Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 09:54 PM GMT

PDB ID	:	5BUT
Title	:	Crystal structure of inactive conformation of KtrAB K+ transporter
Authors	:	Vieira-Pires, R.S.; Morais-Cabral, J.H.
Deposited on	:	2015-06-04
Resolution	:	5.97 Å(reported)

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

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

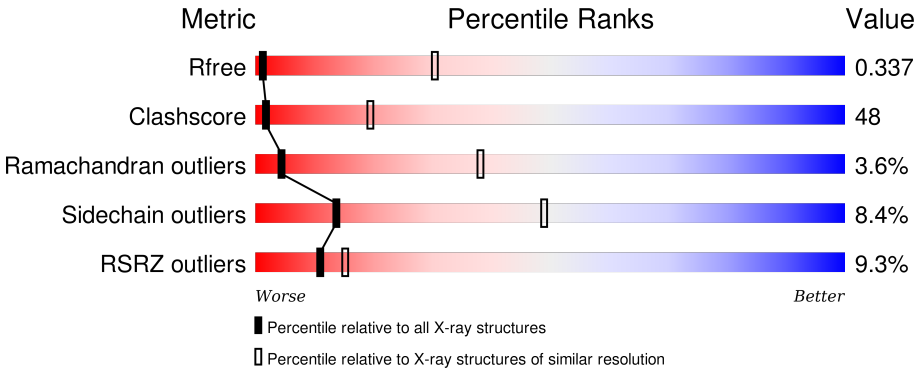
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 5.97 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1002 (8.30-3.66)
Clashscore	102246	1049 (8.20-3.70)
Ramachandran outliers	100387	1023 (8.30-3.66)
Sidechain outliers	100360	1012 (8.30-3.64)
RSRZ outliers	91569	1001 (8.30-3.66)

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

Mol	Chain	Length	Quality of chain
1	A	288	12% 38% 47% 8% 7%
1	C	288	5% 37% 48% 8% 7%
1	E	288	10% 40% 45% 8% • 7%
1	G	288	14% 38% 47% 8% 7%
2	I	445	5% 30% 60% 7% •

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Mol	Chain	Length	Quality of chain
2	J	445	8% 31% 58% 7%
2	K	445	12% 27% 62% 7%
2	L	445	7% 29% 60% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	K	I	501	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 21476 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 Ktr system potassium uptake protein A,Ktr system potassium uptake protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2096	1336	362	394	4			
1	C	268	Total	C	N	O	S	0	0	0
			2096	1336	362	394	4			
1	E	268	Total	C	N	O	S	0	0	0
			2096	1336	362	394	4			
1	G	268	Total	C	N	O	S	0	0	0
			2096	1336	362	394	4			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	145	LEU	-	linker	UNP O32080
A	146	GLU	-	linker	UNP O32080
A	147	GLY	-	linker	UNP O32080
A	148	SER	-	linker	UNP O32080
A	283	LEU	-	expression tag	UNP O32080
A	284	GLU	-	expression tag	UNP O32080
A	285	LEU	-	expression tag	UNP O32080
A	286	VAL	-	expression tag	UNP O32080
A	287	PRO	-	expression tag	UNP O32080
A	288	ARG	-	expression tag	UNP O32080
A	22	VAL	CYS	engineered mutation	UNP O32080
C	145	LEU	-	linker	UNP O32080
C	146	GLU	-	linker	UNP O32080
C	147	GLY	-	linker	UNP O32080
C	148	SER	-	linker	UNP O32080
C	283	LEU	-	expression tag	UNP O32080
C	284	GLU	-	expression tag	UNP O32080
C	285	LEU	-	expression tag	UNP O32080
C	286	VAL	-	expression tag	UNP O32080
C	287	PRO	-	expression tag	UNP O32080

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Chain	Residue	Modelled	Actual	Comment	Reference
C	288	ARG	-	expression tag	UNP O32080
C	22	VAL	CYS	engineered mutation	UNP O32080
E	145	LEU	-	linker	UNP O32080
E	146	GLU	-	linker	UNP O32080
E	147	GLY	-	linker	UNP O32080
E	148	SER	-	linker	UNP O32080
E	283	LEU	-	expression tag	UNP O32080
E	284	GLU	-	expression tag	UNP O32080
E	285	LEU	-	expression tag	UNP O32080
E	286	VAL	-	expression tag	UNP O32080
E	287	PRO	-	expression tag	UNP O32080
E	288	ARG	-	expression tag	UNP O32080
E	22	VAL	CYS	engineered mutation	UNP O32080
G	145	LEU	-	linker	UNP O32080
G	146	GLU	-	linker	UNP O32080
G	147	GLY	-	linker	UNP O32080
G	148	SER	-	linker	UNP O32080
G	283	LEU	-	expression tag	UNP O32080
G	284	GLU	-	expression tag	UNP O32080
G	285	LEU	-	expression tag	UNP O32080
G	286	VAL	-	expression tag	UNP O32080
G	287	PRO	-	expression tag	UNP O32080
G	288	ARG	-	expression tag	UNP O32080
G	22	VAL	CYS	engineered mutation	UNP O32080

- Molecule 2 is a protein called Ktr system potassium uptake protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	431	Total	C	N	O	S	0	0	0
			3272	2180	507	570	15			
2	J	431	Total	C	N	O	S	0	0	0
			3272	2180	507	570	15			
2	K	431	Total	C	N	O	S	0	0	0
			3272	2180	507	570	15			
2	L	431	Total	C	N	O	S	0	0	0
			3272	2180	507	570	15			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	103	ALA	GLY	conflict	UNP O32081
I	104	ALA	LYS	conflict	UNP O32081

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Chain	Residue	Modelled	Actual	Comment	Reference
I	105	ALA	LYS	conflict	UNP O32081
I	218	GLN	ASN	conflict	UNP O32081
I	229	ALA	LYS	conflict	UNP O32081
I	261	ALA	HIS	conflict	UNP O32081
I	262	ALA	ILE	conflict	UNP O32081
I	429	ALA	LYS	conflict	UNP O32081
J	103	ALA	GLY	conflict	UNP O32081
J	104	ALA	LYS	conflict	UNP O32081
J	105	ALA	LYS	conflict	UNP O32081
J	218	GLN	ASN	conflict	UNP O32081
J	229	ALA	LYS	conflict	UNP O32081
J	261	ALA	HIS	conflict	UNP O32081
J	262	ALA	ILE	conflict	UNP O32081
J	429	ALA	LYS	conflict	UNP O32081
K	103	ALA	GLY	conflict	UNP O32081
K	104	ALA	LYS	conflict	UNP O32081
K	105	ALA	LYS	conflict	UNP O32081
K	218	GLN	ASN	conflict	UNP O32081
K	229	ALA	LYS	conflict	UNP O32081
K	261	ALA	HIS	conflict	UNP O32081
K	262	ALA	ILE	conflict	UNP O32081
K	429	ALA	LYS	conflict	UNP O32081
L	103	ALA	GLY	conflict	UNP O32081
L	104	ALA	LYS	conflict	UNP O32081
L	105	ALA	LYS	conflict	UNP O32081
L	218	GLN	ASN	conflict	UNP O32081
L	229	ALA	LYS	conflict	UNP O32081
L	261	ALA	HIS	conflict	UNP O32081
L	262	ALA	ILE	conflict	UNP O32081
L	429	ALA	LYS	conflict	UNP O32081

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

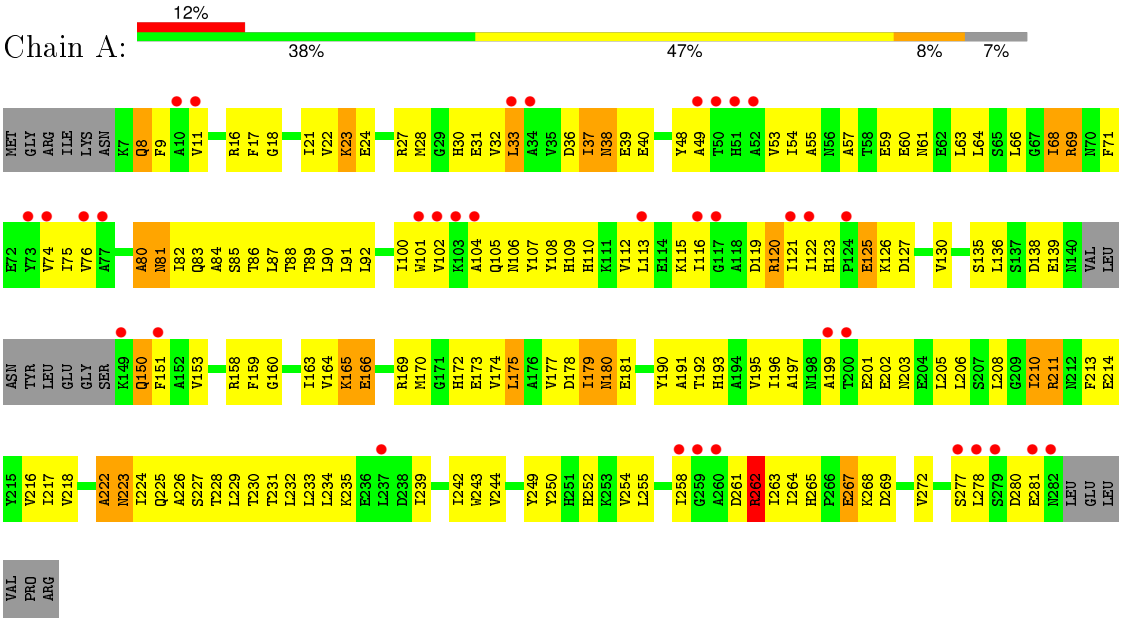
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	1	Total K 1 1	0	0
3	I	1	Total K 1 1	0	0
3	L	1	Total K 1 1	0	0
3	K	1	Total K 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

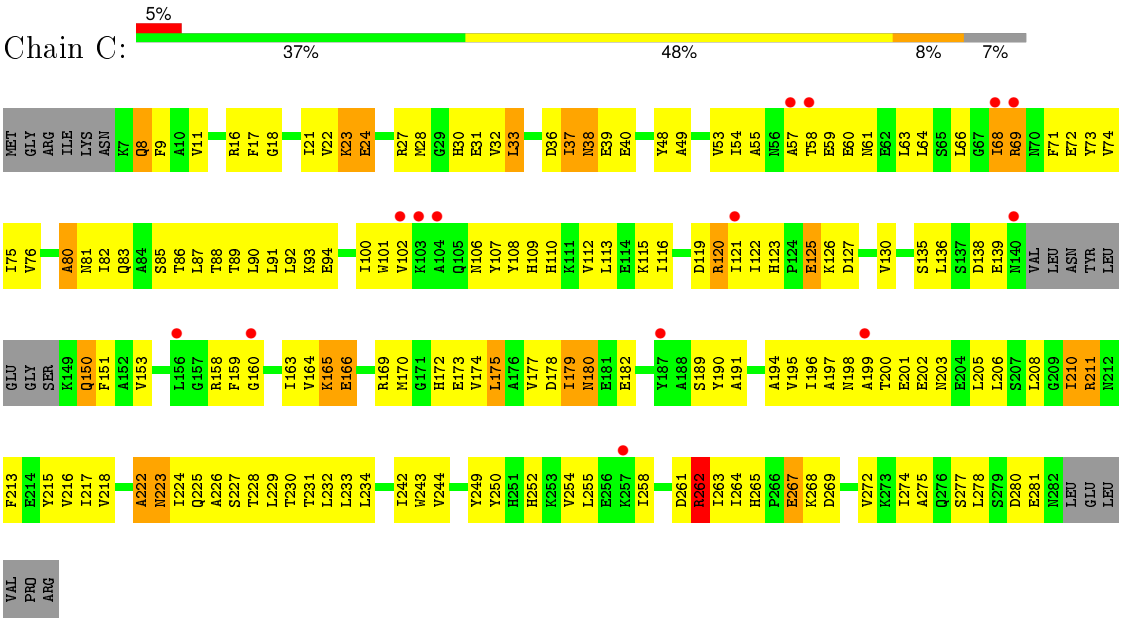
• Molecule 1: Ktr system potassium uptake protein A,Ktr system potassium uptake protein A

Chain A:



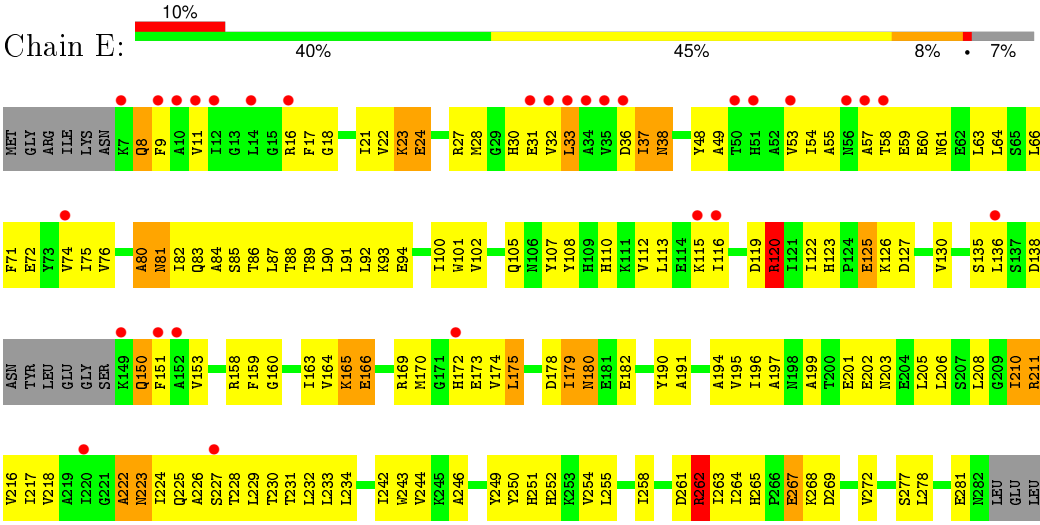
• Molecule 1: Ktr system potassium uptake protein A,Ktr system potassium uptake protein A

Chain C:



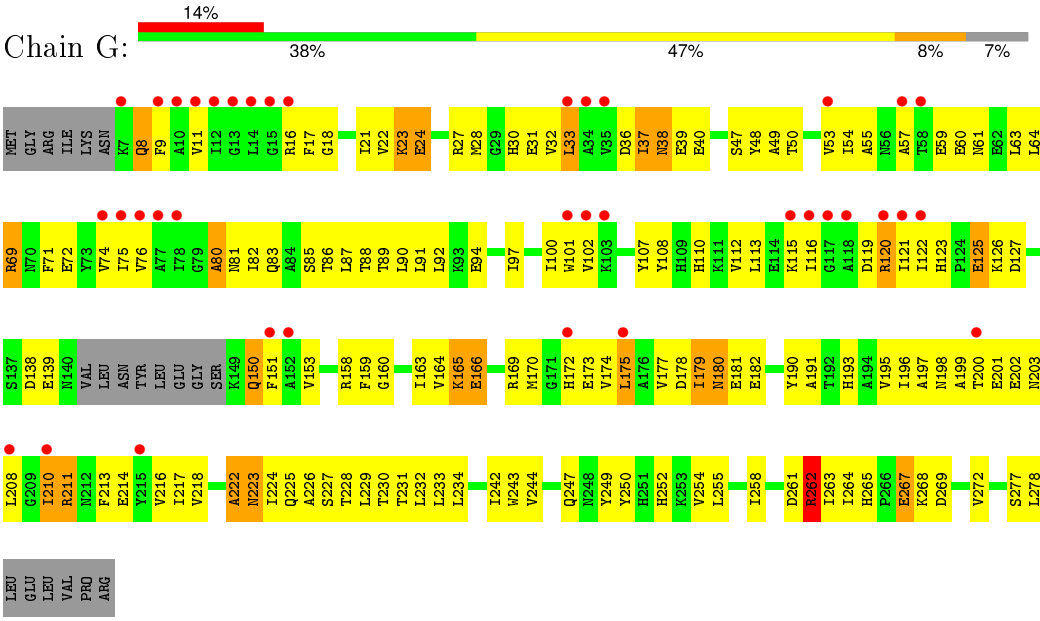
• Molecule 1: Ktr system potassium uptake protein A,Ktr system potassium uptake protein A

Chain E:



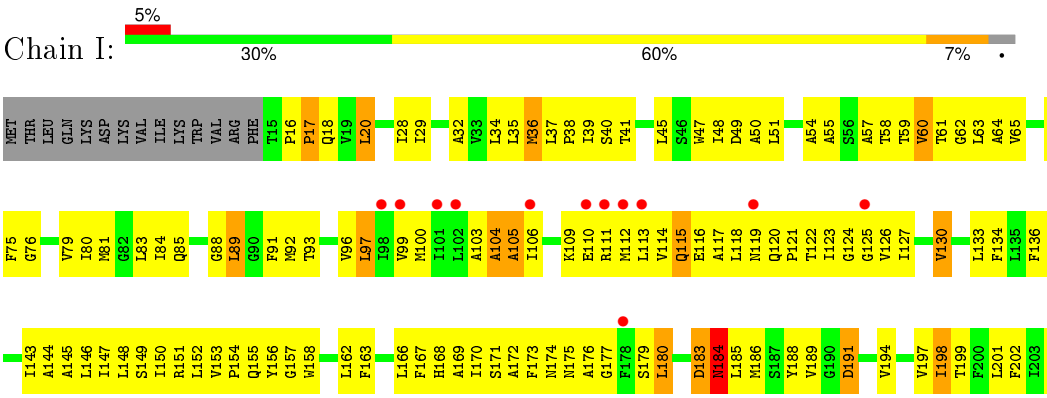
• Molecule 1: Ktr system potassium uptake protein A,Ktr system potassium uptake protein A

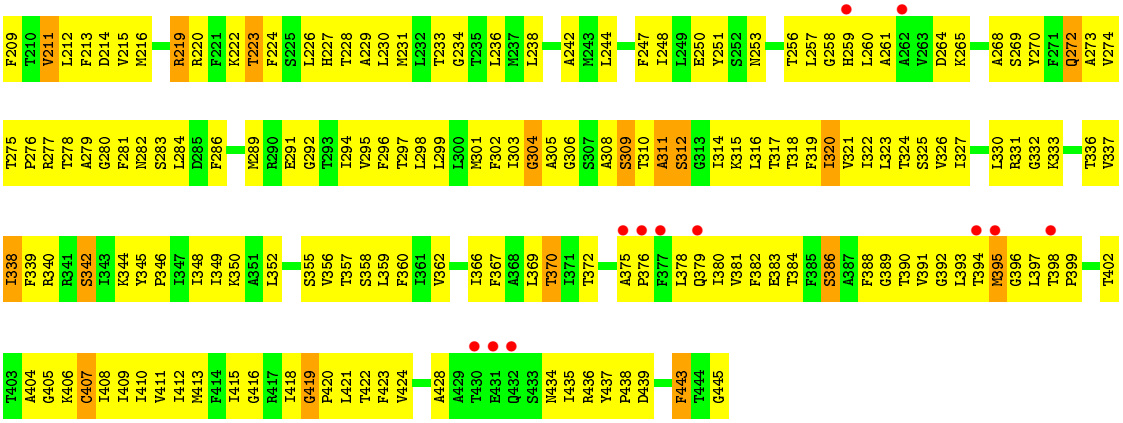
Chain G:



• Molecule 2: Ktr system potassium uptake protein B

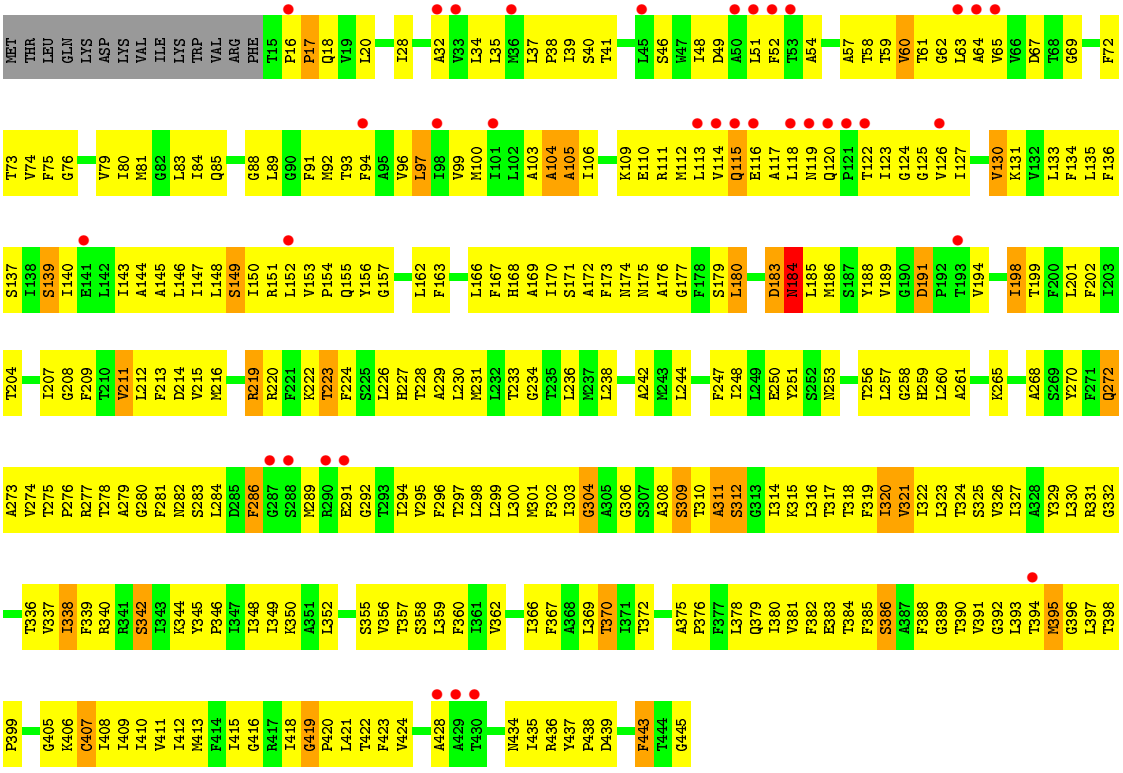
Chain I:





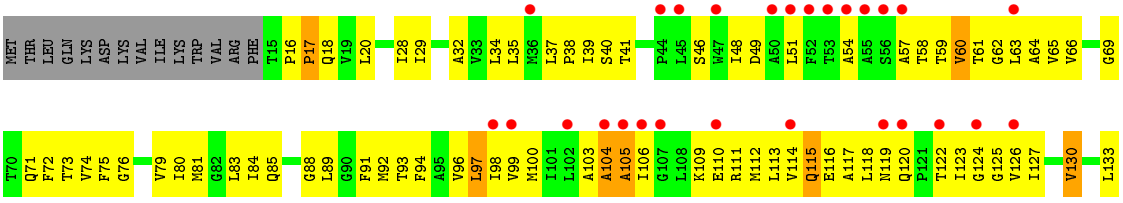
• Molecule 2: Ktr system potassium uptake protein B

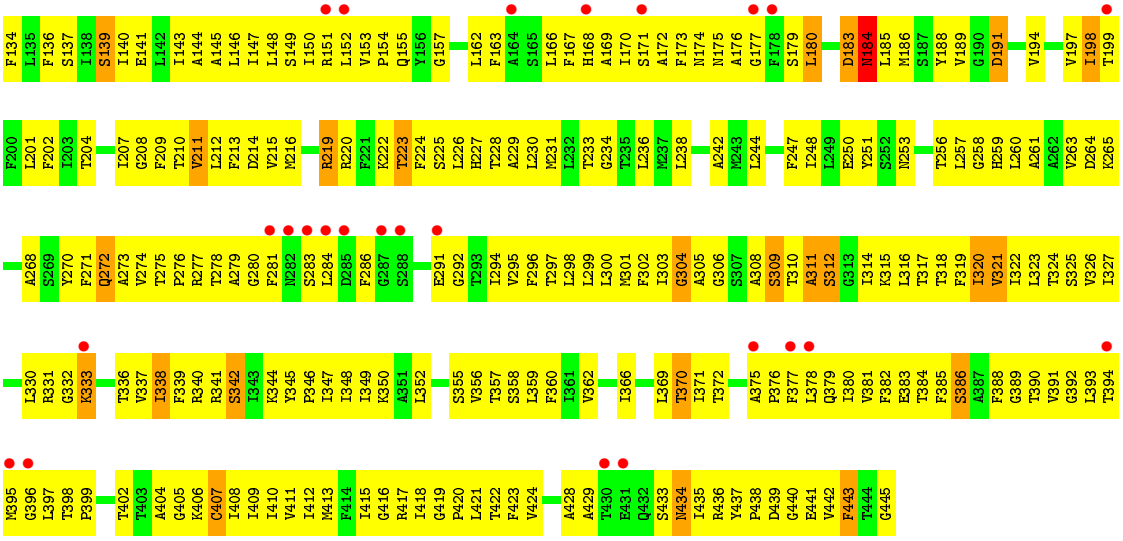
Chain J:



• Molecule 2: Ktr system potassium uptake protein B

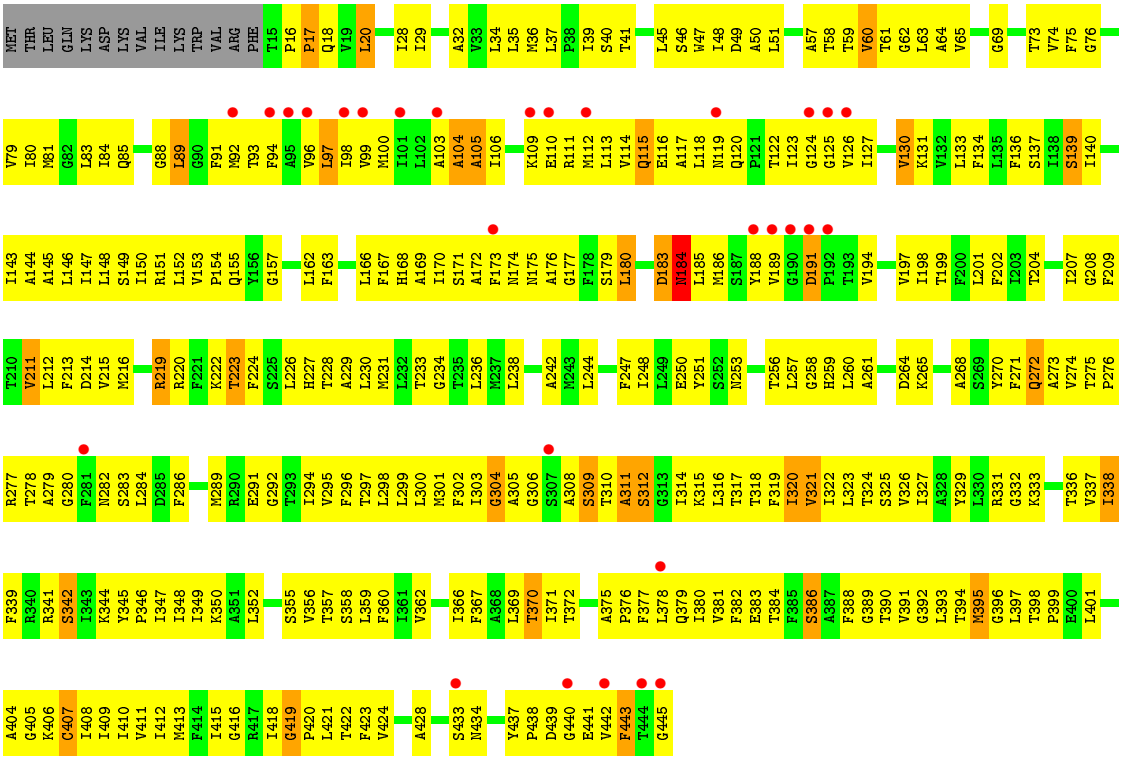
Chain K:





• Molecule 2: Ktr system potassium uptake protein B

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	307.06Å 79.41Å 205.65Å 90.00° 98.10° 90.00°	Depositor
Resolution (Å)	200.00 – 5.97 58.35 – 5.97	Depositor EDS
% Data completeness (in resolution range)	96.7 (200.00-5.97) 98.1 (58.35-5.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 6.17Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.325 , 0.339 0.338 , 0.337	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	316.7	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 272.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Outliers	0 of 23607 reflections	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	21476	wwPDB-VP
Average B, all atoms (Å^2)	342.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.23	0/2130	0.52	4/2882 (0.1%)
1	C	0.25	0/2130	0.75	5/2882 (0.2%)
1	E	0.23	0/2130	0.52	4/2882 (0.1%)
1	G	0.25	0/2130	0.75	5/2882 (0.2%)
2	I	0.28	0/3343	0.50	0/4550
2	J	0.28	0/3343	0.50	0/4550
2	K	0.28	0/3343	0.50	0/4550
2	L	0.28	0/3343	0.50	0/4550
All	All	0.27	0/21892	0.56	18/29728 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	120	ARG	NE-CZ-NH1	-21.01	109.80	120.30
1	G	120	ARG	NE-CZ-NH1	-20.98	109.81	120.30
1	C	120	ARG	NE-CZ-NH2	19.76	130.18	120.30
1	G	120	ARG	NE-CZ-NH2	19.75	130.18	120.30
1	C	120	ARG	CD-NE-CZ	9.78	137.29	123.60
1	G	120	ARG	CD-NE-CZ	9.77	137.28	123.60
1	E	120	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	A	120	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	G	262	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	C	262	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	E	262	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	A	262	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	E	120	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	C	262	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	G	262	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	E	262	ARG	NE-CZ-NH1	6.67	123.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	120	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	A	262	ARG	NE-CZ-NH1	6.61	123.60	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2096	0	2120	181	0
1	C	2096	0	2120	177	0
1	E	2096	0	2120	145	0
1	G	2096	0	2120	156	0
2	I	3272	0	3442	384	0
2	J	3272	0	3442	379	0
2	K	3272	0	3442	405	0
2	L	3272	0	3442	386	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
All	All	21476	0	22248	2100	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 48.

All (2100) 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)
2:J:28:ILE:HG12	2:J:58:THR:HG21	1.37	1.05
2:K:28:ILE:HG12	2:K:58:THR:HG21	1.38	1.04
1:C:194:ALA:O	2:K:438:PRO:HD3	1.63	0.99
2:J:227:HIS:HA	2:J:230:LEU:HD12	1.46	0.96
2:L:133:LEU:HD12	2:L:134:PHE:H	1.29	0.96
2:I:133:LEU:HD12	2:I:134:PHE:H	1.31	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:227:HIS:HA	2:K:230:LEU:HD12	1.47	0.95
2:K:133:LEU:HD12	2:K:134:PHE:H	1.31	0.95
2:L:227:HIS:HA	2:L:230:LEU:HD12	1.49	0.95
2:J:173:PHE:HB2	2:J:201:LEU:HD22	1.47	0.94
2:I:209:PHE:HA	2:I:212:LEU:HD12	1.49	0.94
2:I:28:ILE:HG12	2:I:58:THR:HG21	1.49	0.94
2:I:61:THR:HG23	2:I:390:THR:HA	1.46	0.94
2:J:133:LEU:HD12	2:J:134:PHE:H	1.33	0.93
2:K:61:THR:HG23	2:K:390:THR:HA	1.49	0.93
2:L:209:PHE:HA	2:L:212:LEU:HD12	1.48	0.93
2:L:28:ILE:HG12	2:L:58:THR:HG21	1.46	0.93
2:K:370:THR:HG23	2:K:380:ILE:HG21	1.52	0.92
1:A:83:GLN:NE2	1:C:108:TYR:HB2	1.84	0.92
2:I:278:THR:HA	2:I:391:VAL:HA	1.52	0.92
2:I:227:HIS:HA	2:I:230:LEU:HD12	1.52	0.91
2:K:61:THR:HA	2:K:390:THR:HB	1.53	0.91
2:L:409:ILE:HD13	2:L:412:ILE:HD12	1.52	0.91
2:L:278:THR:HA	2:L:391:VAL:HA	1.52	0.90
2:J:409:ILE:HD13	2:J:412:ILE:HD12	1.53	0.90
2:K:173:PHE:HB2	2:K:201:LEU:HD22	1.52	0.90
2:K:209:PHE:HA	2:K:212:LEU:HD12	1.53	0.90
1:A:125:GLU:HG3	1:A:159:PHE:HB2	1.55	0.88
2:I:61:THR:HA	2:I:390:THR:HB	1.55	0.88
2:I:409:ILE:HD13	2:I:412:ILE:HD12	1.54	0.88
1:G:196:ILE:HB	2:I:436:ARG:HB2	1.53	0.88
2:I:173:PHE:HB2	2:I:201:LEU:HD22	1.56	0.88
2:K:140:ILE:HD12	2:K:143:ILE:HD11	1.53	0.88
2:J:278:THR:HA	2:J:391:VAL:HA	1.55	0.87
2:J:209:PHE:HA	2:J:212:LEU:HD12	1.55	0.87
2:J:379:GLN:HE21	2:J:397:LEU:HB2	1.39	0.87
2:I:370:THR:HG23	2:I:380:ILE:HG21	1.57	0.86
2:L:61:THR:HG23	2:L:390:THR:HA	1.55	0.86
2:J:370:THR:HG23	2:J:380:ILE:HG21	1.57	0.86
2:K:97:LEU:HG	2:K:130:VAL:HG13	1.56	0.86
2:I:379:GLN:HE21	2:I:397:LEU:HB2	1.40	0.86
2:I:146:LEU:HD13	2:I:166:LEU:HD23	1.58	0.86
2:K:379:GLN:NE2	2:K:397:LEU:HB2	1.91	0.85
2:K:409:ILE:HD13	2:K:412:ILE:HD12	1.58	0.85
2:K:379:GLN:HE21	2:K:397:LEU:HB2	1.37	0.85
2:J:209:PHE:H	2:J:308:ALA:HB3	1.39	0.85
1:E:76:VAL:HB	1:E:102:VAL:HG13	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:97:LEU:HG	2:I:130:VAL:HG13	1.57	0.85
2:I:379:GLN:NE2	2:I:397:LEU:HB2	1.91	0.85
2:L:64:ALA:H	2:L:398:THR:HG21	1.41	0.84
1:C:218:VAL:HB	1:C:244:VAL:HG13	1.60	0.84
2:J:60:VAL:HG13	2:J:84:ILE:HG23	1.58	0.84
1:G:125:GLU:HG3	1:G:159:PHE:HB2	1.59	0.83
2:I:140:ILE:HD12	2:I:143:ILE:HD11	1.58	0.83
2:J:81:MET:SD	2:J:167:PHE:HA	2.18	0.83
1:A:17:PHE:HB2	1:A:267:GLU:HG3	1.60	0.83
1:A:76:VAL:HB	1:A:102:VAL:HG13	1.60	0.83
2:L:370:THR:HG23	2:L:380:ILE:HG21	1.61	0.83
2:J:175:ASN:HB3	2:J:278:THR:O	1.79	0.83
1:E:83:GLN:OE1	1:G:82:ILE:HD13	1.79	0.83
2:I:352:LEU:HD23	2:J:352:LEU:HD23	1.58	0.82
2:J:303:ILE:HA	2:J:314:ILE:HG23	1.58	0.82
2:L:173:PHE:HB2	2:L:201:LEU:HD22	1.59	0.82
1:A:196:ILE:HB	2:J:436:ARG:HB2	1.59	0.82
2:J:97:LEU:HG	2:J:130:VAL:HG13	1.61	0.82
2:K:303:ILE:HA	2:K:314:ILE:HG23	1.60	0.82
2:K:60:VAL:HG13	2:K:84:ILE:HG23	1.60	0.82
1:E:150:GLN:HB3	1:E:213:PHE:HA	1.61	0.81
1:A:90:LEU:HD21	1:C:115:LYS:HB2	1.60	0.81
2:J:61:THR:HG23	2:J:390:THR:HA	1.62	0.81
2:J:146:LEU:HD13	2:J:166:LEU:HD23	1.61	0.81
2:L:97:LEU:HG	2:L:130:VAL:HG13	1.62	0.81
1:C:17:PHE:HB2	1:C:267:GLU:HG3	1.62	0.81
1:G:218:VAL:HB	1:G:244:VAL:HG13	1.63	0.81
2:J:150:ILE:HD11	2:J:162:LEU:HD23	1.62	0.81
1:G:8:GLN:HB3	1:G:71:PHE:HA	1.62	0.81
2:I:175:ASN:HB3	2:I:278:THR:O	1.81	0.81
2:K:64:ALA:H	2:K:398:THR:HG21	1.44	0.81
2:J:379:GLN:NE2	2:J:397:LEU:HB2	1.96	0.81
2:L:202:PHE:HE1	2:L:274:VAL:HG12	1.47	0.80
2:L:60:VAL:HG13	2:L:84:ILE:HG23	1.61	0.80
1:E:8:GLN:HB3	1:E:71:PHE:HA	1.62	0.80
2:J:140:ILE:HD12	2:J:143:ILE:HD11	1.62	0.80
2:L:379:GLN:HE21	2:L:397:LEU:HB2	1.45	0.80
2:J:437:TYR:HB3	2:J:438:PRO:HD2	1.61	0.80
2:K:437:TYR:HB3	2:K:438:PRO:HD2	1.62	0.80
2:L:175:ASN:HB3	2:L:278:THR:O	1.82	0.80
1:G:17:PHE:HB2	1:G:267:GLU:HG3	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:437:TYR:HB3	2:L:438:PRO:HD2	1.62	0.80
2:I:303:ILE:HA	2:I:314:ILE:HG23	1.64	0.80
2:J:61:THR:HA	2:J:390:THR:HB	1.62	0.80
2:J:106:ILE:HD12	2:J:127:ILE:HG23	1.63	0.79
1:A:108:TYR:HB2	1:C:83:GLN:NE2	1.97	0.79
2:J:96:VAL:HG22	2:J:110:GLU:OE1	1.83	0.79
1:A:85:SER:O	1:A:89:THR:HG23	1.82	0.79
1:A:202:GLU:HG2	1:A:203:ASN:H	1.47	0.79
1:E:227:SER:O	1:E:231:THR:HG23	1.82	0.79
2:I:60:VAL:HG13	2:I:84:ILE:HG23	1.62	0.79
2:K:322:ILE:O	2:K:326:VAL:HG23	1.82	0.79
2:L:106:ILE:HD12	2:L:127:ILE:HG23	1.64	0.79
2:I:437:TYR:HB3	2:I:438:PRO:HD2	1.63	0.79
2:K:244:LEU:O	2:K:248:ILE:HG12	1.83	0.79
2:K:106:ILE:HD12	2:K:127:ILE:HG23	1.65	0.79
2:L:146:LEU:HD13	2:L:166:LEU:HD23	1.65	0.79
2:L:133:LEU:HD12	2:L:134:PHE:N	1.98	0.79
2:I:202:PHE:HE1	2:I:274:VAL:HG12	1.46	0.79
2:I:64:ALA:H	2:I:398:THR:HG21	1.45	0.79
2:L:61:THR:HA	2:L:390:THR:HB	1.64	0.79
2:J:317:THR:HA	2:J:320:ILE:HD12	1.63	0.79
2:I:106:ILE:HD12	2:I:127:ILE:HG23	1.64	0.78
2:K:146:LEU:HD13	2:K:166:LEU:HD23	1.63	0.78
1:E:85:SER:O	1:E:89:THR:HG23	1.84	0.78
2:I:317:THR:HA	2:I:320:ILE:HD12	1.63	0.78
2:L:322:ILE:O	2:L:326:VAL:HG23	1.83	0.78
1:A:227:SER:O	1:A:231:THR:HG23	1.82	0.78
2:L:244:LEU:O	2:L:248:ILE:HG12	1.84	0.78
2:J:168:HIS:HE1	2:J:180:LEU:HB2	1.48	0.78
1:A:218:VAL:HB	1:A:244:VAL:HG13	1.64	0.78
1:G:227:SER:O	1:G:231:THR:HG23	1.84	0.78
2:K:337:VAL:HA	2:K:342:SER:HA	1.66	0.78
1:C:85:SER:O	1:C:89:THR:HG23	1.83	0.78
2:L:337:VAL:HA	2:L:342:SER:HA	1.64	0.78
2:J:35:LEU:HD21	2:J:79:VAL:HB	1.66	0.78
2:I:209:PHE:H	2:I:308:ALA:HB3	1.48	0.78
2:K:292:GLY:HA3	2:L:371:ILE:HD11	1.65	0.78
1:A:8:GLN:HB3	1:A:71:PHE:HA	1.66	0.78
2:L:379:GLN:NE2	2:L:397:LEU:HB2	1.99	0.77
2:I:133:LEU:HD12	2:I:134:PHE:N	1.99	0.77
1:C:8:GLN:HB3	1:C:71:PHE:HA	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:85:SER:O	1:G:89:THR:HG23	1.84	0.77
1:C:227:SER:O	1:C:231:THR:HG23	1.83	0.77
1:A:150:GLN:HB3	1:A:213:PHE:HA	1.66	0.77
2:L:303:ILE:HA	2:L:314:ILE:HG23	1.64	0.77
1:E:202:GLU:HG2	1:E:203:ASN:H	1.50	0.77
1:A:115:LYS:HB2	1:C:90:LEU:HD21	1.67	0.77
2:I:168:HIS:HE1	2:I:180:LEU:HB2	1.50	0.77
2:J:133:LEU:HD12	2:J:134:PHE:N	2.00	0.77
2:L:96:VAL:HG22	2:L:110:GLU:OE1	1.85	0.77
1:C:202:GLU:HG2	1:C:203:ASN:H	1.50	0.77
2:I:337:VAL:HA	2:I:342:SER:HA	1.66	0.77
2:I:115:GLN:HG2	2:I:120:GLN:O	1.85	0.77
2:L:140:ILE:HD12	2:L:143:ILE:HD11	1.65	0.77
2:K:133:LEU:HD12	2:K:134:PHE:N	2.00	0.76
2:K:175:ASN:HB3	2:K:278:THR:O	1.85	0.76
1:G:202:GLU:HG2	1:G:203:ASN:H	1.49	0.76
2:L:168:HIS:HE1	2:L:180:LEU:HB2	1.49	0.76
2:I:73:THR:HG22	2:I:74:VAL:H	1.50	0.76
2:I:62:GLY:HA3	2:I:392:GLY:HA2	1.68	0.76
2:K:341:ARG:HA	2:L:438:PRO:HG2	1.67	0.76
2:J:337:VAL:HA	2:J:342:SER:HA	1.66	0.76
2:K:278:THR:HA	2:K:391:VAL:HA	1.67	0.76
1:C:76:VAL:HB	1:C:102:VAL:HG13	1.67	0.76
2:K:150:ILE:HD11	2:K:162:LEU:HD23	1.67	0.76
1:G:150:GLN:HB3	1:G:213:PHE:HA	1.66	0.76
2:I:93:THR:OG1	2:I:118:LEU:HD21	1.85	0.76
2:L:391:VAL:HG12	2:L:393:LEU:HD23	1.67	0.76
1:E:218:VAL:HB	1:E:244:VAL:HG13	1.67	0.76
1:C:195:VAL:HG21	1:C:208:LEU:HD11	1.68	0.76
1:C:60:GLU:HG2	1:C:61:ASN:H	1.51	0.76
2:K:391:VAL:HG12	2:K:393:LEU:HD23	1.67	0.76
1:G:76:VAL:HB	1:G:102:VAL:HG13	1.67	0.76
2:K:35:LEU:HD21	2:K:79:VAL:HB	1.68	0.76
2:J:202:PHE:HE1	2:J:274:VAL:HG12	1.51	0.76
1:C:150:GLN:HB3	1:C:213:PHE:HA	1.66	0.76
2:I:322:ILE:O	2:I:326:VAL:HG23	1.85	0.76
2:L:81:MET:SD	2:L:167:PHE:HA	2.26	0.75
2:L:73:THR:HG22	2:L:74:VAL:H	1.51	0.75
2:J:244:LEU:O	2:J:248:ILE:HG12	1.86	0.75
2:J:64:ALA:H	2:J:398:THR:HG21	1.49	0.75
2:I:244:LEU:O	2:I:248:ILE:HG12	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:226:LEU:HD21	2:J:338:ILE:HG22	1.67	0.75
2:L:317:THR:HA	2:L:320:ILE:HD12	1.66	0.75
2:J:322:ILE:O	2:J:326:VAL:HG23	1.85	0.75
2:L:115:GLN:HG2	2:L:120:GLN:O	1.87	0.75
2:I:92:MET:HB2	2:I:117:ALA:CB	2.17	0.74
2:K:62:GLY:HA3	2:K:392:GLY:HA2	1.68	0.74
2:K:73:THR:HG22	2:K:74:VAL:H	1.51	0.74
2:I:35:LEU:HD21	2:I:79:VAL:HB	1.68	0.74
2:K:96:VAL:HG22	2:K:110:GLU:OE1	1.88	0.74
2:J:93:THR:OG1	2:J:118:LEU:HD21	1.88	0.74
2:I:226:LEU:HD21	2:I:338:ILE:HG22	1.68	0.74
2:L:242:ALA:HB1	2:L:273:ALA:HB1	1.68	0.74
2:J:73:THR:HG22	2:J:74:VAL:H	1.51	0.74
2:K:317:THR:HA	2:K:320:ILE:HD12	1.69	0.74
2:I:391:VAL:HG12	2:I:393:LEU:HD23	1.70	0.74
2:I:153:VAL:N	2:I:154:PRO:HD2	2.03	0.74
2:K:438:PRO:HG2	2:L:341:ARG:HA	1.70	0.74
2:I:168:HIS:CE1	2:I:180:LEU:HB2	2.23	0.74
2:K:153:VAL:N	2:K:154:PRO:HD2	2.03	0.74
1:C:125:GLU:HG3	1:C:159:PHE:HB2	1.68	0.74
2:I:81:MET:SD	2:I:167:PHE:HA	2.28	0.74
2:L:209:PHE:H	2:L:308:ALA:HB3	1.52	0.74
2:K:226:LEU:HD21	2:K:338:ILE:HG22	1.70	0.74
2:K:242:ALA:HB1	2:K:273:ALA:HB1	1.70	0.73
2:L:58:THR:HA	2:L:83:LEU:O	1.89	0.73
2:L:168:HIS:CE1	2:L:180:LEU:HB2	2.23	0.73
1:E:195:VAL:HG21	1:E:208:LEU:HD11	1.70	0.73
1:G:195:VAL:HG21	1:G:208:LEU:HD11	1.69	0.73
1:A:120:ARG:HD3	1:A:122:ILE:HD11	1.69	0.73
1:G:53:VAL:HG21	1:G:66:LEU:HD11	1.69	0.73
1:G:60:GLU:HG2	1:G:61:ASN:H	1.51	0.73
1:A:60:GLU:HG2	1:A:61:ASN:H	1.52	0.73
2:L:150:ILE:HD11	2:L:162:LEU:HD23	1.70	0.73
2:L:226:LEU:HD21	2:L:338:ILE:HG22	1.69	0.73
1:A:53:VAL:HG21	1:A:66:LEU:HD11	1.70	0.73
1:A:115:LYS:HD2	1:C:90:LEU:HG	1.68	0.73
2:K:445:GLY:HA3	2:L:119:ASN:HD21	1.53	0.73
2:K:202:PHE:HE1	2:K:274:VAL:HG12	1.53	0.73
2:L:153:VAL:N	2:L:154:PRO:HD2	2.03	0.73
2:I:445:GLY:HA3	2:J:119:ASN:HD21	1.52	0.73
2:L:35:LEU:HD21	2:L:79:VAL:HB	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:262:ARG:HD3	1:E:264:ILE:HD11	1.71	0.73
2:I:96:VAL:HG22	2:I:110:GLU:OE1	1.89	0.73
2:K:81:MET:SD	2:K:167:PHE:HA	2.28	0.73
1:A:262:ARG:HD3	1:A:264:ILE:HD11	1.70	0.73
2:K:440:GLY:N	2:L:342:SER:O	2.22	0.72
1:E:53:VAL:HG21	1:E:66:LEU:HD11	1.71	0.72
2:J:242:ALA:HB1	2:J:273:ALA:HB1	1.71	0.72
2:L:93:THR:OG1	2:L:118:LEU:HD21	1.89	0.72
2:J:153:VAL:N	2:J:154:PRO:HD2	2.03	0.72
2:I:150:ILE:HD11	2:I:162:LEU:HD23	1.71	0.72
2:J:320:ILE:O	2:J:324:THR:HG22	1.89	0.72
2:L:111:ARG:HB3	2:L:123:ILE:O	1.90	0.72
1:E:60:GLU:HG2	1:E:61:ASN:H	1.54	0.72
2:K:168:HIS:HE1	2:K:180:LEU:HB2	1.55	0.72
2:J:60:VAL:HG12	2:J:176:ALA:HA	1.71	0.72
2:J:168:HIS:CE1	2:J:180:LEU:HB2	2.24	0.72
1:C:53:VAL:HG21	1:C:66:LEU:HD11	1.72	0.72
2:L:272:GLN:NE2	2:L:283:SER:HB3	2.03	0.71
1:G:179:ILE:H	1:G:179:ILE:HD13	1.56	0.71
2:I:330:LEU:HD13	2:J:424:VAL:HG11	1.70	0.71
2:K:209:PHE:H	2:K:308:ALA:HB3	1.54	0.71
2:L:320:ILE:O	2:L:324:THR:HG22	1.90	0.71
2:I:242:ALA:HB1	2:I:273:ALA:HB1	1.72	0.71
2:K:242:ALA:CB	2:K:273:ALA:HB1	2.20	0.71
1:G:127:ASP:O	1:G:130:VAL:HG22	1.90	0.71
2:I:251:TYR:O	2:I:258:GLY:HA2	1.90	0.71
2:L:62:GLY:HA3	2:L:392:GLY:HA2	1.73	0.71
2:J:62:GLY:HA3	2:J:392:GLY:HA2	1.70	0.71
2:J:88:GLY:O	2:J:310:THR:HG22	1.90	0.71
2:L:251:TYR:O	2:L:258:GLY:HA2	1.91	0.70
2:K:115:GLN:HG2	2:K:120:GLN:O	1.91	0.70
2:I:379:GLN:HA	2:I:395:MET:HE2	1.72	0.70
1:A:195:VAL:HG21	1:A:208:LEU:HD11	1.70	0.70
2:L:199:THR:HG21	2:L:270:TYR:HE2	1.56	0.70
2:J:272:GLN:NE2	2:J:283:SER:HB3	2.06	0.70
2:J:106:ILE:HD12	2:J:127:ILE:CG2	2.22	0.70
2:K:16:PRO:HA	2:K:113:LEU:HD23	1.74	0.70
2:J:92:MET:HB2	2:J:117:ALA:CB	2.21	0.70
2:K:320:ILE:O	2:K:324:THR:HG22	1.90	0.70
1:E:120:ARG:HD3	1:E:122:ILE:HD11	1.74	0.70
2:L:242:ALA:CB	2:L:273:ALA:HB1	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:153:VAL:N	2:I:154:PRO:CD	2.55	0.70
2:I:96:VAL:HG21	2:I:114:VAL:CG2	2.22	0.69
2:K:93:THR:OG1	2:K:118:LEU:HD21	1.91	0.69
2:L:270:TYR:O	2:L:274:VAL:HG23	1.91	0.69
2:L:60:VAL:HG12	2:L:176:ALA:HA	1.72	0.69
2:I:88:GLY:O	2:I:310:THR:HG22	1.92	0.69
2:I:148:LEU:HG	2:I:151:ARG:CZ	2.22	0.69
2:I:60:VAL:HG12	2:I:176:ALA:HA	1.73	0.69
2:J:153:VAL:N	2:J:154:PRO:CD	2.55	0.69
2:J:242:ALA:CB	2:J:273:ALA:HB1	2.23	0.69
1:G:64:LEU:HA	1:G:69:ARG:HH12	1.57	0.69
2:L:153:VAL:N	2:L:154:PRO:CD	2.55	0.69
2:J:115:GLN:HG2	2:J:120:GLN:O	1.93	0.69
2:L:48:ILE:HG22	2:L:406:LYS:HD3	1.72	0.69
2:J:391:VAL:HG12	2:J:393:LEU:HD23	1.73	0.69
2:K:88:GLY:O	2:K:310:THR:HG22	1.93	0.69
2:I:272:GLN:NE2	2:I:283:SER:HB3	2.08	0.69
2:L:220:ARG:HB2	2:L:223:THR:OG1	1.93	0.69
2:L:93:THR:HG22	2:L:133:LEU:HD13	1.74	0.69
2:J:93:THR:HG22	2:J:133:LEU:HD13	1.75	0.69
2:I:320:ILE:O	2:I:324:THR:HG22	1.93	0.69
2:K:153:VAL:N	2:K:154:PRO:CD	2.55	0.69
2:K:92:MET:HB2	2:K:117:ALA:CB	2.23	0.69
2:J:172:ALA:O	2:J:202:PHE:HB3	1.93	0.69
2:J:183:ASP:O	2:J:185:LEU:N	2.26	0.69
2:K:172:ALA:O	2:K:202:PHE:HB3	1.93	0.68
2:I:242:ALA:CB	2:I:273:ALA:HB1	2.23	0.68
1:E:37:ILE:HD13	1:E:37:ILE:H	1.58	0.68
2:K:324:THR:HA	2:K:327:ILE:HD12	1.74	0.68
2:K:96:VAL:HG21	2:K:114:VAL:CG2	2.22	0.68
2:K:272:GLN:NE2	2:K:283:SER:HB3	2.08	0.68
2:L:183:ASP:O	2:L:185:LEU:N	2.26	0.68
2:J:324:THR:HA	2:J:327:ILE:HD12	1.76	0.68
1:A:202:GLU:HG2	1:A:203:ASN:N	2.08	0.68
2:J:111:ARG:HB3	2:J:123:ILE:O	1.93	0.68
1:C:127:ASP:O	1:C:130:VAL:HG22	1.93	0.68
2:J:148:LEU:HG	2:J:151:ARG:CZ	2.23	0.68
2:I:199:THR:HA	2:I:202:PHE:CE2	2.29	0.68
2:K:60:VAL:HG12	2:K:176:ALA:HA	1.75	0.68
2:I:215:VAL:HG22	2:I:224:PHE:CE2	2.28	0.68
2:L:199:THR:HA	2:L:202:PHE:CE2	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LEU:HG	1:C:115:LYS:HD2	1.75	0.68
2:I:209:PHE:CD2	2:I:308:ALA:HB1	2.28	0.68
2:I:220:ARG:HB2	2:I:223:THR:OG1	1.92	0.68
1:E:127:ASP:O	1:E:130:VAL:HG22	1.92	0.68
2:I:324:THR:HA	2:I:327:ILE:HD12	1.76	0.68
2:J:209:PHE:CD2	2:J:308:ALA:HB1	2.29	0.68
2:L:96:VAL:HG21	2:L:114:VAL:CG2	2.23	0.67
1:G:269:ASP:O	1:G:272:VAL:HG22	1.94	0.67
2:K:48:ILE:HG22	2:K:406:LYS:HD3	1.76	0.67
2:J:96:VAL:HG21	2:J:114:VAL:CG2	2.23	0.67
1:A:193:HIS:CD2	2:I:340:ARG:HD3	2.30	0.67
2:J:270:TYR:O	2:J:274:VAL:HG23	1.94	0.67
2:I:270:TYR:O	2:I:274:VAL:HG23	1.93	0.67
2:J:209:PHE:N	2:J:308:ALA:HB3	2.08	0.67
1:C:269:ASP:O	1:C:272:VAL:HG22	1.93	0.67
2:I:16:PRO:HA	2:I:113:LEU:HD23	1.76	0.67
2:K:247:PHE:O	2:K:251:TYR:HB2	1.95	0.67
1:A:201:GLU:O	1:A:205:LEU:HD13	1.95	0.67
2:K:93:THR:HG22	2:K:133:LEU:HD13	1.74	0.67
2:L:32:ALA:CB	2:L:51:LEU:HD12	2.24	0.67
2:J:247:PHE:O	2:J:251:TYR:HB2	1.95	0.67
2:I:183:ASP:O	2:I:185:LEU:N	2.26	0.67
2:J:58:THR:HA	2:J:83:LEU:O	1.94	0.67
2:K:199:THR:HG21	2:K:270:TYR:HE2	1.59	0.67
2:K:220:ARG:HB2	2:K:223:THR:OG1	1.95	0.67
2:L:16:PRO:HA	2:L:113:LEU:HD23	1.77	0.67
2:K:168:HIS:CE1	2:K:180:LEU:HB2	2.30	0.67
2:J:215:VAL:HG22	2:J:224:PHE:CE2	2.29	0.67
2:K:58:THR:HA	2:K:83:LEU:O	1.94	0.67
2:J:199:THR:HG21	2:J:270:TYR:HE2	1.60	0.67
2:K:251:TYR:O	2:K:258:GLY:HA2	1.95	0.67
1:E:179:ILE:HD13	1:E:179:ILE:H	1.59	0.66
1:C:262:ARG:HD3	1:C:264:ILE:HD11	1.76	0.66
1:E:201:GLU:O	1:E:205:LEU:HD13	1.95	0.66
2:L:88:GLY:O	2:L:310:THR:HG22	1.95	0.66
2:L:92:MET:HB2	2:L:117:ALA:CB	2.25	0.66
2:K:148:LEU:HG	2:K:151:ARG:CZ	2.26	0.66
2:L:209:PHE:CD2	2:L:308:ALA:HB1	2.31	0.66
2:K:215:VAL:HG22	2:K:224:PHE:CE2	2.30	0.66
1:A:127:ASP:O	1:A:130:VAL:HG22	1.95	0.66
2:K:183:ASP:O	2:K:185:LEU:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:251:TYR:O	2:J:258:GLY:HA2	1.95	0.66
2:J:220:ARG:HB2	2:J:223:THR:OG1	1.96	0.66
2:I:93:THR:HG22	2:I:133:LEU:HD13	1.76	0.66
2:J:148:LEU:HG	2:J:151:ARG:NH2	2.10	0.66
2:I:199:THR:HG21	2:I:270:TYR:HE2	1.61	0.66
2:J:16:PRO:HA	2:J:113:LEU:HD23	1.78	0.66
1:G:87:LEU:O	1:G:91:LEU:HG	1.96	0.66
2:K:330:LEU:HD13	2:L:424:VAL:HG11	1.78	0.66
2:L:391:VAL:HG12	2:L:393:LEU:CD2	2.26	0.65
1:E:202:GLU:HG2	1:E:203:ASN:N	2.11	0.65
1:E:64:LEU:HA	1:E:69:ARG:HH12	1.60	0.65
2:K:406:LYS:O	2:K:410:ILE:HG13	1.97	0.65
2:I:48:ILE:HG22	2:I:406:LYS:HD3	1.79	0.65
2:I:58:THR:HA	2:I:83:LEU:O	1.96	0.65
2:J:379:GLN:HA	2:J:395:MET:HE2	1.79	0.65
2:K:352:LEU:HD23	2:L:352:LEU:HD23	1.77	0.65
2:K:270:TYR:O	2:K:274:VAL:HG23	1.96	0.65
2:K:88:GLY:HA3	2:K:174:ASN:ND2	2.11	0.65
2:K:209:PHE:CD2	2:K:308:ALA:HB1	2.31	0.65
2:J:60:VAL:HG12	2:J:176:ALA:CA	2.26	0.65
2:K:111:ARG:HB3	2:K:123:ILE:O	1.95	0.65
1:E:125:GLU:HG2	1:E:158:ARG:HB2	1.78	0.65
2:J:106:ILE:HD13	2:J:110:GLU:OE2	1.96	0.65
1:C:89:THR:HA	1:C:92:LEU:HD12	1.78	0.65
1:C:201:GLU:O	1:C:205:LEU:HD13	1.96	0.65
2:L:379:GLN:HA	2:L:395:MET:HE2	1.79	0.65
2:L:406:LYS:O	2:L:410:ILE:HG13	1.96	0.65
1:G:202:GLU:HG2	1:G:203:ASN:N	2.11	0.65
2:K:106:ILE:HD13	2:K:110:GLU:OE2	1.97	0.65
1:C:231:THR:HA	1:C:234:LEU:HD12	1.79	0.65
1:C:60:GLU:HG2	1:C:61:ASN:N	2.12	0.65
2:L:324:THR:HA	2:L:327:ILE:HD12	1.78	0.65
1:A:269:ASP:O	1:A:272:VAL:HG22	1.97	0.65
1:A:90:LEU:CD2	1:C:115:LYS:HD2	2.27	0.64
2:I:119:ASN:HD21	2:J:445:GLY:HA3	1.63	0.64
2:L:106:ILE:HD13	2:L:110:GLU:OE2	1.97	0.64
2:L:61:THR:HG22	2:L:63:LEU:HG	1.80	0.64
2:I:424:VAL:HG11	2:J:330:LEU:HD13	1.80	0.64
2:I:230:LEU:HD23	2:I:339:PHE:CE2	2.32	0.64
2:K:60:VAL:HG12	2:K:176:ALA:CA	2.28	0.64
1:A:64:LEU:HA	1:A:69:ARG:HH12	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LEU:HD21	1:C:115:LYS:CB	2.28	0.64
1:C:37:ILE:H	1:C:37:ILE:HD13	1.62	0.64
1:C:202:GLU:HG2	1:C:203:ASN:N	2.12	0.64
1:E:175:LEU:HD12	1:E:213:PHE:CE1	2.33	0.64
1:A:231:THR:HA	1:A:234:LEU:HD12	1.79	0.64
1:C:175:LEU:HD12	1:C:213:PHE:CE1	2.32	0.64
2:K:391:VAL:HG12	2:K:393:LEU:CD2	2.27	0.64
2:K:377:PHE:CD2	2:L:378:LEU:HA	2.33	0.64
1:A:60:GLU:HG2	1:A:61:ASN:N	2.13	0.64
2:L:148:LEU:HG	2:L:151:ARG:CZ	2.28	0.64
1:C:151:PHE:HB2	1:C:173:GLU:O	1.98	0.64
2:I:296:PHE:HB2	2:J:367:PHE:HE1	1.63	0.64
2:J:143:ILE:HA	2:J:147:ILE:HD12	1.78	0.63
2:L:49:ASP:OD1	2:L:65:VAL:HG11	1.98	0.63
1:G:262:ARG:HD3	1:G:264:ILE:HD11	1.80	0.63
1:E:82:ILE:HD13	1:G:83:GLN:OE1	1.98	0.63
2:J:345:TYR:O	2:J:348:ILE:HG12	1.97	0.63
2:I:106:ILE:HD12	2:I:127:ILE:CG2	2.27	0.63
2:K:306:GLY:O	2:K:315:LYS:HB3	1.97	0.63
2:I:111:ARG:HB3	2:I:123:ILE:O	1.98	0.63
2:K:116:GLU:OE2	2:K:422:THR:HG22	1.98	0.63
2:K:230:LEU:HD23	2:K:339:PHE:CE2	2.34	0.63
2:L:202:PHE:CE1	2:L:274:VAL:HG12	2.31	0.63
2:L:247:PHE:O	2:L:251:TYR:HB2	1.98	0.63
2:I:148:LEU:HG	2:I:151:ARG:NH2	2.13	0.63
1:G:59:GLU:O	1:G:63:LEU:HD13	1.98	0.63
2:I:116:GLU:OE2	2:I:422:THR:HG22	1.98	0.63
2:I:209:PHE:N	2:I:308:ALA:HB3	2.14	0.63
2:K:106:ILE:HD12	2:K:127:ILE:CG2	2.27	0.63
2:K:63:LEU:HD22	2:K:394:THR:CG2	2.29	0.63
1:G:60:GLU:HG2	1:G:61:ASN:N	2.12	0.63
2:J:116:GLU:OE2	2:J:422:THR:HG22	1.98	0.63
1:A:37:ILE:HD13	1:A:37:ILE:H	1.63	0.63
2:I:92:MET:HB2	2:I:117:ALA:HB2	1.79	0.63
2:I:63:LEU:HD22	2:I:394:THR:CG2	2.29	0.63
2:K:49:ASP:OD1	2:K:65:VAL:HG11	1.98	0.63
2:K:378:LEU:HA	2:L:377:PHE:CD2	2.34	0.63
1:A:115:LYS:HD2	1:C:90:LEU:CG	2.29	0.63
1:E:125:GLU:HG2	1:E:158:ARG:CB	2.29	0.63
1:G:201:GLU:O	1:G:205:LEU:HD13	1.98	0.63
2:J:32:ALA:CB	2:J:51:LEU:HD12	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:406:LYS:O	2:J:410:ILE:HG13	1.99	0.63
2:J:48:ILE:HG22	2:J:406:LYS:HD3	1.79	0.63
2:L:114:VAL:HB	2:L:126:VAL:CG2	2.28	0.63
2:I:386:SER:OG	2:I:391:VAL:HB	1.99	0.63
1:A:175:LEU:HD12	1:A:213:PHE:CE1	2.33	0.63
1:A:166:GLU:OE2	1:A:169:ARG:HD3	1.99	0.63
1:A:179:ILE:H	1:A:179:ILE:HD13	1.64	0.63
1:A:135:SER:O	1:A:139:GLU:HB2	1.99	0.63
1:G:206:LEU:HA	1:G:211:ARG:HH12	1.63	0.63
1:A:9:PHE:HB2	1:A:31:GLU:O	1.99	0.63
2:I:247:PHE:O	2:I:251:TYR:HB2	1.98	0.62
2:I:391:VAL:HG12	2:I:393:LEU:CD2	2.30	0.62
1:E:87:LEU:O	1:E:91:LEU:HG	1.99	0.62
2:J:61:THR:HG21	2:J:413:MET:HG2	1.81	0.62
2:I:257:LEU:O	2:I:265:LYS:HE3	2.00	0.62
1:C:24:GLU:OE2	1:C:27:ARG:HD3	1.99	0.62
2:I:375:ALA:HB1	2:I:376:PRO:HD2	1.81	0.62
1:A:87:LEU:O	1:A:91:LEU:HG	1.98	0.62
2:K:388:PHE:O	2:K:416:GLY:HA3	1.99	0.62
2:J:20:LEU:HD22	2:J:92:MET:HG2	1.81	0.62
1:G:277:SER:O	1:G:281:GLU:HB2	2.00	0.62
1:E:135:SER:O	1:E:139:GLU:HB2	2.00	0.62
1:E:151:PHE:HB2	1:E:173:GLU:O	1.99	0.62
1:C:87:LEU:O	1:C:91:LEU:HG	2.00	0.62
2:J:63:LEU:HD22	2:J:394:THR:CG2	2.29	0.62
2:J:92:MET:HB2	2:J:117:ALA:HB2	1.81	0.62
2:J:114:VAL:HB	2:J:126:VAL:CG2	2.30	0.62
2:L:106:ILE:HD12	2:L:127:ILE:CG2	2.28	0.62
2:J:61:THR:HG22	2:J:63:LEU:HG	1.80	0.62
1:C:16:ARG:HB2	1:C:267:GLU:HG2	1.82	0.62
1:A:229:LEU:O	1:A:233:LEU:HG	2.00	0.62
1:G:249:TYR:O	1:G:252:HIS:HB3	2.00	0.62
1:C:136:LEU:CD1	1:C:163:ILE:HD11	2.30	0.62
1:C:179:ILE:H	1:C:179:ILE:HD13	1.64	0.62
2:J:88:GLY:HA3	2:J:174:ASN:ND2	2.14	0.62
1:E:277:SER:O	1:E:281:GLU:HB2	1.99	0.62
2:J:145:ALA:HB2	2:J:169:ALA:CB	2.30	0.62
2:J:226:LEU:O	2:J:230:LEU:HG	2.00	0.61
1:C:277:SER:O	1:C:281:GLU:HB2	2.01	0.61
1:G:151:PHE:HB2	1:G:173:GLU:O	2.00	0.61
2:I:20:LEU:HD22	2:I:92:MET:HG2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:391:VAL:HG12	2:J:393:LEU:CD2	2.29	0.61
2:L:268:ALA:O	2:L:272:GLN:HB2	2.00	0.61
2:J:378:LEU:HG	2:J:395:MET:HE3	1.82	0.61
1:C:9:PHE:HB2	1:C:31:GLU:O	2.00	0.61
2:L:17:PRO:HG2	2:L:18:GLN:H	1.64	0.61
2:K:20:LEU:HD22	2:K:92:MET:HG2	1.82	0.61
2:L:386:SER:OG	2:L:391:VAL:HB	2.00	0.61
2:L:60:VAL:HG12	2:L:176:ALA:CA	2.30	0.61
2:L:148:LEU:HG	2:L:151:ARG:NH2	2.15	0.61
2:J:49:ASP:OD1	2:J:65:VAL:HG11	2.00	0.61
1:C:135:SER:O	1:C:139:GLU:HB2	2.01	0.61
1:G:22:VAL:CG1	1:G:49:ALA:HB2	2.31	0.61
1:E:269:ASP:O	1:E:272:VAL:HG22	2.01	0.61
2:L:145:ALA:HB2	2:L:169:ALA:CB	2.30	0.61
2:L:116:GLU:OE2	2:L:422:THR:HG22	2.00	0.61
2:K:226:LEU:O	2:K:230:LEU:HG	2.00	0.61
2:L:375:ALA:HB1	2:L:376:PRO:HD2	1.82	0.61
2:I:17:PRO:HG2	2:I:18:GLN:H	1.66	0.61
2:J:215:VAL:HG13	2:J:224:PHE:HZ	1.65	0.61
1:E:9:PHE:HB2	1:E:31:GLU:O	2.00	0.61
1:A:277:SER:O	1:A:281:GLU:HB2	2.00	0.61
2:J:407:CYS:O	2:J:411:VAL:HG23	2.01	0.61
2:I:92:MET:HE3	2:I:96:VAL:HG23	1.83	0.61
2:J:272:GLN:HE22	2:J:283:SER:CB	2.13	0.61
2:J:17:PRO:HG2	2:J:18:GLN:H	1.65	0.61
2:K:238:LEU:HD23	2:K:277:ARG:NH2	2.16	0.61
1:C:33:LEU:HD12	1:C:71:PHE:CE1	2.35	0.61
1:C:166:GLU:OE2	1:C:169:ARG:HD3	2.01	0.61
2:L:96:VAL:HG12	2:L:96:VAL:O	2.00	0.61
2:I:202:PHE:CE1	2:I:274:VAL:HG12	2.33	0.61
1:G:135:SER:O	1:G:139:GLU:HB2	2.00	0.61
2:K:204:THR:O	2:K:207:ILE:HG12	2.01	0.61
2:K:345:TYR:O	2:K:348:ILE:HG12	2.01	0.61
2:J:272:GLN:HE22	2:J:283:SER:HB3	1.64	0.60
2:I:60:VAL:HG12	2:I:176:ALA:CA	2.30	0.60
2:I:310:THR:O	2:I:311:ALA:HB2	2.00	0.60
2:J:204:THR:O	2:J:207:ILE:HG12	2.01	0.60
1:E:60:GLU:HG2	1:E:61:ASN:N	2.15	0.60
2:L:278:THR:HB	2:L:390:THR:O	2.00	0.60
2:J:375:ALA:HB1	2:J:376:PRO:HD2	1.83	0.60
1:G:33:LEU:HD12	1:G:71:PHE:CE1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ASN:OD1	1:C:83:GLN:NE2	2.25	0.60
1:A:206:LEU:HA	1:A:211:ARG:HH12	1.66	0.60
1:G:89:THR:HA	1:G:92:LEU:HD12	1.81	0.60
2:L:310:THR:O	2:L:311:ALA:HB2	2.01	0.60
2:J:325:SER:OG	2:J:336:THR:HG21	2.01	0.60
2:L:215:VAL:HG22	2:L:224:PHE:CE2	2.35	0.60
2:I:96:VAL:O	2:I:96:VAL:HG12	2.00	0.60
2:J:268:ALA:O	2:J:272:GLN:HB2	2.01	0.60
1:E:231:THR:HA	1:E:234:LEU:HD12	1.82	0.60
2:L:88:GLY:HA3	2:L:174:ASN:ND2	2.16	0.60
2:J:388:PHE:O	2:J:416:GLY:HA3	2.01	0.60
2:I:106:ILE:HD13	2:I:110:GLU:OE2	2.01	0.60
2:K:61:THR:HG21	2:K:413:MET:HG2	1.83	0.60
2:K:407:CYS:O	2:K:411:VAL:HG23	2.02	0.60
2:K:92:MET:HB2	2:K:117:ALA:HB2	1.83	0.60
2:L:272:GLN:HE22	2:L:283:SER:CB	2.14	0.60
2:J:199:THR:HA	2:J:202:PHE:CE2	2.37	0.60
1:E:59:GLU:O	1:E:63:LEU:HD13	2.00	0.60
2:K:17:PRO:HG2	2:K:18:GLN:H	1.66	0.60
2:K:441:GLU:O	2:L:226:LEU:HB3	2.02	0.60
2:J:93:THR:HG1	2:J:118:LEU:HD21	1.66	0.60
2:L:172:ALA:O	2:L:202:PHE:HB3	2.01	0.60
2:K:148:LEU:HG	2:K:151:ARG:NH2	2.17	0.60
1:A:90:LEU:CG	1:C:115:LYS:HD2	2.31	0.60
1:C:107:TYR:O	1:C:110:HIS:HB3	2.01	0.60
2:L:93:THR:CG2	2:L:133:LEU:HD13	2.31	0.60
2:K:375:ALA:HB1	2:K:376:PRO:HD2	1.84	0.60
2:L:378:LEU:HG	2:L:395:MET:CE	2.32	0.60
1:E:249:TYR:O	1:E:252:HIS:HB3	2.02	0.60
2:J:96:VAL:HG12	2:J:96:VAL:O	2.02	0.60
2:K:238:LEU:HD23	2:K:277:ARG:HH21	1.66	0.60
2:K:378:LEU:HG	2:K:395:MET:HE3	1.83	0.60
2:L:61:THR:HG21	2:L:413:MET:HG2	1.84	0.60
1:A:59:GLU:O	1:A:63:LEU:HD13	2.02	0.60
1:G:231:THR:HA	1:G:234:LEU:HD12	1.84	0.60
2:I:188:TYR:CG	2:I:194:VAL:HG21	2.37	0.60
2:K:96:VAL:O	2:K:96:VAL:HG12	2.02	0.60
1:E:22:VAL:CG1	1:E:49:ALA:HB2	2.31	0.60
1:C:164:VAL:CG1	1:C:191:ALA:HB2	2.32	0.60
1:A:82:ILE:HD13	1:C:83:GLN:OE1	2.02	0.59
1:C:206:LEU:HA	1:C:211:ARG:HH12	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:175:LEU:HD12	1:G:213:PHE:CE1	2.37	0.59
2:L:257:LEU:O	2:L:265:LYS:HE3	2.02	0.59
1:G:166:GLU:OE2	1:G:169:ARG:HD3	2.01	0.59
2:L:306:GLY:O	2:L:315:LYS:HB3	2.02	0.59
2:I:32:ALA:CB	2:I:51:LEU:HD12	2.31	0.59
2:I:204:THR:O	2:I:207:ILE:HG12	2.02	0.59
2:K:310:THR:O	2:K:311:ALA:HB2	2.02	0.59
2:I:145:ALA:HB2	2:I:169:ALA:CB	2.32	0.59
2:J:16:PRO:O	2:J:20:LEU:HG	2.01	0.59
2:L:398:THR:HB	2:L:399:PRO:HD3	1.84	0.59
2:I:103:ALA:O	2:I:104:ALA:CB	2.51	0.59
2:I:172:ALA:O	2:I:202:PHE:HB3	2.02	0.59
2:I:16:PRO:O	2:I:20:LEU:HG	2.02	0.59
2:I:226:LEU:O	2:I:230:LEU:HG	2.02	0.59
2:J:257:LEU:O	2:J:265:LYS:HE3	2.02	0.59
2:L:103:ALA:O	2:L:104:ALA:CB	2.51	0.59
1:E:164:VAL:CG1	1:E:191:ALA:HB2	2.32	0.59
2:I:398:THR:HB	2:I:399:PRO:HD3	1.84	0.59
2:K:88:GLY:C	2:K:89:LEU:HD23	2.23	0.59
2:I:247:PHE:HE1	2:I:265:LYS:HB3	1.66	0.59
1:E:229:LEU:O	1:E:233:LEU:HG	2.03	0.59
2:I:272:GLN:HE22	2:I:283:SER:HB3	1.68	0.59
1:E:136:LEU:CD1	1:E:163:ILE:HD11	2.33	0.59
2:L:112:MET:HG2	2:L:123:ILE:HG21	1.83	0.59
2:I:88:GLY:HA3	2:I:174:ASN:ND2	2.17	0.59
2:K:268:ALA:O	2:K:272:GLN:HB2	2.02	0.59
2:I:143:ILE:HA	2:I:147:ILE:HD12	1.84	0.59
1:E:33:LEU:HD12	1:E:71:PHE:CE1	2.38	0.59
2:I:407:CYS:O	2:I:411:VAL:HG23	2.03	0.59
1:C:64:LEU:HA	1:C:69:ARG:HH12	1.66	0.59
2:I:114:VAL:HB	2:I:126:VAL:CG2	2.33	0.59
2:L:272:GLN:HE22	2:L:283:SER:HB3	1.64	0.59
2:J:376:PRO:HG2	2:J:379:GLN:HB3	1.85	0.59
1:C:21:ILE:HD11	1:C:278:LEU:CD1	2.32	0.59
2:L:226:LEU:O	2:L:230:LEU:HG	2.03	0.58
2:J:93:THR:CG2	2:J:133:LEU:HD13	2.33	0.58
2:J:378:LEU:HG	2:J:395:MET:CE	2.33	0.58
2:J:358:SER:O	2:J:362:VAL:HG23	2.03	0.58
2:K:32:ALA:CB	2:K:51:LEU:HD12	2.32	0.58
1:A:164:VAL:CG1	1:A:191:ALA:HB2	2.32	0.58
1:G:107:TYR:O	1:G:110:HIS:HB3	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:VAL:CG1	1:C:49:ALA:HB2	2.33	0.58
2:L:20:LEU:HD22	2:L:92:MET:HG2	1.85	0.58
2:I:100:MET:HE3	2:I:127:ILE:HG22	1.83	0.58
2:K:16:PRO:O	2:K:20:LEU:HG	2.02	0.58
2:K:294:ILE:HG21	2:K:378:LEU:HD11	1.85	0.58
2:K:386:SER:OG	2:K:391:VAL:HB	2.03	0.58
2:K:57:ALA:HB1	2:K:84:ILE:HG13	1.85	0.58
2:K:370:THR:HA	2:K:380:ILE:HD13	1.85	0.58
1:E:206:LEU:HA	1:E:211:ARG:HH12	1.68	0.58
2:I:268:ALA:O	2:I:272:GLN:HB2	2.02	0.58
2:K:103:ALA:O	2:K:104:ALA:CB	2.50	0.58
2:L:63:LEU:HD22	2:L:394:THR:CG2	2.33	0.58
1:A:89:THR:HA	1:A:92:LEU:HD12	1.85	0.58
2:I:123:ILE:HG13	2:I:124:GLY:N	2.17	0.58
2:L:16:PRO:O	2:L:20:LEU:HG	2.03	0.58
2:J:398:THR:HB	2:J:399:PRO:HD3	1.85	0.58
2:J:208:GLY:HA2	2:J:309:SER:N	2.17	0.58
1:A:107:TYR:O	1:A:110:HIS:HB3	2.03	0.58
2:I:211:VAL:HG21	2:I:231:MET:HG3	1.85	0.58
2:K:92:MET:HE3	2:K:96:VAL:HG23	1.85	0.58
2:L:230:LEU:HD23	2:L:339:PHE:CE2	2.38	0.58
1:C:249:TYR:O	1:C:252:HIS:HB3	2.04	0.58
2:L:345:TYR:O	2:L:348:ILE:HG12	2.02	0.58
2:I:272:GLN:HE22	2:I:283:SER:CB	2.17	0.58
2:J:103:ALA:O	2:J:104:ALA:CB	2.50	0.58
2:K:96:VAL:HB	2:K:130:VAL:HG21	1.85	0.58
2:L:34:LEU:HD22	2:L:79:VAL:HG21	1.86	0.58
2:K:257:LEU:O	2:K:265:LYS:HE3	2.04	0.58
2:I:424:VAL:HG11	2:J:330:LEU:HD22	1.85	0.58
2:K:350:LYS:HE3	2:K:421:LEU:CD1	2.33	0.58
2:K:268:ALA:HB1	2:K:284:LEU:HD11	1.85	0.58
1:A:243:TRP:CD2	1:A:262:ARG:HD2	2.39	0.58
2:J:310:THR:O	2:J:311:ALA:HB2	2.03	0.58
2:K:93:THR:CG2	2:K:133:LEU:HD13	2.33	0.58
2:J:278:THR:HB	2:J:390:THR:O	2.03	0.58
2:K:370:THR:HG22	2:K:380:ILE:HD13	1.85	0.58
1:E:17:PHE:HB2	1:E:267:GLU:HG3	1.85	0.58
2:K:211:VAL:HG21	2:K:231:MET:HG3	1.85	0.58
2:J:96:VAL:HB	2:J:130:VAL:HG21	1.85	0.58
2:K:379:GLN:HA	2:K:395:MET:HE2	1.86	0.58
2:K:341:ARG:HG2	2:L:438:PRO:HG2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:123:ILE:HG13	2:K:124:GLY:N	2.18	0.58
2:I:112:MET:HG2	2:I:123:ILE:HG21	1.86	0.58
2:K:188:TYR:CG	2:K:194:VAL:HG21	2.39	0.58
1:E:107:TYR:O	1:E:110:HIS:HB3	2.03	0.58
2:K:88:GLY:O	2:K:89:LEU:HD23	2.04	0.57
2:I:358:SER:O	2:I:362:VAL:HG23	2.04	0.57
2:J:253:ASN:O	2:J:258:GLY:HA3	2.03	0.57
2:I:306:GLY:O	2:I:315:LYS:HB3	2.04	0.57
2:L:388:PHE:O	2:L:416:GLY:HA3	2.03	0.57
2:J:268:ALA:HB1	2:J:284:LEU:HD11	1.85	0.57
2:K:398:THR:HB	2:K:399:PRO:HD3	1.84	0.57
2:L:394:THR:HG21	2:L:398:THR:OG1	2.04	0.57
2:L:358:SER:O	2:L:362:VAL:HG23	2.04	0.57
2:J:247:PHE:HE1	2:J:265:LYS:HB3	1.69	0.57
2:I:49:ASP:OD1	2:I:65:VAL:HG11	2.04	0.57
2:L:123:ILE:HG13	2:L:124:GLY:N	2.17	0.57
2:J:35:LEU:CD2	2:J:79:VAL:HB	2.35	0.57
1:A:197:ALA:HB2	2:J:435:ILE:HG22	1.86	0.57
2:K:199:THR:HA	2:K:202:PHE:CE2	2.39	0.57
2:J:294:ILE:O	2:J:298:LEU:HD13	2.04	0.57
2:I:185:LEU:HD23	2:I:185:LEU:O	2.04	0.57
2:L:209:PHE:N	2:L:308:ALA:HB3	2.20	0.57
2:K:189:VAL:HG11	2:K:260:LEU:HD21	1.86	0.57
2:J:306:GLY:O	2:J:315:LYS:HB3	2.04	0.57
2:L:350:LYS:HE3	2:L:421:LEU:CD1	2.35	0.57
2:J:379:GLN:HG3	2:J:395:MET:HB2	1.86	0.57
1:A:22:VAL:CG1	1:A:49:ALA:HB2	2.34	0.57
2:L:204:THR:O	2:L:207:ILE:HG12	2.04	0.57
2:L:407:CYS:O	2:L:411:VAL:HG23	2.05	0.57
1:E:179:ILE:HA	1:E:197:ALA:O	2.05	0.57
1:A:21:ILE:HD11	1:A:278:LEU:CD1	2.35	0.57
2:L:419:GLY:O	2:L:423:PHE:HB3	2.05	0.57
2:I:357:THR:HG21	2:I:420:PRO:HB2	1.85	0.57
1:G:164:VAL:CG1	1:G:191:ALA:HB2	2.35	0.57
2:I:345:TYR:O	2:I:348:ILE:HG12	2.05	0.57
1:E:60:GLU:O	1:E:64:LEU:HG	2.04	0.57
2:I:330:LEU:HD22	2:J:424:VAL:HG11	1.87	0.57
1:A:24:GLU:OE2	1:A:27:ARG:HD3	2.05	0.57
2:K:208:GLY:HA2	2:K:309:SER:N	2.20	0.57
2:K:378:LEU:HD13	2:L:377:PHE:CE1	2.40	0.57
2:L:376:PRO:HG2	2:L:379:GLN:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:ASN:O	1:E:54:ILE:HG23	2.05	0.57
2:J:188:TYR:CG	2:J:194:VAL:HG21	2.39	0.57
2:I:93:THR:CG2	2:I:133:LEU:HD13	2.34	0.56
1:E:89:THR:HA	1:E:92:LEU:HD12	1.86	0.56
1:A:106:ASN:CG	1:C:83:GLN:HE22	2.06	0.56
2:K:247:PHE:HE1	2:K:265:LYS:HB3	1.70	0.56
1:G:37:ILE:H	1:G:37:ILE:HD13	1.69	0.56
2:J:350:LYS:HG3	2:J:421:LEU:HD11	1.87	0.56
2:L:92:MET:HE3	2:L:96:VAL:HG23	1.87	0.56
2:J:394:THR:HG21	2:J:398:THR:OG1	2.06	0.56
2:L:379:GLN:HG3	2:L:395:MET:HB2	1.87	0.56
2:K:143:ILE:HA	2:K:147:ILE:HD12	1.85	0.56
1:C:202:GLU:O	1:C:206:LEU:HG	2.05	0.56
2:K:350:LYS:HG3	2:K:421:LEU:HD11	1.86	0.56
2:K:145:ALA:HB2	2:K:169:ALA:CB	2.35	0.56
2:L:92:MET:HB2	2:L:117:ALA:HB2	1.87	0.56
2:K:114:VAL:HB	2:K:126:VAL:CG2	2.35	0.56
2:I:278:THR:HB	2:I:390:THR:O	2.05	0.56
2:K:378:LEU:HG	2:K:395:MET:CE	2.35	0.56
2:J:123:ILE:HG13	2:J:124:GLY:N	2.19	0.56
2:K:394:THR:HG21	2:K:398:THR:OG1	2.04	0.56
1:C:88:THR:O	1:C:92:LEU:HG	2.05	0.56
2:J:34:LEU:HD22	2:J:79:VAL:HG21	1.86	0.56
1:A:33:LEU:HD12	1:A:71:PHE:CE1	2.39	0.56
2:L:253:ASN:O	2:L:258:GLY:HA3	2.05	0.56
2:K:185:LEU:O	2:K:185:LEU:HD23	2.03	0.56
2:K:357:THR:HG21	2:K:420:PRO:HB2	1.87	0.56
2:L:96:VAL:HB	2:L:130:VAL:HG21	1.86	0.56
1:C:229:LEU:O	1:C:233:LEU:HG	2.06	0.56
1:E:166:GLU:OE2	1:E:169:ARG:HD3	2.05	0.56
2:L:114:VAL:HB	2:L:126:VAL:HG21	1.85	0.56
2:I:383:GLU:OE2	2:I:397:LEU:HB3	2.05	0.56
2:J:100:MET:SD	2:J:127:ILE:HG22	2.45	0.56
2:J:369:LEU:HD11	2:J:409:ILE:HD11	1.88	0.56
1:G:181:GLU:HB3	1:G:196:ILE:HD13	1.87	0.56
2:I:238:LEU:HD23	2:I:277:ARG:HH21	1.70	0.56
2:L:208:GLY:HA2	2:L:309:SER:N	2.21	0.56
2:L:383:GLU:OE2	2:L:397:LEU:HB3	2.05	0.56
2:J:211:VAL:HG21	2:J:231:MET:HG3	1.88	0.56
2:L:359:LEU:HD23	2:L:360:PHE:N	2.21	0.56
2:I:88:GLY:C	2:I:89:LEU:HD23	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:92:MET:HE3	2:J:96:VAL:HG23	1.86	0.56
2:K:272:GLN:HE22	2:K:283:SER:CB	2.19	0.56
2:J:370:THR:HG22	2:J:380:ILE:HD13	1.87	0.56
2:L:143:ILE:HA	2:L:147:ILE:HD12	1.87	0.56
1:E:101:TRP:CD2	1:E:120:ARG:HD2	2.41	0.56
1:E:94:GLU:OE1	1:G:115:LYS:HD3	2.06	0.56
2:I:238:LEU:HD23	2:I:277:ARG:NH2	2.21	0.56
2:I:294:ILE:O	2:I:298:LEU:HD13	2.06	0.56
1:C:112:VAL:O	1:C:116:ILE:HG12	2.06	0.56
1:A:249:TYR:O	1:A:252:HIS:HB3	2.06	0.56
2:J:316:LEU:HG	2:J:320:ILE:HD11	1.88	0.56
2:K:376:PRO:HG2	2:K:379:GLN:HB3	1.86	0.56
1:C:22:VAL:HG13	1:C:49:ALA:HB2	1.88	0.56
2:L:188:TYR:CG	2:L:194:VAL:HG21	2.41	0.56
1:G:24:GLU:OE2	1:G:27:ARG:HD3	2.06	0.56
2:I:419:GLY:O	2:I:423:PHE:HB3	2.06	0.56
2:K:294:ILE:O	2:K:298:LEU:HD13	2.06	0.56
1:C:60:GLU:O	1:C:64:LEU:HG	2.05	0.56
1:G:229:LEU:O	1:G:232:LEU:HB3	2.05	0.56
1:G:22:VAL:HG13	1:G:49:ALA:HB2	1.89	0.56
2:J:350:LYS:HE3	2:J:421:LEU:CD1	2.36	0.56
2:I:350:LYS:HE3	2:I:421:LEU:CD1	2.35	0.56
2:L:96:VAL:O	2:L:130:VAL:HG11	2.07	0.55
2:I:394:THR:HG21	2:I:398:THR:OG1	2.06	0.55
1:A:60:GLU:O	1:A:64:LEU:HG	2.06	0.55
2:L:357:THR:HG21	2:L:420:PRO:HB2	1.86	0.55
2:I:406:LYS:O	2:I:410:ILE:HG13	2.07	0.55
2:I:96:VAL:HB	2:I:130:VAL:HG21	1.87	0.55
1:A:115:LYS:HD2	1:C:90:LEU:CD2	2.36	0.55
2:J:88:GLY:C	2:J:89:LEU:HD23	2.27	0.55
2:I:208:GLY:HA2	2:I:309:SER:N	2.20	0.55
2:K:275:THR:O	2:K:279:ALA:HB3	2.07	0.55
2:I:215:VAL:HG13	2:I:224:PHE:HZ	1.71	0.55
2:I:378:LEU:HG	2:I:395:MET:CE	2.37	0.55
2:L:378:LEU:HG	2:L:395:MET:HE3	1.89	0.55
2:J:366:ILE:HG13	2:J:384:THR:HG21	1.87	0.55
2:K:35:LEU:CD2	2:K:79:VAL:HB	2.37	0.55
1:G:60:GLU:O	1:G:64:LEU:HG	2.07	0.55
2:J:419:GLY:O	2:J:423:PHE:HB3	2.07	0.55
2:J:202:PHE:CE1	2:J:274:VAL:HG12	2.37	0.55
2:J:96:VAL:HG11	2:J:127:ILE:HD13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:370:THR:HG22	2:I:380:ILE:HD13	1.88	0.55
1:E:194:ALA:O	2:L:438:PRO:HD3	2.07	0.55
1:G:243:TRP:CD2	1:G:262:ARG:HD2	2.42	0.55
2:L:93:THR:HG23	2:L:133:LEU:HD22	1.88	0.55
2:I:226:LEU:HD13	2:I:230:LEU:HD11	1.89	0.55
2:L:60:VAL:HG12	2:L:175:ASN:O	2.07	0.55
2:K:291:GLU:CB	2:L:370:THR:HB	2.37	0.55
1:C:59:GLU:O	1:C:63:LEU:HD13	2.07	0.55
1:E:57:ALA:O	1:E:91:LEU:HD12	2.06	0.55
1:E:24:GLU:OE2	1:E:27:ARG:HD3	2.06	0.55
2:K:333:LYS:HG2	2:L:433:SER:HB2	1.89	0.55
2:K:100:MET:SD	2:K:127:ILE:HG22	2.46	0.55
2:I:163:PHE:CD2	2:I:180:LEU:HD11	2.42	0.55
1:A:125:GLU:HG3	1:A:159:PHE:CB	2.34	0.55
2:I:272:GLN:HA	2:I:275:THR:HG22	1.89	0.55
1:C:164:VAL:HG13	1:C:191:ALA:HB2	1.88	0.55
2:J:230:LEU:HD23	2:J:339:PHE:CE2	2.42	0.55
2:I:60:VAL:HG12	2:I:175:ASN:O	2.07	0.55
2:J:112:MET:HG2	2:J:123:ILE:HG21	1.88	0.55
2:L:268:ALA:HB1	2:L:284:LEU:HD11	1.89	0.55
2:L:238:LEU:HD23	2:L:277:ARG:NH2	2.22	0.55
1:G:112:VAL:O	1:G:116:ILE:HG12	2.07	0.55
2:K:419:GLY:O	2:K:423:PHE:HB3	2.07	0.55
2:J:226:LEU:HD13	2:J:230:LEU:HD11	1.89	0.55
2:J:386:SER:OG	2:J:391:VAL:HB	2.06	0.55
2:L:294:ILE:O	2:L:298:LEU:HD13	2.07	0.55
2:L:247:PHE:HE1	2:L:265:LYS:HB3	1.72	0.55
2:J:257:LEU:HA	2:J:260:LEU:HD22	1.89	0.55
1:G:9:PHE:HB2	1:G:31:GLU:O	2.06	0.55
2:K:100:MET:HE3	2:K:127:ILE:HG22	1.88	0.54
2:J:280:GLY:HA2	2:J:392:GLY:HA3	1.89	0.54
1:C:125:GLU:HG2	1:C:158:ARG:CB	2.37	0.54
1:A:229:LEU:O	1:A:232:LEU:HB3	2.07	0.54
1:E:125:GLU:HG3	1:E:159:PHE:HB2	1.87	0.54
2:I:296:PHE:HB2	2:J:367:PHE:CE1	2.42	0.54
2:L:350:LYS:HG3	2:L:421:LEU:HD11	1.88	0.54
2:L:215:VAL:HG13	2:L:224:PHE:HZ	1.71	0.54
2:I:379:GLN:HG3	2:I:395:MET:HB2	1.88	0.54
2:K:61:THR:HG22	2:K:63:LEU:HG	1.88	0.54
2:I:257:LEU:HA	2:I:260:LEU:HD22	1.88	0.54
2:J:411:VAL:HG12	2:J:415:ILE:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:211:VAL:O	2:L:215:VAL:HG23	2.06	0.54
2:I:211:VAL:HG13	2:I:228:THR:HG23	1.89	0.54
2:I:215:VAL:HA	2:I:224:PHE:CZ	2.43	0.54
1:E:202:GLU:O	1:E:206:LEU:HG	2.08	0.54
1:A:151:PHE:HB2	1:A:173:GLU:O	2.06	0.54
2:I:97:LEU:HD11	2:I:130:VAL:O	2.08	0.54
2:J:294:ILE:HG21	2:J:378:LEU:HD11	1.89	0.54
2:J:185:LEU:HD23	2:J:185:LEU:O	2.07	0.54
2:J:211:VAL:HG13	2:J:228:THR:HG23	1.89	0.54
2:I:360:PHE:CE1	2:J:323:LEU:HD11	2.42	0.54
2:I:96:VAL:O	2:I:130:VAL:HG11	2.08	0.54
2:I:383:GLU:HG3	2:I:397:LEU:HD23	1.90	0.54
2:J:114:VAL:HB	2:J:126:VAL:HG21	1.89	0.54
2:L:275:THR:N	2:L:276:PRO:CD	2.71	0.54
2:K:296:PHE:HB2	2:L:367:PHE:CE1	2.43	0.54
2:I:316:LEU:HG	2:I:320:ILE:HD11	1.89	0.54
1:G:229:LEU:O	1:G:233:LEU:HG	2.07	0.54
1:A:254:VAL:O	1:A:258:ILE:HG12	2.07	0.54
2:J:324:THR:HA	2:J:327:ILE:CD1	2.38	0.54
2:K:85:GLN:HA	2:K:174:ASN:ND2	2.23	0.54
2:I:324:THR:HA	2:I:327:ILE:CD1	2.37	0.54
2:J:359:LEU:HD23	2:J:360:PHE:N	2.23	0.54
2:I:253:ASN:O	2:I:258:GLY:HA3	2.08	0.54
1:E:265:HIS:HB3	1:E:268:LYS:HB2	1.89	0.54
2:I:359:LEU:HD23	2:I:360:PHE:N	2.22	0.54
2:K:93:THR:HG23	2:K:133:LEU:HD22	1.88	0.54
2:K:272:GLN:HE22	2:K:283:SER:HB3	1.73	0.54
1:A:83:GLN:HE21	1:C:108:TYR:HB2	1.72	0.54
1:A:180:ASN:O	1:A:196:ILE:HG23	2.08	0.54
1:C:265:HIS:HB3	1:C:268:LYS:HB2	1.89	0.54
2:I:388:PHE:O	2:I:416:GLY:HA3	2.07	0.54
2:K:275:THR:N	2:K:276:PRO:CD	2.71	0.54
2:K:304:GLY:HA3	2:K:312:SER:OG	2.08	0.54
2:L:405:GLY:HA2	2:L:408:ILE:HD11	1.90	0.54
2:K:291:GLU:O	2:K:295:VAL:HG23	2.08	0.54
2:K:318:THR:HG22	2:K:322:ILE:HD11	1.89	0.54
2:L:88:GLY:C	2:L:89:LEU:HD23	2.28	0.54
2:K:440:GLY:HA3	2:L:341:ARG:O	2.08	0.54
2:J:208:GLY:HA2	2:J:309:SER:H	1.73	0.54
2:J:370:THR:HA	2:J:380:ILE:HD13	1.90	0.54
2:J:357:THR:HG21	2:J:420:PRO:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:57:ALA:O	1:G:91:LEU:HD12	2.08	0.54
2:I:36:MET:HG3	2:I:50:ALA:CB	2.37	0.54
1:A:230:THR:O	1:A:234:LEU:HG	2.08	0.54
2:J:65:VAL:CG2	2:J:406:LYS:HE2	2.38	0.54
2:K:383:GLU:OE2	2:K:397:LEU:HB3	2.08	0.53
2:J:322:ILE:CD1	2:J:355:SER:HB2	2.38	0.53
1:G:180:ASN:O	1:G:196:ILE:HG23	2.08	0.53
2:K:358:SER:O	2:K:362:VAL:HG23	2.08	0.53
2:L:324:THR:HA	2:L:327:ILE:CD1	2.38	0.53
1:A:164:VAL:HG13	1:A:191:ALA:HB2	1.90	0.53
1:A:38:ASN:O	1:A:54:ILE:HG23	2.08	0.53
2:I:199:THR:HA	2:I:202:PHE:CZ	2.44	0.53
2:K:370:THR:CG2	2:K:380:ILE:HD13	2.39	0.53
2:L:185:LEU:HD23	2:L:185:LEU:O	2.08	0.53
2:K:16:PRO:HA	2:K:113:LEU:CD2	2.38	0.53
2:L:369:LEU:HD11	2:L:409:ILE:HD11	1.90	0.53
1:A:57:ALA:O	1:A:91:LEU:HD12	2.09	0.53
1:C:57:ALA:O	1:C:91:LEU:HD12	2.08	0.53
2:L:81:MET:SD	2:L:170:ILE:HD12	2.48	0.53
2:I:275:THR:N	2:I:276:PRO:CD	2.71	0.53
2:J:211:VAL:O	2:J:215:VAL:HG23	2.08	0.53
2:K:344:LYS:HG2	2:K:346:PRO:HD2	1.91	0.53
2:L:41:THR:O	2:L:41:THR:HG23	2.09	0.53
2:I:93:THR:HG23	2:I:133:LEU:HD22	1.91	0.53
2:I:208:GLY:HA2	2:I:309:SER:H	1.73	0.53
2:I:362:VAL:HG13	2:I:384:THR:HG22	1.90	0.53
1:C:229:LEU:O	1:C:232:LEU:HB3	2.08	0.53
1:E:164:VAL:HG13	1:E:191:ALA:HB2	1.90	0.53
1:E:112:VAL:O	1:E:116:ILE:HG12	2.08	0.53
2:J:96:VAL:O	2:J:130:VAL:HG11	2.09	0.53
1:A:125:GLU:CG	1:A:159:PHE:HB2	2.35	0.53
2:L:316:LEU:HG	2:L:320:ILE:HD11	1.90	0.53
2:J:238:LEU:HD23	2:J:277:ARG:NH2	2.24	0.53
2:K:96:VAL:HG11	2:K:127:ILE:HD13	1.90	0.53
2:K:294:ILE:HG23	2:K:382:PHE:CD2	2.43	0.53
1:A:16:ARG:HB2	1:A:267:GLU:HG2	1.90	0.53
1:C:199:ALA:O	1:C:233:LEU:HD12	2.08	0.53
2:K:324:THR:HA	2:K:327:ILE:CD1	2.38	0.53
2:K:202:PHE:CE1	2:K:274:VAL:HG12	2.39	0.53
1:C:230:THR:O	1:C:234:LEU:HG	2.09	0.53
2:L:150:ILE:O	2:L:154:PRO:HD3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:250:GLU:O	2:L:257:LEU:HD22	2.08	0.53
1:A:193:HIS:NE2	2:I:340:ARG:CD	2.71	0.53
2:J:215:VAL:HA	2:J:224:PHE:CZ	2.44	0.53
2:I:346:PRO:O	2:I:349:ILE:HG22	2.09	0.53
1:A:225:GLN:HA	1:A:228:THR:OG1	2.08	0.53
2:L:199:THR:HA	2:L:202:PHE:CZ	2.44	0.53
1:E:230:THR:O	1:E:234:LEU:HG	2.09	0.53
2:I:268:ALA:HB1	2:I:284:LEU:HD11	1.91	0.53
2:I:20:LEU:HA	2:I:91:PHE:CD2	2.44	0.53
2:J:275:THR:N	2:J:276:PRO:CD	2.72	0.53
2:L:370:THR:HA	2:L:380:ILE:HD13	1.90	0.53
2:J:229:ALA:O	2:J:233:THR:HG23	2.09	0.53
1:A:202:GLU:O	1:A:206:LEU:HG	2.08	0.52
1:C:24:GLU:O	1:C:27:ARG:HB3	2.09	0.52
1:A:22:VAL:HG13	1:A:49:ALA:HB2	1.91	0.52
2:I:277:ARG:HG3	2:I:277:ARG:NH1	2.23	0.52
2:L:280:GLY:HA2	2:L:392:GLY:HA3	1.91	0.52
2:K:40:SER:HB3	2:K:75:PHE:CD2	2.43	0.52
2:I:350:LYS:HG3	2:I:421:LEU:HD11	1.91	0.52
2:L:272:GLN:HA	2:L:275:THR:HG22	1.90	0.52
2:I:370:THR:HA	2:I:380:ILE:HD13	1.92	0.52
2:J:257:LEU:HD23	2:J:265:LYS:HG2	1.91	0.52
2:K:215:VAL:HG13	2:K:224:PHE:HZ	1.75	0.52
2:K:93:THR:HG1	2:K:118:LEU:HD21	1.73	0.52
1:E:37:ILE:HA	1:E:55:ALA:O	2.08	0.52
1:E:199:ALA:O	1:E:233:LEU:HD12	2.10	0.52
1:G:199:ALA:O	1:G:233:LEU:HD12	2.09	0.52
1:G:23:LYS:HG2	1:G:48:TYR:HD2	1.75	0.52
2:I:37:LEU:HD12	2:I:38:PRO:HD2	1.92	0.52
2:K:316:LEU:HG	2:K:320:ILE:HD11	1.92	0.52
2:K:96:VAL:O	2:K:130:VAL:HG11	2.10	0.52
2:I:376:PRO:HG2	2:I:379:GLN:HB3	1.91	0.52
1:C:16:ARG:CB	1:C:267:GLU:HG2	2.39	0.52
2:J:73:THR:HG22	2:J:74:VAL:N	2.24	0.52
1:E:22:VAL:HG13	1:E:49:ALA:HB2	1.91	0.52
1:E:108:TYR:O	1:E:112:VAL:HG12	2.09	0.52
2:I:61:THR:HG22	2:I:63:LEU:HG	1.90	0.52
2:K:383:GLU:HG3	2:K:397:LEU:HD23	1.90	0.52
2:L:294:ILE:HG21	2:L:378:LEU:HD11	1.91	0.52
1:G:230:THR:O	1:G:234:LEU:HG	2.09	0.52
1:A:112:VAL:O	1:A:116:ILE:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:318:THR:HG22	2:L:322:ILE:HD11	1.91	0.52
1:C:196:ILE:HB	2:K:436:ARG:HB2	1.91	0.52
2:K:272:GLN:N	2:K:272:GLN:NE2	2.58	0.52
1:E:180:ASN:O	1:E:196:ILE:HG23	2.10	0.52
2:J:150:ILE:O	2:J:154:PRO:HD3	2.10	0.52
1:G:202:GLU:O	1:G:206:LEU:HG	2.09	0.52
1:A:199:ALA:O	1:A:233:LEU:HD12	2.10	0.52
1:C:250:TYR:O	1:C:254:VAL:HG12	2.09	0.52
2:K:179:SER:HB2	2:K:184:ASN:OD1	2.09	0.52
2:I:100:MET:SD	2:I:127:ILE:HG22	2.49	0.52
2:I:211:VAL:O	2:I:215:VAL:HG23	2.09	0.52
2:J:362:VAL:HG13	2:J:384:THR:HG22	1.91	0.52
2:K:34:LEU:HD22	2:K:79:VAL:HG21	1.91	0.52
2:I:35:LEU:CD2	2:I:79:VAL:HB	2.38	0.52
1:E:58:THR:HG1	1:G:108:TYR:HE1	1.57	0.52
2:L:327:ILE:O	2:L:331:ARG:HG3	2.10	0.51
2:I:421:LEU:HD21	2:J:329:TYR:CE1	2.45	0.51
1:E:250:TYR:O	1:E:254:VAL:HG12	2.11	0.51
2:I:367:PHE:HE1	2:J:296:PHE:HB2	1.76	0.51
2:J:37:LEU:CD2	2:J:39:ILE:HD13	2.40	0.51
1:C:38:ASN:O	1:C:54:ILE:HG23	2.10	0.51
2:I:250:GLU:O	2:I:257:LEU:HD22	2.11	0.51
1:G:22:VAL:HA	1:G:32:VAL:HG11	1.91	0.51
1:E:153:VAL:HG22	1:E:217:ILE:HB	1.92	0.51
2:K:359:LEU:HD23	2:K:360:PHE:N	2.25	0.51
2:K:226:LEU:HD13	2:K:230:LEU:HD11	1.91	0.51
2:K:215:VAL:HA	2:K:224:PHE:CZ	2.45	0.51
2:K:60:VAL:HG12	2:K:175:ASN:O	2.10	0.51
2:L:177:GLY:HA3	2:L:280:GLY:HA3	1.93	0.51
2:L:294:ILE:HG23	2:L:382:PHE:CD2	2.44	0.51
2:L:362:VAL:HG13	2:L:384:THR:HG22	1.92	0.51
2:L:325:SER:OG	2:L:336:THR:HG21	2.11	0.51
1:E:243:TRP:CD2	1:E:262:ARG:HD2	2.45	0.51
1:G:254:VAL:O	1:G:258:ILE:HG12	2.10	0.51
1:G:164:VAL:HG13	1:G:191:ALA:HB2	1.92	0.51
2:I:114:VAL:HB	2:I:126:VAL:HG21	1.91	0.51
2:K:352:LEU:CD1	2:L:326:VAL:HG22	2.41	0.51
2:J:322:ILE:HD13	2:J:355:SER:HB2	1.93	0.51
1:E:64:LEU:HA	1:E:69:ARG:NH1	2.26	0.51
2:K:257:LEU:HD23	2:K:265:LYS:HG2	1.92	0.51
1:G:23:LYS:HG2	1:G:48:TYR:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:209:PHE:N	2:K:308:ALA:HB3	2.23	0.51
2:I:280:GLY:HA2	2:I:392:GLY:HA3	1.91	0.51
2:I:143:ILE:O	2:I:147:ILE:HB	2.10	0.51
1:A:179:ILE:HA	1:A:197:ALA:O	2.10	0.51
1:C:166:GLU:O	1:C:169:ARG:HB3	2.11	0.51
1:E:164:VAL:HA	1:E:174:VAL:HG11	1.91	0.51
2:J:41:THR:O	2:J:41:THR:HG23	2.11	0.51
2:K:97:LEU:HD11	2:K:130:VAL:O	2.11	0.51
2:K:136:PHE:O	2:K:139:SER:HB3	2.10	0.51
1:A:64:LEU:HD23	1:A:69:ARG:HH22	1.74	0.51
2:J:411:VAL:O	2:J:415:ILE:HG13	2.11	0.51
2:J:291:GLU:O	2:J:295:VAL:HG23	2.11	0.51
2:L:229:ALA:O	2:L:233:THR:HG23	2.11	0.51
2:J:226:LEU:CD1	2:J:230:LEU:HD11	2.40	0.51
2:I:294:ILE:HG23	2:I:382:PHE:CD2	2.45	0.51
2:I:166:LEU:O	2:I:166:LEU:HD13	2.10	0.51
2:J:366:ILE:HD13	2:J:381:VAL:HG13	1.93	0.51
2:I:323:LEU:HD11	2:J:360:PHE:CE1	2.46	0.51
1:C:175:LEU:HD12	1:C:213:PHE:CZ	2.46	0.51
1:G:64:LEU:HA	1:G:69:ARG:NH1	2.25	0.51
1:G:179:ILE:HA	1:G:197:ALA:O	2.11	0.51
2:K:350:LYS:HE3	2:K:421:LEU:HD12	1.93	0.51
1:A:24:GLU:O	1:A:27:ARG:HB3	2.11	0.51
2:J:37:LEU:HD12	2:J:38:PRO:HD2	1.91	0.51
2:K:229:ALA:O	2:K:233:THR:HG23	2.10	0.51
2:K:211:VAL:HG13	2:K:228:THR:HG23	1.92	0.51
2:J:59:THR:C	2:J:60:VAL:HG23	2.30	0.51
2:I:304:GLY:HA3	2:I:312:SER:OG	2.11	0.51
2:I:34:LEU:HD22	2:I:79:VAL:HG21	1.92	0.51
2:J:65:VAL:HG21	2:J:406:LYS:HE2	1.93	0.51
1:C:216:VAL:C	1:C:217:ILE:HD12	2.31	0.51
2:L:145:ALA:O	2:L:149:SER:HB2	2.11	0.51
1:G:38:ASN:O	1:G:54:ILE:HG23	2.10	0.51
2:J:177:GLY:HA3	2:J:280:GLY:HA3	1.93	0.51
2:J:272:GLN:HA	2:J:275:THR:HG22	1.92	0.51
2:J:60:VAL:HG12	2:J:175:ASN:O	2.11	0.51
2:I:301:MET:HB2	2:I:391:VAL:HG21	1.93	0.51
1:G:196:ILE:HD12	2:I:436:ARG:HB3	1.91	0.51
2:K:143:ILE:O	2:K:147:ILE:HB	2.11	0.51
2:I:325:SER:OG	2:I:336:THR:HG21	2.11	0.51
2:K:81:MET:SD	2:K:170:ILE:HD12	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:TRP:CD2	1:C:262:ARG:HD2	2.45	0.51
1:C:178:ASP:OD1	1:C:179:ILE:HG12	2.11	0.51
2:J:145:ALA:O	2:J:149:SER:HB2	2.10	0.51
2:K:97:LEU:HD11	2:K:134:PHE:HB3	1.93	0.51
2:J:99:VAL:HG12	2:J:99:VAL:O	2.11	0.51
2:K:62:GLY:HA3	2:K:392:GLY:CA	2.39	0.51
1:A:175:LEU:HD12	1:A:213:PHE:CZ	2.46	0.51
1:C:87:LEU:O	1:C:90:LEU:HB3	2.10	0.51
1:E:87:LEU:O	1:E:90:LEU:HB3	2.11	0.51
2:L:226:LEU:HD13	2:L:230:LEU:HD11	1.92	0.50
2:K:238:LEU:CD2	2:K:277:ARG:HH21	2.24	0.50
1:A:87:LEU:O	1:A:90:LEU:HB3	2.11	0.50
1:A:115:LYS:HD3	1:C:94:GLU:OE1	2.11	0.50
2:L:153:VAL:O	2:L:153:VAL:HG12	2.11	0.50
1:C:37:ILE:HA	1:C:55:ALA:O	2.11	0.50
2:L:346:PRO:O	2:L:349:ILE:HG22	2.11	0.50
2:K:369:LEU:HD11	2:K:409:ILE:HD11	1.92	0.50
2:L:143:ILE:O	2:L:147:ILE:HB	2.12	0.50
1:E:229:LEU:O	1:E:232:LEU:HB3	2.10	0.50
2:J:163:PHE:CD2	2:J:180:LEU:HD11	2.46	0.50
2:I:177:GLY:HA3	2:I:280:GLY:HA3	1.93	0.50
2:I:59:THR:C	2:I:60:VAL:HG23	2.31	0.50
2:J:93:THR:HG23	2:J:133:LEU:HD22	1.93	0.50
1:A:83:GLN:HA	1:A:86:THR:OG1	2.11	0.50
2:L:189:VAL:HG11	2:L:260:LEU:HD21	1.93	0.50
2:J:344:LYS:HG2	2:J:346:PRO:HD2	1.94	0.50
2:L:238:LEU:HD23	2:L:277:ARG:HH21	1.76	0.50
1:G:39:GLU:HB3	1:G:54:ILE:HD13	1.93	0.50
1:G:21:ILE:HD11	1:G:278:LEU:CD1	2.41	0.50
2:L:291:GLU:O	2:L:295:VAL:HG23	2.11	0.50
2:L:214:ASP:OD2	2:L:228:THR:HG21	2.11	0.50
2:I:96:VAL:C	2:I:130:VAL:HG21	2.32	0.50
2:I:92:MET:HB2	2:I:117:ALA:HB3	1.91	0.50
2:K:272:GLN:HA	2:K:275:THR:HG22	1.94	0.50
2:I:226:LEU:CD1	2:I:230:LEU:HD11	2.42	0.50
1:A:90:LEU:HD21	1:C:115:LYS:HD2	1.91	0.50
2:K:322:ILE:CD1	2:K:355:SER:HB2	2.41	0.50
2:L:302:PHE:HE1	2:L:358:SER:HB2	1.77	0.50
2:I:272:GLN:N	2:I:272:GLN:NE2	2.59	0.50
1:A:164:VAL:HA	1:A:174:VAL:HG11	1.92	0.50
1:C:11:VAL:HG22	1:C:75:ILE:HB	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:35:LEU:CD2	2:L:79:VAL:HB	2.40	0.50
1:E:211:ARG:CZ	1:E:211:ARG:HB3	2.41	0.50
1:C:69:ARG:CZ	1:C:69:ARG:HB3	2.42	0.50
1:A:101:TRP:CD2	1:A:120:ARG:HD2	2.46	0.50
1:E:254:VAL:O	1:E:258:ILE:HG12	2.11	0.50
2:K:41:THR:O	2:K:41:THR:HG23	2.12	0.50
2:J:383:GLU:OE2	2:J:397:LEU:HB3	2.12	0.50
2:K:366:ILE:HD13	2:K:381:VAL:HG13	1.94	0.50
1:G:33:LEU:HD12	1:G:71:PHE:CZ	2.46	0.50
2:K:346:PRO:O	2:K:349:ILE:HG22	2.12	0.50
2:J:350:LYS:HE3	2:J:421:LEU:HD12	1.93	0.50
2:K:184:ASN:C	2:K:186:MET:H	2.15	0.50
2:J:40:SER:HB3	2:J:75:PHE:CD2	2.46	0.50
2:J:57:ALA:O	2:J:84:ILE:HA	2.12	0.50
2:J:20:LEU:CD2	2:J:92:MET:HG2	2.41	0.50
2:K:143:ILE:HG13	2:K:144:ALA:N	2.26	0.50
1:E:175:LEU:HD12	1:E:213:PHE:CZ	2.47	0.50
1:G:88:THR:O	1:G:92:LEU:HG	2.12	0.50
1:C:254:VAL:O	1:C:258:ILE:HG12	2.11	0.50
1:A:166:GLU:O	1:A:169:ARG:HB3	2.11	0.50
2:I:229:ALA:O	2:I:233:THR:HG23	2.12	0.50
2:L:100:MET:HE3	2:L:127:ILE:HG22	1.94	0.50
2:K:294:ILE:CG2	2:K:378:LEU:HD11	2.42	0.50
2:K:59:THR:C	2:K:60:VAL:HG23	2.31	0.50
2:L:59:THR:C	2:L:60:VAL:HG23	2.32	0.50
2:J:115:GLN:O	2:J:115:GLN:HG2	2.10	0.50
1:C:153:VAL:HG22	1:C:217:ILE:HB	1.92	0.50
1:G:166:GLU:O	1:G:169:ARG:HB3	2.12	0.50
2:I:411:VAL:HG12	2:I:415:ILE:HD11	1.94	0.50
2:I:277:ARG:HH11	2:I:277:ARG:HG3	1.76	0.50
2:I:20:LEU:HD23	2:I:20:LEU:N	2.27	0.50
2:K:277:ARG:NH1	2:K:277:ARG:HG3	2.27	0.50
2:J:153:VAL:HG12	2:J:153:VAL:O	2.11	0.50
2:L:257:LEU:HA	2:L:260:LEU:HD22	1.92	0.50
2:I:420:PRO:O	2:I:424:VAL:HG23	2.11	0.50
1:A:178:ASP:OD1	1:A:179:ILE:HG12	2.12	0.50
2:K:349:ILE:HG12	2:L:329:TYR:CD2	2.46	0.50
1:A:250:TYR:O	1:A:254:VAL:HG12	2.11	0.50
1:G:216:VAL:C	1:G:217:ILE:HD12	2.32	0.50
2:K:294:ILE:HG23	2:K:382:PHE:HD2	1.76	0.49
2:K:291:GLU:HB2	2:L:370:THR:HB	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:136:PHE:O	2:L:139:SER:HB3	2.12	0.49
2:K:150:ILE:O	2:K:154:PRO:HD3	2.11	0.49
1:G:36:ASP:OD1	1:G:37:ILE:HG12	2.11	0.49
1:G:37:ILE:HA	1:G:55:ALA:O	2.12	0.49
1:C:74:VAL:C	1:C:75:ILE:HD12	2.32	0.49
2:K:114:VAL:HB	2:K:126:VAL:HG21	1.92	0.49
2:J:209:PHE:H	2:J:308:ALA:CB	2.17	0.49
2:J:97:LEU:HD11	2:J:134:PHE:HB3	1.93	0.49
2:K:304:GLY:HA3	2:K:312:SER:CB	2.41	0.49
2:K:326:VAL:HG22	2:L:352:LEU:CD1	2.42	0.49
2:L:411:VAL:HG12	2:L:415:ILE:HD11	1.92	0.49
1:G:108:TYR:O	1:G:112:VAL:HG12	2.12	0.49
1:E:265:HIS:CB	1:E:268:LYS:HB2	2.42	0.49
1:E:254:VAL:HG13	1:E:255:LEU:N	2.27	0.49
2:K:37:LEU:CD2	2:K:39:ILE:HD13	2.42	0.49
2:K:207:ILE:HD12	2:K:211:VAL:HB	1.93	0.49
2:I:62:GLY:C	2:I:63:LEU:HD23	2.33	0.49
1:A:125:GLU:HG2	1:A:159:PHE:N	2.27	0.49
2:K:153:VAL:O	2:K:153:VAL:HG12	2.11	0.49
2:I:257:LEU:HD23	2:I:265:LYS:HG2	1.94	0.49
2:K:92:MET:HE2	2:K:113:LEU:HB3	1.94	0.49
2:I:62:GLY:HA3	2:I:392:GLY:CA	2.39	0.49
1:C:108:TYR:O	1:C:112:VAL:HG12	2.12	0.49
2:I:405:GLY:HA2	2:I:408:ILE:HD11	1.95	0.49
2:I:81:MET:SD	2:I:170:ILE:HD12	2.52	0.49
1:G:64:LEU:HD23	1:G:69:ARG:HH22	1.77	0.49
1:C:164:VAL:HA	1:C:174:VAL:HG11	1.93	0.49
1:E:172:HIS:O	1:E:174:VAL:HG23	2.13	0.49
1:A:242:ILE:HG13	1:A:261:ASP:H	1.77	0.49
1:E:74:VAL:C	1:E:75:ILE:HD12	2.32	0.49
2:K:393:LEU:HD22	2:K:393:LEU:H	1.78	0.49
2:L:272:GLN:N	2:L:272:GLN:NE2	2.60	0.49
2:I:352:LEU:HD23	2:J:352:LEU:CD2	2.37	0.49
1:A:206:LEU:HD23	1:A:211:ARG:HH22	1.78	0.49
2:I:73:THR:HG22	2:I:74:VAL:N	2.23	0.49
2:I:322:ILE:CD1	2:I:355:SER:HB2	2.42	0.49
2:I:445:GLY:CA	2:J:119:ASN:HD21	2.22	0.49
2:I:256:THR:HB	2:I:284:LEU:HD13	1.95	0.49
2:K:253:ASN:O	2:K:258:GLY:HA3	2.12	0.49
1:E:16:ARG:CB	1:E:267:GLU:HG2	2.42	0.49
2:L:350:LYS:HE3	2:L:421:LEU:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:92:MET:HE2	2:L:113:LEU:HB3	1.93	0.49
2:I:97:LEU:HD11	2:I:134:PHE:HB3	1.94	0.49
2:J:100:MET:HE3	2:J:127:ILE:HG22	1.94	0.49
2:J:136:PHE:O	2:J:139:SER:HB3	2.12	0.49
2:L:294:ILE:HG23	2:L:382:PHE:HD2	1.76	0.49
2:J:294:ILE:HG23	2:J:382:PHE:CD2	2.47	0.49
2:I:318:THR:HG22	2:I:322:ILE:HD11	1.94	0.49
2:I:153:VAL:HG12	2:I:153:VAL:O	2.12	0.49
2:J:346:PRO:O	2:J:349:ILE:HG22	2.13	0.49
2:I:344:LYS:HG2	2:I:346:PRO:HD2	1.94	0.49
2:I:20:LEU:HA	2:I:91:PHE:HD2	1.77	0.49
2:K:96:VAL:C	2:K:130:VAL:HG21	2.33	0.49
2:J:394:THR:C	2:J:396:GLY:H	2.16	0.49
2:I:378:LEU:HG	2:I:395:MET:HE3	1.95	0.49
2:L:57:ALA:O	2:L:84:ILE:HA	2.13	0.49
1:E:88:THR:O	1:E:92:LEU:HG	2.12	0.49
1:A:192:THR:HG22	1:A:193:HIS:HD1	1.77	0.49
2:J:189:VAL:HG11	2:J:260:LEU:HD21	1.95	0.49
1:E:22:VAL:HA	1:E:32:VAL:HG11	1.95	0.49
1:E:216:VAL:C	1:E:217:ILE:HD12	2.33	0.49
2:L:212:LEU:O	2:L:216:MET:HG3	2.13	0.49
2:K:20:LEU:CD2	2:K:92:MET:HG2	2.42	0.49
2:J:20:LEU:HA	2:J:91:PHE:CD2	2.46	0.49
1:C:211:ARG:CZ	1:C:211:ARG:HB3	2.42	0.49
1:G:206:LEU:HA	1:G:211:ARG:NH1	2.28	0.49
2:L:304:GLY:HA3	2:L:312:SER:CB	2.43	0.49
1:E:174:VAL:O	1:E:191:ALA:HB1	2.12	0.49
2:K:349:ILE:HG12	2:L:329:TYR:HD2	1.78	0.49
1:A:216:VAL:C	1:A:217:ILE:HD12	2.33	0.49
2:I:213:PHE:O	2:I:216:MET:HB2	2.13	0.49
2:K:168:HIS:O	2:K:172:ALA:HB2	2.13	0.49
2:K:378:LEU:HD13	2:L:377:PHE:CZ	2.48	0.49
2:I:327:ILE:O	2:I:331:ARG:HG3	2.12	0.49
2:L:304:GLY:HA3	2:L:312:SER:OG	2.13	0.49
2:L:103:ALA:O	2:L:104:ALA:HB2	2.13	0.49
2:I:350:LYS:HE3	2:I:421:LEU:HD12	1.95	0.49
2:I:37:LEU:CD2	2:I:39:ILE:HD13	2.43	0.49
1:G:265:HIS:HB3	1:G:268:LYS:HB2	1.94	0.49
2:L:20:LEU:HA	2:L:91:PHE:CD2	2.48	0.49
2:K:163:PHE:CD2	2:K:180:LEU:HD11	2.48	0.49
2:L:163:PHE:CD2	2:L:180:LEU:HD11	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:189:VAL:HG11	2:I:260:LEU:HD21	1.95	0.49
2:K:104:ALA:O	2:K:105:ALA:HB3	2.12	0.49
1:A:74:VAL:C	1:A:75:ILE:HD12	2.34	0.49
1:G:172:HIS:O	1:G:174:VAL:HG23	2.13	0.49
2:K:233:THR:OG1	2:K:234:GLY:N	2.46	0.49
2:L:184:ASN:C	2:L:186:MET:H	2.16	0.49
2:I:352:LEU:CD2	2:J:352:LEU:HD23	2.37	0.48
2:K:302:PHE:HE1	2:K:358:SER:HB2	1.78	0.48
2:K:318:THR:HG22	2:K:322:ILE:CD1	2.43	0.48
2:L:73:THR:HG22	2:L:74:VAL:N	2.24	0.48
2:I:36:MET:HE2	2:I:47:TRP:HA	1.95	0.48
2:I:103:ALA:O	2:I:104:ALA:HB2	2.13	0.48
2:I:16:PRO:HA	2:I:113:LEU:CD2	2.42	0.48
2:J:275:THR:O	2:J:279:ALA:HB3	2.13	0.48
2:I:369:LEU:HD11	2:I:409:ILE:HD11	1.94	0.48
2:J:383:GLU:HG3	2:J:397:LEU:HD23	1.95	0.48
1:A:172:HIS:O	1:A:174:VAL:HG23	2.13	0.48
2:K:211:VAL:O	2:K:215:VAL:HG23	2.13	0.48
2:K:208:GLY:HA2	2:K:309:SER:H	1.78	0.48
1:G:196:ILE:HD11	2:I:437:TYR:O	2.13	0.48
2:K:296:PHE:HB2	2:L:367:PHE:HE1	1.77	0.48
2:L:318:THR:HG22	2:L:322:ILE:CD1	2.43	0.48
2:L:322:ILE:CD1	2:L:355:SER:HB2	2.43	0.48
2:L:143:ILE:HG13	2:L:144:ALA:N	2.28	0.48
1:C:125:GLU:HG2	1:C:159:PHE:N	2.28	0.48
1:A:64:LEU:HA	1:A:69:ARG:NH1	2.27	0.48
2:J:304:GLY:HA3	2:J:312:SER:OG	2.13	0.48
2:J:88:GLY:O	2:J:89:LEU:HD23	2.13	0.48
2:L:304:GLY:HA3	2:L:312:SER:HB3	1.94	0.48
2:K:411:VAL:HG12	2:K:415:ILE:HD11	1.94	0.48
1:C:225:GLN:HA	1:C:228:THR:OG1	2.14	0.48
1:G:225:GLN:HA	1:G:228:THR:OG1	2.12	0.48
2:L:16:PRO:HA	2:L:113:LEU:CD2	2.42	0.48
2:J:62:GLY:C	2:J:63:LEU:HD23	2.33	0.48
2:I:294:ILE:HG23	2:I:382:PHE:HD2	1.78	0.48
2:L:40:SER:HB3	2:L:75:PHE:CD2	2.48	0.48
2:K:362:VAL:HG13	2:K:384:THR:HG22	1.95	0.48
1:A:193:HIS:NE2	2:I:340:ARG:HD3	2.27	0.48
2:J:104:ALA:O	2:J:105:ALA:HB3	2.14	0.48
1:G:164:VAL:HA	1:G:174:VAL:HG11	1.95	0.48
2:L:99:VAL:HG12	2:L:99:VAL:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:20:LEU:HD23	2:L:20:LEU:N	2.29	0.48
2:L:208:GLY:HA2	2:L:309:SER:H	1.78	0.48
2:K:325:SER:OG	2:K:336:THR:HG21	2.13	0.48
2:J:57:ALA:HB1	2:J:84:ILE:HG13	1.95	0.48
2:L:152:LEU:HD23	2:L:191:ASP:OD2	2.13	0.48
2:L:65:VAL:HG21	2:L:406:LYS:HE2	1.94	0.48
1:C:18:GLY:O	1:C:21:ILE:HG22	2.13	0.48
1:E:166:GLU:O	1:E:169:ARG:HB3	2.13	0.48
2:J:184:ASN:C	2:J:186:MET:H	2.16	0.48
2:I:41:THR:O	2:I:41:THR:HG23	2.13	0.48
2:I:286:PHE:HA	2:I:289:MET:SD	2.53	0.48
2:L:211:VAL:HG21	2:L:231:MET:HG3	1.95	0.48
2:K:276:PRO:O	2:K:391:VAL:HG13	2.14	0.48
2:K:89:LEU:HD12	2:K:94:PHE:CE1	2.49	0.48
2:K:296:PHE:CE2	2:K:300:LEU:HD22	2.49	0.48
2:L:370:THR:HG22	2:L:380:ILE:HD13	1.94	0.48
2:L:65:VAL:CG2	2:L:406:LYS:HE2	2.43	0.48
2:J:411:VAL:HG12	2:J:415:ILE:CD1	2.43	0.48
1:E:160:GLY:O	1:E:163:ILE:HG22	2.13	0.48
1:C:265:HIS:CB	1:C:268:LYS:HB2	2.44	0.48
2:I:37:LEU:HG	2:I:39:ILE:HD13	1.96	0.48
1:G:153:VAL:HG22	1:G:217:ILE:HB	1.94	0.48
2:K:37:LEU:HD12	2:K:38:PRO:HD2	1.96	0.48
1:G:242:ILE:HG13	1:G:261:ASP:H	1.79	0.48
2:L:96:VAL:C	2:L:130:VAL:HG21	2.34	0.48
2:L:92:MET:HB2	2:L:117:ALA:HB3	1.96	0.48
1:A:211:ARG:CZ	1:A:211:ARG:HB3	2.43	0.48
2:K:115:GLN:HG2	2:K:115:GLN:O	2.13	0.48
2:I:184:ASN:C	2:I:186:MET:H	2.17	0.48
2:K:99:VAL:O	2:K:99:VAL:HG12	2.13	0.48
2:L:92:MET:CE	2:L:113:LEU:HB3	2.43	0.48
2:L:213:PHE:O	2:L:216:MET:HB2	2.13	0.48
2:J:389:GLY:O	2:J:390:THR:C	2.52	0.48
2:I:393:LEU:HD22	2:I:393:LEU:H	1.79	0.48
2:I:80:ILE:O	2:I:84:ILE:HG13	2.14	0.48
2:J:92:MET:HB2	2:J:117:ALA:HB3	1.95	0.48
2:L:57:ALA:HB1	2:L:84:ILE:HG13	1.96	0.48
2:K:445:GLY:CA	2:L:119:ASN:HD21	2.26	0.48
1:G:83:GLN:HA	1:G:86:THR:OG1	2.14	0.48
1:G:250:TYR:O	1:G:254:VAL:HG12	2.13	0.48
2:I:145:ALA:O	2:I:149:SER:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:VAL:HG22	1:E:174:VAL:CG1	2.43	0.48
1:G:24:GLU:O	1:G:27:ARG:HB3	2.13	0.48
1:C:123:HIS:HB3	1:C:126:LYS:HB2	1.96	0.48
2:J:299:LEU:C	2:J:299:LEU:HD13	2.34	0.48
2:L:100:MET:SD	2:L:127:ILE:HG22	2.54	0.48
2:L:209:PHE:HA	2:L:212:LEU:CD1	2.32	0.48
2:K:20:LEU:HA	2:K:91:PHE:CD2	2.48	0.48
2:L:226:LEU:CD1	2:L:230:LEU:HD11	2.44	0.48
2:I:294:ILE:HG21	2:I:378:LEU:HD11	1.95	0.48
1:A:88:THR:O	1:A:92:LEU:HG	2.14	0.48
1:G:211:ARG:CZ	1:G:211:ARG:HB3	2.43	0.48
1:C:100:ILE:O	1:C:100:ILE:HG13	2.14	0.48
1:C:100:ILE:HG13	1:C:119:ASP:H	1.78	0.48
2:K:119:ASN:HD21	2:L:445:GLY:HA3	1.79	0.48
1:A:123:HIS:HB3	1:A:126:LYS:HB2	1.96	0.48
2:L:207:ILE:HD12	2:L:211:VAL:HB	1.94	0.48
2:J:92:MET:HE2	2:J:113:LEU:HB3	1.96	0.48
2:L:199:THR:HG21	2:L:270:TYR:CE2	2.43	0.48
2:I:136:PHE:O	2:I:139:SER:HB3	2.13	0.48
2:I:143:ILE:HG13	2:I:144:ALA:N	2.28	0.48
1:G:206:LEU:HD23	1:G:211:ARG:HH22	1.79	0.48
1:C:139:GLU:HG3	1:C:215:TYR:OH	2.14	0.48
2:K:420:PRO:O	2:K:424:VAL:HG23	2.14	0.48
1:A:265:HIS:HB3	1:A:268:LYS:HB2	1.96	0.48
2:L:96:VAL:HG11	2:L:127:ILE:HD13	1.96	0.47
2:I:168:HIS:O	2:I:172:ALA:N	2.47	0.47
2:J:106:ILE:HG21	2:J:127:ILE:CD1	2.44	0.47
2:J:143:ILE:O	2:J:147:ILE:HB	2.14	0.47
1:A:196:ILE:HD12	2:J:436:ARG:HB3	1.96	0.47
1:A:121:ILE:C	1:A:122:ILE:HD12	2.34	0.47
1:C:22:VAL:HA	1:C:32:VAL:HG11	1.96	0.47
1:A:153:VAL:HG22	1:A:217:ILE:HB	1.96	0.47
1:E:123:HIS:HB3	1:E:126:LYS:HB2	1.96	0.47
2:I:61:THR:O	2:I:392:GLY:N	2.47	0.47
2:J:213:PHE:O	2:J:216:MET:HB2	2.15	0.47
2:K:62:GLY:CA	2:K:392:GLY:HA2	2.41	0.47
2:L:34:LEU:HD22	2:L:79:VAL:CG2	2.44	0.47
2:L:61:THR:O	2:L:392:GLY:N	2.47	0.47
2:I:370:THR:CG2	2:I:380:ILE:HD13	2.43	0.47
1:C:125:GLU:HG2	1:C:158:ARG:HB2	1.95	0.47
1:E:69:ARG:CZ	1:E:69:ARG:HB3	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:250:GLU:O	2:J:257:LEU:HD22	2.14	0.47
1:E:30:HIS:O	1:E:32:VAL:HG23	2.14	0.47
1:C:21:ILE:HG13	1:C:275:ALA:HB2	1.95	0.47
1:G:101:TRP:CD2	1:G:120:ARG:HD3	2.49	0.47
2:L:100:MET:SD	2:L:127:ILE:O	2.71	0.47
2:L:215:VAL:HA	2:L:224:PHE:CZ	2.49	0.47
2:I:100:MET:SD	2:I:127:ILE:O	2.71	0.47
2:I:61:THR:HA	2:I:390:THR:CB	2.37	0.47
2:K:304:GLY:HA3	2:K:312:SER:HB3	1.96	0.47
2:K:389:GLY:O	2:K:390:THR:C	2.53	0.47
1:C:112:VAL:HG13	1:C:113:LEU:N	2.30	0.47
1:E:150:GLN:HB2	1:E:214:GLU:OE1	2.13	0.47
1:E:178:ASP:OD1	1:E:179:ILE:HG12	2.14	0.47
2:I:36:MET:HG3	2:I:50:ALA:HB1	1.96	0.47
1:C:165:LYS:HG2	1:C:190:TYR:HD2	1.79	0.47
1:A:165:LYS:HG2	1:A:190:TYR:CD2	2.50	0.47
2:J:227:HIS:CE1	2:J:317:THR:HG21	2.49	0.47
2:L:275:THR:O	2:L:279:ALA:HB3	2.14	0.47
1:A:89:THR:HG21	1:A:102:VAL:HG11	1.96	0.47
2:I:362:VAL:O	2:I:366:ILE:HG13	2.15	0.47
2:K:411:VAL:HG12	2:K:415:ILE:CD1	2.45	0.47
2:I:149:SER:OG	2:I:197:VAL:HG11	2.14	0.47
1:G:100:ILE:HG13	1:G:100:ILE:O	2.14	0.47
2:I:99:VAL:HG12	2:I:99:VAL:O	2.15	0.47
2:I:62:GLY:CA	2:I:392:GLY:HA2	2.41	0.47
1:A:83:GLN:NE2	1:C:106:ASN:OD1	2.38	0.47
2:J:370:THR:CG2	2:J:380:ILE:HD13	2.44	0.47
2:K:341:ARG:HG2	2:L:438:PRO:CG	2.44	0.47
2:I:302:PHE:HE1	2:I:358:SER:HB2	1.79	0.47
2:J:34:LEU:HD22	2:J:79:VAL:CG2	2.44	0.47
1:G:254:VAL:HG13	1:G:255:LEU:N	2.30	0.47
2:I:198:ILE:HD13	2:I:281:PHE:CE2	2.49	0.47
1:E:21:ILE:HD11	1:E:278:LEU:CD1	2.44	0.47
2:K:226:LEU:CD1	2:K:230:LEU:HD11	2.44	0.47
1:C:17:PHE:N	1:C:267:GLU:HG2	2.29	0.47
2:K:166:LEU:HD13	2:K:166:LEU:O	2.14	0.47
1:C:33:LEU:HD12	1:C:71:PHE:CZ	2.48	0.47
1:A:37:ILE:HA	1:A:55:ALA:O	2.14	0.47
1:A:23:LYS:HG2	1:A:48:TYR:CD2	2.49	0.47
1:E:23:LYS:HG2	1:E:48:TYR:CD2	2.49	0.47
2:J:319:PHE:CZ	2:J:323:LEU:HD22	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:172:ALA:HB3	2:J:201:LEU:HD13	1.96	0.47
2:J:62:GLY:HA3	2:J:392:GLY:CA	2.43	0.47
2:K:61:THR:O	2:K:392:GLY:N	2.47	0.47
1:A:181:GLU:HB3	1:A:196:ILE:HD13	1.96	0.47
1:A:108:TYR:O	1:A:112:VAL:HG12	2.13	0.47
2:L:366:ILE:HD13	2:L:381:VAL:HG13	1.97	0.47
2:I:318:THR:HG22	2:I:322:ILE:CD1	2.45	0.47
1:C:250:TYR:CD1	1:G:229:LEU:HD11	2.50	0.47
2:I:233:THR:OG1	2:I:234:GLY:N	2.48	0.47
1:A:165:LYS:HG2	1:A:190:TYR:HD2	1.79	0.47
2:L:296:PHE:CE2	2:L:300:LEU:HD22	2.50	0.47
1:E:242:ILE:HG13	1:E:261:ASP:H	1.78	0.47
2:K:327:ILE:O	2:K:331:ARG:HG3	2.14	0.47
2:K:96:VAL:HG21	2:K:114:VAL:HG21	1.96	0.47
2:L:394:THR:C	2:L:396:GLY:H	2.18	0.47
1:G:16:ARG:HB2	1:G:267:GLU:HG2	1.97	0.47
2:K:342:SER:O	2:L:440:GLY:N	2.48	0.47
2:K:257:LEU:HA	2:K:260:LEU:HD22	1.97	0.47
1:C:160:GLY:O	1:C:163:ILE:HG22	2.14	0.47
1:G:123:HIS:HB3	1:G:126:LYS:HB2	1.96	0.47
1:C:242:ILE:HG13	1:C:242:ILE:O	2.15	0.47
2:K:227:HIS:O	2:K:230:LEU:HB2	2.14	0.47
2:J:275:THR:CG2	2:J:276:PRO:HD3	2.45	0.47
2:K:297:THR:HG22	2:K:301:MET:CE	2.45	0.47
2:L:383:GLU:HG3	2:L:397:LEU:HD23	1.96	0.47
1:A:17:PHE:CB	1:A:267:GLU:HG3	2.40	0.47
2:I:40:SER:HB3	2:I:75:PHE:CD2	2.50	0.47
2:L:411:VAL:HG12	2:L:415:ILE:CD1	2.45	0.47
2:L:85:GLN:HA	2:L:174:ASN:ND2	2.30	0.47
2:I:238:LEU:CD2	2:I:277:ARG:HH21	2.27	0.47
1:E:23:LYS:HG2	1:E:48:TYR:HD2	1.79	0.47
1:A:100:ILE:HG13	1:A:119:ASP:H	1.80	0.47
2:J:323:LEU:O	2:J:327:ILE:HG13	2.15	0.47
2:I:304:GLY:HA3	2:I:312:SER:CB	2.44	0.47
2:I:379:GLN:HA	2:I:395:MET:CE	2.42	0.47
2:K:301:MET:HB2	2:K:391:VAL:HG21	1.97	0.47
2:K:60:VAL:CG1	2:K:176:ALA:HB2	2.45	0.47
2:K:62:GLY:C	2:K:63:LEU:HD23	2.36	0.47
1:A:112:VAL:HG13	1:A:113:LEU:N	2.30	0.47
2:L:322:ILE:HD13	2:L:355:SER:HB2	1.97	0.47
2:I:308:ALA:O	2:I:309:SER:O	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:227:HIS:O	2:L:230:LEU:HB2	2.15	0.46
2:J:100:MET:SD	2:J:127:ILE:O	2.73	0.46
2:J:294:ILE:CG2	2:J:378:LEU:HD11	2.44	0.46
1:A:16:ARG:CB	1:A:267:GLU:HG2	2.45	0.46
2:I:115:GLN:O	2:I:115:GLN:HG2	2.16	0.46
2:L:115:GLN:O	2:L:115:GLN:HG2	2.13	0.46
2:K:402:THR:O	2:K:406:LYS:HD2	2.16	0.46
1:C:179:ILE:HA	1:C:197:ALA:O	2.15	0.46
2:I:188:TYR:CD1	2:I:194:VAL:HG21	2.49	0.46
1:E:164:VAL:HG22	1:E:174:VAL:HG11	1.97	0.46
2:L:233:THR:OG1	2:L:234:GLY:N	2.48	0.46
1:A:242:ILE:O	1:A:242:ILE:HG13	2.15	0.46
2:L:97:LEU:HD11	2:L:134:PHE:HB3	1.96	0.46
2:I:114:VAL:HG12	2:I:118:LEU:HD12	1.97	0.46
2:L:378:LEU:HG	2:L:395:MET:HE1	1.98	0.46
2:J:85:GLN:HA	2:J:174:ASN:ND2	2.30	0.46
2:L:36:MET:HG3	2:L:50:ALA:CB	2.45	0.46
1:C:172:HIS:O	1:C:174:VAL:HG23	2.14	0.46
1:A:23:LYS:HG2	1:A:48:TYR:HD2	1.79	0.46
2:I:299:LEU:C	2:I:299:LEU:HD13	2.35	0.46
2:L:299:LEU:HD13	2:L:299:LEU:C	2.35	0.46
2:J:227:HIS:O	2:J:230:LEU:HB2	2.14	0.46
2:L:100:MET:HE1	2:L:131:LYS:HE3	1.96	0.46
2:K:80:ILE:O	2:K:84:ILE:HG13	2.15	0.46
2:L:64:ALA:N	2:L:398:THR:HG21	2.20	0.46
2:L:62:GLY:HA3	2:L:392:GLY:CA	2.43	0.46
2:I:115:GLN:HA	2:I:120:GLN:HB3	1.97	0.46
2:J:420:PRO:O	2:J:424:VAL:HG23	2.15	0.46
1:E:90:LEU:HD21	1:G:115:LYS:HB2	1.96	0.46
1:G:30:HIS:O	1:G:32:VAL:HG23	2.15	0.46
1:E:32:VAL:O	1:E:49:ALA:HB1	2.16	0.46
2:K:188:TYR:CD1	2:K:194:VAL:HG21	2.50	0.46
1:E:24:GLU:O	1:E:27:ARG:HB3	2.14	0.46
2:L:37:LEU:CD2	2:L:39:ILE:HD13	2.45	0.46
2:K:118:LEU:HD22	2:K:209:PHE:CE2	2.51	0.46
2:J:272:GLN:N	2:J:272:GLN:NE2	2.63	0.46
2:I:298:LEU:HA	2:I:301:MET:HE2	1.97	0.46
2:K:276:PRO:O	2:K:278:THR:N	2.45	0.46
2:L:301:MET:HB2	2:L:391:VAL:HG21	1.97	0.46
1:G:89:THR:HG21	1:G:102:VAL:HG21	1.98	0.46
1:C:263:ILE:C	1:C:264:ILE:HD12	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:HIS:O	1:C:32:VAL:HG23	2.15	0.46
2:K:103:ALA:O	2:K:104:ALA:HB2	2.15	0.46
2:J:238:LEU:HD23	2:J:277:ARG:HH21	1.80	0.46
2:L:292:GLY:O	2:L:295:VAL:HB	2.15	0.46
1:C:165:LYS:HG2	1:C:190:TYR:CD2	2.51	0.46
1:G:165:LYS:HG2	1:G:190:TYR:HD2	1.80	0.46
2:I:61:THR:HG21	2:I:413:MET:HG2	1.96	0.46
2:J:16:PRO:HA	2:J:113:LEU:CD2	2.43	0.46
2:K:172:ALA:HB3	2:K:201:LEU:HD13	1.98	0.46
1:E:83:GLN:OE1	1:G:82:ILE:HG21	2.15	0.46
1:C:254:VAL:HG13	1:C:255:LEU:N	2.31	0.46
1:C:258:ILE:HD11	1:G:254:VAL:HG23	1.97	0.46
1:G:136:LEU:CD1	1:G:163:ILE:HD11	2.45	0.46
2:K:297:THR:HG22	2:K:301:MET:HE2	1.96	0.46
2:J:294:ILE:HG23	2:J:382:PHE:HD2	1.80	0.46
1:A:108:TYR:CE1	1:C:58:THR:HG21	2.50	0.46
1:E:231:THR:HG21	1:E:244:VAL:HG21	1.98	0.46
1:A:115:LYS:CB	1:C:90:LEU:HD21	2.40	0.46
1:G:263:ILE:C	1:G:264:ILE:HD12	2.36	0.46
1:A:174:VAL:O	1:A:191:ALA:HB1	2.15	0.46
2:J:418:ILE:HG12	2:J:418:ILE:O	2.16	0.46
2:K:66:VAL:HG11	2:K:71:GLN:OE1	2.16	0.46
2:I:291:GLU:O	2:I:295:VAL:HG23	2.15	0.46
2:K:96:VAL:CB	2:K:130:VAL:HG21	2.46	0.46
2:I:310:THR:O	2:I:311:ALA:CB	2.63	0.46
2:I:389:GLY:O	2:I:390:THR:C	2.54	0.46
2:J:100:MET:HE1	2:J:131:LYS:HE3	1.98	0.46
1:E:83:GLN:HA	1:E:86:THR:OG1	2.15	0.46
2:K:322:ILE:HD13	2:K:355:SER:HB2	1.98	0.46
1:G:89:THR:CG2	1:G:102:VAL:HG21	2.46	0.46
2:I:322:ILE:HD13	2:I:355:SER:HB2	1.98	0.46
1:C:21:ILE:HD11	1:C:278:LEU:HD12	1.97	0.46
1:A:18:GLY:O	1:A:21:ILE:HG22	2.15	0.46
2:K:371:ILE:HD11	2:L:292:GLY:HA3	1.97	0.46
2:I:286:PHE:N	2:I:286:PHE:CD1	2.84	0.46
2:K:92:MET:HB2	2:K:117:ALA:HB3	1.98	0.46
2:K:57:ALA:O	2:K:84:ILE:HA	2.15	0.46
2:K:292:GLY:HA3	2:L:371:ILE:CD1	2.42	0.46
1:G:231:THR:CG2	1:G:244:VAL:HG21	2.46	0.46
2:J:318:THR:HG22	2:J:322:ILE:CD1	2.46	0.46
2:J:318:THR:HG22	2:J:322:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:LEU:HD23	1:E:69:ARG:HH22	1.80	0.46
2:K:112:MET:HG2	2:K:123:ILE:HG21	1.96	0.46
2:I:119:ASN:HD21	2:J:445:GLY:CA	2.29	0.46
1:A:36:ASP:OD1	1:A:37:ILE:HG12	2.15	0.46
2:I:96:VAL:HG21	2:I:114:VAL:HG21	1.97	0.46
2:K:280:GLY:HA2	2:K:392:GLY:HA3	1.97	0.46
2:L:64:ALA:H	2:L:398:THR:CG2	2.21	0.46
2:K:337:VAL:HG21	2:L:437:TYR:CD1	2.51	0.46
1:A:22:VAL:HA	1:A:32:VAL:HG11	1.98	0.46
2:K:418:ILE:O	2:K:418:ILE:HG12	2.16	0.46
1:C:68:ILE:O	1:C:68:ILE:HD13	2.16	0.46
2:J:324:THR:HG23	2:J:325:SER:N	2.31	0.46
2:I:118:LEU:HD22	2:I:209:PHE:CE2	2.51	0.46
2:K:100:MET:SD	2:K:127:ILE:O	2.73	0.46
2:L:294:ILE:CG2	2:L:378:LEU:HD11	2.46	0.46
2:K:291:GLU:HB3	2:L:370:THR:HB	1.98	0.46
2:L:88:GLY:O	2:L:89:LEU:HD23	2.15	0.46
1:C:36:ASP:OD1	1:C:37:ILE:HG12	2.16	0.46
1:G:112:VAL:HG13	1:G:113:LEU:N	2.31	0.46
2:J:233:THR:OG1	2:J:234:GLY:N	2.48	0.46
1:A:123:HIS:CB	1:A:126:LYS:HB2	2.46	0.46
1:A:100:ILE:HG13	1:A:100:ILE:O	2.16	0.46
1:G:165:LYS:HG2	1:G:190:TYR:CD2	2.51	0.46
2:I:155:GLN:C	2:I:157:GLY:H	2.19	0.46
2:K:212:LEU:O	2:K:216:MET:HG3	2.16	0.45
2:J:80:ILE:O	2:J:84:ILE:HG13	2.16	0.45
2:I:304:GLY:HA3	2:I:312:SER:HB3	1.97	0.45
2:L:393:LEU:H	2:L:393:LEU:HD22	1.80	0.45
2:K:250:GLU:O	2:K:257:LEU:HD22	2.16	0.45
1:C:199:ALA:HA	1:C:205:LEU:HD11	1.98	0.45
2:I:145:ALA:HB2	2:I:169:ALA:HB2	1.98	0.45
1:E:112:VAL:HG13	1:E:113:LEU:N	2.31	0.45
2:J:286:PHE:HA	2:J:289:MET:SD	2.56	0.45
2:J:64:ALA:N	2:J:398:THR:HG21	2.25	0.45
2:J:143:ILE:HG13	2:J:144:ALA:N	2.31	0.45
2:L:391:VAL:CG1	2:L:393:LEU:HD23	2.43	0.45
2:K:137:SER:C	2:K:139:SER:H	2.19	0.45
1:C:83:GLN:HA	1:C:86:THR:OG1	2.17	0.45
2:L:89:LEU:HD12	2:L:94:PHE:CE1	2.52	0.45
1:G:87:LEU:O	1:G:90:LEU:HB3	2.15	0.45
2:L:145:ALA:HB2	2:L:169:ALA:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:VAL:O	1:C:191:ALA:HB1	2.16	0.45
2:K:299:LEU:C	2:K:299:LEU:HD13	2.36	0.45
2:L:112:MET:HG2	2:L:123:ILE:CG2	2.45	0.45
2:K:106:ILE:HG21	2:K:127:ILE:CD1	2.46	0.45
2:J:60:VAL:CG1	2:J:176:ALA:HB2	2.46	0.45
2:J:393:LEU:H	2:J:393:LEU:HD22	1.80	0.45
2:I:408:ILE:HG13	2:I:409:ILE:N	2.31	0.45
1:A:89:THR:CG2	1:A:102:VAL:HG21	2.46	0.45
2:I:366:ILE:HG13	2:I:384:THR:HG21	1.99	0.45
1:E:231:THR:CG2	1:E:244:VAL:HG21	2.46	0.45
1:E:231:THR:HG21	1:E:244:VAL:HG11	1.98	0.45
1:C:64:LEU:HA	1:C:69:ARG:NH1	2.32	0.45
2:L:323:LEU:O	2:L:327:ILE:HG13	2.16	0.45
2:L:104:ALA:O	2:L:105:ALA:HB3	2.16	0.45
2:L:344:LYS:HG2	2:L:346:PRO:HD2	1.97	0.45
2:L:418:ILE:O	2:L:418:ILE:HG12	2.17	0.45
2:I:39:ILE:HD12	2:I:39:ILE:N	2.31	0.45
1:C:242:ILE:HG13	1:C:261:ASP:H	1.81	0.45
2:J:286:PHE:N	2:J:286:PHE:CD1	2.84	0.45
1:C:210:ILE:HD13	1:C:210:ILE:O	2.16	0.45
2:J:96:VAL:C	2:J:130:VAL:HG21	2.37	0.45
2:K:370:THR:HG22	2:K:380:ILE:CD1	2.47	0.45
2:L:256:THR:HB	2:L:284:LEU:HD13	1.97	0.45
2:I:137:SER:C	2:I:139:SER:H	2.19	0.45
2:J:352:LEU:HD22	2:J:356:VAL:HG23	1.99	0.45
2:J:362:VAL:O	2:J:366:ILE:HG13	2.17	0.45
1:C:89:THR:HG21	1:C:102:VAL:HG11	1.98	0.45
1:E:206:LEU:HD23	1:E:211:ARG:HH22	1.80	0.45
1:A:69:ARG:HB3	1:A:69:ARG:CZ	2.46	0.45
1:G:197:ALA:HB2	2:I:435:ILE:HG22	1.98	0.45
2:J:188:TYR:CD1	2:J:194:VAL:HG21	2.52	0.45
2:L:277:ARG:HG3	2:L:277:ARG:NH1	2.31	0.45
1:A:254:VAL:HG13	1:A:255:LEU:N	2.32	0.45
2:I:100:MET:CE	2:I:127:ILE:HG22	2.47	0.45
2:I:96:VAL:CB	2:I:130:VAL:HG21	2.47	0.45
2:K:89:LEU:HD12	2:K:94:PHE:HE1	1.81	0.45
2:K:302:PHE:HZ	2:K:358:SER:HG	1.65	0.45
1:E:199:ALA:HA	1:E:205:LEU:HD11	1.99	0.45
2:L:310:THR:O	2:L:311:ALA:CB	2.64	0.45
1:G:32:VAL:O	1:G:49:ALA:HB1	2.15	0.45
2:J:103:ALA:O	2:J:104:ALA:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:418:ILE:HG23	2:K:423:PHE:HB2	1.98	0.45
1:C:180:ASN:O	1:C:196:ILE:HG23	2.16	0.45
1:C:180:ASN:OD1	1:C:182:GLU:HB2	2.17	0.45
1:G:11:VAL:HG22	1:G:75:ILE:HB	1.99	0.45
2:J:155:GLN:C	2:J:157:GLY:H	2.18	0.45
1:A:210:ILE:O	1:A:210:ILE:HD13	2.16	0.45
2:I:96:VAL:HG11	2:I:127:ILE:HD13	1.97	0.45
2:J:139:SER:O	2:J:143:ILE:HG12	2.17	0.45
2:K:311:ALA:O	2:K:312:SER:CB	2.64	0.45
2:K:312:SER:O	2:K:315:LYS:HE2	2.15	0.45
2:L:62:GLY:C	2:L:63:LEU:HD23	2.37	0.45
1:E:89:THR:HG21	1:E:102:VAL:HG11	1.98	0.45
2:L:366:ILE:HG13	2:L:384:THR:HG21	1.98	0.45
2:L:115:GLN:HA	2:L:120:GLN:HB3	1.99	0.45
1:A:193:HIS:NE2	2:I:340:ARG:HD2	2.31	0.45
1:G:22:VAL:HG22	1:G:32:VAL:CG1	2.46	0.45
1:G:100:ILE:HG13	1:G:119:ASP:H	1.81	0.45
2:L:286:PHE:HA	2:L:289:MET:SD	2.56	0.45
2:J:118:LEU:HD22	2:J:209:PHE:CE2	2.51	0.45
2:J:137:SER:C	2:J:139:SER:H	2.20	0.45
2:K:61:THR:OG1	2:K:390:THR:HG22	2.17	0.45
2:J:166:LEU:O	2:J:166:LEU:HD13	2.17	0.45
2:L:137:SER:C	2:L:139:SER:H	2.19	0.45
2:L:29:ILE:HD13	2:L:51:LEU:HD11	1.98	0.45
1:E:115:LYS:HD3	1:G:94:GLU:OE1	2.16	0.45
2:K:32:ALA:HA	2:K:54:ALA:CB	2.47	0.45
1:G:153:VAL:HG13	1:G:217:ILE:HG22	1.99	0.45
1:G:210:ILE:HD13	1:G:210:ILE:O	2.16	0.45
2:I:418:ILE:O	2:I:418:ILE:HG12	2.16	0.45
2:L:111:ARG:HA	2:L:126:VAL:HG12	1.99	0.45
2:J:199:THR:HG21	2:J:270:TYR:CE2	2.48	0.45
2:J:297:THR:HG22	2:J:301:MET:HE2	1.98	0.45
2:J:62:GLY:CA	2:J:392:GLY:HA2	2.45	0.45
1:G:196:ILE:HD12	2:I:436:ARG:CB	2.47	0.45
1:E:89:THR:HG21	1:E:102:VAL:HG21	1.98	0.45
1:A:109:HIS:HB2	1:C:83:GLN:OE1	2.16	0.45
1:G:64:LEU:CD2	1:G:69:ARG:HH22	2.29	0.45
2:L:411:VAL:O	2:L:415:ILE:HG13	2.17	0.45
2:J:65:VAL:HG11	2:J:406:LYS:HZ3	1.82	0.45
1:A:164:VAL:HG22	1:A:174:VAL:HG11	1.99	0.45
2:I:175:ASN:ND2	2:I:202:PHE:HB2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:20:LEU:HA	2:J:91:PHE:HD2	1.82	0.45
2:K:294:ILE:HD13	2:K:395:MET:SD	2.57	0.45
2:I:227:HIS:O	2:I:230:LEU:HB2	2.17	0.45
2:I:366:ILE:HD13	2:I:381:VAL:HG13	1.98	0.45
1:A:231:THR:CG2	1:A:244:VAL:HG21	2.47	0.45
2:I:75:PHE:O	2:I:79:VAL:HG23	2.17	0.45
2:K:242:ALA:C	2:K:273:ALA:HB1	2.36	0.45
2:J:214:ASP:OD2	2:J:228:THR:HG21	2.17	0.45
1:C:73:TYR:OH	1:C:281:GLU:HG3	2.16	0.45
2:I:104:ALA:O	2:I:105:ALA:HB3	2.16	0.45
1:G:174:VAL:O	1:G:191:ALA:HB1	2.16	0.45
2:L:179:SER:HB2	2:L:184:ASN:OD1	2.17	0.45
2:I:386:SER:HA	2:I:391:VAL:CG2	2.47	0.45
2:I:88:GLY:O	2:I:89:LEU:HD23	2.16	0.45
2:I:372:THR:HG21	2:I:405:GLY:N	2.32	0.45
1:G:16:ARG:NH1	1:G:247:GLN:O	2.50	0.45
1:E:37:ILE:CD1	1:E:37:ILE:H	2.21	0.45
2:I:45:LEU:HG	2:I:50:ALA:HB2	1.99	0.45
2:J:65:VAL:HG11	2:J:406:LYS:NZ	2.32	0.45
1:C:178:ASP:OD1	1:C:179:ILE:N	2.50	0.45
1:C:38:ASN:OD1	1:C:40:GLU:HB2	2.17	0.45
2:J:292:GLY:O	2:J:295:VAL:HB	2.17	0.45
1:E:123:HIS:CB	1:E:126:LYS:HB2	2.47	0.45
1:G:160:GLY:O	1:G:163:ILE:HG22	2.17	0.45
2:K:317:THR:O	2:K:321:VAL:HG23	2.17	0.44
2:J:199:THR:HA	2:J:202:PHE:CZ	2.52	0.44
1:A:89:THR:HG21	1:A:102:VAL:HG21	1.99	0.44
2:J:222:LYS:O	2:J:224:PHE:N	2.45	0.44
2:I:424:VAL:O	2:I:428:ALA:HB2	2.16	0.44
2:J:145:ALA:HB2	2:J:169:ALA:HB2	1.99	0.44
2:L:149:SER:OG	2:L:197:VAL:HG11	2.16	0.44
2:L:211:VAL:HG13	2:L:228:THR:HG23	2.00	0.44
2:I:209:PHE:HA	2:I:212:LEU:CD1	2.35	0.44
2:I:211:VAL:HA	2:I:228:THR:HG23	1.98	0.44
2:I:57:ALA:HB1	2:I:84:ILE:HG13	1.99	0.44
2:J:96:VAL:HG21	2:J:114:VAL:HG21	1.99	0.44
2:K:139:SER:O	2:K:143:ILE:HG12	2.17	0.44
2:I:275:THR:O	2:I:279:ALA:HB3	2.16	0.44
2:I:65:VAL:CG2	2:I:406:LYS:HE2	2.47	0.44
2:J:418:ILE:HG23	2:J:423:PHE:HB2	1.99	0.44
1:G:242:ILE:O	1:G:242:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ASN:OD1	1:C:226:ALA:N	2.47	0.44
1:E:225:GLN:HA	1:E:228:THR:OG1	2.17	0.44
2:I:443:PHE:CD1	2:I:443:PHE:N	2.86	0.44
1:A:68:ILE:HD13	1:A:68:ILE:O	2.17	0.44
2:L:20:LEU:HA	2:L:91:PHE:HD2	1.82	0.44
2:I:85:GLN:HA	2:I:174:ASN:ND2	2.33	0.44
2:J:308:ALA:O	2:J:309:SER:O	2.35	0.44
2:K:199:THR:HA	2:K:202:PHE:CZ	2.52	0.44
2:K:271:PHE:O	2:K:275:THR:HG22	2.16	0.44
2:L:175:ASN:ND2	2:L:202:PHE:HB2	2.32	0.44
2:L:62:GLY:CA	2:L:392:GLY:HA2	2.45	0.44
2:J:408:ILE:HG13	2:J:409:ILE:N	2.32	0.44
2:K:48:ILE:CG2	2:K:406:LYS:HD3	2.46	0.44
1:A:199:ALA:HA	1:A:205:LEU:HD11	1.99	0.44
1:G:22:VAL:HG22	1:G:32:VAL:HG11	2.00	0.44
1:A:164:VAL:HG22	1:A:174:VAL:CG1	2.47	0.44
2:L:238:LEU:CD2	2:L:277:ARG:HH21	2.29	0.44
1:E:165:LYS:HG2	1:E:190:TYR:CD2	2.52	0.44
1:E:165:LYS:HG2	1:E:190:TYR:HD2	1.82	0.44
2:I:92:MET:CE	2:I:113:LEU:HB3	2.48	0.44
2:I:214:ASP:OD2	2:I:228:THR:HG21	2.17	0.44
2:J:97:LEU:HD11	2:J:130:VAL:O	2.18	0.44
2:K:352:LEU:HD22	2:K:356:VAL:HG23	1.98	0.44
1:E:206:LEU:HA	1:E:211:ARG:NH1	2.32	0.44
2:J:304:GLY:HA3	2:J:312:SER:CB	2.46	0.44
1:G:57:ALA:HA	1:G:63:LEU:HD11	1.99	0.44
2:J:296:PHE:CE2	2:J:300:LEU:HD22	2.52	0.44
1:G:38:ASN:ND2	1:G:38:ASN:C	2.70	0.44
2:L:286:PHE:N	2:L:286:PHE:CD1	2.85	0.44
2:K:72:PHE:HB3	2:K:76:GLY:HA3	2.00	0.44
2:K:211:VAL:HA	2:K:228:THR:HG23	1.99	0.44
2:I:57:ALA:O	2:I:84:ILE:HA	2.18	0.44
2:J:92:MET:CE	2:J:113:LEU:HB3	2.46	0.44
2:L:45:LEU:HD11	2:L:49:ASP:O	2.17	0.44
2:J:37:LEU:HG	2:J:39:ILE:HD13	1.99	0.44
1:E:11:VAL:HG22	1:E:75:ILE:HB	1.98	0.44
1:C:123:HIS:CB	1:C:126:LYS:HB2	2.47	0.44
2:J:96:VAL:CB	2:J:130:VAL:HG21	2.48	0.44
2:L:168:HIS:O	2:L:172:ALA:N	2.50	0.44
2:K:405:GLY:HA2	2:K:408:ILE:HD11	1.99	0.44
2:K:408:ILE:HG13	2:K:409:ILE:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:THR:CG2	1:E:102:VAL:HG21	2.48	0.44
2:J:302:PHE:O	2:J:314:ILE:HG22	2.17	0.44
2:K:362:VAL:O	2:K:366:ILE:HG13	2.17	0.44
1:G:178:ASP:OD1	1:G:179:ILE:HG12	2.16	0.44
1:A:179:ILE:H	1:A:179:ILE:CD1	2.25	0.44
1:E:22:VAL:HG22	1:E:32:VAL:HG11	1.99	0.44
1:C:32:VAL:O	1:C:49:ALA:HB1	2.17	0.44
2:J:39:ILE:N	2:J:39:ILE:HD12	2.33	0.44
1:E:100:ILE:HG13	1:E:119:ASP:H	1.82	0.44
1:E:100:ILE:HG13	1:E:100:ILE:O	2.17	0.44
2:J:61:THR:O	2:J:392:GLY:N	2.51	0.44
2:J:204:THR:O	2:J:212:LEU:HD21	2.18	0.44
1:A:83:GLN:OE1	1:C:109:HIS:CA	2.66	0.44
2:I:352:LEU:HD22	2:I:356:VAL:HG23	1.99	0.44
2:L:139:SER:O	2:L:143:ILE:HG12	2.17	0.44
1:C:64:LEU:HD23	1:C:69:ARG:HH22	1.83	0.44
1:E:22:VAL:HG22	1:E:32:VAL:CG1	2.48	0.44
2:K:149:SER:OG	2:K:197:VAL:HG11	2.18	0.44
2:K:436:ARG:HA	2:K:436:ARG:HD3	1.88	0.44
2:J:327:ILE:O	2:J:331:ARG:HG3	2.18	0.44
2:I:126:VAL:HG13	2:I:126:VAL:O	2.16	0.44
2:I:163:PHE:CE2	2:I:180:LEU:HD11	2.53	0.44
2:L:298:LEU:HA	2:L:301:MET:HE2	1.99	0.44
2:I:150:ILE:O	2:I:154:PRO:HD3	2.16	0.44
2:K:120:GLN:CG	2:K:122:THR:HG22	2.48	0.44
2:L:420:PRO:O	2:L:424:VAL:HG23	2.17	0.44
2:L:424:VAL:O	2:L:428:ALA:HB2	2.17	0.44
2:J:145:ALA:HA	2:J:149:SER:HB2	1.99	0.44
2:J:179:SER:HB2	2:J:184:ASN:OD1	2.17	0.44
2:L:155:GLN:C	2:L:157:GLY:H	2.21	0.44
2:K:215:VAL:O	2:K:219:ARG:HG3	2.18	0.44
2:K:222:LYS:O	2:K:224:PHE:N	2.46	0.44
2:I:199:THR:HG21	2:I:270:TYR:CE2	2.47	0.44
2:L:297:THR:HG22	2:L:301:MET:CE	2.48	0.44
2:L:389:GLY:O	2:L:390:THR:C	2.55	0.44
2:K:366:ILE:HG13	2:K:384:THR:HG21	1.98	0.44
1:G:8:GLN:HB2	1:G:72:GLU:OE1	2.18	0.44
1:A:150:GLN:HB2	1:A:214:GLU:OE1	2.18	0.44
1:C:206:LEU:HA	1:C:211:ARG:NH1	2.31	0.44
1:E:36:ASP:OD1	1:E:37:ILE:HG12	2.18	0.44
2:K:65:VAL:CG2	2:K:406:LYS:HE2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:265:HIS:CB	1:G:268:LYS:HB2	2.47	0.44
1:A:265:HIS:CB	1:A:268:LYS:HB2	2.48	0.44
2:L:443:PHE:CD1	2:L:443:PHE:N	2.86	0.44
1:E:68:ILE:HD13	1:E:68:ILE:O	2.18	0.44
2:L:114:VAL:HG12	2:L:118:LEU:HD12	2.00	0.43
2:L:308:ALA:O	2:L:309:SER:O	2.36	0.43
2:I:212:LEU:O	2:I:216:MET:HG3	2.18	0.43
2:K:310:THR:O	2:K:311:ALA:CB	2.65	0.43
2:L:408:ILE:HG13	2:L:409:ILE:N	2.33	0.43
1:G:231:THR:HG21	1:G:244:VAL:HG21	2.00	0.43
1:A:231:THR:HG21	1:A:244:VAL:HG11	2.00	0.43
1:A:263:ILE:C	1:A:264:ILE:HD12	2.38	0.43
2:J:89:LEU:HD12	2:J:94:PHE:CE1	2.52	0.43
2:I:65:VAL:HG21	2:I:406:LYS:HE2	2.00	0.43
1:E:222:ALA:O	1:E:224:ILE:N	2.51	0.43
2:L:106:ILE:HG21	2:L:127:ILE:CD1	2.47	0.43
2:L:93:THR:O	2:L:97:LEU:HD12	2.18	0.43
2:I:394:THR:C	2:I:396:GLY:H	2.21	0.43
2:K:275:THR:CG2	2:K:276:PRO:HD3	2.48	0.43
2:K:60:VAL:HG11	2:K:174:ASN:O	2.18	0.43
2:J:153:VAL:H	2:J:154:PRO:CD	2.31	0.43
2:J:304:GLY:HA3	2:J:312:SER:HB3	2.00	0.43
2:L:89:LEU:HD12	2:L:94:PHE:HE1	1.83	0.43
1:C:22:VAL:HG22	1:C:32:VAL:CG1	2.48	0.43
2:K:20:LEU:HA	2:K:91:PHE:HD2	1.83	0.43
2:I:55:ALA:HA	2:I:58:THR:HG22	2.00	0.43
2:K:199:THR:HG21	2:K:270:TYR:CE2	2.46	0.43
2:K:292:GLY:O	2:L:367:PHE:CE1	2.71	0.43
2:I:324:THR:HG23	2:I:325:SER:N	2.33	0.43
1:C:89:THR:HG21	1:C:102:VAL:HG21	2.00	0.43
2:K:73:THR:HG22	2:K:74:VAL:N	2.26	0.43
1:G:199:ALA:HA	1:G:205:LEU:HD11	2.00	0.43
2:K:349:ILE:HG23	2:K:350:LYS:N	2.33	0.43
2:I:121:PRO:HD3	2:J:443:PHE:HE2	1.82	0.43
2:J:319:PHE:CE1	2:J:323:LEU:HD13	2.53	0.43
2:L:126:VAL:HG13	2:L:126:VAL:O	2.17	0.43
2:K:213:PHE:O	2:K:216:MET:HB2	2.18	0.43
2:J:256:THR:HB	2:J:284:LEU:HD13	2.00	0.43
2:L:80:ILE:O	2:L:84:ILE:HG13	2.18	0.43
2:K:302:PHE:O	2:K:314:ILE:HG22	2.19	0.43
2:K:340:ARG:O	2:L:438:PRO:HD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:146:LEU:HA	2:K:146:LEU:HD12	1.86	0.43
1:C:206:LEU:HD23	1:C:211:ARG:HH22	1.83	0.43
1:G:175:LEU:HD12	1:G:213:PHE:CZ	2.53	0.43
2:I:34:LEU:HD22	2:I:79:VAL:CG2	2.47	0.43
2:I:152:LEU:HD23	2:I:191:ASP:OD2	2.17	0.43
1:E:242:ILE:HG13	1:E:242:ILE:O	2.18	0.43
1:E:223:ASN:OD1	1:E:226:ALA:N	2.50	0.43
2:J:317:THR:O	2:J:321:VAL:HG23	2.18	0.43
2:K:210:THR:O	2:K:214:ASP:HB2	2.18	0.43
2:J:168:HIS:O	2:J:172:ALA:HB2	2.18	0.43
1:A:17:PHE:N	1:A:267:GLU:HG2	2.34	0.43
1:A:57:ALA:HA	1:A:63:LEU:HD11	2.01	0.43
2:L:45:LEU:HG	2:L:50:ALA:HB2	1.99	0.43
2:I:411:VAL:HG12	2:I:415:ILE:CD1	2.48	0.43
2:K:198:ILE:HD13	2:K:281:PHE:CE2	2.53	0.43
2:L:100:MET:CE	2:L:131:LYS:HE3	2.48	0.43
2:L:96:VAL:HG21	2:L:114:VAL:HG21	1.99	0.43
2:I:64:ALA:N	2:I:398:THR:HG21	2.22	0.43
2:J:310:THR:O	2:J:311:ALA:CB	2.66	0.43
2:J:120:GLN:CG	2:J:122:THR:HG22	2.49	0.43
2:J:215:VAL:HG13	2:J:224:PHE:CZ	2.51	0.43
2:K:357:THR:CG2	2:K:420:PRO:HB2	2.47	0.43
2:K:424:VAL:O	2:K:428:ALA:HB2	2.18	0.43
1:C:122:ILE:HG12	1:C:274:ILE:HD11	2.00	0.43
2:I:222:LYS:C	2:I:224:PHE:H	2.22	0.43
2:I:311:ALA:O	2:I:312:SER:CB	2.65	0.43
1:C:89:THR:CG2	1:C:102:VAL:HG21	2.48	0.43
1:C:203:ASN:HD22	2:K:434:ASN:CB	2.32	0.43
2:J:222:LYS:C	2:J:224:PHE:H	2.21	0.43
1:C:22:VAL:HG22	1:C:32:VAL:HG11	2.00	0.43
2:L:418:ILE:HG23	2:L:423:PHE:HB2	2.00	0.43
1:A:38:ASN:OD1	1:A:40:GLU:HB2	2.19	0.43
1:C:38:ASN:ND2	1:C:38:ASN:C	2.72	0.43
2:L:211:VAL:HA	2:L:228:THR:HG23	2.00	0.43
2:J:173:PHE:HA	2:J:201:LEU:O	2.19	0.43
2:J:175:ASN:ND2	2:J:202:PHE:HB2	2.33	0.43
2:K:277:ARG:HH11	2:K:277:ARG:HG3	1.82	0.43
2:K:379:GLN:HG3	2:K:395:MET:HB2	2.00	0.43
2:L:372:THR:HG23	2:L:404:ALA:HB3	2.01	0.43
1:C:23:LYS:HG2	1:C:48:TYR:CD2	2.54	0.43
2:L:118:LEU:HD22	2:L:209:PHE:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:294:ILE:CG2	2:I:378:LEU:HD11	2.49	0.43
2:K:85:GLN:HE22	2:K:141:GLU:CD	2.21	0.43
2:K:177:GLY:HA3	2:K:280:GLY:HA3	2.00	0.43
1:A:206:LEU:HA	1:A:211:ARG:NH1	2.31	0.43
2:K:352:LEU:HD13	2:K:352:LEU:C	2.39	0.43
2:L:317:THR:O	2:L:321:VAL:HG23	2.19	0.43
1:A:64:LEU:CD2	1:A:69:ARG:HH22	2.31	0.43
1:E:80:ALA:O	1:E:82:ILE:N	2.52	0.43
2:I:349:ILE:HG23	2:I:350:LYS:N	2.33	0.43
2:I:209:PHE:O	2:I:212:LEU:HB2	2.18	0.43
2:I:204:THR:O	2:I:212:LEU:HD21	2.19	0.43
2:K:114:VAL:HG12	2:K:118:LEU:HD12	2.01	0.43
2:J:386:SER:HA	2:J:391:VAL:CG2	2.49	0.43
2:L:311:ALA:O	2:L:312:SER:CB	2.66	0.43
1:G:164:VAL:HG22	1:G:174:VAL:HG11	2.01	0.43
1:G:123:HIS:CB	1:G:126:LYS:HB2	2.49	0.43
2:K:225:SER:HB2	2:L:441:GLU:OE2	2.18	0.43
2:I:106:ILE:HG21	2:I:127:ILE:CD1	2.49	0.42
2:K:324:THR:HG23	2:K:325:SER:N	2.33	0.42
2:K:20:LEU:N	2:K:20:LEU:HD23	2.34	0.42
2:K:222:LYS:C	2:K:224:PHE:H	2.23	0.42
2:J:276:PRO:O	2:J:391:VAL:HG13	2.18	0.42
2:K:175:ASN:ND2	2:K:202:PHE:HB2	2.33	0.42
2:I:226:LEU:HD21	2:I:338:ILE:CG2	2.45	0.42
2:L:35:LEU:HD23	2:L:76:GLY:HA2	2.01	0.42
2:J:152:LEU:HD23	2:J:191:ASP:OD2	2.19	0.42
2:K:152:LEU:C	2:K:154:PRO:HD2	2.40	0.42
1:G:37:ILE:CD1	1:G:37:ILE:H	2.28	0.42
2:I:292:GLY:O	2:I:295:VAL:HB	2.18	0.42
2:K:443:PHE:N	2:K:443:PHE:CD1	2.87	0.42
2:L:96:VAL:CB	2:L:130:VAL:HG21	2.49	0.42
2:I:20:LEU:CD2	2:I:92:MET:HG2	2.49	0.42
2:J:297:THR:HG22	2:J:301:MET:CE	2.48	0.42
2:I:378:LEU:HG	2:I:395:MET:HE1	2.01	0.42
2:J:110:GLU:HG2	2:J:110:GLU:O	2.19	0.42
2:L:370:THR:CG2	2:L:380:ILE:HD13	2.49	0.42
2:J:366:ILE:HD11	2:J:385:PHE:CE1	2.54	0.42
1:A:231:THR:HG21	1:A:244:VAL:HG21	2.01	0.42
1:A:115:LYS:HD2	1:C:90:LEU:HD21	2.00	0.42
1:G:153:VAL:HG13	1:G:217:ILE:CG2	2.48	0.42
1:E:18:GLY:O	1:E:21:ILE:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:442:VAL:HG13	2:L:347:ILE:HG21	2.00	0.42
2:L:222:LYS:O	2:L:224:PHE:N	2.44	0.42
2:I:282:ASN:OD1	2:I:393:LEU:HD12	2.19	0.42
2:J:212:LEU:O	2:J:216:MET:HG3	2.18	0.42
1:A:83:GLN:NE2	1:C:108:TYR:CB	2.71	0.42
2:L:152:LEU:C	2:L:154:PRO:HD2	2.40	0.42
1:E:263:ILE:C	1:E:264:ILE:HD12	2.39	0.42
2:J:89:LEU:HD12	2:J:94:PHE:HE1	1.82	0.42
2:J:32:ALA:HA	2:J:54:ALA:CB	2.49	0.42
1:E:153:VAL:HG13	1:E:217:ILE:HG22	2.00	0.42
1:C:222:ALA:O	1:C:224:ILE:N	2.52	0.42
2:L:215:VAL:O	2:L:219:ARG:HG3	2.19	0.42
2:I:96:VAL:O	2:I:96:VAL:CG1	2.67	0.42
2:K:278:THR:HB	2:K:390:THR:O	2.19	0.42
1:A:125:GLU:HG2	1:A:158:ARG:HB2	2.00	0.42
2:J:35:LEU:HD23	2:J:76:GLY:HA2	2.01	0.42
2:I:153:VAL:H	2:I:154:PRO:CD	2.29	0.42
1:G:179:ILE:H	1:G:179:ILE:CD1	2.19	0.42
2:I:330:LEU:HD22	2:J:424:VAL:CG1	2.49	0.42
2:J:311:ALA:O	2:J:312:SER:CB	2.67	0.42
2:I:48:ILE:CG2	2:I:406:LYS:HD3	2.46	0.42
1:A:30:HIS:O	1:A:32:VAL:HG23	2.19	0.42
1:G:38:ASN:OD1	1:G:40:GLU:HB2	2.20	0.42
2:J:443:PHE:CD1	2:J:443:PHE:N	2.87	0.42
1:C:121:ILE:C	1:C:122:ILE:HD12	2.40	0.42
2:L:271:PHE:O	2:L:275:THR:HG22	2.19	0.42
1:E:33:LEU:HD12	1:E:71:PHE:CZ	2.53	0.42
1:A:206:LEU:CD2	1:A:211:ARG:HH22	2.32	0.42
2:I:320:ILE:H	2:I:320:ILE:HG13	1.58	0.42
1:G:92:LEU:O	1:G:97:ILE:HG12	2.20	0.42
1:A:11:VAL:HG22	1:A:75:ILE:HB	2.01	0.42
2:K:145:ALA:O	2:K:149:SER:HB2	2.20	0.42
1:G:18:GLY:O	1:G:21:ILE:HG22	2.19	0.42
1:A:160:GLY:O	1:A:163:ILE:HG22	2.20	0.42
2:K:286:PHE:CD1	2:K:286:PHE:N	2.87	0.42
2:J:163:PHE:CE2	2:J:180:LEU:HD11	2.55	0.42
2:J:301:MET:HB2	2:J:391:VAL:HG21	2.00	0.42
2:I:382:PHE:HB3	2:I:395:MET:HE2	2.02	0.42
2:J:106:ILE:CG2	2:J:110:GLU:HB3	2.50	0.42
2:K:386:SER:HA	2:K:391:VAL:CG2	2.49	0.42
2:L:60:VAL:CG1	2:L:176:ALA:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:372:THR:HG23	2:I:404:ALA:HB3	2.01	0.42
2:I:437:TYR:HB3	2:I:438:PRO:CD	2.43	0.42
2:K:147:ILE:O	2:K:151:ARG:HG3	2.20	0.42
2:J:152:LEU:C	2:J:154:PRO:HD2	2.40	0.42
2:K:65:VAL:HG21	2:K:406:LYS:HE2	2.02	0.42
2:I:402:THR:O	2:I:406:LYS:HD2	2.19	0.42
2:I:172:ALA:HB3	2:I:201:LEU:HD13	2.01	0.42
2:I:60:VAL:HG11	2:I:174:ASN:O	2.20	0.42
2:J:20:LEU:N	2:J:20:LEU:HD23	2.35	0.42
2:L:372:THR:HG21	2:L:405:GLY:N	2.34	0.42
1:C:231:THR:HG21	1:C:244:VAL:HG11	2.02	0.42
2:J:437:TYR:HB3	2:J:438:PRO:CD	2.41	0.42
2:L:166:LEU:O	2:L:166:LEU:HD13	2.20	0.42
2:K:153:VAL:H	2:K:154:PRO:CD	2.31	0.42
2:I:150:ILE:HG23	2:I:150:ILE:O	2.19	0.42
1:C:125:GLU:HG3	1:C:159:PHE:CB	2.43	0.42
2:L:260:LEU:HB3	2:L:264:ASP:HB2	2.02	0.42
1:E:115:LYS:HB2	1:G:90:LEU:HD21	2.01	0.42
1:A:38:ASN:ND2	1:A:38:ASN:C	2.71	0.42
2:J:238:LEU:CD2	2:J:277:ARG:HH21	2.32	0.42
1:C:101:TRP:CD2	1:C:120:ARG:HD3	2.54	0.42
2:L:98:ILE:HG22	2:L:98:ILE:O	2.19	0.42
1:E:210:ILE:O	1:E:210:ILE:HD13	2.20	0.42
2:K:98:ILE:O	2:K:98:ILE:HG22	2.20	0.42
2:K:372:THR:HG23	2:K:404:ALA:HB3	2.02	0.42
2:L:352:LEU:C	2:L:352:LEU:HD13	2.39	0.42
2:I:319:PHE:CE1	2:I:323:LEU:HD13	2.55	0.42
2:L:302:PHE:HZ	2:L:358:SER:HG	1.66	0.42
2:L:324:THR:HG23	2:L:325:SER:N	2.34	0.42
2:I:275:THR:CG2	2:I:276:PRO:HD3	2.49	0.42
2:I:411:VAL:O	2:I:415:ILE:HG13	2.19	0.42
1:G:164:VAL:HG22	1:G:174:VAL:CG1	2.49	0.42
1:A:136:LEU:CD1	1:A:163:ILE:HD11	2.49	0.42
1:A:222:ALA:O	1:A:224:ILE:N	2.53	0.42
2:I:207:ILE:HD12	2:I:211:VAL:HB	2.02	0.42
2:K:207:ILE:HD11	2:K:212:LEU:HD23	2.02	0.42
2:J:177:GLY:CA	2:J:280:GLY:HA3	2.50	0.42
2:J:112:MET:CG	2:J:123:ILE:HD13	2.50	0.42
2:L:272:GLN:CD	2:L:283:SER:HB3	2.39	0.42
2:I:247:PHE:HD1	2:I:269:SER:OG	2.02	0.42
2:K:435:ILE:C	2:K:436:ARG:HH11	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:11:VAL:HG21	1:G:21:ILE:HG23	2.02	0.42
2:I:179:SER:HB2	2:I:184:ASN:OD1	2.19	0.42
2:K:347:ILE:HG21	2:L:442:VAL:CG1	2.50	0.42
2:L:204:THR:O	2:L:212:LEU:HD21	2.20	0.42
2:L:222:LYS:C	2:L:224:PHE:H	2.22	0.42
2:K:308:ALA:O	2:K:309:SER:O	2.38	0.42
2:J:282:ASN:OD1	2:J:393:LEU:HD12	2.19	0.42
2:K:277:ARG:O	2:K:278:THR:C	2.59	0.42
2:L:280:GLY:CA	2:L:392:GLY:HA3	2.49	0.42
2:L:75:PHE:O	2:L:79:VAL:HG23	2.20	0.42
2:I:323:LEU:O	2:I:327:ILE:HG13	2.20	0.42
1:G:89:THR:HG21	1:G:102:VAL:HG11	2.01	0.42
1:G:150:GLN:HB2	1:G:214:GLU:OE1	2.20	0.42
2:L:407:CYS:HA	2:L:410:ILE:HD12	2.01	0.42
2:K:48:ILE:HD12	2:K:48:ILE:H	1.85	0.42
2:I:45:LEU:HD11	2:I:49:ASP:O	2.20	0.42
2:J:52:PHE:CD2	2:J:406:LYS:HG2	2.55	0.42
1:E:38:ASN:C	1:E:38:ASN:ND2	2.73	0.42
2:K:145:ALA:HB2	2:K:169:ALA:HB2	2.02	0.42
1:G:11:VAL:HG21	1:G:21:ILE:CG2	2.50	0.42
1:G:74:VAL:C	1:G:75:ILE:HD12	2.40	0.42
1:C:23:LYS:HG2	1:C:48:TYR:HD2	1.84	0.42
1:C:93:LYS:HD2	1:C:93:LYS:HA	1.92	0.42
1:G:222:ALA:O	1:G:224:ILE:N	2.53	0.42
2:J:198:ILE:HD13	2:J:281:PHE:CE2	2.55	0.42
2:L:96:VAL:CG1	2:L:96:VAL:O	2.68	0.41
2:K:323:LEU:O	2:K:327:ILE:HG13	2.19	0.41
2:I:76:GLY:O	2:I:80:ILE:HG12	2.20	0.41
2:L:276:PRO:O	2:L:391:VAL:HG13	2.20	0.41
2:L:84:ILE:HG22	2:L:84:ILE:O	2.20	0.41
2:J:405:GLY:HA2	2:J:408:ILE:HD11	2.01	0.41
2:L:277:ARG:HG3	2:L:277:ARG:HH11	1.85	0.41
1:G:223:ASN:OD1	1:G:226:ALA:N	2.47	0.41
2:K:204:THR:O	2:K:212:LEU:HD21	2.20	0.41
2:J:278:THR:OG1	2:J:278:THR:O	2.35	0.41
2:J:280:GLY:CA	2:J:392:GLY:HA3	2.49	0.41
2:I:393:LEU:HD22	2:I:393:LEU:N	2.35	0.41
2:J:114:VAL:HG12	2:J:118:LEU:HD12	2.02	0.41
1:C:231:THR:CG2	1:C:244:VAL:HG21	2.50	0.41
2:L:349:ILE:HG23	2:L:350:LYS:N	2.34	0.41
2:J:421:LEU:HA	2:J:421:LEU:HD23	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:277:ARG:HG3	2:J:277:ARG:NH1	2.35	0.41
1:A:223:ASN:OD1	1:A:226:ALA:N	2.48	0.41
1:C:80:ALA:O	1:C:82:ILE:N	2.53	0.41
1:G:68:ILE:O	1:G:68:ILE:HD13	2.19	0.41
2:K:379:GLN:HE21	2:K:397:LEU:CB	2.22	0.41
2:K:391:VAL:CG1	2:K:393:LEU:HD23	2.44	0.41
2:J:372:THR:HG21	2:J:405:GLY:N	2.36	0.41
1:E:8:GLN:HB2	1:E:72:GLU:OE1	2.20	0.41
1:A:211:ARG:HG2	1:A:211:ARG:HH11	1.85	0.41
2:K:34:LEU:HD22	2:K:79:VAL:CG2	2.49	0.41
2:J:424:VAL:O	2:J:428:ALA:HB2	2.20	0.41
2:L:48:ILE:CG2	2:L:406:LYS:HD3	2.45	0.41
2:L:36:MET:HE2	2:L:47:TRP:HA	2.02	0.41
2:L:65:VAL:HG11	2:L:406:LYS:NZ	2.35	0.41
1:A:11:VAL:HG21	1:A:21:ILE:HG23	2.02	0.41
1:E:222:ALA:O	1:E:223:ASN:C	2.59	0.41
2:K:155:GLN:C	2:K:157:GLY:H	2.24	0.41
2:K:301:MET:HB2	2:K:391:VAL:HG11	2.01	0.41
2:K:394:THR:C	2:K:396:GLY:H	2.23	0.41
1:A:234:LEU:O	1:A:239:ILE:HG12	2.20	0.41
2:L:302:PHE:CE1	2:L:358:SER:HB2	2.56	0.41
2:L:319:PHE:O	2:L:320:ILE:C	2.59	0.41
2:J:215:VAL:HG22	2:J:224:PHE:CZ	2.55	0.41
1:C:264:ILE:HD12	1:C:264:ILE:N	2.35	0.41
1:E:81:ASN:OD1	1:E:84:ALA:N	2.51	0.41
1:A:235:LYS:HA	1:A:235:LYS:HD2	1.90	0.41
2:K:437:TYR:HB3	2:K:438:PRO:CD	2.42	0.41
2:J:126:VAL:HG13	2:J:126:VAL:O	2.19	0.41
2:L:297:THR:HG22	2:L:301:MET:HE2	2.01	0.41
2:K:372:THR:HG21	2:K:405:GLY:N	2.36	0.41
2:I:139:SER:O	2:I:143:ILE:HG12	2.20	0.41
1:C:8:GLN:HB2	1:C:72:GLU:OE1	2.21	0.41
2:J:357:THR:CG2	2:J:420:PRO:HB2	2.51	0.41
1:E:180:ASN:OD1	1:E:182:GLU:HB2	2.20	0.41
1:C:39:GLU:HB3	1:C:54:ILE:HD13	2.01	0.41
2:K:433:SER:HB2	2:L:333:LYS:HG2	2.02	0.41
2:I:280:GLY:CA	2:I:392:GLY:HA3	2.50	0.41
2:K:85:GLN:HA	2:K:174:ASN:HD21	1.83	0.41
2:L:163:PHE:CE2	2:L:180:LEU:HD11	2.56	0.41
2:J:150:ILE:O	2:J:150:ILE:HG23	2.21	0.41
1:A:108:TYR:HB2	1:C:83:GLN:HE21	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:302:PHE:O	2:L:314:ILE:HG22	2.20	0.41
2:K:152:LEU:HD23	2:K:191:ASP:OD2	2.20	0.41
1:C:177:VAL:HG23	1:C:195:VAL:O	2.20	0.41
2:I:257:LEU:HD11	2:I:269:SER:OG	2.21	0.41
2:J:115:GLN:HA	2:J:120:GLN:HB3	2.03	0.41
1:E:82:ILE:HD11	1:E:105:GLN:HB2	2.01	0.41
1:E:153:VAL:HG13	1:E:217:ILE:CG2	2.50	0.41
1:C:222:ALA:O	1:C:223:ASN:C	2.58	0.41
2:I:222:LYS:O	2:I:224:PHE:N	2.47	0.41
2:K:106:ILE:CG2	2:K:110:GLU:HB3	2.51	0.41
2:K:96:VAL:O	2:K:96:VAL:CG1	2.68	0.41
2:J:301:MET:HB2	2:J:391:VAL:HG11	2.03	0.41
2:J:134:PHE:O	2:J:137:SER:HB2	2.21	0.41
2:K:64:ALA:H	2:K:398:THR:CG2	2.24	0.41
2:L:379:GLN:HA	2:L:395:MET:CE	2.50	0.41
2:K:292:GLY:O	2:K:295:VAL:HB	2.20	0.41
2:K:366:ILE:HD11	2:K:385:PHE:CE1	2.56	0.41
1:A:80:ALA:O	1:A:82:ILE:N	2.53	0.41
2:L:352:LEU:HD22	2:L:356:VAL:HG23	2.02	0.41
2:I:319:PHE:CZ	2:I:323:LEU:HD22	2.54	0.41
1:G:264:ILE:N	1:G:264:ILE:HD12	2.35	0.41
2:I:32:ALA:HA	2:I:54:ALA:CB	2.50	0.41
2:J:349:ILE:HG23	2:J:350:LYS:N	2.35	0.41
2:L:97:LEU:HD11	2:L:130:VAL:O	2.20	0.41
2:J:168:HIS:CE1	2:J:180:LEU:H	2.38	0.41
2:J:131:LYS:O	2:J:135:LEU:HB2	2.21	0.41
2:J:16:PRO:HB2	2:J:17:PRO:HD3	2.03	0.41
2:K:390:THR:HG21	2:K:417:ARG:HB2	2.03	0.41
2:L:393:LEU:HD22	2:L:393:LEU:N	2.34	0.41
1:G:125:GLU:HG2	1:G:158:ARG:HB2	2.02	0.41
1:A:104:ALA:HA	1:A:109:HIS:ND1	2.36	0.41
2:J:72:PHE:HB3	2:J:76:GLY:HA3	2.03	0.41
2:I:154:PRO:CB	2:I:158:TRP:HZ3	2.33	0.41
2:I:260:LEU:HB3	2:I:264:ASP:HB2	2.03	0.41
1:A:177:VAL:HG23	1:A:195:VAL:O	2.20	0.41
1:C:153:VAL:HG21	1:C:163:ILE:CG2	2.50	0.41
2:K:29:ILE:HD13	2:K:51:LEU:HD11	2.03	0.41
1:C:180:ASN:ND2	1:C:180:ASN:C	2.74	0.41
1:C:11:VAL:HG13	1:C:75:ILE:HG22	2.02	0.41
1:G:198:ASN:OD1	1:G:200:THR:HG23	2.21	0.41
1:C:194:ALA:HB3	2:K:438:PRO:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:ALA:O	2:K:438:PRO:CD	2.51	0.41
2:I:209:PHE:H	2:I:308:ALA:CB	2.25	0.41
2:K:226:LEU:HD21	2:K:338:ILE:CG2	2.47	0.41
2:K:20:LEU:HD11	2:K:116:GLU:HB3	2.03	0.41
2:I:84:ILE:O	2:I:84:ILE:HG22	2.21	0.41
2:J:99:VAL:HB	2:J:106:ILE:HD11	2.03	0.41
2:L:275:THR:CG2	2:L:276:PRO:HD3	2.50	0.41
2:K:377:PHE:CE1	2:L:378:LEU:HD13	2.56	0.41
2:L:386:SER:HA	2:L:391:VAL:CG2	2.51	0.41
2:J:294:ILE:HD13	2:J:395:MET:SD	2.61	0.41
2:J:302:PHE:HE1	2:J:358:SER:HB2	1.85	0.41
2:I:302:PHE:O	2:I:314:ILE:HG22	2.20	0.41
1:C:57:ALA:HA	1:C:63:LEU:HD11	2.02	0.41
2:K:263:VAL:HG13	2:K:264:ASP:N	2.36	0.41
2:L:357:THR:CG2	2:L:420:PRO:HB2	2.49	0.41
2:I:29:ILE:HD13	2:I:51:LEU:HD11	2.03	0.41
1:C:120:ARG:HG2	1:C:122:ILE:HD11	2.02	0.41
2:K:319:PHE:O	2:K:320:ILE:C	2.59	0.41
2:I:297:THR:HG22	2:I:301:MET:CE	2.51	0.41
2:K:84:ILE:O	2:K:84:ILE:HG22	2.19	0.41
1:A:105:GLN:O	1:A:158:ARG:NH1	2.54	0.41
1:G:180:ASN:OD1	1:G:182:GLU:HB2	2.20	0.41
1:A:122:ILE:HD12	1:A:122:ILE:N	2.36	0.41
2:L:36:MET:HA	2:L:45:LEU:HD23	2.03	0.41
2:K:411:VAL:O	2:K:415:ILE:HG13	2.20	0.41
2:I:145:ALA:HA	2:I:149:SER:HB2	2.03	0.41
1:E:180:ASN:C	1:E:180:ASN:ND2	2.73	0.41
1:G:121:ILE:C	1:G:122:ILE:HD12	2.42	0.41
2:K:214:ASP:OD2	2:K:228:THR:HG21	2.21	0.40
2:I:319:PHE:O	2:I:320:ILE:C	2.59	0.40
2:J:46:SER:HB3	2:J:48:ILE:HD12	2.03	0.40
1:A:32:VAL:O	1:A:49:ALA:HB1	2.21	0.40
1:A:39:GLU:HB3	1:A:54:ILE:HD13	2.03	0.40
1:E:246:ALA:HA	1:E:251:HIS:ND1	2.35	0.40
1:A:81:ASN:OD1	1:A:84:ALA:N	2.49	0.40
2:I:215:VAL:O	2:I:219:ARG:HG3	2.22	0.40
2:K:227:HIS:CE1	2:K:317:THR:HG21	2.56	0.40
2:K:126:VAL:O	2:K:126:VAL:HG13	2.21	0.40
2:J:61:THR:CG2	2:J:63:LEU:HG	2.48	0.40
2:I:60:VAL:CG1	2:I:176:ALA:HB2	2.52	0.40
2:J:111:ARG:HA	2:J:126:VAL:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:298:LEU:HA	2:K:301:MET:HE2	2.03	0.40
2:L:397:LEU:O	2:L:401:LEU:HG	2.21	0.40
2:I:436:ARG:HD3	2:I:436:ARG:HA	1.94	0.40
1:A:33:LEU:HD12	1:A:71:PHE:CZ	2.57	0.40
2:L:120:GLN:CG	2:L:122:THR:HG22	2.51	0.40
2:K:260:LEU:HB3	2:K:264:ASP:HB2	2.03	0.40
2:K:421:LEU:HD23	2:K:421:LEU:HA	1.92	0.40
2:L:188:TYR:CD1	2:L:194:VAL:HG21	2.55	0.40
2:I:16:PRO:HB2	2:I:17:PRO:HD3	2.03	0.40
2:K:168:HIS:CE1	2:K:180:LEU:H	2.39	0.40
2:L:282:ASN:OD1	2:L:393:LEU:HD12	2.21	0.40
1:G:80:ALA:O	1:G:82:ILE:N	2.54	0.40
2:K:314:ILE:O	2:K:314:ILE:HG23	2.22	0.40
2:K:75:PHE:O	2:K:79:VAL:HG23	2.21	0.40
2:J:257:LEU:CD2	2:J:265:LYS:HG2	2.50	0.40
2:J:211:VAL:HA	2:J:228:THR:HG23	2.03	0.40
2:I:357:THR:CG2	2:I:420:PRO:HB2	2.50	0.40
2:J:37:LEU:HG	2:J:39:ILE:CD1	2.51	0.40
1:G:193:HIS:HE2	2:J:340:ARG:CD	2.33	0.40
1:E:93:LYS:HD2	1:E:93:LYS:HA	1.90	0.40
2:J:227:HIS:HE1	2:J:317:THR:HG21	1.86	0.40
2:I:209:PHE:HD1	2:I:212:LEU:HD12	1.87	0.40
2:I:215:VAL:HG22	2:I:224:PHE:CZ	2.56	0.40
2:K:256:THR:HB	2:K:284:LEU:HD13	2.03	0.40
2:I:137:SER:C	2:I:139:SER:N	2.75	0.40
1:A:196:ILE:HD12	2:J:436:ARG:CB	2.51	0.40
2:I:120:GLN:CG	2:I:122:THR:HG22	2.51	0.40
2:J:215:VAL:O	2:J:219:ARG:HG3	2.21	0.40
1:E:80:ALA:O	1:E:81:ASN:C	2.60	0.40
1:A:178:ASP:OD1	1:A:179:ILE:N	2.54	0.40
1:A:222:ALA:O	1:A:223:ASN:C	2.59	0.40
1:C:198:ASN:OD1	1:C:200:THR:HG23	2.21	0.40
2:J:84:ILE:HG22	2:J:84:ILE:O	2.20	0.40
2:K:378:LEU:O	2:K:378:LEU:HD12	2.21	0.40
2:L:76:GLY:O	2:L:80:ILE:HG12	2.21	0.40
2:J:81:MET:SD	2:J:170:ILE:HD12	2.61	0.40
1:G:231:THR:HG21	1:G:244:VAL:HG11	2.03	0.40
2:I:314:ILE:O	2:I:314:ILE:HG23	2.22	0.40
2:I:302:PHE:HZ	2:I:358:SER:HG	1.66	0.40
2:I:152:LEU:C	2:I:154:PRO:HD2	2.42	0.40
1:G:177:VAL:HG23	1:G:195:VAL:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:VAL:HG22	1:C:174:VAL:HG11	2.04	0.40
1:A:11:VAL:HG21	1:A:21:ILE:CG2	2.52	0.40
2:K:347:ILE:HD12	2:L:442:VAL:O	2.21	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	264/288 (92%)	228 (86%)	32 (12%)	4 (2%)	13	57
1	C	264/288 (92%)	232 (88%)	28 (11%)	4 (2%)	13	57
1	E	264/288 (92%)	230 (87%)	30 (11%)	4 (2%)	13	57
1	G	264/288 (92%)	231 (88%)	29 (11%)	4 (2%)	13	57
2	I	429/445 (96%)	323 (75%)	84 (20%)	22 (5%)	2	30
2	J	429/445 (96%)	330 (77%)	78 (18%)	21 (5%)	3	31
2	K	429/445 (96%)	329 (77%)	80 (19%)	20 (5%)	3	32
2	L	429/445 (96%)	325 (76%)	83 (19%)	21 (5%)	3	31
All	All	2772/2932 (94%)	2228 (80%)	444 (16%)	100 (4%)	4	38

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	223	ASN
1	C	81	ASN
1	C	223	ASN
1	E	81	ASN
1	E	223	ASN
1	G	223	ASN

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Mol	Chain	Res	Type
2	I	104	ALA
2	I	184	ASN
2	I	261	ALA
2	I	309	SER
2	I	342	SER
2	J	104	ALA
2	J	184	ASN
2	J	261	ALA
2	J	309	SER
2	J	342	SER
2	K	104	ALA
2	K	184	ASN
2	K	261	ALA
2	K	309	SER
2	K	312	SER
2	K	342	SER
2	L	104	ALA
2	L	184	ASN
2	L	261	ALA
2	L	309	SER
2	L	342	SER
1	A	222	ALA
1	G	81	ASN
2	I	125	GLY
2	I	223	THR
2	I	304	GLY
2	I	311	ALA
2	I	312	SER
2	J	125	GLY
2	J	219	ARG
2	J	223	THR
2	J	304	GLY
2	J	311	ALA
2	J	312	SER
2	K	125	GLY
2	K	219	ARG
2	K	223	THR
2	K	304	GLY
2	K	311	ALA
2	L	125	GLY
2	L	223	THR
2	L	304	GLY

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Mol	Chain	Res	Type
2	L	311	ALA
2	L	312	SER
1	A	80	ALA
1	C	80	ALA
1	C	222	ALA
1	E	80	ALA
1	E	222	ALA
1	G	80	ALA
1	G	222	ALA
2	L	219	ARG
2	I	17	PRO
2	I	69	GLY
2	I	219	ARG
2	I	305	ALA
2	J	17	PRO
2	J	67	ASP
2	J	156	TYR
2	J	395	MET
2	K	17	PRO
2	L	17	PRO
2	L	69	GLY
2	L	395	MET
2	I	105	ALA
2	I	156	TYR
2	J	105	ALA
2	K	105	ALA
2	K	305	ALA
2	K	429	ALA
2	L	105	ALA
2	L	305	ALA
2	I	333	LYS
2	I	395	MET
2	K	69	GLY
2	K	321	VAL
2	K	333	LYS
2	L	46	SER
2	L	321	VAL
2	I	320	ILE
2	I	321	VAL
2	J	69	GLY
2	J	321	VAL
2	K	320	ILE

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Mol	Chain	Res	Type
2	J	419	GLY
2	L	320	ILE
2	L	332	GLY
2	I	332	GLY
2	I	419	GLY
2	J	320	ILE
2	J	332	GLY
2	K	332	GLY
2	L	419	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	222/240 (92%)	200 (90%)	22 (10%)	10 39
1	C	222/240 (92%)	198 (89%)	24 (11%)	8 36
1	E	222/240 (92%)	199 (90%)	23 (10%)	9 37
1	G	222/240 (92%)	197 (89%)	25 (11%)	7 33
2	I	354/368 (96%)	328 (93%)	26 (7%)	17 55
2	J	354/368 (96%)	329 (93%)	25 (7%)	18 55
2	K	354/368 (96%)	330 (93%)	24 (7%)	20 57
2	L	354/368 (96%)	329 (93%)	25 (7%)	18 55
All	All	2304/2432 (95%)	2110 (92%)	194 (8%)	14 49

All (194) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	23	LYS
1	A	28	MET
1	A	33	LEU
1	A	37	ILE
1	A	38	ASN

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Mol	Chain	Res	Type
1	A	68	ILE
1	A	69	ARG
1	A	125	GLU
1	A	138	ASP
1	A	150	GLN
1	A	165	LYS
1	A	166	GLU
1	A	170	MET
1	A	175	LEU
1	A	179	ILE
1	A	180	ASN
1	A	210	ILE
1	A	211	ARG
1	A	262	ARG
1	A	267	GLU
1	A	280	ASP
1	C	8	GLN
1	C	23	LYS
1	C	24	GLU
1	C	28	MET
1	C	33	LEU
1	C	37	ILE
1	C	38	ASN
1	C	68	ILE
1	C	69	ARG
1	C	125	GLU
1	C	138	ASP
1	C	150	GLN
1	C	165	LYS
1	C	166	GLU
1	C	170	MET
1	C	175	LEU
1	C	179	ILE
1	C	180	ASN
1	C	189	SER
1	C	210	ILE
1	C	211	ARG
1	C	262	ARG
1	C	267	GLU
1	C	280	ASP
1	E	8	GLN
1	E	23	LYS

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Mol	Chain	Res	Type
1	E	24	GLU
1	E	28	MET
1	E	33	LEU
1	E	37	ILE
1	E	38	ASN
1	E	68	ILE
1	E	69	ARG
1	E	120	ARG
1	E	125	GLU
1	E	138	ASP
1	E	150	GLN
1	E	165	LYS
1	E	166	GLU
1	E	170	MET
1	E	175	LEU
1	E	179	ILE
1	E	180	ASN
1	E	210	ILE
1	E	211	ARG
1	E	262	ARG
1	E	267	GLU
1	G	8	GLN
1	G	23	LYS
1	G	24	GLU
1	G	28	MET
1	G	33	LEU
1	G	37	ILE
1	G	38	ASN
1	G	47	SER
1	G	50	THR
1	G	68	ILE
1	G	69	ARG
1	G	125	GLU
1	G	138	ASP
1	G	150	GLN
1	G	165	LYS
1	G	166	GLU
1	G	170	MET
1	G	175	LEU
1	G	179	ILE
1	G	180	ASN
1	G	210	ILE

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Mol	Chain	Res	Type
1	G	211	ARG
1	G	262	ARG
1	G	267	GLU
1	G	280	ASP
2	I	20	LEU
2	I	36	MET
2	I	60	VAL
2	I	89	LEU
2	I	97	LEU
2	I	109	LYS
2	I	115	GLN
2	I	130	VAL
2	I	139	SER
2	I	171	SER
2	I	180	LEU
2	I	183	ASP
2	I	184	ASN
2	I	191	ASP
2	I	198	ILE
2	I	211	VAL
2	I	236	LEU
2	I	259	HIS
2	I	272	GLN
2	I	338	ILE
2	I	370	THR
2	I	386	SER
2	I	407	CYS
2	I	434	ASN
2	I	439	ASP
2	I	443	PHE
2	J	60	VAL
2	J	97	LEU
2	J	109	LYS
2	J	115	GLN
2	J	130	VAL
2	J	139	SER
2	J	149	SER
2	J	171	SER
2	J	180	LEU
2	J	183	ASP
2	J	184	ASN
2	J	191	ASP

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Mol	Chain	Res	Type
2	J	198	ILE
2	J	211	VAL
2	J	236	LEU
2	J	259	HIS
2	J	272	GLN
2	J	286	PHE
2	J	338	ILE
2	J	370	THR
2	J	386	SER
2	J	407	CYS
2	J	434	ASN
2	J	439	ASP
2	J	443	PHE
2	K	46	SER
2	K	60	VAL
2	K	97	LEU
2	K	109	LYS
2	K	115	GLN
2	K	130	VAL
2	K	139	SER
2	K	171	SER
2	K	180	LEU
2	K	183	ASP
2	K	184	ASN
2	K	191	ASP
2	K	198	ILE
2	K	211	VAL
2	K	236	LEU
2	K	259	HIS
2	K	272	GLN
2	K	338	ILE
2	K	370	THR
2	K	386	SER
2	K	407	CYS
2	K	434	ASN
2	K	439	ASP
2	K	443	PHE
2	L	20	LEU
2	L	60	VAL
2	L	89	LEU
2	L	97	LEU
2	L	109	LYS

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Mol	Chain	Res	Type
2	L	115	GLN
2	L	130	VAL
2	L	139	SER
2	L	171	SER
2	L	180	LEU
2	L	183	ASP
2	L	184	ASN
2	L	191	ASP
2	L	198	ILE
2	L	211	VAL
2	L	236	LEU
2	L	259	HIS
2	L	272	GLN
2	L	338	ILE
2	L	370	THR
2	L	386	SER
2	L	407	CYS
2	L	434	ASN
2	L	439	ASP
2	L	443	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	43	ASN
1	A	150	GLN
1	A	185	ASN
1	A	198	ASN
1	A	225	GLN
1	C	8	GLN
1	C	43	ASN
1	C	56	ASN
1	C	150	GLN
1	C	185	ASN
1	C	198	ASN
1	C	203	ASN
1	C	225	GLN
1	E	8	GLN
1	E	43	ASN
1	E	56	ASN
1	E	150	GLN

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Mol	Chain	Res	Type
1	E	198	ASN
1	E	225	GLN
1	G	8	GLN
1	G	43	ASN
1	G	56	ASN
1	G	150	GLN
1	G	198	ASN
1	G	225	GLN
2	I	119	ASN
2	I	175	ASN
2	I	195	ASN
2	I	239	ASN
2	I	379	GLN
2	J	119	ASN
2	J	175	ASN
2	J	195	ASN
2	J	379	GLN
2	K	119	ASN
2	K	195	ASN
2	K	379	GLN
2	L	119	ASN
2	L	175	ASN
2	L	195	ASN
2	L	379	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	268/288 (93%)	0.58	35 (13%) 5 10	343, 343, 343, 343	0
1	C	268/288 (93%)	0.25	14 (5%) 31 31	343, 343, 343, 343	0
1	E	268/288 (93%)	0.65	29 (10%) 8 12	343, 343, 343, 343	0
1	G	268/288 (93%)	0.65	40 (14%) 3 8	343, 343, 343, 343	0
2	I	431/445 (96%)	0.39	24 (5%) 28 28	343, 343, 343, 343	0
2	J	431/445 (96%)	0.34	36 (8%) 14 17	343, 343, 343, 343	0
2	K	431/445 (96%)	0.54	52 (12%) 6 11	343, 343, 343, 343	0
2	L	431/445 (96%)	0.29	29 (6%) 21 22	343, 343, 343, 343	0
All	All	2796/2932 (95%)	0.45	259 (9%) 11 15	343, 343, 343, 343	0

All (259) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	105	ALA	7.1
2	J	119	ASN	7.0
2	I	431	GLU	6.3
2	K	104	ALA	5.8
1	A	281	GLU	5.5
1	E	58	THR	5.5
1	G	103	LYS	5.5
1	A	282	ASN	5.3
2	J	429	ALA	5.3
1	E	10	ALA	5.1
2	K	106	ILE	5.1
1	E	57	ALA	5.0
1	E	33	LEU	5.0
1	C	103	LYS	5.0
2	K	394	THR	4.9
1	A	260	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	G	14	LEU	4.8
1	G	77	ALA	4.8
1	C	156	LEU	4.6
1	E	53	VAL	4.6
1	A	50	THR	4.6
2	K	56	SER	4.5
2	J	120	GLN	4.5
1	C	102	VAL	4.4
2	I	394	THR	4.3
1	A	49	ALA	4.3
1	G	75	ILE	4.3
2	J	116	GLU	4.3
1	G	102	VAL	4.3
2	L	95	ALA	4.2
1	E	35	VAL	4.2
1	G	120	ARG	4.2
1	A	103	LYS	4.2
2	J	64	ALA	4.1
2	I	102	LEU	4.1
2	J	52	PHE	4.1
2	I	98	ILE	4.0
1	G	121	ILE	4.0
1	E	34	ALA	4.0
1	G	9	PHE	4.0
2	L	190	GLY	4.0
2	L	98	ILE	3.9
2	K	110	GLU	3.9
2	J	16	PRO	3.9
2	K	395	MET	3.9
1	G	10	ALA	3.8
1	A	259	GLY	3.8
2	L	109	LYS	3.8
2	K	287	GLY	3.8
2	K	54	ALA	3.8
2	K	55	ALA	3.8
2	K	178	PHE	3.8
2	J	193	THR	3.8
2	J	430	THR	3.7
1	A	51	HIS	3.7
2	I	110	GLU	3.7
1	E	50	THR	3.7
2	K	98	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	7	LYS	3.7
2	L	99	VAL	3.7
1	A	278	LEU	3.7
1	A	116	ILE	3.6
2	K	99	VAL	3.6
2	J	115	GLN	3.6
2	J	98	ILE	3.6
2	I	112	MET	3.6
1	G	11	VAL	3.6
2	J	51	LEU	3.6
1	A	73	TYR	3.5
1	G	116	ILE	3.5
1	A	149	LYS	3.5
2	L	125	GLY	3.5
2	J	291	GLU	3.5
2	J	53	THR	3.5
2	J	50	ALA	3.5
1	C	121	ILE	3.5
2	K	281	PHE	3.4
2	K	288	SER	3.4
2	L	189	VAL	3.4
2	K	282	ASN	3.4
1	G	74	VAL	3.4
2	K	396	GLY	3.4
1	G	152	ALA	3.3
1	G	208	LEU	3.3
2	L	126	VAL	3.3
1	E	32	VAL	3.3
1	E	31	GLU	3.2
2	J	122	THR	3.2
2	K	45	LEU	3.2
2	J	141	GLU	3.2
1	G	101	TRP	3.2
2	J	114	VAL	3.2
1	A	52	ALA	3.2
1	G	118	ALA	3.2
2	L	112	MET	3.2
1	E	9	PHE	3.1
1	A	113	LEU	3.1
1	A	10	ALA	3.1
1	G	57	ALA	3.1
2	K	50	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	K	36	MET	3.1
2	I	113	LEU	3.1
2	L	444	THR	3.1
1	G	58	THR	3.0
2	K	285	ASP	3.0
2	I	376	PRO	3.0
1	E	12	ILE	3.0
2	L	191	ASP	3.0
1	A	199	ALA	3.0
2	K	168	HIS	3.0
2	L	119	ASN	3.0
1	G	172	HIS	3.0
2	K	126	VAL	3.0
1	E	11	VAL	2.9
1	G	13	GLY	2.9
2	K	119	ASN	2.9
2	K	431	GLU	2.9
2	J	45	LEU	2.9
1	G	76	VAL	2.9
1	A	77	ALA	2.9
2	L	192	PRO	2.9
2	K	57	ALA	2.9
2	K	375	ALA	2.9
1	E	51	HIS	2.9
2	K	47	TRP	2.9
2	I	262	ALA	2.8
2	J	287	GLY	2.8
2	L	442	VAL	2.8
1	G	78	ILE	2.8
2	L	94	PHE	2.8
2	K	291	GLU	2.8
2	L	433	SER	2.8
1	G	200	THR	2.8
2	K	44	PRO	2.8
1	E	220	ILE	2.8
2	L	110	GLU	2.7
2	K	51	LEU	2.7
2	L	445	GLY	2.7
2	K	171	SER	2.7
1	G	215	TYR	2.7
1	G	53	VAL	2.7
1	E	115	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	J	113	LEU	2.7
1	C	68	ILE	2.7
1	A	104	ALA	2.7
1	A	76	VAL	2.7
1	A	151	PHE	2.7
1	E	56	ASN	2.7
2	L	281	PHE	2.6
1	A	122	ILE	2.6
2	I	259	HIS	2.6
2	K	283	SER	2.6
2	J	121	PRO	2.6
2	I	430	THR	2.6
1	G	12	ILE	2.6
2	K	53	THR	2.6
2	L	188	TYR	2.6
1	A	200	THR	2.6
1	G	122	ILE	2.6
2	K	430	THR	2.6
1	E	172	HIS	2.5
2	L	101	ILE	2.5
1	A	277	SER	2.5
1	E	7	LYS	2.5
2	J	118	LEU	2.5
1	C	104	ALA	2.5
1	C	160	GLY	2.5
1	G	35	VAL	2.5
1	A	124	PRO	2.5
1	E	116	ILE	2.5
2	K	107	GLY	2.5
1	A	279	SER	2.5
2	J	101	ILE	2.5
2	I	379	GLN	2.5
2	I	99	VAL	2.4
1	A	74	VAL	2.4
1	A	101	TRP	2.4
1	G	136	LEU	2.4
1	A	258	ILE	2.4
2	J	394	THR	2.4
1	C	57	ALA	2.4
2	J	428	ALA	2.4
1	E	14	LEU	2.4
2	K	114	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	34	ALA	2.4
2	I	375	ALA	2.4
2	K	52	PHE	2.4
2	K	124	GLY	2.4
2	L	96	VAL	2.3
1	G	33	LEU	2.3
2	K	102	LEU	2.3
1	E	74	VAL	2.3
2	J	152	LEU	2.3
2	I	111	ARG	2.3
2	I	101	ILE	2.3
2	I	119	ASN	2.3
2	I	395	MET	2.3
2	I	377	PHE	2.3
1	C	69	ARG	2.3
1	G	115	LYS	2.3
2	I	106	ILE	2.3
2	J	32	ALA	2.3
2	K	377	PHE	2.3
2	L	124	GLY	2.3
1	A	102	VAL	2.2
2	J	36	MET	2.2
2	L	103	ALA	2.2
1	G	282	ASN	2.2
1	A	121	ILE	2.2
2	K	151	ARG	2.2
2	I	125	GLY	2.2
2	K	122	THR	2.2
2	J	126	VAL	2.2
2	K	284	LEU	2.2
1	E	149	LYS	2.2
1	G	16	ARG	2.2
1	E	151	PHE	2.2
1	C	187	TYR	2.2
2	J	290	ARG	2.2
1	E	16	ARG	2.2
1	A	33	LEU	2.2
1	C	257	LYS	2.1
1	E	227	SER	2.1
1	A	11	VAL	2.1
2	K	199	THR	2.1
2	L	378	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	L	307	SER	2.1
1	G	210	ILE	2.1
1	G	117	GLY	2.1
2	K	177	GLY	2.1
2	J	63	LEU	2.1
2	J	94	PHE	2.1
1	A	117	GLY	2.1
2	I	432	GLN	2.1
2	K	63	LEU	2.1
1	E	152	ALA	2.1
2	L	92	MET	2.1
2	J	288	SER	2.1
1	A	34	ALA	2.1
1	C	58	THR	2.1
1	C	199	ALA	2.1
2	K	164	ALA	2.1
1	G	15	GLY	2.1
2	K	378	LEU	2.1
2	J	65	VAL	2.1
2	K	120	GLN	2.1
1	A	237	LEU	2.0
2	L	440	GLY	2.0
1	G	151	PHE	2.0
1	G	175	LEU	2.0
2	I	398	THR	2.0
2	I	178	PHE	2.0
2	K	333	LYS	2.0
1	C	140	ASN	2.0
2	J	33	VAL	2.0
1	E	36	ASP	2.0
2	L	173	PHE	2.0
2	K	152	LEU	2.0
1	E	136	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	K	J	501	1/1	0.94	0.34	1.20	342,342,342,342	0
3	K	I	501	1/1	0.88	0.46	0.95	342,342,342,342	0
3	K	K	501	1/1	0.89	0.24	-0.58	342,342,342,342	0
3	K	L	501	1/1	0.92	0.25	-3.77	342,342,342,342	0

6.5 Other polymers

There are no such residues in this entry.