



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jan 16, 2017 – 02:24 PM EST

PDB ID : 5H37
EMDB ID: : EMD-9575
Title : Cryo-EM structure of zika virus complexed with Fab C10 at pH 8.0
Authors : Zhang, S.; Kostyuchenko, V.; Ng, T.-S.; Lim, X.-N.; Ooi, J.S.G.; Lambert, S.;
Tan, T.Y.; Widman, D.; Shi, J.; Baric, R.S.; Lok, S.-M.
Deposited on : 2016-10-20
Resolution : 4.00 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

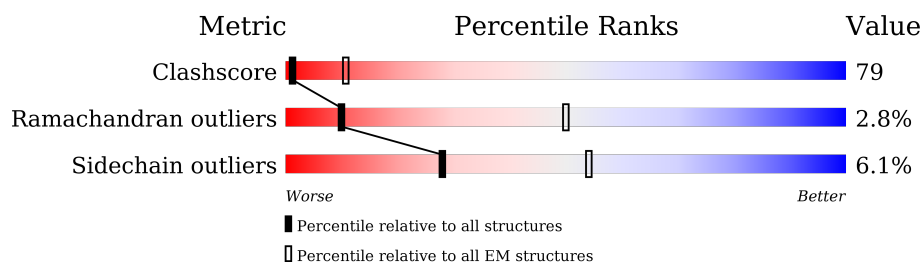
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	504	37% 54% 8% .
1	B	504	43% 49% . . .
1	C	504	31% 59% 7% .
2	D	75	32% 59% 9%
2	E	75	39% 45% 13% .
2	F	75	36% 59% 5%
3	G	127	36% 53% 11%
3	I	127	28% 63% 9%
3	K	127	35% 59% . .

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Mol	Chain	Length	Quality of chain
4	H	109	<div><div></div><div>41%51%5%</div><div></div></div>
4	L	109	<div><div></div><div>42%46%10%</div><div></div></div>
4	M	109	<div><div></div><div>27%61%13%</div><div></div></div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 18517 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 structural protein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	504	Total	C	N	O	S	0	0
			3798	2395	660	712	31		
1	C	494	Total	C	N	O	S	0	0
			3731	2350	647	704	30		
1	B	494	Total	C	N	O	S	0	0
			3732	2350	647	705	30		

- Molecule 2 is a protein called strutral protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	75	Total	C	N	O	S	0	0
			600	391	105	103	1		
2	E	75	Total	C	N	O	S	0	0
			600	391	105	103	1		
2	F	75	Total	C	N	O	S	0	0
			600	391	105	103	1		

- Molecule 3 is a protein called C10 IgG heavy chain variable region.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	127	Total	C	N	O	S	0	0
			1021	650	169	197	5		
3	K	127	Total	C	N	O	S	0	0
			1021	650	169	197	5		
3	I	127	Total	C	N	O	S	0	0
			1021	650	169	197	5		

- Molecule 4 is a protein called C10 IgG light chain variable region.

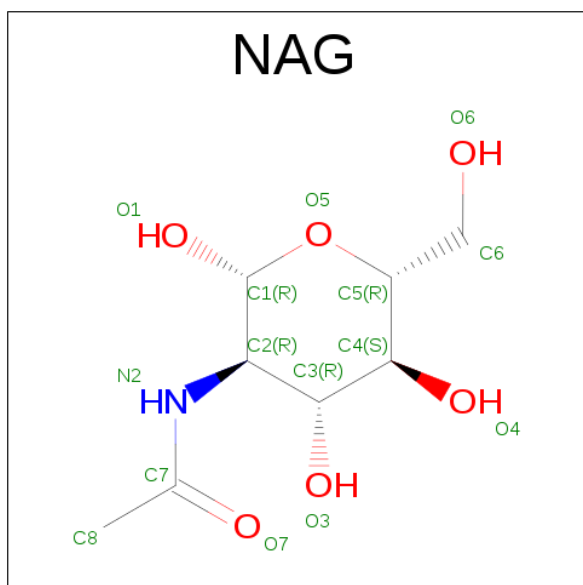
Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	109	Total	C	N	O	S	0	0
			793	491	135	164	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	109	Total	C	N	O	S	0	0
			793	491	135	164	3		
4	M	109	Total	C	N	O	S	0	0
			793	491	135	164	3		

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

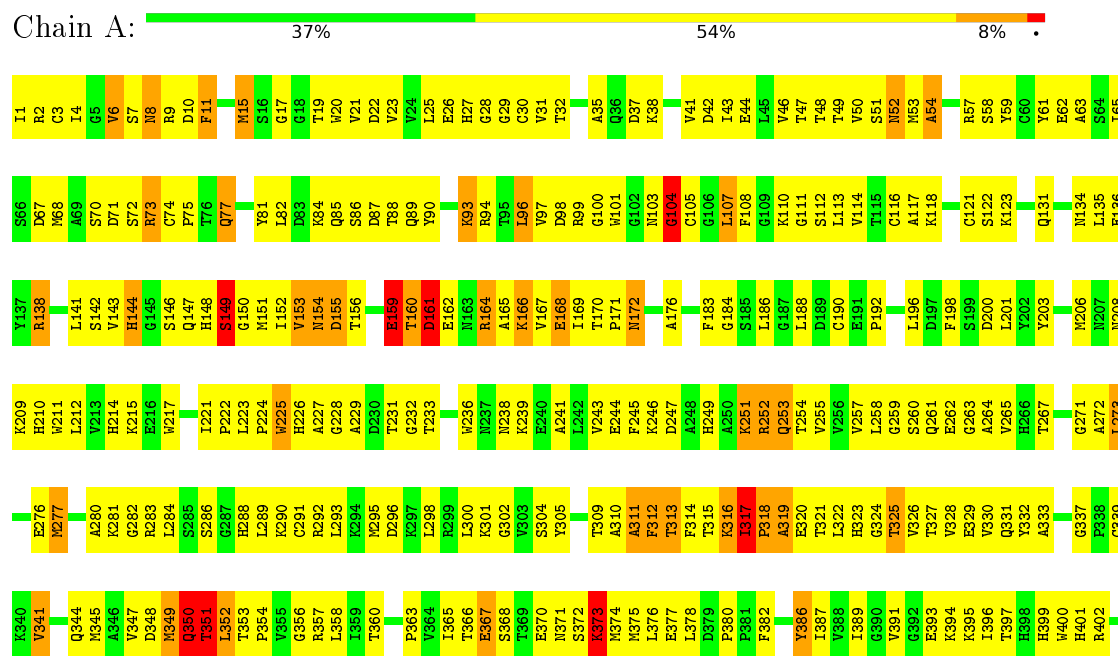


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	

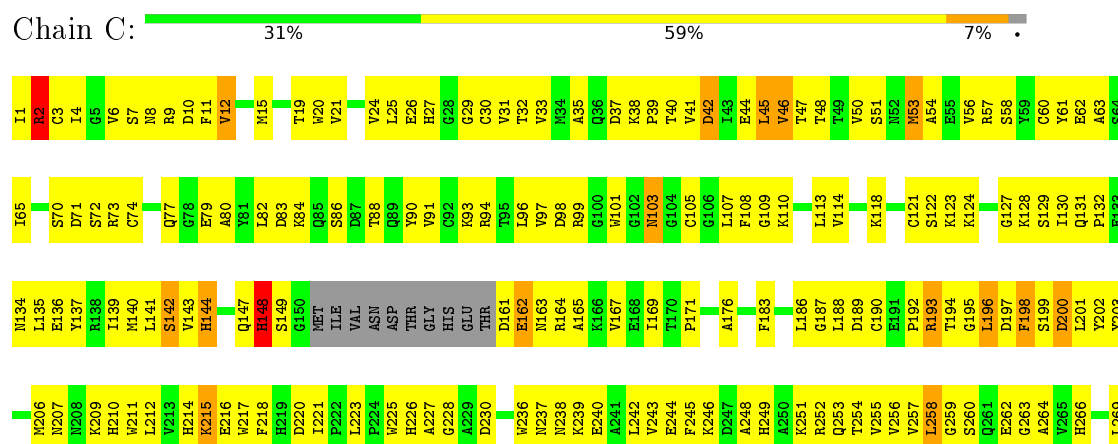
3 Residue-property plots

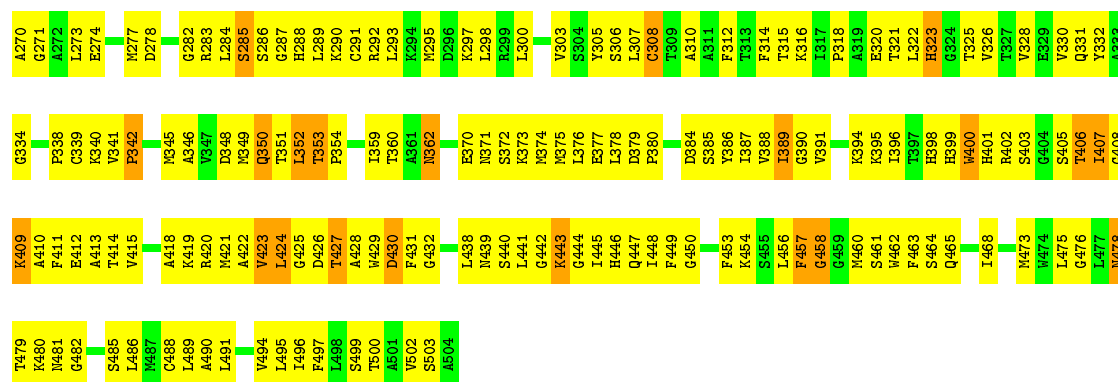
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. 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: structural protein E



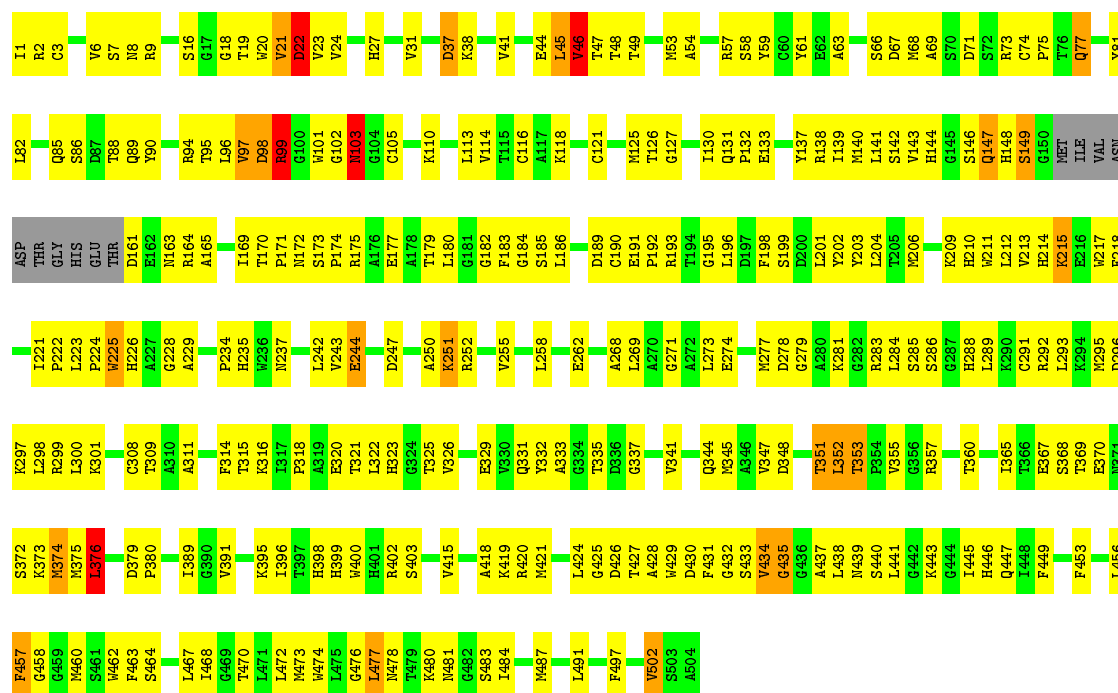
• Molecule 1: structural protein E





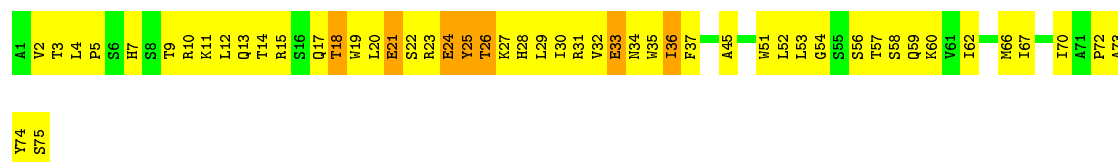
• Molecule 1: structural protein E

Chain B: 43% 49%



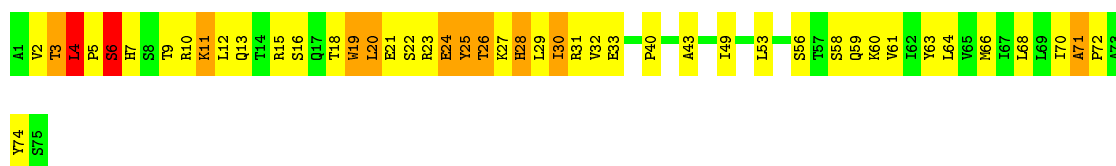
• Molecule 2: strutral protein M

Chain D: 32% 59% 9%



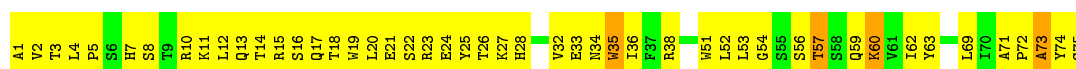
• Molecule 2: strutral protein M

Chain E: 39% 45% 13%



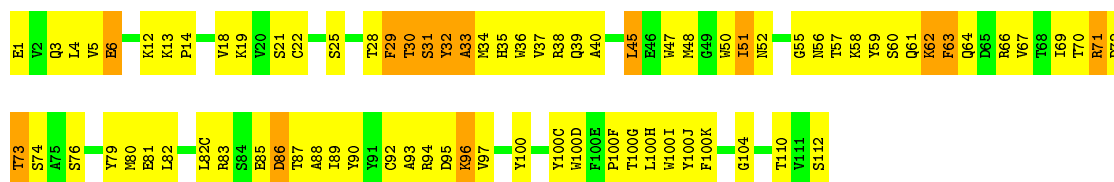
- Molecule 2: strutral protein M

Chain F: 36% 59% 5%



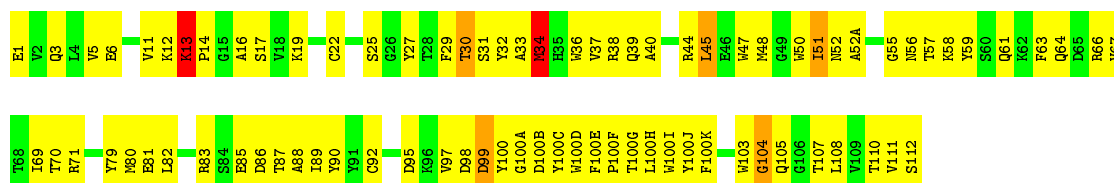
- Molecule 3: C10 IgG heavy chain variable region

Chain G: 36% 53% 11%



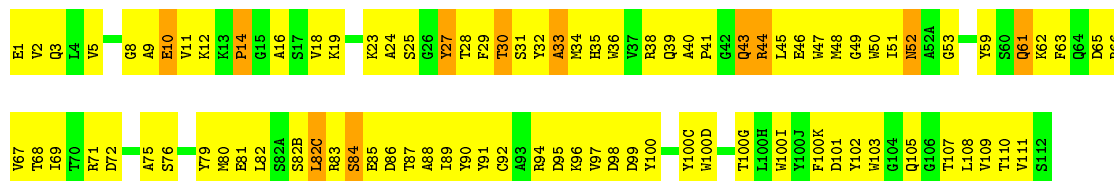
- Molecule 3: C10 IgG heavy chain variable region

Chain K: 35% 59% . .



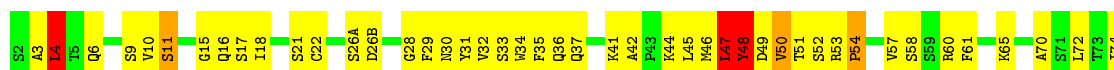
- Molecule 3: C10 IgG heavy chain variable region

Chain I: 28% 63% 9%



- Molecule 4: C10 IgG light chain variable region

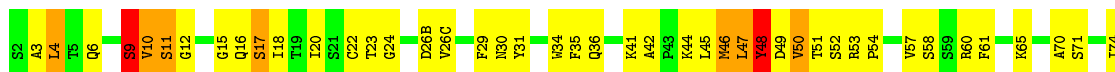
Chain H: 41% 51% 5%





- Molecule 4: C10 IgG light chain variable region

Chain L: 42% 46% 10%



- Molecule 4: C10 IgG light chain variable region

Chain M: 27% 61% 13%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	49100	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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 > 2$	RMSZ	# $ Z > 2$
1	A	0.62	2/3877 (0.1%)	0.92	17/5239 (0.3%)
1	B	0.56	2/3809 (0.1%)	0.84	8/5152 (0.2%)
1	C	0.57	2/3808 (0.1%)	0.91	17/5152 (0.3%)
2	D	0.43	0/615	0.85	2/838 (0.2%)
2	E	0.52	0/615	1.09	5/838 (0.6%)
2	F	0.44	0/615	0.95	5/838 (0.6%)
3	G	0.50	0/1050	0.87	5/1427 (0.4%)
3	I	0.59	1/1050 (0.1%)	0.96	4/1427 (0.3%)
3	K	0.47	0/1050	0.88	6/1427 (0.4%)
4	H	0.60	1/811 (0.1%)	0.88	3/1101 (0.3%)
4	L	0.62	0/811	0.95	6/1101 (0.5%)
4	M	0.47	0/811	0.82	2/1101 (0.2%)
All	All	0.56	8/18922 (0.0%)	0.90	80/25641 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
2	E	0	2
All	All	0	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	342	PRO	N-CD	-11.89	1.31	1.47
1	A	341	VAL	C-N	11.35	1.55	1.34
3	I	14	PRO	N-CD	-9.73	1.34	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	GLU	C-N	9.39	1.55	1.34
1	C	400	TRP	CB-CG	-5.66	1.40	1.50
1	B	318	PRO	N-CD	-5.28	1.40	1.47
4	H	54	PRO	N-CD	5.27	1.55	1.47
1	B	225	TRP	CB-CG	-5.02	1.41	1.50

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	ILE	C-N-CD	-16.95	83.31	120.60
1	C	148	HIS	N-CA-CB	16.02	139.44	110.60
3	K	51	ILE	N-CA-C	12.34	144.32	111.00
3	G	51	ILE	N-CA-C	12.33	144.30	111.00
1	A	325	THR	N-CA-C	9.40	136.38	111.00
4	L	46	MET	N-CA-C	9.12	135.62	111.00
1	A	351	THR	N-CA-C	8.07	132.78	111.00
1	A	144	HIS	C-N-CA	-8.00	105.49	122.30
1	B	103	ASN	N-CA-C	7.93	132.42	111.00
1	A	273	LEU	N-CA-C	-7.90	89.66	111.00
2	E	11	LYS	N-CA-C	7.59	131.48	111.00
3	I	84	SER	N-CA-CB	-7.37	99.44	110.50
1	B	435	GLY	N-CA-C	7.37	131.51	113.10
4	H	83	ALA	N-CA-C	-6.98	92.15	111.00
2	F	35	TRP	N-CA-CB	6.98	123.17	110.60
1	C	389	ILE	CB-CA-C	-6.97	97.66	111.60
4	L	11	SER	N-CA-C	6.97	129.82	111.00
1	A	104	GLY	N-CA-C	6.73	129.92	113.10
2	F	60	LYS	N-CA-CB	6.58	122.44	110.60
1	B	395	LYS	N-CA-C	-6.57	93.27	111.00
4	L	47	LEU	N-CA-C	6.56	128.72	111.00
4	H	82	GLU	N-CA-CB	6.52	122.33	110.60
1	C	228	GLY	N-CA-C	6.51	129.38	113.10
1	C	54	ALA	N-CA-CB	6.45	119.13	110.10
1	C	195	GLY	N-CA-C	-6.24	97.50	113.10
1	A	77	GLN	CA-C-N	-6.23	103.74	116.20
2	E	16	SER	N-CA-C	-6.20	94.25	111.00
3	K	104	GLY	N-CA-C	-6.15	97.72	113.10
4	H	82	GLU	N-CA-C	-6.08	94.57	111.00
2	D	18	THR	N-CA-CB	6.08	121.86	110.30
2	F	73	ALA	N-CA-C	6.07	127.40	111.00
3	I	43	GLN	N-CA-C	6.06	127.37	111.00
1	A	96	LEU	CA-CB-CG	6.06	129.23	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	88	THR	N-CA-C	5.96	127.08	111.00
2	F	1	ALA	CB-CA-C	5.95	119.02	110.10
1	A	150	GLY	CA-C-N	-5.93	104.15	117.20
1	A	77	GLN	CA-C-O	5.93	132.55	120.10
1	A	341	VAL	O-C-N	-5.84	110.00	121.10
1	C	193	ARG	N-CA-C	5.84	126.77	111.00
1	C	390	GLY	N-CA-C	5.83	127.67	113.10
1	A	149	SER	N-CA-C	-5.80	95.34	111.00
2	E	25	TYR	N-CA-CB	5.77	120.99	110.60
1	C	458	GLY	N-CA-C	-5.77	98.67	113.10
1	B	45	LEU	N-CA-C	5.75	126.53	111.00
2	E	6	SER	N-CA-C	5.75	126.52	111.00
1	C	342	PRO	CA-N-CD	5.74	119.74	111.70
3	I	14	PRO	CA-N-CD	5.71	119.69	111.70
1	C	200	ASP	CB-CA-C	-5.70	99.00	110.40
2	D	33	GLU	N-CA-C	5.68	126.34	111.00
4	M	40	GLY	N-CA-C	5.68	127.29	113.10
1	C	342	PRO	N-CA-CB	-5.64	96.39	102.60
1	B	351	THR	N-CA-C	-5.64	95.77	111.00
1	C	389	ILE	N-CA-C	5.63	126.21	111.00
2	E	3	THR	N-CA-C	5.52	125.91	111.00
3	I	84	SER	N-CA-C	5.52	125.91	111.00
3	G	86	ASP	N-CA-C	5.52	125.89	111.00
1	A	159	GLU	C-N-CA	-5.50	107.96	121.70
1	C	400	TRP	CA-CB-CG	-5.49	103.26	113.70
1	A	164	ARG	N-CA-CB	-5.47	100.76	110.60
2	F	60	LYS	N-CA-C	-5.45	96.28	111.00
1	C	306	SER	CB-CA-C	5.45	120.45	110.10
1	A	458	GLY	N-CA-C	-5.37	99.67	113.10
1	A	313	THR	N-CA-C	-5.36	96.52	111.00
1	C	430	ASP	C-N-CA	-5.36	108.31	121.70
1	B	432	GLY	N-CA-C	-5.35	99.73	113.10
3	K	51	ILE	N-CA-CB	-5.33	98.55	110.80
4	L	11	SER	CA-C-N	5.32	126.83	116.20
3	G	51	ILE	N-CA-CB	-5.30	98.60	110.80
1	A	424	LEU	CA-CB-CG	5.29	127.46	115.30
4	M	15	GLY	N-CA-C	5.26	126.26	113.10
1	C	53	MET	N-CA-C	5.22	125.10	111.00
1	B	37	ASP	N-CA-CB	-5.22	101.21	110.60
4	L	47	LEU	N-CA-CB	-5.20	100.00	110.40
3	K	13	LYS	N-CA-C	5.19	125.01	111.00
3	G	51	ILE	CB-CA-C	-5.18	101.24	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	51	ILE	CB-CA-C	-5.17	101.26	111.60
1	B	457	PHE	N-CA-CB	5.16	119.89	110.60
3	G	45	LEU	CA-CB-CG	5.06	126.95	115.30
3	K	45	LEU	CA-CB-CG	5.05	126.92	115.30
4	L	9	SER	N-CA-C	5.05	124.64	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	349	MET	Peptide
1	C	427	THR	Mainchain
2	E	20	LEU	Mainchain
2	E	71	ALA	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3798	0	3759	615	0
1	B	3732	0	3693	436	0
1	C	3731	0	3690	673	0
2	D	600	0	624	145	0
2	E	600	0	624	115	0
2	F	600	0	624	153	0
3	G	1021	0	960	166	0
3	I	1021	0	960	333	0
3	K	1021	0	960	130	0
4	H	793	0	754	144	0
4	L	793	0	755	122	0
4	M	793	0	753	201	0
5	A	14	0	13	6	0
All	All	18517	0	18169	2881	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 79.

All (2881) 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)
3:I:11:VAL:HG12	3:I:110:THR:CB	1.26	1.63
4:M:4:LEU:HB3	4:M:98:GLY:CA	1.22	1.59
1:A:108:PHE:CZ	1:C:4:ILE:CD1	1.87	1.58
3:I:11:VAL:CG1	3:I:110:THR:HB	1.30	1.58
1:C:320:GLU:HB2	1:C:400:TRP:CH2	1.10	1.58
1:C:320:GLU:CG	1:C:400:TRP:HZ2	1.17	1.57
1:A:311:ALA:HB1	1:A:332:TYR:CA	1.28	1.56
1:A:311:ALA:CB	1:A:332:TYR:CA	1.77	1.56
1:A:108:PHE:HZ	1:C:4:ILE:CD1	1.12	1.56
1:A:311:ALA:CB	1:A:332:TYR:HA	1.15	1.56
1:A:183:PHE:CE1	1:A:301:LYS:HD3	1.40	1.56
1:C:201:LEU:CD2	1:C:212:LEU:HD13	1.18	1.55
1:C:320:GLU:HB2	1:C:400:TRP:CZ2	1.40	1.55
4:M:4:LEU:CB	4:M:98:GLY:HA2	1.33	1.55
1:C:201:LEU:HD23	1:C:212:LEU:CD1	1.31	1.54
1:A:148:HIS:CE1	1:A:373:LYS:CB	1.90	1.53
4:M:53:ARG:CD	4:M:57:VAL:HG13	1.36	1.53
3:I:50:TRP:CD1	3:I:59:TYR:HE1	1.26	1.53
4:M:88:SER:HB2	4:M:97:PHE:CE1	1.02	1.53
3:I:67:VAL:HG12	3:I:82:LEU:CA	1.39	1.53
3:I:67:VAL:CG1	3:I:82:LEU:HA	1.29	1.52
1:A:148:HIS:CE1	1:A:373:LYS:HB2	1.42	1.51
4:M:53:ARG:HD2	4:M:57:VAL:CG1	1.37	1.50
4:M:88:SER:CB	4:M:97:PHE:CE1	1.91	1.49
4:M:88:SER:CB	4:M:97:PHE:HE1	1.22	1.48
4:L:15:GLY:CA	4:L:76:GLY:HA2	1.39	1.47
1:A:108:PHE:CZ	1:C:4:ILE:HD13	1.48	1.46
3:I:69:ILE:HG22	3:I:80:MET:CA	1.42	1.46
1:B:148:HIS:ND1	1:B:373:LYS:HB3	1.32	1.45
1:C:27:HIS:CE1	3:G:100:TYR:HE1	1.34	1.44
1:C:320:GLU:CB	1:C:400:TRP:CZ2	2.01	1.44
1:C:420:ARG:HD3	1:C:431:PHE:CD2	1.50	1.44
3:I:50:TRP:CD1	3:I:59:TYR:CE1	2.07	1.43
1:A:151:MET:SD	1:A:373:LYS:HD2	1.59	1.42
4:L:15:GLY:HA2	4:L:76:GLY:CA	1.50	1.42
1:A:148:HIS:ND1	1:A:373:LYS:HB3	1.10	1.42
1:C:12:VAL:CG2	1:C:33:VAL:HG12	1.49	1.41
4:H:88:SER:CB	4:H:97:PHE:CD1	2.06	1.39
3:I:50:TRP:CH2	3:I:80:MET:SD	2.14	1.39
1:C:320:GLU:CB	1:C:400:TRP:CH2	2.06	1.38
1:A:252:ARG:HD2	3:G:100(D):TRP:CD1	1.57	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:GLU:CG	1:C:400:TRP:CZ2	2.07	1.37
1:C:101:TRP:NE1	1:C:108:PHE:HZ	1.20	1.37
1:B:456:LEU:CD1	1:B:457:PHE:CD1	2.08	1.36
1:A:148:HIS:ND1	1:A:373:LYS:CB	1.86	1.35
1:A:74:CYS:CB	1:A:77:GLN:OE1	1.74	1.35
1:A:252:ARG:CD	3:G:100(D):TRP:NE1	1.87	1.35
1:C:47:THR:CG2	1:C:283:ARG:HH21	1.41	1.34
1:B:217:TRP:NE1	2:E:5:PRO:HB2	1.41	1.33
1:C:101:TRP:NE1	1:C:108:PHE:CZ	1.97	1.33
1:A:252:ARG:HD2	3:G:100(D):TRP:NE1	1.36	1.33
3:G:100(H):LEU:HD23	4:H:49:ASP:OD2	1.22	1.33
3:I:69:ILE:CG2	3:I:80:MET:HA	1.58	1.33
4:H:88:SER:HB3	4:H:97:PHE:CD1	1.59	1.32
1:A:1:ILE:N	1:A:144:HIS:NE2	1.74	1.32
4:M:11:SER:OG	4:M:104:THR:HG21	1.22	1.32
1:C:26:GLU:HA	1:C:45:LEU:CD1	1.58	1.30
1:C:27:HIS:CE1	3:G:100:TYR:CE1	2.18	1.29
1:A:324:GLY:O	1:A:402:ARG:NH2	1.61	1.29
1:C:11:PHE:CD2	1:C:32:THR:OG1	1.82	1.29
4:H:60:ARG:NH1	4:H:81:ASP:OD2	1.64	1.29
4:M:4:LEU:CB	4:M:98:GLY:CA	1.97	1.29
1:A:252:ARG:NE	3:G:100(D):TRP:HE1	1.28	1.28
1:C:295:MET:SD	1:C:298:LEU:HD12	1.73	1.28
3:G:28:THR:CG2	3:G:30:THR:OG1	1.81	1.28
4:L:36:GLN:HG3	4:L:83:ALA:CB	1.63	1.27
4:M:11:SER:OG	4:M:104:THR:CG2	1.83	1.27
1:A:345:MET:O	1:A:354:PRO:HB3	1.23	1.26
1:C:47:THR:CG2	1:C:283:ARG:NH2	1.97	1.26
1:C:27:HIS:HE1	3:G:100:TYR:CE1	1.51	1.26
3:I:12:LYS:HG3	3:I:82(C):LEU:CD1	1.63	1.26
1:A:312:PHE:CE2	1:A:389:ILE:HG13	1.71	1.25
3:I:9:ALA:O	3:I:109:VAL:HA	1.16	1.25
4:L:50:VAL:CG2	4:L:51:THR:H	1.39	1.25
1:A:345:MET:O	1:A:354:PRO:CB	1.84	1.24
3:G:29:PHE:CE1	3:G:32:TYR:CD1	2.25	1.24
1:C:47:THR:HG21	1:C:283:ARG:NH2	1.52	1.24
1:C:214:HIS:CD2	2:F:7:HIS:HE1	1.56	1.24
1:B:148:HIS:CE1	1:B:373:LYS:CB	2.21	1.24
3:I:83:ARG:O	3:I:111:VAL:CG2	1.86	1.24
1:B:148:HIS:CE1	1:B:373:LYS:HB3	1.73	1.23
3:I:16:ALA:O	3:I:82(C):LEU:HG	1.36	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:THR:HG21	1:A:164:ARG:C	1.57	1.23
3:G:28:THR:HG22	3:G:30:THR:OG1	1.29	1.23
3:I:50:TRP:CZ3	3:I:80:MET:SD	2.30	1.23
4:M:53:ARG:CD	4:M:57:VAL:CG1	2.04	1.23
1:A:74:CYS:HB2	1:A:77:GLN:OE1	1.10	1.23
1:C:331:GLN:HG3	1:C:371:ASN:CB	1.67	1.23
1:C:9:ARG:NH1	1:C:11:PHE:HZ	1.34	1.22
4:M:59:SER:O	4:M:60:ARG:HG3	1.35	1.22
4:M:11:SER:CB	4:M:104:THR:CG2	2.17	1.21
1:A:71:ASP:O	1:A:113:LEU:HD12	1.36	1.21
4:H:4:LEU:CD1	4:H:22:CYS:SG	2.28	1.21
3:I:84:SER:N	3:I:111:VAL:HG11	1.55	1.21
1:A:108:PHE:CZ	1:C:4:ILE:HD12	1.59	1.20
1:A:46:VAL:HG23	3:I:100:TYR:CE1	1.75	1.19
4:H:88:SER:HB2	4:H:97:PHE:CE1	1.77	1.19
1:A:101:TRP:HD1	1:A:108:PHE:CE1	1.59	1.19
1:A:277:MET:HA	1:A:282:GLY:HA2	1.20	1.19
1:B:344:GLN:HE21	1:B:352:LEU:CD1	1.56	1.19
2:D:74:TYR:CE1	2:F:32:VAL:HG21	1.77	1.18
4:L:4:LEU:HD21	4:L:24:GLY:CA	1.72	1.18
4:M:53:ARG:HD3	4:M:57:VAL:CA	1.72	1.18
4:H:88:SER:CB	4:H:97:PHE:CE1	2.25	1.18
1:A:50:VAL:CG1	1:A:53:MET:SD	2.31	1.18
1:C:464:SER:OG	2:D:75:SER:O	1.57	1.18
2:D:56:SER:O	2:D:57:THR:HG22	1.39	1.18
3:I:67:VAL:HG11	3:I:82:LEU:CB	1.73	1.17
1:C:214:HIS:CD2	2:F:7:HIS:CE1	2.31	1.17
4:M:9:SER:HA	4:M:102:LYS:O	1.41	1.17
4:M:48:TYR:CE2	4:M:52:SER:O	1.98	1.17
1:C:350:GLN:CD	1:B:175:ARG:HE	1.48	1.17
1:C:15:MET:CE	1:C:19:THR:HA	1.75	1.16
1:C:424:LEU:HB3	1:C:428:ALA:HB2	1.28	1.16
4:H:88:SER:HB2	4:H:97:PHE:CD1	1.76	1.16
1:A:464:SER:HB3	2:F:75:SER:HB2	1.26	1.16
3:I:38:ARG:HD3	3:I:48:MET:SD	1.85	1.16
1:B:288:HIS:NE2	1:B:424:LEU:HG	1.60	1.16
1:B:148:HIS:CE1	1:B:373:LYS:HG3	1.81	1.16
1:B:186:LEU:CD1	1:B:293:LEU:HD11	1.76	1.16
1:C:407:ILE:O	1:C:411:PHE:HB3	1.43	1.16
4:H:9:SER:HB3	4:H:102:LYS:HB3	1.26	1.15
1:B:98:ASP:OD2	1:B:251:LYS:HB3	0.98	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:4:LEU:HD21	4:L:24:GLY:HA2	1.21	1.15
2:F:54:GLY:HA3	2:F:59:GLN:NE2	1.59	1.15
3:I:28:THR:CG2	3:I:30:THR:HG23	1.75	1.15
3:I:67:VAL:CG1	3:I:82:LEU:CA	2.07	1.15
1:A:151:MET:SD	1:A:373:LYS:CD	2.35	1.15
1:C:331:GLN:HG3	1:C:371:ASN:HB3	1.18	1.15
1:C:202:TYR:CE2	1:C:215:LYS:HD3	1.78	1.15
2:F:56:SER:O	2:F:57:THR:OG1	1.63	1.15
3:I:12:LYS:CG	3:I:82(C):LEU:CD1	2.24	1.15
1:C:101:TRP:CD1	1:C:108:PHE:CZ	2.32	1.15
1:B:443:LYS:O	1:B:447:GLN:HB2	1.46	1.14
4:L:44:LYS:HE3	4:L:46:MET:CE	1.76	1.14
4:L:50:VAL:HG23	4:L:51:THR:N	1.37	1.14
1:B:98:ASP:OD2	1:B:251:LYS:CB	1.95	1.14
2:E:32:VAL:HG23	2:E:72:PRO:HG2	1.19	1.14
3:I:24:ALA:HB3	3:I:76:SER:OG	1.45	1.14
3:I:66:ARG:HD3	3:I:82:LEU:HD11	1.21	1.14
3:I:9:ALA:CB	3:I:109:VAL:HB	1.75	1.14
1:A:252:ARG:NE	3:G:100(D):TRP:NE1	1.89	1.14
1:C:320:GLU:HG3	1:C:400:TRP:CZ2	1.74	1.14
4:H:36:GLN:HG3	4:H:83:ALA:HB3	1.29	1.14
1:A:159:GLU:HG2	1:A:160:THR:N	1.62	1.14
3:I:50:TRP:CH2	3:I:80:MET:HG3	1.81	1.14
1:B:102:GLY:O	3:K:100(H):LEU:HD21	1.48	1.14
2:F:54:GLY:HA3	2:F:59:GLN:HE21	1.04	1.13
3:I:84:SER:HA	3:I:111:VAL:HB	1.24	1.13
1:C:15:MET:HE3	1:C:19:THR:HA	1.30	1.13
4:H:88:SER:CB	4:H:97:PHE:HD1	1.49	1.13
3:I:29:PHE:CD2	3:I:76:SER:HB2	1.82	1.13
1:A:101:TRP:CD1	1:A:108:PHE:CE1	2.36	1.13
3:I:83:ARG:O	3:I:111:VAL:HG21	0.97	1.13
1:A:312:PHE:CG	1:A:396:ILE:HG13	1.84	1.12
3:I:50:TRP:CH2	3:I:80:MET:CG	2.32	1.12
2:D:27:LYS:HB3	2:F:2:VAL:HG11	1.23	1.12
1:B:456:LEU:HD12	1:B:457:PHE:CD1	1.81	1.12
1:A:183:PHE:HE1	1:A:301:LYS:CD	1.63	1.12
1:A:280:ALA:O	1:A:281:LYS:CD	1.97	1.12
2:D:75:SER:OG	2:F:28:HIS:CE1	2.02	1.12
3:I:9:ALA:HB1	3:I:109:VAL:HB	1.15	1.12
1:A:160:THR:HG21	5:A:601:NAG:C2	1.79	1.12
1:C:478:ASN:O	1:C:478:ASN:ND2	1.80	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:HIS:CE1	1:A:373:LYS:HB3	1.67	1.12
1:C:331:GLN:CG	1:C:371:ASN:HB3	1.80	1.11
1:C:312:PHE:CZ	1:C:341:VAL:HG21	1.85	1.11
4:M:4:LEU:CD1	4:M:22:CYS:SG	2.38	1.11
3:K:38:ARG:HH22	3:K:86:ASP:HA	1.05	1.11
1:A:217:TRP:CH2	1:A:221:ILE:HD11	1.84	1.11
1:A:249:HIS:CE1	2:F:16:SER:HB3	1.84	1.11
4:H:4:LEU:HD12	4:H:22:CYS:SG	1.91	1.11
1:A:311:ALA:CB	1:A:332:TYR:CB	2.27	1.11
2:D:74:TYR:CE1	2:F:32:VAL:CG2	2.34	1.11
1:A:252:ARG:CD	3:G:100(D):TRP:CD1	2.26	1.11
1:B:148:HIS:NE2	1:B:373:LYS:HG3	1.64	1.11
3:I:50:TRP:HB2	3:I:69:ILE:HD11	1.27	1.11
1:C:129:SER:OG	1:C:202:TYR:CE1	2.03	1.11
3:I:9:ALA:O	3:I:108:LEU:O	1.69	1.11
1:A:311:ALA:HB3	1:A:332:TYR:CB	1.81	1.10
2:D:74:TYR:HE1	2:F:32:VAL:CG2	1.65	1.10
2:E:53:LEU:HD11	2:E:63:TYR:CD2	1.86	1.10
1:A:183:PHE:CE1	1:A:301:LYS:CD	2.34	1.10
4:L:36:GLN:HG3	4:L:83:ALA:HB3	1.21	1.10
1:A:148:HIS:CG	1:A:151:MET:HB2	1.85	1.10
1:A:167:VAL:CG1	1:A:176:ALA:HB1	1.82	1.10
1:A:73:ARG:NH2	4:H:26(A):SER:HA	1.66	1.10
1:A:463:PHE:CE2	2:F:74:TYR:CE2	2.39	1.10
1:B:102:GLY:O	3:K:100(H):LEU:CD2	2.00	1.10
3:G:29:PHE:HE1	3:G:32:TYR:CE1	1.69	1.09
1:B:148:HIS:CE1	1:B:373:LYS:CG	2.34	1.09
1:A:59:TYR:HB3	1:A:223:LEU:HD23	1.33	1.09
1:B:268:ALA:O	2:E:5:PRO:O	1.70	1.09
3:I:9:ALA:O	3:I:109:VAL:CA	2.00	1.09
1:C:252:ARG:HG2	3:I:100(D):TRP:CH2	1.87	1.09
4:L:36:GLN:CG	4:L:83:ALA:CB	2.30	1.09
1:C:26:GLU:CA	1:C:45:LEU:HD13	1.82	1.09
1:C:252:ARG:HG3	1:C:253:GLN:H	1.15	1.09
3:I:66:ARG:HG2	3:I:82:LEU:CD1	1.82	1.08
1:A:280:ALA:O	1:A:281:LYS:HD3	1.52	1.08
3:G:29:PHE:CE1	3:G:32:TYR:CE1	2.42	1.08
3:I:67:VAL:HG11	3:I:82:LEU:HB2	1.20	1.08
1:C:214:HIS:HD2	2:F:7:HIS:CE1	1.68	1.08
1:C:46:VAL:HG12	1:C:47:THR:H	1.17	1.08
1:B:344:GLN:NE2	1:B:352:LEU:HD11	1.68	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:LEU:O	1:C:340:LYS:O	1.72	1.08
1:C:143:VAL:HG13	1:C:163:ASN:HB3	1.26	1.08
1:C:211:TRP:HE1	1:C:269:LEU:HD13	1.19	1.07
1:A:169:ILE:HG22	1:A:176:ALA:HB2	1.36	1.07
3:I:38:ARG:HB3	3:I:90:TYR:CD1	1.90	1.07
2:D:2:VAL:CG2	2:F:27:LYS:HD2	1.84	1.07
1:A:350:GLN:HG3	1:A:351:THR:N	1.70	1.06
1:C:99:ARG:HH11	1:C:103:ASN:CB	1.68	1.06
4:H:4:LEU:HD13	4:H:22:CYS:SG	1.94	1.06
3:I:50:TRP:HH2	3:I:80:MET:SD	1.62	1.06
4:M:53:ARG:HD3	4:M:57:VAL:HA	1.34	1.06
1:C:202:TYR:CE2	1:C:215:LYS:CD	2.38	1.06
2:D:57:THR:HG23	2:D:58:SER:N	1.67	1.06
3:I:18:VAL:N	3:I:82(C):LEU:HD21	1.70	1.06
1:A:249:HIS:CE1	2:F:16:SER:CB	2.38	1.06
1:C:9:ARG:CZ	1:C:11:PHE:HZ	1.69	1.06
1:C:99:ARG:HH11	1:C:103:ASN:CG	1.58	1.06
3:I:12:LYS:HB2	3:I:82(C):LEU:HD12	1.38	1.06
1:C:90:TYR:CE1	1:C:118:LYS:HB2	1.90	1.06
3:I:38:ARG:CB	3:I:90:TYR:CD1	2.39	1.06
1:C:420:ARG:CD	1:C:431:PHE:HD2	1.69	1.05
2:D:2:VAL:HG21	2:F:27:LYS:CD	1.85	1.05
1:C:42:ASP:OD1	1:C:142:SER:CB	2.05	1.05
1:C:346:ALA:HB1	1:C:351:THR:O	1.55	1.05
1:C:460:MET:CE	1:C:464:SER:HB3	1.87	1.05
1:C:65:ILE:HD11	1:C:243:VAL:HG22	1.10	1.05
1:A:312:PHE:CZ	1:A:389:ILE:HG13	1.92	1.05
3:I:67:VAL:HG13	3:I:82:LEU:HD13	1.37	1.05
1:C:99:ARG:NH1	1:C:103:ASN:HB2	1.70	1.05
2:E:4:LEU:N	2:E:5:PRO:HD3	1.68	1.05
1:B:186:LEU:HD11	1:B:293:LEU:HD11	1.37	1.04
4:M:49:ASP:O	4:M:50:VAL:HG23	1.54	1.04
1:A:160:THR:HG21	5:A:601:NAG:H2	1.11	1.04
2:F:54:GLY:CA	2:F:59:GLN:NE2	2.20	1.04
3:K:52:ASN:HD22	3:K:56:ASN:HB2	1.23	1.04
1:A:87:ASP:O	1:A:88:THR:HG22	1.56	1.04
1:C:12:VAL:HG21	1:C:33:VAL:CG1	1.86	1.04
2:D:33:GLU:O	2:D:36:ILE:HG13	1.56	1.04
1:A:312:PHE:CZ	1:A:389:ILE:CG1	2.41	1.04
1:C:65:ILE:HD11	1:C:243:VAL:CG2	1.88	1.04
1:C:47:THR:HG22	1:C:283:ARG:NH2	1.72	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:VAL:HG23	2:F:74:TYR:CE1	1.93	1.03
1:C:420:ARG:CD	1:C:431:PHE:CD2	2.41	1.03
4:L:46:MET:O	4:L:47:LEU:HD13	1.58	1.03
1:A:344:GLN:HB2	1:A:354:PRO:HG3	1.05	1.03
1:C:460:MET:HE1	1:C:464:SER:HB3	1.38	1.03
1:A:318:PRO:HB2	1:A:400:TRP:HZ3	1.21	1.03
1:B:99:ARG:NH2	1:B:105:CYS:SG	2.30	1.03
1:C:315:THR:HG21	1:C:373:LYS:HD2	1.39	1.03
3:I:84:SER:HA	3:I:111:VAL:CB	1.87	1.03
3:I:83:ARG:C	3:I:111:VAL:HG11	1.78	1.03
4:M:4:LEU:HB3	4:M:98:GLY:HA3	1.34	1.03
2:D:57:THR:HG23	2:D:58:SER:H	0.86	1.03
2:E:27:LYS:HE3	2:E:31:ARG:HH11	1.23	1.02
4:M:88:SER:HB2	4:M:97:PHE:CD1	1.94	1.02
3:I:28:THR:HG22	3:I:30:THR:HG23	1.04	1.02
1:A:252:ARG:HD2	3:G:100(D):TRP:CE2	1.94	1.02
1:B:217:TRP:CD1	2:E:5:PRO:CB	2.42	1.02
1:A:160:THR:CG2	5:A:601:NAG:H2	1.89	1.02
1:C:9:ARG:NH1	1:C:11:PHE:CZ	2.27	1.02
3:I:12:LYS:CG	3:I:82(C):LEU:HD13	1.87	1.02
3:I:27:TYR:CD1	3:I:94:ARG:NH1	2.27	1.02
1:C:430:ASP:O	1:C:431:PHE:C	1.96	1.02
3:I:16:ALA:O	3:I:82(C):LEU:CG	2.08	1.02
3:I:9:ALA:N	3:I:107:THR:HG23	1.75	1.02
1:A:108:PHE:CE1	1:C:4:ILE:HD12	1.95	1.01
1:B:374:MET:O	1:B:375:MET:HG2	1.60	1.01
1:C:143:VAL:CG1	1:C:163:ASN:HB3	1.89	1.01
1:C:42:ASP:OD1	1:C:142:SER:HB3	1.57	1.01
1:B:148:HIS:ND1	1:B:373:LYS:CB	2.23	1.01
3:I:38:ARG:HD2	3:I:90:TYR:HE1	1.26	1.01
3:K:12:LYS:O	3:K:16:ALA:HB3	1.59	1.01
2:D:75:SER:HG	2:F:28:HIS:CE1	1.76	1.01
1:A:312:PHE:CE1	1:A:389:ILE:HG12	1.95	1.01
3:G:52:ASN:HD22	3:G:56:ASN:HB2	1.23	1.01
1:B:99:ARG:CZ	1:B:105:CYS:SG	2.48	1.01
1:C:389:ILE:HG22	1:C:395:LYS:HB2	1.42	1.01
2:F:18:THR:HG22	2:F:19:TRP:H	1.22	1.01
4:M:49:ASP:OD1	4:M:50:VAL:HG22	1.59	1.01
1:B:456:LEU:HD12	1:B:457:PHE:N	1.75	1.01
3:G:32:TYR:CZ	3:G:33:ALA:O	2.14	1.01
1:A:46:VAL:HG23	3:I:100:TYR:CD1	1.96	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:ARG:CZ	1:C:11:PHE:CZ	2.43	1.00
4:M:9:SER:CA	4:M:102:LYS:O	2.08	1.00
2:D:57:THR:CG2	2:D:58:SER:H	1.74	1.00
3:I:69:ILE:HA	3:I:79:TYR:O	1.60	1.00
4:L:4:LEU:CD2	4:L:24:GLY:HA2	1.92	1.00
1:A:172:ASN:O	1:A:172:ASN:ND2	1.94	1.00
1:C:101:TRP:CD1	1:C:108:PHE:CE1	2.50	1.00
1:C:9:ARG:NE	1:C:11:PHE:CZ	2.30	1.00
3:G:29:PHE:CD1	3:G:32:TYR:CD1	2.50	1.00
1:A:151:MET:HG2	4:M:48:TYR:OH	1.60	1.00
1:A:367:GLU:HG2	1:A:368:SER:N	1.77	0.99
1:A:50:VAL:O	1:A:281:LYS:HA	1.61	0.99
3:I:66:ARG:CD	3:I:82:LEU:HD11	1.91	0.99
1:C:202:TYR:HE2	1:C:215:LYS:CD	1.72	0.99
1:B:73:ARG:HB3	1:B:77:GLN:OE1	1.63	0.99
1:B:217:TRP:NE1	2:E:5:PRO:CB	2.25	0.99
2:D:27:LYS:CB	2:F:2:VAL:HG11	1.91	0.99
1:C:99:ARG:NH1	1:C:103:ASN:CB	2.24	0.99
3:G:6:GLU:HB3	3:G:21:SER:O	1.63	0.99
3:I:50:TRP:HD1	3:I:59:TYR:CE1	1.62	0.99
1:A:318:PRO:HB2	1:A:400:TRP:CZ3	1.96	0.99
1:C:320:GLU:CB	1:C:400:TRP:HZ2	1.57	0.99
1:B:344:GLN:HE21	1:B:352:LEU:HD11	0.82	0.99
1:C:456:LEU:HD12	2:D:45:ALA:HB2	1.40	0.98
1:C:47:THR:HG21	1:C:283:ARG:HH21	0.83	0.98
3:I:38:ARG:CB	3:I:90:TYR:CE1	2.45	0.98
1:C:271:GLY:HA2	2:F:18:THR:HG21	1.42	0.98
3:I:67:VAL:CG1	3:I:82:LEU:CB	2.37	0.98
2:E:9:THR:O	2:E:10:ARG:HG3	1.63	0.98
1:A:155:ASP:HA	1:A:164:ARG:HH21	1.28	0.98
2:D:2:VAL:HG21	2:F:27:LYS:HD2	1.01	0.98
1:B:463:PHE:CE2	2:E:28:HIS:HB3	1.98	0.98
4:H:33:SER:HA	4:H:47:LEU:HD22	1.46	0.98
3:G:100(H):LEU:CD2	4:H:49:ASP:OD2	2.11	0.98
1:C:99:ARG:CG	1:C:103:ASN:OD1	2.10	0.97
1:B:211:TRP:HB3	1:B:274:GLU:HA	1.46	0.97
3:K:6:GLU:N	3:K:105:GLN:HE22	1.62	0.97
1:C:139:ILE:HD12	1:C:169:ILE:CD1	1.93	0.97
1:C:252:ARG:HG2	3:I:100(D):TRP:CZ3	2.00	0.97
1:A:27:HIS:NE2	3:I:100:TYR:HE1	1.61	0.97
4:H:34:TRP:CD1	4:H:47:LEU:CD1	2.47	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:VAL:HB	1:A:281:LYS:O	1.65	0.97
1:B:217:TRP:HE1	2:E:5:PRO:HB2	1.15	0.97
1:A:311:ALA:HB3	1:A:332:TYR:HA	1.42	0.97
4:M:48:TYR:HE2	4:M:52:SER:O	1.37	0.97
1:A:97:VAL:O	1:A:98:ASP:OD1	1.83	0.97
1:A:1:ILE:CG1	1:A:144:HIS:HD2	1.76	0.97
4:L:44:LYS:HE3	4:L:46:MET:HE1	1.45	0.97
2:E:32:VAL:HG23	2:E:72:PRO:CG	1.93	0.97
3:I:1:GLU:HG3	3:I:2:VAL:H	1.29	0.97
1:A:312:PHE:CE2	1:A:389:ILE:CG1	2.47	0.96
1:C:441:LEU:O	1:C:445:ILE:HG12	1.65	0.96
1:A:148:HIS:HD2	1:A:152:ILE:HG13	1.26	0.96
1:C:129:SER:OG	1:C:202:TYR:CD1	2.16	0.96
1:C:463:PHE:HE2	2:D:74:TYR:CE2	1.81	0.96
2:F:54:GLY:CA	2:F:59:GLN:HE21	1.76	0.96
1:A:311:ALA:HB2	1:A:332:TYR:CA	1.94	0.96
1:C:26:GLU:HA	1:C:45:LEU:HD13	0.98	0.96
3:I:18:VAL:HB	3:I:82(C):LEU:HD22	1.44	0.96
3:I:9:ALA:N	3:I:107:THR:CG2	2.29	0.96
3:K:38:ARG:HH22	3:K:86:ASP:CA	1.78	0.96
4:M:11:SER:HB3	4:M:104:THR:CG2	1.93	0.96
3:I:12:LYS:HG3	3:I:82(C):LEU:HD11	1.46	0.96
1:A:475:LEU:HD21	2:F:53:LEU:HD11	1.45	0.96
2:D:4:LEU:HD21	2:F:34:ASN:HD21	1.30	0.96
1:C:12:VAL:HG21	1:C:33:VAL:HG12	1.00	0.96
1:B:225:TRP:HB2	1:B:237:ASN:HB2	1.46	0.96
1:C:201:LEU:CD2	1:C:212:LEU:CD1	2.07	0.96
3:I:28:THR:HG22	3:I:30:THR:CG2	1.96	0.96
2:E:7:HIS:NE2	2:E:24:GLU:CG	2.29	0.96
3:G:38:ARG:HH22	3:G:86:ASP:HA	1.29	0.96
4:H:46:MET:SD	4:H:57:VAL:HG13	2.06	0.95
3:I:32:TYR:O	3:I:33:ALA:HB2	1.66	0.95
1:B:59:TYR:CE2	1:B:221:ILE:HD11	2.00	0.95
1:C:20:TRP:HZ2	1:C:292:ARG:HH11	1.07	0.95
1:A:67:ASP:O	1:A:68:MET:HG2	1.66	0.95
1:C:420:ARG:HD3	1:C:431:PHE:CE2	1.99	0.95
1:C:26:GLU:CA	1:C:45:LEU:CD1	2.41	0.95
1:C:295:MET:SD	1:C:298:LEU:CD1	2.54	0.95
3:I:69:ILE:CG2	3:I:80:MET:CA	2.25	0.95
4:M:4:LEU:CB	4:M:98:GLY:N	2.29	0.95
1:A:331:GLN:HG3	1:A:372:SER:OG	1.64	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ASP:O	1:A:113:LEU:CD1	2.15	0.95
1:B:225:TRP:HE3	1:B:237:ASN:HD22	1.14	0.95
2:D:52:LEU:HD13	2:D:52:LEU:O	1.65	0.95
3:I:9:ALA:H	3:I:107:THR:HG23	1.30	0.95
1:C:423:VAL:HG13	1:C:424:LEU:H	1.28	0.95
1:A:311:ALA:CB	1:A:333:ALA:N	2.30	0.95
1:A:46:VAL:CG2	3:I:100:TYR:CD1	2.50	0.95
1:B:202:TYR:OH	1:B:215:LYS:HG3	1.66	0.94
1:B:21:VAL:O	1:B:22:ASP:HB3	1.60	0.94
1:B:148:HIS:HA	1:B:375:MET:SD	2.07	0.94
2:E:7:HIS:NE2	2:E:24:GLU:HG3	1.81	0.94
4:H:34:TRP:HD1	4:H:47:LEU:CD1	1.80	0.94
1:B:102:GLY:O	3:K:100(H):LEU:CG	2.15	0.94
1:B:456:LEU:CD1	1:B:457:PHE:CE1	2.50	0.94
2:D:32:VAL:CG2	2:F:74:TYR:CE1	2.49	0.94
1:B:365:ILE:HG22	1:B:367:GLU:H	1.33	0.94
4:L:46:MET:O	4:L:47:LEU:CD1	2.16	0.94
1:C:20:TRP:HZ2	1:C:292:ARG:NH1	1.66	0.94
3:I:9:ALA:CB	3:I:107:THR:HG22	1.97	0.94
3:I:38:ARG:HB2	3:I:90:TYR:CE1	2.01	0.94
3:K:52:ASN:ND2	3:K:56:ASN:ND2	2.16	0.94
4:M:36:GLN:OE1	4:M:46:MET:SD	2.26	0.94
1:C:143:VAL:HG13	1:C:163:ASN:CB	1.98	0.94
1:C:46:VAL:HG12	1:C:47:THR:N	1.82	0.93
3:I:29:PHE:HA	3:I:32:TYR:HB3	1.47	0.93
3:I:9:ALA:HB1	3:I:109:VAL:CB	1.96	0.93
2:E:18:THR:HG22	2:E:21:GLU:HB2	1.51	0.93
1:A:2:ARG:HG3	1:A:44:GLU:OE1	1.67	0.93
3:I:50:TRP:NE1	3:I:59:TYR:CE1	2.35	0.93
1:A:463:PHE:CE2	2:F:74:TYR:HE2	1.85	0.93
1:B:217:TRP:CD1	2:E:5:PRO:HB2	2.04	0.93
2:E:4:LEU:N	2:E:5:PRO:CD	2.31	0.93
3:G:30:THR:O	3:G:32:TYR:N	2.01	0.93
3:K:33:ALA:O	3:K:34:MET:HB2	1.69	0.93
1:A:27:HIS:HE2	3:I:100:TYR:HE1	1.03	0.93
1:A:311:ALA:HB2	1:A:333:ALA:N	1.82	0.93
3:I:3:GLN:HB2	3:I:25:SER:HB2	1.49	0.93
3:G:52:ASN:ND2	3:G:56:ASN:HD22	1.67	0.93
3:I:66:ARG:CG	3:I:82:LEU:CD1	2.47	0.93
4:L:49:ASP:O	4:L:50:VAL:HG22	1.68	0.93
3:G:52:ASN:ND2	3:G:56:ASN:ND2	2.16	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:83:ARG:C	3:I:111:VAL:HG21	1.88	0.93
1:A:222:PRO:CG	2:D:3:THR:HA	1.99	0.93
1:A:311:ALA:CB	1:A:332:TYR:C	2.36	0.92
1:B:98:ASP:HB3	1:B:250:ALA:HB1	1.47	0.92
1:C:99:ARG:HG2	1:C:103:ASN:OD1	1.68	0.92
1:C:135:LEU:HD11	1:C:198:PHE:CE2	2.03	0.92
3:I:12:LYS:CB	3:I:82(C):LEU:HD12	2.00	0.92
1:C:135:LEU:HD11	1:C:198:PHE:HE2	1.32	0.92
1:B:148:HIS:CD2	1:B:373:LYS:HD2	2.04	0.92
1:C:12:VAL:CG2	1:C:33:VAL:CG1	2.43	0.92
3:K:52:ASN:HD22	3:K:56:ASN:CB	1.83	0.92
1:A:326:VAL:HG11	1:A:400:TRP:CE2	2.04	0.92
1:C:351:THR:HG22	1:C:388:VAL:HG11	1.50	0.92
4:H:36:GLN:HG3	4:H:83:ALA:CB	2.00	0.92
4:M:4:LEU:HB2	4:M:98:GLY:HA2	1.48	0.92
1:A:81:TYR:CE2	1:B:229:ALA:HB1	2.04	0.91
1:C:351:THR:HG22	1:C:388:VAL:CG1	1.98	0.91
3:I:16:ALA:HB3	3:I:82(C):LEU:HD12	1.51	0.91
4:L:4:LEU:HD13	4:L:22:CYS:SG	2.10	0.91
1:A:321:THR:HG22	1:A:325:THR:O	1.71	0.91
1:C:341:VAL:CG1	1:C:374:MET:SD	2.58	0.91
2:E:7:HIS:CE1	2:E:24:GLU:HG3	2.05	0.91
1:C:350:GLN:NE2	1:B:175:ARG:HE	1.67	0.91
1:B:133:GLU:OE2	1:B:193:ARG:NH2	2.03	0.91
2:D:74:TYR:HB2	2:F:73:ALA:HB3	1.53	0.91
4:L:77:LEU:HB3	4:L:81:ASP:OD1	1.70	0.91
1:A:15:MET:HE2	1:A:35:ALA:HB2	1.50	0.91
4:M:8:ALA:O	4:M:102:LYS:N	2.03	0.91
2:D:74:TYR:CE2	2:F:69:LEU:HG	2.06	0.91
3:G:52:ASN:HD22	3:G:56:ASN:CB	1.84	0.91
4:M:11:SER:CB	4:M:104:THR:HG22	1.99	0.91
1:A:101:TRP:HD1	1:A:108:PHE:CD1	1.87	0.91
1:A:214:HIS:CE1	2:D:10:ARG:HB3	2.06	0.91
4:H:82:GLU:HA	4:H:103:LEU:HD22	1.50	0.91
3:I:39:GLN:C	3:I:88:ALA:HB1	1.90	0.91
4:M:48:TYR:OH	4:M:52:SER:HB3	1.71	0.91
1:B:186:LEU:HD12	1:B:293:LEU:HD11	1.50	0.90
1:B:456:LEU:HD13	1:B:457:PHE:CD1	2.04	0.90
1:C:9:ARG:NE	1:C:11:PHE:CE2	2.39	0.90
3:G:32:TYR:CG	3:G:33:ALA:N	2.39	0.90
1:B:333:ALA:HA	1:B:370:GLU:HG2	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:69:ILE:CG2	3:I:80:MET:CB	2.49	0.90
3:I:50:TRP:HZ3	3:I:80:MET:SD	1.95	0.90
1:A:222:PRO:HG2	2:D:3:THR:HA	1.54	0.90
1:A:344:GLN:HE22	1:A:352:LEU:HG	1.34	0.90
2:E:53:LEU:CD1	2:E:63:TYR:CD2	2.54	0.90
3:G:32:TYR:OH	3:G:34:MET:HB2	1.69	0.90
4:M:17:SER:HB3	4:M:75:SER:HB2	1.54	0.90
1:A:74:CYS:HB3	1:A:77:GLN:OE1	1.71	0.90
1:B:148:HIS:HD1	1:B:373:LYS:HB3	1.36	0.90
1:C:225:TRP:HB2	1:C:237:ASN:HB3	1.51	0.90
2:D:32:VAL:HG21	2:F:74:TYR:CZ	2.07	0.90
2:D:56:SER:O	2:D:57:THR:CG2	2.20	0.90
3:I:36:TRP:CD1	3:I:50:TRP:CE3	2.59	0.90
3:I:12:LYS:HG3	3:I:82(C):LEU:HD13	1.43	0.90
1:C:99:ARG:HD3	1:C:103:ASN:ND2	1.86	0.90
3:K:11:VAL:HA	3:K:110:THR:O	1.72	0.90
1:A:312:PHE:CD1	1:A:389:ILE:HG12	2.06	0.90
1:A:50:VAL:HG12	1:A:53:MET:SD	2.08	0.90
3:I:69:ILE:HG21	3:I:80:MET:HB2	1.53	0.90
1:C:407:ILE:O	1:C:411:PHE:CB	2.19	0.89
3:I:18:VAL:CG1	3:I:82(C):LEU:HD22	2.01	0.89
3:I:11:VAL:CB	3:I:110:THR:HB	2.02	0.89
2:F:20:LEU:O	2:F:24:GLU:HB2	1.72	0.89
4:H:60:ARG:HH12	4:H:81:ASP:CG	1.75	0.89
3:K:52:ASN:ND2	3:K:56:ASN:HD22	1.68	0.89
1:A:148:HIS:CD2	1:A:152:ILE:HG13	2.08	0.89
1:A:1:ILE:HG13	1:A:144:HIS:CD2	2.06	0.89
1:C:398:HIS:CE1	1:B:172:ASN:HA	2.07	0.89
4:M:11:SER:HG	4:M:104:THR:HG21	1.18	0.89
1:A:15:MET:CE	1:A:35:ALA:HB2	2.02	0.89
2:E:20:LEU:O	2:E:23:ARG:N	2.06	0.89
1:B:462:TRP:CE2	2:E:25:TYR:HD2	1.91	0.89
2:D:4:LEU:CD2	2:F:34:ASN:HD21	1.84	0.89
4:L:50:VAL:CG2	4:L:51:THR:N	2.11	0.89
2:E:7:HIS:NE2	2:E:24:GLU:CD	2.26	0.89
2:D:22:SER:HA	2:D:25:TYR:CZ	2.08	0.88
3:G:66:ARG:NH1	3:G:82:LEU:HD11	1.87	0.88
4:M:11:SER:CB	4:M:104:THR:HG21	1.92	0.88
1:A:280:ALA:O	1:A:281:LYS:HD2	1.74	0.88
3:I:18:VAL:CB	3:I:82(C):LEU:HD22	2.01	0.88
1:A:148:HIS:CD2	1:A:151:MET:HB2	2.09	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:VAL:CG1	1:A:176:ALA:CB	2.51	0.88
1:B:456:LEU:HD13	1:B:457:PHE:CE1	2.09	0.88
1:C:9:ARG:HH11	1:C:11:PHE:HZ	1.16	0.88
2:F:56:SER:C	2:F:57:THR:HG1	1.73	0.88
4:H:34:TRP:N	4:H:47:LEU:HD13	1.89	0.88
1:A:1:ILE:HD12	1:A:144:HIS:HA	1.53	0.88
1:C:341:VAL:HG11	1:C:374:MET:SD	2.14	0.88
2:D:20:LEU:O	2:D:24:GLU:HB2	1.72	0.88
3:G:39:GLN:O	3:G:89:ILE:N	2.06	0.88
3:I:84:SER:HA	3:I:111:VAL:CG1	2.01	0.88
3:I:38:ARG:CB	3:I:90:TYR:HD1	1.83	0.88
3:K:27:TYR:HE1	3:K:32:TYR:HB3	1.39	0.88
1:A:93:LYS:HB3	1:A:245:PHE:HD2	1.38	0.88
1:A:389:ILE:HD12	1:A:391:VAL:HG12	1.55	0.88
3:K:38:ARG:NH2	3:K:86:ASP:HA	1.89	0.88
4:M:9:SER:CB	4:M:102:LYS:O	2.20	0.88
1:B:456:LEU:HD11	1:B:457:PHE:CD1	2.09	0.88
1:C:331:GLN:HG3	1:C:371:ASN:HB2	1.55	0.88
2:D:74:TYR:HB2	2:F:73:ALA:CB	2.02	0.88
3:I:28:THR:CG2	3:I:30:THR:CG2	2.49	0.88
1:C:252:ARG:NH1	3:I:100(D):TRP:HZ3	1.71	0.88
3:K:12:LYS:O	3:K:16:ALA:CB	2.20	0.88
4:M:59:SER:O	4:M:60:ARG:CG	2.21	0.88
1:B:217:TRP:CD1	2:E:5:PRO:HB3	2.09	0.88
2:D:11:LYS:HG2	2:D:12:LEU:H	1.36	0.88
2:F:18:THR:HG22	2:F:19:TRP:N	1.88	0.87
2:D:23:ARG:HH12	2:F:2:VAL:HG23	1.40	0.87
2:D:23:ARG:NH1	2:F:2:VAL:HG23	1.89	0.87
4:L:105:VAL:HG12	4:L:106:LEU:HD13	1.55	0.87
1:C:11:PHE:HD2	1:C:32:THR:OG1	1.31	0.87
1:C:12:VAL:HG22	1:C:33:VAL:HG12	1.53	0.87
1:C:48:THR:HG23	1:C:48:THR:O	1.73	0.87
3:I:50:TRP:CB	3:I:69:ILE:HD11	2.04	0.87
2:D:22:SER:O	2:D:25:TYR:CE1	2.27	0.87
3:I:67:VAL:CG1	3:I:82:LEU:HD13	2.05	0.87
4:M:49:ASP:O	4:M:50:VAL:CG2	2.23	0.87
1:A:217:TRP:CZ3	1:A:221:ILE:HD11	2.08	0.87
1:A:101:TRP:CD1	1:A:108:PHE:CZ	2.63	0.87
1:A:345:MET:SD	1:A:387:ILE:HG12	2.14	0.87
1:A:411:PHE:O	1:A:415:VAL:HG23	1.75	0.87
1:C:446:HIS:O	1:C:450:GLY:N	2.06	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:50:VAL:HG12	4:H:51:THR:N	1.90	0.87
3:I:18:VAL:HB	3:I:82(C):LEU:CD2	2.04	0.87
3:I:66:ARG:HG2	3:I:82:LEU:HD13	1.56	0.87
1:A:249:HIS:NE2	2:F:16:SER:HB3	1.89	0.87
1:A:326:VAL:CG1	1:A:400:TRP:CZ2	2.59	0.86
1:A:344:GLN:HB2	1:A:354:PRO:CG	2.00	0.86
1:C:252:ARG:NH1	3:I:100(D):TRP:CZ3	2.43	0.86
1:C:351:THR:CG2	1:C:395:LYS:HE3	2.05	0.86
3:I:1:GLU:HG3	3:I:2:VAL:N	1.86	0.86
1:A:312:PHE:CZ	1:A:396:ILE:O	2.28	0.86
3:G:61:GLN:O	3:G:62:LYS:C	2.14	0.86
3:I:38:ARG:HD2	3:I:90:TYR:CE1	2.10	0.86
1:B:374:MET:HG3	1:B:375:MET:H	1.38	0.86
2:E:11:LYS:HG2	2:E:12:LEU:N	1.89	0.86
4:L:44:LYS:HE3	4:L:46:MET:HE3	1.55	0.86
1:A:1:ILE:CG1	1:A:144:HIS:CD2	2.57	0.86
1:B:27:HIS:HB2	1:B:45:LEU:HD23	1.55	0.86
1:B:66:SER:HB2	1:B:118:LYS:HB3	1.57	0.86
3:G:14:PRO:HD3	3:G:112:SER:OG	1.74	0.86
4:M:51:THR:CG2	4:M:63:GLY:H	1.88	0.86
1:B:23:VAL:HG21	1:B:31:VAL:HG11	1.56	0.86
1:C:94:ARG:HA	1:C:114:VAL:HB	1.57	0.86
4:M:7:PRO:O	4:M:101:THR:OG1	1.91	0.86
3:I:66:ARG:CD	3:I:82:LEU:CD1	2.54	0.86
1:C:463:PHE:CE2	2:D:74:TYR:CE2	2.63	0.86
2:E:32:VAL:CG2	2:E:72:PRO:HG2	2.05	0.86
4:M:53:ARG:HD3	4:M:57:VAL:C	1.95	0.86
3:I:9:ALA:HB3	3:I:107:THR:HG22	1.58	0.86
1:C:27:HIS:HA	1:C:45:LEU:HB3	1.56	0.85
1:A:138:ARG:HG2	1:A:138:ARG:HH11	1.39	0.85
3:G:31:SER:O	3:G:32:TYR:O	1.93	0.85
1:A:317:ILE:O	1:A:319:ALA:N	2.09	0.85
1:B:344:GLN:NE2	1:B:352:LEU:CD1	2.30	0.85
1:C:214:HIS:CE1	1:C:217:TRP:H	1.94	0.85
2:E:3:THR:OG1	2:E:5:PRO:HD2	1.76	0.85
3:I:38:ARG:HB2	3:I:90:TYR:CD1	2.08	0.85
1:C:202:TYR:CZ	1:C:215:LYS:HD3	2.10	0.85
3:G:28:THR:HG21	3:G:30:THR:OG1	1.72	0.85
1:A:183:PHE:CD1	1:A:301:LYS:HD3	2.12	0.85
1:A:249:HIS:CE1	2:F:16:SER:HB2	2.10	0.85
3:I:38:ARG:CD	3:I:90:TYR:HE1	1.89	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:TYR:HB3	1:A:223:LEU:CD2	2.06	0.85
1:C:252:ARG:HG3	1:C:253:GLN:N	1.91	0.85
1:A:312:PHE:CD2	1:A:396:ILE:N	2.45	0.84
1:B:21:VAL:HG13	1:B:22:ASP:N	1.92	0.84
1:B:434:VAL:HG12	1:B:435:GLY:H	1.41	0.84
1:C:411:PHE:O	1:C:414:THR:OG1	1.94	0.84
1:C:424:LEU:CB	1:C:428:ALA:HB2	2.07	0.84
3:I:9:ALA:H	3:I:107:THR:CG2	1.86	0.84
3:I:50:TRP:CD1	3:I:59:TYR:CD1	2.64	0.84
2:D:62:ILE:O	2:D:66:MET:HG2	1.77	0.84
1:A:50:VAL:HG11	1:A:53:MET:SD	2.17	0.84
1:C:203:TYR:CD1	1:C:277:MET:CE	2.60	0.84
1:A:73:ARG:HH22	4:H:26(A):SER:HA	1.40	0.84
1:A:159:GLU:HG2	1:A:160:THR:H	1.40	0.84
1:C:3:CYS:SG	1:C:42:ASP:HB2	2.17	0.84
4:M:33:SER:HA	4:M:47:LEU:HD22	1.58	0.84
1:C:286:SER:O	2:F:14:THR:HG21	1.76	0.84
1:C:350:GLN:CD	1:B:175:ARG:NE	2.30	0.84
2:D:35:TRP:CG	2:D:72:PRO:HB3	2.13	0.84
1:C:286:SER:HB2	2:F:14:THR:HG21	1.59	0.84
4:H:33:SER:OG	4:H:88:SER:OG	1.94	0.84
1:C:186:LEU:HD21	1:C:293:LEU:HD22	1.57	0.84
3:G:30:THR:C	3:G:32:TYR:H	1.82	0.84
1:C:27:HIS:HE1	3:G:100:TYR:CD1	1.96	0.83
1:C:212:LEU:HD11	1:C:284:LEU:HD21	1.60	0.83
1:C:320:GLU:HG2	1:C:400:TRP:HZ2	1.37	0.83
3:K:32:TYR:CE1	3:K:52(A):ALA:HB1	2.13	0.83
2:F:51:TRP:HA	2:F:60:LYS:HD2	1.60	0.83
3:I:18:VAL:H	3:I:82(C):LEU:HD21	1.37	0.83
4:H:34:TRP:HD1	4:H:47:LEU:HD11	1.42	0.83
3:K:6:GLU:H	3:K:105:GLN:HE22	1.24	0.83
4:M:53:ARG:HD3	4:M:57:VAL:O	1.79	0.83
1:A:311:ALA:CB	1:A:333:ALA:H	1.90	0.83
1:A:311:ALA:CB	1:A:332:TYR:HB3	2.08	0.83
4:M:11:SER:OG	4:M:104:THR:HG22	1.78	0.83
1:A:367:GLU:CG	1:A:368:SER:N	2.38	0.83
1:C:244:GLU:OE2	1:C:246:LYS:NZ	2.11	0.83
4:L:22:CYS:HB3	4:L:70:ALA:HB3	1.58	0.83
1:C:90:TYR:CD1	1:C:118:LYS:HB2	2.13	0.83
1:A:312:PHE:CD2	1:A:396:ILE:HG13	2.13	0.83
1:B:418:ALA:HB1	1:B:497:PHE:HZ	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:34:MET:SD	3:G:92:CYS:HB2	2.19	0.82
3:K:32:TYR:CE1	3:K:52(A):ALA:CB	2.62	0.82
1:A:203:TYR:OH	1:A:277:MET:HG3	1.79	0.82
1:B:171:PRO:HB3	1:B:192:PRO:HG2	1.59	0.82
1:C:402:ARG:HH22	1:C:409:LYS:HZ2	1.25	0.82
1:C:42:ASP:OD1	1:C:142:SER:HB2	1.76	0.82
1:A:311:ALA:HB2	1:A:332:TYR:C	1.95	0.82
1:A:320:GLU:HG3	1:A:400:TRP:HZ2	1.42	0.82
3:G:32:TYR:OH	3:G:34:MET:CB	2.28	0.82
3:I:67:VAL:HG13	3:I:82:LEU:CD1	2.09	0.82
3:K:52:ASN:HD22	3:K:56:ASN:ND2	1.77	0.82
1:B:99:ARG:NH2	4:L:29:PHE:CE1	2.48	0.82
4:M:4:LEU:HB2	4:M:98:GLY:N	1.94	0.82
1:A:160:THR:HG21	5:A:601:NAG:C1	2.09	0.82
1:C:101:TRP:CD1	1:C:108:PHE:HZ	1.83	0.82
3:G:52:ASN:HD22	3:G:56:ASN:ND2	1.78	0.82
3:G:31:SER:C	3:G:97:VAL:HG12	1.99	0.82
3:I:29:PHE:O	3:I:32:TYR:N	2.13	0.82
1:A:81:TYR:CE2	1:B:229:ALA:CB	2.62	0.82
2:D:33:GLU:O	2:D:36:ILE:CG1	2.26	0.82
3:G:32:TYR:CD2	3:G:33:ALA:N	2.47	0.82
1:A:326:VAL:HG11	1:A:400:TRP:CZ2	2.15	0.82
1:A:417:GLY:HA2	1:A:420:ARG:HE	1.41	0.82
1:B:103:ASN:HD22	1:B:103:ASN:H	1.27	0.82
1:C:286:SER:HB2	2:F:14:THR:CG2	2.09	0.82
3:G:22:CYS:SG	3:G:34:MET:CE	2.68	0.82
1:B:462:TRP:CE2	2:E:25:TYR:CD2	2.68	0.82
1:C:147:GLN:NE2	1:C:163:ASN:HB2	1.95	0.82
1:C:206:MET:CE	1:C:262:GLU:HG2	2.09	0.82
1:C:320:GLU:CB	1:C:400:TRP:HH2	1.64	0.82
4:H:36:GLN:CG	4:H:83:ALA:CB	2.58	0.82
3:I:33:ALA:O	3:I:52:ASN:O	1.97	0.82
3:G:50:TRP:HZ3	3:G:52:ASN:O	1.63	0.82
1:B:68:MET:HE2	1:B:255:VAL:HG13	1.60	0.81
1:C:423:VAL:HG13	1:C:424:LEU:N	1.94	0.81
4:H:4:LEU:HB2	4:H:98:GLY:HA2	1.62	0.81
2:E:20:LEU:HD12	2:E:23:ARG:O	1.80	0.81
3:I:69:ILE:HG22	3:I:80:MET:N	1.96	0.81
1:C:312:PHE:CZ	1:C:341:VAL:CG2	2.63	0.81
3:I:50:TRP:CG	3:I:69:ILE:HG12	2.15	0.81
1:C:478:ASN:C	1:C:478:ASN:HD22	1.83	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:51:TRP:HA	2:D:60:LYS:HD2	1.60	0.81
3:I:39:GLN:O	3:I:88:ALA:HB1	1.79	0.81
3:K:50:TRP:HZ3	3:K:52:ASN:O	1.63	0.81
1:A:312:PHE:CD1	1:A:396:ILE:HG13	2.16	0.81
1:A:68:MET:HA	1:A:116:CYS:O	1.81	0.81
1:C:139:ILE:HD12	1:C:169:ILE:HD12	1.60	0.81
1:B:102:GLY:O	3:K:100(H):LEU:HG	1.79	0.81
1:B:41:VAL:HG12	1:B:143:VAL:HG12	1.62	0.81
4:H:80:GLU:O	4:H:81:ASP:OD1	1.99	0.81
1:A:350:GLN:HG3	1:A:351:THR:H	1.40	0.81
2:E:53:LEU:CD1	2:E:63:TYR:CE2	2.64	0.81
3:I:67:VAL:CG1	3:I:82:LEU:CD1	2.58	0.81
3:I:69:ILE:HG22	3:I:80:MET:HA	0.82	0.81
1:B:252:ARG:CZ	3:K:100(B):ASP:OD2	2.29	0.81
2:E:18:THR:CG2	2:E:21:GLU:HB2	2.10	0.81
1:A:148:HIS:HE1	1:A:373:LYS:HB2	0.81	0.81
1:C:20:TRP:CZ2	1:C:292:ARG:NH1	2.49	0.81
2:D:74:TYR:HE1	2:F:32:VAL:HG23	1.46	0.81
3:I:11:VAL:CG1	3:I:110:THR:CB	2.15	0.81
1:A:389:ILE:CD1	1:A:391:VAL:HG12	2.10	0.80
1:C:101:TRP:HD1	1:C:108:PHE:CE1	1.97	0.80
1:B:20:TRP:HD1	1:B:434:VAL:HA	1.46	0.80
1:B:463:PHE:CD2	2:E:28:HIS:HB3	2.16	0.80
3:G:22:CYS:SG	3:G:34:MET:HE1	2.21	0.80
1:C:65:ILE:CD1	1:C:243:VAL:HG22	2.04	0.80
1:C:351:THR:HG21	1:C:395:LYS:HE3	1.63	0.80
1:B:344:GLN:HG3	1:B:352:LEU:CD1	2.12	0.80
1:C:202:TYR:CE2	1:C:215:LYS:CG	2.65	0.80
1:C:176:ALA:HB3	1:C:188:LEU:HG	1.63	0.80
1:C:56:VAL:CG1	1:C:129:SER:HB2	2.12	0.80
1:C:99:ARG:HD3	1:C:103:ASN:CG	2.00	0.80
1:B:21:VAL:HG13	1:B:22:ASP:H	1.43	0.80
1:C:350:GLN:HG2	1:B:175:ARG:HD2	1.64	0.80
2:D:19:TRP:CD1	2:D:20:LEU:HG	2.16	0.80
2:F:19:TRP:CD1	2:F:20:LEU:HG	2.16	0.80
3:I:16:ALA:HB3	3:I:82(C):LEU:CD1	2.11	0.80
1:A:214:HIS:CE1	2:D:10:ARG:CB	2.65	0.80
1:A:93:LYS:HB3	1:A:245:PHE:CD2	2.16	0.80
1:A:311:ALA:HB3	1:A:332:TYR:HB3	1.64	0.80
2:E:53:LEU:O	2:E:53:LEU:HD12	1.81	0.80
1:A:311:ALA:HB1	1:A:332:TYR:C	2.00	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:PHE:CE2	1:A:396:ILE:O	2.35	0.80
1:A:46:VAL:HG11	3:I:99:ASP:OD2	1.82	0.80
2:E:27:LYS:HE3	2:E:31:ARG:NH1	1.95	0.80
3:I:84:SER:CA	3:I:111:VAL:CG1	2.60	0.80
3:I:29:PHE:O	3:I:30:THR:C	2.20	0.80
3:I:69:ILE:CG2	3:I:80:MET:HB2	2.12	0.80
3:I:32:TYR:O	3:I:96:LYS:HA	1.82	0.80
3:K:100(F):PRO:HG2	4:L:31:TYR:HE1	1.47	0.80
4:M:34:TRP:H	4:M:47:LEU:HB3	1.45	0.80
1:A:312:PHE:CG	1:A:396:ILE:CG1	2.63	0.79
1:A:350:GLN:CG	1:A:351:THR:N	2.45	0.79
1:A:72:SER:HB3	1:A:113:LEU:HD13	1.63	0.79
1:C:143:VAL:HG21	1:C:183:PHE:HZ	1.46	0.79
4:M:49:ASP:OD1	4:M:50:VAL:CG2	2.30	0.79
1:C:454:LYS:O	1:C:458:GLY:HA3	1.80	0.79
2:E:29:LEU:O	2:E:32:VAL:HG12	1.81	0.79
3:G:29:PHE:CD1	3:G:32:TYR:HD1	1.97	0.79
1:C:312:PHE:CG	1:C:389:ILE:HG12	2.18	0.79
1:A:153:VAL:HB	3:I:100(I):TRP:CZ3	2.18	0.79
3:I:66:ARG:HD3	3:I:82:LEU:CD1	2.06	0.79
3:I:16:ALA:O	3:I:82(C):LEU:CD2	2.29	0.79
1:B:344:GLN:CG	1:B:352:LEU:CD1	2.60	0.79
3:I:9:ALA:C	3:I:108:LEU:O	2.21	0.79
4:L:11:SER:HA	4:L:104:THR:O	1.82	0.79
1:C:143:VAL:CG1	1:C:163:ASN:CB	2.57	0.79
2:D:32:VAL:CG2	2:F:74:TYR:CZ	2.64	0.79
2:E:9:THR:O	2:E:10:ARG:CG	2.31	0.79
3:G:52:ASN:ND2	3:G:56:ASN:HB2	1.97	0.79
4:H:34:TRP:CD1	4:H:47:LEU:HD11	2.15	0.79
3:I:40:ALA:HA	3:I:88:ALA:HA	1.65	0.79
4:M:51:THR:HG22	4:M:63:GLY:H	1.47	0.79
1:A:169:ILE:HD12	1:A:190:CYS:HB2	1.63	0.79
4:H:33:SER:HB2	4:H:35:PHE:CE2	2.16	0.79
1:A:27:HIS:NE2	3:I:100:TYR:CE1	2.44	0.79
3:I:32:TYR:O	3:I:33:ALA:CB	2.30	0.79
4:M:4:LEU:HB2	4:M:98:GLY:CA	2.02	0.79
2:D:34:ASN:HD21	2:F:4:LEU:HD21	1.46	0.79
4:M:34:TRP:CZ3	4:M:87:CYS:SG	2.75	0.79
1:A:345:MET:C	1:A:354:PRO:HB3	2.02	0.79
1:C:27:HIS:HB2	1:C:285:SER:O	1.83	0.79
2:E:20:LEU:CD1	2:E:23:ARG:O	2.31	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:32:TYR:CE1	3:G:33:ALA:O	2.35	0.79
3:I:36:TRP:HD1	3:I:50:TRP:CE3	1.99	0.79
4:H:50:VAL:HG12	4:H:51:THR:H	1.47	0.79
4:M:4:LEU:HD13	4:M:22:CYS:SG	2.20	0.79
1:C:196:LEU:CD2	1:C:287:GLY:HA2	2.13	0.78
2:E:4:LEU:H	2:E:5:PRO:HD3	1.47	0.78
4:H:22:CYS:HB3	4:H:70:ALA:HB3	1.64	0.78
3:K:52:ASN:ND2	3:K:56:ASN:HB2	1.97	0.78
1:A:167:VAL:HG13	1:A:176:ALA:HB1	1.63	0.78
1:A:311:ALA:HB3	1:A:332:TYR:CG	2.17	0.78
1:C:99:ARG:HH12	1:C:103:ASN:HB2	1.47	0.78
3:I:84:SER:N	3:I:111:VAL:CG1	2.43	0.78
1:A:246:LYS:HE3	2:F:17:GLN:HB3	1.66	0.78
1:A:252:ARG:HE	3:G:100(D):TRP:HE1	0.80	0.78
1:C:273:LEU:HD23	1:C:286:SER:OG	1.82	0.78
4:L:4:LEU:HD22	4:L:23:THR:O	1.84	0.78
4:M:47:LEU:O	4:M:48:TYR:CD2	2.37	0.78
3:I:50:TRP:HD1	3:I:59:TYR:HE1	0.82	0.78
4:M:11:SER:CA	4:M:104:THR:HG22	2.13	0.78
1:A:350:GLN:CG	1:A:351:THR:H	1.96	0.78
1:C:26:GLU:HA	1:C:45:LEU:HD12	1.63	0.78
1:C:349:MET:SD	1:C:352:LEU:HD13	2.22	0.78
1:C:400:TRP:O	1:C:400:TRP:CG	2.36	0.78
3:G:100(H):LEU:HD23	4:H:49:ASP:CG	2.03	0.78
1:A:67:ASP:O	1:A:68:MET:CG	2.31	0.78
1:C:161:ASP:CG	1:C:162:GLU:H	1.87	0.78
3:I:16:ALA:C	3:I:82(C):LEU:HG	2.04	0.78
1:A:311:ALA:HB3	1:A:332:TYR:CD1	2.19	0.78
1:A:476:GLY:HA3	1:A:489:LEU:HB2	1.65	0.78
1:A:108:PHE:HZ	1:C:4:ILE:HD13	0.61	0.78
1:A:310:ALA:O	1:A:333:ALA:O	2.00	0.78
1:C:203:TYR:CD1	1:C:277:MET:HE3	2.18	0.78
1:B:251:LYS:O	1:B:252:ARG:HG2	1.83	0.78
1:A:312:PHE:HZ	1:A:389:ILE:H	1.32	0.77
1:B:202:TYR:CZ	1:B:215:LYS:HG3	2.19	0.77
1:B:429:TRP:O	1:B:430:ASP:OD1	2.02	0.77
1:C:15:MET:HE2	1:C:19:THR:HA	1.66	0.77
1:C:419:LYS:HA	1:C:422:ALA:HB3	1.66	0.77
4:M:11:SER:HB3	4:M:104:THR:HG23	1.64	0.77
1:A:88:THR:HG21	1:B:86:SER:O	1.84	0.77
3:I:1:GLU:OE2	3:I:102:TYR:OH	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:34:MET:O	3:I:35:HIS:CD2	2.37	0.77
3:I:38:ARG:HB3	3:I:90:TYR:CE1	2.14	0.77
4:L:10:VAL:O	4:L:104:THR:N	2.16	0.77
1:A:155:ASP:HA	1:A:164:ARG:NH2	1.99	0.77
1:A:156:THR:HG21	1:A:164:ARG:CB	2.13	0.77
1:B:352:LEU:O	1:B:353:THR:HG23	1.85	0.77
1:B:457:PHE:CZ	1:B:491:LEU:HD21	2.20	0.77
1:B:148:HIS:NE2	1:B:373:LYS:CG	2.43	0.77
1:C:312:PHE:CE2	1:C:391:VAL:HG23	2.20	0.77
3:I:50:TRP:CZ2	3:I:67:VAL:HG23	2.19	0.77
1:B:252:ARG:NH2	3:K:100(B):ASP:OD2	2.17	0.77
4:M:53:ARG:CD	4:M:57:VAL:HA	2.14	0.77
1:A:156:THR:HG21	1:A:164:ARG:CA	2.15	0.77
1:B:21:VAL:HG22	1:B:22:ASP:N	2.00	0.77
2:E:7:HIS:NE2	2:E:24:GLU:OE2	2.17	0.77
3:G:32:TYR:CE2	3:G:33:ALA:O	2.37	0.77
4:M:48:TYR:CZ	4:M:52:SER:HB3	2.19	0.77
1:A:249:HIS:ND1	2:F:16:SER:HB2	2.00	0.77
1:A:50:VAL:HG11	1:A:53:MET:CE	2.14	0.77
4:L:36:GLN:CG	4:L:83:ALA:HB1	2.14	0.77
1:A:328:VAL:O	1:A:376:LEU:N	2.18	0.77
3:I:50:TRP:HZ2	3:I:67:VAL:HG23	1.49	0.77
3:I:18:VAL:HG12	3:I:82(C):LEU:CD2	2.14	0.77
1:B:252:ARG:HB2	3:K:100(D):TRP:NE1	2.00	0.76
1:C:203:TYR:OH	1:C:284:LEU:HD13	1.84	0.76
3:I:44:ARG:O	3:I:45:LEU:C	2.24	0.76
3:I:69:ILE:CA	3:I:79:TYR:O	2.33	0.76
3:K:33:ALA:O	3:K:34:MET:CB	2.32	0.76
4:L:53:ARG:NH2	4:L:61:PHE:O	2.18	0.76
1:A:159:GLU:CG	1:A:160:THR:N	2.42	0.76
1:A:326:VAL:HG12	1:A:400:TRP:CZ2	2.21	0.76
1:B:211:TRP:CB	1:B:274:GLU:HA	2.15	0.76
2:F:18:THR:CG2	2:F:19:TRP:H	1.96	0.76
4:H:88:SER:HB3	4:H:97:PHE:HD1	1.04	0.76
4:M:6:GLN:HB3	4:M:87:CYS:SG	2.25	0.76
1:B:23:VAL:HA	1:B:431:PHE:O	1.84	0.76
4:L:30:ASN:HA	4:L:65:LYS:NZ	2.01	0.76
1:A:201:LEU:HD23	1:A:212:LEU:HD23	1.67	0.76
2:D:26:THR:O	2:D:29:LEU:N	2.19	0.76
2:D:27:LYS:HB3	2:F:2:VAL:CG1	2.11	0.76
4:M:4:LEU:HB3	4:M:98:GLY:HA2	0.77	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:VAL:HG22	1:B:22:ASP:H	1.49	0.76
1:C:148:HIS:CD2	4:H:48:TYR:OH	2.37	0.76
3:I:9:ALA:CB	3:I:107:THR:CG2	2.63	0.76
1:A:332:TYR:HE1	1:A:389:ILE:HD13	1.51	0.76
1:B:252:ARG:HB2	3:K:100(D):TRP:CE2	2.21	0.76
1:B:47:THR:HG21	1:B:283:ARG:HD2	1.68	0.76
4:M:53:ARG:CD	4:M:57:VAL:HG12	2.13	0.76
1:A:226:HIS:O	1:A:227:ALA:HB3	1.85	0.75
1:C:3:CYS:HB2	1:C:42:ASP:OD2	1.86	0.75
2:F:74:TYR:O	2:F:75:SER:CB	2.33	0.75
1:C:307:LEU:C	1:C:340:LYS:O	2.24	0.75
2:D:73:ALA:CB	2:F:74:TYR:HB2	2.17	0.75
3:I:24:ALA:HB3	3:I:76:SER:HG	1.47	0.75
3:I:12:LYS:HG2	3:I:82(C):LEU:HD13	1.66	0.75
3:K:27:TYR:CE1	3:K:32:TYR:HB3	2.20	0.75
3:K:5:VAL:HA	3:K:105:GLN:OE1	1.86	0.75
3:I:39:GLN:HE22	4:M:37:GLN:NE2	1.84	0.75
1:B:372:SER:O	1:B:373:LYS:HB2	1.85	0.75
3:G:100(G):THR:OG1	3:G:100(I):TRP:O	2.05	0.75
4:M:80:GLU:N	4:M:80:GLU:OE1	2.13	0.75
4:L:15:GLY:C	4:L:76:GLY:HA2	2.05	0.75
1:B:98:ASP:HB3	1:B:250:ALA:CB	2.17	0.75
1:C:196:LEU:O	1:C:197:ASP:OD2	2.03	0.75
4:H:47:LEU:O	4:H:52:SER:O	2.03	0.75
1:A:15:MET:SD	1:A:295:MET:HG3	2.27	0.75
1:A:156:THR:HB	1:A:161:ASP:OD2	1.87	0.75
1:A:252:ARG:HD2	3:G:100(D):TRP:CG	2.21	0.75
2:D:4:LEU:HD21	2:F:34:ASN:ND2	2.00	0.75
3:I:36:TRP:HD1	3:I:50:TRP:HE3	1.30	0.75
1:C:56:VAL:HG11	1:C:129:SER:HB2	1.69	0.75
1:C:389:ILE:CG2	1:C:395:LYS:HB2	2.16	0.75
4:M:35:PHE:CE2	4:M:97:PHE:CZ	2.75	0.75
1:C:47:THR:HG21	1:C:283:ARG:CZ	2.16	0.75
1:C:2:ARG:HH22	1:C:44:GLU:HB2	1.52	0.75
3:I:29:PHE:CE2	3:I:76:SER:HB2	2.22	0.75
1:C:26:GLU:C	1:C:45:LEU:HB2	2.06	0.74
2:D:35:TRP:CD2	2:D:72:PRO:HB3	2.22	0.74
2:E:71:ALA:HA	2:E:74:TYR:HA	1.69	0.74
4:H:41:LYS:HG2	4:H:42:ALA:H	1.51	0.74
3:I:18:VAL:CB	3:I:82(C):LEU:CD2	2.62	0.74
1:A:367:GLU:CG	1:A:368:SER:H	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:TRP:O	1:B:21:VAL:HG12	1.85	0.74
1:B:24:VAL:HG11	1:B:424:LEU:HD21	1.69	0.74
3:I:40:ALA:HB3	3:I:43:GLN:HB2	1.69	0.74
4:M:79:ALA:O	4:M:105:VAL:HG21	1.87	0.74
4:M:88:SER:CB	4:M:97:PHE:CD1	2.64	0.74
3:I:33:ALA:HB2	3:I:96:LYS:HA	1.67	0.74
1:C:418:ALA:HB1	1:C:497:PHE:CZ	2.22	0.74
1:C:419:LYS:HA	1:C:422:ALA:CB	2.18	0.74
1:C:96:LEU:HB3	1:C:110:LYS:HB3	1.69	0.74
3:G:61:GLN:HA	3:G:64:GLN:HB2	1.70	0.74
1:A:87:ASP:O	1:A:88:THR:CG2	2.35	0.74
1:C:346:ALA:CB	1:C:351:THR:O	2.35	0.74
1:C:420:ARG:HD3	1:C:431:PHE:HD2	0.87	0.74
3:I:11:VAL:HG12	3:I:110:THR:OG1	1.85	0.74
1:A:103:ASN:O	4:H:31:TYR:CE2	2.41	0.74
1:A:249:HIS:ND1	2:F:16:SER:CB	2.50	0.74
2:D:22:SER:O	2:D:25:TYR:CD1	2.40	0.74
4:M:4:LEU:HD11	4:M:22:CYS:SG	2.28	0.74
3:G:32:TYR:CE2	3:G:33:ALA:C	2.61	0.74
4:L:48:TYR:CE2	4:L:52:SER:HB3	2.22	0.74
1:B:352:LEU:O	1:B:353:THR:CG2	2.36	0.74
4:H:60:ARG:CZ	4:H:81:ASP:OD2	2.36	0.74
4:M:105:VAL:HG22	4:M:106:LEU:HB3	1.69	0.74
1:A:257:VAL:HG12	1:A:259:GLY:H	1.52	0.74
2:E:71:ALA:HA	2:E:74:TYR:H	1.51	0.74
4:H:10:VAL:O	4:H:104:THR:HB	1.87	0.74
4:H:88:SER:CB	4:H:97:PHE:HE1	1.91	0.74
3:K:100(G):THR:OG1	3:K:100(I):TRP:O	2.05	0.74
3:I:43:GLN:HG3	3:I:44:ARG:N	2.01	0.73
1:B:99:ARG:HD2	3:K:100(E):PHE:CE1	2.23	0.73
4:M:7:PRO:O	4:M:101:THR:HA	1.88	0.73
1:B:456:LEU:HD12	1:B:457:PHE:HD1	1.49	0.73
1:C:445:ILE:O	1:C:448:ILE:HG12	1.88	0.73
2:D:74:TYR:CE2	2:F:69:LEU:CD2	2.71	0.73
1:C:148:HIS:CD2	4:H:48:TYR:HH	2.07	0.73
1:B:309:THR:HG22	1:B:391:VAL:HG11	1.70	0.73
1:A:101:TRP:CZ3	1:C:316:LYS:HD2	2.24	0.73
1:A:85:GLN:OE1	1:A:94:ARG:NH2	2.21	0.73
1:B:148:HIS:CG	1:B:373:LYS:HD2	2.23	0.73
1:C:189:ASP:O	1:C:189:ASP:OD1	2.06	0.73
3:I:84:SER:CA	3:I:111:VAL:HG11	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:100(K):PHE:HE2	4:H:97:PHE:HZ	1.35	0.73
1:A:148:HIS:HB3	1:A:151:MET:SD	2.29	0.73
2:D:74:TYR:CZ	2:F:32:VAL:HG21	2.23	0.73
3:I:12:LYS:CG	3:I:82(C):LEU:HD12	2.19	0.73
4:L:4:LEU:HD11	4:L:26(C):VAL:HG21	1.70	0.73
1:A:167:VAL:HG11	1:A:176:ALA:CB	2.17	0.73
1:B:460:MET:HE2	1:B:468:ILE:HD12	1.71	0.73
1:A:261:GLN:HA	1:C:263:GLY:HA3	1.71	0.73
1:C:321:THR:HG22	1:C:323:HIS:H	1.54	0.73
4:H:60:ARG:HG2	4:H:75:SER:O	1.88	0.73
3:I:27:TYR:HD1	3:I:94:ARG:NH1	1.86	0.73
3:I:50:TRP:CZ2	3:I:80:MET:HG3	2.23	0.73
1:A:23:VAL:HG21	1:A:31:VAL:HG11	1.69	0.73
3:G:38:ARG:NH2	3:G:86:ASP:HA	2.02	0.73
3:I:38:ARG:CB	3:I:90:TYR:HE1	1.97	0.73
3:I:100(I):TRP:HA	4:M:48:TYR:HB2	1.71	0.73
1:B:169:ILE:HG21	1:B:190:CYS:HB2	1.71	0.73
1:C:341:VAL:HG13	1:C:374:MET:HE1	1.71	0.73
1:C:271:GLY:CA	2:F:18:THR:HG21	2.19	0.73
1:B:344:GLN:CG	1:B:352:LEU:HD13	2.19	0.72
3:I:18:VAL:CG1	3:I:82(C):LEU:CD2	2.67	0.72
4:M:4:LEU:CA	4:M:98:GLY:HA2	2.18	0.72
1:C:201:LEU:HD23	1:C:212:LEU:CG	2.15	0.72
1:A:312:PHE:CZ	1:A:389:ILE:HG12	2.16	0.72
1:C:200:ASP:O	1:C:214:HIS:HA	1.88	0.72
1:C:189:ASP:OD1	1:C:292:ARG:CG	2.36	0.72
3:K:29:PHE:O	3:K:30:THR:HB	1.88	0.72
3:I:103:TRP:CE2	4:M:43:PRO:O	2.42	0.72
1:A:15:MET:SD	1:A:295:MET:HB2	2.29	0.72
1:A:20:TRP:HZ3	1:A:434:VAL:H	1.35	0.72
1:B:170:THR:HG22	1:B:172:ASN:H	1.54	0.72
1:B:212:LEU:HD11	1:B:284:LEU:HD22	1.72	0.72
1:B:443:LYS:O	1:B:447:GLN:CB	2.33	0.72
1:A:463:PHE:CZ	2:F:74:TYR:HE2	2.06	0.72
4:L:36:GLN:HG2	4:L:83:ALA:CB	2.19	0.72
1:A:168:GLU:HG2	1:A:168:GLU:O	1.89	0.72
1:C:321:THR:HG22	1:C:322:LEU:N	2.05	0.72
4:H:33:SER:CA	4:H:47:LEU:HD22	2.18	0.72
3:K:89:ILE:HG13	3:K:108:LEU:HA	1.72	0.72
3:K:100(I):TRP:HB3	4:L:48:TYR:CD1	2.24	0.72
1:A:156:THR:CG2	1:A:164:ARG:HB2	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:18:THR:OG1	2:D:21:GLU:HG2	1.90	0.72
1:A:314:PHE:CD2	1:A:396:ILE:HD13	2.24	0.72
1:C:93:LYS:HB3	1:C:245:PHE:CE1	2.24	0.72
1:B:8:ASN:OD1	2:E:15:ARG:CD	2.37	0.72
2:D:74:TYR:CE2	2:F:69:LEU:CG	2.72	0.72
4:M:49:ASP:C	4:M:50:VAL:CG2	2.57	0.72
1:A:172:ASN:HD22	1:A:172:ASN:C	1.89	0.72
3:I:24:ALA:HB1	3:I:27:TYR:HE2	1.55	0.72
3:I:29:PHE:CA	3:I:32:TYR:HB3	2.20	0.72
4:M:38:HIS:HD2	4:M:83:ALA:HB2	1.55	0.72
1:A:1:ILE:CD1	1:A:144:HIS:HD2	2.02	0.72
1:B:434:VAL:HG12	1:B:435:GLY:N	2.04	0.72
1:C:71:ASP:O	4:M:92:SER:HB2	1.89	0.72
4:L:30:ASN:HA	4:L:65:LYS:HZ2	1.52	0.72
1:A:136:GLU:HB3	1:A:170:THR:HB	1.72	0.71
1:A:151:MET:CE	1:A:373:LYS:HD2	2.21	0.71
1:B:421:MET:HA	1:B:428:ALA:HB2	1.71	0.71
1:C:252:ARG:CG	1:C:253:GLN:H	1.92	0.71
1:C:351:THR:CG2	1:C:388:VAL:HG11	2.20	0.71
3:I:36:TRP:CD1	3:I:69:ILE:HD13	2.25	0.71
1:B:460:MET:CE	1:B:468:ILE:HD12	2.21	0.71
1:C:96:LEU:HD13	1:C:110:LYS:HD2	1.71	0.71
2:D:74:TYR:HE2	2:F:69:LEU:CD2	2.03	0.71
3:I:40:ALA:HA	3:I:88:ALA:CB	2.20	0.71
3:I:12:LYS:CB	3:I:82(C):LEU:CD1	2.64	0.71
4:M:48:TYR:CZ	4:M:52:SER:CB	2.73	0.71
1:B:59:TYR:CZ	1:B:221:ILE:HD11	2.24	0.71
1:B:71:ASP:OD2	1:B:82:LEU:N	2.23	0.71
1:A:320:GLU:HG3	1:A:400:TRP:CZ2	2.24	0.71
3:I:29:PHE:CD2	3:I:76:SER:CB	2.69	0.71
1:B:472:LEU:HD13	1:B:491:LEU:HD23	1.73	0.71
1:C:48:THR:CG2	1:C:48:THR:O	2.38	0.71
3:I:29:PHE:O	3:I:30:THR:O	2.08	0.71
4:M:47:LEU:HD23	4:M:48:TYR:N	2.06	0.71
1:A:345:MET:HE2	1:A:380:PRO:HB3	1.72	0.71
1:B:48:THR:HG23	1:B:137:TYR:CD1	2.25	0.71
1:C:149:SER:HB2	4:H:48:TYR:OH	1.90	0.71
2:E:71:ALA:HA	2:E:74:TYR:N	2.06	0.71
1:B:458:GLY:O	1:B:460:MET:HG2	1.91	0.71
3:I:86:ASP:O	3:I:88:ALA:N	2.24	0.71
4:M:25:THR:OG1	4:M:26(B):ASP:OD1	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:PHE:CD2	1:C:391:VAL:HG23	2.25	0.71
3:G:96:LYS:HB3	3:G:96:LYS:NZ	2.05	0.71
1:A:151:MET:CG	4:M:48:TYR:OH	2.39	0.70
2:D:34:ASN:HD21	2:F:4:LEU:CD2	2.04	0.70
1:B:222:PRO:HD2	2:E:3:THR:HB	1.73	0.70
1:C:312:PHE:CE1	1:C:341:VAL:HG21	2.26	0.70
1:C:453:PHE:CE2	1:C:495:LEU:HD21	2.26	0.70
4:L:11:SER:HB2	4:L:106:LEU:C	2.11	0.70
4:H:36:GLN:CG	4:H:83:ALA:HB3	2.13	0.70
3:I:30:THR:OG1	3:I:31:SER:N	2.21	0.70
4:M:4:LEU:HD12	4:M:22:CYS:SG	2.28	0.70
3:K:6:GLU:H	3:K:105:GLN:NE2	1.90	0.70
4:H:10:VAL:O	4:H:104:THR:CB	2.39	0.70
1:A:196:LEU:HD13	1:A:288:HIS:CE1	2.27	0.70
1:A:97:VAL:O	1:A:98:ASP:CG	2.29	0.70
1:C:325:THR:HG21	1:C:377:GLU:HG3	1.73	0.70
3:K:44:ARG:NH1	4:L:3:ALA:HB2	2.05	0.70
1:A:365:ILE:HG22	1:A:366:THR:N	2.05	0.70
1:C:90:TYR:HE1	1:C:118:LYS:HB2	1.53	0.70
1:B:8:ASN:OD1	2:E:15:ARG:HD2	1.91	0.70
2:E:3:THR:HA	2:E:5:PRO:HD3	1.73	0.70
4:H:10:VAL:O	4:H:104:THR:N	2.23	0.70
3:I:38:ARG:CD	3:I:90:TYR:CE1	2.74	0.70
4:M:6:GLN:OE1	4:M:85:TYR:O	2.10	0.70
4:M:88:SER:OG	4:M:97:PHE:CE1	2.44	0.70
1:B:333:ALA:CB	1:B:370:GLU:HG3	2.22	0.70
1:B:102:GLY:C	3:K:100(H):LEU:HD21	2.12	0.70
1:B:273:LEU:HD23	2:E:12:LEU:HD13	1.74	0.70
1:A:1:ILE:CB	1:A:144:HIS:CD2	2.75	0.70
2:D:27:LYS:HA	2:D:30:ILE:HG22	1.74	0.70
3:K:100(J):TYR:OH	4:L:31:TYR:HB3	1.92	0.70
1:C:410:ALA:O	1:C:413:ALA:HB3	1.92	0.69
1:C:71:ASP:OD2	1:C:114:VAL:N	2.24	0.69
4:M:6:GLN:OE1	4:M:100:GLY:HA2	1.92	0.69
1:A:74:CYS:SG	4:H:28:GLY:O	2.50	0.69
1:C:448:ILE:HG13	1:C:449:PHE:N	2.05	0.69
3:I:9:ALA:O	3:I:10:GLU:O	2.09	0.69
1:A:51:SER:OG	1:A:134:ASN:HB3	1.91	0.69
1:A:37:ASP:HB3	1:A:300:LEU:HD11	1.74	0.69
4:L:77:LEU:HD23	4:L:77:LEU:N	2.07	0.69
1:A:320:GLU:CG	1:A:400:TRP:HZ2	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:THR:HG23	1:B:137:TYR:CE1	2.28	0.69
1:C:290:LYS:HE3	1:C:430:ASP:CB	2.23	0.69
3:I:84:SER:CA	3:I:111:VAL:HB	2.14	0.69
1:A:151:MET:HA	4:M:48:TYR:OH	1.91	0.69
1:C:147:GLN:O	1:C:148:HIS:ND1	2.25	0.69
1:C:320:GLU:HB2	1:C:400:TRP:HH2	0.90	0.69
1:C:430:ASP:O	1:C:432:GLY:N	2.24	0.69
1:A:156:THR:CG2	1:A:164:ARG:C	2.50	0.69
3:I:34:MET:O	3:I:35:HIS:CG	2.46	0.69
1:B:217:TRP:HE1	2:E:5:PRO:CB	1.98	0.69
1:C:206:MET:HE1	1:C:262:GLU:HG2	1.75	0.69
1:C:3:CYS:SG	1:C:30:CYS:CB	2.80	0.69
1:A:208:ASN:O	1:A:210:HIS:CD2	2.46	0.69
1:C:310:ALA:O	1:C:391:VAL:HG21	1.93	0.69
3:I:18:VAL:HG21	3:I:109:VAL:HG21	1.75	0.69
4:L:83:ALA:O	4:L:85:TYR:CD2	2.45	0.69
1:C:129:SER:CB	1:C:202:TYR:CD1	2.76	0.69
4:L:44:LYS:HG2	4:L:46:MET:HE3	1.75	0.69
1:B:457:PHE:HZ	1:B:491:LEU:HD21	1.56	0.68
1:B:88:THR:HG23	1:B:89:GLN:HG3	1.75	0.68
1:C:419:LYS:O	1:C:423:VAL:HG12	1.93	0.68
4:L:45:LEU:HD23	4:L:45:LEU:O	1.93	0.68
1:B:341:VAL:HG21	1:B:374:MET:SD	2.33	0.68
1:C:245:PHE:HB3	1:C:255:VAL:HA	1.74	0.68
1:C:244:GLU:HG2	2:D:20:LEU:CD2	2.23	0.68
1:A:156:THR:CG2	1:A:164:ARG:CB	2.71	0.68
3:G:31:SER:O	3:G:97:VAL:HG12	1.92	0.68
3:I:96:LYS:NZ	3:I:101:ASP:OD2	2.26	0.68
2:F:35:TRP:CG	2:F:72:PRO:HB3	2.28	0.68
4:M:34:TRP:CH2	4:M:87:CYS:SG	2.86	0.68
1:C:325:THR:CG2	1:C:377:GLU:HG3	2.23	0.68
1:C:11:PHE:HD2	1:C:32:THR:HG1	0.99	0.68
1:C:41:VAL:HG12	1:C:143:VAL:HB	1.76	0.68
3:I:9:ALA:HB2	3:I:107:THR:CG2	2.24	0.68
1:C:42:ASP:N	1:C:42:ASP:OD1	2.25	0.68
4:M:5:THR:O	4:M:6:GLN:O	2.12	0.68
4:M:7:PRO:HD3	4:M:21:SER:O	1.94	0.68
1:A:41:VAL:HG22	1:A:143:VAL:HG22	1.73	0.68
1:B:347:VAL:HG23	1:B:355:VAL:HG11	1.76	0.68
1:C:246:LYS:O	1:C:254:THR:OG1	2.12	0.68
3:I:36:TRP:CD1	3:I:50:TRP:CZ3	2.82	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:VAL:HG13	1:A:53:MET:SD	2.31	0.68
3:I:38:ARG:NH1	3:I:63:PHE:HZ	1.91	0.68
4:L:50:VAL:HG23	4:L:51:THR:H	0.57	0.68
1:A:1:ILE:N	1:A:144:HIS:CD2	2.59	0.68
1:B:61:TYR:CD1	1:B:262:GLU:HB2	2.29	0.68
1:B:398:HIS:ND1	1:B:399:HIS:O	2.27	0.68
1:B:441:LEU:O	1:B:445:ILE:HG12	1.93	0.68
1:C:90:TYR:CE1	1:C:118:LYS:CB	2.74	0.68
2:D:35:TRP:NE1	2:D:72:PRO:HA	2.09	0.68
1:B:99:ARG:NH2	4:L:29:PHE:HE1	1.92	0.68
1:A:26:GLU:HG3	2:D:15:ARG:HG3	1.75	0.68
1:A:148:HIS:ND1	1:A:373:LYS:CG	2.56	0.67
1:C:203:TYR:HD1	1:C:277:MET:HE3	1.58	0.67
1:C:444:GLY:O	1:C:448:ILE:HG23	1.93	0.67
1:C:465:GLN:HA	1:C:468:ILE:HG22	1.75	0.67
4:H:11:SER:HB2	4:H:104:THR:HB	1.77	0.67
4:M:53:ARG:CD	4:M:57:VAL:O	2.41	0.67
1:C:189:ASP:OD1	1:C:292:ARG:HG2	1.94	0.67
2:E:9:THR:C	2:E:10:ARG:HG3	2.13	0.67
4:L:47:LEU:O	4:L:52:SER:O	2.11	0.67
1:A:200:ASP:OD1	1:A:215:LYS:NZ	2.25	0.67
1:A:463:PHE:HE2	2:F:74:TYR:CE2	2.02	0.67
1:B:95:THR:O	1:B:97:VAL:HG13	1.94	0.67
1:A:312:PHE:CE1	1:A:389:ILE:CG1	2.68	0.67
1:C:47:THR:CG2	1:C:283:ARG:CZ	2.72	0.67
2:D:32:VAL:O	2:D:36:ILE:HG23	1.95	0.67
1:A:332:TYR:CE1	1:A:389:ILE:HD13	2.29	0.67
1:B:463:PHE:HE2	2:E:28:HIS:C	1.98	0.67
1:C:439:ASN:O	1:C:442:GLY:N	2.28	0.67
1:A:214:HIS:HE1	2:D:11:LYS:O	1.77	0.67
1:C:26:GLU:CA	1:C:45:LEU:HD12	2.21	0.67
1:C:384:ASP:HB2	1:C:399:HIS:CE1	2.29	0.67
1:A:71:ASP:C	1:A:113:LEU:CD1	2.62	0.67
1:C:91:VAL:HG11	1:C:243:VAL:HG11	1.75	0.67
1:C:8:ASN:HD21	2:F:15:ARG:HD2	1.60	0.67
1:A:312:PHE:CD2	1:A:389:ILE:CG1	2.78	0.67
1:B:344:GLN:HG3	1:B:352:LEU:HD13	1.77	0.67
1:B:146:SER:HA	1:B:374:MET:HA	1.77	0.67
1:C:331:GLN:CG	1:C:371:ASN:CB	2.52	0.67
1:C:462:TRP:HZ3	1:C:499:SER:O	1.77	0.67
1:C:214:HIS:HD2	2:F:7:HIS:HE1	0.80	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:66:ARG:HG2	3:I:82:LEU:HD12	1.74	0.67
3:K:52:ASN:HD22	3:K:56:ASN:CG	1.97	0.67
1:B:196:LEU:HB3	1:B:198:PHE:CE2	2.29	0.67
1:C:412:GLU:O	1:C:415:VAL:HG12	1.94	0.67
3:G:100(J):TYR:OH	4:H:31:TYR:HB3	1.95	0.67
3:I:2:VAL:HG22	3:I:27:TYR:HB3	1.76	0.67
1:A:246:LYS:O	1:A:254:THR:OG1	2.11	0.67
3:I:10:GLU:O	3:I:110:THR:N	2.28	0.67
4:M:11:SER:HA	4:M:104:THR:HG22	1.76	0.67
1:A:317:ILE:H	1:A:317:ILE:HD12	1.60	0.66
1:A:386:TYR:CE1	1:A:399:HIS:HB2	2.30	0.66
1:C:57:ARG:CD	1:C:225:TRP:HE3	2.08	0.66
4:L:11:SER:HB3	4:L:104:THR:HB	1.77	0.66
4:L:36:GLN:HG2	4:L:83:ALA:HB1	1.77	0.66
1:C:248:ALA:HB2	2:D:17:GLN:HB2	1.76	0.66
3:G:52:ASN:HD22	3:G:56:ASN:CG	1.98	0.66
3:I:43:GLN:CG	3:I:44:ARG:N	2.58	0.66
1:A:273:LEU:HD11	2:D:12:LEU:HD22	1.76	0.66
1:C:345:MET:HE2	1:C:378:LEU:HD23	1.75	0.66
2:E:26:THR:O	2:E:30:ILE:HG12	1.95	0.66
4:H:82:GLU:HB3	4:H:105:VAL:HG13	1.75	0.66
4:H:82:GLU:CA	4:H:103:LEU:HD22	2.23	0.66
3:I:40:ALA:HA	3:I:88:ALA:CA	2.25	0.66
4:M:53:ARG:CD	4:M:57:VAL:CA	2.62	0.66
1:A:190:CYS:HB3	1:A:289:LEU:HD21	1.77	0.66
1:B:481:ASN:ND2	1:B:483:SER:OG	2.28	0.66
1:C:41:VAL:HG12	1:C:143:VAL:CA	2.25	0.66
2:D:26:THR:O	2:D:27:LYS:C	2.31	0.66
2:D:29:LEU:HD21	2:D:33:GLU:OE2	1.96	0.66
1:C:464:SER:CB	2:D:75:SER:O	2.42	0.66
1:A:344:GLN:NE2	1:A:352:LEU:HG	2.10	0.66
4:H:83:ALA:O	4:H:85:TYR:CD2	2.48	0.66
3:I:9:ALA:HB3	3:I:109:VAL:HB	1.74	0.66
3:I:51:ILE:HG13	3:I:51:ILE:O	1.93	0.66
4:L:106:LEU:HD13	4:L:106:LEU:N	2.10	0.66
1:B:171:PRO:HA	1:B:192:PRO:HG3	1.76	0.66
1:C:202:TYR:HE2	1:C:215:LYS:CG	2.07	0.66
2:E:71:ALA:HA	2:E:74:TYR:CA	2.26	0.66
1:A:252:ARG:HD3	3:G:100(D):TRP:CD1	2.29	0.66
4:H:10:VAL:HG21	4:H:18:ILE:HD11	1.76	0.66
1:A:108:PHE:CD2	1:C:321:THR:OG1	2.49	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:MET:O	1:B:375:MET:CG	2.42	0.66
4:M:29:PHE:O	4:M:65:LYS:NZ	2.28	0.66
2:D:20:LEU:O	2:D:24:GLU:CB	2.44	0.65
2:D:25:TYR:HD1	2:D:26:THR:N	1.93	0.65
3:G:30:THR:C	3:G:32:TYR:N	2.43	0.65
4:H:4:LEU:HD12	4:H:87:CYS:SG	2.34	0.65
3:I:50:TRP:HB2	3:I:69:ILE:CD1	2.16	0.65
3:K:89:ILE:HD11	3:K:108:LEU:HD12	1.78	0.65
4:L:11:SER:HB2	4:L:106:LEU:O	1.96	0.65
4:M:14:PRO:HA	4:M:77:LEU:HB2	1.77	0.65
1:C:211:TRP:NE1	1:C:269:LEU:HD13	2.03	0.65
3:I:63:PHE:CE1	3:I:66:ARG:HD2	2.32	0.65
1:A:496:ILE:O	1:A:499:SER:OG	2.13	0.65
1:B:333:ALA:HA	1:B:370:GLU:CG	2.26	0.65
3:K:29:PHE:O	3:K:30:THR:CB	2.44	0.65
4:M:53:ARG:HD3	4:M:57:VAL:CB	2.26	0.65
1:A:226:HIS:O	1:A:227:ALA:CB	2.44	0.65
1:B:103:ASN:H	1:B:103:ASN:ND2	1.93	0.65
1:C:198:PHE:C	1:C:200:ASP:H	2.00	0.65
1:C:190:CYS:HA	1:C:291:CYS:HA	1.76	0.65
3:I:50:TRP:CD2	3:I:69:ILE:HG12	2.32	0.65
4:M:7:PRO:O	4:M:101:THR:CB	2.45	0.65
1:A:169:ILE:HG22	1:A:176:ALA:CB	2.18	0.65
1:C:143:VAL:HG21	1:C:183:PHE:CZ	2.28	0.65
1:A:231:THR:OG1	1:A:232:GLY:N	2.29	0.65
1:C:41:VAL:HG12	1:C:143:VAL:CB	2.27	0.65
4:L:41:LYS:HG2	4:L:42:ALA:H	1.62	0.65
1:A:156:THR:HG21	1:A:165:ALA:N	2.11	0.65
2:E:26:THR:HG23	2:E:26:THR:O	1.96	0.65
3:G:61:GLN:O	3:G:64:GLN:N	2.29	0.65
3:I:38:ARG:CZ	3:I:63:PHE:HZ	2.10	0.65
1:B:165:ALA:HB2	1:B:180:LEU:HD21	1.78	0.65
1:A:108:PHE:CE1	1:C:4:ILE:CD1	2.60	0.65
3:I:86:ASP:O	3:I:87:THR:C	2.29	0.65
3:I:97:VAL:HG22	3:I:98:ASP:N	2.12	0.65
1:B:472:LEU:CD1	1:B:491:LEU:HD23	2.26	0.65
4:L:4:LEU:CD2	4:L:23:THR:O	2.44	0.65
1:A:63:ALA:HB3	1:A:257:VAL:HG13	1.79	0.65
1:B:146:SER:O	1:B:147:GLN:C	2.32	0.65
4:M:10:VAL:CG2	4:M:18:ILE:HD11	2.27	0.65
1:A:420:ARG:HA	2:D:15:ARG:HH22	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:VAL:HB	1:C:394:LYS:O	1.98	0.64
1:C:407:ILE:HD12	1:C:407:ILE:C	2.18	0.64
1:C:441:LEU:O	1:C:445:ILE:CG1	2.41	0.64
3:I:10:GLU:HA	3:I:10:GLU:OE2	1.97	0.64
1:C:148:HIS:NE2	4:H:48:TYR:OH	2.26	0.64
1:C:380:PRO:HG2	1:C:400:TRP:CD1	2.32	0.64
3:K:51:ILE:O	3:K:51:ILE:HD12	1.98	0.64
4:L:11:SER:CA	4:L:104:THR:O	2.44	0.64
2:F:20:LEU:O	2:F:24:GLU:CB	2.44	0.64
3:G:14:PRO:CG	3:G:112:SER:O	2.46	0.64
3:I:83:ARG:C	3:I:111:VAL:CG1	2.59	0.64
1:A:156:THR:HG21	1:A:164:ARG:O	1.96	0.64
1:B:203:TYR:OH	1:B:277:MET:O	2.16	0.64
1:B:434:VAL:CG1	1:B:435:GLY:H	2.08	0.64
3:I:9:ALA:O	3:I:108:LEU:C	2.34	0.64
1:A:312:PHE:CD1	1:A:396:ILE:CG1	2.79	0.64
1:C:161:ASP:CG	1:C:162:GLU:N	2.50	0.64
1:C:312:PHE:CB	1:C:389:ILE:HG12	2.27	0.64
1:C:460:MET:HE3	1:C:464:SER:HB3	1.74	0.64
4:H:82:GLU:HG2	4:H:82:GLU:O	1.95	0.64
3:K:100(F):PRO:HG2	4:L:31:TYR:CE1	2.32	0.64
4:L:10:VAL:O	4:L:104:THR:HB	1.98	0.64
1:A:420:ARG:HA	2:D:15:ARG:NH2	2.13	0.64
1:A:311:ALA:O	1:A:312:PHE:CB	2.46	0.64
1:A:2:ARG:CG	1:A:44:GLU:OE1	2.45	0.64
4:H:44:LYS:HG2	4:H:45:LEU:N	2.13	0.64
1:A:75:PRO:HG2	1:A:107:LEU:HB3	1.79	0.64
1:A:252:ARG:CD	3:G:100(D):TRP:CE2	2.66	0.64
1:A:74:CYS:HB2	1:A:77:GLN:CD	2.09	0.64
1:B:332:TYR:HE1	1:B:335:THR:CG2	2.11	0.64
2:E:24:GLU:OE1	2:E:25:TYR:N	2.31	0.64
4:L:80:GLU:OE1	4:L:80:GLU:HA	1.96	0.64
1:A:210:HIS:ND1	1:A:277:MET:HB2	2.12	0.64
1:B:352:LEU:C	1:B:353:THR:HG22	2.18	0.64
1:B:420:ARG:NH1	1:B:431:PHE:CD2	2.66	0.64
3:K:11:VAL:HG12	3:K:110:THR:O	1.98	0.64
1:A:71:ASP:HB2	1:A:82:LEU:HD23	1.80	0.64
1:A:99:ARG:NH1	1:C:4:ILE:O	2.31	0.64
4:L:58:SER:OG	4:L:60:ARG:NH1	2.30	0.64
1:B:189:ASP:O	1:B:292:ARG:N	2.28	0.63
1:C:147:GLN:HE22	1:C:163:ASN:HB2	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:TRP:CZ2	1:C:292:ARG:HD2	2.33	0.63
4:L:4:LEU:HD21	4:L:24:GLY:HA3	1.75	0.63
4:M:17:SER:CB	4:M:75:SER:HB2	2.26	0.63
1:A:302:GLY:HA3	1:A:305:TYR:CE2	2.33	0.63
1:B:460:MET:HE3	1:B:464:SER:HB3	1.80	0.63
1:C:211:TRP:HB3	1:C:274:GLU:HA	1.80	0.63
3:I:24:ALA:HB1	3:I:27:TYR:CE2	2.32	0.63
3:K:44:ARG:CZ	4:L:3:ALA:HB2	2.28	0.63
3:K:100(K):PHE:HE2	4:L:97:PHE:HZ	1.46	0.63
1:A:65:ILE:HD12	1:A:117:ALA:HB1	1.79	0.63
1:C:273:LEU:CD2	1:C:286:SER:OG	2.46	0.63
1:C:32:THR:HG22	1:C:42:ASP:HB3	1.80	0.63
2:E:24:GLU:O	2:E:27:LYS:N	2.28	0.63
2:F:54:GLY:CA	2:F:59:GLN:HE22	2.11	0.63
1:B:311:ALA:O	1:B:332:TYR:HB2	1.99	0.63
3:G:67:VAL:HG13	3:G:82:LEU:HD13	1.80	0.63
3:K:32:TYR:CZ	3:K:52(A):ALA:HB1	2.32	0.63
4:M:82:GLU:HG3	4:M:103:LEU:O	1.99	0.63
4:M:48:TYR:HH	4:M:52:SER:HB3	1.63	0.63
4:M:78:GLN:HB3	4:M:81:ASP:HB3	1.81	0.63
1:A:167:VAL:HG11	1:A:176:ALA:HB1	1.75	0.63
1:A:345:MET:O	1:A:354:PRO:HB2	1.92	0.63
1:B:225:TRP:HE3	1:B:237:ASN:ND2	1.93	0.63
1:C:374:MET:O	1:C:376:LEU:CD1	2.46	0.63
2:D:26:THR:O	2:D:28:HIS:N	2.31	0.63
1:A:15:MET:CE	1:A:295:MET:HG3	2.28	0.63
1:A:1:ILE:HB	1:A:144:HIS:CD2	2.33	0.63
1:A:320:GLU:CB	1:A:400:TRP:HZ2	2.11	0.63
1:B:148:HIS:CD2	1:B:373:LYS:CD	2.79	0.63
1:B:352:LEU:C	1:B:353:THR:CG2	2.66	0.63
1:C:315:THR:HG21	1:C:373:LYS:CD	2.22	0.63
3:G:51:ILE:HD12	3:G:51:ILE:O	1.97	0.63
3:I:38:ARG:CD	3:I:48:MET:SD	2.77	0.63
4:M:53:ARG:CD	4:M:57:VAL:CB	2.77	0.63
1:A:148:HIS:CG	1:A:151:MET:CB	2.73	0.63
1:A:84:LYS:HB3	1:A:90:TYR:CD2	2.34	0.63
1:B:20:TRP:O	1:B:21:VAL:CG1	2.47	0.63
1:C:169:ILE:HD13	1:C:190:CYS:SG	2.39	0.63
1:C:351:THR:HG22	1:C:388:VAL:HG13	1.77	0.63
1:C:475:LEU:HD21	2:D:53:LEU:HD11	1.80	0.63
3:G:29:PHE:CD2	3:G:29:PHE:O	2.52	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:44:LYS:CG	4:H:45:LEU:N	2.61	0.63
4:L:60:ARG:HD2	4:L:75:SER:O	1.99	0.63
1:A:417:GLY:HA2	1:A:420:ARG:NE	2.12	0.63
1:B:244:GLU:HG3	1:B:258:LEU:HD12	1.80	0.63
2:F:23:ARG:O	2:F:27:LYS:HB3	1.98	0.63
1:A:99:ARG:CD	1:A:251:LYS:HD3	2.29	0.63
1:A:321:THR:CG2	1:A:325:THR:O	2.43	0.63
1:A:360:THR:OG1	1:A:377:GLU:OE1	2.16	0.63
1:B:21:VAL:CG2	1:B:22:ASP:H	2.10	0.63
1:C:310:ALA:O	1:C:391:VAL:CG2	2.47	0.63
1:C:400:TRP:CD1	1:C:400:TRP:O	2.52	0.63
1:A:241:ALA:HA	2:F:23:ARG:HH12	1.63	0.63
3:K:100(I):TRP:HB3	4:L:48:TYR:HD1	1.64	0.63
1:A:188:LEU:HD13	1:A:190:CYS:SG	2.38	0.62
1:C:320:GLU:CA	1:C:400:TRP:CH2	2.82	0.62
3:I:97:VAL:HG23	3:I:100(C):TYR:HD1	1.63	0.62
3:I:18:VAL:H	3:I:82(C):LEU:CD2	2.10	0.62
1:A:15:MET:SD	1:A:295:MET:CB	2.87	0.62
1:B:74:CYS:SG	1:B:99:ARG:NH2	2.72	0.62
1:B:344:GLN:HG3	1:B:352:LEU:HD12	1.79	0.62
1:B:98:ASP:O	1:B:99:ARG:HB2	1.98	0.62
1:C:143:VAL:HG22	1:C:143:VAL:O	1.99	0.62
2:F:74:TYR:O	2:F:75:SER:HB3	1.99	0.62
1:B:161:ASP:OD1	1:B:163:ASN:HB2	2.00	0.62
1:C:41:VAL:HG12	1:C:143:VAL:HA	1.82	0.62
1:C:349:MET:SD	1:C:352:LEU:CD1	2.87	0.62
2:D:34:ASN:ND2	2:F:4:LEU:HD21	2.14	0.62
1:A:341:VAL:CG2	1:A:365:ILE:HG13	2.29	0.62
3:G:48:MET:HG3	3:G:48:MET:O	2.00	0.62
3:I:29:PHE:O	3:I:32:TYR:HB3	1.99	0.62
1:B:460:MET:CE	1:B:464:SER:HB3	2.29	0.62
1:C:12:VAL:HG23	1:C:33:VAL:HA	1.80	0.62
1:C:189:ASP:OD1	1:C:292:ARG:HG3	1.99	0.62
1:C:427:THR:O	1:C:427:THR:HG22	2.00	0.62
1:C:58:SER:O	1:C:225:TRP:O	2.18	0.62
2:E:3:THR:C	2:E:5:PRO:HD3	2.18	0.62
3:I:27:TYR:OH	3:I:32:TYR:HB2	2.00	0.62
1:A:68:MET:HG3	1:A:68:MET:O	1.98	0.62
1:B:337:GLY:N	1:B:367:GLU:HG3	2.15	0.62
1:C:315:THR:OG1	1:C:316:LYS:N	2.33	0.62
1:C:71:ASP:HB2	1:C:113:LEU:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:13:GLN:OE1	2:F:13:GLN:N	2.32	0.62
3:G:100(F):PRO:HG2	4:H:31:TYR:HE1	1.65	0.62
1:A:1:ILE:HD12	1:A:144:HIS:HD2	1.63	0.62
1:B:288:HIS:CD2	1:B:424:LEU:HG	2.35	0.62
1:C:186:LEU:HD21	1:C:293:LEU:CD2	2.29	0.62
1:A:8:ASN:HB3	1:A:29:GLY:HA3	1.81	0.61
1:B:357:ARG:NH2	1:B:379:ASP:OD2	2.32	0.61
1:C:176:ALA:CB	1:C:188:LEU:HG	2.29	0.61
4:M:4:LEU:HB2	4:M:97:PHE:C	2.21	0.61
1:A:46:VAL:HG22	1:A:47:THR:HG23	1.82	0.61
1:B:171:PRO:CB	1:B:192:PRO:HG2	2.29	0.61
1:C:196:LEU:HD22	1:C:287:GLY:HA2	1.82	0.61
1:C:46:VAL:HG21	1:C:140:MET:HG2	1.83	0.61
1:A:1:ILE:CB	1:A:144:HIS:HD2	2.11	0.61
3:G:51:ILE:HD13	3:G:100(C):TYR:HD2	1.66	0.61
3:I:83:ARG:HD2	3:I:85:GLU:OE2	1.99	0.61
4:M:53:ARG:NE	4:M:57:VAL:O	2.33	0.61
1:B:315:THR:OG1	1:B:329:GLU:OE1	2.15	0.61
1:C:56:VAL:HG12	1:C:129:SER:HB2	1.81	0.61
1:C:1:ILE:HG13	1:C:147:GLN:OE1	2.00	0.61
1:C:214:HIS:H	1:C:214:HIS:CD2	2.17	0.61
3:K:11:VAL:CA	3:K:110:THR:O	2.45	0.61
1:B:21:VAL:CG1	1:B:22:ASP:H	2.05	0.61
2:D:57:THR:O	2:D:60:LYS:N	2.31	0.61
1:A:244:GLU:HG3	2:F:20:LEU:HD23	1.82	0.61
1:B:137:TYR:HE2	1:B:192:PRO:HA	1.65	0.61
1:B:196:LEU:HD23	1:B:198:PHE:CZ	2.35	0.61
1:C:149:SER:HB3	3:G:100(I):TRP:HZ3	1.66	0.61
1:C:401:HIS:CG	1:C:401:HIS:O	2.51	0.61
1:C:457:PHE:CD2	1:C:468:ILE:HD13	2.36	0.61
3:G:48:MET:HE2	3:G:67:VAL:HG11	1.81	0.61
3:I:39:GLN:NE2	4:M:37:GLN:HE22	1.99	0.61
1:A:154:ASN:ND2	1:A:160:THR:HG21	2.15	0.61
4:L:46:MET:O	4:L:47:LEU:HD12	2.00	0.61
4:M:6:GLN:HA	4:M:21:SER:O	2.00	0.61
1:A:345:MET:CE	1:A:380:PRO:HB3	2.30	0.61
4:H:41:LYS:HG2	4:H:42:ALA:N	2.14	0.61
3:I:66:ARG:CG	3:I:82:LEU:HD13	2.26	0.61
4:L:36:GLN:CG	4:L:83:ALA:HB2	2.26	0.61
1:A:214:HIS:NE2	2:D:10:ARG:HB3	2.15	0.61
1:B:456:LEU:HD11	1:B:457:PHE:CE1	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:MET:HG2	1:C:130:ILE:HG22	1.83	0.61
1:C:37:ASP:HB2	1:C:300:LEU:HD11	1.81	0.61
3:I:38:ARG:HB3	3:I:90:TYR:HD1	1.43	0.61
1:B:59:TYR:HA	1:B:224:PRO:O	2.01	0.60
1:B:429:TRP:O	1:B:430:ASP:CG	2.38	0.60
1:C:72:SER:O	4:M:29:PHE:HZ	1.83	0.60
4:M:80:GLU:H	4:M:80:GLU:CD	2.04	0.60
1:C:143:VAL:HG12	1:C:163:ASN:O	2.01	0.60
1:C:30:CYS:SG	1:C:44:GLU:OE1	2.59	0.60
1:A:331:GLN:O	1:A:331:GLN:HG2	2.00	0.60
1:A:160:THR:CG2	5:A:601:NAG:O7	2.50	0.60
1:B:171:PRO:HA	1:B:192:PRO:CG	2.31	0.60
1:A:273:LEU:CD1	2:D:12:LEU:HD22	2.31	0.60
4:H:88:SER:HB2	4:H:97:PHE:HE1	1.47	0.60
1:A:103:ASN:HA	4:H:31:TYR:OH	2.01	0.60
1:A:105:CYS:HB3	1:A:107:LEU:HB2	1.83	0.60
4:H:82:GLU:CB	4:H:103:LEU:HD22	2.31	0.60
4:M:57:VAL:O	4:M:58:SER:C	2.40	0.60
1:A:135:LEU:HD12	1:A:135:LEU:O	2.00	0.60
1:C:214:HIS:NE2	2:F:7:HIS:CE1	2.70	0.60
1:C:237:ASN:OD1	1:C:238:ASN:N	2.34	0.60
1:C:330:VAL:HG21	1:C:389:ILE:CD1	2.30	0.60
2:E:3:THR:C	2:E:5:PRO:CD	2.70	0.60
4:H:21:SER:HA	4:H:70:ALA:O	2.01	0.60
4:H:34:TRP:CD1	4:H:47:LEU:HD12	2.35	0.60
4:M:17:SER:HB3	4:M:75:SER:CB	2.30	0.60
4:M:7:PRO:CD	4:M:21:SER:O	2.50	0.60
1:C:252:ARG:CZ	3:I:100(D):TRP:CZ3	2.85	0.60
1:C:321:THR:HB	1:C:325:THR:HB	1.83	0.60
2:D:24:GLU:OE1	2:D:25:TYR:N	2.35	0.60
3:K:12:LYS:O	3:K:13:LYS:O	2.20	0.60
1:B:252:ARG:NH2	3:K:100(B):ASP:CG	2.55	0.60
1:B:374:MET:HG3	1:B:375:MET:N	2.12	0.60
2:D:73:ALA:HB3	2:F:74:TYR:HB2	1.84	0.60
4:M:5:THR:O	4:M:6:GLN:C	2.39	0.60
1:A:314:PHE:CE2	1:A:396:ILE:HD13	2.36	0.60
1:B:171:PRO:CA	1:B:192:PRO:HG3	2.32	0.60
1:B:95:THR:HG22	1:B:95:THR:O	2.01	0.60
1:C:71:ASP:HB3	1:C:80:ALA:CB	2.32	0.60
2:E:2:VAL:HG12	2:E:2:VAL:O	2.02	0.60
2:E:3:THR:OG1	2:E:5:PRO:CD	2.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:48:TYR:HE2	4:L:52:SER:HB3	1.67	0.60
4:M:78:GLN:HA	4:M:78:GLN:NE2	2.16	0.60
1:A:17:GLY:HA3	1:A:434:VAL:HG11	1.84	0.60
1:B:96:LEU:HD12	1:B:96:LEU:O	2.01	0.60
1:C:121:CYS:SG	1:C:122:SER:N	2.73	0.60
3:G:39:GLN:CD	4:H:37:GLN:HE22	2.04	0.60
3:I:40:ALA:CA	3:I:88:ALA:CB	2.79	0.60
1:A:188:LEU:HD13	1:A:291:CYS:SG	2.42	0.60
1:B:101:TRP:O	1:B:103:ASN:ND2	2.34	0.60
1:A:108:PHE:HD2	1:C:321:THR:OG1	1.85	0.60
2:E:3:THR:CA	2:E:5:PRO:HD3	2.32	0.60
3:I:48:MET:HB3	3:I:63:PHE:CE2	2.37	0.60
3:K:85:GLU:OE1	3:K:86:ASP:OD1	2.19	0.60
1:A:35:ALA:HB3	1:A:37:ASP:O	2.00	0.59
1:B:314:PHE:CE2	1:B:396:ILE:HG12	2.37	0.59
1:C:350:GLN:NE2	1:B:175:ARG:NE	2.46	0.59
2:D:57:THR:CG2	2:D:58:SER:N	2.43	0.59
2:F:59:GLN:O	2:F:62:ILE:N	2.34	0.59
1:B:415:VAL:HG12	1:B:419:LYS:NZ	2.18	0.59
1:C:15:MET:SD	1:C:38:LYS:NZ	2.64	0.59
1:C:389:ILE:O	1:C:389:ILE:HG13	2.02	0.59
3:I:38:ARG:HB2	3:I:90:TYR:HE1	1.59	0.59
4:M:50:VAL:O	4:M:63:GLY:HA3	2.02	0.59
4:M:7:PRO:O	4:M:101:THR:CA	2.49	0.59
1:A:311:ALA:HB1	1:A:333:ALA:N	2.09	0.59
1:A:418:ALA:HB1	1:A:497:PHE:HZ	1.67	0.59
1:B:314:PHE:HE2	1:B:396:ILE:HG12	1.67	0.59
1:C:270:ALA:HB3	2:F:8:SER:OG	2.02	0.59
3:K:51:ILE:HD13	3:K:100(C):TYR:HD2	1.65	0.59
1:A:15:MET:SD	1:A:295:MET:CG	2.90	0.59
1:B:308:CYS:HB2	1:B:335:THR:HG21	1.83	0.59
1:C:384:ASP:HB3	1:C:401:HIS:HA	1.82	0.59
4:M:49:ASP:O	4:M:51:THR:N	2.34	0.59
1:A:348:ASP:OD1	1:A:348:ASP:O	2.20	0.59
1:B:2:ARG:HH21	1:B:140:MET:HB2	1.68	0.59
1:B:47:THR:HG21	1:B:283:ARG:CD	2.32	0.59
1:C:312:PHE:HZ	1:C:341:VAL:CG2	2.15	0.59
2:E:53:LEU:HD12	2:E:53:LEU:C	2.22	0.59
1:A:311:ALA:HB2	1:A:332:TYR:HB3	1.83	0.59
1:C:328:VAL:O	1:C:375:MET:HA	2.02	0.59
3:G:96:LYS:HB3	3:G:96:LYS:HZ2	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:ARG:CZ	3:I:100(D):TRP:CE3	2.85	0.59
1:A:400:TRP:CD1	1:A:401:HIS:N	2.71	0.59
1:A:4:ILE:HD13	1:A:9:ARG:HH22	1.67	0.59
1:C:359:ILE:HD11	1:C:379:ASP:HB2	1.83	0.59
3:I:11:VAL:HA	3:I:110:THR:O	2.03	0.59
3:K:95:ASP:OD1	3:K:100(G):THR:OG1	2.20	0.59
4:L:10:VAL:O	4:L:104:THR:CB	2.51	0.59
1:A:353:THR:O	1:A:353:THR:HG22	2.03	0.59
2:E:27:LYS:HG3	2:E:27:LYS:O	2.02	0.59
2:F:3:THR:HG23	2:F:3:THR:O	2.02	0.59
3:I:83:ARG:O	3:I:111:VAL:CB	2.51	0.59
3:K:27:TYR:OH	3:K:32:TYR:HB2	2.02	0.59
1:A:26:GLU:OE1	1:A:26:GLU:N	2.36	0.59
1:B:456:LEU:CD1	1:B:457:PHE:CG	2.81	0.59
1:A:314:PHE:HD2	1:A:396:ILE:HD13	1.68	0.59
1:B:179:THR:O	1:B:180:LEU:HD23	2.01	0.59
1:B:20:TRP:CD1	1:B:434:VAL:HA	2.35	0.59
1:C:131:GLN:OE1	1:C:131:GLN:N	2.36	0.59
1:C:82:LEU:O	1:C:84:LYS:N	2.36	0.59
2:D:36:ILE:HG13	2:D:37:PHE:N	2.18	0.59
4:M:106:LEU:HD12	4:M:106:LEU:O	2.02	0.59
1:B:217:TRP:CD1	2:E:6:SER:N	2.71	0.58
1:B:329:GLU:HA	1:B:375:MET:HA	1.85	0.58
1:C:101:TRP:CD1	1:C:108:PHE:HE1	2.19	0.58
1:C:402:ARG:NH2	1:C:409:LYS:HZ2	1.98	0.58
1:A:73:ARG:HH21	4:H:26(A):SER:HA	1.59	0.58
4:L:17:SER:HA	4:L:74:ILE:O	2.02	0.58
4:M:49:ASP:C	4:M:50:VAL:HG22	2.22	0.58
1:A:101:TRP:CD1	1:A:108:PHE:CD1	2.80	0.58
1:A:61:TYR:OH	1:A:265:VAL:HG11	2.03	0.58
1:A:312:PHE:CG	1:A:389:ILE:HG12	2.37	0.58
1:A:365:ILE:CG2	1:A:366:THR:N	2.65	0.58
1:A:418:ALA:HB1	1:A:497:PHE:CZ	2.37	0.58
1:B:21:VAL:O	1:B:22:ASP:CB	2.44	0.58
1:A:81:TYR:HE2	1:B:229:ALA:HB1	1.65	0.58
1:A:28:GLY:HA2	1:C:249:HIS:CD2	2.37	0.58
3:I:95:ASP:OD2	3:I:100(C):TYR:OH	2.18	0.58
1:B:127:GLY:HA3	1:B:218:PHE:CZ	2.38	0.58
1:B:183:PHE:O	1:B:299:ARG:N	2.26	0.58
1:B:186:LEU:HD12	1:B:293:LEU:CD1	2.29	0.58
1:B:226:HIS:CD2	1:B:229:ALA:HB3	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:63:PHE:CD1	3:I:66:ARG:HD2	2.38	0.58
3:K:29:PHE:HA	3:K:32:TYR:HD2	1.68	0.58
3:K:52:ASN:CB	3:K:56:ASN:HB2	2.32	0.58
1:A:252:ARG:HD2	3:G:100(D):TRP:CD2	2.38	0.58
4:H:36:GLN:HG2	4:H:83:ALA:CB	2.33	0.58
4:M:53:ARG:HB3	4:M:57:VAL:HA	1.85	0.58
1:B:24:VAL:HG11	1:B:424:LEU:CD2	2.33	0.58
1:B:47:THR:CG2	1:B:283:ARG:HG3	2.33	0.58
1:B:288:HIS:NE2	1:B:424:LEU:CG	2.53	0.58
1:B:69:ALA:HB3	1:B:82:LEU:HD21	1.84	0.58
1:C:312:PHE:HE2	1:C:391:VAL:HG23	1.69	0.58
4:H:29:PHE:O	4:H:65:LYS:NZ	2.35	0.58
4:H:4:LEU:CB	4:H:98:GLY:HA2	2.31	0.58
3:I:28:THR:HG21	3:I:30:THR:CG2	2.31	0.58
1:A:411:PHE:O	1:A:414:THR:HG22	2.04	0.58
1:C:206:MET:HE2	1:C:262:GLU:HG2	1.85	0.58
1:C:405:SER:O	1:C:406:THR:C	2.41	0.58
1:C:423:VAL:CG1	1:C:424:LEU:H	2.10	0.58
1:C:445:ILE:O	1:C:448:ILE:CG1	2.52	0.58
1:A:214:HIS:CE1	2:D:10:ARG:HB2	2.38	0.58
2:D:74:TYR:CE2	2:F:69:LEU:HD23	2.37	0.58
3:G:52:ASN:CB	3:G:56:ASN:HB2	2.32	0.58
4:L:48:TYR:O	4:L:48:TYR:CD2	2.57	0.58
4:M:35:PHE:CE2	4:M:97:PHE:HZ	2.20	0.58
1:C:221:ILE:HG22	1:C:223:LEU:H	1.68	0.58
2:D:67:ILE:HA	2:D:70:ILE:HG22	1.85	0.58
4:L:4:LEU:CD2	4:L:24:GLY:CA	2.61	0.58
1:B:331:GLN:HA	1:B:372:SER:HB3	1.84	0.58
1:B:456:LEU:C	1:B:456:LEU:HD12	2.24	0.58
3:G:4:LEU:CD2	3:G:34:MET:HE1	2.34	0.58
3:G:40:ALA:HB2	3:G:88:ALA:HA	1.85	0.58
4:L:88:SER:HB2	4:L:97:PHE:CD1	2.38	0.58
4:M:48:TYR:OH	4:M:52:SER:CB	2.50	0.58
1:B:38:LYS:HD2	1:B:298:LEU:HB2	1.85	0.58
1:B:74:CYS:HB3	1:B:75:PRO:HD2	1.85	0.58
1:C:214:HIS:ND1	1:C:216:GLU:HB2	2.18	0.58
1:C:330:VAL:O	1:C:373:LYS:HA	2.04	0.58
3:G:28:THR:C	3:G:30:THR:H	2.07	0.58
3:G:32:TYR:CZ	3:G:34:MET:HB2	2.39	0.58
3:K:87:THR:HG23	3:K:87:THR:O	2.02	0.58
1:C:26:GLU:O	1:C:45:LEU:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:50:TRP:HZ3	3:K:52:ASN:C	2.07	0.58
4:M:48:TYR:CZ	4:M:52:SER:HB2	2.39	0.58
4:M:6:GLN:NE2	4:M:87:CYS:N	2.52	0.58
1:A:138:ARG:CG	1:A:138:ARG:HH11	2.14	0.57
1:B:171:PRO:CA	1:B:192:PRO:CG	2.82	0.57
1:B:426:ASP:OD2	1:B:447:GLN:NE2	2.35	0.57
1:B:456:LEU:HD12	1:B:457:PHE:CG	2.36	0.57
1:C:331:GLN:HG2	1:C:371:ASN:HB3	1.80	0.57
1:A:463:PHE:CZ	2:F:74:TYR:CE2	2.86	0.57
1:A:101:TRP:HB2	1:A:108:PHE:HE1	1.67	0.57
1:A:154:ASN:ND2	1:A:160:THR:CG2	2.66	0.57
1:A:15:MET:CE	1:A:35:ALA:CB	2.78	0.57
1:A:1:ILE:HG21	1:A:147:GLN:OE1	2.04	0.57
2:D:34:ASN:OD1	2:D:35:TRP:N	2.37	0.57
3:I:32:TYR:CD1	3:I:33:ALA:N	2.71	0.57
3:I:33:ALA:O	3:I:34:MET:HB2	2.03	0.57
1:A:167:VAL:HG11	1:A:176:ALA:HB3	1.85	0.57
1:A:231:THR:O	1:A:233:THR:N	2.36	0.57
1:A:276:GLU:O	1:A:283:ARG:N	2.37	0.57
3:G:100(K):PHE:HD2	4:H:35:PHE:HE1	1.52	0.57
3:I:16:ALA:CB	3:I:82(C):LEU:CD1	2.83	0.57
4:M:15:GLY:HA2	4:M:76:GLY:HA2	1.85	0.57
1:A:49:THR:OG1	1:A:136:GLU:O	2.21	0.57
1:C:103:ASN:ND2	1:C:105:CYS:SG	2.62	0.57
3:G:50:TRP:HZ3	3:G:52:ASN:C	2.07	0.57
4:H:6:GLN:NE2	4:H:34:TRP:HZ3	2.02	0.57
1:A:148:HIS:ND1	1:A:151:MET:SD	2.78	0.57
1:A:27:HIS:ND1	1:C:249:HIS:HE1	2.02	0.57
1:C:312:PHE:CE2	1:C:391:VAL:CG2	2.88	0.57
2:E:24:GLU:O	2:E:25:TYR:C	2.42	0.57
3:I:3:GLN:HB2	3:I:25:SER:CB	2.27	0.57
1:C:359:ILE:HD11	1:C:379:ASP:CB	2.35	0.57
1:C:384:ASP:OD1	1:C:384:ASP:N	2.35	0.57
3:G:61:GLN:O	3:G:63:PHE:N	2.38	0.57
3:I:66:ARG:CG	3:I:82:LEU:HD11	2.22	0.57
1:A:358:LEU:HD13	1:A:360:THR:O	2.04	0.57
1:B:297:LYS:O	1:B:298:LEU:HD12	2.04	0.57
1:B:53:MET:HG2	1:B:130:ILE:HG22	1.87	0.57
1:C:99:ARG:CD	1:C:103:ASN:CG	2.71	0.57
1:C:262:GLU:O	1:C:266:HIS:ND1	2.37	0.57
1:C:212:LEU:HD21	1:C:284:LEU:HD11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:TRP:CH2	1:C:316:LYS:HD2	2.39	0.57
1:C:332:TYR:O	1:C:332:TYR:CG	2.58	0.57
1:C:99:ARG:HH11	1:C:103:ASN:ND2	2.03	0.57
3:G:31:SER:CA	3:G:97:VAL:HG12	2.35	0.57
1:B:99:ARG:HD2	3:K:100(E):PHE:CZ	2.39	0.57
2:E:27:LYS:CE	2:E:31:ARG:HH11	2.09	0.57
1:C:264:ALA:HB1	2:F:3:THR:HG21	1.87	0.57
1:C:226:HIS:ND1	1:C:226:HIS:O	2.37	0.57
1:C:286:SER:HB2	2:F:14:THR:HG22	1.86	0.57
2:F:74:TYR:O	2:F:75:SER:OG	2.23	0.57
4:M:6:GLN:NE2	4:M:87:CYS:H	2.01	0.57
1:A:245:PHE:CE1	1:A:255:VAL:HG12	2.39	0.57
1:A:96:LEU:HA	1:A:111:GLY:O	2.05	0.57
1:C:453:PHE:CZ	1:C:495:LEU:HD21	2.40	0.57
1:C:460:MET:CE	1:C:464:SER:CB	2.73	0.57
1:C:271:GLY:HA3	2:F:11:LYS:HA	1.87	0.57
4:H:50:VAL:CG1	4:H:51:THR:N	2.61	0.57
1:B:68:MET:CE	1:B:255:VAL:HG13	2.33	0.56
1:C:139:ILE:CD1	1:C:169:ILE:HD12	2.34	0.56
3:I:61:GLN:OE1	3:I:61:GLN:HA	2.03	0.56
3:K:52:ASN:HD21	3:K:56:ASN:ND2	2.00	0.56
1:A:271:GLY:HA2	2:D:18:THR:HB	1.87	0.56
1:C:51:SER:O	1:C:134:ASN:HB3	2.05	0.56
1:A:244:GLU:HG3	2:F:20:LEU:CD2	2.35	0.56
3:I:39:GLN:O	3:I:89:ILE:N	2.36	0.56
4:L:15:GLY:CA	4:L:76:GLY:CA	2.35	0.56
1:A:331:GLN:O	1:A:332:TYR:C	2.42	0.56
1:C:46:VAL:CG1	1:C:47:THR:N	2.56	0.56
2:D:31:ARG:HG3	2:F:4:LEU:HB2	1.86	0.56
4:L:44:LYS:CE	4:L:46:MET:HE1	2.29	0.56
1:A:122:SER:OG	1:A:123:LYS:N	2.38	0.56
1:A:426:ASP:OD2	1:A:447:GLN:HG3	2.05	0.56
1:C:385:SER:O	1:C:399:HIS:HA	2.05	0.56
1:C:288:HIS:CG	1:C:424:LEU:HD11	2.41	0.56
1:C:496:ILE:O	1:C:499:SER:OG	2.22	0.56
2:E:20:LEU:HD13	2:E:23:ARG:O	2.06	0.56
3:G:95:ASP:OD1	3:G:100(G):THR:OG1	2.20	0.56
3:I:65:ASP:O	3:I:65:ASP:CG	2.43	0.56
3:I:24:ALA:CB	3:I:76:SER:OG	2.38	0.56
1:A:15:MET:HE3	1:A:35:ALA:CB	2.36	0.56
1:B:456:LEU:HD12	1:B:457:PHE:CA	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:TYR:CD2	1:B:221:ILE:HD11	2.40	0.56
1:C:9:ARG:CZ	1:C:11:PHE:CE2	2.84	0.56
1:C:277:MET:HG3	1:C:282:GLY:HA2	1.86	0.56
3:I:40:ALA:CA	3:I:88:ALA:HB2	2.36	0.56
2:E:11:LYS:HD2	2:E:13:GLN:OE1	2.06	0.56
4:H:44:LYS:CG	4:H:45:LEU:H	2.18	0.56
3:I:50:TRP:HZ2	3:I:67:VAL:CG2	2.18	0.56
3:K:50:TRP:CZ3	3:K:52:ASN:O	2.53	0.56
4:M:53:ARG:HD3	4:M:57:VAL:CG1	2.05	0.56
4:M:17:SER:HA	4:M:75:SER:HA	1.87	0.56
1:A:101:TRP:HZ3	1:C:316:LYS:HD2	1.70	0.56
1:C:20:TRP:CE2	1:C:292:ARG:HD2	2.41	0.56
1:A:263:GLY:HA3	1:C:260:SER:O	2.04	0.56
1:C:443:LYS:O	1:C:447:GLN:HG2	2.05	0.56
2:F:14:THR:HG22	2:F:15:ARG:N	2.20	0.56
4:H:58:SER:C	4:H:60:ARG:H	2.09	0.56
3:I:9:ALA:CB	3:I:109:VAL:CB	2.65	0.56
3:K:61:GLN:NE2	3:K:64:GLN:OE1	2.39	0.56
4:L:34:TRP:HD1	4:L:47:LEU:CD2	2.19	0.56
1:A:151:MET:CE	4:M:52:SER:OG	2.53	0.56
1:B:367:GLU:OE1	1:B:368:SER:N	2.39	0.56
1:C:342:PRO:O	1:C:389:ILE:O	2.24	0.56
1:C:39:PRO:HG3	1:C:300:LEU:HA	1.87	0.56
3:G:52:ASN:HD22	3:G:56:ASN:HD22	1.39	0.56
3:G:63:PHE:CD2	3:G:63:PHE:N	2.74	0.56
4:H:82:GLU:OE1	4:H:105:VAL:HG11	2.06	0.56
1:B:103:ASN:HA	3:K:100(H):LEU:HD21	1.87	0.56
3:K:39:GLN:HG3	3:K:40:ALA:O	2.05	0.56
4:L:44:LYS:HG2	4:L:46:MET:CE	2.36	0.56
4:M:6:GLN:CB	4:M:87:CYS:SG	2.94	0.56
1:B:226:HIS:NE2	1:B:234:PRO:HB3	2.21	0.56
1:B:456:LEU:CD1	1:B:457:PHE:HD1	1.99	0.56
1:B:46:VAL:HB	1:B:138:ARG:O	2.06	0.56
1:C:90:TYR:CD1	1:C:118:LYS:CB	2.86	0.56
1:C:226:HIS:O	1:C:227:ALA:HB3	2.05	0.56
1:C:321:THR:HG22	1:C:322:LEU:H	1.71	0.56
1:A:217:TRP:CD1	2:D:5:PRO:HB2	2.41	0.56
1:A:249:HIS:CD2	2:F:16:SER:HB3	2.41	0.56
1:A:252:ARG:NE	3:G:100(D):TRP:CE2	2.73	0.56
3:G:52:ASN:HD21	3:G:56:ASN:ND2	2.01	0.56
3:G:66:ARG:CZ	3:G:82:LEU:HD11	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:3:GLN:HB2	3:K:25:SER:HB3	1.87	0.56
4:L:6:GLN:NE2	4:L:34:TRP:HZ3	2.02	0.56
1:B:332:TYR:HE1	1:B:335:THR:HG22	1.71	0.56
1:C:15:MET:HE3	1:C:19:THR:CA	2.21	0.56
1:C:15:MET:HG3	1:C:35:ALA:CB	2.36	0.56
1:C:290:LYS:O	1:C:290:LYS:HG3	2.05	0.56
1:C:57:ARG:HD3	1:C:225:TRP:HE3	1.69	0.56
2:D:2:VAL:HG21	2:F:27:LYS:CE	2.36	0.56
3:G:3:GLN:HB2	3:G:25:SER:HB3	1.87	0.56
3:I:40:ALA:N	3:I:88:ALA:HB1	2.20	0.56
4:L:44:LYS:CE	4:L:46:MET:HE3	2.34	0.56
1:A:160:THR:HG22	5:A:601:NAG:O7	2.07	0.55
1:A:147:GLN:O	1:A:375:MET:HB3	2.05	0.55
1:A:412:GLU:O	1:A:415:VAL:HB	2.06	0.55
2:D:10:ARG:NH1	2:F:38:ARG:HB3	2.21	0.55
4:M:84:ASP:OD1	4:M:102:LYS:HG3	2.06	0.55
1:A:143:VAL:HG11	1:A:183:PHE:CE2	2.41	0.55
1:B:177:GLU:HG3	1:B:185:SER:HB3	1.87	0.55
1:B:38:LYS:H	1:B:300:LEU:HD11	1.72	0.55
1:B:329:GLU:OE2	1:B:373:LYS:HD3	2.06	0.55
1:C:188:LEU:O	1:C:188:LEU:HD12	2.06	0.55
1:C:258:LEU:HD12	1:C:258:LEU:O	2.06	0.55
2:D:32:VAL:HG23	2:F:74:TYR:HE1	1.59	0.55
1:A:148:HIS:CB	1:A:151:MET:HB2	2.35	0.55
1:B:37:ASP:OD1	1:B:37:ASP:N	2.35	0.55
1:C:135:LEU:CD1	1:C:198:PHE:CE2	2.84	0.55
1:C:50:VAL:O	1:C:282:GLY:N	2.39	0.55
1:C:70:SER:O	1:C:82:LEU:CD1	2.55	0.55
1:B:148:HIS:CE1	1:B:373:LYS:HB2	2.35	0.55
1:B:184:GLY:HA3	1:B:297:LYS:O	2.05	0.55
1:C:453:PHE:CZ	1:C:495:LEU:CD2	2.89	0.55
3:K:39:GLN:HE21	3:K:40:ALA:N	2.05	0.55
4:M:10:VAL:HG23	4:M:18:ILE:HD11	1.87	0.55
3:I:39:GLN:NE2	4:M:37:GLN:NE2	2.53	0.55
1:A:324:GLY:O	1:A:402:ARG:CZ	2.50	0.55
1:A:337:GLY:O	1:A:339:CYS:N	2.39	0.55
1:C:99:ARG:CD	1:C:103:ASN:OD1	2.53	0.55
1:B:271:GLY:HA3	2:E:6:SER:O	2.06	0.55
3:G:50:TRP:CE2	3:G:69:ILE:HG21	2.42	0.55
3:I:9:ALA:HB2	3:I:107:THR:HG21	1.88	0.55
3:I:69:ILE:HG23	3:I:80:MET:HA	1.77	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:40:ALA:HB2	3:K:88:ALA:HA	1.88	0.55
1:A:188:LEU:CD1	1:A:190:CYS:SG	2.94	0.55
1:A:317:ILE:HD12	1:A:317:ILE:N	2.22	0.55
1:B:58:SER:HA	1:B:126:THR:HA	1.88	0.55
1:C:142:SER:O	1:C:143:VAL:HG12	2.07	0.55
1:C:201:LEU:HD21	1:C:212:LEU:CD1	2.23	0.55
1:C:457:PHE:HB3	1:C:460:MET:HG3	1.88	0.55
1:C:3:CYS:O	1:C:9:ARG:NH2	2.39	0.55
1:A:331:GLN:CG	1:A:372:SER:OG	2.48	0.55
1:B:148:HIS:CG	1:B:373:LYS:HB3	2.31	0.55
1:B:9:ARG:HG2	1:B:323:HIS:CD2	2.42	0.55
1:C:351:THR:HG23	1:C:395:LYS:HE3	1.87	0.55
1:C:482:GLY:N	1:C:485:SER:OG	2.38	0.55
3:G:35:HIS:N	3:G:93:ALA:O	2.40	0.55
4:H:53:ARG:HD2	4:H:57:VAL:HG11	1.89	0.55
3:I:29:PHE:HB2	3:I:32:TYR:CD2	2.41	0.55
4:L:77:LEU:HD23	4:L:77:LEU:H	1.72	0.55
1:A:3:CYS:O	1:A:9:ARG:NH2	2.39	0.55
1:B:131:GLN:OE1	1:B:131:GLN:N	2.40	0.55
1:B:132:PRO:HD3	1:B:199:SER:HB3	1.89	0.55
1:B:21:VAL:CG1	1:B:293:LEU:O	2.55	0.55
1:B:211:TRP:HB2	1:B:273:LEU:O	2.05	0.55
1:B:333:ALA:HB2	1:B:370:GLU:HG3	1.89	0.55
1:C:65:ILE:CD1	1:C:243:VAL:CG2	2.75	0.55
1:C:321:THR:CG2	1:C:322:LEU:N	2.70	0.55
1:C:42:ASP:O	1:C:142:SER:HB2	2.07	0.55
2:D:33:GLU:HA	2:D:36:ILE:HG12	1.87	0.55
2:F:22:SER:OG	2:F:23:ARG:N	2.39	0.55
4:H:34:TRP:CH2	4:H:87:CYS:HB3	2.42	0.55
4:L:4:LEU:HD11	4:L:26(C):VAL:CG2	2.37	0.55
4:M:12:GLY:O	4:M:105:VAL:O	2.24	0.55
1:A:148:HIS:CE1	1:A:373:LYS:CG	2.86	0.55
1:A:1:ILE:HD12	1:A:144:HIS:CD2	2.42	0.55
1:A:277:MET:HA	1:A:282:GLY:CA	2.14	0.55
1:A:365:ILE:CG2	1:A:366:THR:H	2.20	0.55
1:B:82:LEU:HB2	1:B:114:VAL:HG11	1.89	0.55
1:C:460:MET:HE1	1:C:464:SER:CB	2.27	0.55
3:G:5:VAL:C	3:G:6:GLU:HG3	2.26	0.55
4:L:49:ASP:O	4:L:50:VAL:CG2	2.51	0.55
4:L:34:TRP:CH2	4:L:87:CYS:HB3	2.42	0.55
1:C:308:CYS:HB2	1:C:340:LYS:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:MET:C	1:C:376:LEU:HD12	2.28	0.54
1:C:488:CYS:SG	1:C:489:LEU:N	2.81	0.54
1:A:101:TRP:CZ3	1:C:316:LYS:CD	2.90	0.54
2:E:53:LEU:HD11	2:E:63:TYR:CE2	2.32	0.54
4:H:58:SER:C	4:H:60:ARG:N	2.60	0.54
4:L:29:PHE:O	4:L:65:LYS:NZ	2.40	0.54
4:M:6:GLN:HB3	4:M:22:CYS:SG	2.47	0.54
1:A:344:GLN:HE22	1:A:352:LEU:CG	2.15	0.54
1:C:326:VAL:HG22	1:C:400:TRP:CZ2	2.43	0.54
1:C:462:TRP:CZ3	1:C:499:SER:O	2.58	0.54
3:G:4:LEU:HD23	3:G:34:MET:HE1	1.90	0.54
3:I:39:GLN:HE22	4:M:37:GLN:HE22	1.53	0.54
4:M:58:SER:O	4:M:59:SER:C	2.45	0.54
1:B:101:TRP:O	1:B:103:ASN:N	2.37	0.54
1:B:190:CYS:HA	1:B:291:CYS:HA	1.89	0.54
1:B:73:ARG:HD2	1:B:77:GLN:OE1	2.07	0.54
2:D:35:TRP:CE2	2:D:72:PRO:HA	2.42	0.54
3:I:14:PRO:HG3	3:I:111:VAL:HG12	1.90	0.54
3:I:40:ALA:HB3	3:I:43:GLN:CB	2.37	0.54
1:A:38:LYS:HD2	1:A:298:LEU:HD12	1.89	0.54
1:A:84:LYS:HD2	1:A:90:TYR:HE2	1.72	0.54
1:B:103:ASN:HA	3:K:100(H):LEU:CD2	2.36	0.54
1:C:398:HIS:ND1	1:B:171:PRO:O	2.36	0.54
1:B:332:TYR:H	1:B:372:SER:CB	2.20	0.54
1:C:257:VAL:O	1:C:258:LEU:CB	2.56	0.54
1:C:60:CYS:HB2	1:C:236:TRP:CH2	2.42	0.54
2:E:5:PRO:O	2:E:6:SER:CB	2.56	0.54
2:D:75:SER:OG	2:F:28:HIS:ND1	2.14	0.54
2:F:59:GLN:O	2:F:63:TYR:N	2.38	0.54
3:I:10:GLU:O	3:I:109:VAL:HA	2.07	0.54
4:L:41:LYS:HG2	4:L:42:ALA:N	2.23	0.54
4:M:4:LEU:CG	4:M:98:GLY:N	2.71	0.54
1:A:475:LEU:HD21	2:F:53:LEU:CD1	2.29	0.54
1:C:26:GLU:C	1:C:45:LEU:HD13	2.28	0.54
2:F:71:ALA:O	2:F:75:SER:OG	2.26	0.54
3:K:50:TRP:CE2	3:K:69:ILE:HG21	2.42	0.54
1:A:96:LEU:HD22	1:A:112:SER:HB3	1.89	0.54
1:A:345:MET:HG2	1:A:378:LEU:HD23	1.89	0.54
1:A:477:LEU:O	1:A:478:ASN:OD1	2.26	0.54
1:B:463:PHE:CZ	2:E:29:LEU:HB2	2.42	0.54
3:I:36:TRP:CB	3:I:50:TRP:HZ3	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:LEU:HD13	2:F:52:LEU:HD22	1.90	0.54
1:C:290:LYS:HE3	1:C:430:ASP:HB3	1.90	0.54
2:D:17:GLN:HG3	2:D:18:THR:O	2.08	0.54
3:G:48:MET:HB3	3:G:63:PHE:CE2	2.43	0.54
4:H:33:SER:HB2	4:H:35:PHE:HE2	1.69	0.54
3:K:11:VAL:HG12	3:K:110:THR:C	2.28	0.54
4:M:79:ALA:HB3	4:M:80:GLU:OE1	2.08	0.54
1:A:1:ILE:H1	1:A:144:HIS:CD2	2.21	0.54
1:A:20:TRP:HE1	1:A:292:ARG:HD3	1.73	0.54
1:C:420:ARG:CD	1:C:431:PHE:CE2	2.81	0.54
1:C:486:LEU:HD23	1:C:489:LEU:HD11	1.89	0.54
1:C:453:PHE:CE2	1:C:495:LEU:CD2	2.91	0.54
2:F:34:ASN:OD1	2:F:34:ASN:C	2.45	0.54
1:C:252:ARG:CG	3:I:100(D):TRP:CH2	2.79	0.54
3:I:29:PHE:O	3:I:32:TYR:CB	2.56	0.54
3:I:36:TRP:CG	3:I:50:TRP:HZ3	2.26	0.54
1:A:15:MET:HE3	1:A:38:LYS:CE	2.37	0.54
1:B:9:ARG:O	1:B:323:HIS:CE1	2.61	0.54
1:C:426:ASP:C	1:C:428:ALA:H	2.07	0.54
1:A:464:SER:CB	2:F:75:SER:HB2	2.18	0.54
3:G:22:CYS:SG	3:G:34:MET:HE3	2.46	0.54
3:G:37:VAL:HG11	3:G:45:LEU:HD23	1.90	0.54
4:H:4:LEU:HB2	4:H:98:GLY:CA	2.37	0.54
3:I:36:TRP:CG	3:I:50:TRP:CZ3	2.95	0.54
3:K:44:ARG:HD2	4:L:3:ALA:HB2	1.90	0.54
4:M:26(B):ASP:HB3	4:M:91:THR:HG22	1.89	0.54
4:M:79:ALA:CB	4:M:80:GLU:OE1	2.56	0.54
1:A:156:THR:HG22	1:A:164:ARG:HB2	1.90	0.53
1:B:186:LEU:CD1	1:B:293:LEU:CD1	2.69	0.53
1:B:252:ARG:HB2	3:K:100(D):TRP:CD1	2.43	0.53
1:C:99:ARG:HG3	1:C:103:ASN:OD1	2.01	0.53
1:C:202:TYR:HE2	1:C:215:LYS:HD2	1.68	0.53
1:C:71:ASP:HB3	1:C:80:ALA:HB1	1.88	0.53
3:G:87:THR:HG23	3:G:110:THR:HA	1.90	0.53
4:L:9:SER:HB2	4:L:102:LYS:O	2.08	0.53
4:M:34:TRP:H	4:M:47:LEU:CB	2.17	0.53
1:A:100:GLY:O	1:A:108:PHE:CE1	2.61	0.53
1:C:326:VAL:CG2	1:C:400:TRP:CE2	2.91	0.53
1:C:244:GLU:HG2	2:D:20:LEU:HD22	1.89	0.53
1:A:475:LEU:CD2	2:F:53:LEU:HD11	2.27	0.53
4:H:10:VAL:CG2	4:H:18:ILE:HD11	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:78:GLN:CA	4:M:78:GLN:NE2	2.70	0.53
1:A:341:VAL:HG22	1:A:365:ILE:HG13	1.89	0.53
1:B:45:LEU:O	1:B:45:LEU:HD12	2.09	0.53
1:C:209:LYS:HG3	1:C:211:TRP:HZ3	1.73	0.53
3:K:37:VAL:HG11	3:K:45:LEU:HD23	1.90	0.53
4:L:48:TYR:CE2	4:L:52:SER:CB	2.90	0.53
4:M:76:GLY:O	4:M:77:LEU:C	2.45	0.53
4:M:80:GLU:O	4:M:80:GLU:HG2	2.08	0.53
1:A:320:GLU:N	1:A:400:TRP:HH2	2.06	0.53
1:A:330:VAL:HG21	1:A:332:TYR:CE2	2.43	0.53
1:C:290:LYS:HE3	1:C:430:ASP:CG	2.29	0.53
3:G:63:PHE:HD1	3:G:66:ARG:HH11	1.56	0.53
3:I:40:ALA:N	3:I:43:GLN:HB3	2.23	0.53
1:A:72:SER:CB	1:A:113:LEU:HD13	2.35	0.53
1:A:314:PHE:HD2	1:A:396:ILE:CD1	2.20	0.53
1:C:143:VAL:HG13	1:C:163:ASN:CG	2.28	0.53
1:A:420:ARG:CA	2:D:15:ARG:HH22	2.21	0.53
3:K:44:ARG:HD2	4:L:3:ALA:CB	2.39	0.53
1:C:399:HIS:CD2	1:B:191:GLU:HB3	2.44	0.53
1:B:20:TRP:C	1:B:21:VAL:HG12	2.28	0.53
3:G:28:THR:O	3:G:30:THR:N	2.41	0.53
3:G:33:ALA:HB3	3:G:94:ARG:HB2	1.91	0.53
3:I:66:ARG:CD	3:I:82:LEU:HD13	2.39	0.53
1:A:131:GLN:OE1	1:A:131:GLN:N	2.42	0.53
1:B:326:VAL:HG12	1:B:380:PRO:HD3	1.90	0.53
1:C:446:HIS:HA	1:C:449:PHE:HB2	1.91	0.53
2:F:59:GLN:O	2:F:60:LYS:C	2.47	0.53
4:H:82:GLU:CB	4:H:103:LEU:CD2	2.87	0.53
3:K:98:ASP:OD2	3:K:100:TYR:HD2	1.92	0.53
4:L:105:VAL:HG12	4:L:106:LEU:CD1	2.34	0.53
1:A:15:MET:HE1	1:A:295:MET:HG3	1.90	0.53
1:A:198:PHE:C	1:A:200:ASP:H	2.12	0.53
1:A:314:PHE:CD2	1:A:396:ILE:CD1	2.92	0.53
1:B:141:LEU:HD22	1:B:186:LEU:HD21	1.91	0.53
1:B:201:LEU:HD21	2:E:12:LEU:HD21	1.90	0.53
1:C:330:VAL:HG21	1:C:389:ILE:HD11	1.91	0.53
1:C:463:PHE:CE2	2:D:74:TYR:CZ	2.96	0.53
3:G:32:TYR:OH	3:G:34:MET:HB3	2.08	0.53
4:H:34:TRP:HB2	4:H:47:LEU:HD12	1.91	0.53
3:I:38:ARG:NH1	3:I:63:PHE:CZ	2.75	0.53
4:L:10:VAL:O	4:L:104:THR:O	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:50:VAL:HG23	4:L:51:THR:HG23	1.91	0.53
4:M:35:PHE:CE2	4:M:97:PHE:CE1	2.97	0.53
1:B:48:THR:CG2	1:B:137:TYR:CE1	2.92	0.52
1:C:71:ASP:CG	1:C:114:VAL:H	2.10	0.52
1:C:137:TYR:HE2	1:C:192:PRO:HB3	1.75	0.52
1:C:453:PHE:C	1:C:453:PHE:CD1	2.81	0.52
3:I:50:TRP:CG	3:I:69:ILE:CG1	2.90	0.52
1:A:206:MET:HB2	1:A:211:TRP:HZ3	1.74	0.52
1:C:210:HIS:CD2	1:C:277:MET:HB3	2.43	0.52
1:C:196:LEU:HD23	1:C:287:GLY:HA2	1.88	0.52
3:G:36:TRP:CZ3	3:G:92:CYS:HB3	2.44	0.52
3:I:50:TRP:CZ2	3:I:67:VAL:CG2	2.92	0.52
1:A:167:VAL:HG12	1:A:176:ALA:CB	2.38	0.52
1:B:99:ARG:HG3	1:B:103:ASN:OD1	2.09	0.52
1:B:344:GLN:HG2	1:B:352:LEU:HD13	1.91	0.52
1:B:2:ARG:CZ	1:B:44:GLU:OE2	2.57	0.52
1:A:229:ALA:HB3	1:B:81:TYR:HB2	1.91	0.52
1:C:3:CYS:CB	1:C:42:ASP:OD2	2.57	0.52
3:I:48:MET:HB3	3:I:63:PHE:CD2	2.44	0.52
1:A:151:MET:SD	1:A:373:LYS:HD3	2.43	0.52
1:B:345:MET:SD	1:B:380:PRO:HA	2.49	0.52
1:B:341:VAL:HG11	1:B:374:MET:HE2	1.91	0.52
1:B:437:ALA:O	1:B:440:SER:N	2.42	0.52
1:C:21:VAL:O	1:C:292:ARG:HB2	2.10	0.52
1:C:409:LYS:HD2	1:C:409:LYS:C	2.30	0.52
1:C:42:ASP:CG	1:C:142:SER:CB	2.77	0.52
4:H:26(B):ASP:OD1	4:H:26(B):ASP:N	2.41	0.52
4:H:53:ARG:HD2	4:H:57:VAL:CG1	2.39	0.52
3:K:89:ILE:HA	3:K:107:THR:O	2.09	0.52
1:A:311:ALA:HB2	1:A:332:TYR:CB	2.27	0.52
4:H:34:TRP:H	4:H:47:LEU:HB2	1.74	0.52
1:A:46:VAL:CG2	3:I:100:TYR:CE1	2.66	0.52
3:K:36:TRP:CZ3	3:K:92:CYS:HB3	2.44	0.52
1:C:24:VAL:O	1:C:431:PHE:HE1	1.92	0.52
1:C:70:SER:HB3	1:C:252:ARG:HD2	1.91	0.52
1:C:352:LEU:HD23	1:C:353:THR:H	1.74	0.52
2:D:11:LYS:HG2	2:D:12:LEU:N	2.14	0.52
2:E:23:ARG:NH1	2:E:23:ARG:HB2	2.25	0.52
4:L:10:VAL:C	4:L:104:THR:HB	2.30	0.52
1:A:103:ASN:OD1	1:A:104:GLY:N	2.43	0.52
1:A:138:ARG:HG2	1:A:138:ARG:NH1	2.14	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ILE:CG2	1:A:176:ALA:HB2	2.24	0.52
1:A:312:PHE:CE1	1:A:389:ILE:HG23	2.45	0.52
1:A:347:VAL:HG23	1:A:348:ASP:OD1	2.09	0.52
1:B:3:CYS:O	1:B:6:VAL:HG13	2.08	0.52
1:C:290:LYS:HE3	1:C:430:ASP:OD2	2.10	0.52
1:C:460:MET:HE3	1:C:464:SER:CB	2.36	0.52
1:B:462:TRP:NE1	2:E:25:TYR:HD2	2.06	0.52
2:F:57:THR:O	2:F:60:LYS:HB2	2.10	0.52
1:B:49:THR:HG21	1:B:281:LYS:HD3	1.90	0.52
3:I:9:ALA:HB2	3:I:107:THR:HG22	1.84	0.52
1:A:375:MET:O	1:A:376:LEU:HD23	2.10	0.52
1:A:37:ASP:O	1:A:38:LYS:HB2	2.10	0.52
1:A:320:GLU:CB	1:A:400:TRP:CZ2	2.93	0.52
1:B:344:GLN:NE2	1:B:352:LEU:HD12	2.23	0.52
1:C:39:PRO:HG3	1:C:300:LEU:HD23	1.91	0.52
1:C:286:SER:CB	2:F:14:THR:HG21	2.34	0.52
3:I:94:ARG:NH1	3:I:96:LYS:HD3	2.25	0.52
3:K:57:THR:HB	3:K:59:TYR:CE1	2.45	0.52
4:M:4:LEU:HD11	4:M:87:CYS:HB2	1.92	0.52
1:B:186:LEU:HD11	1:B:293:LEU:CD1	2.26	0.52
1:B:426:ASP:HA	1:B:446:HIS:ND1	2.24	0.52
1:B:8:ASN:OD1	2:E:15:ARG:HD3	2.10	0.52
1:C:135:LEU:HD23	1:C:136:GLU:H	1.75	0.52
1:C:386:TYR:HA	1:C:398:HIS:O	2.10	0.52
1:C:490:ALA:C	1:C:491:LEU:HD12	2.30	0.52
2:E:7:HIS:CD2	2:E:24:GLU:OE2	2.63	0.52
3:K:30:THR:O	3:K:30:THR:HG22	2.10	0.52
1:B:211:TRP:HE1	1:B:269:LEU:HD11	1.75	0.51
1:B:137:TYR:CD2	1:B:289:LEU:HD21	2.45	0.51
1:B:8:ASN:CG	2:E:15:ARG:HD3	2.29	0.51
3:I:50:TRP:CD1	3:I:69:ILE:HG12	2.45	0.51
1:A:19:THR:OG1	1:A:296:ASP:OD1	2.22	0.51
1:B:142:SER:HA	1:B:164:ARG:HA	1.92	0.51
1:B:27:HIS:CB	1:B:45:LEU:HD23	2.34	0.51
1:C:198:PHE:C	1:C:200:ASP:N	2.62	0.51
1:C:70:SER:OG	1:C:252:ARG:NH1	2.43	0.51
3:I:8:GLY:HA2	3:I:107:THR:HG23	1.91	0.51
3:K:66:ARG:NH2	3:K:86:ASP:OD2	2.43	0.51
4:M:49:ASP:C	4:M:49:ASP:OD1	2.49	0.51
4:M:90:HIS:ND1	4:M:91:THR:O	2.43	0.51
1:A:100:GLY:O	1:A:108:PHE:HE1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LEU:HD21	1:A:293:LEU:HD11	1.93	0.51
1:B:125:MET:HG2	1:B:204:LEU:HD11	1.92	0.51
3:K:87:THR:CG2	3:K:87:THR:O	2.59	0.51
1:A:252:ARG:HH11	1:A:252:ARG:HG2	1.75	0.51
1:C:99:ARG:NH1	1:C:103:ASN:CG	2.43	0.51
3:G:86:ASP:O	3:G:87:THR:C	2.47	0.51
4:H:61:PHE:N	4:H:61:PHE:CD1	2.76	0.51
4:H:88:SER:OG	4:H:97:PHE:CE1	2.62	0.51
1:B:21:VAL:CG1	1:B:22:ASP:N	2.60	0.51
1:B:58:SER:HB2	1:B:226:HIS:HB2	1.93	0.51
2:D:70:ILE:CD1	2:D:74:TYR:HB3	2.40	0.51
4:H:34:TRP:HD1	4:H:47:LEU:HD12	1.65	0.51
3:I:100(K):PHE:O	4:M:45:LEU:HB2	2.11	0.51
3:I:40:ALA:HA	3:I:88:ALA:HB2	1.91	0.51
1:B:217:TRP:CD1	2:E:5:PRO:C	2.84	0.51
1:C:348:ASP:OD1	1:C:349:MET:N	2.43	0.51
1:C:314:PHE:CE2	1:C:396:ILE:HG23	2.45	0.51
1:A:222:PRO:HG3	2:D:3:THR:HA	1.92	0.51
3:G:50:TRP:HA	3:G:58:LYS:O	2.11	0.51
1:A:27:HIS:ND1	1:C:249:HIS:CE1	2.79	0.51
3:K:33:ALA:HB2	3:K:97:VAL:HG13	1.93	0.51
1:A:101:TRP:HB2	1:A:108:PHE:CE1	2.45	0.51
1:A:217:TRP:CD1	2:D:7:HIS:HA	2.46	0.51
1:A:224:PRO:HA	1:A:238:ASN:HB2	1.93	0.51
1:B:103:ASN:HD22	1:B:103:ASN:N	1.94	0.51
1:B:137:TYR:CE2	1:B:192:PRO:HA	2.44	0.51
1:C:348:ASP:OD2	1:C:352:LEU:HD22	2.11	0.51
4:H:88:SER:OG	4:H:97:PHE:HE1	1.94	0.51
4:L:16:GLN:O	4:L:77:LEU:HD21	2.10	0.51
1:A:90:TYR:CD1	1:A:118:LYS:HA	2.46	0.51
1:A:167:VAL:HG12	1:A:176:ALA:HB1	1.87	0.51
1:C:399:HIS:NE2	1:B:191:GLU:HG2	2.26	0.51
1:C:215:LYS:NZ	1:C:215:LYS:CB	2.73	0.51
1:C:278:ASP:OD1	1:C:278:ASP:N	2.44	0.51
4:M:47:LEU:O	4:M:48:TYR:HD2	1.93	0.51
1:A:312:PHE:CZ	1:A:389:ILE:N	2.73	0.51
1:B:247:ASP:N	1:B:247:ASP:OD1	2.41	0.51
1:B:332:TYR:O	1:B:372:SER:OG	2.28	0.51
1:C:196:LEU:C	1:C:197:ASP:OD2	2.48	0.51
1:C:27:HIS:CE1	3:G:100:TYR:CD1	2.84	0.51
2:D:27:LYS:HD3	2:D:30:ILE:CG2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:15:GLY:HA2	4:L:76:GLY:HA2	0.58	0.51
1:A:311:ALA:HB1	1:A:332:TYR:HA	0.52	0.50
1:B:463:PHE:HZ	2:E:29:LEU:HB2	1.74	0.50
1:B:502:VAL:O	1:B:502:VAL:HG12	2.11	0.50
3:G:48:MET:CE	3:G:67:VAL:HG11	2.41	0.50
3:I:43:GLN:CD	3:I:44:ARG:H	2.12	0.50
3:I:66:ARG:HG2	3:I:67:VAL:HG13	1.92	0.50
4:L:50:VAL:HG23	4:L:51:THR:CA	2.31	0.50
4:M:6:GLN:OE1	4:M:86:TYR:HA	2.11	0.50
1:A:147:GLN:O	1:A:375:MET:CB	2.59	0.50
1:A:148:HIS:CD2	1:A:152:ILE:CG1	2.90	0.50
1:A:345:MET:O	1:A:354:PRO:CA	2.57	0.50
1:A:312:PHE:CD1	1:A:396:ILE:HD11	2.46	0.50
1:C:399:HIS:CD2	1:B:191:GLU:HG2	2.46	0.50
1:C:99:ARG:HD3	1:C:103:ASN:OD1	2.10	0.50
1:C:164:ARG:HG3	1:C:164:ARG:O	2.10	0.50
3:G:29:PHE:CG	3:G:29:PHE:O	2.63	0.50
3:G:50:TRP:CZ3	3:G:52:ASN:O	2.53	0.50
3:I:29:PHE:O	3:I:32:TYR:HD2	1.94	0.50
3:K:37:VAL:HG22	3:K:47:TRP:HD1	1.76	0.50
4:L:10:VAL:O	4:L:104:THR:CA	2.59	0.50
1:A:224:PRO:O	1:A:236:TRP:HE3	1.95	0.50
1:A:386:TYR:HE1	1:A:399:HIS:HB2	1.75	0.50
1:B:456:LEU:CD1	1:B:457:PHE:N	2.62	0.50
1:B:47:THR:HG21	1:B:283:ARG:CG	2.41	0.50
1:C:286:SER:HB3	2:F:16:SER:OG	2.11	0.50
2:D:59:GLN:HE22	2:F:54:GLY:HA2	1.76	0.50
4:L:26(B):ASP:N	4:L:26(B):ASP:OD1	2.41	0.50
1:A:121:CYS:SG	1:A:122:SER:N	2.84	0.50
1:A:21:VAL:O	1:A:293:LEU:N	2.36	0.50
1:A:2:ARG:O	1:A:44:GLU:OE1	2.28	0.50
1:C:312:PHE:HE2	1:C:391:VAL:CG2	2.25	0.50
1:C:473:MET:SD	1:C:488:CYS:HB2	2.51	0.50
2:F:33:GLU:O	2:F:36:ILE:HG13	2.11	0.50
3:G:57:THR:HB	3:G:59:TYR:CE1	2.46	0.50
3:I:36:TRP:HB2	3:I:50:TRP:CZ3	2.46	0.50
1:A:81:TYR:CE2	1:B:229:ALA:HB2	2.43	0.50
2:D:22:SER:HA	2:D:25:TYR:CE1	2.47	0.50
3:G:55:GLY:CA	3:G:71:ARG:HE	2.25	0.50
3:K:39:GLN:HE21	3:K:40:ALA:H	1.60	0.50
1:A:58:SER:HB2	1:A:226:HIS:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:MET:CE	1:A:38:LYS:CE	2.89	0.50
1:A:84:LYS:HB3	1:A:90:TYR:HD2	1.77	0.50
1:A:6:VAL:CG1	1:A:9:ARG:HB3	2.42	0.50
1:B:47:THR:HG21	1:B:283:ARG:HG3	1.93	0.50
1:B:331:GLN:HA	1:B:372:SER:CB	2.41	0.50
1:B:430:ASP:OD2	1:B:443:LYS:HD3	2.12	0.50
1:C:359:ILE:CD1	1:C:379:ASP:N	2.74	0.50
3:G:14:PRO:HG2	3:G:112:SER:O	2.11	0.50
3:K:27:TYR:HE1	3:K:32:TYR:CB	2.20	0.50
1:A:87:ASP:C	1:A:88:THR:HG22	2.27	0.50
1:C:341:VAL:HG13	1:C:374:MET:CE	2.39	0.50
2:E:71:ALA:CA	2:E:74:TYR:HA	2.40	0.50
3:G:100(C):TYR:OH	3:G:100(F):PRO:HB3	2.12	0.50
3:G:50:TRP:NE1	3:G:69:ILE:HG21	2.27	0.50
1:C:251:LYS:HG2	3:I:100(D):TRP:CD1	2.47	0.50
3:K:50:TRP:NE1	3:K:69:ILE:HG21	2.27	0.50
3:K:50:TRP:HA	3:K:58:LYS:O	2.11	0.50
3:K:38:ARG:NH2	3:K:86:ASP:CA	2.61	0.50
4:M:59:SER:C	4:M:60:ARG:HG3	2.24	0.50
1:A:90:TYR:HD1	1:A:118:LYS:HA	1.76	0.50
4:H:34:TRP:C	4:H:35:PHE:HD2	2.15	0.50
1:A:11:PHE:CE1	1:A:323:HIS:NE2	2.80	0.50
1:A:349:MET:SD	1:A:386:TYR:CD2	3.05	0.50
1:A:48:THR:HB	1:A:284:LEU:HB3	1.92	0.50
1:B:99:ARG:NH1	1:B:105:CYS:SG	2.84	0.50
1:C:40:THR:O	1:C:143:VAL:HA	2.12	0.50
3:I:47:TRP:CZ2	3:I:49:GLY:HA3	2.46	0.50
1:A:43:ILE:HG12	1:A:141:LEU:CD2	2.42	0.49
1:A:312:PHE:CE2	1:A:395:LYS:HB2	2.47	0.49
1:B:85:GLN:HG2	1:B:86:SER:H	1.76	0.49
1:C:457:PHE:HD2	1:C:468:ILE:HD13	1.77	0.49
3:G:83:ARG:HD2	3:G:85:GLU:HB2	1.94	0.49
3:I:39:GLN:NE2	3:I:91:TYR:HE2	2.09	0.49
4:L:45:LEU:HD21	4:L:48:TYR:HB3	1.94	0.49
1:A:214:HIS:H	2:D:7:HIS:HE1	1.58	0.49
1:A:236:TRP:O	1:A:239:LYS:NZ	2.43	0.49
1:A:73:ARG:NH2	4:H:26(A):SER:CA	2.58	0.49
1:C:402:ARG:HH22	1:C:409:LYS:NZ	2.02	0.49
4:H:46:MET:HG3	4:H:61:PHE:HE2	1.77	0.49
3:I:36:TRP:NE1	3:I:69:ILE:HD13	2.27	0.49
1:A:153:VAL:HG23	3:I:100(I):TRP:CH2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:TYR:OH	1:A:277:MET:CG	2.57	0.49
1:A:484:ILE:O	1:A:488:CYS:CB	2.60	0.49
1:B:59:TYR:CE1	1:B:221:ILE:HG13	2.47	0.49
1:C:421:MET:O	1:C:421:MET:HG3	2.13	0.49
2:E:20:LEU:O	2:E:23:ARG:O	2.30	0.49
3:G:73:THR:O	3:G:74:SER:C	2.46	0.49
3:I:50:TRP:HE1	3:I:68:THR:HA	1.75	0.49
3:I:27:TYR:HD1	3:I:94:ARG:HH12	1.55	0.49
1:A:280:ALA:C	1:A:281:LYS:CD	2.75	0.49
1:A:345:MET:CE	1:A:387:ILE:HG12	2.42	0.49
1:A:229:ALA:CB	1:B:81:TYR:HB2	2.42	0.49
1:C:107:LEU:HG	1:C:108:PHE:H	1.77	0.49
1:C:47:THR:HG21	1:C:283:ARG:NE	2.27	0.49
1:C:351:THR:CG2	1:C:388:VAL:CG1	2.82	0.49
1:C:79:GLU:OE2	1:C:94:ARG:NE	2.40	0.49
3:G:37:VAL:HG22	3:G:47:TRP:HD1	1.76	0.49
4:H:34:TRP:H	4:H:47:LEU:HD13	1.70	0.49
4:H:32:VAL:C	4:H:47:LEU:HD22	2.32	0.49
4:L:35:PHE:CZ	4:L:45:LEU:HD12	2.47	0.49
4:M:22:CYS:CB	4:M:70:ALA:HB3	2.42	0.49
1:A:160:THR:HG22	1:A:161:ASP:N	2.27	0.49
1:A:332:TYR:HE2	1:A:341:VAL:HG13	1.77	0.49
1:A:464:SER:HB3	2:F:75:SER:CB	2.19	0.49
1:B:213:VAL:HG12	1:B:214:HIS:H	1.78	0.49
1:B:348:ASP:OD1	1:B:351:THR:O	2.30	0.49
1:B:45:LEU:C	1:B:46:VAL:HG23	2.32	0.49
1:C:148:HIS:CG	1:C:149:SER:H	2.31	0.49
1:C:167:VAL:HG11	1:C:176:ALA:HB1	1.94	0.49
1:C:198:PHE:HE1	1:C:201:LEU:HD22	1.77	0.49
1:C:439:ASN:O	1:C:440:SER:C	2.51	0.49
1:C:56:VAL:HG12	1:C:129:SER:CB	2.41	0.49
2:D:70:ILE:HD12	2:D:74:TYR:HB3	1.94	0.49
2:D:74:TYR:CZ	2:F:69:LEU:HG	2.47	0.49
3:I:87:THR:HA	3:I:109:VAL:O	2.12	0.49
4:L:36:GLN:HE21	4:L:83:ALA:HB2	1.78	0.49
4:L:34:TRP:CZ3	4:L:87:CYS:HB3	2.48	0.49
4:M:13:SER:O	4:M:77:LEU:HG	2.12	0.49
1:B:21:VAL:HG12	1:B:293:LEU:O	2.11	0.49
1:C:132:PRO:HB2	1:C:193:ARG:NH1	2.28	0.49
1:C:142:SER:O	1:C:143:VAL:CG1	2.60	0.49
2:E:11:LYS:CG	2:E:12:LEU:N	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2:VAL:HG11	2:F:27:LYS:HD2	1.94	0.49
3:G:50:TRP:CD1	3:G:69:ILE:HG12	2.48	0.49
3:I:69:ILE:HG22	3:I:79:TYR:C	2.31	0.49
1:A:329:GLU:OE2	1:A:373:LYS:HE2	2.13	0.49
1:A:3:CYS:SG	1:A:44:GLU:HB2	2.53	0.49
1:C:457:PHE:HB3	1:C:460:MET:CG	2.43	0.49
1:A:419:LYS:HB3	2:D:15:ARG:HH12	1.77	0.49
2:E:56:SER:C	2:E:58:SER:H	2.15	0.49
4:H:35:PHE:CE2	4:H:45:LEU:HD13	2.48	0.49
3:K:83:ARG:O	3:K:111:VAL:HG21	2.12	0.49
4:M:103:LEU:HD23	4:M:104:THR:N	2.28	0.49
1:A:459:GLY:HA2	2:D:9:THR:OG1	2.13	0.49
1:C:90:TYR:CE1	1:C:118:LYS:HD3	2.48	0.49
1:C:245:PHE:CB	1:C:255:VAL:HA	2.40	0.49
1:C:312:PHE:CD1	1:C:330:VAL:HG11	2.47	0.49
1:C:326:VAL:HG22	1:C:400:TRP:CE2	2.48	0.49
1:C:491:LEU:O	1:C:494:VAL:N	2.45	0.49
4:H:22:CYS:N	4:H:70:ALA:O	2.42	0.49
4:M:88:SER:CA	4:M:97:PHE:CD1	2.94	0.49
1:A:142:SER:HA	1:A:164:ARG:HG2	1.94	0.49
1:A:1:ILE:CD1	1:A:144:HIS:CD2	2.92	0.49
1:A:86:SER:HA	1:B:235:HIS:HD2	1.78	0.49
1:B:27:HIS:HB2	1:B:45:LEU:CD2	2.36	0.49
1:B:473:MET:C	1:B:476:GLY:H	2.16	0.49
1:C:225:TRP:HB2	1:C:237:ASN:CB	2.35	0.49
1:C:27:HIS:CB	1:C:285:SER:O	2.58	0.49
2:D:74:TYR:CB	2:F:73:ALA:CB	2.86	0.49
4:L:18:ILE:HG23	4:L:77:LEU:HD11	1.95	0.49
4:M:47:LEU:CD2	4:M:48:TYR:N	2.76	0.49
4:M:45:LEU:HD11	4:M:48:TYR:HB3	1.95	0.49
1:C:11:PHE:CE2	1:C:32:THR:OG1	2.39	0.49
4:M:4:LEU:CD1	4:M:87:CYS:HB2	2.43	0.49
1:A:252:ARG:HH11	1:A:252:ARG:CG	2.26	0.48
1:B:285:SER:O	1:B:286:SER:OG	2.27	0.48
1:C:362:ASN:C	1:C:362:ASN:HD22	2.16	0.48
3:I:100(G):THR:OG1	3:I:100(I):TRP:O	2.27	0.48
4:M:61:PHE:CD1	4:M:74:ILE:HG12	2.48	0.48
1:B:169:ILE:HD13	1:B:190:CYS:SG	2.53	0.48
1:C:207:ASN:N	1:C:207:ASN:OD1	2.46	0.48
1:C:236:TRP:HB2	1:C:239:LYS:HE3	1.94	0.48
1:C:418:ALA:O	1:C:422:ALA:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:THR:O	1:C:137:TYR:O	2.31	0.48
3:K:100(C):TYR:OH	3:K:100(F):PRO:HB3	2.12	0.48
4:L:15:GLY:O	4:L:76:GLY:N	2.45	0.48
4:M:34:TRP:HB2	4:M:47:LEU:HB2	1.96	0.48
1:C:21:VAL:CG2	1:C:293:LEU:HB2	2.43	0.48
1:A:108:PHE:CB	1:C:321:THR:HA	2.43	0.48
1:C:453:PHE:O	1:C:453:PHE:CD1	2.66	0.48
1:C:99:ARG:HD3	1:C:103:ASN:HD21	1.72	0.48
2:D:70:ILE:HD11	2:D:74:TYR:CD2	2.47	0.48
3:G:13:LYS:HA	3:G:112:SER:OG	2.14	0.48
3:I:97:VAL:HG23	3:I:100(C):TYR:CD1	2.46	0.48
1:B:23:VAL:HG21	1:B:31:VAL:CG1	2.38	0.48
1:B:402:ARG:O	1:B:403:SER:OG	2.30	0.48
1:C:148:HIS:HA	1:C:375:MET:SD	2.54	0.48
1:C:209:LYS:HG3	1:C:211:TRP:CZ3	2.48	0.48
1:C:214:HIS:CE1	1:C:216:GLU:HB2	2.49	0.48
1:C:426:ASP:O	1:C:429:TRP:HD1	1.97	0.48
1:C:490:ALA:O	1:C:491:LEU:HD12	2.14	0.48
2:D:31:ARG:HA	2:F:4:LEU:HD22	1.94	0.48
4:H:34:TRP:CZ3	4:H:87:CYS:HB3	2.48	0.48
3:I:29:PHE:CG	3:I:76:SER:HB2	2.44	0.48
4:L:29:PHE:HB3	4:L:31:TYR:HD2	1.78	0.48
1:A:312:PHE:O	1:A:313:THR:C	2.49	0.48
1:C:128:LYS:O	1:C:203:TYR:N	2.46	0.48
1:C:42:ASP:CG	1:C:142:SER:HB2	2.34	0.48
1:C:214:HIS:NE2	2:F:7:HIS:ND1	2.61	0.48
1:C:3:CYS:SG	1:C:42:ASP:CB	2.98	0.48
2:D:9:THR:HG23	2:D:10:ARG:HG2	1.96	0.48
2:E:40:PRO:O	2:E:43:ALA:N	2.45	0.48
2:F:52:LEU:HD23	2:F:52:LEU:O	2.13	0.48
1:A:371:ASN:O	1:A:372:SER:C	2.51	0.48
1:C:314:PHE:CE2	1:C:398:HIS:CD2	3.01	0.48
1:C:405:SER:O	1:C:408:GLY:N	2.46	0.48
3:G:31:SER:CA	3:G:97:VAL:CG1	2.91	0.48
4:H:29:PHE:HB3	4:H:31:TYR:HD2	1.78	0.48
3:I:9:ALA:O	3:I:109:VAL:N	2.47	0.48
4:L:12:GLY:H	4:L:106:LEU:C	2.16	0.48
1:B:1:ILE:C	1:B:3:CYS:H	2.17	0.48
1:C:148:HIS:CD2	1:C:149:SER:H	2.31	0.48
2:E:32:VAL:HG23	2:E:72:PRO:CB	2.41	0.48
3:G:97:VAL:HA	3:G:100(C):TYR:HD1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:77:LEU:N	4:H:77:LEU:HD12	2.29	0.48
4:M:38:HIS:HB3	4:M:39:PRO:HD2	1.96	0.48
1:A:382:PHE:HZ	1:A:409:LYS:HD3	1.77	0.48
1:C:142:SER:C	1:C:143:VAL:HG12	2.34	0.48
1:C:312:PHE:CE1	1:C:332:TYR:HD1	2.31	0.48
1:C:312:PHE:HD1	1:C:330:VAL:HG11	1.78	0.48
3:K:50:TRP:CD1	3:K:69:ILE:HG12	2.48	0.48
1:C:476:GLY:HA3	1:C:488:CYS:SG	2.54	0.48
4:H:60:ARG:HD3	4:H:76:GLY:O	2.14	0.48
3:I:50:TRP:CE3	3:I:69:ILE:HD13	2.49	0.48
3:K:14:PRO:HD3	3:K:112:SER:OG	2.14	0.48
1:B:148:HIS:CD2	1:B:373:LYS:CG	2.97	0.48
1:B:434:VAL:CG1	1:B:435:GLY:N	2.69	0.48
1:C:143:VAL:O	1:C:144:HIS:C	2.52	0.48
1:C:426:ASP:HB3	1:C:446:HIS:CB	2.44	0.48
2:E:53:LEU:CD1	2:E:63:TYR:HD2	2.22	0.48
1:A:82:LEU:HD11	1:A:116:CYS:SG	2.54	0.47
1:B:430:ASP:HA	1:B:439:ASN:HD21	1.76	0.47
1:C:348:ASP:O	1:C:351:THR:O	2.30	0.47
1:C:57:ARG:CD	1:C:225:TRP:CE3	2.93	0.47
4:H:78:GLN:HG2	4:H:78:GLN:O	2.14	0.47
1:A:73:ARG:HH22	4:H:26(A):SER:CA	2.20	0.47
1:A:75:PRO:HG2	1:A:107:LEU:CB	2.44	0.47
3:I:14:PRO:HG3	3:I:111:VAL:CG1	2.44	0.47
3:I:48:MET:CB	3:I:63:PHE:CD2	2.97	0.47
1:A:8:ASN:O	1:A:8:ASN:ND2	2.47	0.47
1:B:251:LYS:C	1:B:252:ARG:HG2	2.34	0.47
1:C:99:ARG:CG	1:C:103:ASN:CG	2.81	0.47
2:E:53:LEU:HD11	2:E:63:TYR:HD2	1.67	0.47
3:G:12:LYS:HZ1	3:G:18:VAL:HA	1.80	0.47
4:H:48:TYR:HB3	4:H:54:PRO:HD3	1.95	0.47
3:I:40:ALA:H	3:I:43:GLN:HB3	1.77	0.47
3:I:87:THR:O	3:I:87:THR:HG23	2.14	0.47
4:L:11:SER:HB3	4:L:104:THR:CB	2.44	0.47
4:L:6:GLN:NE2	4:L:85:TYR:O	2.47	0.47
4:M:88:SER:HA	4:M:97:PHE:CD1	2.49	0.47
1:A:46:VAL:HG23	3:I:100:TYR:CZ	2.41	0.47
1:B:333:ALA:CB	1:B:370:GLU:CG	2.91	0.47
1:C:61:TYR:OH	1:C:123:LYS:HB3	2.15	0.47
1:C:2:ARG:O	1:C:2:ARG:HG3	2.14	0.47
1:C:352:LEU:O	1:C:353:THR:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:GLY:O	1:C:428:ALA:HB3	2.15	0.47
2:D:27:LYS:HD3	2:D:30:ILE:HG21	1.96	0.47
1:C:8:ASN:ND2	2:F:15:ARG:HD2	2.26	0.47
3:G:66:ARG:HH12	3:G:82:LEU:HD11	1.77	0.47
3:I:16:ALA:O	3:I:82(C):LEU:N	2.47	0.47
3:I:43:GLN:CG	3:I:44:ARG:H	2.26	0.47
3:K:19:LYS:NZ	3:K:81:GLU:OE1	2.39	0.47
4:L:35:PHE:CE1	4:L:45:LEU:HB2	2.49	0.47
1:C:63:ALA:HB2	1:C:242:LEU:HD13	1.97	0.47
1:C:9:ARG:NH1	1:C:377:GLU:OE2	2.47	0.47
1:C:389:ILE:CG2	1:C:395:LYS:CB	2.89	0.47
2:F:11:LYS:C	2:F:12:LEU:HD12	2.35	0.47
1:B:196:LEU:HD23	1:B:198:PHE:CE1	2.49	0.47
1:C:167:VAL:HG11	1:C:176:ALA:CB	2.45	0.47
1:A:27:HIS:CE1	1:C:249:HIS:CE1	3.02	0.47
1:C:8:ASN:O	1:C:29:GLY:HA3	2.14	0.47
4:H:6:GLN:NE2	4:H:85:TYR:O	2.47	0.47
3:I:18:VAL:CB	3:I:82(C):LEU:HD21	2.42	0.47
1:B:1:ILE:O	1:B:3:CYS:N	2.47	0.47
1:B:297:LYS:C	1:B:298:LEU:HD12	2.35	0.47
1:B:418:ALA:HB1	1:B:497:PHE:CZ	2.35	0.47
1:C:214:HIS:HE2	1:C:217:TRP:HB2	1.78	0.47
1:C:405:SER:O	1:C:407:ILE:HG13	2.15	0.47
2:E:11:LYS:HG2	2:E:12:LEU:O	2.15	0.47
2:E:23:ARG:O	2:E:24:GLU:HB2	2.14	0.47
3:K:12:LYS:O	3:K:16:ALA:HB2	2.12	0.47
4:L:47:LEU:O	4:L:53:ARG:HA	2.15	0.47
1:A:159:GLU:CG	1:A:160:THR:H	2.13	0.47
1:A:209:LYS:HE3	1:C:256:VAL:HG13	1.96	0.47
1:A:365:ILE:HG22	1:A:366:THR:H	1.73	0.47
1:B:213:VAL:HG12	1:B:214:HIS:N	2.30	0.47
1:C:217:TRP:CH2	1:C:269:LEU:HD21	2.49	0.47
4:H:3:ALA:O	4:H:4:LEU:C	2.53	0.47
4:H:46:MET:SD	4:H:57:VAL:HG22	2.55	0.47
3:I:18:VAL:N	3:I:82(C):LEU:CD2	2.60	0.47
3:I:97:VAL:CG2	3:I:98:ASP:N	2.75	0.47
1:A:239:LYS:O	1:A:243:VAL:HG22	2.15	0.47
1:A:99:ARG:HD2	1:A:251:LYS:HZ3	1.79	0.47
1:B:71:ASP:HB3	1:B:114:VAL:CG1	2.45	0.47
4:H:82:GLU:HB3	4:H:103:LEU:CD2	2.45	0.47
3:I:50:TRP:NE1	3:I:59:TYR:CD1	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:TRP:CH2	1:A:221:ILE:CD1	2.76	0.47
1:C:12:VAL:CG2	1:C:33:VAL:HA	2.44	0.47
1:B:252:ARG:CB	3:K:100(D):TRP:CD1	2.98	0.47
3:K:27:TYR:CE1	3:K:32:TYR:CB	2.96	0.47
3:K:99:ASP:C	3:K:100(A):GLY:H	2.18	0.47
3:K:100(K):PHE:HB2	4:L:35:PHE:CZ	2.50	0.47
4:M:84:ASP:OD1	4:M:102:LYS:CB	2.63	0.47
1:A:262:GLU:OE1	1:C:259:GLY:HA3	2.15	0.47
1:C:97:VAL:HG21	1:C:113:LEU:HD21	1.96	0.47
1:A:249:HIS:CG	2:F:16:SER:CB	2.98	0.47
3:G:39:GLN:NE2	4:H:37:GLN:HE22	2.12	0.47
3:K:48:MET:HB3	3:K:63:PHE:CD2	2.50	0.47
1:A:71:ASP:HB3	1:A:114:VAL:HG12	1.97	0.46
1:A:147:GLN:HE22	1:A:164:ARG:NH1	2.13	0.46
1:A:22:ASP:OD1	1:A:433:SER:OG	2.18	0.46
1:A:21:VAL:HG13	1:A:293:LEU:HB3	1.98	0.46
1:B:7:SER:HB2	1:B:322:LEU:HD22	1.97	0.46
1:A:263:GLY:N	1:C:260:SER:O	2.48	0.46
2:F:59:GLN:HA	2:F:62:ILE:HB	1.97	0.46
1:B:99:ARG:CD	3:K:100(E):PHE:CE1	2.96	0.46
4:M:18:ILE:HG22	4:M:74:ILE:HB	1.96	0.46
1:A:148:HIS:CB	1:A:151:MET:SD	3.02	0.46
1:A:71:ASP:HB3	1:A:114:VAL:CG1	2.45	0.46
1:B:337:GLY:H	1:B:367:GLU:HG3	1.77	0.46
1:B:437:ALA:O	1:B:439:ASN:N	2.49	0.46
2:F:54:GLY:HA2	2:F:59:GLN:HE22	1.75	0.46
3:K:70:THR:OG1	3:K:79:TYR:HB2	2.15	0.46
1:C:271:GLY:CA	2:F:18:THR:CG2	2.93	0.46
1:C:473:MET:HA	1:C:488:CYS:HB2	1.97	0.46
3:K:97:VAL:HA	3:K:100(C):TYR:HD1	1.81	0.46
3:K:52:ASN:HD22	3:K:56:ASN:HD22	1.40	0.46
4:M:4:LEU:HA	4:M:4:LEU:HD22	1.78	0.46
1:A:350:GLN:CD	1:A:351:THR:H	2.18	0.46
1:C:216:GLU:O	1:C:220:ASP:HB2	2.16	0.46
4:H:22:CYS:O	4:H:70:ALA:N	2.48	0.46
4:H:48:TYR:C	4:H:48:TYR:CD1	2.87	0.46
3:I:23:LYS:HE2	3:I:75:ALA:HB1	1.97	0.46
3:K:51:ILE:HG21	4:L:95:TRP:CZ3	2.50	0.46
4:M:38:HIS:CD2	4:M:83:ALA:HB2	2.43	0.46
1:A:22:ASP:HA	1:A:292:ARG:HA	1.98	0.46
1:A:312:PHE:CE1	1:A:389:ILE:CG2	2.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:GLN:O	1:B:86:SER:OG	2.30	0.46
1:C:214:HIS:NE2	1:C:217:TRP:HB2	2.31	0.46
1:C:312:PHE:HD2	1:C:391:VAL:HG23	1.80	0.46
1:C:391:VAL:CB	1:C:394:LYS:O	2.62	0.46
1:C:475:LEU:O	1:C:479:THR:HG23	2.15	0.46
2:D:34:ASN:HA	2:D:37:PHE:HB3	1.98	0.46
3:G:70:THR:OG1	3:G:79:TYR:HB2	2.15	0.46
1:A:15:MET:CE	1:A:38:LYS:HE3	2.46	0.46
1:B:171:PRO:CA	1:B:192:PRO:HG2	2.45	0.46
1:B:217:TRP:HD1	2:E:6:SER:N	2.11	0.46
1:B:27:HIS:HA	1:B:45:LEU:HB3	1.98	0.46
1:C:203:TYR:CD1	1:C:277:MET:HE1	2.47	0.46
3:K:99:ASP:C	3:K:100(A):GLY:N	2.66	0.46
4:L:34:TRP:HD1	4:L:47:LEU:HD23	1.80	0.46
4:L:82:GLU:HA	4:L:103:LEU:HD22	1.98	0.46
1:A:465:GLN:OE1	1:A:498:LEU:HD22	2.16	0.46
1:B:341:VAL:HG21	1:B:374:MET:CE	2.45	0.46
1:C:176:ALA:O	1:C:187:GLY:HA2	2.16	0.46
1:A:108:PHE:HB2	1:C:321:THR:HA	1.98	0.46
1:A:423:VAL:HG23	2:D:13:GLN:HG3	1.97	0.46
2:F:18:THR:CG2	2:F:19:TRP:N	2.58	0.46
3:G:3:GLN:O	3:G:4:LEU:HD12	2.15	0.46
1:C:84:LYS:HZ3	4:M:93:ARG:HH22	1.63	0.46
1:A:312:PHE:CD1	1:A:396:ILE:CD1	2.99	0.46
1:A:453:PHE:HE1	1:A:495:LEU:HD11	1.81	0.46
1:A:98:ASP:O	1:A:110:LYS:O	2.34	0.46
1:B:333:ALA:CA	1:B:370:GLU:HG2	2.38	0.46
1:B:449:PHE:O	1:B:453:PHE:HB2	2.15	0.46
1:C:70:SER:OG	1:C:252:ARG:CZ	2.64	0.46
1:C:96:LEU:HD22	1:C:110:LYS:HB3	1.97	0.46
3:I:11:VAL:HG12	3:I:110:THR:HB	0.53	0.46
1:B:82:LEU:HD12	4:L:93:ARG:NH1	2.31	0.46
4:M:22:CYS:HB3	4:M:70:ALA:HB3	1.96	0.46
1:A:302:GLY:HA3	1:A:305:TYR:HE2	1.80	0.46
1:A:320:GLU:HB2	1:A:400:TRP:CZ2	2.51	0.46
1:A:461:SER:HB3	2:F:75:SER:C	2.36	0.46
1:B:344:GLN:CD	1:B:352:LEU:CD1	2.84	0.46
1:C:214:HIS:H	1:C:214:HIS:HD2	1.62	0.46
2:F:25:TYR:CE1	2:F:26:THR:HG23	2.51	0.46
4:L:4:LEU:HD22	4:L:23:THR:C	2.36	0.46
1:A:62:GLU:HB3	1:A:122:SER:OG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:LEU:O	1:A:380:PRO:HD3	2.16	0.46
1:A:424:LEU:O	1:A:427:THR:HG22	2.15	0.46
1:B:424:LEU:HB3	1:B:427:THR:HB	1.97	0.46
1:B:462:TRP:CZ3	2:E:25:TYR:HE2	2.34	0.46
1:C:215:LYS:HB3	1:C:215:LYS:NZ	2.31	0.46
1:C:33:VAL:HG22	1:C:41:VAL:O	2.16	0.46
3:I:9:ALA:N	3:I:107:THR:HG22	2.27	0.46
3:K:29:PHE:HA	3:K:32:TYR:CD2	2.49	0.46
3:K:6:GLU:OE2	3:K:104:GLY:HA3	2.16	0.46
1:A:25:LEU:O	1:A:289:LEU:N	2.48	0.45
1:B:161:ASP:C	1:B:163:ASN:H	2.18	0.45
1:B:59:TYR:CZ	1:B:221:ILE:CD1	2.95	0.45
1:C:135:LEU:HD23	1:C:136:GLU:N	2.31	0.45
4:H:83:ALA:O	4:H:84:ASP:C	2.54	0.45
3:I:95:ASP:OD1	3:I:100(G):THR:OG1	2.33	0.45
3:K:51:ILE:HD13	3:K:100(C):TYR:CD2	2.50	0.45
4:M:37:GLN:CD	4:M:43:PRO:HG3	2.37	0.45
4:M:78:GLN:O	4:M:79:ALA:C	2.54	0.45
1:A:100:GLY:O	1:A:101:TRP:HB2	2.16	0.45
1:A:3:CYS:HB2	1:A:42:ASP:OD2	2.16	0.45
1:B:137:TYR:CE1	1:B:289:LEU:HD11	2.51	0.45
1:C:20:TRP:NE1	1:C:292:ARG:HD2	2.32	0.45
2:D:19:TRP:CD1	2:D:20:LEU:CG	2.95	0.45
4:L:60:ARG:NH2	4:L:78:GLN:HB3	2.31	0.45
1:B:95:THR:O	1:B:96:LEU:C	2.52	0.45
3:G:67:VAL:CG1	3:G:82:LEU:HD13	2.46	0.45
3:G:100(H):LEU:CG	4:H:49:ASP:OD2	2.64	0.45
3:I:84:SER:CA	3:I:111:VAL:CB	2.75	0.45
4:M:12:GLY:O	4:M:77:LEU:CD1	2.65	0.45
1:A:264:ALA:O	1:A:267:THR:OG1	2.28	0.45
1:A:289:LEU:HD23	1:A:290:LYS:N	2.31	0.45
1:A:30:CYS:SG	1:A:44:GLU:HG3	2.56	0.45
1:A:377:GLU:C	1:A:378:LEU:HD12	2.37	0.45
1:C:386:TYR:O	1:C:387:ILE:C	2.53	0.45
1:C:99:ARG:HD3	1:C:105:CYS:SG	2.56	0.45
4:H:9:SER:CB	4:H:102:LYS:HB3	2.19	0.45
1:A:311:ALA:CA	1:A:333:ALA:H	2.28	0.45
1:B:295:MET:O	1:B:297:LYS:N	2.50	0.45
1:C:214:HIS:CG	2:F:10:ARG:HG2	2.52	0.45
1:B:462:TRP:CD2	2:E:25:TYR:CD2	3.03	0.45
3:G:28:THR:CG2	3:G:30:THR:HG1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:10:VAL:O	4:H:104:THR:CA	2.63	0.45
4:H:48:TYR:CD1	4:H:48:TYR:O	2.70	0.45
3:I:89:ILE:HG21	3:I:91:TYR:CZ	2.51	0.45
1:A:138:ARG:NH1	1:A:138:ARG:CG	2.73	0.45
1:A:247:ASP:HA	1:A:253:GLN:HA	1.99	0.45
1:A:81:TYR:CD2	1:B:229:ALA:CB	3.00	0.45
1:C:196:LEU:HD12	1:C:196:LEU:O	2.16	0.45
1:C:57:ARG:HA	1:C:227:ALA:O	2.16	0.45
1:C:203:TYR:CZ	1:C:284:LEU:HD13	2.51	0.45
2:D:73:ALA:HB2	2:F:74:TYR:HB2	1.94	0.45
3:G:100(K):PHE:HE2	4:H:97:PHE:CZ	2.25	0.45
3:G:97:VAL:HG23	3:G:100(C):TYR:HB2	1.98	0.45
3:I:36:TRP:HB2	3:I:50:TRP:HZ3	1.82	0.45
4:L:22:CYS:O	4:L:70:ALA:N	2.50	0.45
4:M:48:TYR:CD2	4:M:52:SER:O	2.62	0.45
1:A:160:THR:CG2	1:A:161:ASP:N	2.79	0.45
1:A:332:TYR:CE2	1:A:341:VAL:HG13	2.51	0.45
1:A:65:ILE:HG23	1:A:117:ALA:HB1	1.98	0.45
1:B:374:MET:CG	1:B:375:MET:H	2.18	0.45
1:C:176:ALA:HB2	1:C:188:LEU:CD1	2.47	0.45
1:C:127:GLY:HA3	1:C:218:PHE:CZ	2.52	0.45
1:C:419:LYS:HA	1:C:422:ALA:HB2	1.94	0.45
4:H:35:PHE:N	4:H:35:PHE:CD2	2.82	0.45
3:I:39:GLN:O	3:I:88:ALA:CB	2.59	0.45
1:B:226:HIS:CD2	1:B:234:PRO:HB3	2.52	0.45
1:B:352:LEU:HD22	1:B:352:LEU:HA	1.79	0.45
1:B:480:LYS:HB3	1:B:481:ASN:H	1.34	0.45
1:C:149:SER:HB3	3:G:100(I):TRP:CZ3	2.50	0.45
1:C:409:LYS:CD	1:C:409:LYS:C	2.86	0.45
3:G:5:VAL:HG12	3:G:6:GLU:N	2.32	0.45
3:I:5:VAL:HA	3:I:105:GLN:HG2	1.98	0.45
3:I:18:VAL:CA	3:I:82(C):LEU:HD21	2.46	0.45
3:I:9:ALA:H	3:I:107:THR:HG22	1.78	0.45
1:A:110:LYS:HB3	1:A:111:GLY:H	1.40	0.45
1:A:151:MET:SD	1:A:373:LYS:CG	3.05	0.45
1:B:206:MET:CE	1:B:262:GLU:HG3	2.47	0.45
1:B:373:LYS:O	1:B:374:MET:C	2.53	0.45
1:C:25:LEU:O	1:C:45:LEU:HD12	2.17	0.45
2:E:56:SER:OG	2:E:59:GLN:N	2.48	0.45
2:E:66:MET:O	2:E:70:ILE:HG23	2.17	0.45
2:F:54:GLY:HA2	2:F:59:GLN:NE2	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:73:THR:C	3:G:76:SER:H	2.20	0.45
3:I:40:ALA:N	3:I:88:ALA:CB	2.80	0.45
1:A:151:MET:CA	4:M:48:TYR:OH	2.64	0.45
4:M:49:ASP:O	4:M:49:ASP:CG	2.55	0.45
1:A:169:ILE:CG2	1:A:176:ALA:CB	2.92	0.45
1:A:87:ASP:C	1:A:89:GLN:H	2.21	0.45
1:C:132:PRO:O	1:C:171:PRO:HG3	2.17	0.45
1:C:1:ILE:C	1:C:3:CYS:H	2.20	0.45
2:E:60:LYS:HG3	2:E:61:VAL:N	2.32	0.45
3:G:52:ASN:HD21	3:G:56:ASN:HD22	1.53	0.45
4:H:30:ASN:HA	4:H:65:LYS:HZ2	1.82	0.45
3:I:29:PHE:O	3:I:32:TYR:CD2	2.69	0.45
1:A:2:ARG:CD	1:A:44:GLU:OE1	2.65	0.44
1:C:252:ARG:CG	1:C:253:GLN:N	2.59	0.44
1:C:290:LYS:CE	1:C:430:ASP:OD2	2.65	0.44
1:C:62:GLU:OE1	1:C:122:SER:HB2	2.16	0.44
2:D:35:TRP:CE3	2:D:35:TRP:O	2.71	0.44
2:E:60:LYS:O	2:E:64:LEU:N	2.42	0.44
2:F:19:TRP:CD1	2:F:20:LEU:CG	2.95	0.44
4:H:50:VAL:CG1	4:H:51:THR:H	2.15	0.44
3:I:72:ASP:O	3:I:72:ASP:OD1	2.34	0.44
3:I:19:LYS:NZ	3:I:81:GLU:OE1	2.39	0.44
1:A:311:ALA:O	1:A:312:PHE:HB2	2.18	0.44
1:A:70:SER:OG	1:A:113:LEU:HD11	2.17	0.44
1:B:146:SER:O	1:B:374:MET:O	2.34	0.44
1:C:374:MET:O	1:C:376:LEU:HD12	2.16	0.44
2:D:11:LYS:CG	2:D:12:LEU:H	2.17	0.44
1:B:273:LEU:CD2	2:E:12:LEU:HD13	2.45	0.44
3:I:27:TYR:O	3:I:27:TYR:CG	2.70	0.44
3:I:36:TRP:CZ3	3:I:92:CYS:HB3	2.53	0.44
3:K:89:ILE:HG13	3:K:108:LEU:CA	2.46	0.44
1:A:463:PHE:HE2	2:F:74:TYR:CD2	2.35	0.44
1:B:97:VAL:HG21	1:B:113:LEU:HD23	1.98	0.44
1:B:355:VAL:O	1:B:355:VAL:HG13	2.17	0.44
1:A:322:LEU:CD1	1:C:108:PHE:O	2.66	0.44
3:G:31:SER:HA	3:G:97:VAL:CG1	2.46	0.44
4:H:34:TRP:CG	4:H:47:LEU:CD1	3.00	0.44
3:I:29:PHE:C	3:I:32:TYR:HB3	2.38	0.44
3:I:33:ALA:HB2	3:I:96:LYS:CA	2.42	0.44
3:I:50:TRP:HH2	3:I:80:MET:CG	2.01	0.44
4:M:48:TYR:CE2	4:M:52:SER:CB	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:ILE:O	1:A:2:ARG:HB3	2.17	0.44
1:A:356:GLY:O	1:A:357:ARG:C	2.50	0.44
1:C:325:THR:HG23	1:C:377:GLU:HG3	1.99	0.44
1:C:320:GLU:CA	1:C:400:TRP:HH2	2.20	0.44
1:A:153:VAL:HG23	3:I:100(I):TRP:CZ2	2.53	0.44
3:I:1:GLU:OE2	3:I:102:TYR:CZ	2.70	0.44
3:I:9:ALA:HB1	3:I:109:VAL:CG2	2.46	0.44
1:A:15:MET:HB3	1:A:21:VAL:HB	2.00	0.44
1:A:6:VAL:HG12	1:A:9:ARG:HB3	1.99	0.44
1:A:85:GLN:HE22	1:A:94:ARG:CZ	2.31	0.44
1:B:437:ALA:C	1:B:439:ASN:N	2.70	0.44
1:B:425:GLY:C	1:B:446:HIS:HE1	2.21	0.44
1:C:26:GLU:C	1:C:45:LEU:CB	2.82	0.44
2:E:18:THR:O	2:E:19:TRP:C	2.56	0.44
3:G:3:GLN:C	3:G:4:LEU:HD12	2.37	0.44
3:G:48:MET:CE	3:G:67:VAL:CG1	2.95	0.44
3:G:92:CYS:O	3:G:104:GLY:N	2.50	0.44
4:H:17:SER:HA	4:H:74:ILE:O	2.18	0.44
3:K:22:CYS:HB2	3:K:36:TRP:CH2	2.52	0.44
1:A:380:PRO:HG2	1:A:402:ARG:HD3	1.99	0.44
1:C:359:ILE:HD12	1:C:379:ASP:N	2.31	0.44
1:C:457:PHE:CE2	1:C:468:ILE:HD13	2.52	0.44
1:A:108:PHE:CE2	1:C:4:ILE:HD13	2.31	0.44
2:F:2:VAL:HG12	2:F:2:VAL:O	2.17	0.44
1:C:461:SER:HB2	2:F:8:SER:O	2.17	0.44
3:G:60:SER:O	3:G:61:GLN:C	2.53	0.44
3:I:103:TRP:NE1	4:M:43:PRO:O	2.50	0.44
3:K:34:MET:SD	3:K:92:CYS:HB2	2.58	0.44
4:M:48:TYR:O	4:M:48:TYR:CG	2.70	0.44
1:A:341:VAL:O	1:A:363:PRO:HG2	2.17	0.44
1:A:32:THR:OG1	1:A:42:ASP:OD1	2.33	0.44
1:B:375:MET:O	1:B:376:LEU:O	2.35	0.44
1:C:251:LYS:CG	3:I:100(D):TRP:CD1	3.01	0.44
1:C:292:ARG:O	1:C:292:ARG:HG3	2.18	0.44
1:C:83:ASP:O	1:C:86:SER:HB3	2.18	0.44
2:E:32:VAL:HG13	2:E:33:GLU:N	2.33	0.44
3:I:53:GLY:O	3:I:71:ARG:CD	2.66	0.44
1:A:148:HIS:CG	1:A:151:MET:SD	3.10	0.44
1:A:312:PHE:HE2	1:A:395:LYS:HB2	1.83	0.44
1:A:315:THR:HG22	1:A:316:LYS:NZ	2.32	0.44
1:B:182:GLY:O	1:B:301:LYS:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:THR:OG1	1:B:325:THR:HG22	2.18	0.44
1:C:217:TRP:CH2	1:C:221:ILE:HD11	2.53	0.44
1:C:290:LYS:O	1:C:291:CYS:C	2.56	0.44
1:C:308:CYS:CB	1:C:340:LYS:O	2.66	0.44
1:C:418:ALA:HB1	1:C:497:PHE:HZ	1.79	0.44
2:E:20:LEU:O	2:E:22:SER:N	2.51	0.44
3:G:33:ALA:HB1	3:G:95:ASP:H	1.83	0.44
4:H:34:TRP:CD1	4:H:72:LEU:HB2	2.52	0.44
3:I:48:MET:SD	3:I:63:PHE:CE2	3.11	0.44
3:I:53:GLY:O	3:I:71:ARG:NE	2.51	0.44
3:K:92:CYS:O	3:K:104:GLY:N	2.50	0.44
4:M:53:ARG:CB	4:M:57:VAL:HA	2.48	0.44
1:A:136:GLU:HG3	1:A:168:GLU:HG3	1.99	0.44
1:A:151:MET:SD	4:M:52:SER:OG	2.75	0.44
1:B:202:TYR:HH	1:B:215:LYS:HG3	1.78	0.44
1:B:148:HIS:CA	1:B:375:MET:SD	2.95	0.44
1:B:24:VAL:CG1	1:B:424:LEU:HD21	2.42	0.44
1:C:10:ASP:OD2	1:C:431:PHE:CE2	2.71	0.44
1:C:321:THR:CG2	1:C:322:LEU:H	2.28	0.44
1:C:334:GLY:HA3	1:C:370:GLU:HA	1.99	0.44
1:C:62:GLU:HG2	1:C:63:ALA:N	2.33	0.44
3:I:8:GLY:C	3:I:107:THR:HG23	2.33	0.44
1:A:148:HIS:HB2	1:A:149:SER:H	1.65	0.43
1:A:169:ILE:HD12	1:A:190:CYS:CB	2.42	0.43
1:B:320:GLU:HB2	1:B:400:TRP:CZ2	2.52	0.43
1:B:48:THR:CG2	1:B:137:TYR:HE1	2.31	0.43
1:C:486:LEU:HG	1:C:489:LEU:HD21	1.99	0.43
2:D:23:ARG:NH1	2:F:2:VAL:CG2	2.71	0.43
2:D:2:VAL:HG11	2:F:27:LYS:CD	2.48	0.43
1:C:214:HIS:ND1	2:F:10:ARG:HG2	2.33	0.43
4:H:15:GLY:HA2	4:H:76:GLY:HA2	2.00	0.43
3:I:11:VAL:CG1	3:I:110:THR:CG2	2.90	0.43
3:I:35:HIS:CD2	3:I:100(K):PHE:HE1	2.36	0.43
4:M:9:SER:HB3	4:M:102:LYS:O	2.10	0.43
4:M:5:THR:O	4:M:5:THR:HG23	2.18	0.43
4:M:4:LEU:C	4:M:98:GLY:HA2	2.38	0.43
1:A:42:ASP:N	1:A:142:SER:O	2.47	0.43
1:B:90:TYR:CE1	1:B:118:LYS:HB2	2.53	0.43
1:B:16:SER:O	1:B:18:GLY:O	2.36	0.43
1:C:426:ASP:CB	1:C:446:HIS:HB2	2.48	0.43
3:G:19:LYS:NZ	3:G:81:GLU:OE1	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:11:SER:CB	4:H:104:THR:HB	2.44	0.43
4:M:6:GLN:HB2	4:M:7:PRO:HD2	2.01	0.43
1:B:144:HIS:HB3	1:B:360:THR:HG23	2.00	0.43
1:C:295:MET:C	1:C:297:LYS:H	2.21	0.43
1:C:8:ASN:HD21	2:F:15:ARG:CD	2.28	0.43
3:G:31:SER:C	3:G:32:TYR:O	2.57	0.43
3:I:28:THR:HG21	3:I:30:THR:HG21	1.99	0.43
1:A:46:VAL:CG2	3:I:100:TYR:CG	3.01	0.43
1:A:61:TYR:O	1:A:260:SER:HA	2.19	0.43
1:B:332:TYR:CE1	1:B:335:THR:HG22	2.53	0.43
1:C:176:ALA:N	1:C:188:LEU:O	2.40	0.43
1:C:27:HIS:HA	1:C:45:LEU:CB	2.37	0.43
1:A:214:HIS:CE1	2:D:11:LYS:O	2.66	0.43
2:D:56:SER:C	2:D:57:THR:HG22	2.27	0.43
1:B:462:TRP:CZ2	2:E:25:TYR:CD2	3.05	0.43
3:G:22:CYS:HB2	3:G:36:TRP:CH2	2.52	0.43
3:K:103:TRP:C	3:K:104:GLY:O	2.54	0.43
4:L:54:PRO:HD2	4:L:57:VAL:HG21	2.00	0.43
1:A:143:VAL:HG11	1:A:183:PHE:CD2	2.53	0.43
1:A:394:LYS:C	1:A:395:LYS:HG2	2.39	0.43
1:A:484:ILE:O	1:A:488:CYS:HB2	2.18	0.43
1:B:315:THR:OG1	1:B:316:LYS:N	2.51	0.43
2:E:3:THR:CA	2:E:5:PRO:CD	2.97	0.43
4:M:60:ARG:O	4:M:74:ILE:HA	2.18	0.43
1:B:170:THR:O	1:B:173:SER:N	2.36	0.43
1:B:484:ILE:HA	1:B:487:MET:HG2	1.99	0.43
1:C:107:LEU:HG	1:C:108:PHE:N	2.34	0.43
1:C:161:ASP:OD1	1:C:164:ARG:HG2	2.17	0.43
2:D:35:TRP:CG	2:D:72:PRO:CB	2.95	0.43
3:G:48:MET:HB3	3:G:63:PHE:CD2	2.53	0.43
3:I:9:ALA:CA	3:I:107:THR:CG2	2.96	0.43
3:I:31:SER:OG	3:I:31:SER:O	2.34	0.43
4:M:48:TYR:CE2	4:M:52:SER:HB3	2.53	0.43
4:M:53:ARG:HB2	4:M:57:VAL:HG22	2.00	0.43
1:A:210:HIS:CE1	1:A:277:MET:SD	3.12	0.43
1:A:53:MET:O	1:A:54:ALA:HB2	2.18	0.43
1:C:9:ARG:CD	1:C:11:PHE:CE2	3.00	0.43
1:C:269:LEU:O	2:F:19:TRP:CD1	2.72	0.43
3:G:32:TYR:CD2	3:G:33:ALA:CA	3.01	0.43
4:H:48:TYR:CG	4:H:48:TYR:O	2.70	0.43
3:I:29:PHE:CD1	3:I:30:THR:N	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:67:VAL:CG1	3:I:82:LEU:CG	2.96	0.43
4:M:33:SER:OG	4:M:88:SER:HB3	2.19	0.43
1:A:15:MET:HE1	1:A:295:MET:CG	2.48	0.43
1:A:172:ASN:C	1:A:172:ASN:ND2	2.59	0.43
1:A:249:HIS:CG	2:F:16:SER:HA	2.54	0.43
1:A:26:GLU:HG3	2:D:15:ARG:CG	2.46	0.43
1:A:49:THR:O	1:A:135:LEU:HB2	2.19	0.43
1:B:433:SER:O	1:B:434:VAL:HB	2.18	0.43
1:B:458:GLY:O	1:B:460:MET:N	2.52	0.43
1:C:318:PRO:HB3	1:C:328:VAL:HG22	1.99	0.43
1:C:325:THR:HG22	1:C:326:VAL:N	2.33	0.43
1:C:430:ASP:C	1:C:432:GLY:N	2.72	0.43
2:D:2:VAL:CG1	2:F:27:LYS:HD2	2.48	0.43
3:G:51:ILE:HD13	3:G:100(C):TYR:CD2	2.50	0.43
3:G:100(K):PHE:CE2	4:H:97:PHE:HZ	2.24	0.43
3:I:18:VAL:HB	3:I:82(C):LEU:HD21	1.96	0.43
3:I:36:TRP:CB	3:I:50:TRP:CZ3	3.02	0.43
1:A:146:SER:O	1:A:147:GLN:HB2	2.19	0.43
1:A:61:TYR:HE1	1:A:265:VAL:HG21	1.83	0.43
1:A:184:GLY:HA3	1:A:298:LEU:HA	2.01	0.43
1:B:137:TYR:CD1	1:B:289:LEU:HD11	2.54	0.43
1:C:188:LEU:HD13	1:C:291:CYS:HB3	2.00	0.43
1:C:202:TYR:CE2	1:C:215:LYS:HG3	2.51	0.43
1:C:32:THR:HA	1:C:42:ASP:HB3	2.00	0.43
1:C:453:PHE:CZ	1:C:495:LEU:HD23	2.53	0.43
3:G:32:TYR:CD2	3:G:33:ALA:C	2.92	0.43
4:H:18:ILE:HG22	4:H:74:ILE:HB	2.01	0.43
3:I:2:VAL:HG22	3:I:27:TYR:CB	2.48	0.43
1:A:329:GLU:HG2	1:A:374:MET:O	2.19	0.43
1:A:50:VAL:O	1:A:281:LYS:HD2	2.19	0.43
1:B:184:GLY:HA3	1:B:298:LEU:HA	2.00	0.43
1:B:375:MET:O	1:B:376:LEU:C	2.57	0.43
1:B:82:LEU:HB2	1:B:114:VAL:CG1	2.49	0.43
1:C:141:LEU:HB2	1:C:165:ALA:O	2.19	0.43
1:C:194:THR:O	1:C:194:THR:HG23	2.17	0.43
1:C:407:ILE:O	1:C:407:ILE:HD12	2.18	0.43
1:B:463:PHE:CE2	2:E:28:HIS:C	2.85	0.43
3:G:3:GLN:N	3:G:25:SER:O	2.38	0.43
3:G:52:ASN:HB3	3:G:56:ASN:HB2	2.01	0.43
3:K:38:ARG:HD2	3:K:48:MET:SD	2.59	0.43
1:A:1:ILE:HD13	1:A:147:GLN:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:PRO:HG2	1:A:402:ARG:CG	2.48	0.42
1:A:48:THR:HG21	1:A:284:LEU:HD23	2.01	0.42
1:B:97:VAL:HG21	1:B:113:LEU:CD2	2.49	0.42
1:B:114:VAL:HG22	1:B:114:VAL:O	2.18	0.42
1:B:460:MET:HE1	1:B:468:ILE:HD12	2.01	0.42
1:A:77:GLN:HG3	1:B:54:ALA:CB	2.48	0.42
1:C:312:PHE:HD1	1:C:330:VAL:CG1	2.32	0.42
2:E:53:LEU:HD12	2:E:63:TYR:CD2	2.50	0.42
3:G:28:THR:C	3:G:30:THR:N	2.72	0.42
4:M:47:LEU:O	4:M:48:TYR:CG	2.72	0.42
1:C:214:HIS:NE2	1:C:217:TRP:CB	2.82	0.42
4:L:44:LYS:CE	4:L:46:MET:CE	2.70	0.42
1:A:196:LEU:CD1	1:A:288:HIS:CE1	3.00	0.42
1:A:41:VAL:HG22	1:A:143:VAL:CG2	2.45	0.42
1:B:195:GLY:HA3	1:B:288:HIS:O	2.19	0.42
1:B:333:ALA:HB2	1:B:370:GLU:CG	2.50	0.42
1:B:368:SER:OG	1:B:369:THR:N	2.50	0.42
1:C:135:LEU:O	1:C:136:GLU:HB2	2.20	0.42
1:C:217:TRP:CZ2	1:C:269:LEU:HD21	2.54	0.42
1:C:310:ALA:HB3	1:C:332:TYR:CE1	2.54	0.42
1:C:72:SER:O	4:M:29:PHE:CZ	2.66	0.42
2:D:4:LEU:HG	2:D:5:PRO:HD3	2.01	0.42
2:F:25:TYR:O	2:F:26:THR:C	2.56	0.42
3:G:67:VAL:HG12	3:G:82:LEU:HB2	2.01	0.42
3:I:18:VAL:O	3:I:18:VAL:HG13	2.19	0.42
1:A:169:ILE:CD1	1:A:190:CYS:SG	3.07	0.42
1:A:57:ARG:HA	1:A:227:ALA:H	1.83	0.42
1:B:204:LEU:HD13	1:B:218:PHE:CE1	2.54	0.42
1:B:429:TRP:HE3	1:B:439:ASN:OD1	2.03	0.42
1:C:124:LYS:HE3	1:C:230:ASP:HB3	2.01	0.42
3:I:50:TRP:CB	3:I:69:ILE:CD1	2.86	0.42
3:K:100(K):PHE:HE2	4:L:97:PHE:CZ	2.30	0.42
4:L:53:ARG:HD3	4:L:57:VAL:HB	2.00	0.42
4:M:90:HIS:HD2	4:M:95:TRP:CZ2	2.37	0.42
1:A:252:ARG:CG	1:A:252:ARG:NH1	2.82	0.42
1:A:245:PHE:CD1	1:A:255:VAL:HG12	2.55	0.42
1:A:323:HIS:O	1:A:323:HIS:CG	2.70	0.42
1:A:461:SER:N	1:A:464:SER:OG	2.52	0.42
1:A:88:THR:HG21	1:B:86:SER:C	2.39	0.42
1:B:183:PHE:O	1:B:298:LEU:HA	2.19	0.42
1:C:326:VAL:HG11	1:C:387:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:38:ARG:HA	3:G:90:TYR:HD1	1.84	0.42
3:K:38:ARG:HA	3:K:90:TYR:HD1	1.85	0.42
1:A:263:GLY:CA	1:C:260:SER:O	2.67	0.42
1:A:352:LEU:HB3	1:A:353:THR:H	1.55	0.42
1:B:20:TRP:CZ3	1:B:292:ARG:HD3	2.55	0.42
1:B:333:ALA:CA	1:B:370:GLU:CG	2.95	0.42
1:C:10:ASP:O	1:C:31:VAL:HA	2.20	0.42
1:C:412:GLU:O	1:C:413:ALA:C	2.57	0.42
1:C:71:ASP:HB2	1:C:113:LEU:CB	2.48	0.42
2:E:68:LEU:O	2:E:72:PRO:HD3	2.19	0.42
2:D:59:GLN:NE2	2:F:54:GLY:HA2	2.35	0.42
3:G:14:PRO:CD	3:G:112:SER:O	2.67	0.42
3:I:50:TRP:CZ3	3:I:80:MET:CG	2.89	0.42
4:M:27:GLY:CA	4:M:67:GLY:O	2.67	0.42
1:A:10:ASP:OD1	1:A:416:ARG:NE	2.53	0.42
1:A:311:ALA:HA	1:A:333:ALA:H	1.84	0.42
1:A:320:GLU:N	1:A:400:TRP:CH2	2.87	0.42
1:B:278:ASP:OD1	1:B:279:GLY:N	2.45	0.42
1:C:15:MET:SD	1:C:38:LYS:HD2	2.60	0.42
1:C:271:GLY:C	2:F:18:THR:CG2	2.88	0.42
1:C:420:ARG:CG	1:C:431:PHE:CE2	3.03	0.42
1:C:47:THR:HG21	1:C:283:ARG:HE	1.85	0.42
1:C:480:LYS:HG3	1:C:481:ASN:O	2.20	0.42
3:I:44:ARG:O	3:I:46:GLU:N	2.52	0.42
3:K:1:GLU:O	3:K:3:GLN:HG3	2.20	0.42
1:B:180:LEU:HB2	1:B:183:PHE:HB2	2.02	0.42
1:C:25:LEU:C	1:C:45:LEU:HD12	2.40	0.42
2:D:19:TRP:CD1	2:D:20:LEU:CD1	3.03	0.42
3:G:100(K):PHE:CD2	4:H:35:PHE:HE1	2.35	0.42
4:H:36:GLN:HG2	4:H:83:ALA:HB1	2.01	0.42
1:A:224:PRO:O	1:A:236:TRP:CE3	2.73	0.42
1:A:457:PHE:CD2	1:A:457:PHE:N	2.87	0.42
1:B:75:PRO:HD3	1:B:110:LYS:O	2.20	0.42
1:B:173:SER:N	1:B:174:PRO:HD3	2.35	0.42
1:B:206:MET:HE2	1:B:262:GLU:HG3	2.02	0.42
1:B:20:TRP:CH2	1:B:292:ARG:NE	2.88	0.42
1:B:467:LEU:O	1:B:470:THR:N	2.52	0.42
2:D:10:ARG:NH1	2:F:38:ARG:O	2.53	0.42
2:D:26:THR:C	2:D:28:HIS:N	2.73	0.42
2:F:19:TRP:CD1	2:F:20:LEU:CD1	3.03	0.42
1:A:136:GLU:OE1	1:A:136:GLU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:SER:O	1:A:305:TYR:CG	2.73	0.42
1:B:477:LEU:O	1:B:477:LEU:HD12	2.19	0.42
1:C:320:GLU:N	1:C:400:TRP:HH2	2.17	0.42
2:F:4:LEU:HG	2:F:5:PRO:HD3	2.01	0.42
1:A:96:LEU:CA	1:A:111:GLY:O	2.68	0.41
1:A:166:LYS:HB2	1:A:166:LYS:HE3	1.71	0.41
1:B:137:TYR:CZ	1:B:289:LEU:HD11	2.55	0.41
1:B:217:TRP:NE1	2:E:5:PRO:C	2.73	0.41
1:B:374:MET:SD	1:B:376:LEU:CD2	3.08	0.41
1:C:139:ILE:HD12	1:C:169:ILE:HD11	1.93	0.41
1:C:1:ILE:C	1:C:3:CYS:N	2.73	0.41
1:C:499:SER:OG	1:C:500:THR:N	2.53	0.41
2:D:51:TRP:CG	2:D:51:TRP:O	2.73	0.41
3:G:1:GLU:O	3:G:3:GLN:HG3	2.20	0.41
4:H:87:CYS:O	4:H:98:GLY:N	2.25	0.41
3:I:40:ALA:O	3:I:41:PRO:C	2.57	0.41
3:I:46:GLU:OE2	3:I:62:LYS:HD3	2.20	0.41
4:M:26(B):ASP:OD1	4:M:26(B):ASP:N	2.51	0.41
1:A:143:VAL:CG1	1:A:183:PHE:CE2	3.04	0.41
1:A:290:LYS:HE3	1:A:290:LYS:HB3	1.88	0.41
1:A:358:LEU:CD1	1:A:360:THR:O	2.67	0.41
1:A:65:ILE:HA	1:A:65:ILE:HD13	1.86	0.41
1:B:189:ASP:HB2	1:B:292:ARG:HB3	2.01	0.41
1:B:57:ARG:HA	1:B:228:GLY:H	1.85	0.41
1:B:463:PHE:O	1:B:467:LEU:HG	2.19	0.41
1:C:286:SER:CB	2:F:16:SER:OG	2.68	0.41
1:C:305:TYR:CD1	1:C:338:PRO:O	2.73	0.41
2:D:22:SER:OG	2:D:23:ARG:N	2.53	0.41
2:E:26:THR:O	2:E:30:ILE:CG1	2.65	0.41
3:I:38:ARG:CG	3:I:90:TYR:HE1	2.32	0.41
1:A:11:PHE:N	1:A:11:PHE:CD1	2.85	0.41
1:B:63:ALA:HB2	1:B:242:LEU:CD2	2.49	0.41
1:B:374:MET:SD	1:B:376:LEU:HD21	2.61	0.41
1:B:463:PHE:HE2	2:E:29:LEU:N	2.18	0.41
1:C:37:ASP:O	1:C:300:LEU:HG	2.20	0.41
1:B:222:PRO:CD	2:E:3:THR:HB	2.47	0.41
3:I:50:TRP:NE1	3:I:68:THR:HA	2.35	0.41
3:K:52:ASN:HD21	3:K:56:ASN:HD22	1.54	0.41
4:M:4:LEU:O	4:M:99:GLY:N	2.52	0.41
1:A:57:ARG:HD3	1:A:225:TRP:HB2	2.02	0.41
1:A:327:THR:HA	1:A:377:GLU:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:TRP:O	1:B:478:ASN:HB2	2.20	0.41
1:C:341:VAL:CG2	1:C:342:PRO:HD2	2.50	0.41
2:D:54:GLY:O	2:D:56:SER:N	2.53	0.41
2:E:71:ALA:CB	2:E:74:TYR:HA	2.51	0.41
3:G:66:ARG:NH2	3:G:82(C):LEU:HA	2.35	0.41
4:H:41:LYS:CG	4:H:42:ALA:H	2.28	0.41
4:L:15:GLY:C	4:L:76:GLY:CA	2.80	0.41
4:M:12:GLY:O	4:M:77:LEU:HD12	2.21	0.41
1:A:171:PRO:HD3	1:A:192:PRO:CB	2.51	0.41
1:A:395:LYS:O	1:A:396:ILE:CG2	2.68	0.41
1:A:426:ASP:N	1:A:446:HIS:CE1	2.89	0.41
1:B:202:TYR:CE2	1:B:215:LYS:HG3	2.55	0.41
1:C:289:LEU:HD21	1:C:291:CYS:SG	2.61	0.41
1:C:74:CYS:HB2	1:C:77:GLN:CD	2.40	0.41
4:H:30:ASN:HD22	4:H:30:ASN:HA	1.69	0.41
3:G:51:ILE:HG21	4:H:95:TRP:CZ3	2.55	0.41
4:L:48:TYR:O	4:L:52:SER:HB2	2.20	0.41
1:A:258:LEU:HA	1:A:258:LEU:HD23	1.81	0.41
1:B:147:GLN:H	1:B:147:GLN:HG3	1.52	0.41
1:C:350:GLN:OE1	1:B:175:ARG:NE	2.50	0.41
1:C:238:ASN:OD1	1:C:240:GLU:N	2.43	0.41
1:C:26:GLU:N	1:C:45:LEU:HD12	2.35	0.41
1:C:98:ASP:HA	1:C:109:GLY:O	2.21	0.41
1:A:286:SER:HB2	2:D:14:THR:HG21	2.01	0.41
2:D:74:TYR:O	2:D:74:TYR:CG	2.73	0.41
3:K:36:TRP:CE2	3:K:80:MET:HB2	2.56	0.41
4:M:53:ARG:NH1	4:M:59:SER:HA	2.35	0.41
1:A:405:SER:O	1:A:408:GLY:N	2.53	0.41
1:A:52:ASN:HA	1:A:52:ASN:HD22	1.57	0.41
1:A:67:ASP:C	1:A:68:MET:HG2	2.39	0.41
1:B:295:MET:O	1:B:296:ASP:C	2.59	0.41
1:B:46:VAL:HG23	1:B:139:ILE:HA	2.02	0.41
1:C:148:HIS:CG	1:C:149:SER:N	2.88	0.41
1:C:288:HIS:CD2	1:C:424:LEU:HD11	2.56	0.41
4:H:54:PRO:HD2	4:H:57:VAL:HG21	2.02	0.41
1:A:393:GLU:C	1:A:395:LYS:H	2.24	0.41
1:C:398:HIS:C	1:B:174:PRO:HG2	2.41	0.41
1:B:209:LYS:C	1:B:210:HIS:CG	2.93	0.41
2:D:52:LEU:CD1	2:D:52:LEU:O	2.53	0.41
4:M:37:GLN:O	4:M:83:ALA:HB1	2.20	0.41
3:I:103:TRP:CD2	4:M:43:PRO:O	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:53:ARG:NE	4:M:57:VAL:CG1	2.78	0.41
4:M:58:SER:O	4:M:60:ARG:N	2.54	0.41
4:M:5:THR:C	4:M:6:GLN:O	2.58	0.41
1:A:101:TRP:CG	1:A:108:PHE:CE1	3.04	0.41
1:A:84:LYS:HB3	1:A:90:TYR:CE2	2.55	0.41
1:B:20:TRP:HD1	1:B:434:VAL:CA	2.25	0.41
1:B:215:LYS:NZ	1:B:215:LYS:HB3	2.36	0.41
1:C:143:VAL:HG13	1:C:143:VAL:O	2.21	0.41
1:C:1:ILE:O	1:C:3:CYS:N	2.53	0.41
2:D:52:LEU:HD13	2:D:52:LEU:C	2.36	0.41
2:F:14:THR:CG2	2:F:15:ARG:N	2.83	0.41
2:F:35:TRP:CB	2:F:72:PRO:HB3	2.51	0.41
4:H:34:TRP:HB2	4:H:47:LEU:CD1	2.51	0.41
3:I:8:GLY:CA	3:I:107:THR:HG23	2.50	0.41
3:I:12:LYS:HB2	3:I:16:ALA:HB3	2.02	0.41
1:A:103:ASN:O	4:H:31:TYR:CZ	2.74	0.41
1:A:156:THR:CG2	1:A:164:ARG:O	2.64	0.41
1:A:99:ARG:HD3	1:A:251:LYS:HD3	2.01	0.41
1:A:349:MET:HG3	1:A:349:MET:O	2.21	0.41
1:A:382:PHE:HE2	1:A:406:THR:HA	1.86	0.41
1:A:58:SER:HB2	1:A:226:HIS:CB	2.50	0.41
1:B:148:HIS:CG	1:B:373:LYS:CD	3.01	0.41
1:B:141:LEU:HD22	1:B:186:LEU:CD2	2.50	0.41
1:B:185:SER:N	1:B:297:LYS:O	2.54	0.41
1:C:399:HIS:CD2	1:B:191:GLU:CB	3.04	0.41
1:C:423:VAL:CG1	1:C:424:LEU:N	2.65	0.41
1:C:439:ASN:O	1:C:441:LEU:N	2.54	0.41
2:E:12:LEU:HD23	2:E:12:LEU:HA	1.89	0.41
3:G:12:LYS:HG3	3:G:18:VAL:HG12	2.02	0.41
3:K:67:VAL:HG12	3:K:82:LEU:HA	2.02	0.41
3:K:40:ALA:HB2	3:K:87:THR:O	2.21	0.41
1:B:82:LEU:HD23	1:B:116:CYS:SG	2.60	0.41
1:C:201:LEU:HD23	1:C:212:LEU:CB	2.51	0.41
1:C:331:GLN:O	1:C:371:ASN:HA	2.20	0.41
1:C:438:LEU:O	1:C:439:ASN:C	2.59	0.41
1:C:482:GLY:O	1:C:485:SER:N	2.49	0.41
2:E:74:TYR:CD1	2:E:74:TYR:O	2.74	0.41
1:C:214:HIS:CE1	2:F:10:ARG:HG2	2.56	0.41
3:G:48:MET:HE1	3:G:67:VAL:HG13	2.03	0.41
3:G:36:TRP:CE2	3:G:80:MET:HB2	2.56	0.41
3:I:69:ILE:CB	3:I:79:TYR:O	2.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:CYS:O	1:A:192:PRO:HD3	2.21	0.40
1:B:223:LEU:HD23	1:B:223:LEU:HA	1.85	0.40
2:E:49:ILE:O	2:E:53:LEU:HD23	2.21	0.40
3:K:59:TYR:CE1	3:K:69:ILE:HD13	2.56	0.40
1:A:171:PRO:HD3	1:A:192:PRO:HB2	2.02	0.40
1:B:58:SER:HB2	1:B:226:HIS:CB	2.51	0.40
1:C:202:TYR:OH	1:C:215:LYS:HD3	2.19	0.40
2:F:54:GLY:C	2:F:59:GLN:HE21	2.19	0.40
3:K:89:ILE:HD11	3:K:108:LEU:CD1	2.50	0.40
4:L:44:LYS:CG	4:L:46:MET:HE3	2.48	0.40
4:M:66:SER:N	4:M:69:THR:OG1	2.47	0.40
1:A:196:LEU:HD23	1:A:198:PHE:CZ	2.56	0.40
1:A:276:GLU:O	1:A:282:GLY:C	2.60	0.40
1:A:349:MET:SD	1:A:397:THR:HG21	2.62	0.40
1:B:130:ILE:HD11	1:B:198:PHE:HB3	2.03	0.40
1:B:2:ARG:NH2	1:B:140:MET:HB2	2.34	0.40
1:B:415:VAL:HG12	1:B:419:LYS:HZ2	1.87	0.40
1:C:300:LEU:HB2	1:C:303:VAL:HG22	2.03	0.40
1:C:374:MET:HB2	1:C:376:LEU:HD11	2.03	0.40
1:C:360:THR:HG21	1:C:376:LEU:HA	2.03	0.40
1:C:407:ILE:C	1:C:407:ILE:CD1	2.85	0.40
1:C:73:ARG:HG3	1:C:80:ALA:HA	2.04	0.40
2:D:53:LEU:O	2:D:60:LYS:HD3	2.21	0.40
2:E:4:LEU:HA	2:E:4:LEU:HD13	1.77	0.40
3:G:59:TYR:CE1	3:G:69:ILE:HD13	2.56	0.40
4:M:103:LEU:HD23	4:M:103:LEU:C	2.41	0.40
4:M:88:SER:HA	4:M:97:PHE:HD1	1.85	0.40
1:A:99:ARG:HD2	1:A:251:LYS:HD3	2.04	0.40
1:B:130:ILE:CD1	1:B:198:PHE:HB3	2.51	0.40
1:B:217:TRP:NE1	2:E:6:SER:HB2	2.36	0.40
1:C:198:PHE:O	1:C:199:SER:HB2	2.22	0.40
1:C:453:PHE:HZ	1:C:495:LEU:HD23	1.85	0.40
1:C:70:SER:O	1:C:82:LEU:HD13	2.21	0.40
3:G:48:MET:CB	3:G:63:PHE:CD2	3.05	0.40
3:I:83:ARG:C	3:I:111:VAL:CB	2.89	0.40
3:K:39:GLN:OE1	3:K:45:LEU:HA	2.21	0.40
1:B:67:ASP:OD2	3:K:64:GLN:NE2	2.54	0.40
3:K:55:GLY:HA2	3:K:71:ARG:HD3	2.04	0.40
1:A:249:HIS:CG	2:F:16:SER:CA	3.05	0.40
1:A:260:SER:O	1:C:263:GLY:N	2.54	0.40
1:A:317:ILE:HA	1:A:318:PRO:HD3	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:MET:CE	1:A:38:LYS:HE2	2.51	0.40
1:B:314:PHE:HE1	1:B:389:ILE:HD13	1.86	0.40
1:C:330:VAL:HG11	1:C:389:ILE:HD11	2.04	0.40
1:C:6:VAL:HG13	1:C:7:SER:O	2.21	0.40
2:E:29:LEU:O	2:E:32:VAL:CG1	2.60	0.40
2:F:23:ARG:O	2:F:27:LYS:CB	2.67	0.40
1:C:461:SER:OG	2:F:8:SER:HB3	2.20	0.40
4:H:16:GLN:O	4:H:77:LEU:HD13	2.21	0.40
3:K:50:TRP:CZ3	3:K:52:ASN:C	2.92	0.40
4:L:20:ILE:O	4:L:71:SER:HA	2.21	0.40
4:M:9:SER:HB2	4:M:102:LYS:O	2.15	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 PDB entries followed by that with respect to all EM entries.

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	502/504 (100%)	397 (79%)	85 (17%)	20 (4%)	4	37
1	B	490/504 (97%)	402 (82%)	78 (16%)	10 (2%)	9	54
1	C	490/504 (97%)	402 (82%)	79 (16%)	9 (2%)	11	55
2	D	73/75 (97%)	60 (82%)	12 (16%)	1 (1%)	14	59
2	E	73/75 (97%)	60 (82%)	10 (14%)	3 (4%)	3	37
2	F	73/75 (97%)	59 (81%)	13 (18%)	1 (1%)	14	59
3	G	125/127 (98%)	110 (88%)	9 (7%)	6 (5%)	3	32
3	I	125/127 (98%)	99 (79%)	22 (18%)	4 (3%)	5	44
3	K	125/127 (98%)	111 (89%)	11 (9%)	3 (2%)	7	50
4	H	107/109 (98%)	94 (88%)	9 (8%)	4 (4%)	4	40
4	L	107/109 (98%)	99 (92%)	6 (6%)	2 (2%)	10	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	M	107/109 (98%)	87 (81%)	16 (15%)	4 (4%)	4	40
All	All	2397/2445 (98%)	1980 (83%)	350 (15%)	67 (3%)	10	47

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	SER
1	A	153	VAL
1	A	154	ASN
1	A	155	ASP
1	A	159	GLU
1	A	160	THR
1	A	161	ASP
1	A	272	ALA
1	A	311	ALA
1	A	317	ILE
1	A	318	PRO
1	A	351	THR
1	C	148	HIS
1	C	407	ILE
1	B	99	ARG
1	B	434	VAL
2	E	19	TRP
2	E	24	GLU
3	G	31	SER
3	G	32	TYR
3	K	13	LYS
3	K	34	MET
4	L	48	TYR
3	I	10	GLU
3	I	30	THR
3	I	33	ALA
4	M	60	ARG
1	A	225	TRP
1	A	228	GLY
1	A	350	GLN
1	A	373	LYS
1	B	22	ASP
1	B	374	MET
2	F	57	THR
4	H	4	LEU
4	M	47	LEU

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Mol	Chain	Res	Type
4	M	55	SER
1	A	7	SER
1	A	54	ALA
1	A	319	ALA
1	C	2	ARG
1	C	144	HIS
1	C	308	CYS
1	B	376	LEU
3	G	30	THR
3	G	33	ALA
3	G	62	LYS
4	H	48	TYR
4	H	50	VAL
3	K	30	THR
4	M	6	GLN
1	C	46	VAL
1	C	502	VAL
1	B	21	VAL
1	B	46	VAL
1	B	149	SER
1	B	438	LEU
3	G	29	PHE
4	L	50	VAL
1	C	353	THR
4	H	47	LEU
1	A	104	GLY
1	C	354	PRO
2	D	24	GLU
3	I	82(B)	SER
1	B	502	VAL
2	E	4	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	410/410 (100%)	383 (93%)	27 (7%)	21	60
1	B	401/410 (98%)	381 (95%)	20 (5%)	30	68
1	C	401/410 (98%)	374 (93%)	27 (7%)	20	60
2	D	64/64 (100%)	60 (94%)	4 (6%)	22	61
2	E	64/64 (100%)	59 (92%)	5 (8%)	16	54
2	F	64/64 (100%)	63 (98%)	1 (2%)	70	88
3	G	107/107 (100%)	101 (94%)	6 (6%)	26	65
3	I	107/107 (100%)	102 (95%)	5 (5%)	32	70
3	K	107/107 (100%)	103 (96%)	4 (4%)	41	75
4	H	89/89 (100%)	85 (96%)	4 (4%)	34	71
4	L	89/89 (100%)	80 (90%)	9 (10%)	9	41
4	M	89/89 (100%)	79 (89%)	10 (11%)	7	37
All	All	1992/2010 (99%)	1870 (94%)	122 (6%)	28	63

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	8	ASN
1	A	11	PHE
1	A	15	MET
1	A	52	ASN
1	A	73	ARG
1	A	93	LYS
1	A	107	LEU
1	A	138	ARG
1	A	161	ASP
1	A	162	GLU
1	A	166	LYS
1	A	168	GLU
1	A	172	ASN
1	A	251	LYS
1	A	252	ARG
1	A	253	GLN
1	A	277	MET
1	A	309	THR

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Mol	Chain	Res	Type
1	A	312	PHE
1	A	316	LYS
1	A	350	GLN
1	A	352	LEU
1	A	367	GLU
1	A	370	GLU
1	A	373	LYS
1	A	386	TYR
1	C	2	ARG
1	C	12	VAL
1	C	42	ASP
1	C	45	LEU
1	C	103	ASN
1	C	142	SER
1	C	162	GLU
1	C	196	LEU
1	C	198	PHE
1	C	215	LYS
1	C	258	LEU
1	C	285	SER
1	C	323	HIS
1	C	339	CYS
1	C	350	GLN
1	C	352	LEU
1	C	362	ASN
1	C	372	SER
1	C	403	SER
1	C	406	THR
1	C	409	LYS
1	C	423	VAL
1	C	424	LEU
1	C	443	LYS
1	C	457	PHE
1	C	478	ASN
1	C	503	SER
2	D	21	GLU
2	D	25	TYR
2	D	26	THR
2	D	36	ILE
1	B	19	THR
1	B	22	ASP
1	B	46	VAL

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Mol	Chain	Res	Type
1	B	77	GLN
1	B	94	ARG
1	B	97	VAL
1	B	98	ASP
1	B	99	ARG
1	B	103	ASN
1	B	121	CYS
1	B	147	GLN
1	B	149	SER
1	B	215	LYS
1	B	243	VAL
1	B	244	GLU
1	B	251	LYS
1	B	352	LEU
1	B	353	THR
1	B	376	LEU
1	B	477	LEU
2	E	4	LEU
2	E	6	SER
2	E	26	THR
2	E	28	HIS
2	E	30	ILE
2	F	21	GLU
3	G	6	GLU
3	G	63	PHE
3	G	71	ARG
3	G	72	ASP
3	G	73	THR
3	G	96	LYS
4	H	4	LEU
4	H	11	SER
4	H	47	LEU
4	H	48	TYR
3	K	17	SER
3	K	31	SER
3	K	34	MET
3	K	99	ASP
4	L	4	LEU
4	L	9	SER
4	L	10	VAL
4	L	17	SER
4	L	48	TYR

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Mol	Chain	Res	Type
4	L	75	SER
4	L	77	LEU
4	L	80	GLU
4	L	106	LEU
3	I	27	TYR
3	I	44	ARG
3	I	52	ASN
3	I	61	GLN
3	I	82(C)	LEU
4	M	4	LEU
4	M	5	THR
4	M	22	CYS
4	M	48	TYR
4	M	50	VAL
4	M	78	GLN
4	M	87	CYS
4	M	97	PHE
4	M	104	THR
4	M	106	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	HIS
1	A	253	GLN
1	C	27	HIS
1	C	214	HIS
1	C	249	HIS
1	C	253	GLN
1	C	350	GLN
1	C	362	ASN
2	D	7	HIS
1	B	103	ASN
1	B	235	HIS
1	B	323	HIS
1	B	481	ASN
2	F	7	HIS
2	F	59	GLN
3	G	52	ASN
4	H	36	GLN
4	H	37	GLN
4	H	38	HIS

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Mol	Chain	Res	Type
3	K	52	ASN
3	K	105	GLN
4	L	38	HIS
3	I	64	GLN
4	M	36	GLN
4	M	37	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 ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	A	601	1	14,14,15	0.39	0	15,19,21	1.15	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	NAG	C2-N2-C7	-2.36	120.03	123.11
5	A	601	NAG	C8-C7-N2	2.06	120.04	116.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	NAG	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.