
			119	77	16	25	1			
2	N	14	Total	C	N	O	S	0	0	0
			119	77	16	25	1			
2	P	14	Total	C	N	O	S	0	0	0
			119	77	16	25	1			

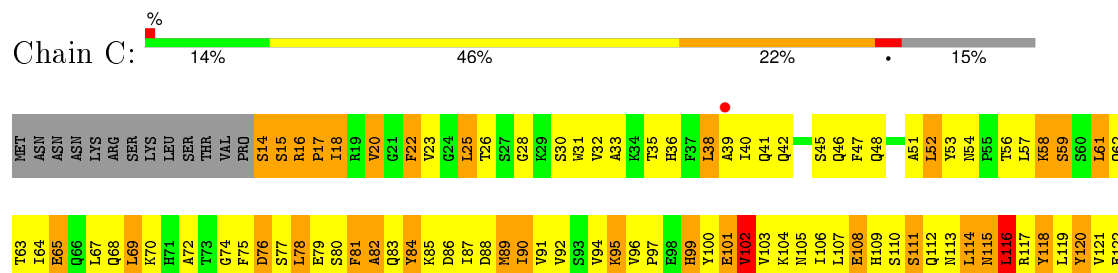
### 3 Residue-property plots

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: Galactose/lactose metabolism regulatory protein GAL80

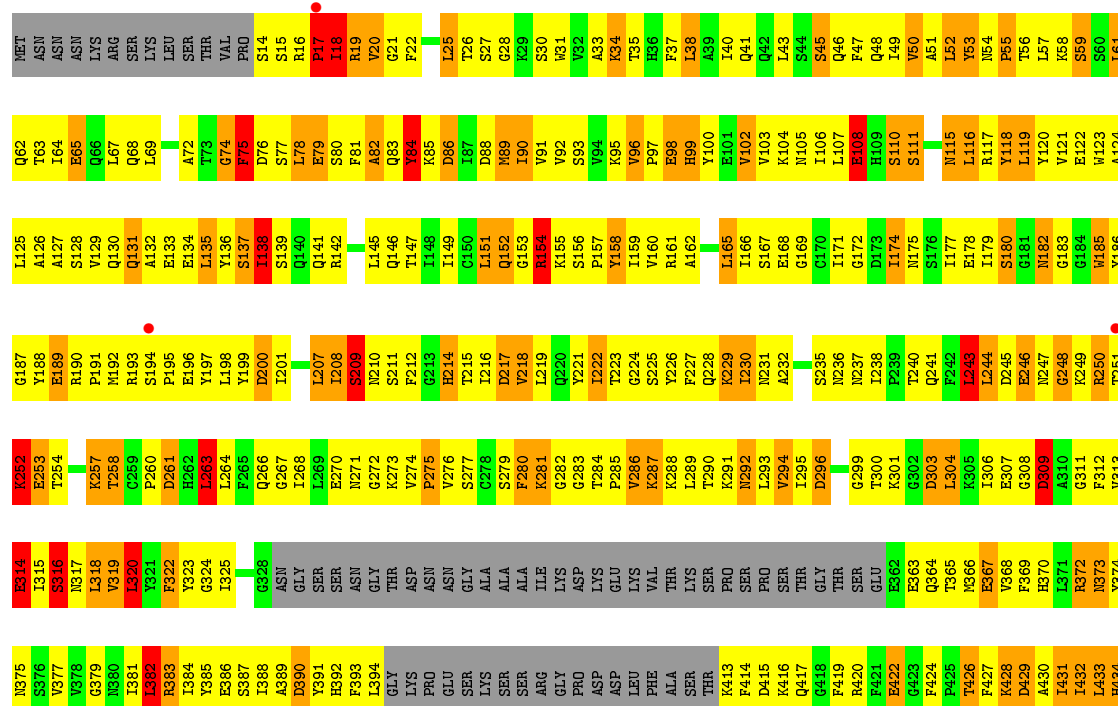


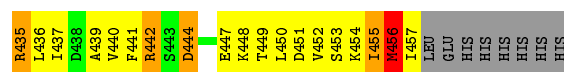
- Molecule 1: Galactose/lactose metabolism regulatory protein GAL80



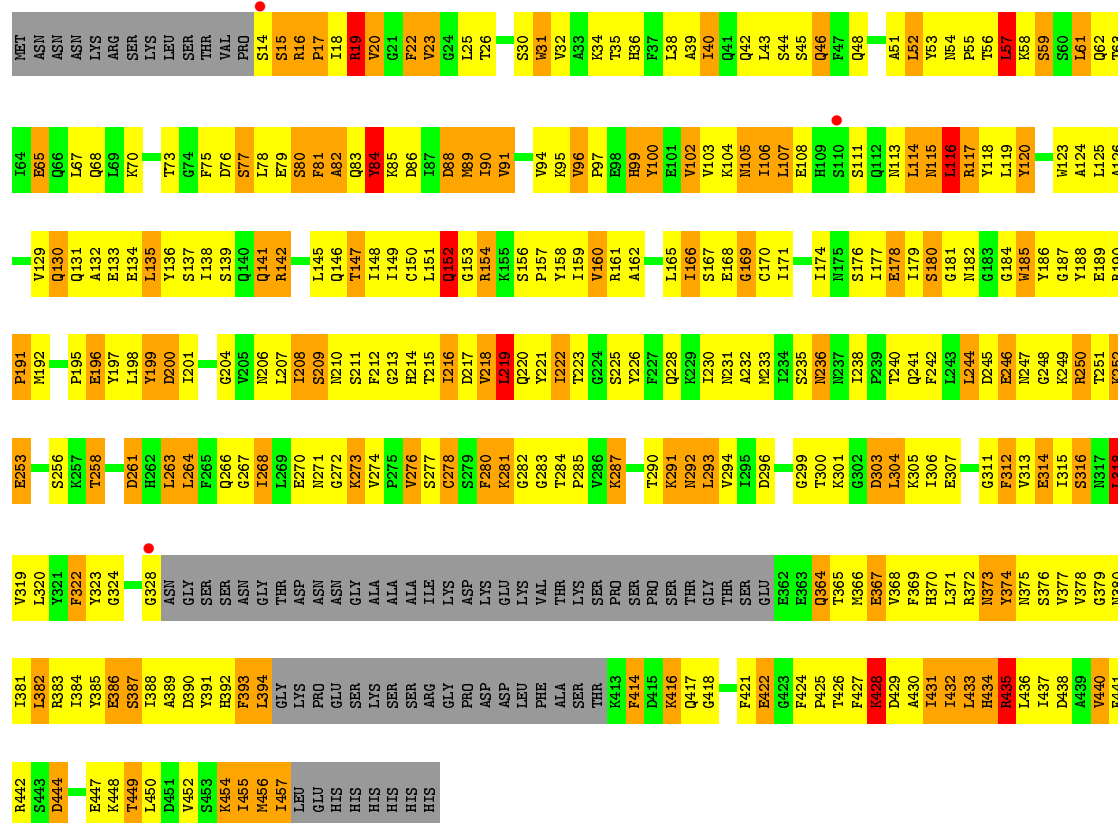
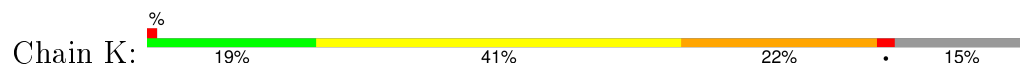




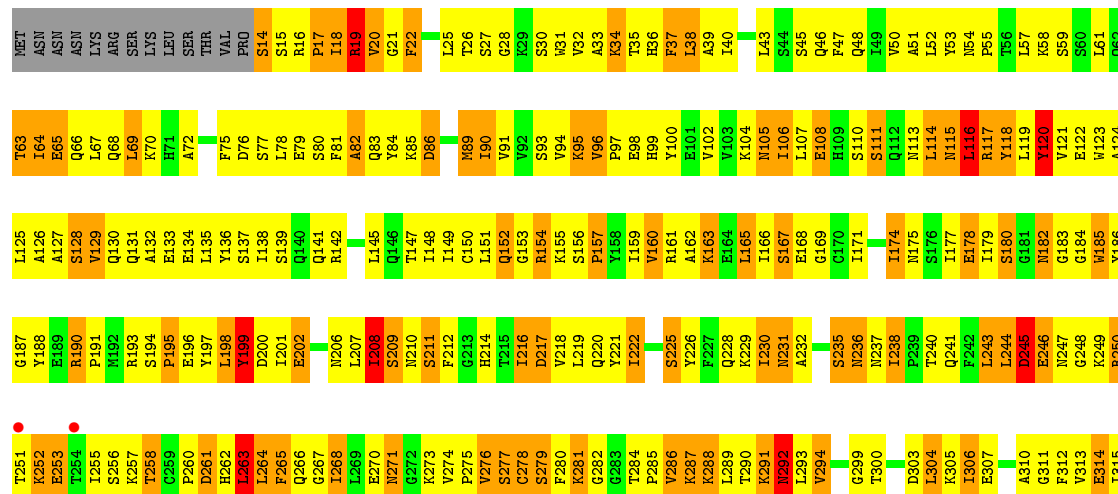
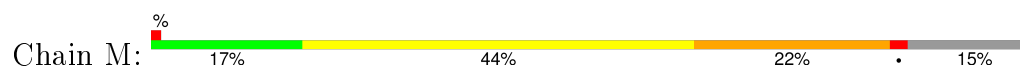




• Molecule 1: Galactose/lactose metabolism regulatory protein GAL80

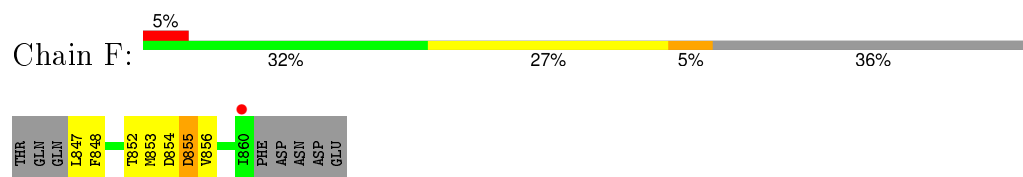


• Molecule 1: Galactose/lactose metabolism regulatory protein GAL80

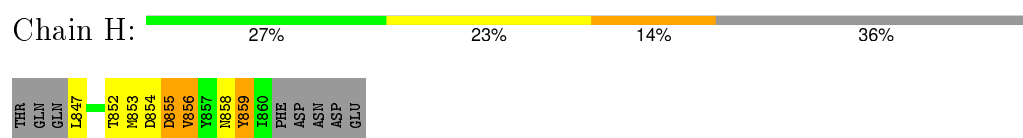




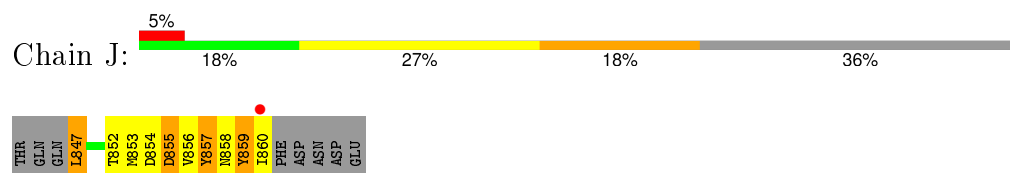
- Molecule 2: Lactose regulatory protein LAC9



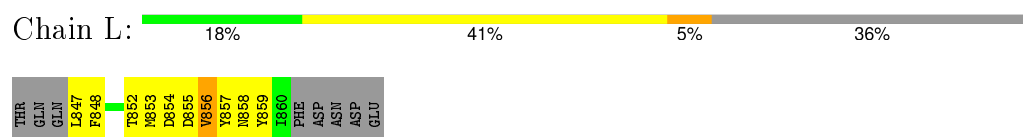
- Molecule 2: Lactose regulatory protein LAC9



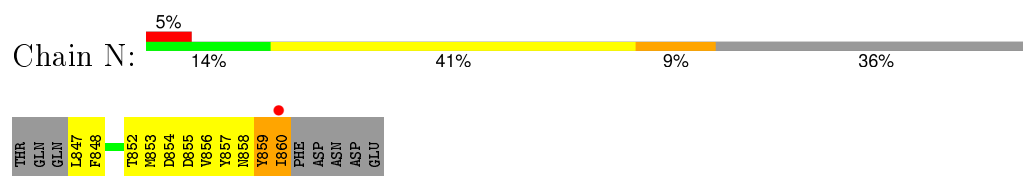
- Molecule 2: Lactose regulatory protein LAC9



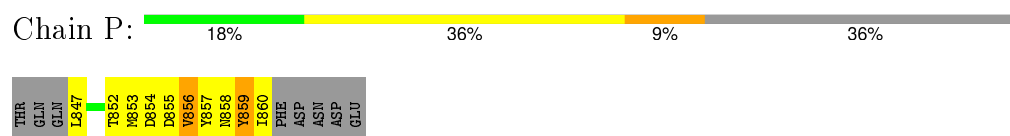
- Molecule 2: Lactose regulatory protein LAC9



- Molecule 2: Lactose regulatory protein LAC9



- Molecule 2: Lactose regulatory protein LAC9



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.10Å 160.50Å 132.60Å 90.00° 94.70° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 48.41 – 2.99	Depositor EDS
% Data completeness (in resolution range)	88.8 (30.00-3.00) 88.3 (48.41-2.99)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.68 (at 3.01Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.228 , 0.289 0.221 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	36.5	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 123.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	4 of 74981 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	26057	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.86 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.8688e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	1.11	7/3215 (0.2%)	1.66	65/4340 (1.5%)
1	C	0.98	7/3198 (0.2%)	1.59	46/4317 (1.1%)
1	E	1.12	5/3198 (0.2%)	1.62	45/4317 (1.0%)
1	G	1.09	11/3198 (0.3%)	1.56	37/4317 (0.9%)
1	I	1.14	8/3198 (0.3%)	1.61	57/4317 (1.3%)
1	K	1.06	4/3198 (0.1%)	1.58	50/4317 (1.2%)
1	M	1.05	4/3198 (0.1%)	1.62	53/4317 (1.2%)
1	O	0.96	1/3198 (0.0%)	1.60	48/4317 (1.1%)
2	B	0.95	0/121	1.63	0/165
2	D	1.07	0/121	1.23	0/165
2	F	0.97	0/121	1.30	1/165 (0.6%)
2	H	0.88	0/121	1.41	0/165
2	J	1.09	0/121	1.32	0/165
2	L	1.01	0/121	1.29	0/165
2	N	0.79	0/121	1.33	0/165
2	P	0.72	0/121	1.39	0/165
All	All	1.06	47/26569 (0.2%)	1.60	402/35879 (1.1%)

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	O	0	1

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	158	TYR	CD2-CE2	-6.72	1.29	1.39
1	G	158	TYR	CD2-CE2	-6.69	1.29	1.39
1	C	158	TYR	CE2-CZ	-6.55	1.30	1.38
1	A	326	LYS	CE-NZ	6.50	1.65	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	84	TYR	CD2-CE2	-6.30	1.29	1.39
1	E	197	TYR	CE1-CZ	-6.26	1.30	1.38
1	G	158	TYR	CE1-CZ	-6.14	1.30	1.38
1	G	84	TYR	CD1-CE1	-6.11	1.30	1.39
1	C	158	TYR	CD1-CE1	-6.09	1.30	1.39
1	E	197	TYR	CD1-CE1	-5.95	1.30	1.39
1	C	120	TYR	CD1-CE1	-5.89	1.30	1.39
1	K	374	TYR	CE1-CZ	-5.88	1.30	1.38
1	M	216	ILE	CA-CB	-5.88	1.41	1.54
1	A	374	TYR	CE1-CZ	-5.80	1.31	1.38
1	I	226	TYR	CD2-CE2	-5.78	1.30	1.39
1	I	229	LYS	CE-NZ	5.74	1.63	1.49
1	A	136	TYR	CD1-CE1	-5.74	1.30	1.39
1	I	226	TYR	CE2-CZ	-5.71	1.31	1.38
1	G	280	PHE	CD1-CE1	-5.69	1.27	1.39
1	G	158	TYR	CE2-CZ	-5.66	1.31	1.38
1	M	120	TYR	CD1-CE1	-5.63	1.30	1.39
1	A	132	ALA	CA-CB	-5.60	1.40	1.52
1	G	185	TRP	CB-CG	-5.58	1.40	1.50
1	M	120	TYR	CE2-CZ	-5.55	1.31	1.38
1	G	158	TYR	CD1-CE1	-5.52	1.31	1.39
1	I	189	GLU	CB-CG	-5.48	1.41	1.52
1	E	197	TYR	CD2-CE2	-5.45	1.31	1.39
1	K	301	LYS	CE-NZ	5.36	1.62	1.49
1	K	421	PHE	CE2-CZ	-5.35	1.27	1.37
1	G	188	TYR	CE2-CZ	-5.34	1.31	1.38
1	E	120	TYR	CE1-CZ	-5.32	1.31	1.38
1	A	120	TYR	CD1-CE1	-5.30	1.31	1.39
1	K	20	VAL	CB-CG2	-5.30	1.41	1.52
1	I	374	TYR	CE1-CZ	-5.20	1.31	1.38
1	C	279	SER	CB-OG	5.14	1.49	1.42
1	C	196	GLU	CG-CD	5.12	1.59	1.51
1	I	189	GLU	CG-CD	-5.12	1.44	1.51
1	M	199	TYR	CD1-CE1	-5.11	1.31	1.39
1	A	452	VAL	CB-CG2	-5.09	1.42	1.52
1	C	120	TYR	CD2-CE2	-5.04	1.31	1.39
1	G	178	GLU	CG-CD	-5.03	1.44	1.51
1	I	280	PHE	CD1-CE1	-5.01	1.29	1.39
1	A	383	ARG	CB-CG	-5.01	1.39	1.52
1	I	314	GLU	CG-CD	-5.01	1.44	1.51
1	O	120	TYR	CE1-CZ	-5.01	1.32	1.38
1	E	102	VAL	CB-CG1	5.00	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	186	TYR	CE2-CZ	-5.00	1.32	1.38

All (402) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	119	LEU	CB-CG-CD2	-14.83	85.79	111.00
1	A	165	LEU	CB-CG-CD2	-12.70	89.41	111.00
1	G	38	LEU	CA-CB-CG	-12.12	87.41	115.30
1	O	38	LEU	CA-CB-CG	-10.97	90.07	115.30
1	M	165	LEU	CB-CG-CD2	-10.97	92.36	111.00
1	M	38	LEU	CA-CB-CG	-10.81	90.43	115.30
1	G	154	ARG	NE-CZ-NH1	10.40	125.50	120.30
1	A	429	ASP	CB-CG-OD1	-10.39	108.94	118.30
1	K	371	LEU	CB-CG-CD1	-10.34	93.42	111.00
1	O	161	ARG	NE-CZ-NH1	-10.29	115.16	120.30
1	I	38	LEU	CA-CB-CG	-9.95	92.42	115.30
1	E	154	ARG	NE-CZ-NH2	9.90	125.25	120.30
1	G	264	LEU	CB-CG-CD2	-9.83	94.29	111.00
1	G	43	LEU	CB-CG-CD1	9.79	127.64	111.00
1	I	243	LEU	CB-CG-CD2	-9.78	94.37	111.00
1	A	61	LEU	CB-CG-CD2	-9.74	94.44	111.00
1	E	38	LEU	CA-CB-CG	-9.71	92.96	115.30
1	E	145	LEU	CB-CG-CD2	-9.50	94.84	111.00
1	C	38	LEU	CA-CB-CG	-9.27	93.97	115.30
1	A	250	ARG	CB-CA-C	-9.27	91.86	110.40
1	G	161	ARG	NE-CZ-NH1	-9.25	115.67	120.30
1	O	320	LEU	CB-CG-CD1	-9.24	95.30	111.00
1	A	217	ASP	CB-CG-OD1	8.96	126.36	118.30
1	A	320	LEU	CB-CG-CD2	-8.95	95.79	111.00
1	A	193	ARG	NE-CZ-NH2	-8.91	115.84	120.30
1	M	116	LEU	CB-CG-CD1	-8.82	96.00	111.00
1	O	145	LEU	CB-CG-CD2	-8.68	96.25	111.00
1	C	198	LEU	CB-CG-CD2	8.67	125.75	111.00
1	M	190	ARG	NE-CZ-NH1	-8.62	115.99	120.30
1	M	119	LEU	CB-CG-CD2	-8.60	96.37	111.00
1	A	154	ARG	NE-CZ-NH1	-8.57	116.02	120.30
1	I	390	ASP	CB-CG-OD1	-8.46	110.68	118.30
1	A	219	LEU	CB-CG-CD2	-8.44	96.66	111.00
1	A	382	LEU	CB-CG-CD2	-8.26	96.96	111.00
1	C	293	LEU	CA-CB-CG	-8.20	96.43	115.30
1	K	294	VAL	CB-CA-C	-8.16	95.89	111.40
1	I	309	ASP	CB-CG-OD2	8.11	125.60	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	38	LEU	CB-CG-CD2	-8.11	97.21	111.00
1	K	57	LEU	CA-CB-CG	-8.11	96.65	115.30
1	O	222	ILE	CB-CA-C	-8.11	95.39	111.60
1	E	420	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	O	244	LEU	CB-CG-CD2	-7.99	97.42	111.00
1	C	38	LEU	CB-CG-CD2	-7.95	97.48	111.00
1	E	16	ARG	NE-CZ-NH1	-7.89	116.35	120.30
1	C	222	ILE	CB-CA-C	-7.89	95.82	111.60
1	E	429	ASP	CB-CG-OD1	-7.89	111.20	118.30
1	K	15	SER	CB-CA-C	7.87	125.06	110.10
1	M	250	ARG	CB-CA-C	-7.87	94.67	110.40
1	O	25	LEU	CA-CB-CG	-7.83	97.29	115.30
1	K	440	VAL	CG1-CB-CG2	7.74	123.29	110.90
1	E	433	LEU	CB-CG-CD1	-7.73	97.86	111.00
1	A	190	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	I	217	ASP	CB-CG-OD1	7.67	125.20	118.30
1	I	74	GLY	N-CA-C	7.66	132.24	113.10
1	A	119	LEU	CB-CG-CD2	-7.61	98.07	111.00
1	I	75	PHE	N-CA-C	7.53	131.32	111.00
1	O	391	TYR	N-CA-CB	-7.51	97.07	110.60
1	K	88	ASP	CB-CG-OD1	-7.49	111.56	118.30
1	E	116	LEU	CB-CG-CD1	-7.47	98.29	111.00
1	I	78	LEU	CB-CG-CD1	-7.45	98.34	111.00
1	E	21	GLY	N-CA-C	-7.42	94.55	113.10
1	E	58	LYS	CD-CE-NZ	7.41	128.75	111.70
1	O	102	VAL	CB-CA-C	-7.41	97.32	111.40
1	E	391	TYR	N-CA-CB	-7.40	97.29	110.60
1	G	43	LEU	CB-CG-CD2	-7.39	98.43	111.00
1	A	62	GLN	CB-CA-C	-7.39	95.63	110.40
1	O	161	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	G	116	LEU	CA-CB-CG	-7.38	98.33	115.30
1	I	391	TYR	N-CA-CB	-7.36	97.36	110.60
1	M	442	ARG	NE-CZ-NH2	-7.35	116.63	120.30
1	I	21	GLY	N-CA-C	-7.30	94.85	113.10
1	K	293	LEU	CA-CB-CG	-7.30	98.51	115.30
1	O	234	ILE	CG1-CB-CG2	-7.29	95.35	111.40
1	M	222	ILE	CB-CA-C	-7.29	97.03	111.60
1	I	222	ILE	CB-CA-C	-7.29	97.03	111.60
1	A	96	VAL	C-N-CD	-7.28	104.58	120.60
1	K	15	SER	N-CA-CB	-7.28	99.58	110.50
1	G	250	ARG	CB-CA-C	-7.27	95.86	110.40
1	M	263	LEU	CB-CG-CD2	7.26	123.33	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	37	PHE	CB-CG-CD1	7.22	125.86	120.80
1	K	391	TYR	N-CA-CB	-7.22	97.61	110.60
1	O	374	TYR	N-CA-C	-7.22	91.51	111.00
1	O	244	LEU	CB-CG-CD1	-7.20	98.75	111.00
1	M	37	PHE	CB-CG-CD2	-7.20	115.76	120.80
1	G	220	GLN	N-CA-C	-7.19	91.60	111.00
1	A	306	ILE	CG1-CB-CG2	7.18	127.20	111.40
1	A	161	ARG	NE-CZ-NH2	7.17	123.89	120.30
1	M	429	ASP	CB-CG-OD1	-7.14	111.87	118.30
1	A	21	GLY	N-CA-C	-7.08	95.41	113.10
1	I	207	LEU	CB-CG-CD2	-7.07	98.98	111.00
1	O	431	ILE	CG1-CB-CG2	-7.06	95.87	111.40
1	O	15	SER	CB-CA-C	7.06	123.51	110.10
1	K	135	LEU	CB-CG-CD1	-7.05	99.01	111.00
1	M	322	PHE	CB-CG-CD2	-7.05	115.86	120.80
1	M	230	ILE	CB-CA-C	-6.97	97.66	111.60
1	A	38	LEU	CA-CB-CG	-6.95	99.31	115.30
1	I	119	LEU	CB-CG-CD2	-6.95	99.18	111.00
1	O	102	VAL	N-CA-C	6.95	129.76	111.00
1	K	16	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	K	222	ILE	CB-CA-C	-6.92	97.75	111.60
1	A	317	ASN	N-CA-C	-6.91	92.34	111.00
1	E	294	VAL	CB-CA-C	-6.89	98.30	111.40
1	C	220	GLN	N-CA-C	-6.86	92.48	111.00
1	A	25	LEU	CA-CB-CG	-6.85	99.55	115.30
1	E	15	SER	N-CA-C	-6.85	92.52	111.00
1	G	222	ILE	CB-CA-C	-6.84	97.92	111.60
1	O	135	LEU	CB-CG-CD1	-6.82	99.40	111.00
1	A	198	LEU	N-CA-C	-6.81	92.60	111.00
1	A	384	ILE	CB-CA-C	-6.81	97.97	111.60
1	M	245	ASP	CB-CG-OD1	-6.81	112.17	118.30
1	O	294	VAL	CB-CA-C	-6.80	98.48	111.40
1	K	106	ILE	CG1-CB-CG2	-6.77	96.50	111.40
1	E	16	ARG	NE-CZ-NH2	6.77	123.69	120.30
1	M	217	ASP	CB-CG-OD2	6.74	124.37	118.30
1	G	96	VAL	C-N-CD	-6.74	105.78	120.60
1	K	428	LYS	CD-CE-NZ	6.73	127.19	111.70
1	C	135	LEU	CB-CG-CD1	-6.73	99.56	111.00
1	M	371	LEU	CB-CG-CD2	-6.73	99.56	111.00
1	K	219	LEU	CB-CG-CD1	-6.72	99.57	111.00
1	O	158	TYR	CB-CG-CD2	-6.72	116.97	121.00
1	A	40	ILE	CG1-CB-CG2	-6.70	96.65	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	320	LEU	CB-CG-CD2	-6.69	99.62	111.00
1	K	77	SER	CA-CB-OG	6.69	129.26	111.20
1	E	250	ARG	CB-CA-C	-6.68	97.03	110.40
1	K	18	ILE	N-CA-C	-6.67	92.98	111.00
1	A	222	ILE	CG1-CB-CG2	-6.66	96.74	111.40
1	E	447	GLU	OE1-CD-OE2	6.64	131.27	123.30
1	I	165	LEU	CB-CG-CD2	-6.62	99.74	111.00
1	I	296	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	C	90	ILE	CB-CA-C	-6.58	98.44	111.60
1	G	90	ILE	CB-CA-C	-6.56	98.49	111.60
1	E	151	LEU	CB-CG-CD1	-6.55	99.86	111.00
1	E	438	ASP	CB-CG-OD2	6.54	124.18	118.30
1	K	43	LEU	CB-CG-CD1	6.54	122.11	111.00
1	K	96	VAL	C-N-CD	-6.53	106.24	120.60
1	E	374	TYR	N-CA-C	-6.51	93.41	111.00
1	G	204	GLY	N-CA-C	-6.51	96.82	113.10
1	M	440	VAL	CB-CA-C	-6.51	99.02	111.40
1	I	38	LEU	CB-CG-CD1	6.50	122.06	111.00
1	O	52	LEU	CA-CB-CG	-6.49	100.38	115.30
1	G	217	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	K	204	GLY	N-CA-C	-6.47	96.93	113.10
1	E	34	LYS	CD-CE-NZ	-6.47	96.82	111.70
1	C	286	VAL	CB-CA-C	-6.46	99.13	111.40
1	I	316	SER	N-CA-C	6.46	128.43	111.00
1	I	288	LYS	CD-CE-NZ	-6.43	96.92	111.70
2	F	855	ASP	CB-CA-C	-6.36	97.67	110.40
1	M	372	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	I	27	SER	CA-CB-OG	-6.33	94.09	111.20
1	I	154	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	M	294	VAL	CB-CA-C	-6.32	99.39	111.40
1	C	391	TYR	N-CA-CB	-6.32	99.22	110.60
1	I	95	LYS	CB-CA-C	-6.32	97.76	110.40
1	C	74	GLY	N-CA-C	6.32	128.89	113.10
1	K	318	LEU	CB-CG-CD2	-6.32	100.26	111.00
1	O	208	ILE	CB-CA-C	-6.31	98.98	111.60
1	A	90	ILE	CB-CA-C	-6.30	99.00	111.60
1	I	433	LEU	CB-CG-CD1	-6.29	100.31	111.00
1	A	173	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	A	25	LEU	CB-CG-CD1	-6.27	100.34	111.00
1	E	263	LEU	CB-CG-CD2	6.26	121.64	111.00
1	A	86	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	E	429	ASP	CB-CG-OD2	6.22	123.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	306	ILE	CG1-CB-CG2	-6.21	97.73	111.40
1	O	219	LEU	CB-CG-CD1	-6.21	100.44	111.00
1	G	371	LEU	CA-CB-CG	6.21	129.57	115.30
1	A	429	ASP	OD1-CG-OD2	6.20	135.09	123.30
1	K	116	LEU	CB-CG-CD2	-6.19	100.48	111.00
1	G	414	PHE	N-CA-CB	-6.19	99.47	110.60
1	C	294	VAL	CB-CA-C	-6.17	99.67	111.40
1	I	456	MET	CG-SD-CE	6.17	110.07	100.20
1	M	18	ILE	N-CA-C	-6.17	94.35	111.00
1	I	18	ILE	N-CA-C	-6.15	94.39	111.00
1	O	204	GLY	N-CA-C	-6.15	97.73	113.10
1	I	317	ASN	N-CA-C	-6.13	94.44	111.00
1	C	76	ASP	CB-CG-OD1	-6.12	112.80	118.30
1	C	116	LEU	CB-CG-CD2	-6.10	100.62	111.00
1	A	15	SER	N-CA-C	-6.10	94.53	111.00
1	A	107	LEU	CB-CG-CD1	-6.09	100.66	111.00
1	A	154	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	I	426	THR	CA-CB-CG2	-6.08	103.89	112.40
1	A	38	LEU	CB-CG-CD1	6.08	121.33	111.00
1	A	376	SER	N-CA-CB	-6.07	101.39	110.50
1	A	391	TYR	N-CA-CB	-6.07	99.67	110.60
1	I	257	LYS	CA-CB-CG	-6.06	100.06	113.40
1	M	391	TYR	N-CA-CB	-6.06	99.69	110.60
1	E	25	LEU	CB-CA-C	6.06	121.71	110.20
1	K	256	SER	CB-CA-C	-6.06	98.59	110.10
1	M	69	LEU	CB-CG-CD2	-6.05	100.72	111.00
1	C	69	LEU	CB-CG-CD2	6.04	121.28	111.00
1	G	89	MET	CB-CG-SD	-6.04	94.28	112.40
1	K	220	GLN	N-CA-C	-6.04	94.69	111.00
1	C	250	ARG	CB-CA-C	-6.04	98.33	110.40
1	K	91	VAL	CA-CB-CG2	-6.03	101.85	110.90
1	E	371	LEU	CB-CG-CD2	-6.03	100.75	111.00
1	I	294	VAL	CB-CA-C	-6.02	99.96	111.40
1	I	18	ILE	CB-CA-C	-6.00	99.60	111.60
1	G	316	SER	N-CA-C	5.99	127.18	111.00
1	G	276	VAL	N-CA-C	5.99	127.17	111.00
1	O	18	ILE	N-CA-C	-5.99	94.82	111.00
1	A	424	PHE	CB-CG-CD1	-5.97	116.62	120.80
1	I	230	ILE	CB-CA-C	-5.97	99.67	111.60
1	C	393	PHE	CB-CG-CD1	-5.96	116.62	120.80
1	E	420	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	212	PHE	CB-CG-CD1	-5.96	116.63	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	390	ASP	CB-CG-OD1	-5.96	112.94	118.30
1	I	442	ARG	CG-CD-NE	-5.95	99.30	111.80
1	C	381	ILE	CG1-CB-CG2	-5.95	98.31	111.40
1	M	414	PHE	N-CA-CB	-5.95	99.90	110.60
1	C	376	SER	N-CA-CB	-5.93	101.61	110.50
1	A	382	LEU	CA-CB-CG	-5.93	101.67	115.30
1	A	18	ILE	N-CA-C	-5.92	95.01	111.00
1	I	17	PRO	N-CA-C	5.92	127.50	112.10
1	I	138	ILE	CG1-CB-CG2	-5.92	98.38	111.40
1	O	304	LEU	CB-CG-CD1	-5.90	100.97	111.00
1	O	316	SER	N-CA-C	5.90	126.92	111.00
1	M	163	LYS	CD-CE-NZ	5.88	125.23	111.70
1	C	200	ASP	CB-CG-OD2	-5.87	113.01	118.30
1	A	243	LEU	CA-CB-CG	-5.87	101.80	115.30
1	C	243	LEU	CA-CB-CG	-5.87	101.80	115.30
1	M	452	VAL	CA-CB-CG2	-5.87	102.10	110.90
1	K	268	ILE	CG1-CB-CG2	-5.87	98.49	111.40
1	O	52	LEU	CB-CG-CD1	-5.86	101.03	111.00
1	A	414	PHE	N-CA-CB	-5.85	100.06	110.60
1	C	372	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	E	320	LEU	CB-CG-CD2	-5.85	101.06	111.00
1	E	256	SER	CB-CA-C	-5.84	99.00	110.10
1	E	276	VAL	N-CA-C	5.83	126.74	111.00
1	A	372	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	294	VAL	CB-CA-C	-5.82	100.34	111.40
1	I	49	ILE	CB-CA-C	-5.82	99.96	111.60
1	E	40	ILE	CG1-CB-CG2	-5.81	98.61	111.40
1	M	21	GLY	N-CA-C	-5.81	98.57	113.10
1	A	64	ILE	CG1-CB-CG2	5.81	124.18	111.40
1	E	317	ASN	N-CA-C	-5.80	95.34	111.00
1	K	316	SER	N-CA-C	5.79	126.65	111.00
1	O	253	GLU	OE1-CD-OE2	5.79	130.25	123.30
1	A	264	LEU	CB-CG-CD1	-5.77	101.19	111.00
1	M	61	LEU	CB-CG-CD2	-5.76	101.20	111.00
1	A	271	ASN	CB-CA-C	-5.76	98.88	110.40
1	C	41	GLN	CB-CA-C	-5.76	98.89	110.40
1	M	211	SER	N-CA-CB	5.76	119.14	110.50
1	E	414	PHE	N-CA-CB	-5.75	100.25	110.60
1	E	151	LEU	CB-CG-CD2	-5.73	101.25	111.00
1	G	384	ILE	CG1-CB-CG2	-5.72	98.81	111.40
1	K	57	LEU	CB-CG-CD2	-5.71	101.28	111.00
1	A	316	SER	N-CA-C	5.71	126.41	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	21	GLY	N-CA-C	-5.71	98.83	113.10
1	O	243	LEU	CA-CB-CG	-5.70	102.19	115.30
1	M	43	LEU	CA-CB-CG	-5.69	102.21	115.30
1	C	264	LEU	CB-CA-C	-5.68	99.41	110.20
1	M	25	LEU	CA-CB-CG	-5.68	102.24	115.30
1	I	308	GLY	N-CA-C	-5.67	98.91	113.10
1	I	325	ILE	N-CA-C	5.66	126.27	111.00
1	I	429	ASP	CB-CG-OD2	5.65	123.39	118.30
1	M	57	LEU	CB-CG-CD1	-5.65	101.39	111.00
1	O	171	ILE	CG1-CB-CG2	5.65	123.84	111.40
1	K	116	LEU	N-CA-C	-5.65	95.75	111.00
1	K	312	PHE	CB-CG-CD2	-5.65	116.84	120.80
1	A	448	LYS	N-CA-CB	-5.65	100.44	110.60
1	M	279	SER	N-CA-CB	5.64	118.96	110.50
1	O	119	LEU	CB-CG-CD1	5.61	120.53	111.00
1	M	286	VAL	CB-CA-C	-5.60	100.76	111.40
1	M	63	THR	CA-CB-CG2	-5.59	104.57	112.40
1	G	18	ILE	N-CA-C	-5.59	95.91	111.00
1	O	212	PHE	CB-CG-CD1	-5.58	116.90	120.80
1	M	243	LEU	CA-CB-CG	-5.55	102.53	115.30
1	E	376	SER	N-CA-CB	-5.55	102.18	110.50
1	O	145	LEU	CB-CG-CD1	-5.54	101.57	111.00
1	C	448	LYS	N-CA-CB	-5.54	100.63	110.60
1	E	316	SER	N-CA-C	5.53	125.92	111.00
1	I	368	VAL	CG1-CB-CG2	-5.52	102.06	110.90
1	E	207	LEU	CA-CB-CG	5.51	127.97	115.30
1	O	96	VAL	C-N-CD	-5.50	108.50	120.60
1	A	371	LEU	CB-CG-CD2	-5.49	101.67	111.00
1	I	248	GLY	C-N-CA	-5.49	107.98	121.70
1	A	314	GLU	OE1-CD-OE2	5.48	129.88	123.30
1	C	435	ARG	CB-CA-C	-5.48	99.44	110.40
1	C	204	GLY	N-CA-C	-5.47	99.43	113.10
1	G	43	LEU	CA-CB-CG	-5.47	102.73	115.30
1	G	374	TYR	N-CA-C	-5.47	96.24	111.00
1	I	110	SER	CB-CA-C	-5.46	99.72	110.10
1	I	243	LEU	CA-CB-CG	-5.46	102.75	115.30
1	O	393	PHE	CB-CG-CD1	-5.46	116.98	120.80
1	M	276	VAL	N-CA-C	5.46	125.73	111.00
1	I	263	LEU	CB-CG-CD2	5.45	120.26	111.00
1	M	96	VAL	C-N-CD	-5.45	108.62	120.60
1	C	25	LEU	CB-CG-CD2	5.44	120.25	111.00
1	I	86	ASP	CB-CG-OD2	5.44	123.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	96	VAL	C-N-CD	-5.43	108.66	120.60
1	E	37	PHE	CB-CG-CD1	5.42	124.59	120.80
1	K	276	VAL	N-CA-C	5.42	125.62	111.00
1	A	204	GLY	N-CA-C	-5.41	99.57	113.10
1	C	69	LEU	CA-CB-CG	-5.41	102.86	115.30
1	K	120	TYR	CB-CG-CD1	-5.41	117.75	121.00
1	G	233	MET	CG-SD-CE	5.40	108.84	100.20
1	M	208	ILE	CA-C-N	-5.40	105.33	117.20
1	G	25	LEU	N-CA-CB	5.39	121.18	110.40
1	I	135	LEU	CB-CG-CD1	-5.38	101.85	111.00
1	C	102	VAL	CG1-CB-CG2	-5.38	102.29	110.90
1	A	394	LEU	CB-CG-CD2	5.37	120.13	111.00
1	K	23	VAL	CG1-CB-CG2	-5.37	102.30	110.90
1	A	222	ILE	CB-CA-C	-5.35	100.90	111.60
1	C	256	SER	CB-CA-C	-5.35	99.93	110.10
1	O	264	LEU	CB-CA-C	-5.33	100.07	110.20
1	G	153	GLY	N-CA-C	-5.33	99.78	113.10
1	O	207	LEU	CA-CB-CG	5.32	127.53	115.30
1	C	15	SER	N-CA-C	5.31	125.34	111.00
1	M	235	SER	N-CA-C	5.31	125.33	111.00
1	A	151	LEU	CB-CG-CD1	-5.31	101.98	111.00
1	K	304	LEU	CB-CA-C	-5.30	100.12	110.20
1	O	297	ILE	CG1-CB-CG2	5.30	123.07	111.40
1	C	419	PHE	CB-CG-CD2	-5.30	117.09	120.80
1	K	100	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	O	183	GLY	N-CA-C	-5.30	99.86	113.10
1	E	86	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	31	TRP	CB-CA-C	-5.29	99.82	110.40
1	G	286	VAL	CG1-CB-CG2	5.29	119.36	110.90
1	K	19	ARG	CG-CD-NE	-5.29	100.70	111.80
1	K	457	ILE	CG1-CB-CG2	5.29	123.03	111.40
1	K	250	ARG	CB-CA-C	-5.28	99.83	110.40
1	I	90	ILE	CG1-CB-CG2	5.28	123.02	111.40
1	A	238	ILE	N-CA-C	-5.28	96.75	111.00
1	A	390	ASP	CB-CG-OD1	5.28	123.05	118.30
1	G	21	GLY	N-CA-C	-5.28	99.91	113.10
1	C	371	LEU	CA-CB-CG	5.27	127.43	115.30
1	I	286	VAL	CB-CA-C	-5.27	101.38	111.40
1	K	414	PHE	N-CA-CB	-5.27	101.11	110.60
1	E	286	VAL	CB-CA-C	-5.27	101.39	111.40
1	I	158	TYR	CB-CG-CD2	-5.26	117.84	121.00
1	A	211	SER	N-CA-C	5.25	125.17	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	238	ILE	N-CA-C	-5.25	96.83	111.00
1	M	238	ILE	N-CA-C	-5.24	96.84	111.00
1	K	90	ILE	CB-CA-C	-5.24	101.12	111.60
1	G	432	ILE	CG1-CB-CG2	-5.23	99.89	111.40
1	M	256	SER	CB-CA-C	-5.22	100.17	110.10
1	E	439	ALA	N-CA-CB	-5.22	102.79	110.10
1	I	382	LEU	CA-CB-CG	-5.22	103.29	115.30
1	I	90	ILE	CB-CA-C	-5.21	101.17	111.60
1	M	371	LEU	CB-CG-CD1	-5.21	102.14	111.00
1	O	190	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	A	389	ALA	N-CA-CB	-5.20	102.83	110.10
1	C	207	LEU	CA-CB-CG	5.20	127.25	115.30
1	M	95	LYS	CB-CA-C	-5.19	100.02	110.40
1	M	19	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	G	444	ASP	CB-CG-OD1	5.17	122.96	118.30
1	A	219	LEU	CA-CB-CG	-5.17	103.42	115.30
1	A	73	THR	N-CA-C	-5.16	97.08	111.00
1	A	188	TYR	N-CA-C	-5.16	97.07	111.00
1	I	420	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	M	190	ARG	NH1-CZ-NH2	5.16	125.07	119.40
1	G	273	LYS	N-CA-C	-5.16	97.08	111.00
1	E	17	PRO	N-CA-C	5.16	125.50	112.10
1	I	374	TYR	N-CA-C	-5.15	97.09	111.00
1	C	317	ASN	N-CA-C	-5.15	97.10	111.00
1	M	90	ILE	CB-CA-C	-5.15	101.30	111.60
1	K	233	MET	CG-SD-CE	5.14	108.43	100.20
1	E	435	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	E	116	LEU	CB-CG-CD2	-5.14	102.26	111.00
1	K	95	LYS	CB-CA-C	-5.14	100.12	110.40
1	K	19	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	M	264	LEU	CB-CG-CD1	-5.12	102.29	111.00
1	K	438	ASP	CB-CG-OD1	-5.11	113.70	118.30
1	G	234	ILE	N-CA-C	5.11	124.80	111.00
1	C	414	PHE	N-CA-CB	-5.11	101.41	110.60
1	K	52	LEU	CB-CG-CD2	-5.11	102.32	111.00
1	C	432	ILE	CG1-CB-CG2	-5.11	100.17	111.40
1	O	252	LYS	CB-CA-C	5.11	120.61	110.40
1	I	108	GLU	OE1-CD-OE2	-5.10	117.17	123.30
1	K	154	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	I	207	LEU	CA-CB-CG	5.10	127.03	115.30
1	O	150	CYS	CA-CB-SG	-5.10	104.82	114.00
1	A	424	PHE	CB-CG-CD2	5.10	124.37	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	151	LEU	CA-CB-CG	-5.10	103.57	115.30
1	O	444	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	M	52	LEU	CB-CG-CD1	-5.09	102.34	111.00
1	G	179	ILE	CB-CA-C	-5.09	101.42	111.60
1	G	292	ASN	CB-CA-C	5.09	120.57	110.40
1	G	256	SER	CB-CA-C	-5.08	100.45	110.10
1	G	277	SER	CB-CA-C	-5.08	100.45	110.10
1	O	318	LEU	CB-CG-CD2	-5.08	102.37	111.00
1	C	273	LYS	N-CA-C	-5.07	97.30	111.00
1	C	276	VAL	N-CA-C	5.07	124.69	111.00
1	I	303	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	K	116	LEU	CB-CG-CD1	-5.07	102.38	111.00
1	C	212	PHE	CB-CG-CD1	-5.07	117.25	120.80
1	K	31	TRP	CB-CA-C	-5.06	100.27	110.40
1	E	271	ASN	CB-CA-C	-5.05	100.29	110.40
1	O	414	PHE	N-CA-CB	-5.05	101.51	110.60
1	C	189	GLU	OE1-CD-OE2	5.05	129.36	123.30
1	I	319	VAL	CB-CA-C	-5.04	101.82	111.40
1	M	317	ASN	N-CA-C	-5.04	97.38	111.00
1	A	374	TYR	N-CA-C	-5.04	97.39	111.00
1	C	116	LEU	CA-CB-CG	-5.04	103.72	115.30
1	E	52	LEU	CB-CG-CD2	-5.03	102.44	111.00
1	A	435	ARG	N-CA-CB	-5.03	101.55	110.60
1	M	292	ASN	CB-CA-C	5.03	120.45	110.40
1	M	374	TYR	N-CA-C	-5.02	97.44	111.00
1	C	78	LEU	CB-CG-CD2	5.02	119.53	111.00
1	O	95	LYS	CB-CA-C	-5.01	100.37	110.40
1	K	120	TYR	CB-CG-CD2	5.01	124.01	121.00
1	K	435	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	O	321	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3153	0	3158	482	0
1	C	3136	0	3141	458	0
1	E	3136	0	3139	465	0
1	G	3136	0	3141	463	0
1	I	3136	0	3141	420	0
1	K	3136	0	3141	391	0
1	M	3136	0	3141	373	0
1	O	3136	0	3141	435	0
2	B	119	0	107	22	0
2	D	119	0	107	9	0
2	F	119	0	107	6	0
2	H	119	0	107	9	0
2	J	119	0	107	12	0
2	L	119	0	107	12	0
2	N	119	0	107	11	0
2	P	119	0	107	10	0
All	All	26057	0	25999	3442	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 66.

All (3442) 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:C:452:VAL:HG13	1:C:455:ILE:CD1	1.46	1.43
1:C:452:VAL:CG1	1:C:455:ILE:HD12	1.47	1.43
1:E:198:LEU:HD13	1:E:199:TYR:CE1	1.57	1.38
1:E:194:SER:HB3	1:E:199:TYR:OH	1.20	1.27
1:I:281:LYS:HD2	1:I:282:GLY:N	1.51	1.23
1:G:392:HIS:CD2	1:G:393:PHE:CE2	2.25	1.23
1:I:228:GLN:NE2	1:I:273:LYS:HE3	1.53	1.21
1:I:390:ASP:O	1:I:394:LEU:HB2	1.41	1.20
1:G:392:HIS:CD2	1:G:393:PHE:CD2	2.32	1.17
1:O:208:ILE:HG22	1:O:209:SER:N	1.35	1.17
1:M:390:ASP:O	1:M:394:LEU:HB2	1.44	1.16
1:E:433:LEU:O	1:E:437:ILE:HD12	1.45	1.15
1:O:68:GLN:HA	1:O:68:GLN:HE21	1.02	1.14
1:E:198:LEU:HD12	1:E:198:LEU:H	1.09	1.14
1:O:390:ASP:O	1:O:394:LEU:HB2	1.49	1.11
1:E:198:LEU:HD13	1:E:199:TYR:CD1	1.84	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:281:LYS:NZ	1:G:285:PRO:O	1.84	1.11
1:G:123:TRP:CD1	1:G:214:HIS:CD2	2.39	1.11
1:I:281:LYS:HD2	1:I:282:GLY:H	1.01	1.10
1:A:244:LEU:HD12	1:A:250:ARG:HA	1.34	1.09
1:G:392:HIS:NE2	1:G:393:PHE:CE2	2.21	1.09
1:K:238:ILE:HD12	1:K:261:ASP:HB2	1.35	1.09
1:E:387:SER:OG	1:E:423:GLY:O	1.71	1.08
1:I:252:LYS:HD2	1:I:252:LYS:H	0.99	1.08
1:M:244:LEU:HD23	1:M:248:GLY:HA2	1.30	1.08
1:G:219:LEU:HA	1:G:222:ILE:HD12	1.30	1.08
1:O:244:LEU:HD12	1:O:250:ARG:HA	1.36	1.08
1:O:68:GLN:CA	1:O:68:GLN:HE21	1.61	1.08
1:A:168:GLU:O	1:A:328:GLY:O	1.70	1.07
1:G:123:TRP:CD1	1:G:214:HIS:HD2	1.74	1.06
1:E:390:ASP:O	1:E:394:LEU:HB2	1.55	1.06
1:K:452:VAL:HG13	1:K:455:ILE:HG13	1.35	1.06
1:O:208:ILE:CG2	1:O:209:SER:N	2.12	1.06
1:E:102:VAL:O	1:E:106:ILE:CD1	2.03	1.06
1:A:145:LEU:O	1:A:413:LYS:HD3	1.55	1.05
1:I:192:MET:CE	1:I:243:LEU:HD22	1.86	1.05
1:A:458:LEU:HG	1:A:459:GLU:H	1.19	1.05
1:O:57:LEU:CD2	1:O:61:LEU:HD11	1.86	1.04
1:E:194:SER:CB	1:E:199:TYR:OH	2.05	1.04
1:G:433:LEU:HG	1:G:437:ILE:HD11	1.35	1.04
1:I:117:ARG:O	1:I:145:LEU:HD12	1.57	1.04
1:I:289:LEU:HD12	1:K:303:ASP:HB3	1.10	1.04
1:E:379:GLY:O	1:E:382:LEU:HB3	1.57	1.04
1:M:289:LEU:HD12	1:O:303:ASP:HB3	1.39	1.04
1:A:266:GLN:HB2	1:C:264:LEU:HD22	1.08	1.03
1:E:384:ILE:O	1:E:388:ILE:HD12	1.56	1.03
1:A:266:GLN:NE2	1:C:231:ASN:HD22	1.56	1.03
1:K:390:ASP:O	1:K:394:LEU:HB2	1.57	1.03
1:C:96:VAL:O	1:C:99:HIS:HB2	1.58	1.03
1:A:65:GLU:HG3	1:A:66:GLN:N	1.72	1.03
1:I:53:TYR:C	1:I:53:TYR:CD2	2.30	1.02
1:G:212:PHE:HD1	1:G:280:PHE:CE1	1.76	1.02
1:I:228:GLN:HE22	1:I:273:LYS:CE	1.72	1.01
1:M:194:SER:HB3	1:M:199:TYR:OH	1.59	1.01
1:I:53:TYR:CD2	1:I:54:ASN:N	2.27	1.01
1:G:177:ILE:C	1:G:178:GLU:HG3	1.79	1.01
1:E:89:MET:HB2	1:E:118:TYR:HB2	1.43	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:ILE:HD12	1:C:261:ASP:HB2	1.41	1.01
1:O:385:TYR:HA	1:O:388:ILE:HD12	1.41	1.01
1:O:68:GLN:NE2	1:O:68:GLN:HA	1.57	1.00
1:M:197:TYR:CE1	1:M:198:LEU:CD1	2.43	1.00
1:A:244:LEU:HD11	1:A:250:ARG:HG3	1.43	1.00
1:G:238:ILE:HD12	1:G:261:ASP:HB2	1.41	1.00
1:I:228:GLN:NE2	1:I:273:LYS:CE	2.23	1.00
1:G:87:ILE:O	1:G:87:ILE:HG22	1.58	0.99
1:A:304:LEU:HD23	1:A:322:PHE:HB2	1.44	0.99
1:I:57:LEU:CD2	1:I:74:GLY:O	2.11	0.99
1:A:42:GLN:O	1:A:43:LEU:HD23	1.61	0.99
1:O:57:LEU:HD23	1:O:61:LEU:CD1	1.93	0.99
1:G:392:HIS:NE2	1:G:393:PHE:HE2	1.59	0.98
1:C:244:LEU:HD12	1:C:250:ARG:HA	1.44	0.98
1:M:152:GLN:HE21	1:M:152:GLN:N	1.60	0.98
1:I:289:LEU:CD1	1:K:303:ASP:HB3	1.94	0.97
1:C:160:VAL:O	1:C:164:GLU:HG3	1.62	0.97
1:A:266:GLN:HE21	1:C:231:ASN:ND2	1.64	0.96
1:E:198:LEU:CD1	1:E:199:TYR:CE1	2.48	0.96
1:I:183:GLY:CA	1:I:207:LEU:CD1	2.43	0.96
1:C:304:LEU:HD23	1:C:322:PHE:HB2	1.46	0.95
1:A:56:THR:OG1	1:A:59:SER:OG	1.84	0.95
1:E:198:LEU:N	1:E:198:LEU:HD12	1.72	0.95
1:I:244:LEU:HD12	1:I:250:ARG:HA	1.48	0.95
1:G:52:LEU:HD21	1:G:63:THR:HG21	1.47	0.95
1:A:266:GLN:CB	1:C:264:LEU:HD22	1.95	0.95
1:E:152:GLN:N	1:E:152:GLN:HE21	1.65	0.95
1:K:452:VAL:CG1	1:K:455:ILE:HG13	1.96	0.95
1:E:156:SER:HB3	1:E:159:ILE:HG12	1.45	0.95
1:G:304:LEU:HD22	1:G:320:LEU:HD11	1.48	0.95
1:E:382:LEU:C	1:E:382:LEU:HD12	1.87	0.95
1:E:382:LEU:O	1:E:382:LEU:HD12	1.67	0.95
1:E:67:LEU:HD12	1:E:69:LEU:HD11	1.49	0.95
1:K:85:LYS:O	1:K:115:ASN:ND2	2.00	0.95
1:E:102:VAL:O	1:E:106:ILE:HD12	1.67	0.95
1:E:381:ILE:HD13	1:E:381:ILE:H	1.32	0.94
1:C:306:ILE:HG12	1:C:320:LEU:HD12	1.48	0.94
1:A:148:ILE:HD13	1:A:388:ILE:HD11	1.46	0.94
1:K:385:TYR:HA	1:K:388:ILE:HD12	1.48	0.94
1:A:145:LEU:O	1:A:413:LYS:CD	2.14	0.94
1:A:192:MET:HE1	1:K:15:SER:HB3	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ALA:HB3	1:A:132:ALA:HB2	1.48	0.94
1:I:252:LYS:HD2	1:I:252:LYS:N	1.82	0.94
1:I:289:LEU:HD12	1:K:303:ASP:CB	1.97	0.94
1:A:194:SER:HB3	1:A:199:TYR:OH	1.67	0.94
1:E:381:ILE:CD1	1:E:381:ILE:H	1.79	0.94
1:A:208:ILE:HD13	1:A:441:PHE:CZ	2.03	0.94
1:A:65:GLU:CG	1:A:66:GLN:N	2.29	0.93
1:I:183:GLY:HA3	1:I:207:LEU:HD13	1.48	0.93
1:O:432:ILE:HG22	1:O:455:ILE:HD12	1.51	0.93
1:A:266:GLN:HE21	1:C:231:ASN:HD22	1.09	0.93
1:M:152:GLN:NE2	1:M:152:GLN:H	1.64	0.93
1:I:57:LEU:HD21	1:I:74:GLY:O	1.69	0.92
1:G:117:ARG:HB3	1:G:118:TYR:CD1	2.04	0.92
1:I:147:THR:HB	1:I:427:PHE:CD1	2.04	0.92
1:C:90:ILE:CD1	1:C:116:LEU:HD13	2.00	0.92
1:G:91:VAL:HG22	1:G:120:TYR:HB3	1.49	0.92
1:I:312:PHE:HB3	1:I:315:ILE:HD12	1.49	0.92
1:O:67:LEU:O	1:O:68:GLN:CB	2.17	0.92
1:G:123:TRP:HD1	1:G:214:HIS:CD2	1.85	0.92
1:G:117:ARG:HB3	1:G:118:TYR:CE1	2.05	0.91
1:M:244:LEU:CD2	1:M:248:GLY:HA2	1.98	0.91
1:C:238:ILE:HD12	1:C:261:ASP:CB	2.01	0.91
1:I:195:PRO:HB2	1:I:198:LEU:HG	1.53	0.91
1:C:52:LEU:HD11	1:C:63:THR:HG21	1.53	0.91
1:A:303:ASP:HB3	1:C:289:LEU:HD12	1.51	0.91
1:C:39:ALA:HA	1:C:382:LEU:HD12	1.53	0.91
1:E:229:LYS:NZ	1:G:447:GLU:OE2	2.03	0.91
1:O:69:LEU:HD23	1:O:72:ALA:CB	2.01	0.91
1:I:228:GLN:HE22	1:I:273:LYS:HE3	1.31	0.90
1:E:322:PHE:HD2	1:E:367:GLU:HB3	1.34	0.90
1:A:266:GLN:HB2	1:C:264:LEU:CD2	1.99	0.90
1:O:67:LEU:O	1:O:68:GLN:HB2	1.71	0.90
1:O:432:ILE:CG2	1:O:455:ILE:HD12	2.01	0.90
1:C:312:PHE:HB3	1:C:315:ILE:HD12	1.52	0.90
1:K:40:ILE:HG22	1:K:40:ILE:O	1.70	0.90
1:C:118:TYR:HH	1:C:392:HIS:HD1	1.05	0.90
1:E:238:ILE:O	1:E:257:LYS:NZ	2.04	0.90
1:A:130:GLN:HA	1:A:133:GLU:HB2	1.53	0.90
1:E:152:GLN:H	1:E:152:GLN:HE21	1.19	0.90
1:I:25:LEU:HD13	1:I:52:LEU:HD11	1.54	0.89
1:A:458:LEU:HG	1:A:459:GLU:N	1.88	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:VAL:HG13	1:E:222:ILE:CD1	2.02	0.89
1:G:244:LEU:HD23	1:G:250:ARG:HA	1.54	0.89
1:K:89:MET:HB2	1:K:118:TYR:HB2	1.55	0.89
1:I:372:ARG:O	1:I:373:ASN:ND2	2.05	0.89
1:M:156:SER:HB3	1:M:159:ILE:HG12	1.53	0.89
1:G:392:HIS:HE2	1:G:393:PHE:HE2	1.15	0.88
1:O:208:ILE:HG22	1:O:209:SER:H	1.36	0.88
1:G:214:HIS:ND1	1:G:314:GLU:HG2	1.87	0.88
1:E:381:ILE:N	1:E:381:ILE:CD1	2.30	0.88
1:O:244:LEU:CD1	1:O:250:ARG:HA	2.01	0.88
1:E:28:GLY:HA2	1:E:67:LEU:HD21	1.54	0.88
1:G:238:ILE:HD12	1:G:261:ASP:CB	2.04	0.88
1:K:238:ILE:HD12	1:K:261:ASP:CB	2.03	0.88
1:G:238:ILE:O	1:G:257:LYS:NZ	2.05	0.88
1:A:77:SER:HB3	1:A:80:SER:CB	2.03	0.88
1:E:198:LEU:HD13	1:E:199:TYR:HE1	1.20	0.88
1:M:168:GLU:O	1:M:328:GLY:O	1.91	0.88
1:O:171:ILE:HD12	1:O:299:GLY:CA	2.03	0.88
1:O:57:LEU:CD2	1:O:61:LEU:CD1	2.50	0.88
1:C:304:LEU:CD2	1:C:322:PHE:HB2	2.03	0.88
1:C:77:SER:HB3	1:C:80:SER:HB2	1.54	0.88
1:I:281:LYS:CD	1:I:282:GLY:H	1.85	0.87
1:M:312:PHE:HB3	1:M:315:ILE:HD12	1.56	0.87
1:E:62:GLN:HG2	1:E:66:GLN:HE21	1.38	0.87
1:I:383:ARG:HG3	1:I:383:ARG:HH11	1.36	0.87
1:E:304:LEU:HD23	1:E:322:PHE:HB2	1.55	0.87
1:O:171:ILE:HD12	1:O:299:GLY:HA3	1.57	0.87
1:E:136:TYR:HB2	1:E:431:ILE:HD11	1.55	0.87
1:I:53:TYR:HD2	1:I:53:TYR:C	1.75	0.87
1:E:381:ILE:N	1:E:381:ILE:HD12	1.87	0.87
1:A:272:GLY:O	1:A:273:LYS:HB2	1.74	0.87
1:K:77:SER:HB3	1:K:80:SER:CB	2.04	0.87
1:I:183:GLY:HA3	1:I:207:LEU:CD1	2.03	0.86
1:A:128:SER:OG	1:A:131:GLN:HB2	1.73	0.86
1:K:57:LEU:O	1:K:61:LEU:HD13	1.76	0.86
1:C:77:SER:HB3	1:C:80:SER:CB	2.05	0.86
1:O:158:TYR:CD1	1:O:318:LEU:HD12	2.09	0.86
1:E:177:ILE:HD13	1:E:219:LEU:HD11	1.58	0.86
1:G:19:ARG:HB3	1:G:50:VAL:HG21	1.58	0.86
1:I:192:MET:HE2	1:I:243:LEU:HD22	1.57	0.86
1:E:195:PRO:CB	1:E:198:LEU:HD11	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:MET:HB2	1:A:118:TYR:HB2	1.57	0.86
1:I:102:VAL:HG12	1:I:106:ILE:HD11	1.56	0.86
1:E:218:VAL:HG13	1:E:222:ILE:HD12	1.58	0.85
1:G:219:LEU:HA	1:G:222:ILE:CD1	2.06	0.85
1:I:102:VAL:HG12	1:I:106:ILE:CD1	2.06	0.85
1:E:152:GLN:H	1:E:152:GLN:NE2	1.73	0.85
1:E:238:ILE:HD12	1:E:261:ASP:CB	2.06	0.85
1:M:225:SER:HB2	1:M:271:ASN:HB2	1.58	0.85
1:A:16:ARG:O	1:A:17:PRO:O	1.94	0.85
1:C:89:MET:HB2	1:C:118:TYR:HB2	1.57	0.85
1:K:88:ASP:HA	1:K:115:ASN:O	1.75	0.85
1:M:161:ARG:O	1:M:161:ARG:HD2	1.77	0.85
1:O:57:LEU:HD23	1:O:61:LEU:HD13	1.59	0.85
1:K:126:ALA:HB3	1:K:132:ALA:HB2	1.57	0.85
1:A:147:THR:HB	1:A:427:PHE:CD1	2.11	0.85
1:E:102:VAL:CG1	1:E:106:ILE:HD11	2.06	0.85
1:K:208:ILE:HD13	1:K:441:PHE:CZ	2.12	0.85
1:O:100:TYR:HB2	1:O:131:GLN:OE1	1.76	0.84
1:I:28:GLY:HA2	1:I:67:LEU:HD21	1.57	0.84
1:A:304:LEU:CD2	1:A:322:PHE:HB2	2.07	0.84
1:O:142:ARG:HB3	1:O:142:ARG:HH11	1.43	0.84
1:G:225:SER:HB2	1:G:271:ASN:HB2	1.60	0.84
1:K:149:ILE:HD13	1:K:430:ALA:HB2	1.58	0.84
1:I:118:TYR:HH	1:I:392:HIS:HD1	0.88	0.84
1:K:192:MET:HG2	1:K:244:LEU:O	1.77	0.84
1:A:77:SER:HB3	1:A:80:SER:HB2	1.60	0.84
1:G:433:LEU:C	1:G:437:ILE:HD12	1.97	0.84
1:A:199:TYR:CD1	1:A:199:TYR:N	2.40	0.84
2:H:852:THR:HG22	2:H:854:ASP:H	1.43	0.84
1:A:148:ILE:CD1	1:A:388:ILE:HD11	2.07	0.83
1:C:90:ILE:HD12	1:C:116:LEU:HD13	1.58	0.83
1:K:77:SER:HB3	1:K:80:SER:HB2	1.59	0.83
1:K:149:ILE:HD13	1:K:430:ALA:CB	2.07	0.83
1:G:212:PHE:HD1	1:G:280:PHE:HE1	1.24	0.83
1:C:433:LEU:HG	1:C:437:ILE:HD11	1.58	0.83
1:M:452:VAL:HG13	1:M:455:ILE:HD12	1.60	0.83
1:O:154:ARG:HD2	1:O:425:PRO:HG3	1.60	0.83
1:E:194:SER:HB3	1:E:199:TYR:HH	1.02	0.83
1:A:244:LEU:CD1	1:A:250:ARG:HA	2.08	0.83
1:O:287:LYS:HG2	1:O:290:THR:HB	1.60	0.83
1:E:384:ILE:O	1:E:388:ILE:CD1	2.25	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:255:ILE:O	1:E:255:ILE:HG23	1.77	0.83
1:C:100:TYR:CD1	1:C:135:LEU:HD21	2.14	0.82
1:E:238:ILE:HD12	1:E:261:ASP:HB2	1.60	0.82
1:G:416:LYS:HD2	1:G:418:GLY:CA	2.08	0.82
1:G:32:VAL:HG13	1:G:36:HIS:HB2	1.61	0.82
1:E:266:GLN:HB2	1:G:264:LEU:HD22	1.61	0.82
1:C:416:LYS:HD2	1:C:418:GLY:CA	2.08	0.82
1:K:165:LEU:O	1:K:170:CYS:HB2	1.80	0.82
1:O:100:TYR:CD1	1:O:135:LEU:HD21	2.14	0.82
1:M:117:ARG:HB3	1:M:118:TYR:CD1	2.14	0.82
1:C:79:GLU:HG2	1:C:109:HIS:CD2	2.14	0.82
1:O:84:TYR:CE1	1:O:86:ASP:HB2	2.15	0.82
1:C:175:ASN:O	1:C:274:VAL:HG13	1.80	0.82
1:A:118:TYR:HH	1:A:392:HIS:HD1	1.28	0.82
1:E:436:LEU:HB2	1:E:455:ILE:HD11	1.60	0.82
1:E:102:VAL:HG12	1:E:106:ILE:HD11	1.61	0.81
1:M:315:ILE:CG2	1:M:377:VAL:HG22	2.09	0.81
1:C:225:SER:HB2	1:C:271:ASN:HB2	1.62	0.81
1:E:198:LEU:CD1	1:E:199:TYR:HE1	1.87	0.81
1:M:185:TRP:HZ3	1:M:186:TYR:HH	1.28	0.81
1:A:62:GLN:O	1:A:66:GLN:HG3	1.79	0.81
1:M:89:MET:HB2	1:M:118:TYR:HB2	1.62	0.81
1:C:219:LEU:HA	1:C:222:ILE:HD12	1.63	0.81
1:E:136:TYR:HB2	1:E:431:ILE:CD1	2.10	0.81
1:E:195:PRO:O	1:E:199:TYR:CE1	2.32	0.81
1:G:116:LEU:HD21	1:G:145:LEU:HD13	1.63	0.81
1:I:252:LYS:CD	1:I:252:LYS:H	1.83	0.81
1:I:228:GLN:HE22	1:I:273:LYS:HE2	1.46	0.80
1:G:212:PHE:CD1	1:G:280:PHE:CE1	2.67	0.80
1:O:52:LEU:HD12	1:O:52:LEU:N	1.92	0.80
1:E:263:LEU:HD12	1:E:264:LEU:N	1.96	0.80
1:G:100:TYR:CD1	1:G:135:LEU:HD21	2.15	0.80
1:A:200:ASP:O	1:A:201:ILE:C	2.14	0.80
1:A:185:TRP:HZ3	1:A:186:TYR:HH	1.27	0.80
1:I:244:LEU:HD11	1:I:250:ARG:HB2	1.62	0.80
1:O:69:LEU:HD23	1:O:72:ALA:HB2	1.64	0.80
1:E:384:ILE:O	1:E:384:ILE:CG2	2.30	0.80
1:K:135:LEU:HA	1:K:138:ILE:HD12	1.63	0.80
1:I:225:SER:HB2	1:I:271:ASN:HB2	1.62	0.80
1:A:191:PRO:HG2	1:A:194:SER:OG	1.81	0.80
1:M:53:TYR:O	1:M:54:ASN:ND2	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:SER:O	1:E:64:ILE:HD12	1.82	0.80
1:I:136:TYR:HB2	1:I:431:ILE:CD1	2.11	0.80
1:G:19:ARG:HB3	1:G:50:VAL:CG2	2.12	0.80
1:M:147:THR:HB	1:M:427:PHE:CD1	2.17	0.80
1:M:117:ARG:HB3	1:M:118:TYR:CE1	2.17	0.80
1:E:273:LYS:N	1:E:273:LYS:HD3	1.95	0.80
1:G:154:ARG:HD2	1:G:425:PRO:HG3	1.64	0.79
1:K:40:ILE:O	1:K:40:ILE:CG2	2.30	0.79
1:A:312:PHE:HB3	1:A:315:ILE:HD12	1.62	0.79
1:I:100:TYR:HB2	1:I:131:GLN:OE1	1.80	0.79
1:C:319:VAL:HG22	1:C:370:HIS:CD2	2.17	0.79
1:G:175:ASN:O	1:G:274:VAL:HG13	1.80	0.79
1:E:433:LEU:O	1:E:437:ILE:CD1	2.29	0.79
1:I:214:HIS:CD2	1:I:314:GLU:HG2	2.17	0.79
1:G:136:TYR:HB2	1:G:431:ILE:HD13	1.63	0.79
1:C:115:ASN:O	1:C:117:ARG:HG2	1.83	0.79
1:A:281:LYS:HD2	1:C:298:HIS:CD2	2.18	0.79
1:E:103:VAL:HA	1:E:106:ILE:HD12	1.64	0.79
1:G:96:VAL:O	1:G:99:HIS:HB2	1.83	0.79
1:E:281:LYS:HE2	1:G:175:ASN:OD1	1.81	0.79
1:K:104:LYS:O	1:K:107:LEU:HB2	1.82	0.79
1:K:312:PHE:HB3	1:K:315:ILE:HD12	1.63	0.79
1:K:147:THR:HB	1:K:427:PHE:CD1	2.18	0.79
1:K:84:TYR:CE1	1:K:86:ASP:HB2	2.18	0.79
1:A:199:TYR:HD1	1:A:199:TYR:H	1.30	0.78
1:G:147:THR:HB	1:G:427:PHE:CD1	2.18	0.78
1:A:195:PRO:O	1:A:199:TYR:CE1	2.35	0.78
1:O:136:TYR:HB2	1:O:431:ILE:HD13	1.65	0.78
1:E:195:PRO:HB2	1:E:198:LEU:HD11	1.66	0.78
1:E:208:ILE:HD13	1:E:441:PHE:CZ	2.18	0.78
1:I:192:MET:HE1	1:I:243:LEU:HD22	1.63	0.78
1:A:136:TYR:HB2	1:A:431:ILE:CD1	2.14	0.78
1:I:294:VAL:HG22	1:I:307:GLU:HG2	1.66	0.78
1:G:433:LEU:O	1:G:437:ILE:HD12	1.82	0.78
1:A:452:VAL:HG12	1:A:455:ILE:HG12	1.63	0.78
1:C:244:LEU:HD11	1:C:250:ARG:HG3	1.65	0.78
1:K:215:THR:O	1:K:218:VAL:HG12	1.84	0.78
1:M:228:GLN:OE1	1:M:229:LYS:HE3	1.82	0.78
1:M:197:TYR:CZ	1:M:198:LEU:HD11	2.19	0.78
1:A:263:LEU:HD12	1:A:264:LEU:N	1.99	0.78
1:G:416:LYS:HG3	1:G:418:GLY:N	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:197:TYR:CE1	1:M:198:LEU:HD11	2.15	0.78
1:O:123:TRP:CD2	1:O:124:ALA:HA	2.19	0.78
1:I:96:VAL:O	1:I:99:HIS:HB2	1.83	0.78
1:C:452:VAL:HG13	1:C:455:ILE:HD12	0.80	0.78
1:A:156:SER:HB3	1:A:159:ILE:HG12	1.66	0.78
1:A:435:ARG:NH1	1:A:455:ILE:O	2.16	0.78
1:I:136:TYR:HB2	1:I:431:ILE:HD13	1.66	0.77
1:A:41:GLN:O	1:A:43:LEU:N	2.17	0.77
1:I:377:VAL:HG11	2:J:859:TYR:CD2	2.18	0.77
1:C:452:VAL:HG13	1:C:455:ILE:HD11	1.61	0.77
2:D:852:THR:HG22	2:D:854:ASP:N	2.00	0.77
1:C:182:ASN:ND2	1:C:283:GLY:HA2	1.99	0.77
1:O:96:VAL:O	1:O:99:HIS:HB2	1.85	0.77
2:D:852:THR:HG22	2:D:854:ASP:H	1.47	0.77
1:C:452:VAL:CG1	1:C:455:ILE:CD1	2.29	0.77
1:M:129:VAL:HG13	1:M:130:GLN:H	1.48	0.77
1:I:183:GLY:CA	1:I:207:LEU:HD11	2.13	0.77
1:G:64:ILE:HG22	1:G:65:GLU:N	1.99	0.77
1:K:225:SER:HB2	1:K:271:ASN:HB2	1.66	0.77
1:E:322:PHE:CD2	1:E:367:GLU:HB3	2.20	0.77
2:H:852:THR:HG22	2:H:854:ASP:N	1.98	0.77
1:M:187:GLY:HA3	1:M:284:THR:H	1.50	0.77
1:E:96:VAL:O	1:E:96:VAL:CG1	2.33	0.77
1:M:212:PHE:O	1:M:216:ILE:HG22	1.85	0.77
1:M:436:LEU:O	1:M:439:ALA:HB3	1.85	0.77
1:G:376:SER:O	1:G:380:ASN:HB2	1.84	0.77
1:G:315:ILE:CG2	1:G:377:VAL:HG22	2.14	0.77
1:M:416:LYS:HB3	1:M:428:LYS:HD2	1.65	0.76
1:A:255:ILE:HG13	1:A:256:SER:N	1.99	0.76
1:G:26:THR:HB	1:G:30:SER:HB3	1.67	0.76
1:K:123:TRP:CD2	1:K:124:ALA:HA	2.21	0.76
1:G:125:LEU:HD13	1:G:430:ALA:CB	2.16	0.76
1:C:416:LYS:HD2	1:C:418:GLY:HA3	1.67	0.76
1:I:287:LYS:HG2	1:I:290:THR:HB	1.66	0.76
1:C:154:ARG:HD2	1:C:425:PRO:HG3	1.66	0.76
1:C:147:THR:HB	1:C:427:PHE:CD1	2.19	0.76
1:K:96:VAL:O	1:K:99:HIS:HB2	1.85	0.76
1:O:51:ALA:C	1:O:52:LEU:HD12	2.06	0.76
1:K:454:LYS:HA	1:K:457:ILE:HD12	1.66	0.76
1:K:180:SER:O	1:K:293:LEU:HD12	1.84	0.76
1:E:384:ILE:O	1:E:384:ILE:HG22	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:377:VAL:HG11	2:J:859:TYR:CE2	2.21	0.76
1:O:180:SER:O	1:O:293:LEU:HD12	1.86	0.76
1:E:64:ILE:HA	1:E:69:LEU:HD12	1.65	0.76
1:I:187:GLY:HA3	1:I:284:THR:H	1.51	0.76
1:E:103:VAL:CA	1:E:106:ILE:HD12	2.16	0.76
1:A:19:ARG:HB3	1:A:50:VAL:HG21	1.68	0.76
1:I:182:ASN:HA	1:I:281:LYS:O	1.85	0.76
1:K:61:LEU:CD1	1:K:61:LEU:H	1.99	0.76
1:A:105:ASN:N	1:A:105:ASN:HD22	1.82	0.76
1:C:179:ILE:HB	1:C:278:CYS:HB2	1.68	0.75
1:E:177:ILE:CD1	1:E:219:LEU:HD11	2.17	0.75
1:G:177:ILE:C	1:G:178:GLU:CG	2.53	0.75
1:G:179:ILE:HD12	1:G:278:CYS:HB2	1.65	0.75
1:I:89:MET:HB2	1:I:118:TYR:HB2	1.67	0.75
1:G:212:PHE:O	1:G:216:ILE:HG22	1.87	0.75
1:O:52:LEU:CD1	1:O:52:LEU:N	2.50	0.75
1:C:136:TYR:HB2	1:C:431:ILE:CD1	2.16	0.75
1:G:322:PHE:HD2	1:G:367:GLU:HB3	1.51	0.75
1:K:136:TYR:HB2	1:K:431:ILE:CD1	2.16	0.75
1:O:142:ARG:CB	1:O:142:ARG:HH11	1.99	0.75
1:E:195:PRO:O	1:E:199:TYR:CD1	2.39	0.75
1:G:96:VAL:HB	1:G:97:PRO:HD3	1.67	0.75
1:C:67:LEU:HD12	1:C:69:LEU:HD11	1.65	0.75
1:E:304:LEU:CD2	1:E:322:PHE:HB2	2.16	0.75
1:A:96:VAL:HB	1:A:97:PRO:HD3	1.69	0.75
1:E:272:GLY:O	1:E:273:LYS:HB2	1.85	0.74
1:K:96:VAL:HA	1:K:99:HIS:CG	2.22	0.74
1:C:123:TRP:CD2	1:C:124:ALA:HA	2.22	0.74
1:M:289:LEU:CD1	1:O:303:ASP:HB3	2.16	0.74
1:M:115:ASN:O	1:M:116:LEU:C	2.23	0.74
1:O:84:TYR:CD1	1:O:86:ASP:HB2	2.22	0.74
1:K:433:LEU:O	1:K:436:LEU:HB3	1.87	0.74
1:M:123:TRP:CD2	1:M:124:ALA:HA	2.21	0.74
1:E:306:ILE:HG12	1:E:320:LEU:HD12	1.68	0.74
1:G:304:LEU:HD23	1:G:322:PHE:HB2	1.70	0.74
1:M:136:TYR:HB2	1:M:431:ILE:CD1	2.17	0.74
1:I:212:PHE:O	1:I:216:ILE:HG22	1.88	0.74
1:O:225:SER:HB2	1:O:271:ASN:HB2	1.70	0.74
1:E:385:TYR:HA	1:E:388:ILE:HD12	1.68	0.74
1:E:436:LEU:O	1:E:436:LEU:HG	1.88	0.74
1:O:149:ILE:HG23	1:O:151:LEU:HD12	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:GLN:HG2	1:E:66:GLN:NE2	2.03	0.74
1:M:194:SER:CB	1:M:199:TYR:OH	2.36	0.73
1:C:390:ASP:O	1:C:394:LEU:HB2	1.87	0.73
1:A:416:LYS:HD2	1:A:418:GLY:CA	2.18	0.73
1:A:26:THR:HB	1:A:30:SER:HB3	1.69	0.73
1:A:286:VAL:O	1:A:288:LYS:HE3	1.88	0.73
1:C:225:SER:CB	1:C:271:ASN:HB2	2.16	0.73
1:O:25:LEU:HD23	1:O:63:THR:CG2	2.18	0.73
1:G:115:ASN:O	1:G:116:LEU:C	2.25	0.73
1:M:319:VAL:HG22	1:M:370:HIS:CD2	2.22	0.73
1:I:383:ARG:HH11	1:I:383:ARG:CG	1.96	0.73
1:I:19:ARG:HA	1:I:48:GLN:O	1.89	0.73
1:G:104:LYS:HA	1:G:107:LEU:HD12	1.69	0.73
1:M:77:SER:HB3	1:M:80:SER:CB	2.18	0.73
1:G:142:ARG:HB3	1:G:145:LEU:CB	2.18	0.73
1:O:68:GLN:NE2	1:O:68:GLN:CA	2.30	0.73
1:C:215:THR:O	1:C:218:VAL:HG12	1.87	0.73
1:G:152:GLN:O	1:G:153:GLY:C	2.23	0.73
1:G:219:LEU:CA	1:G:222:ILE:HD12	2.14	0.73
1:E:428:LYS:O	1:E:432:ILE:HG13	1.89	0.73
1:K:212:PHE:CZ	1:K:216:ILE:HD13	2.22	0.73
1:A:219:LEU:HA	1:A:222:ILE:HD12	1.70	0.73
1:O:57:LEU:O	1:O:58:LYS:C	2.26	0.73
1:M:208:ILE:HD13	1:M:441:PHE:CZ	2.24	0.73
1:O:142:ARG:O	1:O:145:LEU:N	2.18	0.73
1:K:182:ASN:ND2	1:K:283:GLY:HA2	2.03	0.73
1:A:306:ILE:HG12	1:A:320:LEU:HD12	1.71	0.73
1:E:225:SER:HB2	1:E:271:ASN:HB2	1.69	0.73
1:A:84:TYR:CE1	1:A:86:ASP:HB2	2.24	0.73
1:I:393:PHE:O	1:I:394:LEU:HD12	1.89	0.72
1:E:433:LEU:C	1:E:437:ILE:HD12	2.09	0.72
1:E:115:ASN:O	1:E:117:ARG:N	2.22	0.72
1:O:20:VAL:HA	1:O:89:MET:O	1.89	0.72
1:C:322:PHE:HD2	1:C:367:GLU:HB3	1.52	0.72
1:C:115:ASN:O	1:C:116:LEU:C	2.27	0.72
1:G:91:VAL:HG22	1:G:120:TYR:CB	2.18	0.72
1:E:452:VAL:CG1	1:E:455:ILE:HD13	2.19	0.72
1:M:77:SER:HB3	1:M:80:SER:HB2	1.70	0.72
1:I:121:VAL:HG12	1:I:122:GLU:H	1.54	0.72
1:G:67:LEU:HD12	1:G:69:LEU:HD11	1.69	0.72
1:C:64:ILE:HG12	1:C:72:ALA:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:77:SER:HB3	1:I:80:SER:CB	2.19	0.72
1:M:216:ILE:HG23	1:M:217:ASP:N	2.03	0.72
1:C:136:TYR:HB2	1:C:431:ILE:HD13	1.69	0.72
1:O:147:THR:HB	1:O:427:PHE:CD1	2.24	0.72
1:I:270:GLU:OE1	1:I:456:MET:HE3	1.90	0.72
1:C:452:VAL:HG12	1:C:455:ILE:HD12	1.62	0.72
1:O:89:MET:HB2	1:O:118:TYR:HB2	1.70	0.72
1:A:40:ILE:HG23	1:A:47:PHE:HB2	1.70	0.72
1:G:306:ILE:HG12	1:G:320:LEU:HD12	1.70	0.72
1:E:147:THR:HB	1:E:427:PHE:CD1	2.24	0.72
1:I:201:ILE:HB	1:I:258:THR:HB	1.70	0.72
1:A:123:TRP:CH2	1:A:433:LEU:HD23	2.24	0.72
1:C:212:PHE:O	1:C:216:ILE:HG22	1.89	0.72
1:E:298:HIS:HD2	1:G:281:LYS:HD2	1.54	0.72
1:A:41:GLN:O	1:A:44:SER:N	2.21	0.72
1:A:195:PRO:O	1:A:198:LEU:HB2	1.89	0.72
1:A:257:LYS:HD2	1:A:259:CYS:O	1.90	0.72
1:C:208:ILE:HG13	1:C:263:LEU:HD22	1.71	0.72
1:E:375:ASN:O	1:E:379:GLY:N	2.22	0.72
1:E:102:VAL:HG12	1:E:106:ILE:CD1	2.20	0.72
1:K:96:VAL:HB	1:K:97:PRO:HD3	1.71	0.72
1:A:89:MET:CB	1:A:118:TYR:HB2	2.18	0.72
1:K:201:ILE:HB	1:K:258:THR:HB	1.71	0.72
1:C:319:VAL:HG13	1:C:370:HIS:HB2	1.71	0.71
1:O:452:VAL:HG12	1:O:455:ILE:HG12	1.71	0.71
1:O:96:VAL:HA	1:O:99:HIS:CG	2.25	0.71
1:M:26:THR:HB	1:M:30:SER:CB	2.20	0.71
1:G:125:LEU:HB2	1:G:430:ALA:HB1	1.71	0.71
1:I:304:LEU:CD2	1:I:320:LEU:HD11	2.20	0.71
1:G:163:LYS:NZ	1:G:419:PHE:O	2.21	0.71
1:O:120:TYR:CD2	1:O:148:ILE:HG21	2.26	0.71
1:I:322:PHE:HD2	1:I:367:GLU:HB3	1.55	0.71
1:G:214:HIS:ND1	1:G:314:GLU:CG	2.52	0.71
1:E:96:VAL:O	1:E:96:VAL:HG12	1.89	0.71
1:A:231:ASN:HB2	1:A:449:THR:OG1	1.91	0.71
1:A:195:PRO:O	1:A:199:TYR:HE1	1.74	0.71
1:C:62:GLN:O	1:C:63:THR:C	2.26	0.71
1:O:88:ASP:OD1	1:O:115:ASN:HB3	1.91	0.71
1:A:416:LYS:HD2	1:A:418:GLY:HA2	1.72	0.71
1:O:212:PHE:HD1	1:O:280:PHE:CE1	2.09	0.71
1:G:123:TRP:HB3	1:G:214:HIS:HE2	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:231:ASN:ND2	1:K:266:GLN:HE21	1.88	0.71
1:A:281:LYS:HD2	1:C:298:HIS:NE2	2.06	0.71
1:E:436:LEU:HB2	1:E:455:ILE:CD1	2.21	0.71
2:P:853:MET:O	2:P:856:VAL:HB	1.91	0.71
1:I:245:ASP:O	1:I:247:ASN:N	2.23	0.71
1:A:190:ARG:HG3	1:A:191:PRO:HD2	1.71	0.71
1:I:244:LEU:CD1	1:I:250:ARG:HB2	2.21	0.71
1:K:57:LEU:HD23	1:K:61:LEU:HD11	1.72	0.71
1:A:390:ASP:O	1:A:394:LEU:HB2	1.91	0.71
1:A:285:PRO:HG3	1:C:300:THR:O	1.90	0.71
1:A:372:ARG:NH2	2:B:847:LEU:HD23	2.06	0.71
1:A:447:GLU:OE2	1:C:229:LYS:NZ	2.19	0.71
1:G:453:SER:HA	1:G:456:MET:HE3	1.72	0.70
1:O:244:LEU:HD11	1:O:250:ARG:HG3	1.73	0.70
1:C:96:VAL:HA	1:C:99:HIS:CG	2.27	0.70
1:G:113:ASN:O	1:G:114:LEU:HD23	1.92	0.70
1:K:182:ASN:HA	1:K:281:LYS:O	1.91	0.70
1:O:136:TYR:HB2	1:O:431:ILE:CD1	2.21	0.70
1:O:432:ILE:HG22	1:O:455:ILE:CD1	2.21	0.70
1:O:433:LEU:HG	1:O:437:ILE:HD11	1.73	0.70
1:I:270:GLU:OE1	1:I:456:MET:CE	2.39	0.70
1:I:156:SER:HB3	1:I:159:ILE:HG12	1.71	0.70
1:C:112:GLN:O	1:C:114:LEU:HD12	1.92	0.70
1:A:136:TYR:HB2	1:A:431:ILE:HD11	1.71	0.70
1:M:281:LYS:HE2	1:O:175:ASN:OD1	1.91	0.70
1:K:231:ASN:HB2	1:K:449:THR:OG1	1.91	0.70
1:G:436:LEU:HB2	1:G:455:ILE:CD1	2.21	0.70
1:C:115:ASN:O	1:C:117:ARG:N	2.24	0.70
1:K:195:PRO:HB2	1:K:198:LEU:HD13	1.73	0.70
1:O:77:SER:HB3	1:O:80:SER:HB2	1.73	0.70
1:M:201:ILE:HG23	1:M:202:GLU:N	2.05	0.70
1:C:30:SER:O	1:C:33:ALA:HB3	1.91	0.70
1:E:436:LEU:O	1:E:439:ALA:HB3	1.91	0.70
1:E:175:ASN:O	1:E:275:PRO:HD2	1.92	0.70
1:O:195:PRO:O	1:O:198:LEU:HB2	1.91	0.70
1:I:155:LYS:HB3	1:I:383:ARG:HD3	1.72	0.70
1:O:77:SER:HB3	1:O:80:SER:CB	2.20	0.70
1:O:208:ILE:HG22	1:O:209:SER:CA	2.22	0.70
1:G:156:SER:O	1:G:157:PRO:C	2.27	0.70
1:A:126:ALA:CB	1:A:132:ALA:HB2	2.20	0.70
1:I:102:VAL:CG1	1:I:106:ILE:HD11	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:TYR:O	1:A:198:LEU:C	2.25	0.70
1:K:177:ILE:C	1:K:178:GLU:HG3	2.12	0.70
1:I:100:TYR:HB2	1:I:131:GLN:CD	2.12	0.70
1:C:286:VAL:O	1:C:288:LYS:HD2	1.92	0.70
1:M:126:ALA:HB3	1:M:132:ALA:HB2	1.74	0.69
1:G:65:GLU:O	1:G:68:GLN:NE2	2.25	0.69
1:G:89:MET:O	1:G:89:MET:HG3	1.90	0.69
1:E:158:TYR:HB2	1:E:318:LEU:HD12	1.72	0.69
1:M:231:ASN:C	1:M:231:ASN:OD1	2.30	0.69
1:M:201:ILE:HB	1:M:258:THR:HB	1.73	0.69
1:E:159:ILE:N	1:E:159:ILE:HD13	2.04	0.69
1:K:416:LYS:HA	1:K:426:THR:OG1	1.93	0.69
1:E:244:LEU:HD12	1:E:250:ARG:HA	1.74	0.69
1:E:146:GLN:NE2	1:E:146:GLN:HA	2.06	0.69
1:C:290:THR:HG22	1:C:291:LYS:O	1.93	0.69
1:G:375:ASN:O	1:G:379:GLY:N	2.25	0.69
1:K:435:ARG:NH1	1:K:455:ILE:O	2.25	0.69
1:G:118:TYR:N	1:G:118:TYR:CD1	2.60	0.69
1:E:442:ARG:O	1:E:446:GLU:HG3	1.92	0.69
1:E:102:VAL:O	1:E:106:ILE:HD11	1.90	0.69
1:A:64:ILE:HA	1:A:69:LEU:HD12	1.75	0.69
1:I:183:GLY:HA2	1:I:207:LEU:CD1	2.21	0.69
1:G:96:VAL:HA	1:G:99:HIS:CG	2.26	0.69
1:I:30:SER:O	1:I:34:LYS:HG3	1.93	0.69
1:K:156:SER:HB3	1:K:159:ILE:HG12	1.75	0.69
1:G:52:LEU:HD21	1:G:63:THR:CG2	2.20	0.69
1:G:142:ARG:CB	1:G:145:LEU:HB3	2.23	0.69
1:E:19:ARG:HB3	1:E:50:VAL:HG21	1.74	0.69
1:E:208:ILE:O	1:E:212:PHE:HB3	1.93	0.69
1:I:231:ASN:HB2	1:I:449:THR:OG1	1.92	0.69
1:E:192:MET:HE1	1:O:15:SER:HB3	1.75	0.69
1:E:102:VAL:C	1:E:106:ILE:HD12	2.13	0.69
1:O:385:TYR:CA	1:O:388:ILE:HD12	2.20	0.69
1:C:304:LEU:HD21	1:C:320:LEU:HD21	1.75	0.69
1:C:20:VAL:HG23	1:C:48:GLN:O	1.92	0.69
1:A:105:ASN:O	1:A:106:ILE:C	2.29	0.69
1:K:290:THR:HG22	1:K:291:LYS:O	1.93	0.69
1:G:195:PRO:O	1:G:198:LEU:HB2	1.93	0.69
1:M:53:TYR:CG	1:M:54:ASN:N	2.61	0.68
1:O:375:ASN:O	1:O:379:GLY:N	2.24	0.68
1:I:152:GLN:NE2	1:I:152:GLN:H	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:197:TYR:CE1	1:M:198:LEU:HD12	2.29	0.68
1:G:22:PHE:O	1:G:53:TYR:N	2.26	0.68
1:K:75:PHE:HD2	1:K:80:SER:HB3	1.57	0.68
1:C:431:ILE:HG23	1:C:435:ARG:HD2	1.75	0.68
1:C:433:LEU:HG	1:C:437:ILE:CD1	2.22	0.68
1:M:197:TYR:CZ	1:M:198:LEU:CD1	2.75	0.68
1:O:187:GLY:HA3	1:O:284:THR:H	1.58	0.68
1:C:142:ARG:HB3	1:C:145:LEU:HB3	1.75	0.68
1:G:52:LEU:CD2	1:G:63:THR:HG21	2.22	0.68
1:A:238:ILE:HD12	1:A:261:ASP:CB	2.23	0.68
1:E:19:ARG:HA	1:E:48:GLN:O	1.92	0.68
1:M:19:ARG:HA	1:M:48:GLN:O	1.93	0.68
1:E:298:HIS:CD2	1:G:281:LYS:HD2	2.28	0.68
1:A:375:ASN:O	1:A:379:GLY:N	2.26	0.68
1:K:435:ARG:HB3	1:K:455:ILE:HG23	1.74	0.68
1:M:197:TYR:CD1	1:M:198:LEU:CD1	2.76	0.68
1:I:67:LEU:HD12	1:I:69:LEU:HD11	1.74	0.68
1:C:228:GLN:O	1:C:452:VAL:N	2.27	0.68
1:E:198:LEU:CD1	1:E:198:LEU:N	2.44	0.68
1:A:67:LEU:HD12	1:A:69:LEU:HD11	1.73	0.68
1:G:30:SER:O	1:G:34:LYS:HG3	1.93	0.68
1:E:200:ASP:OD1	1:E:200:ASP:C	2.29	0.68
1:K:102:VAL:HG12	1:K:106:ILE:CD1	2.23	0.68
1:K:104:LYS:O	1:K:107:LEU:CB	2.42	0.68
1:M:177:ILE:HB	1:M:276:VAL:HG22	1.76	0.68
1:A:319:VAL:HG22	1:A:370:HIS:CD2	2.29	0.68
1:M:136:TYR:HB2	1:M:431:ILE:HD11	1.75	0.68
1:E:142:ARG:HB3	1:E:145:LEU:CB	2.24	0.68
1:A:436:LEU:O	1:A:439:ALA:HB3	1.94	0.68
1:O:146:GLN:HA	1:O:146:GLN:NE2	2.08	0.68
1:M:324:GLY:O	1:M:365:THR:N	2.26	0.68
1:O:26:THR:HB	1:O:30:SER:HB3	1.76	0.68
1:E:195:PRO:HB2	1:E:198:LEU:CD1	2.23	0.68
1:E:25:LEU:HD23	1:E:63:THR:HG21	1.76	0.68
1:I:312:PHE:O	1:I:316:SER:N	2.27	0.68
1:M:225:SER:CB	1:M:271:ASN:HB2	2.24	0.68
1:I:96:VAL:HA	1:I:99:HIS:CG	2.29	0.68
1:G:312:PHE:O	1:G:316:SER:N	2.27	0.68
1:K:156:SER:O	1:K:157:PRO:C	2.31	0.68
1:I:385:TYR:HA	1:I:388:ILE:HD12	1.74	0.68
1:O:208:ILE:CG2	1:O:209:SER:H	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:96:VAL:HG12	1:E:127:ALA:HB2	1.75	0.67
1:O:155:LYS:HE2	1:O:384:ILE:HD13	1.76	0.67
1:C:90:ILE:HD12	1:C:116:LEU:CD1	2.24	0.67
1:I:372:ARG:O	1:I:373:ASN:CG	2.33	0.67
1:E:125:LEU:HB2	1:E:430:ALA:HB1	1.76	0.67
1:I:107:LEU:HD13	1:I:138:ILE:CG2	2.25	0.67
1:C:159:ILE:HD12	1:C:218:VAL:HG22	1.76	0.67
1:G:30:SER:O	1:G:33:ALA:HB3	1.94	0.67
1:I:26:THR:HB	1:I:30:SER:HB3	1.76	0.67
1:G:452:VAL:HG13	1:G:455:ILE:HG21	1.75	0.67
1:G:182:ASN:ND2	1:G:283:GLY:HA2	2.09	0.67
1:C:293:LEU:HB2	1:C:311:GLY:HA2	1.76	0.67
1:I:216:ILE:HG23	1:I:217:ASP:N	2.09	0.67
1:M:312:PHE:O	1:M:316:SER:N	2.27	0.67
1:E:43:LEU:HB3	1:E:46:GLN:HG3	1.75	0.67
1:A:433:LEU:HG	1:A:437:ILE:HD11	1.75	0.67
1:I:26:THR:HB	1:I:30:SER:CB	2.24	0.67
1:C:100:TYR:HB2	1:C:131:GLN:OE1	1.93	0.67
1:E:142:ARG:HB3	1:E:145:LEU:HB3	1.77	0.67
1:K:136:TYR:HB2	1:K:431:ILE:HD13	1.76	0.67
1:A:62:GLN:HG3	1:O:252:LYS:HD2	1.77	0.67
1:E:291:LYS:HG3	1:E:307:GLU:HB3	1.75	0.67
1:E:370:HIS:CD2	2:F:848:PHE:HD2	2.11	0.67
1:I:142:ARG:HB3	1:I:145:LEU:HB2	1.76	0.67
1:C:177:ILE:HD13	1:C:219:LEU:HD11	1.75	0.67
1:O:263:LEU:O	1:O:263:LEU:HG	1.95	0.67
1:K:251:THR:O	1:K:253:GLU:N	2.27	0.67
1:M:195:PRO:O	1:M:199:TYR:CE1	2.48	0.67
1:G:84:TYR:CE1	1:G:86:ASP:HB2	2.29	0.67
1:K:384:ILE:HG22	1:K:388:ILE:HD11	1.77	0.67
1:K:125:LEU:HB2	1:K:430:ALA:HB1	1.76	0.67
1:A:172:GLY:CA	1:A:301:LYS:HD2	2.25	0.67
1:O:443:SER:HB2	1:O:450:LEU:HD12	1.77	0.67
1:E:89:MET:CB	1:E:118:TYR:HB2	2.22	0.67
1:M:152:GLN:HE21	1:M:152:GLN:H	0.79	0.67
1:C:304:LEU:HD22	1:C:320:LEU:HD11	1.76	0.67
1:G:89:MET:HB2	1:G:118:TYR:HB2	1.76	0.67
1:O:166:ILE:HG22	1:O:167:SER:N	2.10	0.67
1:A:216:ILE:HG23	1:A:217:ASP:N	2.10	0.66
1:I:231:ASN:HD22	1:K:266:GLN:NE2	1.92	0.66
1:K:195:PRO:O	1:K:198:LEU:HB2	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:MET:CE	1:O:15:SER:HB3	2.25	0.66
1:E:78:LEU:O	1:E:81:PHE:HB3	1.95	0.66
1:E:199:TYR:CD1	1:E:199:TYR:N	2.62	0.66
1:G:392:HIS:HD2	1:G:393:PHE:CE2	2.07	0.66
1:O:61:LEU:N	1:O:61:LEU:CD1	2.58	0.66
1:M:315:ILE:HG23	1:M:377:VAL:HG22	1.78	0.66
1:M:26:THR:HB	1:M:30:SER:HB3	1.78	0.66
1:G:212:PHE:CD1	1:G:280:PHE:HE1	2.10	0.66
1:K:196:GLU:HG2	1:O:56:THR:CG2	2.25	0.66
1:O:69:LEU:HB3	1:O:72:ALA:HB3	1.76	0.66
1:I:121:VAL:HG12	1:I:122:GLU:N	2.11	0.66
1:C:85:LYS:O	1:C:115:ASN:ND2	2.28	0.66
1:M:104:LYS:O	1:M:107:LEU:HB2	1.96	0.66
1:E:293:LEU:O	1:E:307:GLU:HA	1.94	0.66
1:K:65:GLU:O	1:K:68:GLN:NE2	2.28	0.66
1:E:100:TYR:OH	1:E:104:LYS:NZ	2.28	0.66
1:I:75:PHE:CD1	1:I:75:PHE:N	2.63	0.66
1:K:129:VAL:HG13	1:K:130:GLN:H	1.60	0.66
1:O:432:ILE:HD13	1:O:456:MET:HA	1.75	0.66
1:K:16:ARG:HB2	1:K:17:PRO:HD3	1.78	0.66
1:O:149:ILE:CG2	1:O:151:LEU:HD12	2.26	0.66
1:O:312:PHE:O	1:O:316:SER:OG	2.10	0.66
1:C:251:THR:O	1:C:253:GLU:N	2.29	0.66
1:K:322:PHE:HD2	1:K:367:GLU:HB3	1.60	0.66
1:A:134:GLU:HA	1:A:137:SER:OG	1.95	0.66
1:K:61:LEU:N	1:K:61:LEU:CD1	2.59	0.66
1:M:142:ARG:HB3	1:M:145:LEU:CB	2.26	0.66
1:O:125:LEU:HB2	1:O:430:ALA:HB1	1.77	0.66
1:A:177:ILE:HD13	1:A:219:LEU:HD11	1.76	0.66
1:G:103:VAL:HG12	1:G:107:LEU:HD11	1.77	0.66
1:K:151:LEU:O	1:K:153:GLY:N	2.29	0.66
1:I:96:VAL:N	1:I:97:PRO:HD2	2.10	0.66
1:A:187:GLY:HA3	1:A:284:THR:H	1.60	0.66
1:C:263:LEU:O	1:C:263:LEU:HG	1.95	0.66
1:G:436:LEU:CD1	1:G:452:VAL:HG11	2.26	0.66
1:M:432:ILE:HD13	1:M:456:MET:HA	1.77	0.66
1:A:195:PRO:HB2	1:A:198:LEU:HD22	1.77	0.66
1:K:177:ILE:HB	1:K:276:VAL:HG22	1.77	0.66
1:G:25:LEU:O	1:G:54:ASN:ND2	2.29	0.66
1:A:77:SER:HB3	1:A:80:SER:OG	1.96	0.66
1:I:192:MET:HE2	1:I:243:LEU:CD2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:229:LYS:HE3	1:I:449:THR:HG21	1.78	0.65
1:M:84:TYR:CE1	1:M:86:ASP:HB2	2.30	0.65
1:G:446:GLU:OE1	1:G:448:LYS:NZ	2.29	0.65
1:C:81:PHE:O	1:C:83:GLN:N	2.29	0.65
1:A:281:LYS:HE2	1:C:298:HIS:CD2	2.31	0.65
1:K:375:ASN:O	1:K:379:GLY:N	2.26	0.65
1:M:322:PHE:HD2	1:M:367:GLU:HB3	1.61	0.65
1:O:61:LEU:H	1:O:61:LEU:CD1	2.09	0.65
1:G:81:PHE:O	1:G:83:GLN:N	2.30	0.65
1:K:116:LEU:HD23	1:K:116:LEU:O	1.97	0.65
1:A:102:VAL:HG12	1:A:106:ILE:CD1	2.26	0.65
1:M:67:LEU:HD12	1:M:69:LEU:HD11	1.78	0.65
1:C:129:VAL:HG13	1:C:130:GLN:H	1.60	0.65
1:I:77:SER:HB3	1:I:80:SER:HB2	1.78	0.65
1:O:22:PHE:CE2	1:O:91:VAL:HB	2.32	0.65
1:E:386:GLU:O	1:E:387:SER:C	2.30	0.65
1:A:322:PHE:CD2	1:A:367:GLU:HG2	2.31	0.65
1:A:117:ARG:NH2	1:A:392:HIS:HE1	1.94	0.65
1:K:123:TRP:CE3	1:K:124:ALA:HA	2.31	0.65
1:G:83:GLN:O	1:G:84:TYR:C	2.35	0.65
1:C:65:GLU:O	1:C:68:GLN:NE2	2.29	0.65
2:D:855:ASP:O	2:D:858:ASN:N	2.27	0.65
1:I:375:ASN:O	1:I:379:GLY:N	2.20	0.65
1:M:372:ARG:O	1:M:373:ASN:ND2	2.29	0.65
1:K:166:ILE:HG22	1:K:167:SER:N	2.12	0.65
1:M:218:VAL:O	1:M:222:ILE:N	2.28	0.65
1:C:216:ILE:HG23	1:C:217:ASP:N	2.11	0.65
1:G:381:ILE:O	1:G:382:LEU:C	2.32	0.65
1:I:103:VAL:HA	1:I:106:ILE:CD1	2.26	0.65
1:G:19:ARG:HA	1:G:48:GLN:O	1.96	0.65
1:E:162:ALA:O	1:E:166:ILE:HD12	1.97	0.65
1:C:123:TRP:CZ2	1:C:433:LEU:HD23	2.32	0.65
1:I:20:VAL:HG23	1:I:48:GLN:O	1.97	0.65
1:G:156:SER:O	1:G:158:TYR:N	2.29	0.65
1:E:266:GLN:CB	1:G:264:LEU:HD22	2.26	0.65
1:G:416:LYS:HD2	1:G:418:GLY:HA2	1.77	0.65
1:E:102:VAL:HG13	1:E:106:ILE:HD11	1.79	0.65
1:E:40:ILE:HG23	1:E:47:PHE:HB2	1.79	0.65
1:M:125:LEU:HB2	1:M:149:ILE:HD13	1.79	0.65
1:M:182:ASN:HA	1:M:281:LYS:O	1.96	0.65
1:M:251:THR:O	1:M:253:GLU:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:206:ASN:C	1:G:206:ASN:OD1	2.34	0.65
1:O:105:ASN:O	1:O:106:ILE:C	2.36	0.65
1:K:228:GLN:O	1:K:452:VAL:N	2.30	0.65
1:O:39:ALA:HA	1:O:382:LEU:HD12	1.78	0.65
1:G:218:VAL:O	1:G:222:ILE:N	2.29	0.65
1:K:187:GLY:HA3	1:K:284:THR:H	1.61	0.65
1:E:18:ILE:HD11	1:E:392:HIS:CD2	2.32	0.65
1:K:26:THR:HB	1:K:30:SER:HB3	1.79	0.65
1:C:14:SER:O	1:C:16:ARG:N	2.30	0.65
1:M:100:TYR:HB2	1:M:131:GLN:NE2	2.12	0.64
1:G:64:ILE:HG12	1:G:72:ALA:HB3	1.79	0.64
1:A:195:PRO:O	1:A:199:TYR:CD1	2.50	0.64
1:G:200:ASP:C	1:G:200:ASP:OD1	2.34	0.64
1:E:201:ILE:HG23	1:E:202:GLU:H	1.62	0.64
1:E:284:THR:HA	1:E:285:PRO:C	2.15	0.64
1:I:228:GLN:O	1:I:451:ASP:OD2	2.15	0.64
1:G:129:VAL:O	1:G:133:GLU:N	2.28	0.64
1:G:136:TYR:HB2	1:G:431:ILE:CD1	2.26	0.64
1:O:452:VAL:CG1	1:O:455:ILE:HG12	2.28	0.64
1:G:20:VAL:HA	1:G:89:MET:O	1.98	0.64
1:M:27:SER:HA	1:M:63:THR:HG23	1.78	0.64
1:M:230:ILE:HA	1:M:267:GLY:HA2	1.80	0.64
1:E:233:MET:HE1	1:G:266:GLN:O	1.96	0.64
1:O:61:LEU:HD12	1:O:61:LEU:N	2.11	0.64
1:A:459:GLU:HG3	1:A:459:GLU:O	1.98	0.64
1:K:385:TYR:CA	1:K:388:ILE:HD12	2.23	0.64
1:A:287:LYS:HG2	1:A:290:THR:HB	1.78	0.64
1:E:192:MET:HG2	1:E:244:LEU:O	1.97	0.64
1:G:102:VAL:HG12	1:G:106:ILE:CD1	2.26	0.64
1:G:389:ALA:O	1:G:392:HIS:HB3	1.98	0.64
1:G:115:ASN:O	1:G:117:ARG:N	2.30	0.64
1:E:238:ILE:HD12	1:E:261:ASP:HB3	1.79	0.64
1:K:312:PHE:O	1:K:316:SER:N	2.26	0.64
1:A:284:THR:HA	1:A:285:PRO:C	2.18	0.64
1:K:17:PRO:HA	1:K:46:GLN:O	1.97	0.64
1:M:28:GLY:HA2	1:M:67:LEU:HD21	1.80	0.64
1:I:142:ARG:HB3	1:I:145:LEU:CB	2.28	0.64
1:C:293:LEU:O	1:C:307:GLU:HA	1.98	0.64
1:C:389:ALA:O	1:C:393:PHE:N	2.30	0.64
1:O:319:VAL:HG22	1:O:370:HIS:CG	2.32	0.64
1:C:201:ILE:HG23	1:C:202:GLU:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:312:PHE:O	1:E:316:SER:N	2.28	0.64
1:A:281:LYS:CD	1:C:298:HIS:CD2	2.80	0.64
1:A:216:ILE:HD11	1:A:227:PHE:HE1	1.61	0.64
1:I:102:VAL:C	1:I:106:ILE:HD12	2.17	0.64
1:G:111:SER:N	1:G:142:ARG:HH22	1.95	0.64
1:G:99:HIS:O	1:G:103:VAL:HG23	1.98	0.64
1:K:102:VAL:HG12	1:K:106:ILE:HD11	1.79	0.64
1:K:323:TYR:OH	1:K:364:GLN:HB2	1.98	0.64
1:E:312:PHE:HB3	1:E:315:ILE:HD12	1.80	0.64
1:E:26:THR:HB	1:E:30:SER:HB3	1.79	0.64
1:M:14:SER:OG	1:M:15:SER:N	2.30	0.64
2:L:852:THR:HG22	2:L:854:ASP:H	1.61	0.64
1:G:450:LEU:HD23	1:G:450:LEU:N	2.13	0.64
1:K:100:TYR:CD1	1:K:135:LEU:HD21	2.32	0.64
1:C:89:MET:HG3	1:C:89:MET:O	1.96	0.64
1:C:64:ILE:HD11	1:C:72:ALA:HB1	1.79	0.64
1:E:452:VAL:HG13	1:E:455:ILE:HD13	1.78	0.64
1:C:287:LYS:HG2	1:C:290:THR:HB	1.78	0.64
1:C:132:ALA:O	1:C:133:GLU:C	2.35	0.64
1:E:198:LEU:CD1	1:E:199:TYR:CD1	2.75	0.64
1:I:115:ASN:O	1:I:116:LEU:C	2.36	0.64
1:O:100:TYR:HB2	1:O:131:GLN:CD	2.17	0.64
1:G:142:ARG:HB3	1:G:145:LEU:HB3	1.77	0.64
1:C:416:LYS:HA	1:C:426:THR:OG1	1.98	0.64
1:I:236:ASN:ND2	1:I:260:PRO:HA	2.13	0.64
1:E:195:PRO:O	1:E:199:TYR:HE1	1.77	0.64
1:O:123:TRP:CE3	1:O:124:ALA:HA	2.32	0.64
1:K:192:MET:CG	1:K:244:LEU:O	2.45	0.64
1:A:36:HIS:O	1:A:39:ALA:N	2.30	0.64
1:K:25:LEU:HB3	1:K:52:LEU:HD21	1.81	0.64
1:K:78:LEU:O	1:K:81:PHE:HB3	1.97	0.64
1:I:92:VAL:HG12	1:I:92:VAL:O	1.98	0.64
1:O:64:ILE:HG22	1:O:65:GLU:N	2.13	0.63
1:O:319:VAL:HG22	1:O:370:HIS:CD2	2.33	0.63
1:I:64:ILE:HG22	1:I:65:GLU:N	2.11	0.63
1:K:142:ARG:HB2	1:K:145:LEU:HB3	1.80	0.63
1:C:152:GLN:O	1:C:153:GLY:C	2.32	0.63
1:C:20:VAL:HA	1:C:89:MET:O	1.98	0.63
1:G:251:THR:O	1:G:253:GLU:N	2.30	0.63
1:M:375:ASN:O	1:M:379:GLY:N	2.22	0.63
1:C:446:GLU:OE1	1:C:448:LYS:NZ	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:182:ASN:ND2	1:O:283:GLY:HA2	2.13	0.63
1:G:324:GLY:O	1:G:365:THR:N	2.30	0.63
1:G:263:LEU:O	1:G:263:LEU:HG	1.98	0.63
1:I:192:MET:CE	1:I:243:LEU:CD2	2.71	0.63
1:C:96:VAL:N	1:C:97:PRO:CD	2.62	0.63
1:M:115:ASN:O	1:M:117:ARG:N	2.31	0.63
1:O:156:SER:O	1:O:157:PRO:C	2.36	0.63
1:I:251:THR:O	1:I:253:GLU:N	2.32	0.63
1:C:103:VAL:O	1:C:107:LEU:HG	1.98	0.63
1:A:58:LYS:HG2	1:O:252:LYS:O	1.98	0.63
1:M:150:CYS:O	1:M:152:GLN:NE2	2.32	0.63
1:C:179:ILE:HD12	1:C:278:CYS:HB2	1.79	0.63
1:E:214:HIS:ND1	1:E:314:GLU:HG2	2.13	0.63
1:C:102:VAL:HG12	1:C:106:ILE:CD1	2.28	0.63
1:K:212:PHE:O	1:K:213:GLY:C	2.35	0.63
1:A:201:ILE:HB	1:A:258:THR:HB	1.80	0.63
1:C:201:ILE:HB	1:C:258:THR:HB	1.80	0.63
1:A:225:SER:HB2	1:A:271:ASN:HB2	1.81	0.63
1:G:165:LEU:O	1:G:170:CYS:HB2	1.97	0.63
1:K:213:GLY:O	1:K:216:ILE:HG22	1.99	0.63
1:E:146:GLN:OE1	1:E:413:LYS:HB2	1.98	0.63
1:O:156:SER:HB3	1:O:159:ILE:HG12	1.80	0.63
1:A:177:ILE:HB	1:A:276:VAL:HG13	1.80	0.63
1:G:129:VAL:HG13	1:G:130:GLN:H	1.64	0.63
1:E:22:PHE:O	1:E:53:TYR:N	2.24	0.63
1:C:375:ASN:O	1:C:379:GLY:N	2.30	0.63
1:K:212:PHE:HD1	1:K:280:PHE:CE1	2.16	0.63
1:M:115:ASN:N	1:M:115:ASN:OD1	2.31	0.63
2:B:852:THR:HG22	2:B:854:ASP:H	1.64	0.63
1:G:228:GLN:O	1:G:451:ASP:OD2	2.16	0.63
1:G:216:ILE:HG23	1:G:217:ASP:N	2.13	0.63
1:M:142:ARG:HG3	1:M:145:LEU:HD23	1.80	0.63
1:K:105:ASN:HD22	1:K:105:ASN:N	1.97	0.63
1:C:110:SER:O	1:C:113:ASN:N	2.32	0.63
1:E:218:VAL:O	1:E:221:TYR:HB3	1.98	0.63
1:A:20:VAL:HG23	1:A:48:GLN:O	1.98	0.63
1:I:130:GLN:O	1:I:131:GLN:C	2.37	0.63
1:M:263:LEU:HD12	1:M:264:LEU:N	2.14	0.63
1:I:284:THR:HA	1:I:285:PRO:C	2.18	0.63
1:M:33:ALA:O	1:M:37:PHE:HB3	1.99	0.63
1:A:125:LEU:HB2	1:A:430:ALA:HB1	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:172:GLY:CA	1:I:301:LYS:HD2	2.29	0.63
1:E:231:ASN:HB2	1:E:449:THR:OG1	1.98	0.63
1:G:416:LYS:HD2	1:G:418:GLY:HA3	1.80	0.63
1:G:436:LEU:HD13	1:G:452:VAL:HG11	1.81	0.63
1:I:107:LEU:HD13	1:I:138:ILE:HG21	1.79	0.63
1:C:148:ILE:HG12	1:C:424:PHE:CE1	2.34	0.63
1:E:442:ARG:HD2	1:E:446:GLU:OE2	1.99	0.63
1:G:416:LYS:HA	1:G:426:THR:OG1	1.99	0.62
1:E:18:ILE:HD11	1:E:392:HIS:CG	2.34	0.62
1:E:142:ARG:CB	1:E:145:LEU:HB3	2.29	0.62
1:C:206:ASN:C	1:C:206:ASN:OD1	2.36	0.62
1:G:181:GLY:HA3	1:G:280:PHE:CE2	2.34	0.62
1:E:62:GLN:O	1:E:65:GLU:N	2.32	0.62
1:A:60:SER:O	1:A:64:ILE:HD12	1.99	0.62
1:K:293:LEU:O	1:K:307:GLU:HA	1.99	0.62
1:E:285:PRO:HG3	1:G:300:THR:O	1.99	0.62
1:G:319:VAL:HG22	1:G:370:HIS:ND1	2.14	0.62
1:K:368:VAL:O	1:K:368:VAL:HG12	1.97	0.62
1:G:313:VAL:HG13	1:G:314:GLU:N	2.14	0.62
1:K:129:VAL:O	1:K:133:GLU:N	2.26	0.62
1:O:228:GLN:O	1:O:452:VAL:N	2.32	0.62
1:I:18:ILE:HB	1:I:47:PHE:CD2	2.34	0.62
1:G:226:TYR:O	1:G:270:GLU:HB2	1.99	0.62
1:C:431:ILE:HG22	1:C:432:ILE:N	2.13	0.62
1:E:218:VAL:HG13	1:E:222:ILE:HD11	1.82	0.62
1:M:195:PRO:HB2	1:M:198:LEU:HD22	1.80	0.62
1:C:324:GLY:O	1:C:365:THR:N	2.31	0.62
1:K:57:LEU:CD2	1:K:61:LEU:HD11	2.29	0.62
1:A:118:TYR:OH	1:A:392:HIS:ND1	2.22	0.62
1:A:182:ASN:ND2	1:A:283:GLY:HA2	2.14	0.62
1:G:26:THR:HB	1:G:30:SER:CB	2.29	0.62
1:M:263:LEU:HG	1:M:263:LEU:O	1.97	0.62
1:I:238:ILE:O	1:I:257:LYS:NZ	2.31	0.62
1:G:126:ALA:HB3	1:G:132:ALA:HB2	1.81	0.62
1:G:218:VAL:O	1:G:221:TYR:HB3	1.98	0.62
1:M:134:GLU:HA	1:M:137:SER:OG	1.98	0.62
1:M:318:LEU:O	1:M:370:HIS:HD2	1.83	0.62
1:A:293:LEU:O	1:A:307:GLU:HA	1.99	0.62
1:O:89:MET:O	1:O:89:MET:HG3	1.99	0.62
1:O:201:ILE:HB	1:O:258:THR:HB	1.82	0.62
1:G:201:ILE:HB	1:G:258:THR:HB	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:134:GLU:HG2	1:K:138:ILE:HD11	1.81	0.62
1:I:427:PHE:O	1:I:428:LYS:C	2.33	0.62
1:C:115:ASN:OD1	1:C:115:ASN:N	2.31	0.62
1:C:22:PHE:O	1:C:53:TYR:N	2.29	0.62
1:C:312:PHE:O	1:C:316:SER:N	2.33	0.62
1:K:91:VAL:HG22	1:K:120:TYR:HB3	1.81	0.62
1:C:26:THR:HB	1:C:30:SER:HB3	1.80	0.62
1:O:26:THR:HB	1:O:30:SER:CB	2.29	0.62
1:C:123:TRP:CE3	1:C:124:ALA:HA	2.34	0.62
1:C:431:ILE:HG23	1:C:435:ARG:CD	2.30	0.62
1:G:148:ILE:HG12	1:G:424:PHE:CE1	2.35	0.62
1:G:28:GLY:HA2	1:G:67:LEU:HD21	1.81	0.62
1:K:306:ILE:HG12	1:K:320:LEU:HD12	1.82	0.62
1:I:134:GLU:HA	1:I:137:SER:OG	2.00	0.62
1:K:61:LEU:HD13	1:K:61:LEU:H	1.63	0.62
1:M:231:ASN:HB2	1:M:449:THR:OG1	1.99	0.62
1:I:177:ILE:HD13	1:I:219:LEU:HD11	1.80	0.62
1:E:154:ARG:NH1	1:E:417:GLN:OE1	2.29	0.62
1:A:447:GLU:HG3	1:C:449:THR:CG2	2.30	0.62
1:A:146:GLN:HA	1:A:146:GLN:NE2	2.14	0.62
1:I:231:ASN:HD22	1:K:266:GLN:HE21	1.47	0.62
1:I:50:VAL:O	1:I:72:ALA:HA	2.00	0.62
2:H:855:ASP:O	2:H:858:ASN:N	2.29	0.62
2:P:855:ASP:O	2:P:858:ASN:N	2.32	0.62
1:E:134:GLU:HA	1:E:137:SER:OG	1.99	0.62
1:C:450:LEU:HD23	1:C:450:LEU:N	2.15	0.62
1:M:148:ILE:HD13	1:M:388:ILE:CD1	2.29	0.62
1:E:96:VAL:HA	1:E:99:HIS:CG	2.35	0.62
1:M:130:GLN:O	1:M:131:GLN:C	2.37	0.62
1:I:208:ILE:HA	1:I:212:PHE:HB3	1.82	0.62
1:C:393:PHE:O	1:C:394:LEU:HD12	1.99	0.62
1:A:294:VAL:HA	1:A:306:ILE:O	2.00	0.62
1:O:324:GLY:O	1:O:365:THR:N	2.29	0.62
1:C:273:LYS:HD3	1:C:273:LYS:N	2.14	0.62
1:C:126:ALA:HB3	1:C:132:ALA:HB2	1.82	0.61
1:C:129:VAL:HG13	1:C:130:GLN:N	2.15	0.61
1:M:194:SER:HB3	1:M:199:TYR:HH	1.65	0.61
1:M:125:LEU:HB2	1:M:430:ALA:HB1	1.81	0.61
1:O:142:ARG:CG	1:O:142:ARG:HH11	2.12	0.61
1:I:188:TYR:N	1:I:284:THR:O	2.32	0.61
1:K:320:LEU:HB3	1:K:369:PHE:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:TRP:HD1	1:C:214:HIS:CD2	2.18	0.61
1:A:266:GLN:NE2	1:C:231:ASN:ND2	2.31	0.61
1:E:96:VAL:HG22	1:E:99:HIS:CE1	2.34	0.61
1:C:148:ILE:HD13	1:C:388:ILE:CD1	2.30	0.61
1:M:319:VAL:HG22	1:M:370:HIS:CG	2.35	0.61
1:E:129:VAL:O	1:E:133:GLU:N	2.25	0.61
1:E:225:SER:HB2	1:E:271:ASN:CB	2.30	0.61
1:K:304:LEU:HD23	1:K:322:PHE:HB2	1.82	0.61
1:K:306:ILE:HG12	1:K:320:LEU:CD1	2.31	0.61
1:E:233:MET:HE1	1:G:266:GLN:HG3	1.81	0.61
1:A:161:ARG:NH2	1:A:367:GLU:OE2	2.32	0.61
1:C:79:GLU:HG2	1:C:109:HIS:CG	2.35	0.61
1:C:91:VAL:HG22	1:C:120:TYR:HB3	1.81	0.61
1:O:96:VAL:HB	1:O:97:PRO:HD3	1.81	0.61
1:I:452:VAL:O	1:I:452:VAL:HG12	2.00	0.61
1:C:244:LEU:CD1	1:C:250:ARG:HA	2.26	0.61
1:A:20:VAL:HA	1:A:89:MET:O	2.00	0.61
1:K:416:LYS:HG3	1:K:418:GLY:N	2.15	0.61
1:O:96:VAL:HG12	1:O:127:ALA:HB2	1.80	0.61
1:A:255:ILE:HG13	1:A:256:SER:H	1.66	0.61
1:I:279:SER:HB2	1:K:277:SER:HB2	1.81	0.61
1:A:123:TRP:CD2	1:A:124:ALA:HA	2.34	0.61
1:E:25:LEU:O	1:E:54:ASN:ND2	2.33	0.61
1:A:129:VAL:O	1:A:133:GLU:N	2.25	0.61
1:A:459:GLU:CG	1:A:459:GLU:O	2.48	0.61
1:O:146:GLN:OE1	1:O:414:PHE:CB	2.48	0.61
1:A:251:THR:O	1:A:253:GLU:N	2.34	0.61
1:E:218:VAL:O	1:E:222:ILE:HD12	1.99	0.61
1:G:208:ILE:CG1	1:G:263:LEU:HD22	2.30	0.61
1:C:148:ILE:HD13	1:C:388:ILE:HD13	1.83	0.61
1:M:188:TYR:N	1:M:284:THR:O	2.32	0.61
1:A:290:THR:HG22	1:A:291:LYS:O	2.00	0.61
1:E:313:VAL:HG23	1:E:318:LEU:HD11	1.82	0.61
1:I:237:ASN:N	1:I:261:ASP:OD2	2.29	0.61
1:G:14:SER:OG	1:G:15:SER:N	2.32	0.61
1:G:372:ARG:O	1:G:373:ASN:ND2	2.33	0.61
1:I:166:ILE:HG22	1:I:167:SER:N	2.16	0.61
1:E:206:ASN:C	1:E:206:ASN:OD1	2.38	0.61
1:G:125:LEU:HD23	1:G:132:ALA:HB1	1.83	0.61
1:I:125:LEU:HB2	1:I:430:ALA:HB1	1.82	0.61
1:I:428:LYS:O	1:I:432:ILE:HG13	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:142:ARG:HB3	1:G:145:LEU:HB2	1.82	0.61
2:B:855:ASP:O	2:B:858:ASN:N	2.33	0.61
1:E:290:THR:HG22	1:E:291:LYS:O	2.00	0.61
1:A:305:LYS:NZ	1:A:307:GLU:OE2	2.23	0.61
1:O:105:ASN:N	1:O:105:ASN:HD22	1.97	0.61
1:G:57:LEU:HD22	1:G:61:LEU:HD21	1.83	0.61
1:O:129:VAL:O	1:O:133:GLU:N	2.29	0.61
1:O:115:ASN:O	1:O:116:LEU:C	2.35	0.61
1:K:83:GLN:O	1:K:84:TYR:C	2.39	0.61
1:A:238:ILE:HD12	1:A:261:ASP:HB2	1.81	0.61
2:F:853:MET:O	2:F:856:VAL:HB	2.01	0.61
1:M:129:VAL:HG13	1:M:130:GLN:N	2.15	0.61
1:A:16:ARG:O	1:A:17:PRO:C	2.37	0.61
1:K:324:GLY:O	1:K:365:THR:N	2.33	0.61
1:A:206:ASN:C	1:A:206:ASN:OD1	2.38	0.61
1:A:152:GLN:HE22	1:A:214:HIS:HE1	1.48	0.61
1:I:78:LEU:O	1:I:81:PHE:HB3	2.00	0.61
1:E:218:VAL:O	1:E:222:ILE:N	2.28	0.61
1:G:166:ILE:HG22	1:G:167:SER:N	2.13	0.61
1:I:57:LEU:HD23	1:I:74:GLY:O	2.00	0.61
1:M:136:TYR:HB2	1:M:431:ILE:HD13	1.83	0.61
1:A:263:LEU:HD12	1:A:264:LEU:C	2.21	0.61
1:M:228:GLN:O	1:M:452:VAL:N	2.31	0.61
1:O:215:THR:O	1:O:218:VAL:HG12	2.00	0.61
1:I:232:ALA:O	1:I:444:ASP:HA	2.01	0.61
1:C:134:GLU:HA	1:C:137:SER:OG	2.00	0.60
1:C:208:ILE:HD12	1:C:208:ILE:H	1.66	0.60
1:I:185:TRP:HZ3	1:I:186:TYR:HH	1.48	0.60
1:M:208:ILE:HA	1:M:212:PHE:HB3	1.83	0.60
1:C:225:SER:HB2	1:C:271:ASN:CB	2.31	0.60
1:G:286:VAL:O	1:G:288:LYS:HE3	2.01	0.60
1:A:22:PHE:O	1:A:53:TYR:N	2.29	0.60
1:I:185:TRP:CE3	1:I:186:TYR:CE1	2.89	0.60
1:E:266:GLN:HA	1:E:276:VAL:O	2.01	0.60
1:I:244:LEU:HD11	1:I:250:ARG:CB	2.30	0.60
1:G:85:LYS:O	1:G:115:ASN:ND2	2.34	0.60
1:K:20:VAL:HA	1:K:89:MET:O	2.01	0.60
1:E:431:ILE:HG22	1:E:432:ILE:N	2.16	0.60
1:O:177:ILE:HB	1:O:276:VAL:HG22	1.83	0.60
1:M:34:LYS:O	1:M:35:THR:HG22	2.01	0.60
1:M:230:ILE:HG22	1:M:267:GLY:HA3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:THR:HB	1:E:30:SER:CB	2.32	0.60
1:A:123:TRP:HD1	1:A:214:HIS:CD2	2.20	0.60
1:E:177:ILE:HB	1:E:276:VAL:HG22	1.82	0.60
1:G:306:ILE:HG12	1:G:320:LEU:CD1	2.32	0.60
1:C:89:MET:CB	1:C:118:TYR:HB2	2.30	0.60
1:E:142:ARG:HG3	1:E:145:LEU:HD23	1.83	0.60
1:E:201:ILE:HB	1:E:258:THR:HB	1.82	0.60
1:A:172:GLY:HA3	1:A:301:LYS:HD2	1.82	0.60
2:L:852:THR:HG22	2:L:853:MET:N	2.15	0.60
1:I:171:ILE:O	1:I:300:THR:N	2.33	0.60
1:K:54:ASN:HB3	1:K:55:PRO:HD2	1.82	0.60
1:O:225:SER:CB	1:O:271:ASN:HB2	2.29	0.60
1:I:319:VAL:HG22	1:I:370:HIS:ND1	2.16	0.60
1:M:96:VAL:HG12	1:M:127:ALA:HB2	1.84	0.60
1:M:389:ALA:O	1:M:393:PHE:N	2.33	0.60
1:I:136:TYR:HB2	1:I:431:ILE:HD11	1.82	0.60
1:O:381:ILE:O	1:O:382:LEU:C	2.38	0.60
1:C:222:ILE:HG22	1:C:223:THR:N	2.12	0.60
1:M:166:ILE:HG22	1:M:167:SER:N	2.14	0.60
1:E:147:THR:O	1:E:426:THR:HG22	2.01	0.60
1:M:435:ARG:HB3	1:M:455:ILE:CG2	2.31	0.60
1:I:177:ILE:HB	1:I:276:VAL:HG22	1.84	0.60
1:C:26:THR:HB	1:C:30:SER:CB	2.32	0.60
1:E:158:TYR:CB	1:E:318:LEU:HD12	2.31	0.60
1:G:161:ARG:HA	1:G:164:GLU:OE1	2.01	0.60
1:E:212:PHE:O	1:E:216:ILE:HG22	2.00	0.60
1:E:123:TRP:CD2	1:E:124:ALA:HA	2.36	0.60
1:K:222:ILE:HG22	1:K:223:THR:N	2.12	0.60
1:O:115:ASN:O	1:O:117:ARG:N	2.34	0.60
1:C:142:ARG:CB	1:C:145:LEU:HB3	2.32	0.60
1:A:62:GLN:HG3	1:O:252:LYS:CD	2.31	0.60
1:G:84:TYR:CZ	1:G:86:ASP:HB2	2.36	0.60
1:G:107:LEU:O	1:G:142:ARG:NH2	2.35	0.60
1:C:125:LEU:HB2	1:C:430:ALA:HB1	1.84	0.60
1:O:293:LEU:HG	1:O:294:VAL:N	2.16	0.60
1:I:33:ALA:O	1:I:37:PHE:HB3	2.00	0.60
1:E:251:THR:O	1:E:253:GLU:N	2.35	0.60
1:G:263:LEU:HD12	1:G:264:LEU:O	2.01	0.60
1:G:322:PHE:CD2	1:G:367:GLU:HB3	2.36	0.60
1:A:136:TYR:HB2	1:A:431:ILE:HD13	1.82	0.60
1:A:229:LYS:NZ	1:C:447:GLU:OE2	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:159:ILE:O	1:E:160:VAL:C	2.39	0.60
1:A:201:ILE:HG23	1:A:202:GLU:H	1.67	0.60
1:I:291:LYS:HG3	1:I:307:GLU:HB3	1.84	0.60
1:A:26:THR:HB	1:A:30:SER:CB	2.31	0.60
1:A:197:TYR:C	1:A:199:TYR:N	2.44	0.60
1:I:199:TYR:N	1:I:199:TYR:CD1	2.70	0.60
1:C:64:ILE:HA	1:C:69:LEU:HD12	1.84	0.60
1:K:61:LEU:N	1:K:61:LEU:HD12	2.17	0.60
1:I:245:ASP:OD1	1:I:249:LYS:HB3	2.02	0.60
1:E:77:SER:CB	1:E:80:SER:HB2	2.32	0.60
1:I:105:ASN:HD22	1:I:105:ASN:N	2.00	0.60
1:M:199:TYR:N	1:M:199:TYR:CD1	2.70	0.60
1:C:25:LEU:O	1:C:54:ASN:ND2	2.35	0.60
1:G:225:SER:CB	1:G:271:ASN:HB2	2.31	0.60
1:E:452:VAL:HG13	1:E:455:ILE:HG21	1.83	0.60
1:C:171:ILE:O	1:C:300:THR:N	2.34	0.60
1:K:158:TYR:CD1	1:K:318:LEU:HD12	2.37	0.60
1:M:64:ILE:O	1:M:68:GLN:N	2.35	0.60
1:I:236:ASN:HA	1:I:261:ASP:OD1	2.01	0.60
1:A:433:LEU:HG	1:A:437:ILE:CD1	2.32	0.59
1:I:89:MET:CB	1:I:118:TYR:HB2	2.31	0.59
1:I:53:TYR:O	1:I:54:ASN:ND2	2.35	0.59
1:K:393:PHE:O	1:K:394:LEU:HD12	2.01	0.59
1:C:320:LEU:HG	1:C:321:TYR:N	2.16	0.59
1:O:229:LYS:HE2	1:O:268:ILE:HG13	1.83	0.59
1:O:318:LEU:O	1:O:370:HIS:HD2	1.85	0.59
1:A:19:ARG:HA	1:A:48:GLN:O	2.02	0.59
1:I:225:SER:CB	1:I:271:ASN:HB2	2.31	0.59
1:G:315:ILE:HG23	1:G:377:VAL:HG22	1.84	0.59
1:K:30:SER:O	1:K:34:LYS:HG3	2.01	0.59
1:E:172:GLY:CA	1:E:301:LYS:HD2	2.32	0.59
1:K:244:LEU:HD12	1:K:250:ARG:HA	1.84	0.59
1:K:431:ILE:HG22	1:K:432:ILE:N	2.17	0.59
1:I:431:ILE:O	1:I:435:ARG:HB2	2.02	0.59
1:G:67:LEU:HB2	1:G:69:LEU:HG	1.83	0.59
1:G:103:VAL:O	1:G:107:LEU:HG	2.02	0.59
1:E:225:SER:CB	1:E:271:ASN:HB2	2.31	0.59
1:C:195:PRO:HB3	1:C:197:TYR:CD2	2.36	0.59
2:J:853:MET:O	2:J:854:ASP:C	2.36	0.59
1:I:53:TYR:CG	1:I:54:ASN:N	2.70	0.59
1:G:209:SER:OG	1:G:210:ASN:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:32:VAL:HG13	1:O:36:HIS:HB2	1.83	0.59
1:G:123:TRP:CD2	1:G:124:ALA:HA	2.36	0.59
1:E:115:ASN:O	1:E:116:LEU:C	2.39	0.59
1:I:117:ARG:O	1:I:145:LEU:CD1	2.43	0.59
1:K:287:LYS:HG2	1:K:290:THR:HB	1.84	0.59
1:M:19:ARG:HB3	1:M:50:VAL:HG21	1.85	0.59
1:I:129:VAL:O	1:I:133:GLU:N	2.31	0.59
1:O:161:ARG:HA	1:O:164:GLU:OE1	2.02	0.59
1:G:188:TYR:N	1:G:284:THR:O	2.31	0.59
1:C:304:LEU:HD23	1:C:322:PHE:CB	2.27	0.59
1:I:290:THR:HG22	1:I:291:LYS:O	2.01	0.59
1:O:227:PHE:CD2	1:O:269:LEU:HD23	2.37	0.59
1:C:110:SER:OG	1:C:142:ARG:NH2	2.36	0.59
1:I:281:LYS:C	1:I:281:LYS:HD2	2.13	0.59
1:O:436:LEU:HG	1:O:436:LEU:O	2.01	0.59
1:C:102:VAL:HG12	1:C:106:ILE:HD12	1.84	0.59
1:E:454:LYS:HA	1:E:457:ILE:HD12	1.83	0.59
1:O:20:VAL:HG21	1:O:40:ILE:HD13	1.85	0.59
2:P:852:THR:HG22	2:P:854:ASP:H	1.66	0.59
1:K:62:GLN:O	1:K:65:GLU:N	2.35	0.59
1:E:96:VAL:HG22	1:E:99:HIS:ND1	2.18	0.59
1:C:158:TYR:HB2	1:C:318:LEU:HD12	1.83	0.59
1:M:264:LEU:HD13	1:O:266:GLN:HB2	1.83	0.59
1:M:96:VAL:HB	1:M:97:PRO:HD3	1.84	0.59
1:E:157:PRO:HG3	1:E:383:ARG:HH22	1.67	0.59
1:O:209:SER:OG	1:O:210:ASN:N	2.34	0.59
1:G:290:THR:HG22	1:G:291:LYS:O	2.02	0.59
1:I:62:GLN:O	1:I:63:THR:C	2.40	0.59
1:M:284:THR:HA	1:M:285:PRO:C	2.22	0.59
1:I:177:ILE:CD1	1:I:219:LEU:HD11	2.32	0.59
1:C:183:GLY:HA3	1:C:207:LEU:HD13	1.84	0.59
1:E:99:HIS:O	1:E:103:VAL:HG23	2.01	0.59
1:C:177:ILE:CD1	1:C:219:LEU:HD11	2.31	0.59
1:O:126:ALA:HB3	1:O:132:ALA:HB2	1.84	0.59
1:A:281:LYS:CE	1:C:298:HIS:CD2	2.86	0.59
1:K:84:TYR:CD1	1:K:86:ASP:HB2	2.37	0.59
1:E:294:VAL:HA	1:E:306:ILE:O	2.03	0.59
1:I:31:TRP:O	1:I:35:THR:HG23	2.01	0.59
1:E:198:LEU:CD1	1:E:198:LEU:H	1.80	0.59
1:G:177:ILE:HG22	1:G:178:GLU:N	2.18	0.59
1:G:208:ILE:HG13	1:G:263:LEU:HD22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:179:ILE:CD1	1:G:278:CYS:HB2	2.32	0.59
1:G:169:GLY:O	1:G:328:GLY:HA3	2.02	0.59
1:O:25:LEU:HD23	1:O:63:THR:HG21	1.83	0.59
1:A:455:ILE:CD1	1:A:455:ILE:N	2.65	0.59
1:M:123:TRP:CH2	1:M:433:LEU:HD23	2.37	0.59
1:I:306:ILE:HG12	1:I:320:LEU:HD12	1.85	0.59
1:O:219:LEU:HG	1:O:219:LEU:O	2.03	0.59
1:G:105:ASN:O	1:G:106:ILE:C	2.40	0.59
1:C:32:VAL:HG13	1:C:36:HIS:HB2	1.85	0.59
1:K:154:ARG:NH1	1:K:425:PRO:HB3	2.17	0.59
1:C:129:VAL:O	1:C:133:GLU:N	2.26	0.59
1:O:192:MET:HG2	1:O:244:LEU:O	2.03	0.59
1:I:103:VAL:HA	1:I:106:ILE:HD12	1.84	0.59
1:C:88:ASP:OD1	1:C:115:ASN:HB3	2.03	0.59
1:K:218:VAL:O	1:K:222:ILE:N	2.34	0.59
1:C:147:THR:O	1:C:426:THR:HG22	2.02	0.59
1:K:142:ARG:CB	1:K:145:LEU:HB3	2.32	0.59
2:F:852:THR:HG22	2:F:854:ASP:H	1.68	0.59
1:I:89:MET:HB2	1:I:118:TYR:O	2.03	0.58
1:G:177:ILE:HB	1:G:276:VAL:HG13	1.85	0.58
1:K:436:LEU:O	1:K:440:VAL:HG23	2.02	0.58
1:I:115:ASN:O	1:I:117:ARG:N	2.36	0.58
1:O:436:LEU:CD1	1:O:452:VAL:HG11	2.32	0.58
1:A:102:VAL:CG1	1:A:106:ILE:HD11	2.32	0.58
1:C:123:TRP:CH2	1:C:433:LEU:HD23	2.38	0.58
1:I:390:ASP:O	1:I:394:LEU:CB	2.35	0.58
1:G:428:LYS:O	1:G:432:ILE:HG13	2.02	0.58
1:A:192:MET:HE1	1:K:15:SER:CB	2.28	0.58
1:M:454:LYS:HA	1:M:457:ILE:HD12	1.85	0.58
1:O:178:GLU:HB2	1:O:296:ASP:HB3	1.84	0.58
1:I:381:ILE:O	1:I:384:ILE:N	2.35	0.58
1:G:304:LEU:HD21	1:G:320:LEU:HD21	1.85	0.58
1:K:131:GLN:O	1:K:135:LEU:HG	2.03	0.58
1:A:129:VAL:O	1:A:132:ALA:N	2.34	0.58
1:G:88:ASP:OD1	1:G:115:ASN:HB3	2.04	0.58
1:K:208:ILE:HG22	1:K:209:SER:N	2.17	0.58
1:M:85:LYS:O	1:M:115:ASN:ND2	2.36	0.58
1:A:238:ILE:O	1:A:257:LYS:NZ	2.34	0.58
1:O:226:TYR:O	1:O:270:GLU:HB2	2.02	0.58
1:C:453:SER:HA	1:C:456:MET:HE3	1.84	0.58
1:M:200:ASP:C	1:M:200:ASP:OD1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ILE:CG2	1:A:276:VAL:HG13	2.34	0.58
1:E:62:GLN:O	1:E:63:THR:C	2.42	0.58
1:C:218:VAL:O	1:C:222:ILE:N	2.35	0.58
1:I:194:SER:HB3	1:I:199:TYR:OH	2.04	0.58
1:O:88:ASP:HA	1:O:115:ASN:O	2.03	0.58
1:M:20:VAL:HA	1:M:89:MET:O	2.03	0.58
1:I:293:LEU:HG	1:I:294:VAL:N	2.18	0.58
1:G:431:ILE:HG22	1:G:432:ILE:N	2.17	0.58
1:E:152:GLN:N	1:E:152:GLN:NE2	2.39	0.58
1:I:96:VAL:HG12	1:I:127:ALA:HB2	1.86	0.58
1:E:78:LEU:O	1:E:82:ALA:N	2.33	0.58
1:E:189:GLU:HB2	1:E:284:THR:OG1	2.03	0.58
1:A:158:TYR:HB2	1:A:318:LEU:HD12	1.85	0.58
2:N:852:THR:HG22	2:N:854:ASP:H	1.69	0.58
1:I:198:LEU:HB2	1:I:199:TYR:CE1	2.39	0.58
1:M:161:ARG:O	1:M:161:ARG:CD	2.49	0.58
1:O:150:CYS:O	1:O:152:GLN:NE2	2.36	0.58
1:A:257:LYS:NZ	1:A:261:ASP:OD1	2.37	0.58
1:M:211:SER:O	1:M:214:HIS:HB2	2.04	0.58
1:M:96:VAL:N	1:M:97:PRO:HD2	2.19	0.58
1:A:104:LYS:HA	1:A:107:LEU:HD12	1.85	0.58
1:A:156:SER:CB	1:A:159:ILE:HG12	2.34	0.58
1:K:432:ILE:O	1:K:433:LEU:C	2.41	0.58
1:K:102:VAL:CG1	1:K:106:ILE:HD11	2.34	0.58
1:O:146:GLN:OE1	1:O:414:PHE:HB3	2.04	0.58
1:O:121:VAL:HG12	1:O:122:GLU:N	2.19	0.58
1:M:105:ASN:N	1:M:105:ASN:HD22	2.00	0.58
1:I:79:GLU:O	1:I:80:SER:C	2.41	0.58
1:E:177:ILE:CG2	1:E:276:VAL:HG13	2.34	0.58
1:G:156:SER:HB3	1:G:159:ILE:HG12	1.86	0.58
1:I:244:LEU:HD12	1:I:250:ARG:CA	2.26	0.58
1:M:90:ILE:HD12	1:M:116:LEU:CD1	2.33	0.58
1:A:200:ASP:O	1:A:202:GLU:N	2.37	0.58
1:A:312:PHE:O	1:A:316:SER:N	2.30	0.58
1:K:22:PHE:CE2	1:K:91:VAL:HB	2.39	0.58
1:O:389:ALA:O	1:O:393:PHE:N	2.35	0.58
1:E:142:ARG:HG3	1:E:145:LEU:CD2	2.34	0.58
1:E:130:GLN:O	1:E:131:GLN:C	2.42	0.58
1:M:94:VAL:O	1:M:99:HIS:CD2	2.57	0.58
1:M:232:ALA:O	1:M:444:ASP:HA	2.03	0.58
1:O:435:ARG:NH1	1:O:455:ILE:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:216:ILE:HG23	1:K:217:ASP:N	2.18	0.58
1:E:225:SER:HB2	1:E:271:ASN:CG	2.23	0.58
1:C:197:TYR:HA	1:C:200:ASP:HB3	1.85	0.58
1:K:129:VAL:HG13	1:K:130:GLN:N	2.18	0.57
1:G:236:ASN:HA	1:G:261:ASP:OD1	2.04	0.57
1:M:273:LYS:HD3	1:M:273:LYS:N	2.19	0.57
1:M:142:ARG:CB	1:M:145:LEU:HB3	2.34	0.57
1:O:179:ILE:HG22	1:O:180:SER:N	2.18	0.57
1:I:257:LYS:O	1:I:257:LYS:HG3	2.03	0.57
1:A:96:VAL:N	1:A:97:PRO:HD2	2.18	0.57
1:I:126:ALA:HB3	1:I:132:ALA:HB2	1.86	0.57
1:E:190:ARG:HG3	1:E:191:PRO:HD2	1.86	0.57
1:A:272:GLY:O	1:A:273:LYS:CB	2.48	0.57
1:M:129:VAL:O	1:M:132:ALA:N	2.37	0.57
1:G:16:ARG:O	1:G:16:ARG:HG2	2.05	0.57
1:C:138:ILE:O	1:C:139:SER:C	2.42	0.57
1:C:142:ARG:HB3	1:C:145:LEU:CB	2.34	0.57
1:G:436:LEU:O	1:G:439:ALA:HB3	2.03	0.57
1:E:148:ILE:HD13	1:E:388:ILE:HG12	1.86	0.57
1:M:198:LEU:N	1:M:198:LEU:CD1	2.67	0.57
1:C:159:ILE:O	1:C:160:VAL:C	2.43	0.57
1:G:20:VAL:HG21	1:G:40:ILE:CD1	2.34	0.57
1:G:89:MET:HB2	1:G:118:TYR:O	2.04	0.57
1:E:237:ASN:O	1:E:239:PRO:HD3	2.04	0.57
1:O:158:TYR:CG	1:O:318:LEU:HD12	2.39	0.57
1:O:85:LYS:O	1:O:115:ASN:ND2	2.37	0.57
1:O:89:MET:HB2	1:O:118:TYR:O	2.04	0.57
1:M:30:SER:O	1:M:34:LYS:HG3	2.04	0.57
1:M:34:LYS:O	1:M:35:THR:CG2	2.52	0.57
1:M:68:GLN:NE2	1:M:68:GLN:HA	2.19	0.57
1:M:64:ILE:HG12	1:M:72:ALA:HB3	1.84	0.57
1:M:294:VAL:HA	1:M:306:ILE:O	2.04	0.57
1:E:230:ILE:HD12	1:E:230:ILE:O	2.04	0.57
1:E:96:VAL:N	1:E:97:PRO:CD	2.66	0.57
1:G:121:VAL:HG12	1:G:122:GLU:N	2.18	0.57
1:K:177:ILE:O	1:K:178:GLU:HG3	2.02	0.57
1:E:19:ARG:HB3	1:E:50:VAL:CG2	2.35	0.57
2:J:852:THR:HG22	2:J:854:ASP:H	1.68	0.57
1:O:192:MET:SD	1:O:243:LEU:HD22	2.43	0.57
1:E:102:VAL:O	1:E:106:ILE:CG1	2.52	0.57
1:I:85:LYS:O	1:I:115:ASN:ND2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:147:THR:HB	1:I:427:PHE:CE1	2.39	0.57
1:M:142:ARG:HB3	1:M:145:LEU:HB3	1.86	0.57
1:E:452:VAL:HG13	1:E:455:ILE:CG2	2.34	0.57
1:O:89:MET:SD	1:O:118:TYR:HB2	2.44	0.57
1:O:195:PRO:HB2	1:O:198:LEU:HD13	1.86	0.57
1:A:132:ALA:O	1:A:133:GLU:C	2.39	0.57
1:K:218:VAL:O	1:K:221:TYR:HB3	2.05	0.57
1:A:102:VAL:C	1:A:106:ILE:HD12	2.24	0.57
1:E:294:VAL:HG22	1:E:307:GLU:HG2	1.85	0.57
1:O:40:ILE:O	1:O:40:ILE:HG22	2.05	0.57
1:C:16:ARG:O	1:C:17:PRO:O	2.22	0.57
1:G:284:THR:HA	1:G:285:PRO:C	2.24	0.57
1:G:96:VAL:N	1:G:97:PRO:HD2	2.19	0.57
1:C:187:GLY:HA3	1:C:284:THR:H	1.70	0.57
1:A:153:GLY:O	1:A:159:ILE:HG13	2.05	0.57
1:C:208:ILE:HD11	1:C:234:ILE:HD13	1.86	0.57
1:I:75:PHE:H	1:I:75:PHE:HD1	1.53	0.57
1:E:75:PHE:CZ	1:E:84:TYR:CD2	2.93	0.57
1:C:56:THR:O	1:C:59:SER:OG	2.22	0.57
1:C:154:ARG:NH1	1:C:417:GLN:OE1	2.32	0.57
1:M:210:ASN:O	1:M:211:SER:C	2.36	0.57
1:G:161:ARG:HG3	1:G:161:ARG:O	2.03	0.57
1:A:175:ASN:O	1:A:275:PRO:HD2	2.05	0.57
1:C:209:SER:OG	1:C:210:ASN:N	2.38	0.57
1:C:208:ILE:HA	1:C:212:PHE:HB3	1.87	0.57
1:G:129:VAL:O	1:G:132:ALA:N	2.37	0.57
1:G:156:SER:O	1:G:159:ILE:N	2.35	0.57
1:O:57:LEU:O	1:O:59:SER:N	2.37	0.57
1:G:244:LEU:HD22	1:G:248:GLY:O	2.05	0.57
1:E:95:LYS:HB3	1:E:97:PRO:HD2	1.86	0.57
1:O:134:GLU:O	1:O:135:LEU:C	2.43	0.57
1:C:84:TYR:CE1	1:C:86:ASP:HB2	2.39	0.57
1:K:57:LEU:HD23	1:K:61:LEU:CD1	2.34	0.57
1:K:315:ILE:CG2	1:K:377:VAL:HG22	2.35	0.57
1:O:152:GLN:H	1:O:152:GLN:NE2	2.03	0.57
1:G:106:ILE:HG21	1:G:119:LEU:HD11	1.86	0.57
1:I:20:VAL:HA	1:I:89:MET:O	2.05	0.57
1:A:138:ILE:O	1:A:141:GLN:HG2	2.05	0.57
1:I:115:ASN:N	1:I:115:ASN:OD1	2.34	0.57
1:C:96:VAL:N	1:C:97:PRO:HD2	2.20	0.57
1:O:431:ILE:HG22	1:O:432:ILE:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:225:SER:HB2	1:M:271:ASN:CB	2.32	0.57
1:A:182:ASN:HA	1:A:281:LYS:O	2.05	0.57
1:M:22:PHE:O	1:M:53:TYR:N	2.37	0.57
1:A:238:ILE:HD12	1:A:261:ASP:HB3	1.87	0.57
1:I:324:GLY:O	1:I:365:THR:N	2.32	0.57
1:A:217:ASP:HB2	1:A:433:LEU:HD13	1.87	0.56
1:G:64:ILE:O	1:G:68:GLN:N	2.38	0.56
1:A:19:ARG:HB3	1:A:50:VAL:CG2	2.34	0.56
1:E:126:ALA:HB1	1:E:131:GLN:OE1	2.05	0.56
1:A:25:LEU:O	1:A:54:ASN:ND2	2.38	0.56
1:E:36:HIS:O	1:E:39:ALA:N	2.37	0.56
1:O:313:VAL:HG13	1:O:314:GLU:N	2.20	0.56
1:I:422:GLU:OE1	1:I:422:GLU:N	2.37	0.56
1:M:304:LEU:CD2	1:M:320:LEU:HD11	2.35	0.56
1:O:384:ILE:HG22	1:O:388:ILE:HD11	1.87	0.56
1:A:88:ASP:HA	1:A:115:ASN:O	2.06	0.56
1:O:142:ARG:O	1:O:144:ASN:N	2.38	0.56
1:M:142:ARG:HB3	1:M:145:LEU:HB2	1.85	0.56
1:M:90:ILE:HG22	1:M:90:ILE:O	2.05	0.56
1:A:96:VAL:HG12	1:A:127:ALA:HB2	1.86	0.56
1:C:16:ARG:HB2	1:C:17:PRO:CD	2.35	0.56
1:A:218:VAL:O	1:A:222:ILE:HD12	2.05	0.56
1:G:132:ALA:O	1:G:133:GLU:C	2.43	0.56
1:G:295:ILE:HD13	1:G:306:ILE:HD12	1.85	0.56
1:A:192:MET:HG2	1:A:244:LEU:O	2.05	0.56
1:A:142:ARG:HB2	1:A:145:LEU:HB2	1.87	0.56
1:M:195:PRO:O	1:M:199:TYR:HE1	1.87	0.56
1:A:194:SER:HB3	1:A:199:TYR:HH	1.70	0.56
1:G:88:ASP:O	1:G:116:LEU:HA	2.05	0.56
1:M:89:MET:HB2	1:M:118:TYR:O	2.06	0.56
1:O:216:ILE:HG23	1:O:217:ASP:N	2.20	0.56
1:E:287:LYS:HE3	1:E:290:THR:HB	1.87	0.56
1:A:40:ILE:HG23	1:A:47:PHE:CB	2.35	0.56
1:K:67:LEU:O	1:K:68:GLN:HB2	2.05	0.56
2:L:853:MET:O	2:L:856:VAL:HB	2.05	0.56
1:K:154:ARG:NH1	1:K:417:GLN:OE1	2.38	0.56
1:C:188:TYR:N	1:C:284:THR:O	2.35	0.56
1:M:102:VAL:HG12	1:M:106:ILE:HD12	1.86	0.56
1:I:230:ILE:HG13	1:I:230:ILE:O	2.04	0.56
1:C:166:ILE:HG22	1:C:167:SER:N	2.18	0.56
1:G:129:VAL:CG1	1:G:130:GLN:OE1	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:TYR:HB2	1:C:81:PHE:CD1	2.40	0.56
1:E:188:TYR:N	1:E:284:THR:O	2.36	0.56
1:A:22:PHE:CE2	1:A:91:VAL:HB	2.41	0.56
1:C:452:VAL:O	1:C:452:VAL:HG12	2.05	0.56
1:I:19:ARG:NE	1:I:86:ASP:O	2.37	0.56
1:M:245:ASP:O	1:M:247:ASN:N	2.39	0.56
1:E:96:VAL:O	1:E:127:ALA:HB2	2.06	0.56
1:O:171:ILE:O	1:O:300:THR:N	2.38	0.56
1:E:255:ILE:O	1:E:255:ILE:CG2	2.47	0.56
1:G:312:PHE:HB3	1:G:315:ILE:HD12	1.88	0.56
1:I:156:SER:O	1:I:157:PRO:C	2.42	0.56
1:G:390:ASP:O	1:G:394:LEU:CB	2.53	0.56
1:C:216:ILE:HG23	1:C:217:ASP:H	1.69	0.56
1:O:68:GLN:O	1:O:69:LEU:C	2.43	0.56
1:E:85:LYS:O	1:E:115:ASN:ND2	2.38	0.56
1:O:436:LEU:HD12	1:O:452:VAL:HG11	1.86	0.56
1:M:293:LEU:HB2	1:M:311:GLY:HA2	1.87	0.56
1:I:383:ARG:CG	1:I:383:ARG:NH1	2.59	0.56
1:A:185:TRP:CE3	1:A:186:TYR:CE1	2.93	0.56
1:I:322:PHE:CG	1:I:323:TYR:N	2.72	0.56
1:M:94:VAL:O	1:M:99:HIS:NE2	2.38	0.56
1:I:174:ILE:HB	1:I:274:VAL:HG21	1.88	0.56
1:G:177:ILE:CG2	1:G:178:GLU:N	2.68	0.56
1:O:120:TYR:CE2	1:O:148:ILE:HG21	2.40	0.56
1:C:304:LEU:CD2	1:C:320:LEU:HD21	2.35	0.56
1:I:183:GLY:N	1:I:207:LEU:HD11	2.19	0.56
1:I:197:TYR:CE1	1:I:198:LEU:HD23	2.40	0.56
1:E:431:ILE:CG2	1:E:432:ILE:N	2.69	0.56
1:A:89:MET:HB2	1:A:118:TYR:O	2.05	0.56
1:K:416:LYS:HD2	1:K:418:GLY:CA	2.35	0.56
1:G:171:ILE:O	1:G:300:THR:N	2.39	0.56
1:O:251:THR:O	1:O:253:GLU:N	2.39	0.56
1:E:245:ASP:O	1:E:248:GLY:N	2.28	0.56
1:E:443:SER:HA	1:E:450:LEU:HD21	1.87	0.56
1:K:179:ILE:HG22	1:K:180:SER:N	2.21	0.56
1:O:290:THR:HG22	1:O:291:LYS:N	2.21	0.56
1:I:222:ILE:HG22	1:I:223:THR:N	2.13	0.56
1:E:195:PRO:HB2	1:E:198:LEU:CG	2.36	0.56
1:E:209:SER:OG	1:E:210:ASN:N	2.39	0.56
1:K:436:LEU:HG	1:K:436:LEU:O	2.03	0.56
1:M:128:SER:O	1:M:129:VAL:C	2.43	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:216:ILE:HG23	1:M:217:ASP:H	1.70	0.56
1:O:223:THR:OG1	1:O:224:GLY:N	2.37	0.56
1:I:218:VAL:HG12	1:I:219:LEU:N	2.20	0.56
1:G:183:GLY:N	1:G:282:GLY:O	2.39	0.56
1:E:176:SER:HB2	1:G:262:HIS:CE1	2.41	0.56
1:G:304:LEU:CD2	1:G:322:PHE:HB2	2.36	0.56
1:K:228:GLN:NE2	1:K:273:LYS:HE3	2.21	0.56
1:E:89:MET:HB2	1:E:118:TYR:O	2.06	0.56
1:C:322:PHE:CD2	1:C:367:GLU:HB3	2.37	0.56
1:I:25:LEU:CD1	1:I:52:LEU:HD11	2.31	0.56
1:K:177:ILE:HG22	1:K:178:GLU:N	2.21	0.56
1:K:149:ILE:HD13	1:K:430:ALA:HB1	1.87	0.56
1:A:105:ASN:N	1:A:105:ASN:ND2	2.54	0.56
1:K:182:ASN:HD21	1:K:283:GLY:HA2	1.70	0.56
1:G:16:ARG:CG	1:G:16:ARG:O	2.54	0.56
1:G:223:THR:OG1	1:G:224:GLY:N	2.40	0.55
1:G:187:GLY:HA3	1:G:284:THR:H	1.71	0.55
1:M:159:ILE:O	1:M:160:VAL:C	2.44	0.55
1:E:77:SER:HB3	1:E:80:SER:H	1.71	0.55
1:G:390:ASP:O	1:G:394:LEU:HB3	2.05	0.55
1:K:226:TYR:O	1:K:270:GLU:HB2	2.06	0.55
1:G:454:LYS:HA	1:G:457:ILE:HD12	1.88	0.55
1:C:124:ALA:HB1	1:C:434:HIS:HE1	1.71	0.55
1:E:208:ILE:HA	1:E:212:PHE:HB3	1.87	0.55
1:G:452:VAL:O	1:G:452:VAL:HG12	2.06	0.55
1:I:431:ILE:HG22	1:I:432:ILE:N	2.20	0.55
1:C:89:MET:HB2	1:C:118:TYR:O	2.06	0.55
1:O:218:VAL:O	1:O:222:ILE:N	2.34	0.55
1:A:102:VAL:HG12	1:A:103:VAL:N	2.21	0.55
1:A:306:ILE:HG12	1:A:320:LEU:CD1	2.36	0.55
1:K:159:ILE:O	1:K:160:VAL:C	2.45	0.55
1:O:186:TYR:OH	1:O:206:ASN:HA	2.06	0.55
1:E:105:ASN:N	1:E:105:ASN:HD22	2.04	0.55
1:M:195:PRO:O	1:M:198:LEU:HB2	2.06	0.55
1:A:281:LYS:HE2	1:C:175:ASN:OD1	2.06	0.55
1:I:218:VAL:O	1:I:221:TYR:HB3	2.05	0.55
2:L:855:ASP:O	2:L:858:ASN:N	2.37	0.55
1:E:230:ILE:C	1:E:230:ILE:HD12	2.27	0.55
1:M:175:ASN:O	1:M:275:PRO:HD2	2.06	0.55
1:K:197:TYR:HA	1:K:200:ASP:HB3	1.88	0.55
1:O:208:ILE:HG13	1:O:263:LEU:HD22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ILE:HG22	1:A:384:ILE:O	2.06	0.55
1:I:216:ILE:HD11	1:I:227:PHE:HE1	1.71	0.55
1:O:177:ILE:HG22	1:O:178:GLU:N	2.20	0.55
1:O:152:GLN:O	1:O:153:GLY:C	2.44	0.55
1:I:453:SER:HA	1:I:456:MET:HE1	1.87	0.55
1:I:322:PHE:CD1	1:I:323:TYR:N	2.74	0.55
1:E:251:THR:C	1:E:253:GLU:H	2.10	0.55
1:C:454:LYS:HA	1:C:457:ILE:HD12	1.88	0.55
1:O:373:ASN:O	1:O:373:ASN:ND2	2.26	0.55
1:O:120:TYR:CD2	1:O:148:ILE:CG2	2.89	0.55
1:M:431:ILE:HG22	1:M:432:ILE:N	2.20	0.55
1:I:207:LEU:O	1:I:208:ILE:O	2.25	0.55
1:E:195:PRO:HD2	1:E:198:LEU:HD21	1.89	0.55
1:I:389:ALA:O	1:I:393:PHE:N	2.39	0.55
1:G:453:SER:HA	1:G:456:MET:CE	2.37	0.55
1:O:61:LEU:H	1:O:61:LEU:HD13	1.72	0.55
1:G:245:ASP:O	1:G:248:GLY:N	2.26	0.55
1:G:313:VAL:HG13	1:G:314:GLU:HG3	1.89	0.55
1:E:21:GLY:HA3	1:E:87:ILE:HD13	1.88	0.55
1:M:124:ALA:O	1:M:125:LEU:C	2.41	0.55
1:O:452:VAL:HG12	1:O:452:VAL:O	2.06	0.55
1:C:386:GLU:O	1:C:388:ILE:N	2.39	0.55
1:G:216:ILE:HG23	1:G:217:ASP:H	1.71	0.55
1:K:284:THR:HA	1:K:285:PRO:C	2.27	0.55
1:A:435:ARG:HH22	1:A:458:LEU:HD13	1.71	0.55
1:I:103:VAL:CA	1:I:106:ILE:HD12	2.37	0.55
1:A:322:PHE:HD2	1:A:367:GLU:HG2	1.71	0.55
1:G:64:ILE:HD11	1:G:72:ALA:HB1	1.89	0.55
1:M:263:LEU:HD12	1:M:264:LEU:C	2.27	0.55
1:O:188:TYR:N	1:O:284:THR:O	2.38	0.55
1:I:452:VAL:HG12	1:I:455:ILE:HG12	1.88	0.55
1:C:195:PRO:CB	1:C:197:TYR:CE2	2.90	0.55
1:M:304:LEU:HD22	1:M:320:LEU:HD11	1.89	0.55
1:E:324:GLY:O	1:E:365:THR:N	2.33	0.55
1:K:436:LEU:HD13	1:K:452:VAL:HG11	1.88	0.55
1:M:123:TRP:CE3	1:M:124:ALA:HA	2.42	0.55
1:M:217:ASP:HB2	1:M:433:LEU:HD13	1.87	0.55
1:O:171:ILE:HD12	1:O:299:GLY:HA2	1.86	0.55
1:K:225:SER:CB	1:K:271:ASN:HB2	2.33	0.55
1:M:187:GLY:HA3	1:M:284:THR:N	2.20	0.55
1:A:318:LEU:O	1:A:370:HIS:HD2	1.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:279:SER:HB2	1:O:277:SER:HB2	1.89	0.55
1:C:152:GLN:H	1:C:152:GLN:NE2	2.04	0.55
1:C:436:LEU:O	1:C:440:VAL:HG23	2.06	0.55
1:G:304:LEU:CD2	1:G:320:LEU:HD11	2.31	0.55
1:M:293:LEU:O	1:M:307:GLU:HA	2.06	0.55
1:M:75:PHE:HD2	1:M:80:SER:HB3	1.72	0.55
1:A:257:LYS:CD	1:A:259:CYS:O	2.55	0.55
1:O:199:TYR:CD1	1:O:199:TYR:N	2.75	0.55
1:O:41:GLN:HG2	1:O:41:GLN:O	2.05	0.55
1:A:123:TRP:CZ2	1:A:433:LEU:HD23	2.42	0.55
1:A:49:ILE:HD12	1:A:69:LEU:HD22	1.89	0.55
1:A:262:HIS:CE1	1:C:176:SER:HB2	2.43	0.55
1:K:416:LYS:HD2	1:K:418:GLY:HA2	1.89	0.55
1:A:257:LYS:HG2	1:A:259:CYS:O	2.07	0.55
1:M:26:THR:HB	1:M:30:SER:HB2	1.89	0.55
1:E:201:ILE:HG23	1:E:202:GLU:N	2.21	0.55
1:G:102:VAL:HG12	1:G:106:ILE:HD11	1.89	0.55
1:E:161:ARG:HA	1:E:164:GLU:OE1	2.07	0.55
1:A:152:GLN:NE2	1:A:214:HIS:HE1	2.05	0.54
1:E:194:SER:HB3	1:E:199:TYR:CZ	2.32	0.54
1:E:22:PHE:CE2	1:E:91:VAL:HB	2.42	0.54
1:M:149:ILE:HG23	1:M:151:LEU:HD12	1.88	0.54
1:C:392:HIS:C	1:C:394:LEU:H	2.10	0.54
1:A:30:SER:OG	1:A:33:ALA:HB2	2.06	0.54
1:K:158:TYR:HB2	1:K:318:LEU:HD12	1.89	0.54
1:C:167:SER:OG	1:C:168:GLU:N	2.38	0.54
1:C:199:TYR:CD1	1:C:199:TYR:N	2.74	0.54
2:H:852:THR:HG22	2:H:853:MET:N	2.21	0.54
1:I:416:LYS:HB3	1:I:428:LYS:HG2	1.89	0.54
1:O:312:PHE:O	1:O:316:SER:N	2.40	0.54
1:M:381:ILE:O	1:M:382:LEU:C	2.45	0.54
1:C:126:ALA:HB1	1:C:131:GLN:OE1	2.05	0.54
1:C:212:PHE:HD1	1:C:280:PHE:CE1	2.26	0.54
1:G:125:LEU:HD13	1:G:430:ALA:HB1	1.89	0.54
1:A:455:ILE:H	1:A:455:ILE:HD13	1.73	0.54
1:I:124:ALA:O	1:I:125:LEU:C	2.42	0.54
1:K:384:ILE:O	1:K:385:TYR:C	2.44	0.54
1:O:427:PHE:O	1:O:428:LYS:C	2.41	0.54
1:I:229:LYS:HE3	1:I:449:THR:CG2	2.37	0.54
1:I:65:GLU:O	1:I:68:GLN:NE2	2.40	0.54
1:O:178:GLU:C	1:O:179:ILE:HG13	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:232:ALA:O	1:K:444:ASP:HA	2.08	0.54
1:C:129:VAL:CG1	1:C:130:GLN:H	2.20	0.54
1:I:250:ARG:HG2	1:I:250:ARG:O	2.05	0.54
1:I:107:LEU:O	1:I:142:ARG:NH2	2.38	0.54
1:O:129:VAL:HG13	1:O:130:GLN:H	1.73	0.54
1:C:77:SER:HB3	1:C:80:SER:OG	2.07	0.54
1:O:215:THR:O	1:O:216:ILE:C	2.42	0.54
1:A:81:PHE:O	1:A:83:GLN:N	2.40	0.54
1:A:188:TYR:N	1:A:284:THR:O	2.34	0.54
1:E:111:SER:N	1:E:142:ARG:HH22	2.06	0.54
1:I:83:GLN:O	1:I:84:TYR:C	2.46	0.54
1:O:132:ALA:O	1:O:133:GLU:C	2.46	0.54
1:G:40:ILE:O	1:G:40:ILE:HG22	2.08	0.54
1:K:149:ILE:CD1	1:K:430:ALA:HB2	2.36	0.54
1:M:435:ARG:CB	1:M:455:ILE:HG23	2.38	0.54
1:A:287:LYS:HZ3	1:A:290:THR:HB	1.72	0.54
1:A:177:ILE:CB	1:A:276:VAL:HG13	2.38	0.54
1:K:196:GLU:HG2	1:O:56:THR:HG21	1.87	0.54
1:K:245:ASP:O	1:K:247:ASN:N	2.40	0.54
1:O:64:ILE:HG12	1:O:72:ALA:HB3	1.89	0.54
1:M:152:GLN:O	1:M:153:GLY:C	2.45	0.54
1:C:159:ILE:HD12	1:C:218:VAL:CG2	2.38	0.54
1:A:25:LEU:HB3	1:A:52:LEU:HD21	1.90	0.54
1:C:195:PRO:CB	1:C:197:TYR:CD2	2.91	0.54
1:K:190:ARG:HG3	1:K:199:TYR:CZ	2.42	0.54
1:C:232:ALA:O	1:C:444:ASP:HA	2.08	0.54
1:C:106:ILE:HG21	1:C:119:LEU:HD11	1.90	0.54
1:K:179:ILE:HD11	1:K:219:LEU:HD13	1.90	0.54
1:A:96:VAL:O	1:A:99:HIS:HB2	2.08	0.54
1:I:201:ILE:HB	1:I:258:THR:CB	2.37	0.54
1:M:171:ILE:O	1:M:300:THR:N	2.41	0.54
1:A:156:SER:O	1:A:157:PRO:C	2.46	0.54
1:A:208:ILE:HA	1:A:212:PHE:HB3	1.90	0.54
1:G:379:GLY:O	1:G:382:LEU:HB3	2.07	0.54
1:G:129:VAL:O	1:G:132:ALA:HB3	2.08	0.54
1:O:56:THR:HG1	1:O:59:SER:HG	1.55	0.54
1:I:138:ILE:O	1:I:139:SER:C	2.44	0.54
1:A:229:LYS:O	1:A:230:ILE:CG2	2.55	0.54
1:O:136:TYR:O	1:O:137:SER:C	2.46	0.54
1:C:389:ALA:O	1:C:390:ASP:O	2.25	0.54
1:O:96:VAL:N	1:O:97:PRO:HD2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:PRO:O	1:C:198:LEU:HB2	2.08	0.54
1:C:432:ILE:HG23	1:C:455:ILE:HG22	1.90	0.54
1:O:123:TRP:HD1	1:O:214:HIS:CD2	2.26	0.54
1:G:62:GLN:O	1:G:63:THR:C	2.46	0.54
1:O:129:VAL:O	1:O:132:ALA:N	2.41	0.54
1:M:313:VAL:HG23	1:M:318:LEU:HD11	1.90	0.54
1:E:431:ILE:O	1:E:432:ILE:C	2.47	0.54
1:E:452:VAL:O	1:E:452:VAL:HG12	2.08	0.54
1:M:84:TYR:CD1	1:M:86:ASP:HB2	2.42	0.54
1:K:56:THR:O	1:K:59:SER:OG	2.25	0.54
1:O:312:PHE:O	1:O:316:SER:CB	2.55	0.54
1:K:322:PHE:CG	1:K:323:TYR:N	2.76	0.54
1:K:31:TRP:O	1:K:35:THR:HG23	2.08	0.54
1:M:39:ALA:HA	1:M:382:LEU:HD12	1.90	0.54
1:C:263:LEU:HD12	1:C:264:LEU:O	2.07	0.53
1:E:191:PRO:HG2	1:E:194:SER:OG	2.07	0.53
1:G:375:ASN:C	1:G:375:ASN:OD1	2.43	0.53
1:O:208:ILE:HG21	1:O:441:PHE:CE1	2.44	0.53
1:E:105:ASN:O	1:E:106:ILE:C	2.45	0.53
1:G:104:LYS:O	1:G:107:LEU:HB2	2.08	0.53
1:G:115:ASN:O	1:G:117:ARG:HB2	2.07	0.53
1:C:52:LEU:HD11	1:C:63:THR:CG2	2.33	0.53
1:A:105:ASN:HA	1:A:108:GLU:HG3	1.90	0.53
1:I:381:ILE:HG22	1:I:385:TYR:CE1	2.44	0.53
1:K:313:VAL:HG13	1:K:314:GLU:N	2.23	0.53
1:A:216:ILE:HG23	1:A:217:ASP:H	1.72	0.53
1:K:436:LEU:CD1	1:K:452:VAL:HG11	2.39	0.53
1:M:129:VAL:O	1:M:133:GLU:N	2.33	0.53
1:A:48:GLN:OE1	1:A:71:HIS:CD2	2.62	0.53
1:I:453:SER:O	1:I:456:MET:HE2	2.08	0.53
1:I:381:ILE:CG2	1:I:385:TYR:HE1	2.20	0.53
1:I:279:SER:HB2	1:K:277:SER:CB	2.38	0.53
1:A:232:ALA:O	1:A:444:ASP:HA	2.07	0.53
1:G:130:GLN:O	1:G:131:GLN:C	2.46	0.53
1:G:435:ARG:NH1	1:G:455:ILE:O	2.40	0.53
1:K:134:GLU:O	1:K:138:ILE:HG13	2.08	0.53
1:C:386:GLU:O	1:C:387:SER:C	2.46	0.53
1:C:78:LEU:O	1:C:82:ALA:N	2.38	0.53
1:K:89:MET:CB	1:K:118:TYR:HB2	2.32	0.53
1:I:218:VAL:O	1:I:222:ILE:N	2.34	0.53
1:M:177:ILE:HG22	1:M:178:GLU:N	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:322:PHE:CG	1:M:323:TYR:N	2.76	0.53
1:I:436:LEU:O	1:I:440:VAL:HG23	2.08	0.53
2:N:853:MET:O	2:N:854:ASP:C	2.47	0.53
1:E:171:ILE:HD12	1:E:299:GLY:HA3	1.90	0.53
1:C:107:LEU:O	1:C:142:ARG:NH2	2.41	0.53
1:C:435:ARG:NH1	1:C:455:ILE:O	2.41	0.53
1:E:195:PRO:O	1:E:199:TYR:HD1	1.91	0.53
1:G:178:GLU:HA	1:G:277:SER:O	2.09	0.53
1:A:228:GLN:HE22	1:A:273:LYS:CE	2.22	0.53
1:I:429:ASP:O	1:I:430:ALA:C	2.47	0.53
1:A:262:HIS:CD2	1:A:263:LEU:N	2.77	0.53
1:C:180:SER:O	1:C:293:LEU:HD12	2.09	0.53
1:E:129:VAL:O	1:E:132:ALA:HB3	2.08	0.53
2:D:856:VAL:O	2:D:860:ILE:HG22	2.08	0.53
1:A:158:TYR:CB	1:A:318:LEU:HD12	2.38	0.53
1:A:149:ILE:CG2	1:A:151:LEU:HD12	2.39	0.53
1:E:14:SER:OG	1:E:15:SER:N	2.42	0.53
1:C:61:LEU:N	1:C:61:LEU:CD1	2.72	0.53
1:K:100:TYR:HB2	1:K:131:GLN:OE1	2.09	0.53
1:M:428:LYS:O	1:M:432:ILE:HG13	2.09	0.53
1:E:166:ILE:HG22	1:E:167:SER:N	2.23	0.53
1:M:156:SER:O	1:M:157:PRO:C	2.43	0.53
1:K:266:GLN:HA	1:K:276:VAL:O	2.08	0.53
1:I:159:ILE:N	1:I:159:ILE:HD13	2.24	0.53
1:E:30:SER:O	1:E:34:LYS:HG3	2.08	0.53
1:O:79:GLU:HG2	1:O:109:HIS:CD2	2.44	0.53
1:E:40:ILE:HG23	1:E:47:PHE:CB	2.39	0.53
1:I:105:ASN:O	1:I:106:ILE:C	2.46	0.53
1:A:38:LEU:O	1:A:39:ALA:C	2.47	0.53
1:A:41:GLN:C	1:A:43:LEU:H	2.11	0.53
1:M:313:VAL:HG13	1:M:314:GLU:N	2.22	0.53
1:M:452:VAL:O	1:M:452:VAL:HG12	2.07	0.53
1:I:96:VAL:HB	1:I:97:PRO:HD3	1.91	0.53
1:O:189:GLU:HB2	1:O:284:THR:OG1	2.09	0.53
1:O:322:PHE:HD2	1:O:367:GLU:HB3	1.73	0.53
1:A:266:GLN:HA	1:A:276:VAL:O	2.09	0.53
1:A:38:LEU:HD23	1:A:41:GLN:OE1	2.09	0.53
1:M:91:VAL:HG22	1:M:120:TYR:HB3	1.89	0.53
1:I:208:ILE:HD13	1:I:441:PHE:CZ	2.44	0.53
1:O:177:ILE:HD13	1:O:219:LEU:HD11	1.91	0.53
1:M:177:ILE:HD13	1:M:219:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:245:ASP:O	1:G:247:ASN:N	2.41	0.53
1:A:39:ALA:HA	1:A:382:LEU:HD12	1.90	0.53
1:M:129:VAL:O	1:M:130:GLN:C	2.47	0.53
1:C:179:ILE:HG22	1:C:180:SER:N	2.23	0.53
1:A:190:ARG:HG3	1:A:191:PRO:CD	2.38	0.53
1:I:28:GLY:HA2	1:I:67:LEU:CD2	2.34	0.53
1:K:125:LEU:HB2	1:K:149:ILE:HD13	1.91	0.53
1:E:370:HIS:CD2	2:F:848:PHE:CD2	2.95	0.53
1:M:64:ILE:HG22	1:M:65:GLU:N	2.23	0.53
1:M:65:GLU:O	1:M:68:GLN:NE2	2.42	0.53
1:K:313:VAL:HG13	1:K:314:GLU:H	1.73	0.53
1:C:263:LEU:HD12	1:C:264:LEU:N	2.24	0.53
1:G:158:TYR:HB2	1:G:318:LEU:HD12	1.91	0.53
1:G:427:PHE:HA	1:G:430:ALA:HB3	1.91	0.53
1:M:128:SER:O	1:M:131:GLN:HB2	2.08	0.53
1:C:389:ALA:O	1:C:390:ASP:C	2.48	0.53
1:M:105:ASN:HA	1:M:108:GLU:HG3	1.89	0.53
1:O:231:ASN:HB2	1:O:449:THR:OG1	2.08	0.53
1:G:148:ILE:HD13	1:G:388:ILE:HD11	1.91	0.52
1:G:222:ILE:HG22	1:G:223:THR:N	2.23	0.52
1:E:389:ALA:O	1:E:392:HIS:HB3	2.09	0.52
1:A:427:PHE:O	1:A:431:ILE:HB	2.09	0.52
1:C:75:PHE:N	1:C:75:PHE:CD1	2.77	0.52
1:C:147:THR:HB	1:C:427:PHE:CE1	2.43	0.52
1:G:174:ILE:HG22	1:G:175:ASN:N	2.23	0.52
2:D:852:THR:O	2:D:856:VAL:HG23	2.09	0.52
1:E:293:LEU:HB2	1:E:311:GLY:HA2	1.91	0.52
1:O:40:ILE:HG23	1:O:47:PHE:HB2	1.91	0.52
1:A:226:TYR:O	1:A:270:GLU:HB2	2.08	0.52
1:C:100:TYR:HB2	1:C:131:GLN:CD	2.29	0.52
1:O:129:VAL:HA	1:O:434:HIS:HD2	1.74	0.52
1:I:218:VAL:CG1	1:I:219:LEU:N	2.70	0.52
1:M:218:VAL:O	1:M:221:TYR:HB3	2.09	0.52
1:I:78:LEU:O	1:I:79:GLU:C	2.47	0.52
1:G:218:VAL:O	1:G:222:ILE:HD12	2.09	0.52
1:M:136:TYR:O	1:M:137:SER:C	2.47	0.52
1:A:89:MET:HG3	1:A:89:MET:O	2.09	0.52
1:A:281:LYS:CE	1:C:298:HIS:NE2	2.72	0.52
1:A:201:ILE:HG23	1:A:202:GLU:N	2.24	0.52
1:A:291:LYS:HG3	1:A:307:GLU:HB3	1.91	0.52
1:I:454:LYS:HA	1:I:457:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:LEU:HD21	1:E:74:GLY:O	2.09	0.52
1:A:208:ILE:HD13	1:A:441:PHE:HZ	1.67	0.52
1:M:120:TYR:HE2	1:M:150:CYS:HB2	1.74	0.52
1:K:115:ASN:O	1:K:116:LEU:C	2.42	0.52
1:M:201:ILE:HG23	1:M:202:GLU:H	1.74	0.52
1:E:232:ALA:O	1:E:444:ASP:HA	2.10	0.52
1:C:226:TYR:O	1:C:270:GLU:HB2	2.09	0.52
1:G:75:PHE:CD1	1:G:75:PHE:N	2.78	0.52
1:M:226:TYR:O	1:M:270:GLU:HB2	2.09	0.52
1:A:123:TRP:CE3	1:A:124:ALA:HA	2.45	0.52
1:E:233:MET:CE	1:G:266:GLN:HG3	2.40	0.52
1:M:197:TYR:CD1	1:M:198:LEU:HD12	2.43	0.52
1:K:151:LEU:C	1:K:153:GLY:N	2.63	0.52
1:O:222:ILE:HG22	1:O:223:THR:N	2.19	0.52
1:A:96:VAL:HA	1:A:99:HIS:CG	2.44	0.52
1:E:142:ARG:HB3	1:E:145:LEU:HB2	1.91	0.52
1:M:64:ILE:HA	1:M:69:LEU:HD12	1.91	0.52
1:G:78:LEU:O	1:G:82:ALA:N	2.38	0.52
1:M:244:LEU:CD2	1:M:248:GLY:CA	2.81	0.52
1:E:103:VAL:HA	1:E:106:ILE:CD1	2.38	0.52
1:E:49:ILE:HD13	1:E:69:LEU:CD2	2.40	0.52
1:A:455:ILE:N	1:A:455:ILE:HD13	2.25	0.52
1:K:77:SER:CB	1:K:80:SER:HB2	2.38	0.52
1:I:128:SER:OG	1:I:131:GLN:HB2	2.10	0.52
1:A:30:SER:O	1:A:34:LYS:HG3	2.10	0.52
1:C:200:ASP:C	1:C:200:ASP:OD1	2.48	0.52
1:O:168:GLU:O	1:O:170:CYS:N	2.42	0.52
1:O:81:PHE:O	1:O:83:GLN:N	2.43	0.52
1:K:431:ILE:HG23	1:K:435:ARG:HD2	1.92	0.52
1:K:389:ALA:O	1:K:393:PHE:N	2.42	0.52
1:M:313:VAL:CG1	1:M:314:GLU:N	2.72	0.52
1:K:123:TRP:HD1	1:K:214:HIS:CD2	2.27	0.52
1:A:290:THR:HG22	1:A:291:LYS:N	2.24	0.52
1:A:238:ILE:O	1:A:257:LYS:CE	2.58	0.52
1:I:154:ARG:NH1	1:I:417:GLN:OE1	2.37	0.52
1:K:272:GLY:O	1:K:273:LYS:HB2	2.10	0.52
1:E:75:PHE:HZ	1:E:84:TYR:CD2	2.28	0.52
1:O:88:ASP:O	1:O:117:ARG:N	2.34	0.52
1:K:426:THR:O	1:K:429:ASP:N	2.43	0.52
1:E:142:ARG:O	1:E:413:LYS:NZ	2.34	0.52
1:C:189:GLU:HB2	1:C:284:THR:OG1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:VAL:C	1:C:264:LEU:HD21	2.29	0.52
1:K:187:GLY:HA3	1:K:284:THR:N	2.25	0.52
1:E:392:HIS:CD2	1:E:393:PHE:CD2	2.97	0.52
1:K:136:TYR:HB2	1:K:431:ILE:HD11	1.91	0.52
1:A:146:GLN:OE1	1:A:413:LYS:HB2	2.09	0.52
1:A:288:LYS:HD2	1:C:323:TYR:CE2	2.44	0.52
1:I:372:ARG:HH21	2:J:847:LEU:HB3	1.74	0.52
1:M:182:ASN:O	1:M:183:GLY:C	2.46	0.52
1:E:177:ILE:HG22	1:E:276:VAL:HG13	1.91	0.52
1:G:152:GLN:O	1:G:153:GLY:O	2.27	0.52
1:O:23:VAL:HG22	1:O:53:TYR:HB3	1.92	0.52
1:M:198:LEU:HB2	1:M:199:TYR:CE1	2.45	0.52
1:M:121:VAL:HG21	1:M:427:PHE:HZ	1.75	0.52
1:I:312:PHE:CB	1:I:315:ILE:HD12	2.31	0.52
1:I:152:GLN:O	1:I:153:GLY:C	2.48	0.52
1:E:77:SER:HB3	1:E:80:SER:HB2	1.92	0.52
1:E:128:SER:OG	1:E:131:GLN:HB2	2.10	0.52
1:C:272:GLY:O	1:C:273:LYS:HB2	2.09	0.52
1:G:147:THR:O	1:G:426:THR:HG22	2.10	0.51
1:G:434:HIS:N	1:G:437:ILE:HD12	2.25	0.51
1:G:456:MET:N	1:G:456:MET:SD	2.83	0.51
1:G:187:GLY:HA3	1:G:284:THR:N	2.25	0.51
1:K:454:LYS:CA	1:K:457:ILE:HD12	2.38	0.51
1:A:138:ILE:O	1:A:139:SER:C	2.49	0.51
1:I:103:VAL:HA	1:I:106:ILE:HD13	1.92	0.51
1:O:427:PHE:O	1:O:431:ILE:HB	2.10	0.51
1:C:90:ILE:HB	1:C:119:LEU:HD12	1.91	0.51
1:K:208:ILE:O	1:K:212:PHE:HB3	2.10	0.51
1:M:201:ILE:CG2	1:M:202:GLU:N	2.73	0.51
1:G:105:ASN:N	1:G:105:ASN:HD22	2.08	0.51
1:A:25:LEU:HD23	1:A:63:THR:CG2	2.39	0.51
1:A:209:SER:OG	1:A:210:ASN:N	2.42	0.51
1:M:286:VAL:HG23	1:M:288:LYS:HE3	1.91	0.51
1:A:313:VAL:HG13	1:A:314:GLU:N	2.25	0.51
1:E:195:PRO:HB2	1:E:198:LEU:HG	1.92	0.51
1:I:53:TYR:CD2	1:I:54:ASN:CA	2.93	0.51
1:G:138:ILE:O	1:G:139:SER:C	2.46	0.51
1:E:266:GLN:NE2	1:G:231:ASN:OD1	2.42	0.51
1:O:64:ILE:O	1:O:68:GLN:N	2.42	0.51
1:E:378:VAL:O	1:E:379:GLY:C	2.46	0.51
1:E:64:ILE:O	1:E:68:GLN:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:381:ILE:O	1:O:384:ILE:N	2.39	0.51
1:C:318:LEU:O	1:C:370:HIS:HD2	1.93	0.51
1:G:142:ARG:HB2	1:G:145:LEU:HB3	1.91	0.51
1:C:64:ILE:HG12	1:C:69:LEU:HB2	1.92	0.51
1:M:107:LEU:O	1:M:142:ARG:NH2	2.41	0.51
1:I:225:SER:HB2	1:I:271:ASN:CB	2.38	0.51
1:K:181:GLY:O	1:K:281:LYS:N	2.41	0.51
1:K:182:ASN:HD21	1:K:283:GLY:CA	2.22	0.51
1:O:188:TYR:CZ	1:O:238:ILE:HG12	2.46	0.51
1:I:375:ASN:C	1:I:375:ASN:OD1	2.48	0.51
1:I:40:ILE:HG22	1:I:40:ILE:O	2.10	0.51
1:G:201:ILE:HG23	1:G:202:GLU:H	1.74	0.51
1:E:451:ASP:O	1:E:451:ASP:OD1	2.28	0.51
1:C:123:TRP:CD1	1:C:214:HIS:CD2	2.98	0.51
1:E:385:TYR:CA	1:E:388:ILE:HD12	2.40	0.51
1:K:134:GLU:HA	1:K:137:SER:OG	2.10	0.51
1:M:198:LEU:N	1:M:198:LEU:HD13	2.25	0.51
1:E:182:ASN:HA	1:E:281:LYS:O	2.10	0.51
1:A:84:TYR:CD1	1:A:86:ASP:HB2	2.46	0.51
1:E:100:TYR:HA	1:E:135:LEU:HD11	1.92	0.51
1:A:237:ASN:O	1:A:239:PRO:HD3	2.10	0.51
1:O:273:LYS:N	1:O:273:LYS:HD3	2.25	0.51
1:M:245:ASP:C	1:M:245:ASP:OD1	2.48	0.51
1:A:161:ARG:HA	1:A:164:GLU:OE1	2.11	0.51
1:M:121:VAL:CG2	1:M:427:PHE:HZ	2.23	0.51
1:A:103:VAL:HG11	1:A:135:LEU:HD13	1.92	0.51
1:I:266:GLN:NE2	1:K:231:ASN:OD1	2.43	0.51
1:O:190:ARG:HH22	1:O:196:GLU:HA	1.76	0.51
1:M:19:ARG:HB3	1:M:50:VAL:CG2	2.40	0.51
1:G:105:ASN:HA	1:G:108:GLU:HG3	1.93	0.51
1:I:211:SER:O	1:I:215:THR:OG1	2.25	0.51
1:G:199:TYR:CD1	1:G:199:TYR:N	2.78	0.51
1:I:185:TRP:CE3	1:I:186:TYR:CZ	2.98	0.51
1:I:185:TRP:CZ3	1:I:186:TYR:OH	2.63	0.51
1:G:436:LEU:O	1:G:436:LEU:HG	2.10	0.51
1:O:53:TYR:CD2	1:O:54:ASN:N	2.78	0.51
1:E:25:LEU:HD23	1:E:63:THR:CG2	2.41	0.51
1:E:51:ALA:HB3	1:E:87:ILE:HD11	1.92	0.51
1:I:244:LEU:CD1	1:I:250:ARG:CB	2.87	0.51
1:M:30:SER:O	1:M:33:ALA:HB3	2.11	0.51
1:I:266:GLN:HA	1:I:276:VAL:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:SER:HA	1:E:142:ARG:NH2	2.25	0.51
1:K:375:ASN:C	1:K:375:ASN:OD1	2.45	0.51
1:G:185:TRP:O	1:G:199:TYR:HE2	1.94	0.51
1:K:292:ASN:HD22	1:K:292:ASN:H	1.57	0.51
1:A:217:ASP:O	1:A:221:TYR:N	2.44	0.51
1:O:62:GLN:O	1:O:63:THR:C	2.49	0.51
1:A:315:ILE:CG2	1:A:377:VAL:HG22	2.41	0.51
1:O:77:SER:CB	1:O:80:SER:HB2	2.39	0.51
1:A:245:ASP:OD1	1:A:249:LYS:HB3	2.10	0.51
1:C:372:ARG:O	1:C:373:ASN:ND2	2.43	0.51
1:O:301:LYS:HD3	1:O:325:ILE:HD11	1.92	0.51
1:E:233:MET:CE	1:G:231:ASN:HB3	2.41	0.51
1:G:436:LEU:HB2	1:G:455:ILE:HD11	1.93	0.51
1:I:110:SER:C	1:I:142:ARG:HH22	2.14	0.51
1:I:197:TYR:CE1	1:I:198:LEU:CD2	2.94	0.51
1:G:32:VAL:CG1	1:G:36:HIS:HB2	2.38	0.51
1:M:179:ILE:HG22	1:M:180:SER:N	2.25	0.51
1:C:453:SER:HA	1:C:456:MET:CE	2.40	0.51
1:A:120:TYR:C	1:A:121:VAL:HG23	2.31	0.51
1:O:104:LYS:O	1:O:107:LEU:HB2	2.10	0.51
1:C:436:LEU:O	1:C:436:LEU:HG	2.08	0.51
1:I:392:HIS:C	1:I:394:LEU:H	2.14	0.51
1:I:84:TYR:CE1	1:I:86:ASP:HB2	2.45	0.51
1:G:218:VAL:HG13	1:G:222:ILE:HD11	1.92	0.51
1:K:452:VAL:HG12	1:K:455:ILE:HG13	1.90	0.51
1:A:62:GLN:CG	1:O:252:LYS:HD2	2.41	0.51
1:M:216:ILE:CG2	1:M:217:ASP:N	2.72	0.51
1:C:218:VAL:O	1:C:221:TYR:HB3	2.10	0.51
1:M:377:VAL:HG11	2:N:859:TYR:CD2	2.46	0.51
1:A:48:GLN:OE1	1:A:71:HIS:CG	2.64	0.51
1:K:179:ILE:HB	1:K:278:CYS:HB2	1.93	0.51
1:I:64:ILE:O	1:I:68:GLN:N	2.43	0.51
1:O:292:ASN:HD22	1:O:292:ASN:H	1.59	0.51
1:E:281:LYS:HD2	1:G:298:HIS:CD2	2.46	0.51
1:I:245:ASP:O	1:I:246:GLU:C	2.49	0.51
1:A:319:VAL:HG22	1:A:370:HIS:CG	2.46	0.51
1:O:146:GLN:HA	1:O:146:GLN:HE21	1.74	0.51
1:E:245:ASP:O	1:E:247:ASN:N	2.44	0.51
1:C:145:LEU:O	1:C:413:LYS:HD2	2.10	0.51
1:G:189:GLU:HB2	1:G:284:THR:OG1	2.11	0.51
1:E:54:ASN:O	1:E:75:PHE:O	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:98:GLU:O	1:I:102:VAL:HG23	2.11	0.51
1:G:116:LEU:HD21	1:G:145:LEU:CD1	2.37	0.51
1:M:89:MET:CB	1:M:118:TYR:HB2	2.37	0.51
1:A:100:TYR:HA	1:A:135:LEU:HD11	1.91	0.51
1:A:158:TYR:CD1	1:A:318:LEU:HD12	2.46	0.51
1:A:245:ASP:N	1:A:249:LYS:O	2.39	0.51
1:G:368:VAL:HG12	1:G:368:VAL:O	2.10	0.51
1:I:54:ASN:O	1:I:75:PHE:O	2.29	0.51
1:E:375:ASN:OD1	1:E:377:VAL:HB	2.10	0.51
1:K:100:TYR:HB2	1:K:131:GLN:CD	2.32	0.51
1:K:431:ILE:CG2	1:K:432:ILE:N	2.74	0.51
1:A:110:SER:OG	1:A:142:ARG:NH2	2.43	0.51
1:I:192:MET:HE1	1:I:243:LEU:CD2	2.37	0.51
1:E:416:LYS:HA	1:E:426:THR:OG1	2.10	0.51
1:O:216:ILE:CG2	1:O:217:ASP:N	2.73	0.51
1:O:227:PHE:CE2	1:O:269:LEU:HD23	2.46	0.51
1:I:266:GLN:CB	1:K:264:LEU:HD22	2.41	0.51
1:G:102:VAL:CG1	1:G:106:ILE:HD11	2.41	0.51
1:K:19:ARG:HA	1:K:48:GLN:O	2.11	0.51
1:G:389:ALA:O	1:G:393:PHE:N	2.35	0.50
1:E:386:GLU:O	1:E:388:ILE:N	2.44	0.50
1:E:102:VAL:C	1:E:106:ILE:CD1	2.73	0.50
1:E:65:GLU:O	1:E:68:GLN:NE2	2.28	0.50
1:E:20:VAL:HA	1:E:89:MET:O	2.11	0.50
1:A:431:ILE:HG22	1:A:432:ILE:N	2.26	0.50
1:A:58:LYS:HA	1:O:252:LYS:O	2.10	0.50
1:A:304:LEU:HD23	1:A:322:PHE:CB	2.29	0.50
1:C:177:ILE:HA	1:C:296:ASP:O	2.11	0.50
1:O:130:GLN:O	1:O:131:GLN:C	2.47	0.50
1:C:52:LEU:CD1	1:C:63:THR:HG21	2.35	0.50
1:I:384:ILE:HG22	1:I:388:ILE:HD11	1.92	0.50
1:O:103:VAL:HA	1:O:106:ILE:HD12	1.94	0.50
1:E:206:ASN:OD1	1:E:206:ASN:O	2.29	0.50
1:I:146:GLN:OE1	1:I:414:PHE:HB3	2.10	0.50
1:A:176:SER:OG	1:A:177:ILE:N	2.44	0.50
1:G:123:TRP:CE3	1:G:124:ALA:HA	2.46	0.50
1:M:195:PRO:O	1:M:199:TYR:CD1	2.64	0.50
1:A:230:ILE:HG22	1:A:267:GLY:HA3	1.93	0.50
1:C:64:ILE:O	1:C:68:GLN:N	2.44	0.50
1:C:67:LEU:O	1:C:68:GLN:HB2	2.11	0.50
1:K:103:VAL:HA	1:K:106:ILE:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:196:GLU:O	1:O:199:TYR:N	2.44	0.50
1:M:174:ILE:HB	1:M:274:VAL:HG21	1.92	0.50
1:M:40:ILE:HG22	1:M:40:ILE:O	2.11	0.50
1:I:185:TRP:HZ3	1:I:186:TYR:OH	1.93	0.50
1:I:53:TYR:CD1	1:I:78:LEU:HD12	2.46	0.50
1:G:307:GLU:OE1	1:G:321:TYR:HE1	1.93	0.50
1:E:40:ILE:HG22	1:E:40:ILE:O	2.10	0.50
1:C:384:ILE:O	1:C:385:TYR:C	2.49	0.50
1:O:142:ARG:O	1:O:143:ALA:C	2.50	0.50
1:E:195:PRO:HB3	1:E:197:TYR:CD2	2.47	0.50
1:M:390:ASP:O	1:M:394:LEU:CB	2.38	0.50
1:G:293:LEU:HB2	1:G:311:GLY:HA2	1.94	0.50
1:O:52:LEU:C	1:O:81:PHE:CE1	2.85	0.50
1:G:182:ASN:HD21	1:G:283:GLY:HA2	1.76	0.50
1:I:102:VAL:O	1:I:106:ILE:HD12	2.12	0.50
1:C:162:ALA:HA	1:C:304:LEU:HD11	1.93	0.50
1:C:177:ILE:HB	1:C:276:VAL:HG22	1.92	0.50
1:C:25:LEU:HB3	1:C:52:LEU:CD1	2.42	0.50
1:C:53:TYR:N	1:C:81:PHE:CE1	2.79	0.50
1:K:77:SER:HB3	1:K:80:SER:OG	2.10	0.50
1:O:115:ASN:N	1:O:115:ASN:OD1	2.45	0.50
1:M:111:SER:N	1:M:142:ARG:HH22	2.10	0.50
1:M:83:GLN:O	1:M:84:TYR:C	2.49	0.50
1:E:273:LYS:H	1:E:273:LYS:HD3	1.74	0.50
1:C:181:GLY:O	1:C:281:LYS:N	2.44	0.50
1:E:100:TYR:HB2	1:E:131:GLN:CD	2.31	0.50
1:G:136:TYR:CB	1:G:431:ILE:HD13	2.39	0.50
1:K:253:GLU:HG2	1:O:61:LEU:HB3	1.91	0.50
1:G:244:LEU:HD23	1:G:250:ARG:CA	2.33	0.50
1:A:142:ARG:O	1:A:143:ALA:C	2.46	0.50
1:A:198:LEU:HB2	1:A:199:TYR:CE1	2.46	0.50
1:G:85:LYS:HB3	1:G:85:LYS:NZ	2.26	0.50
1:C:67:LEU:HD23	1:C:67:LEU:N	2.26	0.50
1:E:236:ASN:HA	1:E:261:ASP:OD1	2.11	0.50
1:A:185:TRP:CD1	2:B:857:TYR:HE1	2.29	0.50
1:K:22:PHE:N	1:K:51:ALA:O	2.28	0.50
1:E:319:VAL:HG12	1:E:320:LEU:N	2.25	0.50
1:I:270:GLU:OE1	1:I:456:MET:HE1	2.11	0.50
1:A:22:PHE:HB2	1:A:52:LEU:HD12	1.94	0.50
1:A:212:PHE:O	1:A:213:GLY:C	2.50	0.50
1:I:55:PRO:O	1:I:76:ASP:OD1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:208:ILE:HA	1:G:212:PHE:HB3	1.92	0.50
1:G:431:ILE:CG2	1:G:432:ILE:N	2.75	0.50
1:O:67:LEU:O	1:O:68:GLN:HB3	2.09	0.50
1:E:375:ASN:C	1:E:375:ASN:OD1	2.50	0.50
1:K:273:LYS:HD3	1:K:273:LYS:N	2.27	0.50
1:A:142:ARG:O	1:A:144:ASN:N	2.45	0.50
1:C:59:SER:O	1:C:63:THR:OG1	2.24	0.50
2:H:855:ASP:OD2	2:H:855:ASP:N	2.43	0.50
1:O:290:THR:CG2	1:O:291:LYS:N	2.75	0.50
1:A:96:VAL:HB	1:A:97:PRO:CD	2.40	0.50
1:O:77:SER:HB3	1:O:80:SER:H	1.76	0.50
1:K:62:GLN:O	1:K:63:THR:C	2.49	0.50
1:M:257:LYS:O	1:M:257:LYS:HG3	2.12	0.50
1:M:265:PHE:CD2	1:M:265:PHE:C	2.85	0.50
1:I:185:TRP:CD1	2:J:857:TYR:HE1	2.30	0.50
1:I:77:SER:O	1:I:80:SER:HB2	2.12	0.50
1:G:151:LEU:C	1:G:153:GLY:N	2.64	0.50
1:I:216:ILE:HG23	1:I:217:ASP:H	1.75	0.50
1:O:416:LYS:HB3	1:O:428:LYS:HG2	1.94	0.50
1:O:319:VAL:HG22	1:O:370:HIS:HB2	1.94	0.50
1:K:208:ILE:O	1:K:209:SER:C	2.50	0.50
1:K:263:LEU:O	1:K:263:LEU:HG	2.04	0.50
1:I:64:ILE:HG12	1:I:72:ALA:HB3	1.93	0.50
1:A:102:VAL:HG13	1:A:106:ILE:HD11	1.93	0.50
1:A:158:TYR:CG	1:A:318:LEU:HD12	2.47	0.50
1:C:57:LEU:O	1:C:58:LYS:C	2.50	0.50
1:I:200:ASP:C	1:I:200:ASP:OD1	2.50	0.50
1:I:161:ARG:O	1:I:161:ARG:HG3	2.11	0.50
1:A:216:ILE:CG2	1:A:217:ASP:N	2.75	0.50
1:E:102:VAL:O	1:E:106:ILE:HG13	2.12	0.50
1:E:118:TYR:CD1	1:E:118:TYR:N	2.80	0.50
1:G:237:ASN:H	1:G:261:ASP:CG	2.14	0.50
1:C:177:ILE:HG22	1:C:178:GLU:N	2.25	0.50
1:I:231:ASN:ND2	1:K:266:GLN:NE2	2.55	0.50
1:M:435:ARG:HD3	1:M:455:ILE:HG23	1.92	0.50
1:M:78:LEU:O	1:M:79:GLU:C	2.50	0.50
1:A:102:VAL:O	1:A:106:ILE:HD12	2.12	0.50
1:A:290:THR:CG2	1:A:291:LYS:N	2.74	0.50
2:P:852:THR:HG22	2:P:854:ASP:N	2.27	0.50
1:E:78:LEU:O	1:E:79:GLU:C	2.49	0.50
1:O:105:ASN:HA	1:O:108:GLU:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:852:THR:HG22	2:L:854:ASP:N	2.27	0.50
1:M:448:LYS:HB3	1:M:450:LEU:HD23	1.94	0.50
1:C:136:TYR:HB2	1:C:431:ILE:HD11	1.90	0.50
1:K:136:TYR:O	1:K:137:SER:C	2.50	0.50
1:E:115:ASN:N	1:E:115:ASN:OD1	2.44	0.50
1:G:19:ARG:CB	1:G:50:VAL:HG21	2.36	0.50
1:O:136:TYR:CB	1:O:431:ILE:HD13	2.36	0.50
1:K:215:THR:O	1:K:216:ILE:C	2.48	0.50
1:I:294:VAL:HG12	1:I:295:ILE:N	2.27	0.50
1:G:215:THR:O	1:G:216:ILE:C	2.50	0.49
1:G:217:ASP:HB2	1:G:433:LEU:HD13	1.94	0.49
1:K:431:ILE:HG23	1:K:435:ARG:CD	2.42	0.49
1:E:25:LEU:HD23	1:E:52:LEU:HD21	1.94	0.49
1:A:229:LYS:C	1:A:230:ILE:HG23	2.32	0.49
1:E:165:LEU:HD13	1:E:322:PHE:CD1	2.47	0.49
1:K:293:LEU:HB2	1:K:311:GLY:HA2	1.93	0.49
1:K:315:ILE:HG23	1:K:377:VAL:HG22	1.93	0.49
1:O:40:ILE:HG23	1:O:47:PHE:CB	2.43	0.49
1:O:272:GLY:O	1:O:273:LYS:HB2	2.12	0.49
1:C:31:TRP:CH2	1:C:35:THR:HG21	2.47	0.49
1:C:101:GLU:HA	1:C:101:GLU:OE1	2.12	0.49
1:C:100:TYR:CE1	1:C:135:LEU:HD21	2.46	0.49
1:G:148:ILE:HD13	1:G:388:ILE:CD1	2.42	0.49
1:I:386:GLU:O	1:I:389:ALA:HB3	2.11	0.49
1:E:218:VAL:C	1:E:222:ILE:HD12	2.32	0.49
1:G:126:ALA:HB1	1:G:131:GLN:OE1	2.11	0.49
1:I:136:TYR:HD1	1:I:139:SER:OG	1.95	0.49
1:O:433:LEU:O	1:O:436:LEU:HB3	2.11	0.49
1:O:142:ARG:CG	1:O:142:ARG:NH1	2.68	0.49
1:I:313:VAL:CG1	1:I:314:GLU:N	2.74	0.49
1:K:16:ARG:HB2	1:K:17:PRO:CD	2.42	0.49
1:A:179:ILE:CG2	1:A:180:SER:N	2.74	0.49
1:E:223:THR:OG1	1:E:224:GLY:N	2.45	0.49
1:O:123:TRP:CD1	1:O:214:HIS:CD2	3.00	0.49
1:G:263:LEU:HD12	1:G:264:LEU:N	2.28	0.49
1:M:197:TYR:CD1	1:M:198:LEU:HD13	2.47	0.49
1:G:68:GLN:NE2	1:G:68:GLN:HA	2.25	0.49
1:A:195:PRO:HB3	1:A:197:TYR:CE2	2.47	0.49
1:I:287:LYS:N	1:I:292:ASN:OD1	2.45	0.49
1:A:236:ASN:HA	1:A:261:ASP:OD1	2.12	0.49
1:K:32:VAL:HG13	1:K:36:HIS:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:443:SER:O	1:E:444:ASP:C	2.50	0.49
1:O:273:LYS:N	1:O:273:LYS:CD	2.74	0.49
1:K:422:GLU:OE1	1:K:422:GLU:N	2.42	0.49
1:I:84:TYR:C	1:I:86:ASP:H	2.15	0.49
1:G:128:SER:O	1:G:129:VAL:C	2.50	0.49
1:G:182:ASN:HA	1:G:281:LYS:O	2.11	0.49
1:E:382:LEU:C	1:E:384:ILE:H	2.15	0.49
1:O:245:ASP:O	1:O:247:ASN:N	2.45	0.49
1:E:64:ILE:HG22	1:E:65:GLU:N	2.26	0.49
1:E:84:TYR:CD1	1:E:86:ASP:HB2	2.48	0.49
1:I:103:VAL:N	1:I:106:ILE:HD12	2.27	0.49
1:I:142:ARG:CB	1:I:145:LEU:HB3	2.42	0.49
1:O:128:SER:O	1:O:129:VAL:C	2.50	0.49
1:G:96:VAL:HG12	1:G:127:ALA:HB2	1.93	0.49
1:M:435:ARG:HB3	1:M:455:ILE:HG23	1.93	0.49
1:I:304:LEU:HD22	1:I:320:LEU:HD11	1.95	0.49
1:O:223:THR:HG21	1:O:269:LEU:HD11	1.94	0.49
1:E:290:THR:HG22	1:E:291:LYS:N	2.28	0.49
1:A:83:GLN:O	1:A:84:TYR:C	2.50	0.49
1:K:142:ARG:HH11	1:K:142:ARG:HB3	1.78	0.49
1:O:182:ASN:HA	1:O:281:LYS:O	2.13	0.49
1:C:245:ASP:O	1:C:247:ASN:N	2.45	0.49
1:A:208:ILE:O	1:A:212:PHE:HB3	2.13	0.49
1:O:83:GLN:O	1:O:84:TYR:C	2.49	0.49
1:K:14:SER:OG	1:K:15:SER:N	2.42	0.49
1:K:236:ASN:HA	1:K:261:ASP:OD1	2.12	0.49
1:K:188:TYR:N	1:K:284:THR:O	2.46	0.49
1:M:245:ASP:OD1	1:M:245:ASP:O	2.30	0.49
1:E:138:ILE:O	1:E:139:SER:C	2.50	0.49
1:K:216:ILE:CG2	1:K:217:ASP:N	2.74	0.49
1:K:149:ILE:HG23	1:K:151:LEU:HD12	1.94	0.49
1:O:373:ASN:HD22	1:O:373:ASN:C	2.12	0.49
1:E:171:ILE:O	1:E:300:THR:N	2.46	0.49
1:A:453:SER:O	1:A:454:LYS:HD3	2.12	0.49
1:C:216:ILE:CG2	1:C:217:ASP:N	2.75	0.49
1:I:393:PHE:C	1:I:394:LEU:HD12	2.33	0.49
1:O:208:ILE:HG21	1:O:441:PHE:HE1	1.77	0.49
1:G:125:LEU:HD11	1:G:427:PHE:CG	2.48	0.49
1:I:134:GLU:O	1:I:135:LEU:C	2.49	0.49
1:G:50:VAL:HG12	1:G:84:TYR:HE2	1.75	0.49
1:M:438:ASP:O	1:M:441:PHE:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:96:VAL:HB	1:G:97:PRO:CD	2.40	0.49
1:M:273:LYS:N	1:M:273:LYS:CD	2.75	0.49
1:M:436:LEU:O	1:M:440:VAL:HG23	2.13	0.49
1:A:103:VAL:HA	1:A:106:ILE:HD12	1.93	0.49
1:O:161:ARG:O	1:O:165:LEU:HG	2.12	0.49
1:E:38:LEU:O	1:E:39:ALA:C	2.51	0.49
1:C:172:GLY:CA	1:C:301:LYS:HD3	2.42	0.49
1:G:146:GLN:NE2	1:G:146:GLN:HA	2.27	0.49
1:E:179:ILE:CG2	1:E:180:SER:N	2.75	0.49
1:C:431:ILE:CG2	1:C:432:ILE:N	2.73	0.49
1:O:212:PHE:HA	1:O:280:PHE:CE1	2.48	0.49
1:I:123:TRP:CD2	1:I:124:ALA:HA	2.47	0.49
1:A:64:ILE:O	1:A:68:GLN:N	2.45	0.49
1:M:149:ILE:CG2	1:M:151:LEU:HD12	2.42	0.49
2:H:852:THR:CG2	2:H:853:MET:N	2.75	0.49
1:K:25:LEU:HB3	1:K:52:LEU:CD2	2.41	0.49
1:M:262:HIS:CD2	1:M:263:LEU:N	2.81	0.49
1:O:159:ILE:O	1:O:160:VAL:C	2.50	0.49
1:O:169:GLY:O	1:O:328:GLY:HA3	2.13	0.49
1:M:287:LYS:HG2	1:M:290:THR:HB	1.94	0.49
1:K:171:ILE:O	1:K:300:THR:N	2.46	0.49
1:M:266:GLN:OE1	1:O:264:LEU:HD22	2.13	0.49
1:E:22:PHE:N	1:E:51:ALA:O	2.39	0.49
1:I:111:SER:HA	1:I:142:ARG:CZ	2.42	0.49
1:C:178:GLU:C	1:C:179:ILE:HG13	2.31	0.49
1:C:105:ASN:O	1:C:106:ILE:C	2.49	0.49
1:M:228:GLN:HB3	1:M:268:ILE:O	2.12	0.49
1:M:89:MET:HG3	1:M:89:MET:O	2.12	0.49
1:O:14:SER:OG	1:O:15:SER:N	2.41	0.49
1:O:156:SER:HB2	1:O:380:ASN:HD21	1.78	0.49
1:G:202:GLU:O	1:G:203:SER:C	2.50	0.49
1:G:214:HIS:ND1	1:G:314:GLU:CD	2.66	0.49
1:C:179:ILE:HB	1:C:278:CYS:CB	2.41	0.49
1:C:223:THR:OG1	1:C:224:GLY:N	2.46	0.49
1:E:136:TYR:HB2	1:E:431:ILE:HD13	1.94	0.49
1:K:53:TYR:CD2	1:K:54:ASN:N	2.81	0.49
1:A:287:LYS:N	1:A:292:ASN:OD1	2.41	0.49
1:A:218:VAL:HG13	1:A:222:ILE:CD1	2.43	0.49
1:C:208:ILE:O	1:C:209:SER:C	2.52	0.49
1:E:84:TYR:CE1	1:E:86:ASP:HB2	2.48	0.49
1:I:192:MET:HG2	1:I:244:LEU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:ASN:O	1:C:117:ARG:CG	2.59	0.49
1:M:22:PHE:N	1:M:51:ALA:O	2.33	0.49
1:G:163:LYS:HD3	1:G:421:PHE:CZ	2.48	0.49
1:G:102:VAL:C	1:G:106:ILE:HD12	2.33	0.49
1:I:319:VAL:HG22	1:I:370:HIS:HB2	1.94	0.49
1:A:210:ASN:OD1	1:A:211:SER:N	2.45	0.49
1:I:56:THR:OG1	1:I:59:SER:OG	2.31	0.48
1:G:212:PHE:O	1:G:213:GLY:C	2.51	0.48
1:G:322:PHE:CG	1:G:323:TYR:N	2.80	0.48
1:G:154:ARG:NH1	1:G:417:GLN:OE1	2.34	0.48
1:K:249:LYS:HE2	1:K:250:ARG:O	2.13	0.48
1:O:57:LEU:HD22	1:O:61:LEU:HD11	1.87	0.48
1:E:54:ASN:HB3	1:E:55:PRO:HD2	1.94	0.48
1:C:322:PHE:CG	1:C:323:TYR:N	2.79	0.48
1:G:115:ASN:N	1:G:115:ASN:OD1	2.43	0.48
1:C:25:LEU:HB3	1:C:52:LEU:HD13	1.94	0.48
1:M:325:ILE:HG13	1:M:325:ILE:O	2.12	0.48
1:A:281:LYS:CD	1:C:298:HIS:NE2	2.75	0.48
1:E:33:ALA:O	1:E:37:PHE:HB3	2.12	0.48
1:O:372:ARG:O	1:O:373:ASN:C	2.51	0.48
1:E:179:ILE:HG22	1:E:180:SER:N	2.26	0.48
1:A:152:GLN:O	1:A:153:GLY:C	2.52	0.48
1:C:150:CYS:O	1:C:152:GLN:NE2	2.47	0.48
1:G:432:ILE:O	1:G:455:ILE:HD12	2.13	0.48
1:A:458:LEU:CG	1:A:459:GLU:H	2.00	0.48
1:G:53:TYR:HB2	1:G:81:PHE:CD1	2.48	0.48
1:A:263:LEU:HD11	1:A:265:PHE:HB2	1.95	0.48
1:A:449:THR:HG21	1:C:233:MET:HE2	1.95	0.48
1:E:237:ASN:H	1:E:261:ASP:CG	2.15	0.48
1:I:187:GLY:HA3	1:I:284:THR:N	2.22	0.48
1:E:56:THR:OG1	1:E:56:THR:O	2.30	0.48
1:I:263:LEU:HG	1:I:263:LEU:O	2.11	0.48
1:C:123:TRP:CE3	1:C:123:TRP:HA	2.48	0.48
1:C:136:TYR:HD1	1:C:139:SER:OG	1.96	0.48
1:I:118:TYR:CD1	1:I:118:TYR:N	2.81	0.48
1:A:431:ILE:O	1:A:435:ARG:HB2	2.13	0.48
1:G:90:ILE:O	1:G:90:ILE:HG22	2.10	0.48
1:M:100:TYR:CD1	1:M:135:LEU:HD21	2.48	0.48
1:M:134:GLU:O	1:M:135:LEU:C	2.51	0.48
1:O:432:ILE:HG23	1:O:455:ILE:HD12	1.91	0.48
1:G:110:SER:O	1:G:113:ASN:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ASN:H	1:A:105:ASN:HD22	1.59	0.48
1:E:290:THR:CG2	1:E:291:LYS:N	2.76	0.48
1:G:251:THR:C	1:G:253:GLU:H	2.15	0.48
1:M:148:ILE:HD13	1:M:388:ILE:HD13	1.94	0.48
1:C:268:ILE:CG2	1:C:273:LYS:HA	2.43	0.48
1:C:284:THR:HA	1:C:285:PRO:C	2.32	0.48
1:C:133:GLU:HA	1:C:133:GLU:OE1	2.13	0.48
1:E:20:VAL:HG21	1:E:40:ILE:CD1	2.43	0.48
1:A:145:LEU:O	1:A:413:LYS:HD2	2.06	0.48
1:M:129:VAL:CG1	1:M:130:GLN:H	2.24	0.48
1:G:60:SER:O	1:G:63:THR:HB	2.12	0.48
1:E:214:HIS:CG	1:E:314:GLU:HG2	2.48	0.48
1:O:138:ILE:O	1:O:139:SER:C	2.51	0.48
1:C:105:ASN:HB3	1:C:109:HIS:CE1	2.48	0.48
1:C:118:TYR:OH	1:C:392:HIS:ND1	2.24	0.48
1:M:185:TRP:CD1	2:N:857:TYR:HE1	2.32	0.48
1:A:377:VAL:HG11	2:B:859:TYR:CD2	2.48	0.48
1:K:53:TYR:CD2	1:K:53:TYR:C	2.86	0.48
1:G:55:PRO:O	1:G:76:ASP:OD1	2.31	0.48
1:G:77:SER:HB3	1:G:80:SER:H	1.78	0.48
1:G:179:ILE:HG22	1:G:180:SER:N	2.28	0.48
1:O:23:VAL:HG12	1:O:94:VAL:CG1	2.44	0.48
1:E:389:ALA:O	1:E:393:PHE:N	2.45	0.48
1:O:248:GLY:O	1:O:249:LYS:C	2.46	0.48
1:K:129:VAL:O	1:K:132:ALA:N	2.46	0.48
1:A:324:GLY:O	1:A:365:THR:N	2.32	0.48
1:K:115:ASN:O	1:K:117:ARG:N	2.47	0.48
1:O:133:GLU:O	1:O:136:TYR:HB3	2.13	0.48
1:M:78:LEU:O	1:M:82:ALA:N	2.42	0.48
1:A:30:SER:HG	1:A:33:ALA:HB2	1.79	0.48
1:I:309:ASP:OD1	1:I:309:ASP:N	2.45	0.48
1:M:244:LEU:O	1:M:245:ASP:C	2.51	0.48
1:K:452:VAL:HG12	1:K:452:VAL:O	2.13	0.48
1:E:25:LEU:HB3	1:E:52:LEU:HG	1.94	0.48
1:G:53:TYR:CD2	1:G:54:ASN:N	2.82	0.48
1:G:84:TYR:CD1	1:G:86:ASP:HB2	2.49	0.48
1:G:113:ASN:O	1:G:114:LEU:CD2	2.61	0.48
1:K:89:MET:HG3	1:K:89:MET:O	2.13	0.48
1:K:179:ILE:CG2	1:K:180:SER:N	2.76	0.48
1:M:78:LEU:O	1:M:81:PHE:HB3	2.13	0.48
1:K:182:ASN:ND2	1:K:283:GLY:CA	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:18:ILE:HD11	1:O:392:HIS:CD2	2.48	0.48
1:A:104:LYS:O	1:A:107:LEU:HB2	2.14	0.48
1:C:61:LEU:CD1	1:C:61:LEU:H	2.27	0.48
1:G:232:ALA:O	1:G:444:ASP:HA	2.13	0.48
1:K:230:ILE:HA	1:K:267:GLY:HA2	1.96	0.48
1:M:113:ASN:OD1	1:M:114:LEU:N	2.47	0.48
1:O:263:LEU:HD12	1:O:264:LEU:N	2.28	0.48
1:A:388:ILE:HG22	1:A:389:ALA:N	2.29	0.48
1:G:62:GLN:O	1:G:65:GLU:N	2.47	0.48
1:O:436:LEU:O	1:O:440:VAL:HG23	2.12	0.48
1:A:79:GLU:HG2	1:A:109:HIS:ND1	2.29	0.48
1:K:77:SER:O	1:K:80:SER:HB2	2.13	0.48
1:O:295:ILE:HD12	1:O:306:ILE:HB	1.96	0.48
1:A:84:TYR:C	1:A:86:ASP:H	2.17	0.48
1:M:201:ILE:HB	1:M:258:THR:CB	2.43	0.48
1:A:428:LYS:O	1:A:429:ASP:C	2.49	0.48
1:E:417:GLN:HB2	1:E:424:PHE:O	2.13	0.48
1:M:174:ILE:HG22	1:M:175:ASN:N	2.29	0.48
1:M:155:LYS:HB3	1:M:383:ARG:HB3	1.95	0.48
1:M:206:ASN:OD1	1:M:206:ASN:C	2.51	0.48
1:I:209:SER:OG	1:I:210:ASN:N	2.43	0.48
1:C:22:PHE:CE2	1:C:91:VAL:HB	2.48	0.48
2:B:853:MET:O	2:B:856:VAL:HB	2.13	0.48
1:M:263:LEU:HD12	1:M:264:LEU:O	2.13	0.48
1:G:16:ARG:O	1:G:17:PRO:O	2.32	0.48
1:G:31:TRP:CH2	1:G:35:THR:HG21	2.49	0.48
1:K:141:GLN:N	1:K:141:GLN:OE1	2.47	0.48
1:C:133:GLU:O	1:C:136:TYR:HB3	2.13	0.48
1:C:433:LEU:O	1:C:436:LEU:HB3	2.13	0.48
1:C:436:LEU:O	1:C:439:ALA:HB3	2.13	0.48
1:E:233:MET:CE	1:G:231:ASN:CB	2.92	0.48
1:O:384:ILE:HG23	1:O:384:ILE:HD12	1.48	0.48
1:A:229:LYS:O	1:A:230:ILE:HG23	2.13	0.48
1:I:201:ILE:HB	1:I:258:THR:CG2	2.42	0.48
1:I:177:ILE:HG22	1:I:178:GLU:N	2.29	0.48
1:G:197:TYR:HA	1:G:200:ASP:HB3	1.95	0.48
1:C:245:ASP:O	1:C:246:GLU:C	2.52	0.48
1:E:372:ARG:O	1:E:373:ASN:ND2	2.47	0.48
1:E:194:SER:CB	1:E:199:TYR:HH	1.96	0.48
1:O:208:ILE:O	1:O:212:PHE:HB3	2.13	0.48
1:M:392:HIS:CD2	1:M:393:PHE:CD2	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:449:THR:O	1:E:449:THR:HG22	2.14	0.48
1:G:219:LEU:HG	1:G:219:LEU:O	2.14	0.48
1:G:231:ASN:HB2	1:G:449:THR:OG1	2.14	0.48
1:O:84:TYR:CE1	1:O:86:ASP:CB	2.91	0.48
1:A:265:PHE:C	1:C:266:GLN:HE22	2.17	0.48
1:K:105:ASN:O	1:K:106:ILE:C	2.52	0.48
1:I:294:VAL:CG1	1:I:295:ILE:N	2.77	0.48
1:M:188:TYR:HB2	1:M:284:THR:O	2.14	0.48
1:O:213:GLY:O	1:O:216:ILE:HG22	2.13	0.48
1:M:236:ASN:OD1	1:M:260:PRO:HA	2.13	0.48
1:G:151:LEU:O	1:G:153:GLY:N	2.47	0.47
1:O:52:LEU:C	1:O:81:PHE:HE1	2.16	0.47
1:E:117:ARG:HB3	1:E:118:TYR:CE1	2.49	0.47
1:E:121:VAL:HG12	1:E:122:GLU:N	2.29	0.47
1:I:216:ILE:CG2	1:I:217:ASP:N	2.77	0.47
1:A:94:VAL:O	1:A:95:LYS:C	2.50	0.47
1:G:96:VAL:N	1:G:97:PRO:CD	2.77	0.47
1:A:312:PHE:CB	1:A:315:ILE:HD12	2.39	0.47
1:A:154:ARG:NH1	1:A:417:GLN:OE1	2.39	0.47
1:A:216:ILE:HD12	1:A:219:LEU:HD23	1.96	0.47
1:C:152:GLN:NE2	1:C:214:HIS:HE1	2.12	0.47
1:A:447:GLU:HG3	1:C:449:THR:HG21	1.96	0.47
1:G:384:ILE:O	1:G:385:TYR:C	2.51	0.47
1:G:208:ILE:HG12	1:G:263:LEU:HD22	1.96	0.47
1:E:298:HIS:NE2	1:G:281:LYS:NZ	2.62	0.47
1:E:382:LEU:O	1:E:384:ILE:N	2.47	0.47
1:A:147:THR:HB	1:A:427:PHE:CE1	2.48	0.47
1:A:228:GLN:NE2	1:A:273:LYS:HE3	2.28	0.47
1:I:105:ASN:HA	1:I:108:GLU:HG3	1.96	0.47
1:A:231:ASN:ND2	1:C:266:GLN:OE1	2.44	0.47
1:C:266:GLN:HA	1:C:276:VAL:O	2.15	0.47
1:K:150:CYS:O	1:K:152:GLN:NE2	2.47	0.47
1:O:389:ALA:O	1:O:392:HIS:HB3	2.14	0.47
1:K:290:THR:CG2	1:K:291:LYS:N	2.77	0.47
1:M:179:ILE:HB	1:M:278:CYS:HB2	1.97	0.47
1:K:323:TYR:CZ	1:K:364:GLN:HB2	2.49	0.47
1:A:425:PRO:HA	1:A:429:ASP:OD2	2.15	0.47
1:O:251:THR:C	1:O:253:GLU:H	2.18	0.47
1:E:224:GLY:HA2	1:E:419:PHE:CD2	2.49	0.47
1:E:185:TRP:CD1	1:E:185:TRP:N	2.75	0.47
1:O:422:GLU:H	1:O:422:GLU:CD	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:251:THR:C	1:K:253:GLU:H	2.16	0.47
1:A:229:LYS:HE3	1:C:233:MET:HE2	1.96	0.47
1:G:67:LEU:O	1:G:68:GLN:HB2	2.14	0.47
1:M:81:PHE:O	1:M:83:GLN:N	2.47	0.47
1:K:147:THR:O	1:K:426:THR:HG22	2.15	0.47
1:I:287:LYS:CB	1:I:287:LYS:NZ	2.77	0.47
1:M:219:LEU:O	1:M:220:GLN:C	2.50	0.47
1:E:30:SER:O	1:E:33:ALA:N	2.46	0.47
1:A:276:VAL:O	1:C:264:LEU:HD21	2.15	0.47
1:I:78:LEU:O	1:I:82:ALA:N	2.40	0.47
1:E:208:ILE:HB	1:E:209:SER:H	1.56	0.47
1:E:263:LEU:HD12	1:E:263:LEU:C	2.34	0.47
1:G:293:LEU:O	1:G:307:GLU:HA	2.14	0.47
1:E:20:VAL:HG21	1:E:40:ILE:HD13	1.97	0.47
1:A:147:THR:C	1:A:148:ILE:HG13	2.33	0.47
1:K:88:ASP:OD1	1:K:115:ASN:HB2	2.15	0.47
1:C:118:TYR:N	1:C:118:TYR:CD1	2.83	0.47
1:C:56:THR:OG1	1:C:59:SER:OG	2.29	0.47
1:K:78:LEU:O	1:K:82:ALA:N	2.40	0.47
1:A:294:VAL:HG22	1:A:307:GLU:HG2	1.96	0.47
1:M:179:ILE:CG2	1:M:180:SER:N	2.77	0.47
1:M:287:LYS:N	1:M:292:ASN:OD1	2.46	0.47
1:M:32:VAL:CG1	1:M:36:HIS:HB2	2.45	0.47
1:E:234:ILE:HG12	1:E:263:LEU:HB2	1.95	0.47
1:C:161:ARG:NH2	1:C:367:GLU:OE1	2.47	0.47
1:O:100:TYR:CE1	1:O:135:LEU:HD21	2.48	0.47
1:C:77:SER:CB	1:C:80:SER:HB2	2.35	0.47
1:E:136:TYR:HD1	1:E:139:SER:OG	1.98	0.47
1:E:136:TYR:CB	1:E:431:ILE:HD11	2.38	0.47
1:K:208:ILE:CG2	1:K:209:SER:N	2.75	0.47
1:A:375:ASN:OD1	1:A:377:VAL:HB	2.14	0.47
1:K:376:SER:OG	1:K:377:VAL:N	2.47	0.47
1:I:379:GLY:O	1:I:382:LEU:HB3	2.14	0.47
1:M:63:THR:O	1:M:67:LEU:HG	2.14	0.47
1:A:22:PHE:N	1:A:51:ALA:O	2.42	0.47
1:M:287:LYS:NZ	1:M:287:LYS:CB	2.77	0.47
1:G:100:TYR:HB2	1:G:131:GLN:CD	2.35	0.47
1:G:177:ILE:O	1:G:178:GLU:CG	2.63	0.47
1:G:149:ILE:HD13	1:G:430:ALA:CB	2.45	0.47
1:A:133:GLU:O	1:A:136:TYR:HB3	2.14	0.47
1:I:136:TYR:O	1:I:137:SER:C	2.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:133:GLU:O	1:M:136:TYR:HB3	2.14	0.47
1:M:136:TYR:HD1	1:M:139:SER:OG	1.98	0.47
1:G:315:ILE:HG22	1:G:315:ILE:O	2.13	0.47
1:C:16:ARG:O	1:C:17:PRO:C	2.53	0.47
1:E:417:GLN:HB2	1:E:424:PHE:C	2.35	0.47
1:M:96:VAL:N	1:M:97:PRO:CD	2.77	0.47
1:O:313:VAL:CG1	1:O:314:GLU:N	2.77	0.47
1:O:78:LEU:O	1:O:82:ALA:N	2.42	0.47
1:I:179:ILE:CG2	1:I:180:SER:N	2.77	0.47
1:A:177:ILE:HG22	1:A:276:VAL:HG13	1.96	0.47
1:O:211:SER:O	1:O:214:HIS:HB2	2.14	0.47
1:E:387:SER:O	1:E:390:ASP:HB2	2.15	0.47
1:K:129:VAL:HA	1:K:434:HIS:HD2	1.80	0.47
1:E:88:ASP:O	1:E:116:LEU:HA	2.14	0.47
1:E:75:PHE:N	1:E:75:PHE:CD1	2.83	0.47
1:A:228:GLN:HB3	1:A:268:ILE:O	2.13	0.47
1:A:432:ILE:HD13	1:A:456:MET:HA	1.96	0.47
1:I:104:LYS:O	1:I:107:LEU:HB2	2.15	0.47
1:C:95:LYS:HB3	1:C:97:PRO:HD2	1.96	0.47
1:A:65:GLU:CG	1:A:66:GLN:H	2.24	0.47
1:G:21:GLY:HA3	1:G:87:ILE:CD1	2.45	0.47
1:A:263:LEU:HD12	1:A:263:LEU:C	2.35	0.47
1:C:276:VAL:HG12	1:C:277:SER:N	2.29	0.47
1:C:389:ALA:O	1:C:392:HIS:HB3	2.15	0.47
1:E:124:ALA:O	1:E:125:LEU:C	2.51	0.47
1:E:182:ASN:ND2	1:E:283:GLY:HA2	2.30	0.47
1:A:96:VAL:N	1:A:97:PRO:CD	2.77	0.47
1:M:30:SER:OG	1:M:33:ALA:HB2	2.15	0.47
1:I:245:ASP:O	1:I:248:GLY:N	2.26	0.47
1:E:192:MET:CE	1:E:243:LEU:HD22	2.45	0.47
1:M:251:THR:C	1:M:253:GLU:H	2.18	0.47
1:I:319:VAL:HG22	1:I:370:HIS:HD1	1.80	0.47
1:C:195:PRO:HB3	1:C:197:TYR:CE2	2.49	0.47
1:I:129:VAL:O	1:I:132:ALA:N	2.48	0.47
1:I:129:VAL:HA	1:I:434:HIS:HD2	1.80	0.47
1:C:188:TYR:O	1:C:242:PHE:HB2	2.15	0.47
1:O:172:GLY:CA	1:O:301:LYS:HD2	2.44	0.47
1:M:110:SER:O	1:M:113:ASN:N	2.47	0.47
1:M:236:ASN:HA	1:M:261:ASP:OD1	2.15	0.47
1:E:422:GLU:N	1:E:422:GLU:OE1	2.48	0.47
1:I:16:ARG:HB2	1:I:17:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:146:GLN:NE2	1:K:146:GLN:HA	2.29	0.47
1:C:104:LYS:O	1:C:107:LEU:HB2	2.15	0.47
1:I:185:TRP:HD1	2:J:857:TYR:HE1	1.62	0.47
1:G:386:GLU:O	1:G:388:ILE:N	2.48	0.47
1:G:136:TYR:O	1:G:137:SER:C	2.53	0.47
1:G:22:PHE:N	1:G:51:ALA:O	2.34	0.47
1:G:53:TYR:CG	1:G:54:ASN:N	2.82	0.47
1:A:42:GLN:C	1:A:43:LEU:HD23	2.31	0.47
1:C:120:TYR:O	1:C:121:VAL:HG23	2.14	0.47
1:O:171:ILE:CD1	1:O:299:GLY:HA3	2.37	0.47
1:O:171:ILE:HB	1:O:299:GLY:HA3	1.97	0.47
1:I:320:LEU:HB3	1:I:369:PHE:HB3	1.96	0.47
2:D:853:MET:HA	2:D:856:VAL:CG2	2.44	0.47
1:A:103:VAL:CA	1:A:106:ILE:HD12	2.44	0.47
1:O:75:PHE:CD1	1:O:75:PHE:N	2.83	0.47
1:O:187:GLY:HA3	1:O:284:THR:N	2.25	0.47
1:I:166:ILE:O	1:I:167:SER:C	2.52	0.47
1:C:187:GLY:HA3	1:C:284:THR:N	2.30	0.47
1:K:422:GLU:CD	1:K:422:GLU:H	2.17	0.47
1:A:31:TRP:HD1	1:A:32:VAL:HG22	1.80	0.47
1:M:277:SER:O	1:M:277:SER:OG	2.31	0.47
1:G:123:TRP:HA	1:G:123:TRP:CE3	2.49	0.47
1:A:134:GLU:O	1:A:137:SER:OG	2.29	0.47
1:C:238:ILE:O	1:C:257:LYS:NZ	2.42	0.47
1:A:372:ARG:O	1:A:373:ASN:C	2.52	0.47
1:O:188:TYR:CE1	1:O:238:ILE:HD11	2.50	0.47
1:I:18:ILE:HD12	1:I:18:ILE:HG21	1.71	0.47
1:C:372:ARG:O	1:C:373:ASN:C	2.53	0.47
1:E:453:SER:HA	1:E:456:MET:CE	2.44	0.47
1:C:134:GLU:HG2	1:C:138:ILE:HD11	1.96	0.47
1:I:53:TYR:CE1	1:I:78:LEU:HD12	2.50	0.47
1:G:177:ILE:CG2	1:G:276:VAL:HG13	2.45	0.47
1:M:100:TYR:HD1	1:M:135:LEU:HD21	1.80	0.47
1:C:368:VAL:HG12	1:C:368:VAL:O	2.15	0.47
1:K:88:ASP:O	1:K:116:LEU:HA	2.15	0.47
1:K:381:ILE:O	1:K:384:ILE:N	2.48	0.47
1:O:129:VAL:O	1:O:132:ALA:HB3	2.15	0.47
1:E:151:LEU:HD12	1:E:151:LEU:N	2.29	0.47
1:K:96:VAL:N	1:K:97:PRO:HD2	2.30	0.47
1:G:195:PRO:HB3	1:G:197:TYR:CD2	2.50	0.47
1:A:277:SER:O	1:A:277:SER:OG	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:ILE:CG2	1:C:217:ASP:H	2.29	0.46
1:A:228:GLN:HE22	1:A:273:LYS:HE2	1.80	0.46
1:A:165:LEU:HD12	1:A:304:LEU:HD21	1.96	0.46
1:C:180:SER:HA	1:C:279:SER:O	2.15	0.46
1:C:321:TYR:HD2	1:C:368:VAL:HG22	1.79	0.46
1:I:207:LEU:O	1:I:208:ILE:C	2.53	0.46
1:O:431:ILE:HG23	1:O:435:ARG:HD2	1.97	0.46
1:E:132:ALA:O	1:E:133:GLU:C	2.52	0.46
1:M:185:TRP:HD1	2:N:857:TYR:CE1	2.33	0.46
1:E:281:LYS:CE	1:G:298:HIS:HD2	2.28	0.46
2:D:853:MET:O	2:D:856:VAL:HB	2.15	0.46
1:C:182:ASN:HA	1:C:281:LYS:O	2.14	0.46
1:M:231:ASN:O	1:M:231:ASN:OD1	2.33	0.46
1:C:291:LYS:HD2	1:C:291:LYS:HA	1.52	0.46
1:M:67:LEU:O	1:M:68:GLN:HB2	2.14	0.46
1:E:26:THR:HG22	1:E:27:SER:OG	2.14	0.46
1:K:313:VAL:CG1	1:K:314:GLU:H	2.28	0.46
1:A:223:THR:OG1	1:A:224:GLY:N	2.47	0.46
1:G:416:LYS:HG3	1:G:417:GLN:N	2.28	0.46
1:G:434:HIS:CA	1:G:437:ILE:HD12	2.45	0.46
1:I:88:ASP:OD1	1:I:115:ASN:HB3	2.16	0.46
1:A:68:GLN:NE2	1:A:68:GLN:HA	2.30	0.46
1:M:190:ARG:HD2	1:M:199:TYR:CE2	2.51	0.46
1:A:230:ILE:HA	1:A:267:GLY:HA2	1.97	0.46
1:C:84:TYR:HB3	1:C:87:ILE:HD12	1.97	0.46
1:E:426:THR:O	1:E:429:ASP:N	2.49	0.46
1:O:115:ASN:O	1:O:117:ARG:HB2	2.15	0.46
1:K:152:GLN:O	1:K:153:GLY:C	2.54	0.46
1:G:269:LEU:HB2	1:G:274:VAL:O	2.15	0.46
1:O:179:ILE:CG2	1:O:180:SER:N	2.78	0.46
1:O:218:VAL:O	1:O:221:TYR:HB3	2.15	0.46
1:I:187:GLY:O	1:I:238:ILE:HD13	2.15	0.46
1:A:293:LEU:HB2	1:A:311:GLY:HA2	1.96	0.46
1:I:178:GLU:HB2	1:I:296:ASP:HB3	1.96	0.46
1:O:232:ALA:O	1:O:444:ASP:HA	2.14	0.46
1:C:201:ILE:HB	1:C:258:THR:CG2	2.45	0.46
1:C:128:SER:OG	1:C:130:GLN:NE2	2.49	0.46
1:C:234:ILE:HG12	1:C:263:LEU:HB2	1.97	0.46
1:G:212:PHE:CD1	1:G:280:PHE:CD1	3.03	0.46
1:G:434:HIS:HA	1:G:437:ILE:HD12	1.97	0.46
1:A:458:LEU:HD12	1:A:458:LEU:HA	1.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLN:HB2	1:A:382:LEU:HD11	1.97	0.46
1:C:158:TYR:CB	1:C:318:LEU:HD12	2.45	0.46
1:C:88:ASP:O	1:C:116:LEU:HA	2.15	0.46
1:M:312:PHE:HA	1:M:314:GLU:OE2	2.15	0.46
1:A:392:HIS:C	1:A:394:LEU:H	2.18	0.46
1:C:125:LEU:HD11	1:C:427:PHE:CE2	2.50	0.46
1:A:185:TRP:HD1	2:B:857:TYR:CE1	2.32	0.46
1:K:53:TYR:CG	1:K:54:ASN:N	2.83	0.46
1:O:20:VAL:HG23	1:O:48:GLN:O	2.15	0.46
1:O:315:ILE:HG23	1:O:377:VAL:HG22	1.96	0.46
2:L:853:MET:O	2:L:854:ASP:C	2.50	0.46
1:E:230:ILE:HA	1:E:267:GLY:HA2	1.97	0.46
1:K:374:TYR:OH	1:K:380:ASN:OD1	2.17	0.46
1:A:166:ILE:HG22	1:A:167:SER:N	2.30	0.46
1:O:368:VAL:O	1:O:368:VAL:HG12	2.16	0.46
1:E:208:ILE:O	1:E:213:GLY:N	2.34	0.46
1:G:129:VAL:HG13	1:G:130:GLN:N	2.28	0.46
1:E:91:VAL:HG13	1:E:120:TYR:HB3	1.97	0.46
1:C:94:VAL:O	1:C:95:LYS:C	2.54	0.46
1:M:121:VAL:HG21	1:M:427:PHE:CZ	2.50	0.46
1:C:294:VAL:HG22	1:C:307:GLU:HG2	1.96	0.46
1:G:121:VAL:CG1	1:G:122:GLU:N	2.78	0.46
1:C:62:GLN:O	1:C:65:GLU:N	2.48	0.46
1:E:304:LEU:HD23	1:E:322:PHE:CB	2.38	0.46
1:A:118:TYR:CD1	1:A:118:TYR:N	2.84	0.46
1:K:208:ILE:HA	1:K:212:PHE:HB3	1.97	0.46
1:A:184:GLY:HA2	2:B:853:MET:HE3	1.98	0.46
1:I:294:VAL:HA	1:I:306:ILE:O	2.14	0.46
1:I:26:THR:HB	1:I:30:SER:HB2	1.98	0.46
1:O:146:GLN:OE1	1:O:414:PHE:N	2.40	0.46
2:L:852:THR:CG2	2:L:853:MET:N	2.78	0.46
1:M:290:THR:CG2	1:M:291:LYS:N	2.78	0.46
1:E:289:LEU:HD12	1:G:303:ASP:HB3	1.96	0.46
1:A:309:ASP:OD2	2:B:850:THR:OG1	2.31	0.46
1:O:244:LEU:HA	1:O:244:LEU:HD12	1.43	0.46
1:K:136:TYR:HD1	1:K:139:SER:OG	1.98	0.46
1:E:53:TYR:O	1:E:54:ASN:ND2	2.49	0.46
1:M:190:ARG:HA	1:M:191:PRO:HD3	1.63	0.46
1:O:100:TYR:CG	1:O:131:GLN:HG2	2.51	0.46
1:C:105:ASN:HA	1:C:108:GLU:HG3	1.98	0.46
1:C:22:PHE:N	1:C:51:ALA:O	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:PHE:HB3	1:C:315:ILE:CD1	2.35	0.46
1:C:125:LEU:HD11	1:C:427:PHE:CD2	2.50	0.46
1:M:54:ASN:HB3	1:M:55:PRO:HD2	1.96	0.46
1:K:22:PHE:O	1:K:53:TYR:N	2.36	0.46
1:O:95:LYS:HE2	1:O:197:TYR:CE2	2.51	0.46
1:K:156:SER:O	1:K:158:TYR:N	2.48	0.46
1:G:198:LEU:HD12	1:G:198:LEU:HA	1.56	0.46
1:E:79:GLU:O	1:E:80:SER:C	2.53	0.46
1:I:14:SER:O	1:I:16:ARG:N	2.45	0.46
1:O:184:GLY:N	1:O:282:GLY:O	2.48	0.46
1:A:123:TRP:HA	1:A:123:TRP:CE3	2.50	0.46
1:C:134:GLU:O	1:C:138:ILE:HG13	2.16	0.46
1:C:313:VAL:CG1	1:C:314:GLU:N	2.79	0.46
1:G:152:GLN:H	1:G:152:GLN:NE2	2.13	0.46
1:G:123:TRP:CD1	1:G:214:HIS:NE2	2.82	0.46
1:A:36:HIS:O	1:A:38:LEU:N	2.48	0.46
1:M:431:ILE:CG2	1:M:432:ILE:N	2.79	0.46
1:C:179:ILE:CG2	1:C:180:SER:N	2.78	0.46
1:A:23:VAL:HG12	1:A:94:VAL:CG1	2.45	0.46
1:O:431:ILE:CG2	1:O:432:ILE:N	2.77	0.46
2:H:855:ASP:O	2:H:856:VAL:C	2.53	0.46
1:K:81:PHE:O	1:K:83:GLN:N	2.49	0.46
1:I:188:TYR:HB2	1:I:284:THR:O	2.16	0.46
1:A:40:ILE:HD13	1:A:40:ILE:HG21	1.63	0.46
1:A:40:ILE:HG22	1:A:40:ILE:O	2.15	0.46
1:M:201:ILE:HB	1:M:258:THR:CG2	2.46	0.46
1:E:78:LEU:O	1:E:81:PHE:CB	2.63	0.46
1:M:14:SER:O	1:M:16:ARG:N	2.45	0.46
2:L:855:ASP:O	2:L:856:VAL:C	2.53	0.46
1:A:163:LYS:HE3	1:A:421:PHE:CE1	2.51	0.46
1:A:57:LEU:HD21	1:A:74:GLY:O	2.14	0.46
1:C:146:GLN:HA	1:C:146:GLN:NE2	2.30	0.46
1:C:136:TYR:O	1:C:137:SER:C	2.54	0.46
1:C:437:ILE:O	1:C:438:ASP:C	2.54	0.46
1:I:51:ALA:HB1	1:I:75:PHE:CE1	2.51	0.46
1:G:136:TYR:HD1	1:G:139:SER:OG	1.99	0.46
1:G:151:LEU:C	1:G:153:GLY:H	2.19	0.46
1:A:458:LEU:CG	1:A:459:GLU:N	2.63	0.46
1:A:65:GLU:O	1:A:66:GLN:C	2.53	0.46
1:G:79:GLU:HG2	1:G:109:HIS:CD2	2.50	0.46
1:C:304:LEU:HD21	1:C:322:PHE:HB2	1.90	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:ILE:O	1:E:257:LYS:CE	2.63	0.46
1:M:78:LEU:O	1:M:81:PHE:N	2.49	0.46
1:K:147:THR:C	1:K:148:ILE:HG13	2.36	0.46
1:A:102:VAL:CG1	1:A:106:ILE:CD1	2.92	0.46
1:E:100:TYR:HB2	1:E:131:GLN:OE1	2.16	0.46
1:K:185:TRP:HD1	2:L:857:TYR:CE1	2.33	0.46
1:I:77:SER:HB3	1:I:80:SER:H	1.80	0.46
1:G:168:GLU:O	1:G:169:GLY:C	2.54	0.46
1:O:57:LEU:O	1:O:60:SER:N	2.48	0.46
1:I:252:LYS:CD	1:I:252:LYS:N	2.59	0.46
1:K:136:TYR:CB	1:K:431:ILE:HD13	2.43	0.46
1:A:147:THR:HG21	1:A:427:PHE:CD2	2.51	0.46
1:I:134:GLU:HA	1:I:137:SER:HG	1.81	0.46
1:O:384:ILE:O	1:O:385:TYR:C	2.54	0.46
1:E:165:LEU:HA	1:E:165:LEU:HD23	1.44	0.46
1:O:142:ARG:HG3	1:O:142:ARG:NH1	2.31	0.46
1:M:118:TYR:CD1	1:M:118:TYR:N	2.83	0.46
1:A:185:TRP:HD1	2:B:857:TYR:HE1	1.64	0.46
1:A:184:GLY:HA2	2:B:853:MET:CE	2.45	0.46
1:K:105:ASN:HA	1:K:108:GLU:HG3	1.97	0.46
1:K:427:PHE:O	1:K:428:LYS:C	2.51	0.46
1:O:238:ILE:H	1:O:261:ASP:CG	2.20	0.46
1:O:443:SER:HB2	1:O:450:LEU:CD1	2.45	0.46
1:K:68:GLN:NE2	1:K:68:GLN:HA	2.30	0.46
1:K:119:LEU:HB2	1:K:145:LEU:HD11	1.97	0.46
1:C:32:VAL:CG1	1:C:36:HIS:HB2	2.44	0.46
1:I:175:ASN:O	1:I:275:PRO:HD2	2.14	0.46
1:M:38:LEU:H	1:M:38:LEU:HG	1.36	0.46
1:O:273:LYS:HD2	1:O:273:LYS:HA	1.74	0.46
1:A:120:TYR:O	1:A:121:VAL:CG2	2.63	0.46
1:C:190:ARG:HA	1:C:191:PRO:HD3	1.74	0.46
1:A:278:CYS:O	1:A:278:CYS:SG	2.73	0.46
1:E:208:ILE:HA	1:E:212:PHE:CB	2.46	0.46
1:E:212:PHE:O	1:E:213:GLY:C	2.54	0.46
1:O:245:ASP:N	1:O:249:LYS:O	2.44	0.46
1:K:392:HIS:C	1:K:394:LEU:H	2.19	0.46
1:G:111:SER:HA	1:G:142:ARG:NH2	2.31	0.46
1:M:188:TYR:CD1	1:M:238:ILE:HD11	2.50	0.46
1:M:187:GLY:O	1:M:238:ILE:HD12	2.16	0.46
1:A:30:SER:O	1:A:33:ALA:HB3	2.15	0.46
1:O:389:ALA:HA	1:O:392:HIS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:19:ARG:HA	1:O:48:GLN:O	2.14	0.46
1:O:284:THR:HA	1:O:285:PRO:C	2.35	0.46
1:M:65:GLU:HG3	1:M:66:GLN:N	2.30	0.46
1:I:172:GLY:HA2	1:I:301:LYS:HD2	1.98	0.46
2:N:852:THR:HG22	2:N:854:ASP:N	2.31	0.46
1:O:121:VAL:CG1	1:O:122:GLU:N	2.79	0.46
1:C:61:LEU:HD13	1:C:61:LEU:H	1.81	0.46
1:M:291:LYS:HA	1:M:291:LYS:HD2	1.48	0.46
1:G:422:GLU:N	1:G:422:GLU:OE1	2.44	0.46
1:E:433:LEU:HA	1:E:433:LEU:HD12	1.54	0.46
1:G:179:ILE:CG2	1:G:180:SER:N	2.78	0.46
1:K:133:GLU:O	1:K:136:TYR:HB3	2.16	0.46
1:I:244:LEU:HD12	1:I:244:LEU:HA	1.57	0.46
1:A:431:ILE:CG2	1:A:432:ILE:N	2.79	0.46
1:G:19:ARG:HB3	1:G:50:VAL:HG23	1.93	0.46
1:C:219:LEU:HA	1:C:222:ILE:CD1	2.41	0.46
1:C:218:VAL:O	1:C:222:ILE:HD12	2.15	0.46
1:C:375:ASN:OD1	1:C:377:VAL:HB	2.16	0.46
1:K:208:ILE:CD1	1:K:441:PHE:CZ	2.94	0.46
1:I:290:THR:CG2	1:I:291:LYS:N	2.79	0.46
1:I:266:GLN:HB2	1:K:264:LEU:HD22	1.98	0.46
1:K:184:GLY:N	1:K:282:GLY:O	2.48	0.46
1:C:131:GLN:O	1:C:135:LEU:HG	2.16	0.45
1:G:386:GLU:O	1:G:389:ALA:N	2.49	0.45
1:I:228:GLN:HE21	1:I:273:LYS:HE3	1.63	0.45
1:I:51:ALA:HB2	1:I:84:TYR:CE2	2.51	0.45
1:G:216:ILE:CG2	1:G:217:ASP:N	2.78	0.45
1:K:189:GLU:HB2	1:K:284:THR:OG1	2.16	0.45
1:I:244:LEU:CD1	1:I:250:ARG:HA	2.34	0.45
1:I:90:ILE:HD12	1:I:116:LEU:CD1	2.46	0.45
1:M:197:TYR:CE1	1:M:198:LEU:HD13	2.46	0.45
1:K:201:ILE:HB	1:K:258:THR:CB	2.43	0.45
1:M:31:TRP:O	1:M:35:THR:HG23	2.16	0.45
1:C:290:THR:CG2	1:C:291:LYS:N	2.79	0.45
1:E:200:ASP:O	1:E:201:ILE:C	2.51	0.45
1:A:25:LEU:HD12	1:A:25:LEU:HA	1.76	0.45
1:M:381:ILE:O	1:M:384:ILE:N	2.36	0.45
1:K:190:ARG:HG2	1:K:191:PRO:N	2.30	0.45
1:G:43:LEU:HA	1:G:43:LEU:HD23	1.55	0.45
1:I:186:TYR:HB2	1:I:282:GLY:O	2.16	0.45
1:O:148:ILE:HG22	1:O:148:ILE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:314:GLU:HG3	1:G:314:GLU:H	1.49	0.45
1:E:386:GLU:O	1:E:389:ALA:N	2.49	0.45
1:O:244:LEU:N	1:O:244:LEU:HD13	2.31	0.45
1:O:244:LEU:HG	1:O:248:GLY:O	2.16	0.45
1:E:53:TYR:C	1:E:53:TYR:CD2	2.89	0.45
1:M:427:PHE:HA	1:M:430:ALA:HB3	1.98	0.45
1:C:321:TYR:CD2	1:C:368:VAL:HG22	2.51	0.45
1:A:194:SER:CB	1:A:199:TYR:OH	2.52	0.45
1:C:18:ILE:HG23	1:C:18:ILE:HD13	1.47	0.45
1:C:28:GLY:HA2	1:C:67:LEU:HD21	1.98	0.45
1:E:162:ALA:HB1	1:E:304:LEU:CD1	2.46	0.45
1:E:257:LYS:HD2	1:E:259:CYS:O	2.16	0.45
1:K:177:ILE:CG2	1:K:178:GLU:N	2.79	0.45
1:A:184:GLY:CA	2:B:853:MET:HE1	2.46	0.45
1:I:287:LYS:HZ2	1:I:287:LYS:CB	2.28	0.45
1:M:231:ASN:HB3	1:O:233:MET:CE	2.46	0.45
1:I:456:MET:SD	1:I:456:MET:N	2.88	0.45
1:M:171:ILE:HB	1:M:299:GLY:HA3	1.97	0.45
1:K:383:ARG:HA	1:K:386:GLU:HG3	1.99	0.45
1:G:230:ILE:HG22	1:G:267:GLY:HA3	1.97	0.45
1:E:217:ASP:O	1:E:221:TYR:N	2.49	0.45
1:G:129:VAL:HG12	1:G:130:GLN:OE1	2.15	0.45
1:G:415:ASP:O	1:G:426:THR:OG1	2.31	0.45
1:E:89:MET:HA	1:E:118:TYR:O	2.16	0.45
1:K:88:ASP:HA	1:K:115:ASN:C	2.35	0.45
1:M:310:ALA:C	1:M:312:PHE:H	2.19	0.45
1:M:319:VAL:CG2	1:M:370:HIS:CD2	2.97	0.45
1:I:264:LEU:HD22	1:K:266:GLN:HB2	1.97	0.45
2:B:854:ASP:O	2:B:857:TYR:HB2	2.16	0.45
1:O:177:ILE:CG2	1:O:178:GLU:N	2.79	0.45
1:G:272:GLY:O	1:G:273:LYS:HB2	2.16	0.45
2:J:852:THR:HG22	2:J:854:ASP:N	2.30	0.45
1:G:381:ILE:HG22	1:G:385:TYR:CE1	2.52	0.45
1:G:291:LYS:HD2	1:G:291:LYS:HA	1.72	0.45
1:E:103:VAL:N	1:E:106:ILE:HD12	2.31	0.45
1:M:147:THR:HB	1:M:427:PHE:CE1	2.51	0.45
1:E:133:GLU:O	1:E:136:TYR:HB3	2.17	0.45
1:O:319:VAL:CG2	1:O:370:HIS:CD2	2.99	0.45
1:O:294:VAL:HA	1:O:306:ILE:O	2.16	0.45
1:E:294:VAL:HG12	1:E:295:ILE:N	2.32	0.45
1:E:134:GLU:O	1:E:135:LEU:C	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:THR:C	1:C:253:GLU:H	2.18	0.45
1:M:16:ARG:HA	1:M:17:PRO:HD3	1.74	0.45
1:A:417:GLN:HB2	1:A:424:PHE:O	2.16	0.45
1:M:162:ALA:O	1:M:163:LYS:C	2.54	0.45
1:E:54:ASN:CB	1:E:55:PRO:HD2	2.47	0.45
1:E:83:GLN:O	1:E:85:LYS:N	2.50	0.45
1:A:136:TYR:O	1:A:139:SER:OG	2.22	0.45
1:I:121:VAL:CG1	1:I:122:GLU:H	2.26	0.45
1:K:123:TRP:CD1	1:K:214:HIS:CD2	3.05	0.45
1:O:443:SER:O	1:O:444:ASP:C	2.52	0.45
1:K:322:PHE:CD2	1:K:367:GLU:HB3	2.46	0.45
1:O:102:VAL:O	1:O:106:ILE:HD12	2.17	0.45
1:I:167:SER:OG	1:I:168:GLU:N	2.49	0.45
1:G:230:ILE:HA	1:G:267:GLY:HA2	1.98	0.45
1:O:185:TRP:HD1	2:P:857:TYR:CE1	2.35	0.45
1:E:61:LEU:HD21	1:K:242:PHE:HZ	1.82	0.45
1:C:40:ILE:HG23	1:C:47:PHE:HB2	1.98	0.45
1:I:38:LEU:H	1:I:38:LEU:HG	1.41	0.45
1:I:53:TYR:HD2	1:I:53:TYR:O	1.97	0.45
1:E:231:ASN:OD1	1:G:266:GLN:NE2	2.49	0.45
1:G:266:GLN:HA	1:G:276:VAL:O	2.16	0.45
1:A:323:TYR:HA	1:A:365:THR:O	2.16	0.45
1:O:88:ASP:O	1:O:116:LEU:HA	2.17	0.45
1:O:266:GLN:HA	1:O:276:VAL:O	2.16	0.45
1:I:34:LYS:H	1:I:34:LYS:HG3	1.56	0.45
1:A:25:LEU:HD23	1:A:63:THR:HG21	1.99	0.45
1:G:235:SER:O	1:G:260:PRO:HB3	2.17	0.45
1:E:226:TYR:O	1:E:270:GLU:HB2	2.17	0.45
1:K:161:ARG:HG3	1:K:161:ARG:O	2.17	0.45
1:E:163:LYS:HE3	1:E:421:PHE:CE1	2.52	0.45
1:C:151:LEU:C	1:C:153:GLY:N	2.69	0.45
1:G:208:ILE:O	1:G:209:SER:C	2.54	0.45
1:I:138:ILE:HG21	1:I:138:ILE:HD12	1.76	0.45
1:G:87:ILE:HG21	1:G:90:ILE:HG13	1.98	0.45
1:M:150:CYS:SG	1:M:152:GLN:NE2	2.90	0.45
1:E:129:VAL:HA	1:E:434:HIS:HD2	1.82	0.45
1:I:63:THR:O	1:I:67:LEU:HG	2.17	0.45
1:A:372:ARG:HH21	2:B:847:LEU:HD23	1.80	0.45
1:I:381:ILE:CG2	1:I:385:TYR:CE1	2.98	0.45
1:E:187:GLY:HA3	1:E:284:THR:N	2.32	0.45
1:E:171:ILE:HD12	1:E:299:GLY:CA	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:TRP:CD1	1:A:214:HIS:CD2	3.02	0.45
1:A:159:ILE:O	1:A:160:VAL:C	2.55	0.45
1:O:262:HIS:CD2	1:O:263:LEU:N	2.84	0.45
1:K:454:LYS:O	1:K:455:ILE:C	2.54	0.45
1:E:120:TYR:HD2	1:E:121:VAL:N	2.15	0.45
1:C:381:ILE:HG22	1:C:385:TYR:CE1	2.52	0.45
1:E:304:LEU:HD23	1:E:304:LEU:HA	1.77	0.45
1:K:149:ILE:CG2	1:K:151:LEU:HD12	2.46	0.45
1:A:149:ILE:HG21	1:A:151:LEU:HD12	1.97	0.45
1:A:269:LEU:HA	1:A:269:LEU:HD23	1.86	0.45
1:A:123:TRP:CZ2	1:A:433:LEU:CD2	2.99	0.45
1:E:85:LYS:HA	1:E:113:ASN:OD1	2.16	0.45
1:I:208:ILE:O	1:I:209:SER:C	2.55	0.45
1:O:228:GLN:HB3	1:O:268:ILE:O	2.17	0.45
1:C:91:VAL:HG22	1:C:120:TYR:CB	2.47	0.45
1:A:315:ILE:HG23	1:A:377:VAL:HG22	1.98	0.45
1:I:290:THR:HG22	1:I:291:LYS:N	2.31	0.45
1:I:187:GLY:CA	1:I:283:GLY:HA3	2.47	0.45
1:O:375:ASN:C	1:O:375:ASN:OD1	2.53	0.45
1:K:292:ASN:ND2	1:K:292:ASN:N	2.65	0.45
1:A:171:ILE:O	1:A:300:THR:N	2.49	0.45
2:J:854:ASP:O	2:J:857:TYR:HB2	2.17	0.45
1:G:215:THR:O	1:G:218:VAL:HG12	2.16	0.45
1:A:142:ARG:C	1:A:144:ASN:N	2.70	0.45
1:I:121:VAL:CG1	1:I:122:GLU:N	2.80	0.45
1:M:183:GLY:O	1:M:312:PHE:CZ	2.70	0.45
1:A:16:ARG:HE	1:A:16:ARG:HB2	1.45	0.45
1:O:117:ARG:O	1:O:145:LEU:HD12	2.17	0.45
1:M:77:SER:HB3	1:M:80:SER:H	1.82	0.45
1:G:269:LEU:HD23	1:G:269:LEU:HA	1.69	0.45
1:E:78:LEU:O	1:E:81:PHE:N	2.50	0.45
1:C:201:ILE:HG23	1:C:202:GLU:N	2.31	0.45
1:C:258:THR:O	1:C:259:CYS:C	2.53	0.45
1:C:454:LYS:HE2	1:C:454:LYS:HB2	1.71	0.45
1:C:245:ASP:OD1	1:C:249:LYS:HB3	2.16	0.45
1:G:56:THR:OG1	1:G:59:SER:OG	2.28	0.45
1:O:31:TRP:O	1:O:34:LYS:N	2.49	0.45
1:E:32:VAL:H	1:E:32:VAL:HG23	1.24	0.45
1:C:129:VAL:HG12	1:C:130:GLN:OE1	2.17	0.44
1:C:136:TYR:CB	1:C:431:ILE:HD13	2.44	0.44
1:G:166:ILE:HD11	1:G:304:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:453:SER:O	1:G:456:MET:HE1	2.17	0.44
1:E:381:ILE:O	1:E:384:ILE:HB	2.17	0.44
1:C:365:THR:CG2	1:C:366:MET:N	2.80	0.44
1:K:384:ILE:O	1:K:387:SER:N	2.50	0.44
1:C:385:TYR:O	1:C:386:GLU:C	2.55	0.44
1:A:77:SER:CB	1:A:80:SER:HB2	2.40	0.44
1:O:175:ASN:O	1:O:275:PRO:HD2	2.17	0.44
1:I:313:VAL:HG13	1:I:314:GLU:N	2.30	0.44
1:K:104:LYS:O	1:K:107:LEU:N	2.50	0.44
1:O:216:ILE:O	1:O:217:ASP:C	2.55	0.44
1:E:291:LYS:HA	1:E:291:LYS:HD2	1.64	0.44
1:E:134:GLU:O	1:E:137:SER:OG	2.29	0.44
1:K:26:THR:HB	1:K:30:SER:CB	2.46	0.44
1:E:15:SER:O	1:E:16:ARG:HB3	2.17	0.44
1:G:194:SER:HB3	1:G:199:TYR:OH	2.17	0.44
1:C:40:ILE:HG22	1:C:40:ILE:O	2.17	0.44
1:I:162:ALA:O	1:I:165:LEU:N	2.50	0.44
1:A:177:ILE:CD1	1:A:219:LEU:HD11	2.44	0.44
1:C:231:ASN:HB2	1:C:449:THR:OG1	2.15	0.44
1:I:185:TRP:HD1	2:J:857:TYR:CE1	2.35	0.44
1:G:138:ILE:O	1:G:140:GLN:N	2.51	0.44
1:G:436:LEU:HB2	1:G:455:ILE:HD13	1.97	0.44
1:O:382:LEU:O	1:O:386:GLU:HG3	2.17	0.44
1:A:77:SER:O	1:A:80:SER:HB2	2.17	0.44
1:A:79:GLU:O	1:A:80:SER:C	2.55	0.44
1:K:215:THR:HB	1:K:216:ILE:H	1.64	0.44
1:A:184:GLY:HA3	2:B:853:MET:HE1	1.99	0.44
1:K:103:VAL:O	1:K:104:LYS:C	2.55	0.44
1:I:452:VAL:CG1	1:I:455:ILE:HG12	2.47	0.44
1:E:251:THR:C	1:E:253:GLU:N	2.70	0.44
1:I:190:ARG:HA	1:I:191:PRO:HD3	1.57	0.44
1:K:372:ARG:O	1:K:373:ASN:ND2	2.50	0.44
1:G:178:GLU:C	1:G:179:ILE:HG13	2.37	0.44
1:O:53:TYR:HB2	1:O:81:PHE:CD1	2.52	0.44
1:A:192:MET:SD	1:K:15:SER:O	2.76	0.44
1:K:187:GLY:O	1:K:238:ILE:HG21	2.16	0.44
1:M:245:ASP:O	1:M:246:GLU:C	2.55	0.44
1:K:433:LEU:HG	1:K:437:ILE:HD11	1.98	0.44
1:A:43:LEU:O	1:A:44:SER:C	2.55	0.44
1:G:111:SER:CA	1:G:142:ARG:NH2	2.81	0.44
1:K:125:LEU:HB2	1:K:149:ILE:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:96:VAL:N	1:O:97:PRO:CD	2.79	0.44
1:A:257:LYS:HE3	1:A:257:LYS:HB3	1.67	0.44
2:P:855:ASP:O	2:P:856:VAL:C	2.55	0.44
1:A:319:VAL:CG2	1:A:370:HIS:CD2	3.00	0.44
1:C:16:ARG:HB2	1:C:17:PRO:HD3	1.97	0.44
1:E:154:ARG:HD2	1:E:425:PRO:HG3	2.00	0.44
1:K:200:ASP:OD1	1:K:200:ASP:C	2.55	0.44
1:I:16:ARG:HA	1:I:17:PRO:HD3	1.69	0.44
2:N:855:ASP:O	2:N:858:ASN:N	2.46	0.44
1:K:456:MET:N	1:K:456:MET:SD	2.87	0.44
1:A:212:PHE:HA	1:A:280:PHE:CZ	2.52	0.44
1:G:313:VAL:CG1	1:G:314:GLU:HG3	2.47	0.44
1:M:100:TYR:CB	1:M:131:GLN:NE2	2.78	0.44
1:M:134:GLU:O	1:M:137:SER:OG	2.28	0.44
1:K:381:ILE:O	1:K:382:LEU:C	2.54	0.44
1:O:287:LYS:N	1:O:292:ASN:OD1	2.51	0.44
1:K:25:LEU:CB	1:K:52:LEU:HD21	2.46	0.44
1:K:123:TRP:CE3	1:K:123:TRP:HA	2.52	0.44
1:A:98:GLU:O	1:A:102:VAL:HG23	2.17	0.44
1:I:30:SER:O	1:I:33:ALA:HB3	2.17	0.44
1:M:214:HIS:O	1:M:218:VAL:HG23	2.17	0.44
1:K:35:THR:HA	1:K:378:VAL:HG22	2.00	0.44
1:G:319:VAL:HG22	1:G:370:HIS:CG	2.52	0.44
1:O:201:ILE:HB	1:O:258:THR:CB	2.48	0.44
1:A:54:ASN:HA	1:A:55:PRO:HD3	1.82	0.44
1:I:319:VAL:HG22	1:I:370:HIS:CG	2.52	0.44
1:C:245:ASP:O	1:C:248:GLY:N	2.30	0.44
1:E:456:MET:SD	1:E:456:MET:N	2.89	0.44
1:M:266:GLN:CB	1:O:264:LEU:HD22	2.47	0.44
1:O:62:GLN:O	1:O:65:GLU:N	2.50	0.44
1:K:455:ILE:H	1:K:455:ILE:HG12	1.45	0.44
1:E:268:ILE:CG2	1:E:273:LYS:HA	2.48	0.44
1:E:417:GLN:O	1:E:420:ARG:HB2	2.18	0.44
1:A:314:GLU:HG3	1:A:314:GLU:H	1.33	0.44
2:J:855:ASP:O	2:J:858:ASN:N	2.45	0.44
1:A:212:PHE:O	1:A:216:ILE:HG22	2.17	0.44
1:K:432:ILE:HD13	1:K:432:ILE:HG23	1.73	0.44
1:M:132:ALA:O	1:M:133:GLU:C	2.55	0.44
1:C:178:GLU:HB2	1:C:296:ASP:HB3	1.99	0.44
1:C:390:ASP:O	1:C:391:TYR:C	2.56	0.44
1:O:154:ARG:CD	1:O:425:PRO:HG3	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:852:THR:HG22	2:B:854:ASP:N	2.30	0.44
1:A:287:LYS:CB	1:A:287:LYS:NZ	2.79	0.44
1:O:75:PHE:HD2	1:O:80:SER:HB3	1.82	0.44
1:K:185:TRP:CD1	2:L:857:TYR:HE1	2.36	0.44
2:N:856:VAL:O	2:N:860:ILE:HG22	2.18	0.44
1:M:384:ILE:O	1:M:385:TYR:C	2.56	0.44
1:I:61:LEU:N	1:I:61:LEU:CD1	2.80	0.44
1:A:218:VAL:HG13	1:A:222:ILE:HD11	1.99	0.44
2:J:853:MET:O	2:J:856:VAL:N	2.51	0.44
1:I:77:SER:HB3	1:I:80:SER:OG	2.17	0.44
1:G:180:SER:O	1:G:293:LEU:HD12	2.18	0.44
1:G:432:ILE:HD13	1:G:456:MET:HA	2.00	0.44
1:K:244:LEU:N	1:K:244:LEU:CD1	2.81	0.44
1:O:91:VAL:HG13	1:O:120:TYR:HD1	1.83	0.44
1:G:189:GLU:HB3	1:G:244:LEU:HD11	2.00	0.44
1:M:147:THR:HB	1:M:427:PHE:CG	2.52	0.44
1:O:129:VAL:HG13	1:O:130:GLN:N	2.33	0.44
1:O:142:ARG:HB2	1:O:145:LEU:HB3	2.00	0.44
1:A:292:ASN:HD22	1:A:292:ASN:H	1.66	0.44
1:G:201:ILE:HG23	1:G:202:GLU:N	2.32	0.44
1:M:102:VAL:HG12	1:M:106:ILE:CD1	2.48	0.44
1:I:146:GLN:NE2	1:I:146:GLN:HA	2.33	0.44
1:I:244:LEU:CD1	1:I:250:ARG:CA	2.96	0.44
1:A:141:GLN:H	1:A:141:GLN:HG2	1.37	0.44
1:O:381:ILE:HG22	1:O:385:TYR:CE1	2.53	0.44
1:A:381:ILE:O	1:A:384:ILE:N	2.43	0.44
1:I:151:LEU:HD23	1:I:217:ASP:OD2	2.18	0.44
1:O:133:GLU:HA	1:O:133:GLU:OE2	2.18	0.44
1:C:389:ALA:O	1:C:392:HIS:N	2.51	0.44
1:E:426:THR:O	1:E:429:ASP:HB2	2.18	0.44
1:O:292:ASN:N	1:O:292:ASN:ND2	2.66	0.44
1:A:312:PHE:HE1	2:B:853:MET:HE1	1.83	0.44
1:M:188:TYR:CD1	1:M:238:ILE:CD1	3.01	0.44
1:I:188:TYR:CZ	1:I:238:ILE:HG12	2.52	0.44
1:O:152:GLN:NE2	1:O:152:GLN:N	2.65	0.44
1:A:438:ASP:O	1:A:439:ALA:C	2.56	0.44
1:C:448:LYS:O	1:C:450:LEU:CD2	2.66	0.44
2:F:852:THR:O	2:F:855:ASP:HB2	2.18	0.44
1:M:237:ASN:H	1:M:261:ASP:CG	2.21	0.44
1:C:262:HIS:CD2	1:C:263:LEU:N	2.86	0.44
1:I:55:PRO:HB2	1:I:56:THR:H	1.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:126:ALA:HB2	1:G:135:LEU:HD12	1.99	0.44
1:G:452:VAL:HG13	1:G:455:ILE:CG2	2.45	0.44
1:G:313:VAL:CG1	1:G:314:GLU:N	2.80	0.44
1:K:126:ALA:CB	1:K:132:ALA:HB2	2.40	0.44
1:A:67:LEU:O	1:A:68:GLN:HB2	2.17	0.44
1:K:293:LEU:HA	1:K:293:LEU:HD12	1.75	0.44
2:B:855:ASP:O	2:B:856:VAL:C	2.57	0.44
1:I:314:GLU:H	1:I:314:GLU:HG3	1.06	0.44
1:O:20:VAL:HG21	1:O:40:ILE:CD1	2.48	0.44
1:O:198:LEU:HB2	1:O:199:TYR:CE1	2.53	0.44
1:I:158:TYR:HB2	1:I:318:LEU:HD12	1.99	0.44
1:A:422:GLU:N	1:A:422:GLU:OE1	2.49	0.44
1:E:218:VAL:HG12	1:E:219:LEU:N	2.33	0.43
1:K:192:MET:O	1:O:58:LYS:HD3	2.18	0.43
1:M:208:ILE:O	1:M:212:PHE:HB3	2.17	0.43
1:M:427:PHE:O	1:M:428:LYS:C	2.53	0.43
1:I:183:GLY:HA2	1:I:207:LEU:HD12	1.99	0.43
1:O:135:LEU:O	1:O:138:ILE:HB	2.18	0.43
1:C:84:TYR:CD1	1:C:86:ASP:HB2	2.53	0.43
1:K:156:SER:O	1:K:159:ILE:N	2.45	0.43
1:E:30:SER:O	1:E:31:TRP:C	2.56	0.43
1:I:437:ILE:HA	1:I:440:VAL:HG23	2.00	0.43
1:M:96:VAL:O	1:M:99:HIS:HB2	2.18	0.43
1:I:230:ILE:HA	1:I:267:GLY:HA2	2.00	0.43
1:K:199:TYR:N	1:K:199:TYR:CD1	2.85	0.43
1:M:290:THR:HG22	1:M:291:LYS:O	2.18	0.43
1:I:38:LEU:HA	1:I:38:LEU:HD23	1.60	0.43
1:C:313:VAL:HG12	1:C:314:GLU:HG3	2.01	0.43
1:G:432:ILE:CG2	1:G:455:ILE:HG13	2.48	0.43
1:K:132:ALA:O	1:K:133:GLU:C	2.55	0.43
1:K:134:GLU:O	1:K:137:SER:OG	2.24	0.43
1:E:85:LYS:HE2	1:E:113:ASN:HA	1.99	0.43
1:A:268:ILE:CG2	1:A:273:LYS:HA	2.49	0.43
1:A:65:GLU:HG2	1:A:66:GLN:N	2.26	0.43
1:O:100:TYR:HA	1:O:135:LEU:HD11	2.00	0.43
1:M:293:LEU:HD23	1:M:318:LEU:HD22	2.00	0.43
1:M:315:ILE:O	1:M:376:SER:HB2	2.18	0.43
1:I:155:LYS:O	1:I:383:ARG:HD3	2.18	0.43
1:O:377:VAL:HG11	2:P:859:TYR:CD2	2.53	0.43
1:I:152:GLN:H	1:I:152:GLN:HE21	1.62	0.43
1:O:156:SER:HB3	1:O:159:ILE:CG1	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:436:LEU:O	1:I:439:ALA:HB3	2.18	0.43
1:C:195:PRO:HB2	1:C:197:TYR:CE2	2.54	0.43
1:K:319:VAL:HG22	1:K:370:HIS:CG	2.53	0.43
1:O:424:PHE:CD1	1:O:424:PHE:O	2.71	0.43
1:G:216:ILE:O	1:G:217:ASP:C	2.54	0.43
1:G:177:ILE:CB	1:G:276:VAL:HG13	2.48	0.43
1:O:54:ASN:HA	1:O:55:PRO:HD3	1.70	0.43
1:E:375:ASN:HD21	1:E:378:VAL:HG23	1.83	0.43
1:K:432:ILE:O	1:K:433:LEU:O	2.36	0.43
1:I:107:LEU:HD13	1:I:138:ILE:HG22	1.98	0.43
1:M:138:ILE:O	1:M:139:SER:C	2.55	0.43
1:G:118:TYR:N	1:G:118:TYR:HD1	2.16	0.43
1:E:129:VAL:O	1:E:132:ALA:N	2.51	0.43
1:M:161:ARG:HA	1:M:161:ARG:HD3	1.73	0.43
1:A:53:TYR:CD2	1:A:54:ASN:N	2.87	0.43
1:E:172:GLY:HA3	1:E:301:LYS:HD2	2.00	0.43
1:C:195:PRO:HB3	1:C:197:TYR:HD2	1.80	0.43
1:M:38:LEU:O	1:M:39:ALA:C	2.56	0.43
1:A:120:TYR:O	1:A:121:VAL:HG23	2.18	0.43
1:K:146:GLN:OE1	1:K:424:PHE:CZ	2.71	0.43
1:C:428:LYS:O	1:C:432:ILE:HG13	2.18	0.43
1:G:381:ILE:CG2	1:G:385:TYR:CE1	3.01	0.43
1:G:381:ILE:O	1:G:384:ILE:N	2.48	0.43
1:K:136:TYR:CD2	1:K:431:ILE:HD13	2.53	0.43
1:E:62:GLN:CG	1:E:66:GLN:NE2	2.78	0.43
1:M:150:CYS:SG	1:M:150:CYS:O	2.76	0.43
1:C:64:ILE:HD11	1:C:72:ALA:CB	2.48	0.43
1:K:77:SER:HB3	1:K:80:SER:H	1.82	0.43
1:I:67:LEU:HB2	1:I:69:LEU:HG	2.00	0.43
1:M:20:VAL:H	1:M:20:VAL:HG23	1.51	0.43
1:G:197:TYR:CE1	1:G:198:LEU:HD13	2.54	0.43
1:E:77:SER:O	1:E:80:SER:HB2	2.18	0.43
1:M:322:PHE:CD1	1:M:323:TYR:N	2.86	0.43
1:G:365:THR:CG2	1:G:366:MET:N	2.80	0.43
1:I:251:THR:C	1:I:253:GLU:H	2.22	0.43
1:O:442:ARG:O	1:O:446:GLU:HB2	2.17	0.43
1:E:252:LYS:HG3	1:E:252:LYS:H	1.19	0.43
1:C:152:GLN:HG3	1:C:314:GLU:O	2.17	0.43
1:O:68:GLN:HE21	1:O:68:GLN:N	2.13	0.43
1:A:389:ALA:O	1:A:393:PHE:N	2.50	0.43
1:G:104:LYS:CA	1:G:107:LEU:HD12	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:69:LEU:HD23	1:I:69:LEU:HA	1.74	0.43
1:C:174:ILE:HG22	1:C:175:ASN:N	2.34	0.43
1:O:269:LEU:HD23	1:O:269:LEU:HA	1.77	0.43
1:O:293:LEU:O	1:O:307:GLU:HA	2.18	0.43
1:K:158:TYR:CB	1:K:318:LEU:HD12	2.48	0.43
1:M:179:ILE:HD11	1:M:219:LEU:HD22	2.00	0.43
1:K:304:LEU:HD21	1:K:320:LEU:HD21	2.00	0.43
1:I:436:LEU:HB2	1:I:455:ILE:HD13	2.01	0.43
1:A:313:VAL:CG1	1:A:314:GLU:N	2.81	0.43
1:C:230:ILE:HA	1:C:267:GLY:HA2	2.01	0.43
1:I:51:ALA:HB2	1:I:84:TYR:HE2	1.83	0.43
1:O:59:SER:O	1:O:63:THR:OG1	2.26	0.43
1:A:165:LEU:HD13	1:A:322:PHE:CD1	2.53	0.43
1:E:427:PHE:O	1:E:428:LYS:C	2.56	0.43
1:O:197:TYR:HA	1:O:200:ASP:HB3	2.01	0.43
1:E:187:GLY:HA3	1:E:284:THR:H	1.84	0.43
1:E:58:LYS:HG2	1:K:252:LYS:O	2.18	0.43
1:I:286:VAL:O	1:I:286:VAL:HG23	2.17	0.43
1:M:154:ARG:NH1	1:M:417:GLN:OE1	2.44	0.43
1:C:432:ILE:HG21	1:C:432:ILE:HD13	1.53	0.43
1:G:208:ILE:HG13	1:G:263:LEU:CD2	2.48	0.43
1:G:436:LEU:HD12	1:G:452:VAL:HG11	2.00	0.43
1:O:57:LEU:HD21	1:O:61:LEU:HD11	1.89	0.43
1:O:79:GLU:O	1:O:83:GLN:HG3	2.18	0.43
1:O:91:VAL:HG22	1:O:120:TYR:HB3	2.01	0.43
1:E:53:TYR:CG	1:E:54:ASN:N	2.86	0.43
1:I:416:LYS:HA	1:I:426:THR:OG1	2.19	0.43
1:C:120:TYR:C	1:C:121:VAL:HG23	2.39	0.43
1:C:25:LEU:HD12	1:C:25:LEU:HA	1.61	0.43
1:E:431:ILE:HG22	1:E:432:ILE:H	1.83	0.43
1:A:118:TYR:HH	1:A:392:HIS:CG	2.30	0.43
1:A:185:TRP:HZ3	1:A:186:TYR:OH	1.94	0.43
1:M:79:GLU:O	1:M:80:SER:C	2.57	0.43
1:E:111:SER:N	1:E:142:ARG:NH2	2.67	0.43
1:G:252:LYS:HG3	1:G:252:LYS:H	1.23	0.43
1:I:129:VAL:O	1:I:132:ALA:HB3	2.19	0.43
1:O:220:GLN:HB2	1:O:220:GLN:HE21	1.55	0.43
1:C:194:SER:HB3	1:C:199:TYR:OH	2.18	0.43
1:A:245:ASP:O	1:A:247:ASN:N	2.51	0.43
1:E:453:SER:HA	1:E:456:MET:HE3	2.01	0.43
1:K:23:VAL:HG12	1:K:94:VAL:CG1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:159:ILE:O	1:G:162:ALA:N	2.51	0.43
1:E:382:LEU:C	1:E:384:ILE:N	2.72	0.43
1:K:129:VAL:CG1	1:K:130:GLN:H	2.29	0.43
1:K:133:GLU:HA	1:K:133:GLU:OE2	2.19	0.43
1:E:84:TYR:C	1:E:86:ASP:H	2.21	0.43
1:A:273:LYS:HA	1:A:273:LYS:HD3	1.64	0.43
1:I:135:LEU:O	1:I:138:ILE:HB	2.19	0.43
1:M:149:ILE:HB	1:M:430:ALA:HB2	2.01	0.43
1:A:190:ARG:HA	1:A:191:PRO:HD3	1.73	0.43
1:I:315:ILE:CG2	1:I:377:VAL:HG22	2.48	0.43
1:M:436:LEU:HD12	1:M:452:VAL:HG11	2.00	0.43
1:K:35:THR:OG1	1:K:36:HIS:N	2.50	0.43
2:L:854:ASP:O	2:L:857:TYR:HB2	2.19	0.43
1:I:40:ILE:HG23	1:I:47:PHE:CB	2.48	0.43
1:I:171:ILE:HB	1:I:299:GLY:HA3	2.01	0.43
1:E:38:LEU:HA	1:E:38:LEU:HD23	1.73	0.43
1:C:61:LEU:HD12	1:C:61:LEU:N	2.34	0.43
1:C:325:ILE:O	1:C:326:LYS:C	2.56	0.43
1:C:455:ILE:HG21	1:C:455:ILE:HD13	1.77	0.43
1:G:168:GLU:O	1:G:170:CYS:N	2.52	0.43
1:K:245:ASP:O	1:K:248:GLY:N	2.27	0.43
1:I:105:ASN:N	1:I:105:ASN:ND2	2.66	0.43
1:A:262:HIS:HE1	1:C:176:SER:OG	2.02	0.43
1:C:218:VAL:CG1	1:C:219:LEU:N	2.82	0.43
1:A:95:LYS:HE2	1:A:197:TYR:CE2	2.54	0.43
1:C:121:VAL:HG12	1:C:122:GLU:N	2.34	0.43
1:K:89:MET:HB2	1:K:118:TYR:O	2.18	0.43
1:E:138:ILE:O	1:E:140:GLN:N	2.52	0.43
2:D:855:ASP:O	2:D:856:VAL:C	2.56	0.43
1:C:292:ASN:N	1:C:292:ASN:HD22	2.17	0.43
1:E:284:THR:H	1:E:284:THR:HG23	1.48	0.43
1:C:183:GLY:CA	1:C:207:LEU:HD13	2.48	0.43
1:O:313:VAL:HG12	1:O:314:GLU:HG3	2.01	0.43
1:M:381:ILE:HG22	1:M:385:TYR:CE1	2.53	0.43
1:O:255:ILE:HG23	1:O:255:ILE:O	2.19	0.43
1:A:295:ILE:HG22	1:A:295:ILE:O	2.19	0.43
1:O:25:LEU:O	1:O:54:ASN:ND2	2.50	0.43
1:O:22:PHE:N	1:O:51:ALA:O	2.35	0.43
1:O:51:ALA:O	1:O:52:LEU:HD12	2.17	0.43
1:I:431:ILE:CG2	1:I:432:ILE:N	2.81	0.43
1:C:236:ASN:HA	1:C:261:ASP:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:ILE:HG21	1:C:218:VAL:HG22	2.01	0.43
1:A:195:PRO:CB	1:A:198:LEU:HD22	2.48	0.43
1:A:88:ASP:O	1:A:117:ARG:N	2.50	0.43
1:E:192:MET:HE3	1:O:15:SER:HB3	1.99	0.43
1:M:365:THR:CG2	1:M:366:MET:N	2.82	0.43
1:O:105:ASN:N	1:O:105:ASN:ND2	2.64	0.43
1:C:201:ILE:HB	1:C:258:THR:CB	2.47	0.43
1:A:417:GLN:HB2	1:A:424:PHE:C	2.39	0.43
1:M:451:ASP:OD1	1:M:453:SER:OG	2.35	0.43
1:C:431:ILE:O	1:C:432:ILE:C	2.57	0.42
1:O:208:ILE:HA	1:O:212:PHE:HB3	2.01	0.42
1:G:291:LYS:HG3	1:G:307:GLU:HB3	2.01	0.42
1:A:192:MET:CE	1:K:15:SER:CB	2.96	0.42
1:K:228:GLN:HE22	1:K:273:LYS:HE3	1.83	0.42
1:I:147:THR:HG21	1:I:427:PHE:CD2	2.54	0.42
1:K:39:ALA:HB1	1:K:382:LEU:HA	2.01	0.42
1:C:39:ALA:HB1	1:C:382:LEU:HA	2.01	0.42
1:K:57:LEU:HD23	1:K:61:LEU:HD21	2.01	0.42
1:M:115:ASN:O	1:M:117:ARG:HB2	2.19	0.42
1:M:142:ARG:HG3	1:M:145:LEU:CD2	2.47	0.42
1:O:216:ILE:HA	1:O:216:ILE:HD12	1.75	0.42
1:A:187:GLY:O	1:A:238:ILE:HG21	2.19	0.42
1:O:195:PRO:HB2	1:O:198:LEU:HD22	2.01	0.42
1:E:192:MET:HE1	1:E:243:LEU:HD22	2.00	0.42
1:C:290:THR:HG22	1:C:291:LYS:N	2.34	0.42
1:G:372:ARG:O	1:G:373:ASN:C	2.57	0.42
1:C:168:GLU:O	1:C:328:GLY:O	2.37	0.42
1:K:292:ASN:HD22	1:K:292:ASN:N	2.17	0.42
1:O:325:ILE:O	1:O:326:LYS:C	2.57	0.42
1:O:38:LEU:HD23	1:O:38:LEU:HA	1.30	0.42
1:G:23:VAL:HG12	1:G:94:VAL:CG1	2.50	0.42
1:G:94:VAL:O	1:G:95:LYS:C	2.57	0.42
1:A:212:PHE:CZ	1:A:216:ILE:HB	2.54	0.42
1:A:218:VAL:O	1:A:222:ILE:N	2.37	0.42
1:G:427:PHE:HA	1:G:430:ALA:CB	2.48	0.42
1:K:244:LEU:HA	1:K:244:LEU:HD12	1.83	0.42
1:K:130:GLN:O	1:K:131:GLN:C	2.57	0.42
1:E:152:GLN:NE2	1:E:214:HIS:HE1	2.17	0.42
1:M:77:SER:CB	1:M:80:SER:HB2	2.43	0.42
1:A:225:SER:HB2	1:A:271:ASN:CB	2.47	0.42
1:A:251:THR:C	1:A:253:GLU:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:LEU:HA	1:C:198:LEU:HD12	1.46	0.42
1:O:165:LEU:O	1:O:170:CYS:SG	2.78	0.42
1:I:174:ILE:HG22	1:I:175:ASN:N	2.34	0.42
1:E:161:ARG:HG3	1:E:161:ARG:O	2.18	0.42
1:A:211:SER:O	1:A:215:THR:OG1	2.33	0.42
1:O:273:LYS:O	1:O:274:VAL:C	2.53	0.42
1:A:300:THR:HG22	1:A:300:THR:O	2.19	0.42
1:G:301:LYS:O	1:G:364:GLN:NE2	2.51	0.42
1:C:156:SER:O	1:C:157:PRO:C	2.55	0.42
1:G:190:ARG:HA	1:G:191:PRO:HD3	1.79	0.42
1:A:297:ILE:HD13	1:A:297:ILE:HG21	1.61	0.42
1:K:174:ILE:HB	1:K:274:VAL:HG21	2.01	0.42
1:C:314:GLU:HG3	1:C:314:GLU:H	1.19	0.42
1:O:50:VAL:HG13	1:O:84:TYR:CE2	2.55	0.42
1:A:228:GLN:O	1:A:452:VAL:N	2.47	0.42
1:A:262:HIS:ND1	1:C:176:SER:HB2	2.34	0.42
1:O:416:LYS:HA	1:O:426:THR:OG1	2.20	0.42
1:C:386:GLU:O	1:C:389:ALA:N	2.52	0.42
1:E:149:ILE:HD12	1:E:149:ILE:HA	1.87	0.42
1:E:416:LYS:HD2	1:E:418:GLY:CA	2.49	0.42
1:M:435:ARG:HB3	1:M:455:ILE:HG21	2.00	0.42
1:C:426:THR:O	1:C:429:ASP:N	2.52	0.42
1:E:228:GLN:O	1:E:452:VAL:N	2.52	0.42
1:A:30:SER:H	1:A:33:ALA:HB3	1.84	0.42
1:E:200:ASP:OD1	1:E:201:ILE:N	2.51	0.42
1:M:94:VAL:O	1:M:95:LYS:C	2.56	0.42
1:I:91:VAL:HG22	1:I:120:TYR:HB3	2.00	0.42
1:C:217:ASP:HB2	1:C:433:LEU:HD13	2.01	0.42
1:O:212:PHE:HA	1:O:280:PHE:CZ	2.54	0.42
1:K:273:LYS:CD	1:K:273:LYS:N	2.82	0.42
1:K:136:TYR:CG	1:K:431:ILE:HD13	2.54	0.42
1:I:111:SER:N	1:I:142:ARG:HH22	2.18	0.42
1:I:111:SER:HA	1:I:142:ARG:NH2	2.35	0.42
1:C:177:ILE:CG2	1:C:178:GLU:N	2.81	0.42
1:C:211:SER:O	1:C:215:THR:OG1	2.33	0.42
1:C:323:TYR:HA	1:C:365:THR:O	2.20	0.42
1:G:64:ILE:CG1	1:G:72:ALA:HB3	2.46	0.42
1:C:79:GLU:HG2	1:C:109:HIS:NE2	2.34	0.42
1:C:92:VAL:HB	1:C:121:VAL:HG22	2.01	0.42
1:I:67:LEU:O	1:I:68:GLN:HB2	2.18	0.42
1:K:152:GLN:H	1:K:152:GLN:HE21	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:103:VAL:CA	1:K:106:ILE:HD12	2.49	0.42
1:K:25:LEU:O	1:K:54:ASN:ND2	2.51	0.42
2:P:853:MET:O	2:P:854:ASP:C	2.57	0.42
1:O:165:LEU:HD23	1:O:165:LEU:HA	1.87	0.42
1:G:16:ARG:HA	1:G:17:PRO:HD3	1.90	0.42
1:A:149:ILE:HG23	1:A:151:LEU:HD12	2.01	0.42
1:O:304:LEU:HD23	1:O:322:PHE:HB2	2.01	0.42
1:G:392:HIS:HD2	1:G:393:PHE:CD2	2.17	0.42
1:G:216:ILE:CG2	1:G:217:ASP:H	2.32	0.42
1:G:294:VAL:HG22	1:G:307:GLU:HG2	2.00	0.42
1:G:294:VAL:HA	1:G:306:ILE:O	2.19	0.42
1:K:244:LEU:HD11	1:K:250:ARG:HG3	2.02	0.42
1:K:245:ASP:O	1:K:246:GLU:C	2.58	0.42
1:O:69:LEU:HB3	1:O:72:ALA:CB	2.46	0.42
1:E:110:SER:HB2	1:E:116:LEU:HD22	2.01	0.42
1:E:28:GLY:HA2	1:E:67:LEU:CD2	2.39	0.42
1:O:381:ILE:CG2	1:O:385:TYR:HE1	2.33	0.42
1:A:381:ILE:CG2	1:A:385:TYR:CE1	3.03	0.42
1:C:178:GLU:OE2	1:C:296:ASP:HB3	2.20	0.42
1:C:319:VAL:HG12	1:C:320:LEU:N	2.34	0.42
1:K:105:ASN:ND2	1:K:105:ASN:N	2.65	0.42
1:G:377:VAL:HG11	2:H:859:TYR:CD2	2.55	0.42
1:O:215:THR:HB	1:O:216:ILE:H	1.66	0.42
1:A:103:VAL:HA	1:A:106:ILE:CD1	2.50	0.42
1:K:201:ILE:HG21	1:K:258:THR:HG21	2.00	0.42
1:A:53:TYR:CG	1:A:54:ASN:N	2.87	0.42
1:A:154:ARG:HH11	1:A:154:ARG:HD3	1.60	0.42
1:E:286:VAL:O	1:E:286:VAL:HG23	2.19	0.42
1:G:160:VAL:O	1:G:160:VAL:HG12	2.19	0.42
1:O:230:ILE:HG13	1:O:230:ILE:O	2.19	0.42
1:C:134:GLU:O	1:C:137:SER:OG	2.26	0.42
1:I:185:TRP:CZ3	1:I:186:TYR:CE1	3.08	0.42
1:M:389:ALA:O	1:M:392:HIS:HB3	2.18	0.42
1:E:88:ASP:O	1:E:117:ARG:N	2.47	0.42
1:A:161:ARG:HD2	1:A:161:ARG:HH11	1.66	0.42
1:K:42:GLN:CD	1:K:382:LEU:HD11	2.40	0.42
1:O:129:VAL:O	1:O:130:GLN:C	2.58	0.42
2:H:853:MET:O	2:H:856:VAL:HB	2.17	0.42
1:M:436:LEU:O	1:M:439:ALA:CB	2.63	0.42
1:M:231:ASN:OD1	1:O:266:GLN:NE2	2.52	0.42
1:A:292:ASN:N	1:A:292:ASN:ND2	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:77:SER:O	1:O:80:SER:HB2	2.19	0.42
1:I:375:ASN:O	1:I:375:ASN:OD1	2.38	0.42
1:E:30:SER:OG	1:E:33:ALA:HB2	2.18	0.42
1:I:18:ILE:HG23	1:I:18:ILE:HD13	1.71	0.42
1:O:313:VAL:CG1	1:O:314:GLU:HG3	2.49	0.42
1:O:185:TRP:CD1	2:P:857:TYR:HE1	2.38	0.42
1:G:24:GLY:HA3	1:G:93:SER:O	2.19	0.42
1:G:290:THR:CG2	1:G:291:LYS:N	2.82	0.42
1:E:106:ILE:O	1:E:110:SER:OG	2.24	0.42
1:I:104:LYS:O	1:I:105:ASN:C	2.58	0.42
1:G:111:SER:N	1:G:142:ARG:NH2	2.66	0.42
1:K:209:SER:OG	1:K:210:ASN:N	2.53	0.42
1:O:306:ILE:HG12	1:O:320:LEU:HD12	2.01	0.42
1:A:96:VAL:HG12	1:A:96:VAL:O	2.19	0.42
1:A:33:ALA:O	1:A:37:PHE:HB3	2.20	0.42
1:E:315:ILE:HG22	1:E:315:ILE:O	2.19	0.42
1:E:30:SER:O	1:E:33:ALA:HB3	2.20	0.42
1:I:436:LEU:HG	1:I:436:LEU:O	2.07	0.42
1:O:220:GLN:HG2	1:O:226:TYR:HA	2.01	0.42
1:G:385:TYR:O	1:G:386:GLU:C	2.57	0.42
1:E:231:ASN:O	1:E:265:PHE:HA	2.20	0.42
1:A:244:LEU:CD1	1:A:250:ARG:HG3	2.30	0.42
1:E:83:GLN:O	1:E:84:TYR:C	2.57	0.42
1:C:23:VAL:HG12	1:C:94:VAL:HG11	2.00	0.42
1:O:384:ILE:HA	1:O:384:ILE:HD13	1.84	0.42
1:M:100:TYR:HB2	1:M:131:GLN:CD	2.39	0.42
1:I:197:TYR:CZ	1:I:198:LEU:HD21	2.55	0.42
1:E:125:LEU:HD11	1:E:427:PHE:CE2	2.55	0.42
1:I:62:GLN:O	1:I:65:GLU:N	2.53	0.42
1:C:174:ILE:HB	1:C:274:VAL:HG21	2.02	0.42
1:A:185:TRP:N	1:A:185:TRP:CD1	2.82	0.42
1:I:293:LEU:HB2	1:I:311:GLY:HA2	2.02	0.42
1:E:31:TRP:CH2	1:E:35:THR:HG21	2.55	0.42
1:A:53:TYR:O	1:A:54:ASN:ND2	2.52	0.42
1:G:184:GLY:N	1:G:282:GLY:O	2.50	0.42
1:I:43:LEU:C	1:I:45:SER:N	2.73	0.42
1:I:424:PHE:CD1	1:I:424:PHE:O	2.73	0.42
1:E:197:TYR:C	1:E:199:TYR:N	2.72	0.42
1:E:437:ILE:O	1:E:438:ASP:C	2.56	0.42
1:K:251:THR:C	1:K:253:GLU:N	2.73	0.42
1:I:103:VAL:O	1:I:104:LYS:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:VAL:HB	1:C:97:PRO:HD3	2.02	0.42
1:M:122:GLU:HA	1:M:150:CYS:HB3	2.01	0.42
1:A:195:PRO:HB3	1:A:197:TYR:CD2	2.55	0.42
1:G:20:VAL:HG21	1:G:40:ILE:HD12	2.01	0.42
1:C:75:PHE:HB2	1:C:81:PHE:HD1	1.84	0.42
1:M:166:ILE:O	1:M:168:GLU:N	2.52	0.42
1:M:313:VAL:HG12	1:M:314:GLU:HG3	2.02	0.42
1:E:149:ILE:HG23	1:E:151:LEU:HD13	2.01	0.42
1:E:430:ALA:O	1:E:434:HIS:HB2	2.19	0.42
1:K:151:LEU:C	1:K:153:GLY:H	2.22	0.42
1:G:310:ALA:C	1:G:312:PHE:H	2.24	0.42
1:A:257:LYS:CG	1:A:259:CYS:O	2.68	0.42
1:G:251:THR:HG22	1:G:252:LYS:N	2.35	0.42
1:I:454:LYS:O	1:I:455:ILE:C	2.57	0.42
1:A:179:ILE:HG22	1:A:180:SER:N	2.34	0.42
1:A:216:ILE:CG2	1:A:217:ASP:H	2.32	0.42
1:A:447:GLU:HG3	1:C:449:THR:HG22	2.00	0.42
1:C:111:SER:N	1:C:142:ARG:HH22	2.17	0.42
1:C:136:TYR:O	1:C:138:ILE:N	2.53	0.42
1:O:210:ASN:O	1:O:211:SER:C	2.57	0.42
1:G:147:THR:HB	1:G:427:PHE:CE1	2.54	0.42
1:G:213:GLY:O	1:G:216:ILE:HG22	2.19	0.42
1:G:427:PHE:O	1:G:428:LYS:C	2.56	0.42
1:O:381:ILE:CG2	1:O:385:TYR:CE1	3.03	0.42
1:M:138:ILE:HD13	1:M:138:ILE:HG21	1.52	0.42
1:M:325:ILE:HD11	1:M:328:GLY:HA2	2.02	0.42
1:A:185:TRP:CZ3	1:A:186:TYR:OH	2.68	0.42
1:E:281:LYS:CE	1:G:298:HIS:CD2	3.02	0.42
1:A:99:HIS:O	1:A:103:VAL:HG23	2.19	0.42
1:A:188:TYR:CZ	1:A:238:ILE:HG12	2.55	0.42
1:C:292:ASN:H	1:C:292:ASN:HD22	1.67	0.42
1:M:425:PRO:HA	1:M:429:ASP:OD2	2.20	0.42
1:I:224:GLY:HA2	1:I:419:PHE:CD2	2.54	0.42
1:A:218:VAL:HA	1:A:221:TYR:HB3	2.01	0.41
1:M:266:GLN:HB2	1:O:264:LEU:HD22	2.02	0.41
1:G:151:LEU:O	1:G:154:ARG:HG3	2.20	0.41
1:O:54:ASN:HB3	1:O:55:PRO:HD2	2.02	0.41
1:E:384:ILE:O	1:E:384:ILE:HG23	2.15	0.41
1:O:245:ASP:OD1	1:O:245:ASP:C	2.59	0.41
1:I:426:THR:O	1:I:429:ASP:N	2.53	0.41
1:M:120:TYR:HD2	1:M:121:VAL:N	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:176:SER:OG	1:K:177:ILE:N	2.52	0.41
1:K:152:GLN:N	1:K:152:GLN:HE21	2.17	0.41
1:K:96:VAL:N	1:K:97:PRO:CD	2.83	0.41
1:O:219:LEU:O	1:O:223:THR:HG23	2.20	0.41
1:A:320:LEU:HB3	1:A:369:PHE:HB3	2.02	0.41
1:C:171:ILE:HG22	1:C:302:GLY:CA	2.50	0.41
1:K:56:THR:HG21	1:O:196:GLU:HG2	2.02	0.41
1:K:146:GLN:OE1	1:K:424:PHE:HZ	2.03	0.41
1:M:18:ILE:HD12	1:M:47:PHE:CE2	2.55	0.41
1:C:436:LEU:CD1	1:C:452:VAL:HG11	2.50	0.41
1:G:216:ILE:O	1:G:219:LEU:N	2.51	0.41
1:I:208:ILE:HB	1:I:209:SER:H	1.46	0.41
1:M:314:GLU:HG3	1:M:314:GLU:H	1.28	0.41
1:A:312:PHE:HE1	2:B:853:MET:CE	2.33	0.41
2:B:853:MET:O	2:B:854:ASP:C	2.56	0.41
1:K:53:TYR:HB2	1:K:81:PHE:CD1	2.55	0.41
1:G:34:LYS:HG3	1:G:34:LYS:H	1.60	0.41
1:A:372:ARG:HH21	2:B:847:LEU:HB3	1.85	0.41
1:I:266:GLN:HB3	1:K:264:LEU:HD22	2.01	0.41
1:K:158:TYR:CG	1:K:318:LEU:HD12	2.54	0.41
1:A:245:ASP:O	1:A:246:GLU:C	2.59	0.41
1:A:219:LEU:C	1:A:221:TYR:N	2.71	0.41
1:I:79:GLU:HB3	1:I:80:SER:H	1.65	0.41
1:K:268:ILE:HG23	1:K:273:LYS:O	2.20	0.41
1:O:136:TYR:HD1	1:O:139:SER:OG	2.03	0.41
1:A:287:LYS:CB	1:A:287:LYS:HZ2	2.33	0.41
1:K:201:ILE:CG2	1:K:258:THR:HG21	2.50	0.41
1:C:287:LYS:N	1:C:292:ASN:OD1	2.53	0.41
1:I:165:LEU:HD23	1:I:165:LEU:HA	1.39	0.41
1:C:149:ILE:HD12	1:C:149:ILE:HA	1.88	0.41
1:E:176:SER:OG	1:E:177:ILE:N	2.53	0.41
1:G:135:LEU:HG	1:G:135:LEU:H	1.60	0.41
1:G:437:ILE:O	1:G:440:VAL:HG23	2.20	0.41
1:O:25:LEU:HD12	1:O:32:VAL:HG11	2.02	0.41
1:A:322:PHE:CG	1:A:323:TYR:N	2.87	0.41
1:A:198:LEU:HA	1:A:198:LEU:HD12	1.48	0.41
1:A:198:LEU:CB	1:A:199:TYR:CE1	3.03	0.41
1:O:138:ILE:HG21	1:O:138:ILE:HD13	1.73	0.41
1:C:82:ALA:CB	1:C:109:HIS:HB2	2.50	0.41
1:K:216:ILE:O	1:K:219:LEU:HB3	2.20	0.41
1:M:454:LYS:O	1:M:455:ILE:C	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:147:THR:HB	1:K:427:PHE:CE1	2.55	0.41
1:K:84:TYR:CZ	1:K:86:ASP:HB2	2.54	0.41
1:I:189:GLU:HG3	1:I:284:THR:OG1	2.21	0.41
1:O:190:ARG:HG3	1:O:199:TYR:OH	2.20	0.41
1:A:429:ASP:O	1:A:430:ALA:C	2.57	0.41
1:O:168:GLU:O	1:O:169:GLY:C	2.57	0.41
1:K:313:VAL:CG1	1:K:314:GLU:N	2.84	0.41
1:K:230:ILE:HG13	1:K:230:ILE:O	2.21	0.41
1:K:424:PHE:O	1:K:424:PHE:CD1	2.74	0.41
1:K:370:HIS:CD2	2:L:848:PHE:HD2	2.38	0.41
1:O:202:GLU:O	1:O:203:SER:C	2.58	0.41
1:O:113:ASN:OD1	1:O:114:LEU:N	2.53	0.41
1:K:113:ASN:OD1	1:K:114:LEU:N	2.54	0.41
1:C:100:TYR:O	1:C:104:LYS:HB2	2.20	0.41
1:I:272:GLY:O	1:I:273:LYS:HB2	2.20	0.41
1:O:123:TRP:HA	1:O:123:TRP:CE3	2.54	0.41
1:M:393:PHE:O	1:M:394:LEU:HD12	2.20	0.41
1:E:208:ILE:CA	1:E:212:PHE:HB3	2.51	0.41
1:E:279:SER:HB2	1:G:277:SER:CB	2.50	0.41
1:G:133:GLU:O	1:G:136:TYR:HB3	2.21	0.41
1:G:53:TYR:C	1:G:53:TYR:CD2	2.93	0.41
1:G:85:LYS:HE2	1:G:113:ASN:HA	2.02	0.41
1:I:231:ASN:C	1:I:231:ASN:ND2	2.74	0.41
1:M:54:ASN:O	1:M:75:PHE:O	2.38	0.41
1:K:182:ASN:HD21	1:K:283:GLY:C	2.23	0.41
1:I:322:PHE:CD2	1:I:367:GLU:HB3	2.45	0.41
1:E:318:LEU:H	1:E:318:LEU:HG	1.57	0.41
1:O:315:ILE:CG2	1:O:377:VAL:HG22	2.51	0.41
1:I:384:ILE:O	1:I:388:ILE:HG13	2.21	0.41
1:E:42:GLN:O	1:E:43:LEU:HD23	2.20	0.41
1:C:259:CYS:HA	1:C:260:PRO:HD2	1.91	0.41
1:C:273:LYS:HA	1:C:273:LYS:HD2	1.78	0.41
1:M:184:GLY:N	1:M:282:GLY:O	2.46	0.41
1:C:432:ILE:O	1:C:433:LEU:C	2.57	0.41
1:C:129:VAL:HA	1:C:434:HIS:HD2	1.85	0.41
1:I:54:ASN:HB3	1:I:55:PRO:HD2	2.01	0.41
1:G:216:ILE:HA	1:G:216:ILE:HD12	1.86	0.41
1:G:129:VAL:HA	1:G:434:HIS:HD2	1.86	0.41
1:G:432:ILE:HG22	1:G:455:ILE:HG13	2.02	0.41
1:A:147:THR:O	1:A:148:ILE:HG13	2.21	0.41
1:G:79:GLU:O	1:G:83:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:454:LYS:O	1:O:455:ILE:C	2.59	0.41
1:O:455:ILE:O	1:O:457:ILE:N	2.53	0.41
1:C:69:LEU:HB3	1:C:72:ALA:HB2	2.01	0.41
1:M:273:LYS:HD2	1:M:273:LYS:HA	1.84	0.41
1:E:319:VAL:HG13	1:E:370:HIS:HB2	2.01	0.41
1:O:18:ILE:HB	1:O:47:PHE:CD2	2.55	0.41
1:K:291:LYS:HA	1:K:291:LYS:HD2	1.51	0.41
1:M:148:ILE:HD13	1:M:388:ILE:HD11	2.01	0.41
1:C:301:LYS:N	1:C:301:LYS:HD2	2.36	0.41
1:K:169:GLY:O	1:K:328:GLY:HA3	2.20	0.41
1:I:147:THR:HB	1:I:427:PHE:CG	2.51	0.41
1:M:194:SER:HA	1:M:195:PRO:HD3	1.93	0.41
1:G:51:ALA:HB3	1:G:87:ILE:HD11	2.03	0.41
1:C:161:ARG:HG3	1:C:161:ARG:O	2.19	0.41
1:K:177:ILE:HG21	1:K:219:LEU:HD11	2.03	0.41
1:C:427:PHE:HA	1:C:430:ALA:HB3	2.01	0.41
1:G:274:VAL:HA	1:G:275:PRO:HD3	1.81	0.41
1:A:100:TYR:O	1:A:101:GLU:C	2.57	0.41
1:O:375:ASN:OD1	1:O:377:VAL:HB	2.20	0.41
2:F:853:MET:O	2:F:854:ASP:C	2.59	0.41
1:A:54:ASN:O	1:A:75:PHE:O	2.39	0.41
1:M:279:SER:HB2	1:O:277:SER:CB	2.50	0.41
1:A:90:ILE:HD12	1:A:116:LEU:CD1	2.50	0.41
1:C:252:LYS:H	1:C:252:LYS:HG3	1.41	0.41
1:E:177:ILE:CG2	1:E:178:GLU:N	2.77	0.41
1:E:276:VAL:HG12	1:E:277:SER:N	2.36	0.41
1:E:217:ASP:HB2	1:E:433:LEU:HD22	2.03	0.41
1:G:53:TYR:N	1:G:81:PHE:CE1	2.89	0.41
1:M:208:ILE:HB	1:M:209:SER:H	1.62	0.41
1:C:320:LEU:O	1:C:369:PHE:N	2.46	0.41
1:G:40:ILE:HG23	1:G:47:PHE:HB2	2.02	0.41
1:C:117:ARG:HB2	1:C:118:TYR:CE1	2.56	0.41
1:C:18:ILE:HD11	1:C:392:HIS:CD2	2.55	0.41
1:M:166:ILE:O	1:M:169:GLY:N	2.54	0.41
1:E:427:PHE:O	1:E:431:ILE:HB	2.20	0.41
1:K:208:ILE:HG13	1:K:263:LEU:HD22	2.03	0.41
1:M:268:ILE:CG2	1:M:273:LYS:O	2.68	0.41
1:E:454:LYS:O	1:E:455:ILE:C	2.59	0.41
1:O:151:LEU:C	1:O:153:GLY:N	2.74	0.41
1:M:322:PHE:CD2	1:M:367:GLU:HB3	2.49	0.41
1:K:162:ALA:O	1:K:166:ILE:HD12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:857:TYR:HA	2:P:860:ILE:HG22	2.03	0.41
1:C:432:ILE:CG2	1:C:455:ILE:HG22	2.51	0.41
1:C:152:GLN:HE22	1:C:214:HIS:HE1	1.69	0.41
1:G:389:ALA:O	1:G:392:HIS:N	2.54	0.41
1:I:228:GLN:HB3	1:I:268:ILE:O	2.21	0.41
1:O:234:ILE:HG12	1:O:263:LEU:HB2	2.03	0.41
1:G:437:ILE:O	1:G:438:ASP:C	2.55	0.41
1:E:216:ILE:HG23	1:E:217:ASP:N	2.35	0.41
1:E:263:LEU:HD11	1:E:265:PHE:HB2	2.03	0.41
1:G:100:TYR:O	1:G:101:GLU:C	2.59	0.41
1:G:159:ILE:HG23	1:G:159:ILE:HD12	1.86	0.41
1:E:233:MET:HE1	1:G:231:ASN:HB3	2.02	0.41
1:G:179:ILE:HB	1:G:278:CYS:HB2	2.03	0.41
1:E:392:HIS:C	1:E:394:LEU:H	2.24	0.41
1:A:130:GLN:HA	1:A:133:GLU:CB	2.35	0.41
1:A:134:GLU:C	1:A:136:TYR:N	2.74	0.41
1:I:88:ASP:HA	1:I:115:ASN:O	2.20	0.41
1:I:142:ARG:HB2	1:I:145:LEU:HB3	2.02	0.41
1:A:64:ILE:HG22	1:A:65:GLU:N	2.36	0.41
1:M:198:LEU:HA	1:M:198:LEU:HD12	1.67	0.41
1:G:25:LEU:HA	1:G:25:LEU:HD12	1.60	0.41
1:M:208:ILE:O	1:M:209:SER:C	2.59	0.41
1:M:456:MET:N	1:M:456:MET:SD	2.92	0.41
1:A:229:LYS:HE3	1:C:233:MET:CE	2.50	0.41
1:E:152:GLN:O	1:E:153:GLY:C	2.57	0.41
1:G:104:LYS:O	1:G:107:LEU:N	2.54	0.41
1:C:105:ASN:N	1:C:105:ASN:ND2	2.69	0.41
1:C:315:ILE:CG2	1:C:377:VAL:HG22	2.51	0.41
1:O:319:VAL:HG22	1:O:370:HIS:CB	2.50	0.41
1:K:216:ILE:CG2	1:K:217:ASP:H	2.34	0.41
1:K:79:GLU:O	1:K:83:GLN:HG3	2.21	0.41
1:I:96:VAL:HB	1:I:97:PRO:CD	2.50	0.41
1:O:216:ILE:O	1:O:219:LEU:N	2.50	0.41
1:A:103:VAL:O	1:A:106:ILE:HB	2.20	0.41
1:O:195:PRO:HB3	1:O:197:TYR:CD2	2.56	0.41
1:I:381:ILE:O	1:I:382:LEU:C	2.58	0.41
1:K:30:SER:O	1:K:31:TRP:C	2.58	0.41
1:A:25:LEU:CB	1:A:52:LEU:HD11	2.51	0.41
2:N:853:MET:O	2:N:856:VAL:N	2.54	0.41
1:O:314:GLU:HG3	1:O:314:GLU:H	1.21	0.41
1:E:245:ASP:OD1	1:E:245:ASP:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:450:LEU:N	1:E:450:LEU:HD23	2.36	0.41
1:K:190:ARG:HG3	1:K:199:TYR:CE2	2.55	0.41
1:K:171:ILE:HD12	1:K:299:GLY:HA3	2.03	0.41
1:A:32:VAL:HG23	1:A:32:VAL:H	1.48	0.41
1:G:230:ILE:HG13	1:G:230:ILE:O	2.20	0.41
1:K:23:VAL:HG12	1:K:23:VAL:O	2.20	0.41
1:G:41:GLN:HB3	1:G:41:GLN:HE21	1.73	0.41
1:C:124:ALA:HB1	1:C:434:HIS:CE1	2.53	0.41
1:O:84:TYR:CZ	1:O:86:ASP:HB2	2.54	0.41
1:G:245:ASP:N	1:G:249:LYS:O	2.54	0.41
1:M:245:ASP:N	1:M:249:LYS:O	2.53	0.41
1:E:105:ASN:N	1:E:105:ASN:ND2	2.69	0.41
1:E:88:ASP:OD1	1:E:115:ASN:HB3	2.21	0.41
1:A:36:HIS:ND1	1:A:385:TYR:OH	2.45	0.41
1:I:320:LEU:N	1:I:369:PHE:O	2.29	0.41
1:M:69:LEU:HB3	1:M:72:ALA:HB2	2.03	0.41
1:C:16:ARG:CB	1:C:17:PRO:CD	2.98	0.41
1:G:102:VAL:O	1:G:106:ILE:HD12	2.21	0.41
1:I:230:ILE:HG22	1:I:267:GLY:HA3	2.02	0.41
1:A:90:ILE:HD12	1:A:116:LEU:HD11	2.03	0.41
2:N:848:PHE:N	2:N:848:PHE:CD1	2.89	0.41
1:C:208:ILE:H	1:C:208:ILE:CD1	2.32	0.40
1:E:190:ARG:CG	1:E:191:PRO:N	2.84	0.40
1:G:436:LEU:O	1:G:440:VAL:HG23	2.22	0.40
1:I:149:ILE:HB	1:I:430:ALA:HB2	2.03	0.40
1:G:81:PHE:C	1:G:83:GLN:H	2.25	0.40
1:A:322:PHE:C	1:A:322:PHE:CD2	2.94	0.40
1:K:315:ILE:O	1:K:376:SER:OG	2.25	0.40
1:C:182:ASN:ND2	1:C:283:GLY:CA	2.79	0.40
1:E:111:SER:CA	1:E:142:ARG:NH2	2.85	0.40
1:O:187:GLY:O	1:O:238:ILE:HG21	2.22	0.40
1:C:309:ASP:OD2	2:D:850:THR:OG1	2.32	0.40
1:C:113:ASN:O	1:C:114:LEU:HG	2.21	0.40
1:C:136:TYR:O	1:C:139:SER:N	2.54	0.40
1:M:389:ALA:HA	1:M:392:HIS:HB3	2.02	0.40
1:K:245:ASP:N	1:K:249:LYS:O	2.46	0.40
1:K:433:LEU:O	1:K:436:LEU:N	2.54	0.40
1:C:238:ILE:HD12	1:C:261:ASP:HB3	1.97	0.40
1:O:385:TYR:O	1:O:388:ILE:HB	2.20	0.40
1:C:159:ILE:O	1:C:161:ARG:N	2.55	0.40
1:I:216:ILE:HD11	1:I:227:PHE:CE1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:TYR:CD2	1:C:54:ASN:N	2.90	0.40
1:M:183:GLY:O	1:M:312:PHE:HZ	2.04	0.40
1:O:290:THR:HG22	1:O:291:LYS:O	2.21	0.40
1:E:435:ARG:NH1	1:E:455:ILE:O	2.54	0.40
1:I:96:VAL:N	1:I:97:PRO:CD	2.75	0.40
1:A:291:LYS:HA	1:A:291:LYS:HD2	1.75	0.40
1:O:201:ILE:CG2	1:O:258:THR:HG21	2.51	0.40
1:E:424:PHE:C	1:E:424:PHE:CD1	2.95	0.40
1:I:274:VAL:HA	1:I:275:PRO:HD3	1.77	0.40
1:C:57:LEU:HD22	1:C:61:LEU:CD1	2.51	0.40
1:E:61:LEU:HD21	1:K:242:PHE:CZ	2.56	0.40
1:G:38:LEU:HD23	1:G:38:LEU:HA	1.07	0.40
1:K:90:ILE:HD13	1:K:90:ILE:HG21	1.91	0.40
1:C:38:LEU:HD23	1:C:38:LEU:HA	1.11	0.40
1:A:85:LYS:HD2	1:A:112:GLN:HE22	1.85	0.40
1:O:23:VAL:HG12	1:O:94:VAL:HG13	2.02	0.40
1:K:138:ILE:O	1:K:139:SER:C	2.59	0.40
1:E:84:TYR:C	1:E:86:ASP:N	2.74	0.40
1:I:123:TRP:CE3	1:I:123:TRP:HA	2.57	0.40
1:A:263:LEU:HD12	1:A:264:LEU:CA	2.51	0.40
1:O:100:TYR:CB	1:O:131:GLN:CD	2.88	0.40
1:O:147:THR:HB	1:O:427:PHE:CE1	2.56	0.40
1:G:120:TYR:C	1:G:121:VAL:HG23	2.40	0.40
1:E:162:ALA:HB1	1:E:304:LEU:HD11	2.03	0.40
1:E:149:ILE:HD13	1:E:430:ALA:HB2	2.02	0.40
1:M:117:ARG:O	1:M:145:LEU:HD12	2.21	0.40
1:M:31:TRP:CH2	1:M:35:THR:HG21	2.57	0.40
1:G:195:PRO:HB3	1:G:197:TYR:CE2	2.57	0.40
1:I:237:ASN:H	1:I:261:ASP:CG	2.20	0.40
1:A:225:SER:HB2	1:A:271:ASN:CG	2.42	0.40
1:O:424:PHE:CD1	1:O:424:PHE:C	2.95	0.40
1:M:426:THR:N	1:M:429:ASP:OD2	2.47	0.40
1:K:113:ASN:O	1:K:114:LEU:HG	2.21	0.40
1:G:162:ALA:O	1:G:166:ILE:HD12	2.22	0.40
1:G:166:ILE:O	1:G:169:GLY:N	2.54	0.40
1:G:426:THR:O	1:G:429:ASP:N	2.54	0.40
1:K:454:LYS:O	1:K:457:ILE:HB	2.22	0.40
1:C:244:LEU:HA	1:C:244:LEU:HD12	1.82	0.40
1:A:262:HIS:CE1	1:C:176:SER:CB	3.04	0.40
1:A:195:PRO:CB	1:A:197:TYR:CE2	3.04	0.40
1:C:392:HIS:O	1:C:394:LEU:N	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:177:ILE:HA	1:K:296:ASP:O	2.21	0.40
1:K:78:LEU:O	1:K:81:PHE:CB	2.67	0.40
1:M:263:LEU:C	1:M:263:LEU:HD12	2.42	0.40
1:A:372:ARG:HH22	2:B:847:LEU:HD23	1.80	0.40
1:I:433:LEU:HB3	1:I:434:HIS:H	1.78	0.40
1:K:186:TYR:OH	1:K:206:ASN:HA	2.22	0.40
1:O:438:ASP:O	1:O:439:ALA:C	2.60	0.40
1:C:269:LEU:HD23	1:C:269:LEU:HA	1.94	0.40
1:O:68:GLN:O	1:O:70:LYS:N	2.55	0.40
1:I:121:VAL:CG2	1:I:427:PHE:HZ	2.34	0.40
1:M:134:GLU:O	1:M:136:TYR:N	2.55	0.40
1:C:320:LEU:HB3	1:C:369:PHE:HB3	2.03	0.40
1:O:454:LYS:O	1:O:457:ILE:HB	2.21	0.40
1:C:390:ASP:C	1:C:392:HIS:N	2.71	0.40
1:C:87:ILE:HG21	1:C:90:ILE:HG13	2.03	0.40
1:C:77:SER:O	1:C:80:SER:HB2	2.21	0.40
1:K:201:ILE:HB	1:K:258:THR:CG2	2.51	0.40
1:K:56:THR:CG2	1:O:196:GLU:HG2	2.52	0.40
1:O:190:ARG:HA	1:O:191:PRO:HD3	1.59	0.40
1:K:304:LEU:CD2	1:K:320:LEU:HD21	2.52	0.40
1:M:373:ASN:HD22	1:M:373:ASN:C	2.24	0.40
2:N:852:THR:HG22	2:N:853:MET:N	2.36	0.40
1:M:165:LEU:HA	1:M:165:LEU:HD23	1.17	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	389/465 (84%)	301 (77%)	73 (19%)	15 (4%)	4	21
1	C	387/465 (83%)	299 (77%)	71 (18%)	17 (4%)	3	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	387/465 (83%)	300 (78%)	67 (17%)	20 (5%)	2	15
1	G	387/465 (83%)	301 (78%)	75 (19%)	11 (3%)	6	30
1	I	387/465 (83%)	303 (78%)	70 (18%)	14 (4%)	4	24
1	K	387/465 (83%)	305 (79%)	66 (17%)	16 (4%)	3	20
1	M	387/465 (83%)	308 (80%)	68 (18%)	11 (3%)	6	30
1	O	387/465 (83%)	309 (80%)	67 (17%)	11 (3%)	6	30
2	B	12/22 (54%)	9 (75%)	2 (17%)	1 (8%)	1	5
2	D	12/22 (54%)	10 (83%)	1 (8%)	1 (8%)	1	5
2	F	12/22 (54%)	10 (83%)	2 (17%)	0	100	100
2	H	12/22 (54%)	10 (83%)	1 (8%)	1 (8%)	1	5
2	J	12/22 (54%)	11 (92%)	1 (8%)	0	100	100
2	L	12/22 (54%)	10 (83%)	1 (8%)	1 (8%)	1	5
2	N	12/22 (54%)	11 (92%)	1 (8%)	0	100	100
2	P	12/22 (54%)	9 (75%)	2 (17%)	1 (8%)	1	5
All	All	3194/3896 (82%)	2506 (78%)	568 (18%)	120 (4%)	4	22

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	PRO
1	A	37	PHE
1	A	42	GLN
1	A	82	ALA
1	A	201	ILE
1	A	246	GLU
1	A	252	LYS
1	A	390	ASP
1	C	15	SER
1	C	17	PRO
1	C	82	ALA
1	C	246	GLU
1	C	252	LYS
1	C	390	ASP
1	E	246	GLU
1	E	252	LYS
1	E	326	LYS
1	G	17	PRO

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Mol	Chain	Res	Type
1	G	82	ALA
1	G	102	VAL
1	G	246	GLU
1	G	252	LYS
1	I	17	PRO
1	I	102	VAL
1	I	208	ILE
1	I	246	GLU
1	K	82	ALA
1	K	152	GLN
1	K	208	ILE
1	K	246	GLU
1	K	252	LYS
1	M	17	PRO
1	M	82	ALA
1	M	208	ILE
1	M	246	GLU
1	M	252	LYS
1	O	82	ALA
1	O	246	GLU
1	O	252	LYS
1	A	102	VAL
1	C	102	VAL
1	C	201	ILE
2	D	856	VAL
1	E	17	PRO
1	E	37	PHE
1	E	82	ALA
1	E	84	TYR
1	E	169	GLY
1	E	201	ILE
1	G	154	ARG
1	G	169	GLY
2	H	856	VAL
1	I	82	ALA
1	I	154	ARG
1	I	169	GLY
1	I	209	SER
1	K	102	VAL
1	K	169	GLY
1	K	191	PRO
1	K	455	ILE

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Mol	Chain	Res	Type
1	M	167	SER
1	O	17	PRO
1	O	143	ALA
1	O	169	GLY
1	O	456	MET
1	C	84	TYR
1	C	101	GLU
1	C	387	SER
1	E	207	LEU
1	E	256	SER
1	E	392	HIS
1	E	456	MET
1	G	387	SER
1	I	55	PRO
1	I	252	LYS
2	L	856	VAL
1	O	58	LYS
1	O	208	ILE
1	O	392	HIS
1	A	81	PHE
1	A	326	LYS
1	C	81	PHE
1	C	95	LYS
1	C	391	TYR
1	K	17	PRO
1	K	81	PHE
1	K	209	SER
1	K	433	LEU
2	P	856	VAL
1	A	207	LEU
1	C	215	THR
1	C	393	PHE
1	E	101	GLU
1	E	116	LEU
1	E	160	VAL
1	E	311	GLY
1	E	387	SER
1	G	95	LYS
1	K	84	TYR
1	K	160	VAL
1	M	271	ASN
1	O	271	ASN

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Mol	Chain	Res	Type
1	A	103	VAL
1	A	311	GLY
1	A	372	ARG
1	E	139	SER
1	G	101	GLU
1	I	84	TYR
1	K	393	PHE
1	M	390	ASP
2	B	856	VAL
1	I	160	VAL
1	M	129	VAL
1	M	455	ILE
1	G	201	ILE
1	I	275	PRO
1	I	455	ILE
1	C	208	ILE
1	E	96	VAL
1	M	160	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	350/411 (85%)	251 (72%)	99 (28%)	0	2
1	C	348/411 (85%)	259 (74%)	89 (26%)	0	3
1	E	348/411 (85%)	251 (72%)	97 (28%)	0	2
1	G	348/411 (85%)	247 (71%)	101 (29%)	0	2
1	I	348/411 (85%)	254 (73%)	94 (27%)	0	3
1	K	348/411 (85%)	258 (74%)	90 (26%)	0	3
1	M	348/411 (85%)	248 (71%)	100 (29%)	0	2
1	O	348/411 (85%)	254 (73%)	94 (27%)	0	3
2	B	14/22 (64%)	13 (93%)	1 (7%)	18	54
2	D	14/22 (64%)	11 (79%)	3 (21%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	14/22 (64%)	13 (93%)	1 (7%)	18	54
2	H	14/22 (64%)	11 (79%)	3 (21%)	1	6
2	J	14/22 (64%)	9 (64%)	5 (36%)	0	1
2	L	14/22 (64%)	12 (86%)	2 (14%)	4	19
2	N	14/22 (64%)	11 (79%)	3 (21%)	1	6
2	P	14/22 (64%)	12 (86%)	2 (14%)	4	19
All	All	2898/3464 (84%)	2114 (73%)	784 (27%)	0	2

All (784) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	16	ARG
1	A	19	ARG
1	A	20	VAL
1	A	45	SER
1	A	46	GLN
1	A	48	GLN
1	A	58	LYS
1	A	59	SER
1	A	62	GLN
1	A	65	GLU
1	A	70	LYS
1	A	79	GLU
1	A	84	TYR
1	A	89	MET
1	A	93	SER
1	A	98	GLU
1	A	99	HIS
1	A	105	ASN
1	A	108	GLU
1	A	111	SER
1	A	114	LEU
1	A	115	ASN
1	A	117	ARG
1	A	118	TYR
1	A	130	GLN
1	A	137	SER
1	A	141	GLN
1	A	142	ARG

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Mol	Chain	Res	Type
1	A	145	LEU
1	A	147	THR
1	A	152	GLN
1	A	156	SER
1	A	174	ILE
1	A	180	SER
1	A	182	ASN
1	A	185	TRP
1	A	193	ARG
1	A	196	GLU
1	A	198	LEU
1	A	199	TYR
1	A	201	ILE
1	A	211	SER
1	A	218	VAL
1	A	219	LEU
1	A	225	SER
1	A	235	SER
1	A	236	ASN
1	A	240	THR
1	A	241	GLN
1	A	243	LEU
1	A	244	LEU
1	A	250	ARG
1	A	253	GLU
1	A	256	SER
1	A	258	THR
1	A	261	ASP
1	A	263	LEU
1	A	277	SER
1	A	278	CYS
1	A	279	SER
1	A	280	PHE
1	A	281	LYS
1	A	286	VAL
1	A	287	LYS
1	A	288	LYS
1	A	292	ASN
1	A	303	ASP
1	A	304	LEU
1	A	305	LYS
1	A	314	GLU

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Mol	Chain	Res	Type
1	A	318	LEU
1	A	322	PHE
1	A	364	GLN
1	A	366	MET
1	A	367	GLU
1	A	372	ARG
1	A	373	ASN
1	A	382	LEU
1	A	383	ARG
1	A	387	SER
1	A	394	LEU
1	A	414	PHE
1	A	416	LYS
1	A	422	GLU
1	A	428	LYS
1	A	431	ILE
1	A	432	ILE
1	A	434	HIS
1	A	435	ARG
1	A	442	ARG
1	A	444	ASP
1	A	447	GLU
1	A	448	LYS
1	A	449	THR
1	A	452	VAL
1	A	454	LYS
1	A	455	ILE
1	A	456	MET
2	B	857	TYR
1	C	14	SER
1	C	16	ARG
1	C	18	ILE
1	C	20	VAL
1	C	22	PHE
1	C	42	GLN
1	C	45	SER
1	C	46	GLN
1	C	52	LEU
1	C	58	LYS
1	C	59	SER
1	C	61	LEU
1	C	65	GLU

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Mol	Chain	Res	Type
1	C	70	LYS
1	C	76	ASP
1	C	89	MET
1	C	99	HIS
1	C	108	GLU
1	C	111	SER
1	C	114	LEU
1	C	115	ASN
1	C	116	LEU
1	C	118	TYR
1	C	128	SER
1	C	130	GLN
1	C	131	GLN
1	C	133	GLU
1	C	137	SER
1	C	141	GLN
1	C	152	GLN
1	C	174	ILE
1	C	180	SER
1	C	182	ASN
1	C	185	TRP
1	C	193	ARG
1	C	196	GLU
1	C	198	LEU
1	C	199	TYR
1	C	200	ASP
1	C	202	GLU
1	C	207	LEU
1	C	218	VAL
1	C	219	LEU
1	C	240	THR
1	C	241	GLN
1	C	243	LEU
1	C	244	LEU
1	C	249	LYS
1	C	250	ARG
1	C	253	GLU
1	C	257	LYS
1	C	258	THR
1	C	261	ASP
1	C	263	LEU
1	C	264	LEU

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Mol	Chain	Res	Type
1	C	277	SER
1	C	278	CYS
1	C	280	PHE
1	C	281	LYS
1	C	287	LYS
1	C	288	LYS
1	C	292	ASN
1	C	303	ASP
1	C	304	LEU
1	C	305	LYS
1	C	314	GLU
1	C	318	LEU
1	C	320	LEU
1	C	322	PHE
1	C	364	GLN
1	C	366	MET
1	C	367	GLU
1	C	373	ASN
1	C	382	LEU
1	C	387	SER
1	C	394	LEU
1	C	413	LYS
1	C	414	PHE
1	C	416	LYS
1	C	428	LYS
1	C	431	ILE
1	C	434	HIS
1	C	435	ARG
1	C	442	ARG
1	C	444	ASP
1	C	447	GLU
1	C	448	LYS
1	C	450	LEU
1	C	456	MET
2	D	847	LEU
2	D	849	ASN
2	D	859	TYR
1	E	15	SER
1	E	16	ARG
1	E	18	ILE
1	E	19	ARG
1	E	20	VAL

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Mol	Chain	Res	Type
1	E	22	PHE
1	E	25	LEU
1	E	29	LYS
1	E	45	SER
1	E	46	GLN
1	E	50	VAL
1	E	52	LEU
1	E	58	LYS
1	E	59	SER
1	E	62	GLN
1	E	65	GLU
1	E	70	LYS
1	E	75	PHE
1	E	76	ASP
1	E	77	SER
1	E	78	LEU
1	E	80	SER
1	E	84	TYR
1	E	89	MET
1	E	98	GLU
1	E	99	HIS
1	E	108	GLU
1	E	111	SER
1	E	116	LEU
1	E	117	ARG
1	E	120	TYR
1	E	130	GLN
1	E	131	GLN
1	E	152	GLN
1	E	161	ARG
1	E	173	ASP
1	E	174	ILE
1	E	180	SER
1	E	185	TRP
1	E	193	ARG
1	E	195	PRO
1	E	196	GLU
1	E	198	LEU
1	E	199	TYR
1	E	200	ASP
1	E	202	GLU
1	E	207	LEU

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Mol	Chain	Res	Type
1	E	210	ASN
1	E	214	HIS
1	E	218	VAL
1	E	225	SER
1	E	229	LYS
1	E	235	SER
1	E	236	ASN
1	E	240	THR
1	E	241	GLN
1	E	243	LEU
1	E	244	LEU
1	E	245	ASP
1	E	253	GLU
1	E	257	LYS
1	E	258	THR
1	E	261	ASP
1	E	263	LEU
1	E	273	LYS
1	E	277	SER
1	E	278	CYS
1	E	280	PHE
1	E	281	LYS
1	E	288	LYS
1	E	303	ASP
1	E	304	LEU
1	E	314	GLU
1	E	318	LEU
1	E	320	LEU
1	E	322	PHE
1	E	366	MET
1	E	367	GLU
1	E	373	ASN
1	E	381	ILE
1	E	382	LEU
1	E	384	ILE
1	E	387	SER
1	E	394	LEU
1	E	414	PHE
1	E	422	GLU
1	E	428	LYS
1	E	431	ILE
1	E	434	HIS

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Mol	Chain	Res	Type
1	E	436	LEU
1	E	442	ARG
1	E	443	SER
1	E	447	GLU
1	E	450	LEU
1	E	454	LYS
1	E	455	ILE
1	E	456	MET
2	F	847	LEU
1	G	16	ARG
1	G	19	ARG
1	G	20	VAL
1	G	22	PHE
1	G	40	ILE
1	G	41	GLN
1	G	45	SER
1	G	46	GLN
1	G	52	LEU
1	G	57	LEU
1	G	58	LYS
1	G	59	SER
1	G	61	LEU
1	G	65	GLU
1	G	70	LYS
1	G	75	PHE
1	G	76	ASP
1	G	77	SER
1	G	80	SER
1	G	84	TYR
1	G	86	ASP
1	G	89	MET
1	G	98	GLU
1	G	99	HIS
1	G	108	GLU
1	G	111	SER
1	G	116	LEU
1	G	117	ARG
1	G	118	TYR
1	G	128	SER
1	G	130	GLN
1	G	131	GLN
1	G	147	THR

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Mol	Chain	Res	Type
1	G	151	LEU
1	G	152	GLN
1	G	154	ARG
1	G	163	LYS
1	G	178	GLU
1	G	180	SER
1	G	185	TRP
1	G	188	TYR
1	G	192	MET
1	G	193	ARG
1	G	196	GLU
1	G	198	LEU
1	G	200	ASP
1	G	201	ILE
1	G	202	GLU
1	G	207	LEU
1	G	211	SER
1	G	218	VAL
1	G	225	SER
1	G	228	GLN
1	G	235	SER
1	G	236	ASN
1	G	240	THR
1	G	241	GLN
1	G	250	ARG
1	G	253	GLU
1	G	257	LYS
1	G	258	THR
1	G	261	ASP
1	G	263	LEU
1	G	268	ILE
1	G	276	VAL
1	G	277	SER
1	G	278	CYS
1	G	280	PHE
1	G	281	LYS
1	G	286	VAL
1	G	287	LYS
1	G	288	LYS
1	G	303	ASP
1	G	304	LEU
1	G	305	LYS

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Mol	Chain	Res	Type
1	G	314	GLU
1	G	318	LEU
1	G	322	PHE
1	G	364	GLN
1	G	366	MET
1	G	367	GLU
1	G	372	ARG
1	G	373	ASN
1	G	374	TYR
1	G	382	LEU
1	G	387	SER
1	G	414	PHE
1	G	416	LYS
1	G	422	GLU
1	G	428	LYS
1	G	431	ILE
1	G	432	ILE
1	G	434	HIS
1	G	435	ARG
1	G	442	ARG
1	G	447	GLU
1	G	448	LYS
1	G	450	LEU
1	G	454	LYS
1	G	455	ILE
1	G	456	MET
2	H	847	LEU
2	H	855	ASP
2	H	859	TYR
1	I	15	SER
1	I	18	ILE
1	I	19	ARG
1	I	20	VAL
1	I	22	PHE
1	I	25	LEU
1	I	34	LYS
1	I	41	GLN
1	I	45	SER
1	I	46	GLN
1	I	50	VAL
1	I	52	LEU
1	I	53	TYR

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Mol	Chain	Res	Type
1	I	58	LYS
1	I	59	SER
1	I	61	LEU
1	I	65	GLU
1	I	75	PHE
1	I	79	GLU
1	I	84	TYR
1	I	89	MET
1	I	93	SER
1	I	98	GLU
1	I	99	HIS
1	I	108	GLU
1	I	111	SER
1	I	115	ASN
1	I	116	LEU
1	I	118	TYR
1	I	119	LEU
1	I	131	GLN
1	I	137	SER
1	I	138	ILE
1	I	141	GLN
1	I	151	LEU
1	I	152	GLN
1	I	174	ILE
1	I	180	SER
1	I	182	ASN
1	I	185	TRP
1	I	193	ARG
1	I	196	GLU
1	I	200	ASP
1	I	209	SER
1	I	214	HIS
1	I	218	VAL
1	I	235	SER
1	I	240	THR
1	I	241	GLN
1	I	243	LEU
1	I	244	LEU
1	I	250	ARG
1	I	252	LYS
1	I	253	GLU
1	I	254	THR

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Mol	Chain	Res	Type
1	I	258	THR
1	I	261	ASP
1	I	263	LEU
1	I	277	SER
1	I	280	PHE
1	I	281	LYS
1	I	287	LYS
1	I	292	ASN
1	I	303	ASP
1	I	304	LEU
1	I	309	ASP
1	I	314	GLU
1	I	316	SER
1	I	318	LEU
1	I	320	LEU
1	I	322	PHE
1	I	363	GLU
1	I	364	GLN
1	I	366	MET
1	I	367	GLU
1	I	372	ARG
1	I	373	ASN
1	I	382	LEU
1	I	383	ARG
1	I	387	SER
1	I	413	LYS
1	I	415	ASP
1	I	422	GLU
1	I	428	LYS
1	I	431	ILE
1	I	432	ILE
1	I	434	HIS
1	I	435	ARG
1	I	442	ARG
1	I	444	ASP
1	I	447	GLU
1	I	448	LYS
1	I	450	LEU
1	I	456	MET
2	J	847	LEU
2	J	855	ASP
2	J	857	TYR

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Mol	Chain	Res	Type
2	J	859	TYR
2	J	860	ILE
1	K	19	ARG
1	K	22	PHE
1	K	38	LEU
1	K	40	ILE
1	K	44	SER
1	K	45	SER
1	K	46	GLN
1	K	57	LEU
1	K	58	LYS
1	K	59	SER
1	K	61	LEU
1	K	65	GLU
1	K	70	LYS
1	K	73	THR
1	K	76	ASP
1	K	80	SER
1	K	84	TYR
1	K	89	MET
1	K	99	HIS
1	K	105	ASN
1	K	107	LEU
1	K	111	SER
1	K	114	LEU
1	K	115	ASN
1	K	116	LEU
1	K	117	ARG
1	K	130	GLN
1	K	141	GLN
1	K	142	ARG
1	K	147	THR
1	K	152	GLN
1	K	166	ILE
1	K	168	GLU
1	K	178	GLU
1	K	180	SER
1	K	185	TRP
1	K	196	GLU
1	K	199	TYR
1	K	200	ASP
1	K	207	LEU

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Mol	Chain	Res	Type
1	K	211	SER
1	K	216	ILE
1	K	218	VAL
1	K	219	LEU
1	K	235	SER
1	K	236	ASN
1	K	240	THR
1	K	241	GLN
1	K	244	LEU
1	K	253	GLU
1	K	258	THR
1	K	261	ASP
1	K	263	LEU
1	K	264	LEU
1	K	273	LYS
1	K	278	CYS
1	K	280	PHE
1	K	281	LYS
1	K	287	LYS
1	K	291	LYS
1	K	292	ASN
1	K	303	ASP
1	K	305	LYS
1	K	314	GLU
1	K	318	LEU
1	K	322	PHE
1	K	364	GLN
1	K	366	MET
1	K	367	GLU
1	K	373	ASN
1	K	382	LEU
1	K	386	GLU
1	K	387	SER
1	K	394	LEU
1	K	414	PHE
1	K	416	LYS
1	K	422	GLU
1	K	428	LYS
1	K	431	ILE
1	K	432	ILE
1	K	434	HIS
1	K	435	ARG

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Mol	Chain	Res	Type
1	K	442	ARG
1	K	444	ASP
1	K	447	GLU
1	K	448	LYS
1	K	449	THR
1	K	450	LEU
1	K	454	LYS
1	K	456	MET
2	L	847	LEU
2	L	859	TYR
1	M	14	SER
1	M	19	ARG
1	M	20	VAL
1	M	22	PHE
1	M	34	LYS
1	M	45	SER
1	M	46	GLN
1	M	58	LYS
1	M	59	SER
1	M	64	ILE
1	M	65	GLU
1	M	70	LYS
1	M	76	ASP
1	M	86	ASP
1	M	89	MET
1	M	93	SER
1	M	98	GLU
1	M	105	ASN
1	M	106	ILE
1	M	108	GLU
1	M	111	SER
1	M	114	LEU
1	M	115	ASN
1	M	116	LEU
1	M	117	ARG
1	M	118	TYR
1	M	120	TYR
1	M	128	SER
1	M	141	GLN
1	M	152	GLN
1	M	154	ARG
1	M	157	PRO

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Mol	Chain	Res	Type
1	M	174	ILE
1	M	178	GLU
1	M	180	SER
1	M	182	ASN
1	M	185	TRP
1	M	193	ARG
1	M	195	PRO
1	M	196	GLU
1	M	198	LEU
1	M	199	TYR
1	M	202	GLU
1	M	207	LEU
1	M	209	SER
1	M	225	SER
1	M	231	ASN
1	M	235	SER
1	M	236	ASN
1	M	240	THR
1	M	241	GLN
1	M	243	LEU
1	M	244	LEU
1	M	245	ASP
1	M	250	ARG
1	M	252	LYS
1	M	253	GLU
1	M	255	ILE
1	M	258	THR
1	M	261	ASP
1	M	263	LEU
1	M	265	PHE
1	M	268	ILE
1	M	277	SER
1	M	278	CYS
1	M	280	PHE
1	M	281	LYS
1	M	287	LYS
1	M	288	LYS
1	M	291	LYS
1	M	292	ASN
1	M	303	ASP
1	M	304	LEU
1	M	305	LYS

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Mol	Chain	Res	Type
1	M	306	ILE
1	M	314	GLU
1	M	318	LEU
1	M	322	PHE
1	M	364	GLN
1	M	366	MET
1	M	367	GLU
1	M	373	ASN
1	M	382	LEU
1	M	383	ARG
1	M	387	SER
1	M	394	LEU
1	M	413	LYS
1	M	414	PHE
1	M	416	LYS
1	M	420	ARG
1	M	422	GLU
1	M	431	ILE
1	M	432	ILE
1	M	434	HIS
1	M	442	ARG
1	M	447	GLU
1	M	448	LYS
1	M	449	THR
1	M	450	LEU
1	M	456	MET
2	N	847	LEU
2	N	859	TYR
2	N	860	ILE
1	O	14	SER
1	O	19	ARG
1	O	20	VAL
1	O	22	PHE
1	O	25	LEU
1	O	45	SER
1	O	46	GLN
1	O	50	VAL
1	O	57	LEU
1	O	58	LYS
1	O	59	SER
1	O	61	LEU
1	O	65	GLU

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Mol	Chain	Res	Type
1	O	68	GLN
1	O	70	LYS
1	O	76	ASP
1	O	80	SER
1	O	84	TYR
1	O	89	MET
1	O	98	GLU
1	O	99	HIS
1	O	101	GLU
1	O	108	GLU
1	O	111	SER
1	O	114	LEU
1	O	116	LEU
1	O	117	ARG
1	O	128	SER
1	O	130	GLN
1	O	131	GLN
1	O	141	GLN
1	O	142	ARG
1	O	147	THR
1	O	152	GLN
1	O	157	PRO
1	O	180	SER
1	O	185	TRP
1	O	194	SER
1	O	196	GLU
1	O	198	LEU
1	O	199	TYR
1	O	207	LEU
1	O	208	ILE
1	O	218	VAL
1	O	219	LEU
1	O	220	GLN
1	O	235	SER
1	O	240	THR
1	O	241	GLN
1	O	243	LEU
1	O	244	LEU
1	O	250	ARG
1	O	252	LYS
1	O	253	GLU
1	O	257	LYS

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Mol	Chain	Res	Type
1	O	258	THR
1	O	261	ASP
1	O	263	LEU
1	O	264	LEU
1	O	273	LYS
1	O	278	CYS
1	O	280	PHE
1	O	281	LYS
1	O	287	LYS
1	O	291	LYS
1	O	292	ASN
1	O	303	ASP
1	O	304	LEU
1	O	305	LYS
1	O	314	GLU
1	O	318	LEU
1	O	322	PHE
1	O	364	GLN
1	O	366	MET
1	O	367	GLU
1	O	373	ASN
1	O	382	LEU
1	O	387	SER
1	O	394	LEU
1	O	414	PHE
1	O	420	ARG
1	O	422	GLU
1	O	428	LYS
1	O	431	ILE
1	O	432	ILE
1	O	434	HIS
1	O	435	ARG
1	O	442	ARG
1	O	444	ASP
1	O	447	GLU
1	O	448	LYS
1	O	450	LEU
1	O	455	ILE
1	O	456	MET
2	P	847	LEU
2	P	859	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	62	GLN
1	A	68	GLN
1	A	71	HIS
1	A	105	ASN
1	A	112	GLN
1	A	152	GLN
1	A	182	ASN
1	A	214	HIS
1	A	220	GLN
1	A	228	GLN
1	A	231	ASN
1	A	236	ASN
1	A	262	HIS
1	A	370	HIS
2	B	858	ASN
1	C	42	GLN
1	C	62	GLN
1	C	105	ASN
1	C	130	GLN
1	C	152	GLN
1	C	182	ASN
1	C	214	HIS
1	C	220	GLN
1	C	231	ASN
1	C	262	HIS
1	C	266	GLN
1	C	370	HIS
1	E	62	GLN
1	E	66	GLN
1	E	105	ASN
1	E	152	GLN
1	E	182	ASN
1	E	214	HIS
1	E	228	GLN
1	E	236	ASN
2	F	858	ASN
1	G	41	GLN
1	G	62	GLN
1	G	105	ASN
1	G	152	GLN
1	G	182	ASN

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Mol	Chain	Res	Type
1	G	220	GLN
1	G	392	HIS
1	I	41	GLN
1	I	62	GLN
1	I	71	HIS
1	I	105	ASN
1	I	112	GLN
1	I	152	GLN
1	I	220	GLN
1	I	228	GLN
1	I	231	ASN
1	I	236	ASN
1	I	241	GLN
1	K	41	GLN
1	K	62	GLN
1	K	105	ASN
1	K	115	ASN
1	K	130	GLN
1	K	152	GLN
1	K	182	ASN
1	K	228	GLN
1	K	262	HIS
1	M	62	GLN
1	M	105	ASN
1	M	152	GLN
1	M	220	GLN
1	M	241	GLN
1	M	262	HIS
1	M	370	HIS
1	M	373	ASN
2	N	858	ASN
1	O	62	GLN
1	O	68	GLN
1	O	105	ASN
1	O	130	GLN
1	O	152	GLN
1	O	182	ASN
1	O	220	GLN
1	O	262	HIS
1	O	370	HIS
1	O	434	HIS
2	P	858	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](#)

There are no ligands in this entry.

### 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	395/465 (84%)	-0.18	2 (0%) 91 76	5, 40, 76, 100	0
1	C	393/465 (84%)	-0.37	3 (0%) 87 67	2, 34, 76, 100	0
1	E	393/465 (84%)	-0.10	6 (1%) 76 49	2, 42, 78, 100	0
1	G	393/465 (84%)	-0.41	1 (0%) 94 84	4, 35, 72, 100	0
1	I	393/465 (84%)	-0.15	3 (0%) 87 67	4, 41, 76, 100	0
1	K	393/465 (84%)	-0.30	3 (0%) 87 67	1, 39, 74, 100	0
1	M	393/465 (84%)	-0.22	4 (1%) 84 60	5, 41, 76, 100	0
1	O	393/465 (84%)	-0.28	4 (1%) 84 60	4, 39, 78, 93	0
2	B	14/22 (63%)	0.15	1 (7%) 19 7	42, 59, 84, 85	0
2	D	14/22 (63%)	-0.12	0 100 100	21, 55, 77, 80	0
2	F	14/22 (63%)	0.11	1 (7%) 19 7	29, 59, 77, 91	0
2	H	14/22 (63%)	-0.46	0 100 100	25, 42, 75, 78	0
2	J	14/22 (63%)	0.12	1 (7%) 19 7	13, 54, 74, 90	0
2	L	14/22 (63%)	-0.09	0 100 100	23, 59, 88, 100	0
2	N	14/22 (63%)	0.11	1 (7%) 19 7	15, 53, 71, 81	0
2	P	14/22 (63%)	-0.20	0 100 100	19, 50, 86, 98	0
All	All	3258/3896 (83%)	-0.24	30 (0%) 85 64	1, 39, 77, 100	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	328	GLY	5.3
1	C	328	GLY	5.0
1	K	328	GLY	4.4
1	O	328	GLY	3.4
1	I	251	THR	3.3

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Mol	Chain	Res	Type	RSRZ
2	N	860	ILE	3.3
2	J	860	ILE	3.0
1	K	14	SER	2.9
1	E	413	LYS	2.8
1	E	194	SER	2.7
1	O	14	SER	2.7
1	E	18	ILE	2.7
2	F	860	ILE	2.6
1	M	251	THR	2.6
1	O	43	LEU	2.4
2	B	860	ILE	2.4
1	A	18	ILE	2.4
1	M	254	THR	2.3
1	E	242	PHE	2.3
1	I	17	PRO	2.1
1	M	362	GLU	2.1
1	M	326	LYS	2.1
1	C	39	ALA	2.1
1	I	194	SER	2.0
1	A	459	GLU	2.0
1	E	17	PRO	2.0
1	O	26	THR	2.0
1	E	250	ARG	2.0
1	C	327	ASN	2.0
1	K	110	SER	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.