Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Feb 19, 2018 – 04:39 PM EST

PDB ID	:	6BZE
EMDB ID:	:	EMD-7314
Title	:	Cryo-EM structure of BCL10 CARD filament
Authors	:	David, L.; Li, Y.; Ma, J.; Garner, E.; Zhang, X.; Wu, H.
Deposited on	:	2017-12-23
Resolution	:	4.00 Å(reported)
Based on PDB ID	:	2MB9

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 (i) symbol.

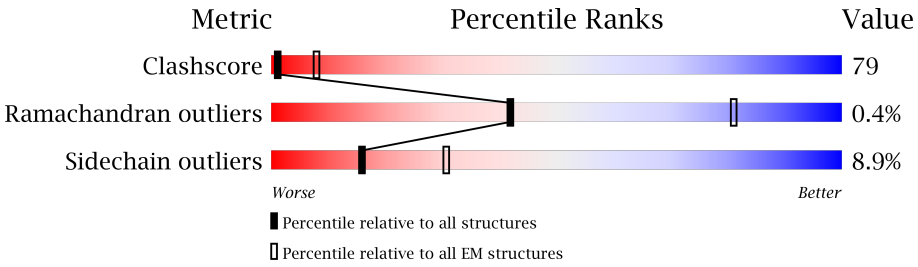
MolProbity	:	4.02b-467
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	106	22% 74% 5%
1	B	106	24% 72% 5%
1	C	106	25% 68% 7%
1	D	106	27% 67% 6%
1	E	106	24% 71% 6%
1	F	106	25% 68% 8%
1	G	106	31% 60% 8%
1	H	106	22% 67% 11%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7072 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 B-cell lymphoma/leukemia 10.

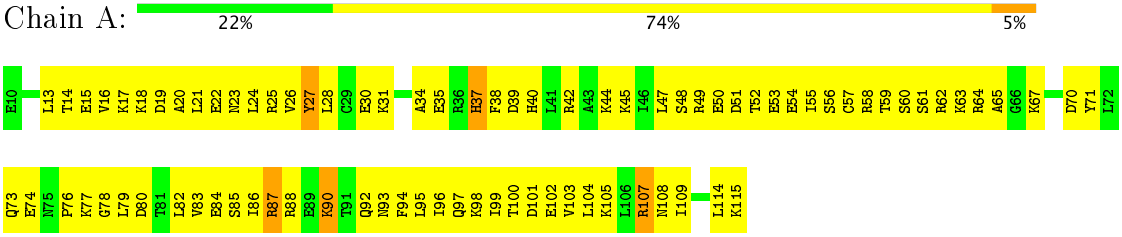
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	106	Total	C	N	O	S	0	0
			884	551	162	169	2		
1	B	106	Total	C	N	O	S	0	0
			884	551	162	169	2		
1	C	106	Total	C	N	O	S	0	0
			884	551	162	169	2		
1	D	106	Total	C	N	O	S	0	0
			884	551	162	169	2		
1	E	106	Total	C	N	O	S	0	0
			884	551	162	169	2		
1	F	106	Total	C	N	O	S	0	0
			884	551	162	169	2		
1	G	106	Total	C	N	O	S	0	0
			884	551	162	169	2		
1	H	106	Total	C	N	O	S	0	0
			884	551	162	169	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

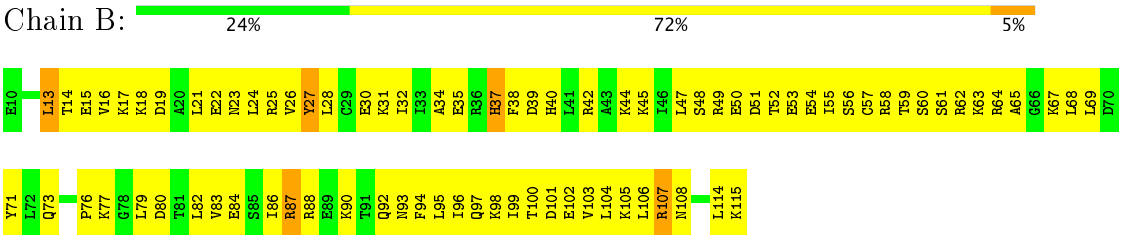
- Molecule 1: B-cell lymphoma/leukemia 10

Chain A:



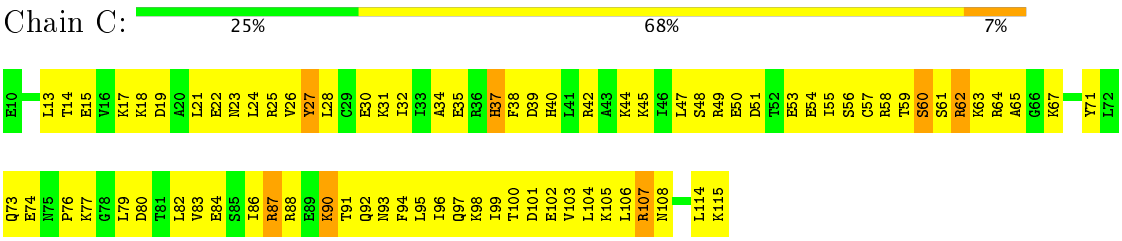
- Molecule 1: B-cell lymphoma/leukemia 10

Chain B:



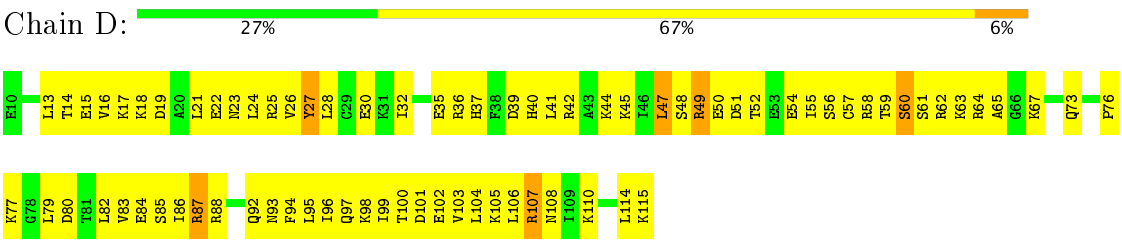
- Molecule 1: B-cell lymphoma/leukemia 10

Chain C:



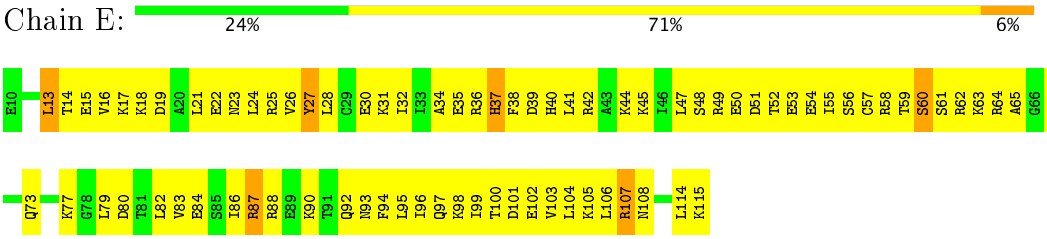
- Molecule 1: B-cell lymphoma/leukemia 10

Chain D:



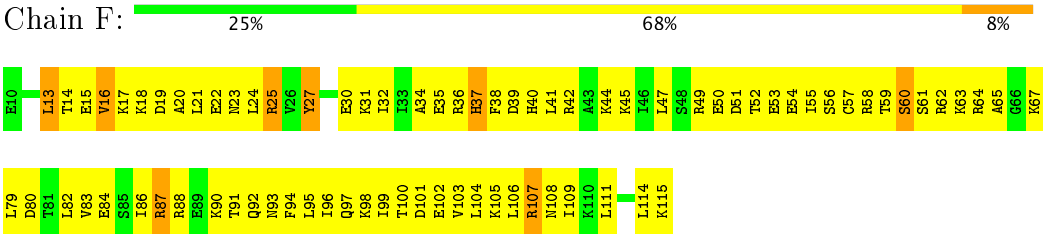
- Molecule 1: B-cell lymphoma/leukemia 10

Chain E:



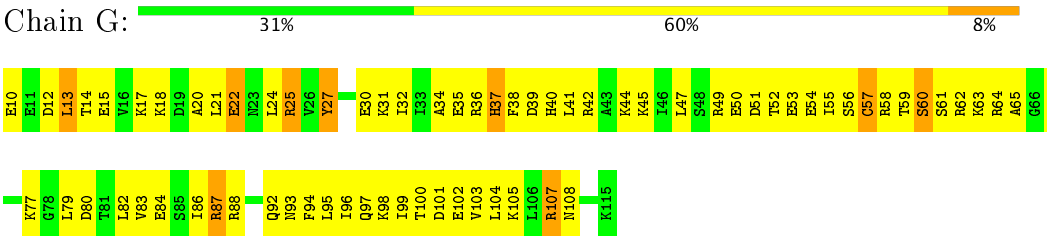
• Molecule 1: B-cell lymphoma/leukemia 10

Chain F:



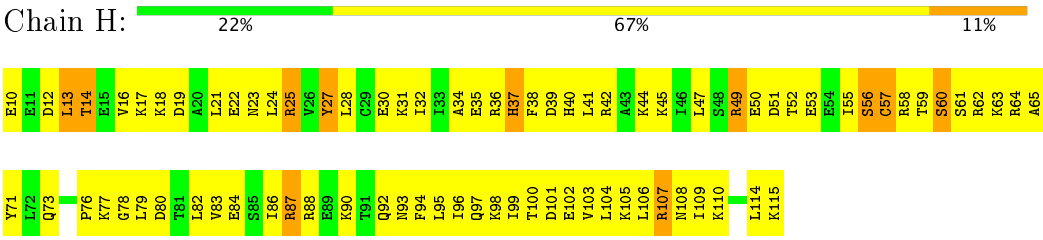
• Molecule 1: B-cell lymphoma/leukemia 10

Chain G:



• Molecule 1: B-cell lymphoma/leukemia 10

Chain H:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-100.8°, rise=5.0 Å, axial sym=C1	Depositor
Number of segments used	39992	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	Not provided	Depositor
Image detector	DIRECT ELECTRON DE-16 (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 2$	RMSZ	$\#\|Z\| > 2$
1	A	0.41	0/891	0.59	0/1188
1	B	0.41	0/891	0.58	0/1188
1	C	0.38	0/891	0.58	0/1188
1	D	0.41	0/891	0.57	0/1188
1	E	0.38	0/891	0.57	0/1188
1	F	0.42	0/891	0.59	0/1188
1	G	0.39	0/891	0.59	0/1188
1	H	0.42	0/891	0.59	0/1188
All	All	0.40	0/7128	0.58	0/9504

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	884	0	925	152	0
1	B	884	0	925	162	0
1	C	884	0	925	154	0
1	D	884	0	925	158	0
1	E	884	0	925	149	0
1	F	884	0	925	165	0
1	G	884	0	925	148	0
1	H	884	0	925	166	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7072	0	7400	1145	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 (1145) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ILE:HG23	1:B:99:ILE:CD1	1.22	1.57
1:A:96:ILE:HG23	1:A:99:ILE:CD1	1.43	1.48
1:B:96:ILE:CG2	1:B:99:ILE:HD11	1.43	1.48
1:G:96:ILE:HG23	1:G:99:ILE:CD1	1.43	1.47
1:H:96:ILE:HG23	1:H:99:ILE:CD1	1.45	1.43
1:G:96:ILE:CG2	1:G:99:ILE:HD11	1.50	1.42
1:H:96:ILE:CG2	1:H:99:ILE:HD11	1.53	1.39
1:E:96:ILE:HG23	1:E:99:ILE:CD1	1.57	1.35
1:A:27:TYR:CE2	1:A:98:LYS:HE2	1.66	1.29
1:C:96:ILE:HG23	1:C:99:ILE:CD1	1.61	1.28
1:A:96:ILE:CG2	1:A:99:ILE:HD11	1.62	1.28
1:H:96:ILE:CA	1:H:99:ILE:HG12	1.66	1.26
1:D:96:ILE:HG23	1:D:99:ILE:CD1	1.63	1.25
1:E:96:ILE:CG2	1:E:99:ILE:HD11	1.66	1.24
1:D:95:LEU:O	1:D:99:ILE:HG23	1.38	1.23
1:G:96:ILE:CA	1:G:99:ILE:HG12	1.69	1.22
1:C:96:ILE:CD1	1:C:99:ILE:HD13	1.69	1.21
1:A:96:ILE:HA	1:A:99:ILE:HG12	1.22	1.20
1:C:96:ILE:CG2	1:C:99:ILE:HD11	1.72	1.20
1:F:96:ILE:O	1:F:99:ILE:HG12	1.42	1.19
1:E:95:LEU:O	1:E:99:ILE:HG23	1.42	1.19
1:A:95:LEU:O	1:A:99:ILE:HG23	1.40	1.19
1:A:96:ILE:CA	1:A:99:ILE:HG12	1.71	1.18
1:D:96:ILE:CG2	1:D:99:ILE:HD11	1.73	1.18
1:E:96:ILE:CA	1:E:99:ILE:HG12	1.72	1.18
1:H:96:ILE:CD1	1:H:99:ILE:HD13	1.72	1.18
1:C:96:ILE:HA	1:C:99:ILE:HG12	1.26	1.17
1:B:96:ILE:CD1	1:B:99:ILE:HD13	1.75	1.16
1:C:27:TYR:CE2	1:C:98:LYS:HE2	1.80	1.16
1:D:96:ILE:CD1	1:D:99:ILE:HD13	1.74	1.16
1:B:96:ILE:O	1:B:99:ILE:HG12	1.44	1.15
1:H:95:LEU:O	1:H:99:ILE:HG23	1.44	1.14
1:D:96:ILE:HA	1:D:99:ILE:HG12	1.26	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ILE:CA	1:B:99:ILE:HG12	1.77	1.14
1:C:96:ILE:CA	1:C:99:ILE:HG12	1.77	1.13
1:G:96:ILE:C	1:G:99:ILE:HG12	1.69	1.13
1:F:96:ILE:C	1:F:99:ILE:HG12	1.68	1.12
1:A:70:ASP:OD2	1:D:49:ARG:NH2	1.79	1.12
1:A:96:ILE:HD12	1:A:99:ILE:HD13	1.15	1.12
1:H:96:ILE:HA	1:H:99:ILE:CG1	1.79	1.12
1:D:96:ILE:HD12	1:D:99:ILE:HD13	1.23	1.11
1:D:27:TYR:CE2	1:D:98:LYS:HE2	1.85	1.11
1:A:96:ILE:O	1:A:99:ILE:HG12	1.50	1.10
1:D:96:ILE:CA	1:D:99:ILE:HG12	1.82	1.10
1:G:96:ILE:HA	1:G:99:ILE:CG1	1.82	1.10
1:G:96:ILE:CD1	1:G:99:ILE:HD13	1.82	1.10
1:E:96:ILE:HD12	1:E:99:ILE:HD13	1.22	1.09
1:H:96:ILE:C	1:H:99:ILE:HG12	1.73	1.09
1:E:96:ILE:HA	1:E:99:ILE:HG12	1.21	1.09
1:G:95:LEU:O	1:G:99:ILE:HG23	1.47	1.09
1:F:96:ILE:CA	1:F:99:ILE:HG12	1.80	1.09
1:A:96:ILE:CD1	1:A:99:ILE:HD13	1.83	1.09
1:E:96:ILE:CD1	1:E:99:ILE:HD13	1.83	1.08
1:B:96:ILE:C	1:B:99:ILE:HG12	1.73	1.08
1:G:96:ILE:HD12	1:G:99:ILE:HD13	1.19	1.08
1:E:96:ILE:HA	1:E:99:ILE:CG1	1.83	1.08
1:G:96:ILE:O	1:G:99:ILE:HG12	1.48	1.07
1:G:96:ILE:HA	1:G:99:ILE:HG12	1.22	1.07
1:F:95:LEU:O	1:F:99:ILE:HG23	1.53	1.07
1:A:27:TYR:HE2	1:A:98:LYS:HE2	0.97	1.07
1:F:96:ILE:O	1:F:99:ILE:CG1	2.01	1.07
1:H:96:ILE:HA	1:H:99:ILE:HG12	1.16	1.07
1:F:96:ILE:HA	1:F:99:ILE:HG12	1.35	1.07
1:A:96:ILE:C	1:A:99:ILE:HG12	1.73	1.06
1:E:96:ILE:O	1:E:99:ILE:HG12	1.55	1.06
1:B:76:PRO:HD3	1:F:94:PHE:CD1	1.91	1.06
1:B:27:TYR:CE2	1:B:98:LYS:HE2	1.90	1.06
1:C:49:ARG:NH1	1:C:49:ARG:O	1.88	1.05
1:C:96:ILE:O	1:C:99:ILE:HG12	1.55	1.05
1:B:96:ILE:HA	1:B:99:ILE:HG12	1.33	1.05
1:F:49:ARG:NH1	1:F:49:ARG:O	1.88	1.04
1:C:96:ILE:HD12	1:C:99:ILE:HD13	1.05	1.04
1:E:49:ARG:O	1:E:49:ARG:NH1	1.89	1.04
1:E:96:ILE:C	1:E:99:ILE:HG12	1.77	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:96:ILE:HD12	1:H:99:ILE:HD13	1.04	1.04
1:G:49:ARG:O	1:G:49:ARG:NH1	1.91	1.04
1:H:96:ILE:O	1:H:99:ILE:HG12	1.55	1.04
1:D:96:ILE:O	1:D:99:ILE:HG12	1.58	1.03
1:D:42:ARG:NH1	1:D:84:GLU:OE1	1.90	1.03
1:E:77:LYS:O	1:E:79:LEU:HG	1.58	1.03
1:F:96:ILE:HG23	1:F:99:ILE:HD11	1.07	1.03
1:H:42:ARG:NH1	1:H:84:GLU:OE1	1.92	1.03
1:A:96:ILE:O	1:A:99:ILE:CG1	2.06	1.03
1:C:95:LEU:O	1:C:99:ILE:HG23	1.58	1.03
1:A:94:PHE:O	1:A:98:LYS:HG2	1.59	1.02
1:C:96:ILE:C	1:C:99:ILE:HG12	1.80	1.02
1:G:96:ILE:O	1:G:99:ILE:CG1	2.07	1.02
1:C:96:ILE:HD12	1:C:99:ILE:CD1	1.90	1.02
1:D:77:LYS:O	1:D:79:LEU:HG	1.60	1.02
1:C:42:ARG:NH1	1:C:84:GLU:OE1	1.92	1.02
1:F:42:ARG:NH1	1:F:84:GLU:OE1	1.92	1.01
1:B:96:ILE:HD12	1:B:99:ILE:HD13	1.03	1.01
1:A:42:ARG:NH1	1:A:84:GLU:OE1	1.92	1.01
1:A:27:TYR:HE2	1:A:98:LYS:CE	1.72	1.01
1:C:94:PHE:O	1:C:98:LYS:HG2	1.60	1.01
1:A:96:ILE:HA	1:A:99:ILE:CG1	1.90	1.00
1:C:96:ILE:HA	1:C:99:ILE:CG1	1.91	1.00
1:B:77:LYS:O	1:B:79:LEU:HG	1.62	1.00
1:F:96:ILE:HA	1:F:99:ILE:CG1	1.91	0.99
1:B:96:ILE:O	1:B:99:ILE:CG1	2.10	0.99
1:B:96:ILE:CG2	1:B:99:ILE:CD1	2.15	0.99
1:D:96:ILE:HA	1:D:99:ILE:CG1	1.92	0.98
1:C:77:LYS:O	1:C:79:LEU:HG	1.62	0.98
1:F:96:ILE:HG23	1:F:99:ILE:CD1	1.93	0.98
1:G:13:LEU:HB2	1:G:17:LYS:HZ1	1.27	0.98
1:E:42:ARG:NH1	1:E:84:GLU:OE1	1.96	0.98
1:H:96:ILE:HD12	1:H:99:ILE:CD1	1.93	0.98
1:B:42:ARG:NH1	1:B:84:GLU:OE1	1.96	0.98
1:A:98:LYS:O	1:A:102:GLU:N	1.96	0.97
1:C:84:GLU:OE2	1:C:88:ARG:NE	1.97	0.97
1:A:27:TYR:CE2	1:A:98:LYS:CE	2.46	0.97
1:E:27:TYR:CE2	1:E:98:LYS:HE2	1.97	0.97
1:B:96:ILE:HA	1:B:99:ILE:CG1	1.94	0.97
1:D:96:ILE:C	1:D:99:ILE:HG12	1.85	0.97
1:D:55:ILE:HG23	1:D:67:LYS:HZ2	1.29	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:GLU:OE2	1:A:73:GLN:NE2	1.98	0.96
1:B:27:TYR:HE2	1:B:98:LYS:HE2	1.28	0.96
1:H:84:GLU:OE2	1:H:88:ARG:NE	1.99	0.96
1:D:76:PRO:HD3	1:H:94:PHE:HB2	1.46	0.96
1:F:96:ILE:HD12	1:F:99:ILE:HD13	1.45	0.96
1:H:96:ILE:O	1:H:99:ILE:CG1	2.13	0.95
1:F:34:ALA:HB2	1:F:38:PHE:CE2	2.01	0.95
1:B:96:ILE:HD12	1:B:99:ILE:CD1	1.97	0.94
1:F:98:LYS:O	1:F:102:GLU:N	2.00	0.94
1:A:70:ASP:CG	1:D:49:ARG:HH21	1.69	0.94
1:B:96:ILE:HD13	1:B:99:ILE:HG21	1.50	0.93
1:C:13:LEU:HB2	1:C:17:LYS:HZ1	1.32	0.93
1:C:96:ILE:O	1:C:99:ILE:CG1	2.17	0.93
1:G:84:GLU:OE2	1:G:88:ARG:NE	2.00	0.93
1:B:22:GLU:OE2	1:B:73:GLN:NE2	2.01	0.93
1:D:44:LYS:HA	1:D:47:LEU:HB3	1.49	0.93
1:F:96:ILE:CG2	1:F:99:ILE:HD11	1.96	0.93
1:B:96:ILE:HG23	1:B:99:ILE:HD13	1.50	0.93
1:G:98:LYS:O	1:G:102:GLU:N	2.00	0.93
1:E:84:GLU:OE2	1:E:88:ARG:NE	2.02	0.93
1:E:96:ILE:O	1:E:99:ILE:CG1	2.16	0.93
1:D:84:GLU:OE2	1:D:88:ARG:NE	2.01	0.93
1:G:27:TYR:CE2	1:G:98:LYS:HE2	2.04	0.92
1:H:98:LYS:O	1:H:102:GLU:N	2.02	0.92
1:D:48:SER:OG	1:H:37:HIS:NE2	1.65	0.92
1:F:77:LYS:O	1:F:79:LEU:HG	1.67	0.92
1:A:84:GLU:OE2	1:A:88:ARG:NE	2.01	0.92
1:A:55:ILE:O	1:A:67:LYS:NZ	2.01	0.92
1:F:34:ALA:CB	1:F:38:PHE:CE2	2.53	0.92
1:C:27:TYR:HE2	1:C:98:LYS:HE2	1.31	0.92
1:C:76:PRO:HD3	1:G:94:PHE:CD1	2.04	0.91
1:D:96:ILE:HD12	1:D:99:ILE:CD1	2.01	0.91
1:F:84:GLU:OE2	1:F:88:ARG:NE	2.02	0.90
1:A:76:PRO:HD3	1:E:94:PHE:HB2	1.53	0.90
1:C:76:PRO:HD3	1:G:94:PHE:HB2	1.52	0.90
1:E:98:LYS:O	1:E:102:GLU:N	2.05	0.90
1:H:77:LYS:O	1:H:79:LEU:HG	1.72	0.90
1:D:49:ARG:HH11	1:D:49:ARG:HG3	1.35	0.90
1:B:54:GLU:OE1	1:F:36:ARG:NH1	2.05	0.90
1:H:27:TYR:CE2	1:H:98:LYS:HE2	2.07	0.89
1:H:22:GLU:OE2	1:H:73:GLN:NE2	2.03	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:ILE:HG23	1:C:67:LYS:HZ2	1.33	0.89
1:D:94:PHE:O	1:D:98:LYS:HG2	1.72	0.89
1:F:55:ILE:O	1:F:67:LYS:NZ	2.06	0.88
1:B:98:LYS:O	1:B:102:GLU:N	2.06	0.88
1:D:96:ILE:O	1:D:99:ILE:CG1	2.22	0.88
1:G:42:ARG:NH1	1:G:84:GLU:OE1	2.06	0.88
1:F:96:ILE:CD1	1:F:99:ILE:HD13	2.03	0.88
1:D:76:PRO:CD	1:H:94:PHE:HB2	2.03	0.88
1:B:55:ILE:O	1:B:67:LYS:NZ	2.06	0.87
1:A:96:ILE:CG2	1:A:99:ILE:CD1	2.35	0.87
1:D:76:PRO:HD3	1:H:94:PHE:CG	2.08	0.87
1:B:95:LEU:O	1:B:99:ILE:HG23	1.72	0.87
1:E:55:ILE:HG23	1:E:67:LYS:HZ2	1.37	0.87
1:E:55:ILE:O	1:E:67:LYS:NZ	2.06	0.87
1:B:55:ILE:HG23	1:B:67:LYS:HZ2	1.39	0.86
1:D:76:PRO:HD3	1:H:94:PHE:CD1	2.10	0.86
1:E:57:CYS:SG	1:E:58:ARG:HG2	2.16	0.86
1:C:98:LYS:O	1:C:102:GLU:N	2.08	0.86
1:D:76:PRO:HD3	1:H:94:PHE:CB	2.04	0.86
1:A:48:SER:OG	1:E:37:HIS:NE2	1.79	0.85
1:D:27:TYR:HE2	1:D:98:LYS:HE2	1.42	0.85
1:B:84:GLU:OE2	1:B:88:ARG:NE	2.09	0.85
1:A:55:ILE:HG23	1:A:67:LYS:HZ2	1.40	0.85
1:C:27:TYR:CE2	1:C:98:LYS:CE	2.59	0.84
1:B:13:LEU:HB2	1:B:17:LYS:HZ1	1.41	0.84
1:G:22:GLU:OE2	1:G:73:GLN:NE2	2.09	0.84
1:F:27:TYR:CE2	1:F:98:LYS:HE2	2.13	0.84
1:C:27:TYR:CZ	1:C:98:LYS:HE2	2.12	0.84
1:F:55:ILE:HG23	1:F:67:LYS:HZ2	1.43	0.83
1:E:13:LEU:HB2	1:E:17:LYS:HZ1	1.42	0.83
1:G:55:ILE:O	1:G:67:LYS:NZ	2.10	0.83
1:B:55:ILE:HG22	1:B:64:ARG:HG3	1.60	0.83
1:B:59:THR:HG21	1:B:64:ARG:HB2	1.60	0.82
1:B:94:PHE:O	1:B:98:LYS:HG2	1.80	0.82
1:B:63:LYS:NZ	1:E:36:ARG:O	2.13	0.82
1:F:59:THR:HG21	1:F:67:LYS:HZ1	1.45	0.82
1:G:55:ILE:HG23	1:G:67:LYS:HZ3	1.43	0.82
1:B:76:PRO:HD3	1:F:94:PHE:CG	2.14	0.82
1:A:13:LEU:HB2	1:A:17:LYS:HZ1	1.44	0.82
1:C:54:GLU:OE1	1:G:36:ARG:NH1	2.13	0.82
1:G:96:ILE:HD12	1:G:99:ILE:CD1	2.06	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:59:THR:HG21	1:E:67:LYS:HZ1	1.45	0.82
1:C:55:ILE:O	1:C:67:LYS:NZ	2.13	0.82
1:C:76:PRO:HD3	1:G:94:PHE:CG	2.15	0.82
1:D:27:TYR:CZ	1:D:98:LYS:HE2	2.14	0.82
1:C:76:PRO:HD3	1:G:94:PHE:CB	2.09	0.82
1:A:96:ILE:HD13	1:A:99:ILE:HG21	1.60	0.81
1:B:48:SER:OG	1:F:37:HIS:NE2	1.88	0.81
1:E:96:ILE:HD12	1:E:99:ILE:CD1	2.07	0.81
1:D:22:GLU:OE2	1:D:73:GLN:NE2	2.14	0.81
1:H:44:LYS:HE3	1:H:49:ARG:CD	2.10	0.81
1:A:54:GLU:OE1	1:E:36:ARG:NH1	2.13	0.81
1:C:76:PRO:CD	1:G:94:PHE:HB2	2.09	0.81
1:D:51:ASP:O	1:D:55:ILE:N	2.13	0.81
1:E:27:TYR:HE2	1:E:98:LYS:HE2	1.46	0.81
1:H:27:TYR:HE2	1:H:98:LYS:HE2	1.45	0.80
1:G:59:THR:HG21	1:G:67:LYS:HZ2	1.46	0.80
1:H:55:ILE:O	1:H:67:LYS:NZ	2.12	0.80
1:F:34:ALA:CB	1:F:38:PHE:CZ	2.64	0.80
1:D:98:LYS:O	1:D:102:GLU:N	2.15	0.80
1:G:49:ARG:C	1:G:49:ARG:HH11	1.84	0.80
1:F:96:ILE:HA	1:F:99:ILE:CD1	2.12	0.80
1:D:54:GLU:OE1	1:H:36:ARG:NH1	2.14	0.79
1:A:51:ASP:O	1:A:55:ILE:N	2.16	0.79
1:A:50:GLU:H	1:E:37:HIS:HE1	1.30	0.79
1:C:27:TYR:HE2	1:C:98:LYS:CE	1.94	0.79
1:C:22:GLU:OE2	1:C:73:GLN:NE2	2.16	0.79
1:C:95:LEU:O	1:C:99:ILE:N	2.15	0.79
1:E:95:LEU:C	1:E:99:ILE:HG23	2.03	0.79
1:D:56:SER:HA	1:D:64:ARG:HD3	1.65	0.78
1:E:49:ARG:HH12	1:E:53:GLU:CG	1.96	0.78
1:B:56:SER:HA	1:B:64:ARG:HD3	1.65	0.78
1:F:97:GLN:O	1:F:100:THR:OG1	1.99	0.78
1:H:56:SER:HA	1:H:64:ARG:HD3	1.65	0.78
1:D:96:ILE:HD13	1:D:99:ILE:HD13	1.65	0.78
1:F:24:LEU:HD22	1:F:102:GLU:HG3	1.66	0.78
1:B:35:GLU:OE2	1:B:64:ARG:HG2	1.84	0.78
1:H:57:CYS:SG	1:H:58:ARG:HG2	2.23	0.78
1:A:49:ARG:HG3	1:A:49:ARG:HH11	1.48	0.78
1:H:49:ARG:O	1:H:49:ARG:NH1	2.16	0.78
1:H:96:ILE:CG2	1:H:99:ILE:CD1	2.34	0.78
1:C:51:ASP:O	1:C:55:ILE:N	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:95:LEU:O	1:H:99:ILE:N	2.16	0.78
1:B:51:ASP:O	1:B:55:ILE:N	2.16	0.77
1:G:96:ILE:CG2	1:G:99:ILE:CD1	2.32	0.77
1:D:27:TYR:CE2	1:D:98:LYS:CE	2.66	0.77
1:A:50:GLU:OE2	1:B:60:SER:OG	2.02	0.77
1:A:59:THR:HG21	1:A:67:LYS:HZ1	1.50	0.76
1:G:96:ILE:CA	1:G:99:ILE:CG1	2.52	0.76
1:H:59:THR:HG21	1:H:67:LYS:HZ1	1.50	0.76
1:B:76:PRO:HD3	1:F:94:PHE:CB	2.16	0.76
1:H:95:LEU:C	1:H:99:ILE:HG23	2.06	0.76
1:D:57:CYS:SG	1:D:58:ARG:HG2	2.26	0.75
1:D:59:THR:HG21	1:D:67:LYS:HZ1	1.51	0.75
1:A:96:ILE:HD12	1:A:99:ILE:CD1	2.07	0.75
1:A:96:ILE:HG23	1:A:99:ILE:HD13	1.66	0.75
1:A:94:PHE:O	1:A:98:LYS:CG	2.33	0.75
1:D:13:LEU:HB2	1:D:17:LYS:HZ1	1.52	0.75
1:F:96:ILE:O	1:F:99:ILE:HG13	1.85	0.75
1:G:77:LYS:O	1:G:79:LEU:HG	1.86	0.75
1:A:18:LYS:O	1:A:22:GLU:N	2.19	0.75
1:B:96:ILE:CD1	1:B:99:ILE:HG21	2.17	0.75
1:C:59:THR:HG21	1:C:67:LYS:HZ1	1.51	0.75
1:G:24:LEU:HD22	1:G:102:GLU:HG3	1.67	0.75
1:B:76:PRO:CD	1:F:94:PHE:HB2	2.16	0.75
1:B:96:ILE:HD13	1:B:99:ILE:CG2	2.17	0.75
1:H:24:LEU:HD22	1:H:102:GLU:HG3	1.67	0.75
1:F:35:GLU:HA	1:F:39:ASP:HB2	1.69	0.74
1:A:96:ILE:O	1:A:99:ILE:HG13	1.87	0.74
1:C:48:SER:OG	1:G:37:HIS:NE2	1.92	0.74
1:B:26:VAL:HG13	1:E:88:ARG:HH22	1.51	0.74
1:G:95:LEU:C	1:G:99:ILE:HG23	2.07	0.74
1:H:93:ASN:OD1	1:H:94:PHE:N	2.20	0.74
1:F:51:ASP:O	1:F:55:ILE:N	2.17	0.74
1:E:95:LEU:O	1:E:99:ILE:N	2.20	0.74
1:H:55:ILE:HG23	1:H:67:LYS:HZ2	1.52	0.74
1:E:22:GLU:OE2	1:E:73:GLN:NE2	2.20	0.74
1:B:50:GLU:H	1:F:37:HIS:HE1	1.36	0.74
1:G:93:ASN:OD1	1:G:94:PHE:N	2.21	0.74
1:C:57:CYS:SG	1:C:58:ARG:HG2	2.27	0.74
1:D:44:LYS:HE3	1:D:49:ARG:HD3	1.69	0.73
1:F:37:HIS:CE1	1:F:90:LYS:HZ3	2.05	0.73
1:D:15:GLU:O	1:D:18:LYS:NZ	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:LEU:O	1:B:99:ILE:N	2.21	0.73
1:B:76:PRO:HD3	1:F:94:PHE:HB2	1.69	0.73
1:G:31:LYS:HE2	1:G:94:PHE:HD2	1.52	0.73
1:A:21:LEU:HD23	1:A:73:GLN:HG2	1.71	0.73
1:F:95:LEU:O	1:F:99:ILE:N	2.22	0.72
1:H:44:LYS:CE	1:H:49:ARG:HD3	2.20	0.72
1:A:93:ASN:OD1	1:A:94:PHE:N	2.21	0.72
1:G:95:LEU:O	1:G:99:ILE:N	2.21	0.72
1:C:56:SER:HA	1:C:64:ARG:HD3	1.71	0.72
1:E:56:SER:HA	1:E:64:ARG:HD3	1.72	0.72
1:A:59:THR:HG21	1:A:64:ARG:HB2	1.72	0.72
1:D:63:LYS:NZ	1:G:36:ARG:HG3	2.05	0.72
1:D:93:ASN:OD1	1:D:94:PHE:N	2.22	0.72
1:F:34:ALA:HB1	1:F:38:PHE:CE2	2.24	0.72
1:G:18:LYS:O	1:G:22:GLU:N	2.21	0.72
1:F:93:ASN:OD1	1:F:94:PHE:N	2.23	0.71
1:H:44:LYS:HE3	1:H:49:ARG:HD3	1.71	0.71
1:H:51:ASP:O	1:H:55:ILE:N	2.18	0.71
1:A:95:LEU:C	1:A:99:ILE:HG23	2.10	0.71
1:B:97:GLN:O	1:B:100:THR:OG1	2.07	0.71
1:G:96:ILE:HA	1:G:99:ILE:CD1	2.19	0.71
1:D:24:LEU:HD22	1:D:102:GLU:HG3	1.72	0.71
1:E:31:LYS:HE2	1:E:94:PHE:HD2	1.55	0.71
1:C:55:ILE:CG2	1:C:67:LYS:HZ2	2.04	0.71
1:D:26:VAL:HG13	1:G:88:ARG:HH22	1.55	0.71
1:F:49:ARG:HH12	1:F:53:GLU:CG	2.02	0.71
1:F:56:SER:HA	1:F:64:ARG:HD3	1.73	0.71
1:E:25:ARG:HE	1:H:44:LYS:HD3	1.56	0.71
1:A:50:GLU:H	1:E:37:HIS:CE1	2.08	0.71
1:F:31:LYS:HE2	1:F:94:PHE:HD2	1.56	0.71
1:D:60:SER:O	1:D:61:SER:OG	2.09	0.70
1:D:50:GLU:H	1:H:37:HIS:HE1	1.39	0.70
1:A:50:GLU:OE2	1:B:63:LYS:HE2	1.92	0.70
1:A:50:GLU:N	1:E:37:HIS:HE1	1.89	0.70
1:E:49:ARG:HH11	1:E:49:ARG:C	1.92	0.70
1:F:49:ARG:HH11	1:F:49:ARG:C	1.95	0.70
1:G:96:ILE:O	1:G:99:ILE:HG13	1.90	0.70
1:H:44:LYS:NZ	1:H:49:ARG:HE	1.88	0.70
1:A:55:ILE:CG2	1:A:67:LYS:HZ2	2.04	0.70
1:F:44:LYS:HA	1:F:47:LEU:HB3	1.73	0.70
1:G:56:SER:HA	1:G:64:ARG:HD3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ARG:HB2	1:A:88:ARG:HH21	1.57	0.70
1:A:70:ASP:CG	1:D:49:ARG:NH2	2.35	0.70
1:H:49:ARG:NH1	1:H:49:ARG:HG3	2.07	0.70
1:E:96:ILE:HA	1:E:99:ILE:CD1	2.22	0.70
1:G:27:TYR:HE2	1:G:98:LYS:HE2	1.51	0.70
1:A:21:LEU:O	1:A:25:ARG:N	2.25	0.69
1:B:59:THR:HG21	1:B:67:LYS:HZ1	1.56	0.69
1:G:44:LYS:HA	1:G:47:LEU:HB3	1.73	0.69
1:H:104:LEU:O	1:H:108:ASN:N	2.20	0.69
1:H:96:ILE:HA	1:H:99:ILE:CD1	2.22	0.69
1:C:96:ILE:HG23	1:C:99:ILE:HD11	0.77	0.69
1:H:44:LYS:HA	1:H:47:LEU:HB3	1.75	0.69
1:B:57:CYS:SG	1:B:58:ARG:HG2	2.32	0.69
1:A:54:GLU:HB2	1:B:60:SER:HB3	1.75	0.69
1:D:50:GLU:N	1:H:37:HIS:HE1	1.91	0.69
1:D:107:ARG:HH11	1:D:107:ARG:HA	1.56	0.69
1:G:13:LEU:HB2	1:G:17:LYS:NZ	2.06	0.69
1:H:96:ILE:O	1:H:99:ILE:HG13	1.93	0.69
1:E:35:GLU:HA	1:E:39:ASP:HB2	1.74	0.69
1:D:51:ASP:H	1:H:37:HIS:CE1	2.11	0.68
1:G:57:CYS:SG	1:G:58:ARG:HG2	2.33	0.68
1:H:13:LEU:C	1:H:17:LYS:HZ3	1.95	0.68
1:F:107:ARG:HH11	1:F:107:ARG:HA	1.58	0.68
1:A:27:TYR:CZ	1:A:98:LYS:HE2	2.26	0.68
1:C:83:VAL:HG23	1:C:87:ARG:HH11	1.58	0.68
1:G:59:THR:HG22	1:G:63:LYS:HB2	1.76	0.68
1:H:104:LEU:HA	1:H:107:ARG:HB3	1.73	0.68
1:A:96:ILE:HG23	1:A:99:ILE:HD11	0.72	0.68
1:H:82:LEU:HD11	1:H:102:GLU:CD	2.14	0.68
1:B:35:GLU:HA	1:B:39:ASP:HB2	1.76	0.68
1:C:96:ILE:CG2	1:C:99:ILE:CD1	2.51	0.68
1:G:104:LEU:HA	1:G:107:ARG:HB3	1.74	0.68
1:E:63:LYS:NZ	1:H:36:ARG:O	2.25	0.68
1:A:24:LEU:HD22	1:A:102:GLU:HG3	1.75	0.68
1:B:55:ILE:CG2	1:B:67:LYS:HZ2	2.06	0.67
1:B:96:ILE:HA	1:B:99:ILE:CG2	2.23	0.67
1:A:15:GLU:O	1:A:18:LYS:NZ	2.27	0.67
1:A:19:ASP:O	1:A:23:ASN:N	2.25	0.67
1:D:59:THR:HG21	1:D:64:ARG:HB2	1.75	0.67
1:E:95:LEU:O	1:E:99:ILE:CG2	2.33	0.67
1:G:60:SER:O	1:G:61:SER:OG	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:SER:HA	1:A:64:ARG:HD3	1.75	0.67
1:D:18:LYS:O	1:D:22:GLU:N	2.24	0.67
1:D:44:LYS:HA	1:D:47:LEU:CB	2.25	0.67
1:D:95:LEU:C	1:D:99:ILE:HG23	2.15	0.67
1:E:24:LEU:HD22	1:E:102:GLU:HG3	1.75	0.67
1:F:104:LEU:HA	1:F:107:ARG:HB3	1.77	0.67
1:A:59:THR:HG22	1:A:63:LYS:HB2	1.77	0.67
1:C:18:LYS:O	1:C:22:GLU:N	2.26	0.67
1:H:38:PHE:CD2	1:H:90:LYS:HD2	2.29	0.67
1:F:59:THR:HG22	1:F:63:LYS:HB2	1.75	0.67
1:F:95:LEU:C	1:F:99:ILE:HG23	2.15	0.67
1:C:50:GLU:H	1:G:37:HIS:HE1	1.41	0.67
1:H:49:ARG:HH11	1:H:49:ARG:HG3	1.59	0.67
1:A:51:ASP:H	1:E:37:HIS:CE1	2.13	0.67
1:D:49:ARG:NH1	1:D:49:ARG:HG3	2.10	0.67
1:C:96:ILE:HD13	1:C:99:ILE:HG21	1.77	0.66
1:D:25:ARG:HE	1:G:44:LYS:HD3	1.58	0.66
1:F:34:ALA:HB1	1:F:38:PHE:CZ	2.31	0.66
1:G:35:GLU:HB3	1:G:68:LEU:HD13	1.77	0.66
1:E:107:ARG:HH11	1:E:107:ARG:HA	1.60	0.66
1:C:25:ARG:HE	1:F:44:LYS:HD3	1.60	0.66
1:B:13:LEU:HB2	1:B:17:LYS:NZ	2.10	0.66
1:B:27:TYR:HE2	1:B:98:LYS:CE	2.07	0.66
1:B:50:GLU:N	1:F:37:HIS:HE1	1.93	0.66
1:C:15:GLU:O	1:C:18:LYS:NZ	2.25	0.66
1:C:60:SER:O	1:C:61:SER:OG	2.08	0.66
1:A:57:CYS:SG	1:A:58:ARG:HG2	2.36	0.66
1:B:17:LYS:HZ2	1:B:106:LEU:HD11	1.61	0.66
1:B:107:ARG:HA	1:B:107:ARG:HH11	1.59	0.66
1:B:96:ILE:CA	1:B:99:ILE:CG1	2.60	0.66
1:E:51:ASP:O	1:E:55:ILE:N	2.21	0.66
1:B:50:GLU:H	1:F:37:HIS:CE1	2.14	0.65
1:F:34:ALA:HB1	1:F:38:PHE:CD2	2.31	0.65
1:D:94:PHE:O	1:D:98:LYS:CG	2.44	0.65
1:E:49:ARG:HH12	1:E:53:GLU:CD	2.00	0.65
1:E:93:ASN:OD1	1:E:94:PHE:N	2.24	0.65
1:H:13:LEU:HB2	1:H:17:LYS:NZ	2.11	0.65
1:D:96:ILE:HG23	1:D:99:ILE:HD11	0.78	0.65
1:E:13:LEU:HB2	1:E:17:LYS:NZ	2.10	0.65
1:E:99:ILE:O	1:E:103:VAL:N	2.25	0.65
1:C:35:GLU:HA	1:C:39:ASP:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:ARG:HH12	1:F:53:GLU:CD	2.00	0.65
1:B:42:ARG:HB2	1:B:88:ARG:HH21	1.60	0.65
1:E:104:LEU:HA	1:E:107:ARG:HB3	1.79	0.65
1:G:50:GLU:OE2	1:H:63:LYS:HE2	1.97	0.65
1:H:96:ILE:HD13	1:H:99:ILE:HG21	1.78	0.65
1:C:24:LEU:HD22	1:C:102:GLU:HG3	1.79	0.65
1:E:18:LYS:O	1:E:22:GLU:N	2.28	0.65
1:F:35:GLU:HB3	1:F:68:LEU:HD13	1.77	0.65
1:B:104:LEU:O	1:B:108:ASN:N	2.20	0.64
1:E:26:VAL:HG13	1:H:88:ARG:HH22	1.62	0.64
1:H:96:ILE:CA	1:H:99:ILE:CG1	2.51	0.64
1:A:18:LYS:HB2	1:A:18:LYS:NZ	2.11	0.64
1:F:60:SER:O	1:F:61:SER:OG	2.10	0.64
1:H:34:ALA:HA	1:H:37:HIS:HB2	1.78	0.64
1:H:59:THR:HG21	1:H:67:LYS:NZ	2.12	0.64
1:E:50:GLU:OE2	1:F:63:LYS:HE2	1.97	0.64
1:G:83:VAL:HG23	1:G:87:ARG:HH11	1.61	0.64
1:B:93:ASN:OD1	1:B:94:PHE:N	2.29	0.64
1:D:96:ILE:HA	1:D:99:ILE:CD1	2.27	0.64
1:E:59:THR:HG22	1:E:63:LYS:HB2	1.80	0.64
1:F:13:LEU:HB2	1:F:17:LYS:HZ1	1.62	0.64
1:B:104:LEU:HA	1:B:107:ARG:HB3	1.79	0.64
1:B:51:ASP:H	1:F:37:HIS:CE1	2.15	0.64
1:F:21:LEU:O	1:F:25:ARG:N	2.31	0.64
1:D:35:GLU:HA	1:D:39:ASP:HB2	1.80	0.64
1:A:95:LEU:O	1:A:99:ILE:CG2	2.31	0.64
1:G:49:ARG:HH12	1:G:53:GLU:CD	2.01	0.64
1:C:51:ASP:H	1:G:37:HIS:CE1	2.16	0.63
1:D:96:ILE:CD1	1:D:99:ILE:CD1	2.64	0.63
1:E:42:ARG:HB2	1:E:88:ARG:HH21	1.63	0.63
1:F:104:LEU:O	1:F:108:ASN:N	2.21	0.63
1:G:49:ARG:HH12	1:G:53:GLU:CG	2.12	0.63
1:D:104:LEU:O	1:D:108:ASN:N	2.21	0.63
1:H:59:THR:HG21	1:H:64:ARG:HB2	1.81	0.63
1:E:96:ILE:HG23	1:E:99:ILE:HD11	0.72	0.63
1:F:19:ASP:OD1	1:F:20:ALA:N	2.31	0.63
1:F:96:ILE:HD12	1:F:99:ILE:CD1	2.25	0.63
1:C:59:THR:HG21	1:C:64:ARG:HB2	1.80	0.63
1:D:55:ILE:CG2	1:D:67:LYS:HZ2	2.07	0.63
1:D:59:THR:HG21	1:D:67:LYS:NZ	2.13	0.63
1:F:31:LYS:HG3	1:F:95:LEU:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:GLU:N	1:G:37:HIS:HE1	1.95	0.63
1:F:17:LYS:HZ2	1:F:106:LEU:HD11	1.63	0.63
1:B:96:ILE:HA	1:B:99:ILE:HG23	1.80	0.63
1:F:19:ASP:O	1:F:23:ASN:N	2.24	0.63
1:E:63:LYS:NZ	1:H:36:ARG:HG3	2.14	0.63
1:D:50:GLU:H	1:H:37:HIS:CE1	2.16	0.63
1:F:57:CYS:SG	1:F:58:ARG:HG2	2.39	0.63
1:F:59:THR:HG21	1:F:67:LYS:NZ	2.14	0.63
1:F:31:LYS:HB2	1:F:95:LEU:HD22	1.80	0.63
1:A:35:GLU:HA	1:A:39:ASP:HB2	1.80	0.62
1:E:44:LYS:HA	1:E:47:LEU:HB3	1.79	0.62
1:B:60:SER:O	1:B:61:SER:OG	2.07	0.62
1:C:96:ILE:HA	1:C:99:ILE:CD1	2.29	0.62
1:C:96:ILE:HD13	1:C:99:ILE:HD13	1.75	0.62
1:H:44:LYS:HE3	1:H:49:ARG:HD2	1.81	0.62
1:A:49:ARG:NH1	1:A:53:GLU:OE2	2.32	0.62
1:B:27:TYR:CE2	1:B:98:LYS:CE	2.76	0.62
1:H:59:THR:HG22	1:H:63:LYS:HB2	1.81	0.62
1:E:55:ILE:CG2	1:E:67:LYS:HZ2	2.12	0.62
1:B:18:LYS:O	1:B:22:GLU:N	2.30	0.62
1:B:76:PRO:HD3	1:F:94:PHE:HD1	1.53	0.62
1:C:31:LYS:HB2	1:C:95:LEU:HD22	1.82	0.62
1:C:94:PHE:O	1:C:98:LYS:CG	2.42	0.62
1:E:59:THR:HG21	1:E:64:ARG:HB2	1.81	0.62
1:G:42:ARG:HB2	1:G:88:ARG:HH21	1.64	0.62
1:H:42:ARG:HB2	1:H:88:ARG:HH21	1.64	0.62
1:F:99:ILE:O	1:F:103:VAL:N	2.28	0.62
1:C:42:ARG:HB2	1:C:88:ARG:NH2	2.15	0.62
1:E:96:ILE:CG2	1:E:99:ILE:CD1	2.46	0.62
1:E:59:THR:HG21	1:E:67:LYS:NZ	2.14	0.62
1:E:96:ILE:O	1:E:99:ILE:HG13	1.98	0.62
1:G:35:GLU:HA	1:G:39:ASP:HB2	1.80	0.62
1:B:59:THR:HG22	1:B:63:LYS:HB2	1.82	0.62
1:G:59:THR:HG21	1:G:64:ARG:HB2	1.82	0.62
1:H:60:SER:O	1:H:61:SER:OG	2.08	0.62
1:H:95:LEU:O	1:H:99:ILE:CG2	2.35	0.62
1:C:59:THR:HG22	1:C:63:LYS:HB2	1.80	0.61
1:D:27:TYR:HE2	1:D:98:LYS:CE	2.08	0.61
1:G:101:ASP:HA	1:G:104:LEU:HB2	1.82	0.61
1:E:63:LYS:HZ2	1:H:36:ARG:HG3	1.63	0.61
1:A:49:ARG:HG3	1:A:49:ARG:NH1	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:THR:HA	1:B:17:LYS:HD2	1.82	0.61
1:B:96:ILE:HG23	1:B:99:ILE:CG1	2.23	0.61
1:F:50:GLU:OE2	1:G:63:LYS:HE2	2.01	0.61
1:A:34:ALA:HA	1:A:37:HIS:HB2	1.81	0.61
1:A:99:ILE:O	1:A:103:VAL:N	2.31	0.61
1:C:21:LEU:HD23	1:C:73:GLN:HG2	1.81	0.61
1:H:107:ARG:HA	1:H:107:ARG:HH11	1.65	0.61
1:F:59:THR:HG21	1:F:64:ARG:HB2	1.82	0.61
1:D:14:THR:HA	1:D:17:LYS:HD2	1.81	0.61
1:D:99:ILE:O	1:D:103:VAL:N	2.31	0.61
1:E:104:LEU:O	1:E:108:ASN:N	2.24	0.61
1:E:35:GLU:HB3	1:E:68:LEU:HD13	1.83	0.61
1:H:97:GLN:O	1:H:100:THR:OG1	2.19	0.61
1:A:25:ARG:HE	1:D:44:LYS:HD3	1.66	0.61
1:C:50:GLU:H	1:G:37:HIS:CE1	2.18	0.61
1:B:44:LYS:HA	1:B:47:LEU:HB3	1.83	0.61
1:C:42:ARG:HG2	1:C:84:GLU:CD	2.20	0.61
1:G:31:LYS:HG3	1:G:95:LEU:HB2	1.82	0.61
1:B:96:ILE:O	1:B:99:ILE:HG13	1.99	0.61
1:C:13:LEU:HB2	1:C:17:LYS:NZ	2.13	0.61
1:E:17:LYS:HZ2	1:E:106:LEU:HD11	1.65	0.61
1:G:97:GLN:O	1:G:100:THR:OG1	2.18	0.61
1:B:37:HIS:HB3	1:B:90:LYS:HZ3	1.66	0.60
1:A:93:ASN:O	1:A:97:GLN:HG3	2.01	0.60
1:C:93:ASN:O	1:C:97:GLN:HG3	2.02	0.60
1:A:70:ASP:OD1	1:D:49:ARG:NH2	2.34	0.60
1:D:59:THR:HG22	1:D:63:LYS:HB2	1.83	0.60
1:F:96:ILE:CA	1:F:99:ILE:CG1	2.61	0.60
1:D:96:ILE:CG2	1:D:99:ILE:CD1	2.53	0.60
1:A:18:LYS:HG2	1:A:73:GLN:HB3	1.84	0.60
1:C:95:LEU:C	1:C:99:ILE:HG23	2.21	0.60
1:E:21:LEU:O	1:E:25:ARG:N	2.35	0.60
1:E:60:SER:O	1:E:61:SER:OG	2.09	0.60
1:C:93:ASN:OD1	1:C:94:PHE:N	2.31	0.60
1:C:107:ARG:HH11	1:C:107:ARG:HA	1.67	0.60
1:H:42:ARG:HB2	1:H:88:ARG:NH2	2.17	0.60
1:A:96:ILE:HA	1:A:99:ILE:CG2	2.32	0.59
1:F:98:LYS:HA	1:F:101:ASP:HB3	1.82	0.59
1:B:21:LEU:HD23	1:B:73:GLN:HG2	1.83	0.59
1:C:27:TYR:OH	1:C:98:LYS:HE2	2.02	0.59
1:B:34:ALA:HA	1:B:37:HIS:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:LEU:O	1:D:86:ILE:HG22	2.02	0.59
1:E:80:ASP:HA	1:E:83:VAL:HG12	1.84	0.59
1:H:44:LYS:NZ	1:H:49:ARG:NE	2.50	0.59
1:B:95:LEU:O	1:B:98:LYS:HB2	2.02	0.59
1:C:59:THR:HG21	1:C:67:LYS:NZ	2.16	0.59
1:G:100:THR:O	1:G:104:LEU:N	2.35	0.59
1:H:49:ARG:HH11	1:H:49:ARG:C	2.06	0.59
1:G:98:LYS:HA	1:G:101:ASP:HB3	1.85	0.59
1:A:63:LYS:O	1:A:67:LYS:N	2.29	0.59
1:A:95:LEU:O	1:A:99:ILE:N	2.36	0.59
1:C:104:LEU:HA	1:C:107:ARG:HB3	1.84	0.59
1:H:49:ARG:HH11	1:H:49:ARG:CG	2.15	0.59
1:C:26:VAL:HG13	1:F:88:ARG:HH22	1.67	0.59
1:D:27:TYR:HE2	1:D:98:LYS:HG3	1.67	0.59
1:H:82:LEU:O	1:H:86:ILE:HG22	2.03	0.59
1:A:14:THR:HA	1:A:17:LYS:HD2	1.85	0.59
1:G:42:ARG:HG2	1:G:42:ARG:HH11	1.66	0.59
1:G:82:LEU:O	1:G:86:ILE:HG22	2.03	0.59
1:C:14:THR:HA	1:C:17:LYS:HD2	1.84	0.59
1:D:18:LYS:NZ	1:D:18:LYS:HB2	2.17	0.59
1:A:98:LYS:HA	1:A:101:ASP:HB3	1.84	0.58
1:A:99:ILE:HG13	1:A:100:THR:N	2.17	0.58
1:D:49:ARG:O	1:D:52:THR:OG1	2.16	0.58
1:G:15:GLU:O	1:G:18:LYS:NZ	2.34	0.58
1:A:31:LYS:HG3	1:A:95:LEU:HB2	1.85	0.58
1:C:99:ILE:O	1:C:103:VAL:N	2.33	0.58
1:E:96:ILE:CA	1:E:99:ILE:CG1	2.56	0.58
1:G:49:ARG:NH1	1:G:53:GLU:OE2	2.36	0.58
1:H:44:LYS:CE	1:H:49:ARG:CD	2.77	0.58
1:F:13:LEU:HB2	1:F:17:LYS:NZ	2.16	0.58
1:F:55:ILE:CG2	1:F:67:LYS:HZ2	2.14	0.58
1:G:21:LEU:O	1:G:25:ARG:N	2.36	0.58
1:H:83:VAL:HG23	1:H:87:ARG:HH11	1.67	0.58
1:C:49:ARG:C	1:C:49:ARG:HH11	2.03	0.58
1:B:95:LEU:C	1:B:99:ILE:HG23	2.24	0.58
1:A:13:LEU:HB2	1:A:17:LYS:NZ	2.18	0.58
1:C:82:LEU:O	1:C:86:ILE:HG22	2.04	0.58
1:D:104:LEU:HA	1:D:107:ARG:HB3	1.85	0.58
1:G:92:GLN:NE2	1:G:96:ILE:HG21	2.18	0.58
1:H:35:GLU:HA	1:H:39:ASP:HB2	1.86	0.58
1:B:35:GLU:HG3	1:B:64:ARG:NH1	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:LYS:NZ	1:F:36:ARG:HG3	2.18	0.58
1:F:34:ALA:O	1:F:38:PHE:N	2.34	0.58
1:G:54:GLU:HB2	1:H:60:SER:HB3	1.84	0.58
1:H:98:LYS:HA	1:H:101:ASP:HB3	1.86	0.58
1:D:42:ARG:HG2	1:D:84:GLU:CD	2.24	0.58
1:F:30:GLU:HB3	1:F:94:PHE:CE2	2.39	0.58
1:G:99:ILE:O	1:G:103:VAL:N	2.32	0.58
1:A:44:LYS:HA	1:A:47:LEU:HB3	1.86	0.57
1:B:99:ILE:HG13	1:B:100:THR:N	2.19	0.57
1:C:96:ILE:O	1:C:99:ILE:HG13	2.00	0.57
1:C:18:LYS:HB2	1:C:18:LYS:NZ	2.19	0.57
1:E:31:LYS:HG3	1:E:95:LEU:HB2	1.86	0.57
1:D:55:ILE:O	1:D:67:LYS:NZ	2.27	0.57
1:D:95:LEU:O	1:D:99:ILE:N	2.36	0.57
1:E:99:ILE:HG13	1:E:100:THR:N	2.20	0.57
1:H:44:LYS:HZ2	1:H:49:ARG:HE	1.52	0.57
1:C:38:PHE:CD2	1:C:90:LYS:HD2	2.40	0.57
1:E:42:ARG:HB2	1:E:88:ARG:NH2	2.20	0.57
1:G:107:ARG:HA	1:G:107:ARG:HH11	1.69	0.57
1:B:18:LYS:HB2	1:B:18:LYS:NZ	2.20	0.57
1:E:27:TYR:HE2	1:E:98:LYS:HG3	1.69	0.57
1:F:37:HIS:CG	1:F:90:LYS:NZ	2.73	0.57
1:G:42:ARG:HH21	1:G:45:LYS:HZ1	1.53	0.57
1:H:99:ILE:O	1:H:103:VAL:N	2.30	0.57
1:G:32:ILE:O	1:G:35:GLU:HG2	2.05	0.56
1:E:96:ILE:HD13	1:E:99:ILE:HG21	1.87	0.56
1:B:76:PRO:HD2	1:F:94:PHE:HB2	1.85	0.56
1:G:59:THR:HG21	1:G:67:LYS:NZ	2.17	0.56
1:F:16:VAL:HA	1:F:19:ASP:OD2	2.06	0.56
1:F:18:LYS:O	1:F:22:GLU:N	2.32	0.56
1:F:96:ILE:HA	1:F:99:ILE:HD13	1.84	0.56
1:D:48:SER:HG	1:H:37:HIS:CD2	2.08	0.56
1:F:18:LYS:HB2	1:F:18:LYS:NZ	2.20	0.56
1:D:50:GLU:OE2	1:E:63:LYS:HE2	2.05	0.56
1:E:97:GLN:O	1:E:100:THR:OG1	2.22	0.56
1:F:92:GLN:HA	1:F:96:ILE:HG13	1.85	0.56
1:C:44:LYS:HA	1:C:47:LEU:HB3	1.87	0.56
1:G:55:ILE:CG2	1:G:67:LYS:HZ3	2.14	0.56
1:D:17:LYS:HZ2	1:D:106:LEU:HD11	1.70	0.56
1:D:85:SER:HB3	1:D:95:LEU:HD23	1.86	0.56
1:D:99:ILE:HG13	1:D:100:THR:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:99:ILE:HG13	1:F:100:THR:N	2.21	0.56
1:F:100:THR:O	1:F:104:LEU:N	2.36	0.56
1:F:27:TYR:HE2	1:F:98:LYS:HG3	1.70	0.56
1:H:18:LYS:O	1:H:22:GLU:N	2.31	0.56
1:B:82:LEU:HD11	1:B:102:GLU:CD	2.26	0.56
1:D:95:LEU:O	1:D:99:ILE:CG2	2.32	0.56
1:E:31:LYS:HB2	1:E:95:LEU:HD22	1.87	0.56
1:F:101:ASP:HA	1:F:104:LEU:HB2	1.87	0.56
1:H:86:ILE:HG23	1:H:87:ARG:HD2	1.88	0.56
1:A:96:ILE:HD13	1:A:99:ILE:CG2	2.31	0.56
1:E:82:LEU:O	1:E:86:ILE:HG22	2.06	0.56
1:A:59:THR:HG21	1:A:67:LYS:NZ	2.19	0.56
1:A:82:LEU:O	1:A:86:ILE:HG22	2.06	0.56
1:B:42:ARG:HB2	1:B:88:ARG:NH2	2.21	0.56
1:E:14:THR:HA	1:E:17:LYS:HD2	1.87	0.56
1:E:27:TYR:CZ	1:E:98:LYS:HE2	2.39	0.56
1:C:98:LYS:HA	1:C:101:ASP:HB3	1.89	0.55
1:B:24:LEU:HD22	1:B:102:GLU:HG3	1.88	0.55
1:B:25:ARG:HE	1:E:44:LYS:HD3	1.71	0.55
1:G:96:ILE:HD13	1:G:99:ILE:HG21	1.87	0.55
1:H:101:ASP:HA	1:H:104:LEU:HB2	1.89	0.55
1:D:96:ILE:O	1:D:99:ILE:HG13	2.06	0.55
1:E:19:ASP:O	1:E:23:ASN:N	2.35	0.55
1:H:99:ILE:HG13	1:H:100:THR:N	2.20	0.55
1:H:64:ARG:HA	1:H:67:LYS:NZ	2.21	0.55
1:B:96:ILE:CB	1:B:99:ILE:CD1	2.85	0.55
1:F:34:ALA:HB2	1:F:38:PHE:CZ	2.36	0.55
1:B:76:PRO:CD	1:F:94:PHE:CD1	2.80	0.55
1:G:42:ARG:HB2	1:G:88:ARG:NH2	2.21	0.55
1:G:99:ILE:HG13	1:G:100:THR:N	2.21	0.55
1:C:35:GLU:HG3	1:C:64:ARG:NH1	2.21	0.55
1:D:77:LYS:O	1:D:79:LEU:CG	2.45	0.55
1:A:49:ARG:O	1:A:52:THR:OG1	2.21	0.55
1:E:101:ASP:HA	1:E:104:LEU:HB2	1.89	0.55
1:F:80:ASP:HA	1:F:83:VAL:HG12	1.87	0.55
1:B:35:GLU:HG3	1:B:64:ARG:HH12	1.70	0.55
1:D:42:ARG:HB2	1:D:88:ARG:NH2	2.22	0.55
1:A:42:ARG:HB2	1:A:88:ARG:NH2	2.21	0.55
1:C:27:TYR:HE2	1:C:98:LYS:HG3	1.72	0.55
1:G:51:ASP:O	1:G:55:ILE:N	2.28	0.55
1:H:55:ILE:CG2	1:H:67:LYS:HZ2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:ILE:HG13	1:C:100:THR:N	2.21	0.55
1:F:82:LEU:O	1:F:86:ILE:HG22	2.07	0.55
1:B:98:LYS:HA	1:B:101:ASP:HB3	1.89	0.55
1:H:30:GLU:HB3	1:H:94:PHE:CE2	2.41	0.55
1:H:31:LYS:HG3	1:H:95:LEU:HB2	1.89	0.54
1:D:96:ILE:HD13	1:D:99:ILE:HG21	1.88	0.54
1:G:30:GLU:HB3	1:G:94:PHE:CE2	2.43	0.54
1:G:96:ILE:CA	1:G:99:ILE:CD1	2.85	0.54
1:H:32:ILE:O	1:H:35:GLU:HG2	2.07	0.54
1:B:101:ASP:HA	1:B:104:LEU:HB2	1.90	0.54
1:G:104:LEU:O	1:G:108:ASN:N	2.26	0.54
1:H:103:VAL:O	1:H:107:ARG:N	2.30	0.54
1:B:31:LYS:HB2	1:B:95:LEU:HD22	1.89	0.54
1:D:27:TYR:OH	1:D:98:LYS:HE2	2.07	0.54
1:E:96:ILE:HD13	1:E:99:ILE:HD13	1.84	0.54
1:H:21:LEU:O	1:H:25:ARG:N	2.40	0.54
1:H:42:ARG:HG2	1:H:42:ARG:HH11	1.71	0.54
1:H:80:ASP:HA	1:H:83:VAL:HG12	1.88	0.54
1:B:55:ILE:CG2	1:B:64:ARG:HG3	2.34	0.54
1:B:80:ASP:HA	1:B:83:VAL:HG12	1.89	0.54
1:D:30:GLU:OE2	1:D:94:PHE:HE2	1.91	0.54
1:B:96:ILE:HG23	1:B:99:ILE:HD11	0.54	0.54
1:B:54:GLU:HB2	1:C:60:SER:HB3	1.89	0.54
1:D:21:LEU:O	1:D:25:ARG:N	2.40	0.54
1:G:82:LEU:HD11	1:G:102:GLU:CD	2.28	0.54
1:D:93:ASN:O	1:D:97:GLN:HG3	2.08	0.54
1:G:49:ARG:O	1:G:52:THR:OG1	2.25	0.54
1:A:47:LEU:HD23	1:A:48:SER:O	2.07	0.53
1:A:97:GLN:O	1:A:100:THR:OG1	2.22	0.53
1:E:27:TYR:CE2	1:E:98:LYS:CE	2.82	0.53
1:F:27:TYR:HE2	1:F:98:LYS:HE2	1.67	0.53
1:H:55:ILE:HG22	1:H:64:ARG:HG3	1.91	0.53
1:A:48:SER:HG	1:E:37:HIS:CD2	2.15	0.53
1:A:30:GLU:OE2	1:A:94:PHE:HE2	1.90	0.53
1:A:63:LYS:NZ	1:D:36:ARG:HG3	2.22	0.53
1:D:55:ILE:HG22	1:D:64:ARG:HG3	1.91	0.53
1:H:13:LEU:HB2	1:H:17:LYS:HZ1	1.72	0.53
1:C:63:LYS:NZ	1:F:36:ARG:O	2.40	0.53
1:E:15:GLU:O	1:E:18:LYS:NZ	2.39	0.53
1:E:38:PHE:CD2	1:E:90:LYS:HD2	2.43	0.53
1:G:42:ARG:HG2	1:G:84:GLU:CD	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:96:ILE:HA	1:G:99:ILE:CG2	2.38	0.53
1:H:49:ARG:O	1:H:52:THR:OG1	2.25	0.53
1:E:30:GLU:HB3	1:E:94:PHE:CE2	2.44	0.53
1:F:42:ARG:HG2	1:F:84:GLU:CD	2.28	0.53
1:C:76:PRO:HD2	1:G:94:PHE:HB2	1.91	0.53
1:G:95:LEU:O	1:G:99:ILE:CG2	2.39	0.53
1:H:96:ILE:CB	1:H:99:ILE:CD1	2.87	0.53
1:B:49:ARG:HH11	1:B:49:ARG:HG3	1.73	0.53
1:C:101:ASP:O	1:C:105:LYS:HG2	2.09	0.53
1:C:55:ILE:HG22	1:C:64:ARG:HG3	1.91	0.53
1:D:19:ASP:O	1:D:23:ASN:N	2.39	0.53
1:F:92:GLN:HA	1:F:96:ILE:CG1	2.38	0.53
1:G:96:ILE:CB	1:G:99:ILE:CD1	2.87	0.53
1:B:79:LEU:HA	1:B:82:LEU:HD23	1.91	0.53
1:B:48:SER:OG	1:F:37:HIS:CE1	2.61	0.53
1:C:21:LEU:O	1:C:25:ARG:N	2.42	0.53
1:H:106:LEU:O	1:H:110:LYS:N	2.28	0.53
1:H:17:LYS:HZ2	1:H:106:LEU:HD11	1.74	0.53
1:A:77:LYS:HG3	1:A:78:GLY:H	1.74	0.53
1:E:37:HIS:CE1	1:E:90:LYS:HZ3	2.27	0.52
1:D:63:LYS:NZ	1:G:36:ARG:O	2.43	0.52
1:E:98:LYS:HA	1:E:101:ASP:HB3	1.91	0.52
1:B:21:LEU:O	1:B:25:ARG:N	2.42	0.52
1:C:97:GLN:O	1:C:100:THR:OG1	2.26	0.52
1:F:14:THR:HA	1:F:17:LYS:HD2	1.91	0.52
1:H:34:ALA:HA	1:H:37:HIS:CB	2.39	0.52
1:F:34:ALA:HB1	1:F:38:PHE:CE1	2.44	0.52
1:G:42:ARG:HH21	1:G:45:LYS:NZ	2.07	0.52
1:B:83:VAL:O	1:B:87:ARG:HD2	2.10	0.52
1:D:92:GLN:NE2	1:D:96:ILE:HG21	2.24	0.52
1:E:34:ALA:HA	1:E:37:HIS:CB	2.39	0.52
1:C:49:ARG:HH12	1:C:53:GLU:CG	2.22	0.52
1:F:42:ARG:HB2	1:F:88:ARG:NH2	2.24	0.52
1:B:49:ARG:NH1	1:B:49:ARG:HG3	2.25	0.52
1:C:104:LEU:O	1:C:108:ASN:N	2.22	0.52
1:C:96:ILE:CD1	1:C:99:ILE:CD1	2.62	0.52
1:F:96:ILE:CA	1:F:99:ILE:CD1	2.86	0.52
1:C:93:ASN:O	1:C:97:GLN:CG	2.58	0.52
1:D:101:ASP:O	1:D:105:LYS:HG2	2.10	0.52
1:C:48:SER:CB	1:G:37:HIS:HE2	2.17	0.52
1:H:10:GLU:HB2	1:H:12:ASP:OD2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:42:ARG:HG2	1:H:84:GLU:CD	2.30	0.52
1:D:80:ASP:HA	1:D:83:VAL:HG12	1.91	0.52
1:E:100:THR:O	1:E:104:LEU:N	2.32	0.52
1:F:19:ASP:OD1	1:F:109:ILE:HG21	2.10	0.52
1:C:96:ILE:CA	1:C:99:ILE:CG1	2.62	0.52
1:H:96:ILE:CA	1:H:99:ILE:CD1	2.87	0.52
1:F:32:ILE:O	1:F:35:GLU:HG2	2.09	0.51
1:B:48:SER:CB	1:F:37:HIS:HE2	2.17	0.51
1:G:34:ALA:HA	1:G:37:HIS:CB	2.40	0.51
1:B:101:ASP:O	1:B:105:LYS:HG2	2.10	0.51
1:D:42:ARG:HE	1:D:45:LYS:HE2	1.76	0.51
1:E:42:ARG:HG2	1:E:42:ARG:HH11	1.74	0.51
1:B:42:ARG:HG2	1:B:84:GLU:CD	2.31	0.51
1:H:96:ILE:HA	1:H:99:ILE:CG2	2.39	0.51
1:A:96:ILE:CA	1:A:99:ILE:CG1	2.59	0.51
1:D:82:LEU:HD11	1:D:102:GLU:CD	2.30	0.51
1:D:28:LEU:HA	1:D:32:ILE:HG13	1.93	0.51
1:E:27:TYR:HE2	1:E:98:LYS:CE	2.18	0.51
1:A:96:ILE:HA	1:A:99:ILE:HG23	1.91	0.51
1:D:50:GLU:HG3	1:E:62:ARG:HB2	1.92	0.51
1:E:83:VAL:O	1:E:87:ARG:HD2	2.11	0.51
1:E:42:ARG:HG2	1:E:84:GLU:CD	2.31	0.51
1:B:35:GLU:HB3	1:B:68:LEU:HD13	1.92	0.51
1:E:34:ALA:O	1:E:38:PHE:N	2.43	0.51
1:F:34:ALA:HB1	1:F:38:PHE:CG	2.46	0.51
1:H:96:ILE:CD1	1:H:99:ILE:CD1	2.65	0.51
1:B:96:ILE:CG2	1:B:99:ILE:CG1	2.87	0.51
1:H:31:LYS:HE2	1:H:94:PHE:HD2	1.76	0.51
1:B:30:GLU:OE2	1:B:94:PHE:HE2	1.94	0.51
1:D:97:GLN:O	1:D:100:THR:OG1	2.29	0.51
1:A:85:SER:HB3	1:A:95:LEU:HD23	1.94	0.50
1:E:18:LYS:HB2	1:E:18:LYS:NZ	2.27	0.50
1:G:80:ASP:HA	1:G:83:VAL:HG12	1.92	0.50
1:G:27:TYR:CZ	1:G:98:LYS:HE2	2.46	0.50
1:A:38:PHE:CD2	1:A:90:LYS:HD2	2.46	0.50
1:G:14:THR:HA	1:G:17:LYS:HD2	1.93	0.50
1:H:42:ARG:HH21	1:H:45:LYS:HZ1	1.58	0.50
1:H:44:LYS:HZ1	1:H:49:ARG:HE	1.58	0.50
1:B:19:ASP:O	1:B:23:ASN:N	2.37	0.50
1:E:30:GLU:OE2	1:E:94:PHE:HE2	1.95	0.50
1:C:100:THR:O	1:C:104:LEU:N	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:VAL:HG23	1:A:87:ARG:HH11	1.76	0.50
1:C:101:ASP:HA	1:C:104:LEU:HB2	1.94	0.50
1:A:22:GLU:CD	1:A:73:GLN:HE22	2.08	0.50
1:F:37:HIS:CG	1:F:90:LYS:HZ3	2.28	0.50
1:C:19:ASP:O	1:C:23:ASN:N	2.37	0.50
1:E:49:ARG:O	1:E:52:THR:OG1	2.26	0.50
1:A:50:GLU:HG2	1:B:60:SER:HB2	1.94	0.49
1:D:47:LEU:HD23	1:D:48:SER:O	2.12	0.49
1:F:34:ALA:HA	1:F:37:HIS:CB	2.42	0.49
1:F:42:ARG:HG2	1:F:42:ARG:HH11	1.75	0.49
1:F:42:ARG:HB2	1:F:88:ARG:HH21	1.77	0.49
1:G:86:ILE:HG23	1:G:87:ARG:HD2	1.94	0.49
1:A:55:ILE:HG22	1:A:64:ARG:HG3	1.94	0.49
1:B:42:ARG:HH11	1:B:42:ARG:HG2	1.76	0.49
1:B:59:THR:HG21	1:B:67:LYS:NZ	2.26	0.49
1:B:96:ILE:HA	1:B:99:ILE:CD1	2.41	0.49
1:D:44:LYS:NZ	1:D:49:ARG:HE	2.10	0.49
1:E:32:ILE:O	1:E:35:GLU:HG2	2.12	0.49
1:B:93:ASN:O	1:B:97:GLN:HG3	2.12	0.49
1:A:18:LYS:HB2	1:A:18:LYS:HZ2	1.76	0.49
1:D:64:ARG:HA	1:D:67:LYS:NZ	2.28	0.49
1:E:49:ARG:HH12	1:E:53:GLU:HG3	1.76	0.49
1:H:50:GLU:HA	1:H:53:GLU:CD	2.32	0.49
1:A:86:ILE:HG23	1:A:87:ARG:HD2	1.95	0.49
1:B:42:ARG:HE	1:B:45:LYS:HE2	1.78	0.49
1:B:18:LYS:HG2	1:B:73:GLN:HB3	1.94	0.49
1:D:96:ILE:CA	1:D:99:ILE:CG1	2.66	0.49
1:E:54:GLU:HB2	1:F:60:SER:HB3	1.94	0.49
1:F:64:ARG:HA	1:F:67:LYS:NZ	2.28	0.49
1:G:101:ASP:O	1:G:105:LYS:N	2.28	0.49
1:A:44:LYS:HE3	1:A:49:ARG:HD3	1.95	0.49
1:B:42:ARG:HH21	1:B:45:LYS:NZ	2.11	0.49
1:D:86:ILE:HG23	1:D:87:ARG:HD2	1.94	0.49
1:D:101:ASP:HA	1:D:104:LEU:HB2	1.95	0.49
1:A:26:VAL:HG13	1:D:88:ARG:HH22	1.78	0.49
1:A:42:ARG:HG2	1:A:84:GLU:CD	2.33	0.49
1:A:42:ARG:HE	1:A:45:LYS:HE2	1.78	0.49
1:E:96:ILE:HA	1:E:99:ILE:CG2	2.43	0.49
1:C:64:ARG:HA	1:C:67:LYS:NZ	2.28	0.48
1:D:100:THR:O	1:D:104:LEU:N	2.40	0.48
1:D:35:GLU:OE1	1:D:65:ALA:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:64:ARG:HA	1:F:67:LYS:HB2	1.95	0.48
1:G:83:VAL:HG23	1:G:87:ARG:NH1	2.26	0.48
1:A:64:ARG:CA	1:A:67:LYS:HZ1	2.27	0.48
1:B:55:ILE:HD11	1:B:71:TYR:CZ	2.47	0.48
1:D:25:ARG:O	1:G:41:LEU:HD11	2.13	0.48
1:D:42:ARG:HG2	1:D:42:ARG:HH11	1.77	0.48
1:E:70:ASP:OD2	1:H:49:ARG:NH2	2.44	0.48
1:F:17:LYS:HG3	1:F:106:LEU:HD13	1.94	0.48
1:F:31:LYS:NZ	1:F:91:THR:HG21	2.28	0.48
1:A:20:ALA:O	1:A:24:LEU:N	2.45	0.48
1:B:59:THR:CG2	1:B:64:ARG:HB2	2.39	0.48
1:D:21:LEU:HD23	1:D:73:GLN:HG2	1.94	0.48
1:E:101:ASP:O	1:E:105:LYS:HG2	2.13	0.48
1:G:100:THR:O	1:G:104:LEU:HG	2.14	0.48
1:G:18:LYS:HG2	1:G:73:GLN:HB3	1.95	0.48
1:A:100:THR:O	1:A:104:LEU:N	2.40	0.48
1:C:30:GLU:OE2	1:C:94:PHE:HE2	1.97	0.48
1:D:49:ARG:NH1	1:D:49:ARG:CG	2.73	0.48
1:G:27:TYR:HE2	1:G:98:LYS:HG3	1.78	0.48
1:G:34:ALA:HA	1:G:37:HIS:HB2	1.95	0.48
1:B:27:TYR:CZ	1:B:98:LYS:HE2	2.46	0.48
1:E:77:LYS:O	1:E:79:LEU:CG	2.48	0.48
1:A:80:ASP:HA	1:A:83:VAL:HG12	1.94	0.48
1:A:96:ILE:HA	1:A:99:ILE:CD1	2.42	0.48
1:F:101:ASP:O	1:F:105:LYS:HG2	2.14	0.48
1:C:51:ASP:OD1	1:G:36:ARG:NH1	2.47	0.48
1:H:17:LYS:HG3	1:H:106:LEU:HD13	1.94	0.48
1:A:101:ASP:O	1:A:105:LYS:HG2	2.14	0.48
1:C:15:GLU:HA	1:C:18:LYS:HE3	1.95	0.48
1:C:42:ARG:HE	1:C:45:LYS:HE2	1.79	0.48
1:A:60:SER:O	1:A:61:SER:CB	2.61	0.48
1:E:82:LEU:HD11	1:E:102:GLU:CD	2.35	0.48
1:E:64:ARG:HA	1:E:67:LYS:NZ	2.29	0.48
1:B:56:SER:HA	1:B:64:ARG:CD	2.39	0.48
1:E:107:ARG:HA	1:E:107:ARG:NH1	2.26	0.48
1:F:38:PHE:CE1	1:F:39:ASP:OD1	2.66	0.48
1:G:31:LYS:HE2	1:G:94:PHE:CD2	2.41	0.48
1:E:34:ALA:HA	1:E:37:HIS:HB2	1.96	0.47
1:D:63:LYS:HZ2	1:G:36:ARG:HG3	1.74	0.47
1:G:31:LYS:HB2	1:G:95:LEU:HD22	1.96	0.47
1:D:48:SER:O	1:D:52:THR:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:HIS:CG	1:E:90:LYS:NZ	2.82	0.47
1:H:77:LYS:O	1:H:79:LEU:CG	2.55	0.47
1:B:50:GLU:OE2	1:C:63:LYS:HE2	2.14	0.47
1:D:51:ASP:H	1:H:37:HIS:HE1	1.62	0.47
1:H:18:LYS:HB2	1:H:18:LYS:NZ	2.28	0.47
1:B:82:LEU:O	1:B:86:ILE:HG22	2.14	0.47
1:A:62:ARG:O	1:A:65:ALA:HB3	2.14	0.47
1:H:100:THR:O	1:H:104:LEU:HG	2.14	0.47
1:A:104:LEU:HA	1:A:107:ARG:HB3	1.96	0.47
1:B:100:THR:O	1:B:104:LEU:N	2.41	0.47
1:B:15:GLU:O	1:B:18:LYS:NZ	2.42	0.47
1:H:24:LEU:HD13	1:H:105:LYS:HG3	1.97	0.47
1:H:82:LEU:HD22	1:H:82:LEU:H	1.80	0.47
1:F:79:LEU:HA	1:F:82:LEU:HD23	1.97	0.47
1:G:42:ARG:HE	1:G:45:LYS:HZ3	1.62	0.47
1:H:64:ARG:HA	1:H:67:LYS:HZ1	1.79	0.47
1:A:92:GLN:HA	1:A:96:ILE:HG13	1.96	0.47
1:B:28:LEU:HD22	1:E:41:LEU:HD13	1.97	0.47
1:C:28:LEU:HD22	1:F:41:LEU:HD13	1.96	0.47
1:D:107:ARG:NH1	1:D:110:LYS:HD3	2.30	0.47
1:F:86:ILE:HG23	1:F:87:ARG:HD2	1.97	0.47
1:H:64:ARG:CA	1:H:67:LYS:HZ1	2.27	0.47
1:C:103:VAL:O	1:C:107:ARG:N	2.36	0.47
1:G:20:ALA:O	1:G:24:LEU:N	2.46	0.47
1:H:79:LEU:HA	1:H:82:LEU:HD23	1.97	0.47
1:A:64:ARG:HA	1:A:67:LYS:NZ	2.31	0.46
1:C:76:PRO:HD3	1:G:94:PHE:HD1	1.73	0.46
1:E:55:ILE:HG22	1:E:64:ARG:HG3	1.98	0.46
1:H:101:ASP:O	1:H:105:LYS:HG2	2.15	0.46
1:H:105:LYS:O	1:H:109:ILE:HB	2.15	0.46
1:E:37:HIS:CD2	1:E:90:LYS:HZ3	2.32	0.46
1:F:49:ARG:O	1:F:52:THR:OG1	2.30	0.46
1:H:38:PHE:CD2	1:H:90:LYS:CD	2.98	0.46
1:D:76:PRO:HD2	1:H:94:PHE:HB2	1.91	0.46
1:F:15:GLU:O	1:F:18:LYS:NZ	2.41	0.46
1:A:16:VAL:HB	1:A:109:ILE:HG22	1.98	0.46
1:A:28:LEU:HD22	1:D:41:LEU:HD13	1.97	0.46
1:C:42:ARG:HG2	1:C:42:ARG:HH11	1.80	0.46
1:H:78:GLY:O	1:H:79:LEU:HD23	2.16	0.46
1:D:15:GLU:HA	1:D:18:LYS:HE3	1.97	0.46
1:C:95:LEU:O	1:C:98:LYS:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:83:VAL:HG23	1:F:87:ARG:HH11	1.81	0.46
1:C:79:LEU:HA	1:C:82:LEU:HD23	1.97	0.46
1:F:44:LYS:HE3	1:F:49:ARG:HD3	1.98	0.46
1:H:44:LYS:HZ2	1:H:49:ARG:NE	2.12	0.46
1:A:18:LYS:O	1:A:22:GLU:HG2	2.16	0.46
1:F:93:ASN:O	1:F:97:GLN:HG3	2.16	0.46
1:H:44:LYS:NZ	1:H:49:ARG:CD	2.79	0.46
1:H:21:LEU:HD23	1:H:73:GLN:HG2	1.97	0.46
1:A:55:ILE:HG12	1:A:67:LYS:HD2	1.98	0.46
1:C:55:ILE:HG12	1:C:67:LYS:HD2	1.98	0.46
1:D:18:LYS:HZ2	1:D:18:LYS:HB2	1.80	0.46
1:D:63:LYS:O	1:D:67:LYS:N	2.40	0.46
1:E:48:SER:OG	1:E:49:ARG:N	2.49	0.46
1:F:64:ARG:CA	1:F:67:LYS:HZ1	2.29	0.46
1:A:64:ARG:HA	1:A:67:LYS:HZ1	1.81	0.45
1:A:59:THR:CG2	1:A:67:LYS:NZ	2.80	0.45
1:C:77:LYS:HB3	1:C:77:LYS:HE2	1.81	0.45
1:E:49:ARG:NH1	1:E:53:GLU:OE2	2.49	0.45
1:G:10:GLU:HB2	1:G:12:ASP:OD2	2.15	0.45
1:F:34:ALA:HB1	1:F:38:PHE:CD1	2.51	0.45
1:F:49:ARG:NH1	1:F:53:GLU:OE2	2.49	0.45
1:F:50:GLU:HG3	1:G:62:ARG:HB2	1.99	0.45
1:B:77:LYS:HE2	1:B:77:LYS:HB3	1.79	0.45
1:F:20:ALA:O	1:F:24:LEU:N	2.49	0.45
1:C:25:ARG:O	1:F:41:LEU:HD11	2.17	0.45
1:G:96:ILE:HA	1:G:99:ILE:HD13	1.96	0.45
1:A:55:ILE:HD11	1:A:71:TYR:CZ	2.51	0.45
1:B:92:GLN:HA	1:B:96:ILE:CG1	2.47	0.45
1:D:93:ASN:O	1:D:97:GLN:CG	2.65	0.45
1:C:96:ILE:HA	1:C:99:ILE:CG2	2.46	0.45
1:D:42:ARG:HH21	1:D:45:LYS:HZ1	1.65	0.45
1:F:96:ILE:HD13	1:F:99:ILE:HD13	1.94	0.45
1:G:34:ALA:O	1:G:38:PHE:N	2.43	0.45
1:G:82:LEU:H	1:G:82:LEU:HD22	1.80	0.45
1:A:35:GLU:HG3	1:A:64:ARG:NH1	2.32	0.45
1:G:42:ARG:NE	1:G:45:LYS:HZ3	2.15	0.45
1:G:55:ILE:HG22	1:G:64:ARG:HG3	1.98	0.45
1:G:64:ARG:HA	1:G:67:LYS:NZ	2.31	0.45
1:A:47:LEU:HG	1:A:48:SER:H	1.82	0.45
1:E:96:ILE:CA	1:E:99:ILE:CD1	2.91	0.45
1:F:107:ARG:NH1	1:F:107:ARG:HA	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:LYS:HZ2	1:F:18:LYS:HB2	1.81	0.45
1:A:98:LYS:HA	1:A:98:LYS:HD2	1.74	0.44
1:B:100:THR:O	1:B:104:LEU:HG	2.17	0.44
1:C:51:ASP:HA	1:C:54:GLU:HB3	1.98	0.44
1:D:114:LEU:O	1:D:115:LYS:OXT	2.34	0.44
1:E:37:HIS:CG	1:E:90:LYS:HZ3	2.35	0.44
1:F:111:LEU:HA	1:F:111:LEU:HD23	1.81	0.44
1:H:62:ARG:O	1:H:65:ALA:HB3	2.17	0.44
1:C:90:LYS:HB3	1:C:91:THR:H	1.58	0.44
1:D:42:ARG:HH21	1:D:45:LYS:NZ	2.15	0.44
1:F:82:LEU:HD11	1:F:102:GLU:CD	2.37	0.44
1:F:27:TYR:CZ	1:F:98:LYS:HE2	2.50	0.44
1:A:50:GLU:HA	1:A:53:GLU:CD	2.38	0.44
1:B:82:LEU:HD22	1:B:82:LEU:H	1.81	0.44
1:D:98:LYS:O	1:D:101:ASP:HB3	2.17	0.44
1:C:76:PRO:CD	1:G:94:PHE:CD1	2.91	0.44
1:B:103:VAL:O	1:B:107:ARG:N	2.35	0.44
1:C:18:LYS:HZ2	1:C:18:LYS:HB2	1.81	0.44
1:C:18:LYS:HG2	1:C:73:GLN:HB3	2.00	0.44
1:F:77:LYS:O	1:F:79:LEU:CG	2.54	0.44
1:D:77:LYS:C	1:D:79:LEU:HG	2.34	0.44
1:E:35:GLU:CD	1:E:64:ARG:HG2	2.38	0.44
1:F:101:ASP:O	1:F:105:LYS:N	2.31	0.44
1:D:59:THR:CG2	1:D:67:LYS:NZ	2.81	0.44
1:F:92:GLN:NE2	1:F:96:ILE:HG21	2.33	0.44
1:G:42:ARG:HG2	1:G:42:ARG:NH1	2.32	0.44
1:A:55:ILE:HG23	1:A:67:LYS:HD2	2.00	0.44
1:C:64:ARG:HA	1:C:67:LYS:HZ1	1.83	0.44
1:D:62:ARG:O	1:D:65:ALA:HB3	2.18	0.44
1:F:34:ALA:CB	1:F:38:PHE:CD2	2.92	0.44
1:A:79:LEU:HA	1:A:82:LEU:HD23	2.00	0.44
1:B:37:HIS:HB3	1:B:90:LYS:NZ	2.33	0.44
1:C:48:SER:OG	1:G:37:HIS:CE1	2.66	0.44
1:C:83:VAL:HG23	1:C:87:ARG:NH1	2.31	0.44
1:D:82:LEU:HD22	1:D:82:LEU:H	1.83	0.44
1:F:13:LEU:C	1:F:17:LYS:HZ3	2.21	0.44
1:A:92:GLN:NE2	1:A:96:ILE:HG21	2.32	0.43
1:B:51:ASP:O	1:B:54:GLU:N	2.50	0.43
1:D:114:LEU:HA	1:D:114:LEU:HD13	1.79	0.43
1:C:50:GLU:OE2	1:D:63:LYS:HE2	2.17	0.43
1:F:100:THR:O	1:F:104:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:49:ARG:HA	1:G:49:ARG:HD2	1.75	0.43
1:C:31:LYS:NZ	1:C:91:THR:HG21	2.33	0.43
1:F:114:LEU:O	1:F:115:LYS:OXT	2.35	0.43
1:F:98:LYS:O	1:F:101:ASP:HB3	2.17	0.43
1:G:64:ARG:HA	1:G:67:LYS:HB2	1.99	0.43
1:A:99:ILE:HA	1:A:102:GLU:HB3	2.00	0.43
1:C:77:LYS:O	1:C:79:LEU:CG	2.50	0.43
1:C:95:LEU:HA	1:C:98:LYS:HB2	2.00	0.43
1:F:64:ARG:HA	1:F:67:LYS:HZ1	1.83	0.43
1:H:98:LYS:O	1:H:101:ASP:HB3	2.18	0.43
1:B:107:ARG:HA	1:B:107:ARG:NH1	2.32	0.43
1:B:32:ILE:HD12	1:B:69:LEU:HD11	2.01	0.43
1:D:98:LYS:HD2	1:D:98:LYS:HA	1.78	0.43
1:H:114:LEU:O	1:H:115:LYS:OXT	2.35	0.43
1:H:42:ARG:HG2	1:H:42:ARG:NH1	2.33	0.43
1:A:34:ALA:HA	1:A:37:HIS:CB	2.48	0.43
1:A:38:PHE:CD2	1:A:90:LYS:CD	3.01	0.43
1:D:47:LEU:HG	1:D:48:SER:H	1.82	0.43
1:E:114:LEU:O	1:E:115:LYS:OXT	2.37	0.43
1:C:63:LYS:HZ2	1:F:36:ARG:HG3	1.83	0.43
1:H:42:ARG:HH21	1:H:45:LYS:NZ	2.16	0.43
1:H:35:GLU:HB3	1:H:68:LEU:HD13	1.99	0.43
1:A:114:LEU:O	1:A:115:LYS:OXT	2.37	0.43
1:A:67:LYS:O	1:A:71:TYR:HD1	2.00	0.43
1:A:96:ILE:CD1	1:A:99:ILE:HG21	2.39	0.43
1:C:35:GLU:OE1	1:C:65:ALA:HA	2.19	0.43
1:C:80:ASP:HA	1:C:83:VAL:HG12	2.00	0.43
1:A:17:LYS:O	1:A:21:LEU:N	2.41	0.43
1:A:42:ARG:HH21	1:A:45:LYS:NZ	2.17	0.43
1:B:114:LEU:O	1:B:115:LYS:OXT	2.37	0.43
1:C:34:ALA:HA	1:C:37:HIS:HB2	2.00	0.43
1:A:100:THR:O	1:A:104:LEU:HG	2.19	0.43
1:B:77:LYS:O	1:B:79:LEU:CG	2.52	0.43
1:D:55:ILE:HG23	1:D:67:LYS:NZ	2.14	0.43
1:G:92:GLN:O	1:G:96:ILE:HB	2.18	0.43
1:H:49:ARG:HA	1:H:49:ARG:HD2	1.61	0.43
1:H:97:GLN:HE21	1:H:97:GLN:HB2	1.64	0.43
1:C:62:ARG:O	1:C:65:ALA:HB3	2.19	0.43
1:D:35:GLU:HG3	1:D:64:ARG:NH1	2.33	0.43
1:E:62:ARG:O	1:E:65:ALA:HB3	2.19	0.43
1:E:79:LEU:HA	1:E:82:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:62:ARG:O	1:G:65:ALA:HB3	2.18	0.43
1:H:13:LEU:HD12	1:H:14:THR:N	2.33	0.43
1:H:96:ILE:HG23	1:H:99:ILE:HD11	0.57	0.43
1:A:101:ASP:HA	1:A:104:LEU:HB2	2.01	0.42
1:A:25:ARG:O	1:D:41:LEU:HD11	2.19	0.42
1:B:34:ALA:O	1:B:38:PHE:N	2.37	0.42
1:C:114:LEU:O	1:C:115:LYS:OXT	2.36	0.42
1:F:34:ALA:HA	1:F:37:HIS:HB3	2.00	0.42
1:D:63:LYS:HZ1	1:G:36:ARG:HG3	1.83	0.42
1:G:98:LYS:HA	1:G:98:LYS:HD2	1.72	0.42
1:B:18:LYS:O	1:B:22:GLU:HG2	2.19	0.42
1:C:17:LYS:HZ2	1:C:106:LEU:HD11	1.83	0.42
1:E:31:LYS:HE2	1:E:94:PHE:CD2	2.44	0.42
1:A:107:ARG:HA	1:A:107:ARG:HH11	1.84	0.42
1:B:28:LEU:HA	1:B:32:ILE:HG13	2.00	0.42
1:C:28:LEU:HA	1:C:32:ILE:HG13	2.00	0.42
1:C:92:GLN:HA	1:C:96:ILE:CG1	2.50	0.42
1:D:48:SER:O	1:D:52:THR:CG2	2.67	0.42
1:G:96:ILE:HG23	1:G:99:ILE:HD11	0.56	0.42
1:A:27:TYR:CE2	1:A:98:LYS:HE3	2.47	0.42
1:C:31:LYS:HG3	1:C:95:LEU:HB2	2.00	0.42
1:G:27:TYR:HE2	1:G:98:LYS:CE	2.28	0.42
1:C:26:VAL:O	1:C:28:LEU:N	2.50	0.42
1:E:49:ARG:HA	1:E:49:ARG:HD2	1.82	0.42
1:H:67:LYS:O	1:H:71:TYR:HD1	2.02	0.42
1:B:25:ARG:O	1:E:41:LEU:HD11	2.19	0.42
1:B:96:ILE:HA	1:B:99:ILE:CB	2.47	0.42
1:D:61:SER:O	1:D:65:ALA:HB2	2.20	0.42
1:F:55:ILE:HG22	1:F:64:ARG:HG3	2.01	0.42
1:B:50:GLU:HA	1:B:53:GLU:OE1	2.19	0.42
1:D:44:LYS:CE	1:D:49:ARG:HD3	2.45	0.42
1:D:64:ARG:HA	1:D:67:LYS:HZ1	1.84	0.42
1:G:30:GLU:OE2	1:G:94:PHE:HE2	2.02	0.42
1:C:18:LYS:O	1:C:22:GLU:HG2	2.20	0.42
1:C:59:THR:CG2	1:C:67:LYS:NZ	2.82	0.42
1:C:38:PHE:CD2	1:C:90:LYS:CD	3.02	0.42
1:G:99:ILE:HA	1:G:102:GLU:HB3	2.01	0.42
1:H:77:LYS:HE2	1:H:77:LYS:HB3	1.78	0.42
1:H:95:LEU:HG	1:H:99:ILE:CG2	2.49	0.42
1:B:86:ILE:HG13	1:B:92:GLN:HE22	1.85	0.42
1:C:63:LYS:O	1:C:67:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:ARG:CA	1:C:67:LYS:HZ1	2.32	0.42
1:D:64:ARG:HA	1:D:67:LYS:HB2	2.02	0.42
1:D:79:LEU:HA	1:D:82:LEU:HD23	2.00	0.42
1:E:96:ILE:CD1	1:E:99:ILE:CD1	2.75	0.42
1:G:18:LYS:HB2	1:G:18:LYS:NZ	2.35	0.42
1:B:96:ILE:CG1	1:B:99:ILE:HD13	2.42	0.42
1:C:101:ASP:O	1:C:104:LEU:HB2	2.20	0.42
1:D:24:LEU:HD22	1:D:102:GLU:CG	2.47	0.42
1:D:92:GLN:HA	1:D:96:ILE:CG1	2.50	0.42
1:G:27:TYR:CE2	1:G:98:LYS:CE	2.90	0.42
1:H:57:CYS:O	1:H:58:ARG:HD3	2.20	0.42
1:H:96:ILE:HA	1:H:99:ILE:HD13	2.02	0.42
1:A:101:ASP:O	1:A:104:LEU:HB2	2.20	0.41
1:H:14:THR:HA	1:H:17:LYS:HD2	2.02	0.41
1:A:64:ARG:HA	1:A:67:LYS:HB2	2.02	0.41
1:B:63:LYS:HZ2	1:E:36:ARG:HG3	1.86	0.41
1:E:49:ARG:NH2	1:E:53:GLU:OE2	2.54	0.41
1:F:49:ARG:HD2	1:F:49:ARG:HA	1.77	0.41
1:F:98:LYS:HA	1:F:98:LYS:HD2	1.78	0.41
1:G:51:ASP:O	1:G:54:GLU:N	2.53	0.41
1:A:63:LYS:O	1:A:67:LYS:HG3	2.20	0.41
1:B:93:ASN:O	1:B:97:GLN:CG	2.68	0.41
1:E:103:VAL:O	1:E:107:ARG:N	2.32	0.41
1:E:64:ARG:CA	1:E:67:LYS:HZ1	2.33	0.41
1:F:42:ARG:HE	1:F:45:LYS:HE2	1.85	0.41
1:G:64:ARG:CA	1:G:67:LYS:HZ2	2.33	0.41
1:A:60:SER:OG	1:A:62:ARG:HB2	2.20	0.41
1:B:37:HIS:CG	1:B:90:LYS:NZ	2.88	0.41
1:C:114:LEU:HD13	1:C:114:LEU:HA	1.84	0.41
1:D:18:LYS:O	1:D:22:GLU:HG2	2.20	0.41
1:E:64:ARG:HA	1:E:67:LYS:HZ1	1.84	0.41
1:H:99:ILE:HA	1:H:102:GLU:HB3	2.02	0.41
1:C:95:LEU:O	1:C:99:ILE:CG2	2.49	0.41
1:C:54:GLU:HB2	1:D:60:SER:HB3	2.02	0.41
1:F:37:HIS:CD2	1:F:90:LYS:HZ3	2.38	0.41
1:H:17:LYS:O	1:H:21:LEU:N	2.46	0.41
1:B:101:ASP:O	1:B:104:LEU:HB2	2.21	0.41
1:B:32:ILE:HG21	1:B:65:ALA:HB1	2.02	0.41
1:B:49:ARG:HA	1:B:49:ARG:HD2	1.74	0.41
1:B:64:ARG:HA	1:B:67:LYS:HZ1	1.86	0.41
1:D:98:LYS:HA	1:D:101:ASP:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:ARG:O	1:H:41:LEU:HD11	2.21	0.41
1:F:49:ARG:HH12	1:F:53:GLU:HG3	1.81	0.41
1:H:82:LEU:HD11	1:H:102:GLU:OE2	2.20	0.41
1:H:86:ILE:HG13	1:H:92:GLN:HE22	1.85	0.41
1:B:64:ARG:HA	1:B:67:LYS:NZ	2.36	0.41
1:E:96:ILE:CB	1:E:99:ILE:CD1	2.98	0.41
1:H:92:GLN:O	1:H:96:ILE:HB	2.20	0.41
1:H:28:LEU:HD11	1:H:65:ALA:C	2.41	0.41
1:C:96:ILE:HD13	1:C:99:ILE:CG2	2.46	0.41
1:E:92:GLN:NE2	1:E:96:ILE:HG21	2.36	0.41
1:F:62:ARG:O	1:F:65:ALA:HB3	2.20	0.41
1:C:54:GLU:CD	1:G:36:ARG:NH1	2.74	0.41
1:H:19:ASP:O	1:H:23:ASN:N	2.36	0.41
1:H:98:LYS:HD2	1:H:98:LYS:HA	1.78	0.41
1:A:82:LEU:H	1:A:82:LEU:HD22	1.85	0.41
1:B:49:ARG:O	1:B:52:THR:OG1	2.36	0.41
1:C:24:LEU:HD22	1:C:102:GLU:CG	2.50	0.41
1:E:28:LEU:HD11	1:E:65:ALA:C	2.42	0.41
1:E:42:ARG:HH21	1:E:45:LYS:NZ	2.18	0.41
1:F:31:LYS:HE2	1:F:94:PHE:CD2	2.45	0.41
1:H:100:THR:O	1:H:104:LEU:N	2.46	0.41
1:E:98:LYS:O	1:E:101:ASP:HB3	2.20	0.40
1:E:30:GLU:OE2	1:E:94:PHE:CE2	2.73	0.40
1:E:82:LEU:HD22	1:E:82:LEU:H	1.86	0.40
1:F:99:ILE:HA	1:F:102:GLU:HB3	2.03	0.40
1:G:101:ASP:O	1:G:105:LYS:HG2	2.21	0.40
1:A:18:LYS:HB2	1:A:18:LYS:HZ3	1.84	0.40
1:B:67:LYS:O	1:B:71:TYR:HD1	2.03	0.40
1:H:14:THR:OG1	1:H:76:PRO:HA	2.21	0.40
1:H:18:LYS:O	1:H:22:GLU:HG2	2.20	0.40
1:H:42:ARG:HE	1:H:45:LYS:HZ3	1.69	0.40
1:H:55:ILE:HD11	1:H:71:TYR:CZ	2.55	0.40
1:B:64:ARG:CA	1:B:67:LYS:HZ1	2.34	0.40
1:F:19:ASP:HA	1:F:22:GLU:HB2	2.03	0.40
1:F:54:GLU:HB2	1:G:60:SER:HB3	2.04	0.40
1:A:104:LEU:O	1:A:108:ASN:N	2.26	0.40
1:C:55:ILE:HD11	1:C:71:TYR:CZ	2.56	0.40
1:G:96:ILE:HA	1:G:99:ILE:HG23	2.04	0.40
1:A:13:LEU:O	1:A:17:LYS:NZ	2.47	0.40
1:B:50:GLU:O	1:B:50:GLU:HG2	2.21	0.40
1:B:50:GLU:HA	1:B:53:GLU:CD	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:GLN:NE2	1:B:96:ILE:HG21	2.37	0.40
1:B:96:ILE:CA	1:B:99:ILE:CD1	2.98	0.40
1:C:42:ARG:HH11	1:C:84:GLU:CD	2.20	0.40
1:E:38:PHE:CD2	1:E:90:LYS:CD	3.05	0.40
1:E:37:HIS:CD2	1:E:90:LYS:NZ	2.90	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	104/106 (98%)	92 (88%)	11 (11%)	1 (1%)	18 61
1	B	104/106 (98%)	90 (86%)	14 (14%)	0	100 100
1	C	104/106 (98%)	88 (85%)	15 (14%)	1 (1%)	18 61
1	D	104/106 (98%)	91 (88%)	13 (12%)	0	100 100
1	E	104/106 (98%)	90 (86%)	14 (14%)	0	100 100
1	F	104/106 (98%)	91 (88%)	13 (12%)	0	100 100
1	G	104/106 (98%)	88 (85%)	16 (15%)	0	100 100
1	H	104/106 (98%)	89 (86%)	14 (14%)	1 (1%)	18 61
All	All	832/848 (98%)	719 (86%)	110 (13%)	3 (0%)	42 77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	GLU
1	C	74	GLU
1	H	67	LYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	100/100 (100%)	94 (94%)	6 (6%)	22 59
1	B	100/100 (100%)	92 (92%)	8 (8%)	14 49
1	C	100/100 (100%)	92 (92%)	8 (8%)	14 49
1	D	100/100 (100%)	91 (91%)	9 (9%)	11 43
1	E	100/100 (100%)	92 (92%)	8 (8%)	14 49
1	F	100/100 (100%)	91 (91%)	9 (9%)	11 43
1	G	100/100 (100%)	90 (90%)	10 (10%)	9 38
1	H	100/100 (100%)	87 (87%)	13 (13%)	5 28
All	All	800/800 (100%)	729 (91%)	71 (9%)	16 44

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	TYR
1	A	37	HIS
1	A	40	HIS
1	A	87	ARG
1	A	90	LYS
1	A	107	ARG
1	B	13	LEU
1	B	16	VAL
1	B	27	TYR
1	B	37	HIS
1	B	40	HIS
1	B	62	ARG
1	B	87	ARG
1	B	107	ARG
1	C	27	TYR
1	C	37	HIS
1	C	40	HIS
1	C	60	SER
1	C	62	ARG

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Mol	Chain	Res	Type
1	C	87	ARG
1	C	90	LYS
1	C	107	ARG
1	D	16	VAL
1	D	27	TYR
1	D	37	HIS
1	D	40	HIS
1	D	47	LEU
1	D	49	ARG
1	D	60	SER
1	D	87	ARG
1	D	107	ARG
1	E	13	LEU
1	E	16	VAL
1	E	27	TYR
1	E	37	HIS
1	E	40	HIS
1	E	60	SER
1	E	87	ARG
1	E	107	ARG
1	F	13	LEU
1	F	16	VAL
1	F	25	ARG
1	F	27	TYR
1	F	37	HIS
1	F	40	HIS
1	F	60	SER
1	F	87	ARG
1	F	107	ARG
1	G	13	LEU
1	G	22	GLU
1	G	25	ARG
1	G	27	TYR
1	G	37	HIS
1	G	40	HIS
1	G	57	CYS
1	G	60	SER
1	G	87	ARG
1	G	107	ARG
1	H	13	LEU
1	H	14	THR
1	H	16	VAL

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Mol	Chain	Res	Type
1	H	25	ARG
1	H	27	TYR
1	H	37	HIS
1	H	40	HIS
1	H	49	ARG
1	H	56	SER
1	H	57	CYS
1	H	60	SER
1	H	87	ARG
1	H	107	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	113	HIS
1	B	37	HIS
1	B	92	GLN
1	B	97	GLN
1	B	113	HIS
1	C	97	GLN
1	C	113	HIS
1	D	97	GLN
1	D	113	HIS
1	E	97	GLN
1	E	113	HIS
1	F	97	GLN
1	F	113	HIS
1	G	97	GLN
1	G	113	HIS
1	H	97	GLN
1	H	113	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.