wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:50 PM BST

PDB ID	:	3J82
EMDB ID:	:	EMD-6102
Title	:	Electron cryo-microscopy of DNGR-1 in complex with F-actin
Authors	:	Hanc, P.; Fujii, T.; Yamada, Y.; Huotari, J.; Schulz, O.; Ahrens, S.; Kjaer, S.; Way, M.; Namba, K.; Reis e Sousa, C.
Deposited on	:	2014-09-25
Resolution	:	7.70 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

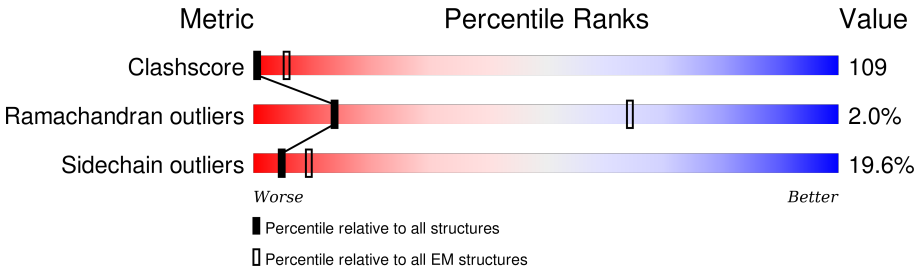
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 7.70 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	131	32% 57% 11%
2	B	374	19% 61% 17% •
2	C	374	21% 61% 17% •
2	D	374	20% 64% 13% •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HIC	C	73	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9884 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 C-type lectin domain family 9 member A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	131	Total	C	N	O	S	0	0
			1050	672	171	197	10		

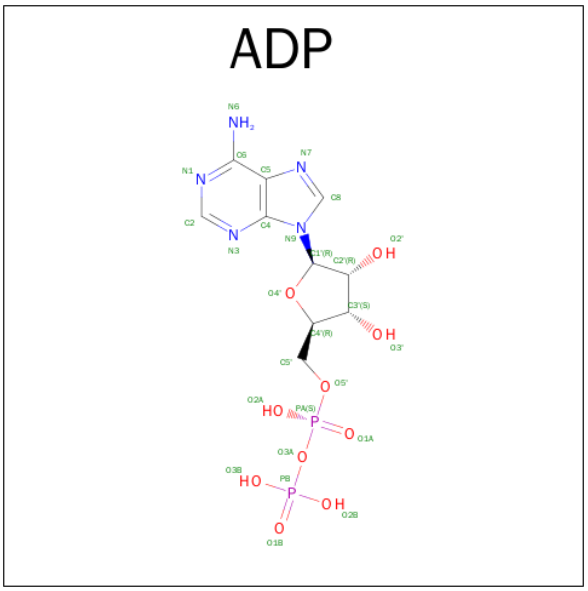
- Molecule 2 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	374	Total	C	N	O	S	0	0
			2917	1846	490	559	22		
2	C	374	Total	C	N	O	S	0	0
			2917	1846	490	559	22		
2	D	374	Total	C	N	O	S	0	0
			2918	1846	490	560	22		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Ca	0
			1	1	

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



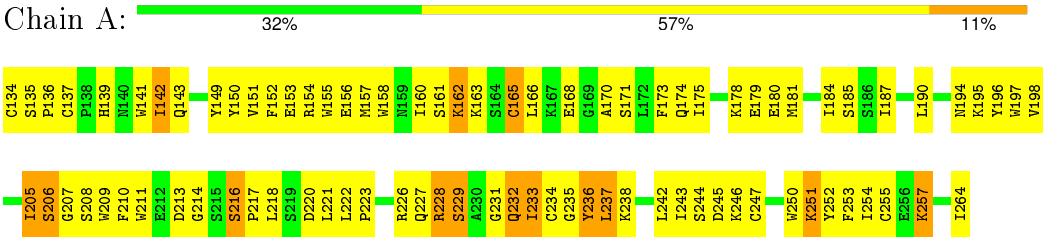
Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

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 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.

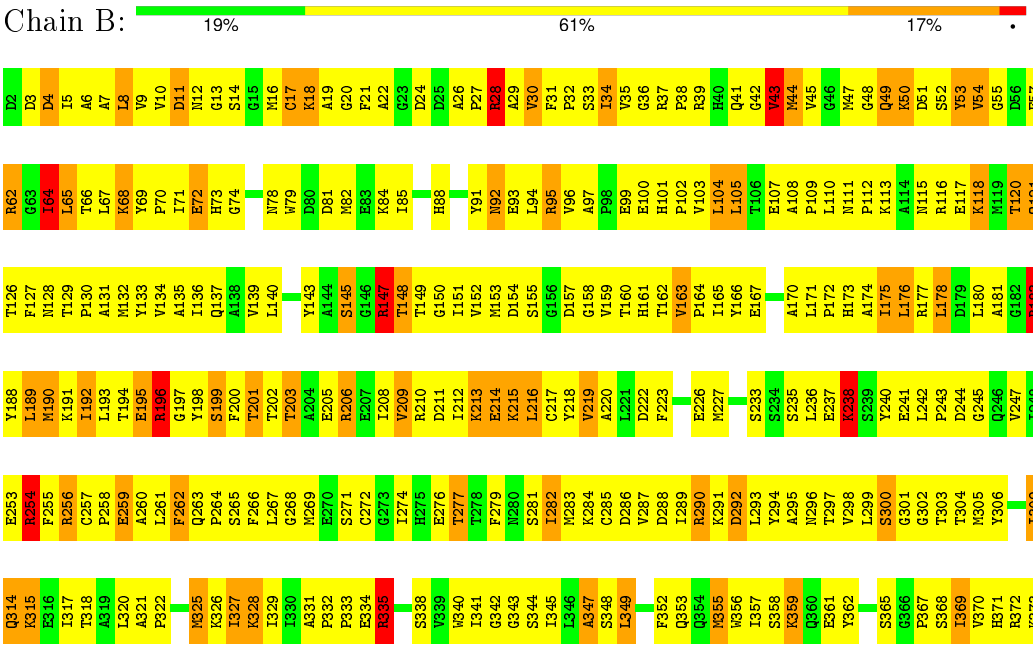
- Molecule 1: C-type lectin domain family 9 member A

Chain A:



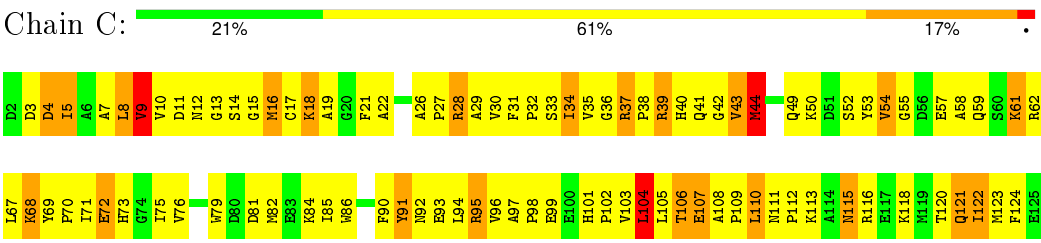
- Molecule 2: Actin, cytoplasmic 1

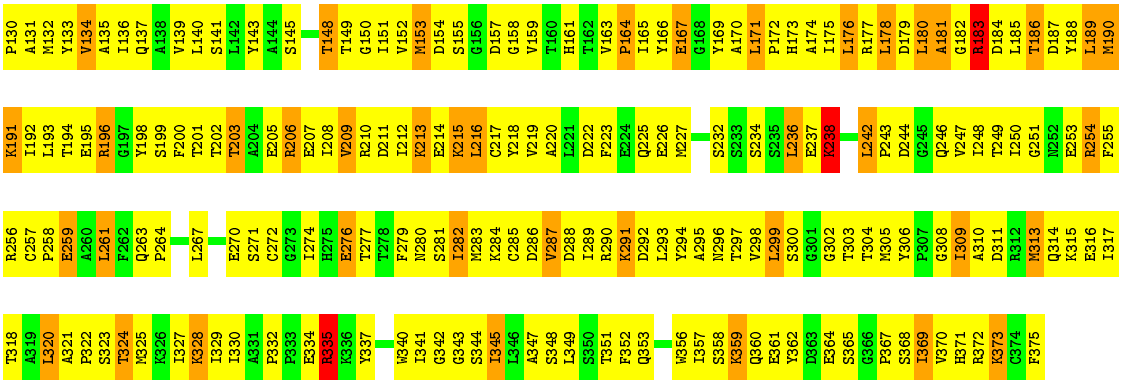
Chain B:



- Molecule 2: Actin, cytoplasmic 1

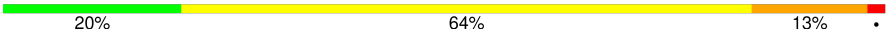
Chain C:

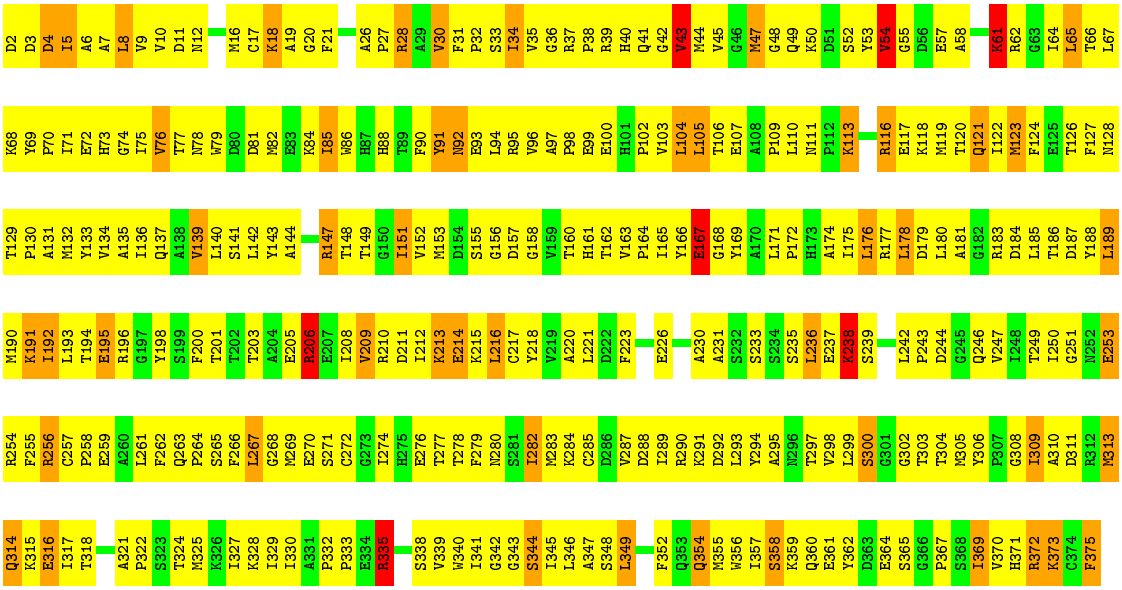




- Molecule 2: Actin, cytoplasmic 1

Chain D:





4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	73608	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each Particle	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	60000	Depositor
Image detector	TVIPS TEMCAM-F416 (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, HIC, ADP

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	0.91	0/1080	1.11	1/1451 (0.1%)
2	B	0.99	0/2967	1.24	11/4017 (0.3%)
2	C	0.99	0/2967	1.23	9/4017 (0.2%)
2	D	0.98	0/2968	1.20	9/4017 (0.2%)
All	All	0.98	0/9982	1.21	30/13502 (0.2%)

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
2	B	0	11
2	C	0	6
2	D	0	3
All	All	0	21

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	277	THR	CA-CB-CG2	-11.90	95.74	112.40
2	C	106	THR	CA-CB-CG2	-8.51	100.49	112.40
2	B	183	ARG	NE-CZ-NH2	-8.40	116.10	120.30
2	D	375	PHE	CB-CG-CD2	-8.10	115.13	120.80
2	B	28	ARG	NE-CZ-NH1	7.84	124.22	120.30
2	C	39	ARG	NE-CZ-NH2	-7.08	116.76	120.30
2	C	104	LEU	CB-CA-C	-7.00	96.91	110.20
2	C	203	THR	CA-CB-CG2	-6.69	103.03	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	292	ASP	CB-CG-OD2	-6.36	112.58	118.30
2	C	167	GLU	CB-CG-CD	-6.34	97.09	114.20
2	D	167	GLU	C-N-CA	6.21	135.35	122.30
2	B	190	MET	CG-SD-CE	-6.09	90.46	100.20
2	D	267	LEU	CB-CA-C	-5.95	98.89	110.20
2	B	91	TYR	CA-CB-CG	-5.93	102.12	113.40
1	A	257	LYS	CB-CA-C	-5.67	99.06	110.40
2	B	262	PHE	CA-CB-CG	-5.66	100.33	113.90
2	B	53	TYR	CA-CB-CG	-5.62	102.73	113.40
2	C	91	TYR	CA-CB-CG	-5.54	102.88	113.40
2	B	28	ARG	NE-CZ-NH2	-5.53	117.54	120.30
2	D	375	PHE	CB-CG-CD1	5.49	124.64	120.80
2	B	325	MET	CG-SD-CE	-5.44	91.49	100.20
2	D	43	VAL	N-CA-C	-5.40	96.42	111.00
2	C	44	MET	N-CA-CB	5.38	120.29	110.60
2	D	91	TYR	CA-CB-CG	-5.38	103.19	113.40
2	B	196	ARG	CD-NE-CZ	-5.36	116.10	123.60
2	C	9	VAL	C-N-CA	5.21	134.73	121.70
2	D	206	ARG	CB-CA-C	-5.20	100.00	110.40
2	C	183	ARG	CB-CA-C	-5.19	100.01	110.40
2	D	54	VAL	CA-CB-CG2	-5.14	103.19	110.90
2	B	347	ALA	CB-CA-C	-5.08	102.48	110.10

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	TYR	Peptide
2	B	147	ARG	Sidechain
2	B	183	ARG	Sidechain
2	B	196	ARG	Sidechain
2	B	197	GLY	Peptide
2	B	245	GLY	Peptide
2	B	254	ARG	Sidechain
2	B	301	GLY	Peptide
2	B	335	ARG	Sidechain
2	B	61	LYS	Peptide
2	B	62	ARG	Sidechain
2	B	64	ILE	Peptide
2	C	181	ALA	Peptide
2	C	232	SER	Peptide
2	C	335	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	C	37	ARG	Sidechain
2	C	61	LYS	Peptide
2	C	9	VAL	Peptide
2	D	167	GLU	Peptide
2	D	335	ARG	Sidechain
2	D	61	LYS	Peptide

5.2 Too-close contacts (i)

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	1050	0	1002	227	0
2	B	2917	0	2880	682	0
2	C	2917	0	2880	606	0
2	D	2918	0	2880	684	0
3	A	1	0	0	0	0
4	B	27	0	12	7	0
4	C	27	0	12	7	0
4	D	27	0	12	8	0
All	All	9884	0	9678	2141	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 109.

All (2141) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:73:HIC:HD2	2:C:183:ARG:NH1	1.50	1.26
2:D:300:SER:HA	2:D:335:ARG:HD3	1.25	1.18
2:B:61:LYS:HD2	2:B:64:ILE:HG21	1.26	1.17
2:D:178:LEU:HD12	2:D:180:LEU:H	1.12	1.14
2:C:189:LEU:HD12	2:C:209:VAL:HG22	1.28	1.14
2:B:216:LEU:HD21	2:B:254:ARG:HG2	1.27	1.14
2:C:8:LEU:HB2	2:C:103:VAL:HG22	1.26	1.13
2:B:253:GLU:HA	2:B:256:ARG:HG2	1.31	1.13
2:C:140:LEU:HD23	2:C:343:GLY:HA2	1.26	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:ASP:HB2	2:D:18:LYS:HD3	1.31	1.12
2:C:7:ALA:HB1	2:C:104:LEU:HD21	1.31	1.11
2:C:163:VAL:HG12	2:C:175:ILE:HG13	1.20	1.11
2:C:35:VAL:HG12	2:C:68:LYS:HB3	1.18	1.11
2:C:9:VAL:HG22	2:C:104:LEU:HD23	1.13	1.11
2:C:135:ALA:HB1	2:C:140:LEU:HD11	1.16	1.10
1:A:142:ILE:HD11	1:A:149:TYR:HB2	1.33	1.10
2:C:34:ILE:HG12	2:C:54:VAL:HG11	1.34	1.10
2:C:191:LYS:HA	2:C:191:LYS:HE3	1.30	1.10
2:B:34:ILE:HG13	2:B:67:LEU:HD22	1.22	1.08
2:B:149:THR:HG22	2:B:166:TYR:HA	1.35	1.08
2:B:251:GLY:HA2	2:B:254:ARG:HD3	1.29	1.08
2:D:7:ALA:HB1	2:D:104:LEU:HD21	1.36	1.08
2:C:34:ILE:HG13	2:C:67:LEU:HD22	1.18	1.07
2:C:37:ARG:HG2	2:C:38:PRO:HD2	1.31	1.07
2:C:251:GLY:HA2	2:C:254:ARG:HD3	1.09	1.07
2:D:176:LEU:HD21	2:D:277:THR:HG23	1.30	1.07
2:C:216:LEU:HD11	2:C:250:ILE:HG21	1.07	1.07
2:C:290:ARG:HD2	2:D:244:ASP:HB2	1.37	1.06
2:B:305:MET:HG3	4:B:401:ADP:C6	1.91	1.06
2:C:285:CYS:HB3	2:C:289:ILE:HD11	1.37	1.05
2:D:8:LEU:HB2	2:D:103:VAL:HG22	1.32	1.05
2:C:35:VAL:HG22	2:C:52:SER:HB3	1.35	1.05
2:D:285:CYS:HB3	2:D:289:ILE:HD11	1.33	1.05
2:C:305:MET:HG3	4:C:401:ADP:C6	1.91	1.05
2:B:176:LEU:HD11	2:B:277:THR:HG22	1.38	1.05
2:D:305:MET:HG3	4:D:401:ADP:C6	1.91	1.04
2:C:216:LEU:HD23	2:C:254:ARG:HG3	1.38	1.04
2:C:272:CYS:HB3	2:C:276:GLU:HG2	1.40	1.03
2:D:116:ARG:HD2	2:D:134:VAL:HG11	1.08	1.03
2:B:216:LEU:HD11	2:B:250:ILE:HG12	1.36	1.03
2:B:220:ALA:HB1	2:B:226:GLU:HG3	1.39	1.02
2:B:8:LEU:HB3	2:B:103:VAL:HG13	1.40	1.00
2:B:7:ALA:HB1	2:B:104:LEU:HD21	1.43	1.00
2:C:153:MET:HG3	2:C:299:LEU:HA	1.43	1.00
2:C:61:LYS:HG3	2:C:64:ILE:HG22	1.44	0.99
2:B:195:GLU:HA	2:C:110:LEU:HD11	1.42	0.99
2:B:35:VAL:HG12	2:B:68:LYS:HB2	1.44	0.99
2:B:250:ILE:HD12	2:B:253:GLU:HG2	1.44	0.99
2:D:349:LEU:HD22	2:D:352:PHE:HD1	1.27	0.98
2:D:139:VAL:HG12	2:D:140:LEU:HD12	1.45	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:PRO:HG2	2:B:335:ARG:HH21	1.24	0.98
2:D:106:THR:HG22	2:D:135:ALA:HB3	1.41	0.98
2:C:11:ASP:HB2	2:C:18:LYS:HG2	1.45	0.98
2:C:39:ARG:HH22	2:C:203:THR:HG21	1.27	0.97
2:C:332:PRO:HG2	2:C:335:ARG:HH21	1.26	0.97
2:B:282:ILE:HD11	2:B:293:LEU:HD13	1.47	0.97
2:C:190:MET:HE1	2:C:206:ARG:HB2	1.45	0.97
2:B:148:THR:HG22	2:B:149:THR:HG23	1.43	0.97
2:B:152:VAL:HG23	2:B:298:VAL:HG12	1.43	0.96
2:B:189:LEU:HA	2:B:192:ILE:HD11	1.47	0.96
2:D:61:LYS:HB3	2:D:65:LEU:HD22	1.46	0.96
2:B:73:HIC:HD2	2:B:183:ARG:NH1	1.80	0.96
2:D:120:THR:HG23	2:D:132:MET:HE2	1.44	0.96
2:D:349:LEU:HD22	2:D:352:PHE:CD1	2.01	0.96
2:D:35:VAL:HG22	2:D:52:SER:HB3	1.47	0.96
2:B:285:CYS:HB3	2:B:289:ILE:HD11	1.45	0.96
2:C:11:ASP:HB3	2:C:18:LYS:HE2	1.46	0.96
2:B:176:LEU:HD21	2:B:277:THR:HG21	1.48	0.96
2:D:166:TYR:HD2	2:D:167:GLU:HG2	1.32	0.95
2:D:54:VAL:HA	2:D:58:ALA:HB2	1.49	0.95
2:C:35:VAL:HA	2:C:54:VAL:HG21	1.48	0.95
2:B:37:ARG:HG3	2:B:38:PRO:HD2	1.48	0.94
2:B:73:HIC:HD2	2:B:183:ARG:HH12	1.30	0.94
2:D:357:ILE:HG12	2:D:370:VAL:HG23	1.47	0.94
2:D:61:LYS:HE2	2:D:64:ILE:HG21	1.48	0.94
2:B:36:GLY:H	2:B:52:SER:HB3	1.30	0.94
2:D:7:ALA:CB	2:D:347:ALA:HB1	1.98	0.94
2:C:216:LEU:HD11	2:C:250:ILE:CG2	1.98	0.94
2:C:34:ILE:HG12	2:C:54:VAL:CG1	1.97	0.94
2:B:82:MET:HA	2:B:82:MET:HE3	1.45	0.94
2:B:34:ILE:HG12	2:B:54:VAL:CG1	1.98	0.93
2:D:134:VAL:HG23	2:D:370:VAL:HG21	1.49	0.93
2:C:140:LEU:HD23	2:C:343:GLY:CA	1.98	0.93
1:A:181:MET:O	1:A:184:ILE:HD13	1.68	0.93
1:A:154:ARG:CZ	2:D:231:ALA:HB1	1.98	0.93
2:D:152:VAL:HG23	2:D:298:VAL:HB	1.50	0.93
2:D:282:ILE:HG23	2:D:290:ARG:HD3	1.49	0.93
2:C:251:GLY:CA	2:C:254:ARG:HD3	1.99	0.93
2:D:34:ILE:HG12	2:D:54:VAL:HG11	1.49	0.92
2:D:11:ASP:HB2	2:D:18:LYS:CD	1.99	0.92
2:C:282:ILE:HG13	2:C:294:TYR:CE2	2.04	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:7:ALA:CB	2:C:347:ALA:HB1	1.99	0.92
2:D:285:CYS:CB	2:D:289:ILE:HD11	1.98	0.92
2:C:43:VAL:HG13	2:C:44:MET:H	1.32	0.92
2:B:140:LEU:HD23	2:B:343:GLY:CA	1.99	0.92
1:A:181:MET:HA	1:A:184:ILE:HD13	1.52	0.92
2:D:9:VAL:HG21	2:D:344:SER:HA	1.51	0.92
2:B:8:LEU:CB	2:B:103:VAL:HG13	1.99	0.91
2:B:294:TYR:HD1	2:B:327:ILE:HD11	1.34	0.91
2:B:9:VAL:HG22	2:B:104:LEU:HD23	1.53	0.91
2:D:41:GLN:HG3	2:D:42:GLY:H	1.33	0.91
2:C:120:THR:HB	2:C:367:PRO:HB3	1.53	0.91
2:B:285:CYS:CB	2:B:289:ILE:HD11	2.01	0.90
1:A:173:PHE:CZ	1:A:198:VAL:HG12	2.07	0.90
2:D:166:TYR:CD2	2:D:167:GLU:HG2	2.07	0.90
2:D:152:VAL:HG23	2:D:298:VAL:CB	2.02	0.90
2:B:193:LEU:HD21	2:B:253:GLU:HG3	1.52	0.89
2:D:37:ARG:H	2:D:66:THR:HG22	1.37	0.89
1:A:173:PHE:CZ	1:A:237:LEU:HD12	2.08	0.89
1:A:181:MET:HA	1:A:184:ILE:CD1	2.03	0.89
2:C:187:ASP:HA	2:C:190:MET:SD	2.13	0.89
2:D:71:ILE:HG23	2:D:75:ILE:C	1.93	0.89
2:D:140:LEU:HD23	2:D:343:GLY:CA	2.03	0.89
2:D:116:ARG:CD	2:D:134:VAL:HG11	2.01	0.88
2:C:73:HIC:HD2	2:C:183:ARG:HH12	1.23	0.88
2:B:349:LEU:HD22	2:B:352:PHE:CD1	2.08	0.88
2:C:34:ILE:CG1	2:C:67:LEU:HD22	2.04	0.88
1:A:151:VAL:HG22	1:A:254:ILE:HD13	1.53	0.88
1:A:181:MET:CA	1:A:184:ILE:HD13	2.03	0.88
2:B:195:GLU:HA	2:C:110:LEU:CD1	2.02	0.88
2:B:251:GLY:HA2	2:B:254:ARG:CD	2.03	0.88
2:D:148:THR:CG2	2:D:167:GLU:HA	2.04	0.88
1:A:155:TRP:HE3	1:A:250:TRP:HB2	1.36	0.87
2:B:110:LEU:CD1	2:D:195:GLU:HA	2.04	0.87
2:C:104:LEU:HD21	2:C:347:ALA:HB1	1.55	0.87
2:B:35:VAL:HG12	2:B:68:LYS:CB	2.04	0.87
2:D:7:ALA:HB3	2:D:347:ALA:HB1	1.56	0.87
2:C:34:ILE:HG13	2:C:67:LEU:CD2	2.03	0.87
2:B:257:CYS:HB3	2:B:258:PRO:HD3	1.54	0.87
2:C:9:VAL:HG22	2:C:104:LEU:CD2	2.03	0.87
2:C:216:LEU:CD2	2:C:254:ARG:HG3	2.03	0.87
2:B:151:ILE:CG2	2:B:297:THR:HG22	2.05	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:MET:C	1:A:184:ILE:HD13	1.94	0.86
2:D:208:ILE:HG21	2:D:242:LEU:CD1	2.05	0.86
2:B:136:ILE:HG23	2:B:139:VAL:H	1.40	0.86
2:C:281:SER:HA	2:C:284:LYS:HD2	1.57	0.86
2:C:58:ALA:HB1	2:C:65:LEU:CD1	2.05	0.86
2:C:7:ALA:HB1	2:C:104:LEU:CD2	2.05	0.86
2:D:133:TYR:CZ	2:D:375:PHE:HB2	2.11	0.86
2:C:287:VAL:HG23	2:D:244:ASP:CB	2.05	0.86
2:D:216:LEU:HD11	2:D:250:ILE:HG21	1.57	0.86
2:D:52:SER:HB2	2:D:84:LYS:HZ1	1.40	0.86
2:D:8:LEU:CB	2:D:103:VAL:HG22	2.06	0.86
2:B:236:LEU:HD12	2:B:237:GLU:N	1.91	0.86
2:C:257:CYS:HB3	2:C:258:PRO:HD3	1.58	0.86
2:C:163:VAL:HG12	2:C:175:ILE:CG1	2.03	0.86
2:B:34:ILE:HG12	2:B:54:VAL:HG11	1.57	0.86
2:C:54:VAL:HA	2:C:58:ALA:HB2	1.56	0.86
2:C:61:LYS:HG3	2:C:64:ILE:CG2	2.06	0.86
2:B:176:LEU:HD21	2:B:277:THR:CG2	2.05	0.85
2:B:35:VAL:HG22	2:B:52:SER:CB	2.06	0.85
2:D:34:ILE:CG1	2:D:54:VAL:HG11	2.05	0.85
2:B:317:ILE:HD11	2:B:329:ILE:HD11	1.59	0.85
2:C:272:CYS:CB	2:C:276:GLU:HG2	2.06	0.85
1:A:202:GLN:HB2	1:A:209:TRP:CZ3	2.10	0.85
2:D:192:ILE:HD12	2:D:256:ARG:HD2	1.58	0.85
1:A:153:GLU:OE1	2:D:236:LEU:HD11	1.77	0.85
2:D:253:GLU:HA	2:D:256:ARG:HG3	1.58	0.85
2:C:106:THR:HB	2:C:137:GLN:HG2	1.58	0.85
2:D:300:SER:CA	2:D:335:ARG:HD3	2.07	0.85
1:A:195:LYS:HB3	1:A:236:TYR:CD1	2.12	0.85
2:D:253:GLU:HA	2:D:256:ARG:CG	2.06	0.85
2:D:148:THR:HG23	2:D:167:GLU:HA	1.59	0.84
2:B:208:ILE:HD11	2:B:243:PRO:HG2	1.59	0.84
1:A:197:TRP:CE2	1:A:251:LYS:HB2	2.11	0.84
2:C:285:CYS:HB3	2:C:289:ILE:CD1	2.06	0.84
2:D:104:LEU:HD21	2:D:347:ALA:HB1	1.56	0.84
2:D:61:LYS:HG3	2:D:64:ILE:CG2	2.07	0.84
2:D:50:LYS:HB3	2:D:53:TYR:CD1	2.12	0.84
2:C:216:LEU:CD1	2:C:250:ILE:HG21	2.01	0.84
1:A:142:ILE:CD1	1:A:149:TYR:HB2	2.07	0.84
2:B:121:GLN:NE2	2:B:122:ILE:HD12	1.93	0.84
2:B:50:LYS:HB3	2:B:53:TYR:CE1	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:250:ILE:HG13	2:D:253:GLU:CG	2.06	0.84
2:D:211:ASP:HA	2:D:214:GLU:OE2	1.78	0.84
2:C:8:LEU:CB	2:C:103:VAL:HG22	2.07	0.84
2:D:140:LEU:HD23	2:D:343:GLY:HA2	1.57	0.84
2:C:290:ARG:HA	2:C:293:LEU:CD1	2.08	0.84
2:C:153:MET:HG3	2:C:299:LEU:CA	2.08	0.84
2:B:143:TYR:CE1	2:B:345:ILE:HG21	2.13	0.84
1:A:233:ILE:HG13	1:A:245:ASP:O	1.78	0.84
2:B:113:LYS:HG2	2:B:371:HIS:NE2	1.92	0.83
2:C:188:TYR:O	2:C:192:ILE:HG13	1.78	0.83
2:D:346:LEU:HA	2:D:349:LEU:HD12	1.59	0.83
1:A:173:PHE:CD1	1:A:254:ILE:HB	2.13	0.83
2:D:140:LEU:O	2:D:342:GLY:HA3	1.77	0.83
2:D:43:VAL:HG22	2:D:44:MET:H	1.42	0.83
2:B:200:PHE:HA	2:B:205:GLU:OE2	1.79	0.83
1:A:233:ILE:HG12	1:A:247:CYS:N	1.93	0.83
1:A:173:PHE:CE1	1:A:254:ILE:HB	2.13	0.83
2:C:189:LEU:HD12	2:C:209:VAL:CG2	2.07	0.83
2:C:39:ARG:NH2	2:C:203:THR:HG21	1.94	0.83
2:C:176:LEU:HD11	2:C:277:THR:CG2	2.09	0.83
2:D:203:THR:O	2:D:206:ARG:HB2	1.78	0.83
2:D:341:ILE:O	2:D:345:ILE:HD12	1.78	0.83
2:C:61:LYS:HE3	2:C:64:ILE:HG21	1.60	0.83
2:D:300:SER:H	2:D:304:THR:HG21	1.44	0.82
2:B:180:LEU:HD12	2:B:184:ASP:HB2	1.59	0.82
2:D:250:ILE:HG13	2:D:253:GLU:HG2	1.59	0.82
1:A:243:ILE:HG22	1:A:244:SER:H	1.42	0.82
2:C:290:ARG:HD2	2:D:244:ASP:CB	2.10	0.82
2:B:216:LEU:CD1	2:B:250:ILE:HG12	2.10	0.82
2:B:250:ILE:HG13	2:B:251:GLY:N	1.95	0.82
2:B:59:GLN:O	2:B:62:ARG:HG2	1.78	0.82
2:D:176:LEU:HD21	2:D:277:THR:CG2	2.10	0.82
2:D:7:ALA:HB1	2:D:104:LEU:CD2	2.08	0.82
2:C:136:ILE:O	2:C:139:VAL:HG12	1.79	0.82
2:C:211:ASP:OD1	2:C:215:LYS:HE2	1.80	0.82
2:D:278:THR:HG21	2:D:313:MET:CE	2.10	0.82
2:C:153:MET:SD	2:C:299:LEU:HG	2.19	0.82
2:C:143:TYR:CE2	2:D:45:VAL:HG11	2.15	0.81
2:D:302:GLY:O	2:D:305:MET:HG2	1.80	0.81
2:C:68:LYS:HD3	2:C:69:TYR:N	1.96	0.81
2:C:302:GLY:O	2:C:305:MET:HG2	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:61:LYS:O	2:D:64:ILE:HG22	1.79	0.81
2:C:118:LYS:HE3	2:C:122:ILE:HD11	1.63	0.81
2:C:164:PRO:O	2:C:165:ILE:HD13	1.81	0.81
2:C:237:GLU:O	2:C:249:THR:HG23	1.80	0.81
2:C:36:GLY:O	2:C:52:SER:HA	1.81	0.81
2:C:176:LEU:HD21	2:C:277:THR:CG2	2.11	0.81
2:B:136:ILE:O	2:B:139:VAL:HG12	1.81	0.81
2:C:57:GLU:O	2:C:61:LYS:HB2	1.79	0.81
2:B:133:TYR:OH	2:B:375:PHE:HB2	1.81	0.81
2:B:135:ALA:HB3	2:B:140:LEU:HD11	1.63	0.80
2:B:36:GLY:N	2:B:52:SER:HB3	1.95	0.80
2:C:11:ASP:OD2	2:C:340:TRP:HA	1.81	0.80
2:C:176:LEU:HD11	2:C:277:THR:HG23	1.60	0.80
2:B:250:ILE:HD12	2:B:253:GLU:CG	2.11	0.80
2:D:180:LEU:CD1	2:D:184:ASP:HB2	2.11	0.80
2:D:164:PRO:HG2	2:D:174:ALA:HB1	1.63	0.80
2:C:367:PRO:O	2:C:370:VAL:HG12	1.80	0.80
2:B:189:LEU:HA	2:B:192:ILE:CD1	2.11	0.80
2:D:180:LEU:HD11	2:D:185:LEU:CD2	2.11	0.80
1:A:200:VAL:O	1:A:234:CYS:HB2	1.81	0.80
2:D:37:ARG:HG3	2:D:38:PRO:HD2	1.64	0.80
2:B:216:LEU:HD21	2:B:254:ARG:CG	2.11	0.80
2:B:12:ASN:HD21	2:B:105:LEU:HD12	1.46	0.80
2:B:8:LEU:HD11	2:B:94:LEU:CD1	2.11	0.80
1:A:157:MET:HG2	1:A:160:ILE:HB	1.62	0.80
2:C:10:VAL:CG2	2:C:105:LEU:HD13	2.12	0.80
2:B:272:CYS:HB3	2:B:276:GLU:CG	2.12	0.80
1:A:155:TRP:CE3	1:A:250:TRP:HB2	2.16	0.80
2:D:58:ALA:HA	2:D:61:LYS:HB2	1.62	0.80
2:B:35:VAL:HG22	2:B:52:SER:HB3	1.64	0.80
2:D:28:ARG:HB3	2:D:28:ARG:NH1	1.97	0.80
2:C:37:ARG:HG2	2:C:38:PRO:CD	2.10	0.80
2:B:16:MET:HG2	2:B:30:VAL:HG22	1.62	0.79
2:C:71:ILE:HD11	2:C:85:ILE:CD1	2.12	0.79
2:D:237:GLU:O	2:D:249:THR:HG23	1.81	0.79
2:C:59:GLN:O	2:C:62:ARG:HG3	1.82	0.79
2:B:358:SER:H	2:B:361:GLU:HG2	1.47	0.79
2:B:110:LEU:HD21	2:D:195:GLU:HB2	1.62	0.79
2:C:206:ARG:O	2:C:209:VAL:HG12	1.83	0.79
2:B:272:CYS:HB3	2:B:276:GLU:CB	2.13	0.79
2:B:190:MET:CE	2:B:206:ARG:HA	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:121:GLN:HE21	2:D:122:ILE:HD12	1.46	0.79
2:B:174:ALA:HA	2:B:284:LYS:HD2	1.63	0.79
2:B:113:LYS:HG2	2:B:371:HIS:CD2	2.18	0.79
2:C:35:VAL:CG2	2:C:52:SER:HB3	2.10	0.79
2:B:262:PHE:CZ	2:B:312:ARG:HD3	2.18	0.79
2:D:358:SER:O	2:D:361:GLU:HG2	1.82	0.79
2:C:73:HIC:HD2	2:C:183:ARG:HH11	1.39	0.79
2:B:10:VAL:HG23	2:B:105:LEU:HD13	1.65	0.79
2:D:121:GLN:NE2	2:D:122:ILE:HD12	1.97	0.79
2:B:104:LEU:HD21	2:B:347:ALA:HB1	1.64	0.79
1:A:184:ILE:H	1:A:184:ILE:HD12	1.48	0.79
2:D:61:LYS:HG3	2:D:64:ILE:HG21	1.65	0.79
2:D:35:VAL:HG12	2:D:68:LYS:CB	2.12	0.79
2:C:143:TYR:HE2	2:D:45:VAL:HG21	1.46	0.79
2:B:107:GLU:O	2:B:137:GLN:HG3	1.83	0.79
2:D:278:THR:HG21	2:D:313:MET:HE1	1.64	0.78
2:D:242:LEU:HG	2:D:243:PRO:HD2	1.64	0.78
2:C:196:ARG:NH2	2:C:250:ILE:HA	1.98	0.78
2:D:106:THR:HG22	2:D:135:ALA:CB	2.13	0.78
2:B:216:LEU:HD11	2:B:250:ILE:HG21	1.65	0.78
2:B:250:ILE:CD1	2:B:253:GLU:HG2	2.14	0.78
2:B:34:ILE:CG1	2:B:67:LEU:HD22	2.10	0.78
2:D:282:ILE:CD1	2:D:293:LEU:HD22	2.14	0.78
2:D:306:TYR:O	2:D:309:ILE:HG23	1.83	0.78
2:C:35:VAL:HG12	2:C:68:LYS:CB	2.08	0.78
2:C:135:ALA:HB1	2:C:140:LEU:CD1	2.08	0.78
2:B:35:VAL:CA	2:B:54:VAL:HG21	2.13	0.78
2:D:257:CYS:HB3	2:D:258:PRO:HD3	1.66	0.78
2:C:238:LYS:O	2:C:250:ILE:HG22	1.84	0.78
2:B:180:LEU:HD13	2:B:267:LEU:HD12	1.66	0.78
2:B:148:THR:CG2	2:B:149:THR:HG23	2.13	0.78
2:B:176:LEU:HD11	2:B:277:THR:CG2	2.14	0.78
2:D:132:MET:O	2:D:357:ILE:HB	1.84	0.78
2:C:238:LYS:HE2	2:C:254:ARG:CZ	2.14	0.78
2:C:143:TYR:CD2	2:D:45:VAL:HG11	2.18	0.78
2:B:190:MET:HE1	2:B:206:ARG:HA	1.67	0.77
2:B:54:VAL:HA	2:B:58:ALA:HB2	1.66	0.77
1:A:157:MET:HG2	1:A:160:ILE:CB	2.14	0.77
1:A:173:PHE:HZ	1:A:237:LEU:HD12	1.47	0.77
1:A:195:LYS:HD3	1:A:251:LYS:HE3	1.65	0.77
2:D:97:ALA:HB3	2:D:100:GLU:OE1	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:LEU:HD11	2:B:67:LEU:CD2	2.14	0.77
2:C:164:PRO:HB3	2:C:293:LEU:CD2	2.14	0.77
2:C:236:LEU:HD12	2:C:237:GLU:N	1.99	0.77
2:D:136:ILE:HG22	2:D:139:VAL:HB	1.67	0.77
2:C:178:LEU:HD12	2:C:180:LEU:H	1.49	0.77
2:B:203:THR:O	2:B:206:ARG:HG2	1.83	0.77
2:B:36:GLY:O	2:B:52:SER:HA	1.83	0.77
2:B:61:LYS:HD2	2:B:64:ILE:CG2	2.10	0.77
2:C:50:LYS:HB3	2:C:53:TYR:CD1	2.19	0.77
2:B:317:ILE:HD12	2:B:327:ILE:HG12	1.64	0.77
2:C:299:LEU:HD21	2:C:309:ILE:HG13	1.67	0.77
1:A:154:ARG:HD3	2:D:231:ALA:O	1.84	0.77
2:B:294:TYR:CD1	2:B:327:ILE:HD11	2.17	0.77
2:B:133:TYR:CZ	2:B:375:PHE:HB2	2.20	0.77
2:B:178:LEU:HD12	2:B:180:LEU:H	1.49	0.77
2:B:211:ASP:HA	2:B:214:GLU:OE2	1.84	0.77
1:A:211:TRP:HB2	1:A:213:ASP:OD1	1.84	0.76
2:D:61:LYS:HE2	2:D:64:ILE:CG2	2.14	0.76
2:C:190:MET:CE	2:C:206:ARG:HB2	2.15	0.76
2:B:14:SER:HA	2:B:71:ILE:HG22	1.67	0.76
2:C:192:ILE:HD12	2:C:193:LEU:N	2.00	0.76
2:C:309:ILE:HG12	2:C:310:ALA:N	1.99	0.76
2:B:242:LEU:HG	2:B:243:PRO:HD2	1.67	0.76
2:C:290:ARG:HA	2:C:293:LEU:HD13	1.67	0.76
2:C:133:TYR:OH	2:C:375:PHE:HB2	1.84	0.76
2:B:293:LEU:H	2:B:293:LEU:HD12	1.50	0.76
2:B:82:MET:CE	2:B:85:ILE:HB	2.15	0.76
2:B:237:GLU:O	2:B:249:THR:HG23	1.86	0.76
2:B:65:LEU:HD12	2:B:66:THR:O	1.85	0.76
2:C:134:VAL:O	2:C:375:PHE:HB3	1.84	0.76
2:B:208:ILE:HD13	2:B:242:LEU:HD11	1.67	0.76
2:D:220:ALA:CB	2:D:226:GLU:HG3	2.16	0.76
2:C:242:LEU:HB3	2:C:244:ASP:OD1	1.84	0.76
2:D:35:VAL:CA	2:D:54:VAL:HG21	2.15	0.76
2:D:236:LEU:O	2:D:251:GLY:HA2	1.85	0.76
2:C:288:ASP:OD2	2:D:62:ARG:HD2	1.86	0.76
2:C:35:VAL:CA	2:C:54:VAL:HG21	2.16	0.76
2:D:8:LEU:HD12	2:D:90:PHE:HE1	1.51	0.76
2:B:361:GLU:OE1	2:B:369:ILE:HD12	1.84	0.76
2:C:279:PHE:O	2:C:282:ILE:HG22	1.86	0.76
2:D:133:TYR:OH	2:D:375:PHE:HB2	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:7:ALA:HB3	2:C:22:ALA:HB2	1.67	0.76
2:B:286:ASP:O	2:B:290:ARG:HG2	1.85	0.76
2:D:300:SER:HA	2:D:335:ARG:CD	2.13	0.75
2:B:50:LYS:HB3	2:B:53:TYR:CD1	2.21	0.75
2:D:105:LEU:HD11	2:D:123:MET:CE	2.14	0.75
2:B:135:ALA:CB	2:B:140:LEU:HD11	2.16	0.75
2:B:164:PRO:HG2	2:B:174:ALA:CB	2.16	0.75
2:B:367:PRO:O	2:B:370:VAL:HG12	1.86	0.75
2:D:35:VAL:CG2	2:D:52:SER:HB3	2.15	0.75
2:D:309:ILE:HG12	2:D:310:ALA:N	2.00	0.75
2:B:196:ARG:NH2	2:B:250:ILE:HA	2.01	0.75
2:B:7:ALA:CB	2:B:347:ALA:HB1	2.16	0.75
2:B:369:ILE:HD13	2:B:369:ILE:O	1.86	0.75
2:B:110:LEU:HD13	2:D:195:GLU:HA	1.68	0.75
2:B:345:ILE:O	2:B:349:LEU:HD12	1.85	0.75
2:B:314:GLN:HG3	2:B:315:LYS:N	2.01	0.75
2:C:14:SER:HA	2:C:71:ILE:HG22	1.67	0.75
2:B:92:ASN:O	2:B:95:ARG:HD3	1.87	0.75
1:A:198:VAL:HG22	1:A:235:GLY:O	1.86	0.75
2:B:110:LEU:HD21	2:D:195:GLU:CB	2.16	0.75
2:B:118:LYS:O	2:B:122:ILE:HD13	1.87	0.75
2:B:68:LYS:HD2	2:B:69:TYR:N	2.02	0.75
2:C:337:TYR:O	2:C:341:ILE:HG12	1.87	0.75
2:B:250:ILE:CG1	2:B:254:ARG:HG2	2.16	0.75
1:A:195:LYS:HD3	1:A:251:LYS:CE	2.15	0.75
2:D:153:MET:CE	2:D:274:ILE:HD13	2.17	0.74
2:C:8:LEU:HB2	2:C:103:VAL:CG2	2.10	0.74
2:D:220:ALA:HB1	2:D:226:GLU:HG3	1.67	0.74
2:B:235:SER:O	2:B:238:LYS:HE2	1.87	0.74
1:A:238:LYS:HB3	1:A:243:ILE:HD11	1.68	0.74
2:D:122:ILE:HG23	2:D:126:THR:CG2	2.17	0.74
2:D:86:TRP:CZ2	2:D:123:MET:HE1	2.22	0.74
2:C:12:ASN:HD21	2:C:105:LEU:HD12	1.51	0.74
2:C:7:ALA:HB3	2:C:347:ALA:HB1	1.67	0.74
2:D:233:SER:HB2	2:D:236:LEU:HG	1.68	0.74
2:C:133:TYR:CZ	2:C:375:PHE:HB2	2.21	0.74
2:C:341:ILE:O	2:C:345:ILE:HD13	1.86	0.74
2:D:261:LEU:HD21	2:D:303:THR:CG2	2.16	0.74
2:D:36:GLY:HA2	2:D:66:THR:HG23	1.70	0.74
2:B:71:ILE:HD12	2:B:71:ILE:H	1.53	0.74
2:C:79:TRP:CE2	2:C:118:LYS:HG2	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:287:VAL:HG21	2:D:242:LEU:HG	1.69	0.74
2:D:7:ALA:CB	2:D:104:LEU:HD21	2.16	0.74
2:C:196:ARG:HH22	2:C:250:ILE:HA	1.52	0.74
2:B:192:ILE:O	2:B:195:GLU:HB3	1.88	0.74
2:D:116:ARG:HD2	2:D:134:VAL:CG1	2.03	0.74
2:D:58:ALA:HB1	2:D:65:LEU:HD13	1.69	0.74
1:A:154:ARG:HD2	2:D:231:ALA:HA	1.69	0.74
2:C:153:MET:HG3	2:C:299:LEU:CB	2.17	0.74
2:D:164:PRO:HG2	2:D:174:ALA:CB	2.17	0.74
2:B:7:ALA:HB1	2:B:104:LEU:CD2	2.15	0.74
2:B:10:VAL:CG2	2:B:105:LEU:HD13	2.17	0.74
1:A:157:MET:CG	1:A:160:ILE:H	2.00	0.74
2:D:216:LEU:CD1	2:D:250:ILE:HG21	2.17	0.74
2:B:152:VAL:HG12	2:B:163:VAL:HG23	1.70	0.74
2:D:113:LYS:HE2	2:D:371:HIS:NE2	2.03	0.74
1:A:174:GLN:HB3	1:A:211:TRP:CD2	2.22	0.74
2:D:36:GLY:O	2:D:52:SER:HA	1.87	0.74
2:C:208:ILE:HD11	2:C:243:PRO:HG2	1.70	0.74
2:B:154:ASP:OD1	2:B:300:SER:HB3	1.88	0.74
2:B:272:CYS:HB3	2:B:276:GLU:HB3	1.69	0.74
2:C:178:LEU:CD1	2:C:180:LEU:H	2.00	0.74
2:B:104:LEU:HG	2:B:347:ALA:HB2	1.69	0.73
2:D:106:THR:CG2	2:D:140:LEU:HD22	2.18	0.73
2:B:314:GLN:O	2:B:318:THR:HG23	1.87	0.73
2:D:61:LYS:CE	2:D:64:ILE:HG21	2.17	0.73
2:D:52:SER:HB2	2:D:84:LYS:NZ	2.03	0.73
2:C:113:LYS:HG2	2:C:371:HIS:CD2	2.23	0.73
2:B:27:PRO:HG3	2:B:340:TRP:CG	2.23	0.73
2:D:20:GLY:HA2	2:D:28:ARG:CD	2.18	0.73
2:B:151:ILE:HG23	2:B:297:THR:HG22	1.70	0.73
2:B:82:MET:HE3	2:B:85:ILE:HB	1.70	0.73
1:A:156:GLU:OE1	1:A:161:SER:HA	1.88	0.73
2:C:256:ARG:O	2:C:259:GLU:HB2	1.89	0.73
2:B:152:VAL:HG23	2:B:298:VAL:CG1	2.16	0.73
1:A:221:LEU:O	1:A:242:LEU:HD22	1.87	0.73
2:D:70:PRO:HB3	2:D:78:ASN:ND2	2.04	0.73
2:C:190:MET:CE	2:C:209:VAL:HG11	2.19	0.73
2:B:151:ILE:O	2:B:297:THR:HA	1.87	0.73
2:D:293:LEU:H	2:D:293:LEU:HD12	1.53	0.73
2:C:171:LEU:HD23	2:C:174:ALA:H	1.54	0.73
2:B:9:VAL:CG2	2:B:104:LEU:HD23	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:302:GLY:O	2:B:305:MET:HG2	1.86	0.73
2:C:369:ILE:O	2:C:369:ILE:HD13	1.88	0.73
1:A:142:ILE:HD13	1:A:142:ILE:H	1.54	0.73
2:B:161:HIS:NE2	2:B:177:ARG:HD2	2.04	0.73
2:B:358:SER:H	2:B:361:GLU:CG	2.01	0.72
2:D:58:ALA:HB1	2:D:65:LEU:CD1	2.19	0.72
2:C:192:ILE:HB	2:C:256:ARG:NH2	2.04	0.72
2:C:65:LEU:HG	2:C:66:THR:O	1.89	0.72
2:D:152:VAL:HG23	2:D:298:VAL:CG1	2.19	0.72
1:A:174:GLN:HA	1:A:211:TRP:CZ3	2.24	0.72
1:A:135:SER:HB2	1:A:136:PRO:HD2	1.71	0.72
2:C:140:LEU:O	2:C:342:GLY:HA3	1.89	0.72
2:D:290:ARG:HA	2:D:293:LEU:HD13	1.71	0.72
2:B:176:LEU:H	2:B:176:LEU:HD13	1.52	0.72
2:B:140:LEU:O	2:B:342:GLY:HA3	1.90	0.72
2:B:7:ALA:HB1	2:B:356:TRP:CH2	2.25	0.72
1:A:157:MET:HG2	1:A:160:ILE:CG2	2.20	0.72
2:C:65:LEU:HD23	2:C:65:LEU:O	1.90	0.72
2:C:118:LYS:HD2	2:C:121:GLN:HG2	1.71	0.72
2:B:21:PHE:CZ	2:B:96:VAL:HG11	2.24	0.72
2:D:134:VAL:HB	2:D:375:PHE:OXT	1.89	0.72
2:D:7:ALA:HB1	2:D:356:TRP:HH2	1.55	0.72
2:C:35:VAL:HA	2:C:54:VAL:CG2	2.18	0.72
2:C:202:THR:OG1	2:C:205:GLU:HG3	1.90	0.72
1:A:195:LYS:CD	1:A:251:LYS:HE3	2.19	0.72
2:D:172:PRO:O	2:D:175:ILE:HG22	1.88	0.72
2:C:285:CYS:CB	2:C:289:ILE:HD11	2.18	0.72
2:D:357:ILE:HD11	2:D:375:PHE:O	1.88	0.72
2:B:164:PRO:HG2	2:B:174:ALA:HB1	1.71	0.72
2:C:143:TYR:CE1	2:C:345:ILE:HG21	2.24	0.72
2:D:208:ILE:HG21	2:D:242:LEU:HD11	1.71	0.71
2:C:10:VAL:HG23	2:C:105:LEU:HD13	1.72	0.71
2:D:157:ASP:H	4:D:401:ADP:PB	2.14	0.71
2:C:8:LEU:O	2:C:103:VAL:HG13	1.91	0.71
2:C:7:ALA:CB	2:C:104:LEU:HD21	2.17	0.71
2:B:136:ILE:CG2	2:B:139:VAL:HB	2.20	0.71
2:D:104:LEU:HD21	2:D:347:ALA:CB	2.19	0.71
1:A:233:ILE:HD12	1:A:234:CYS:O	1.90	0.71
1:A:200:VAL:HG13	1:A:235:GLY:H	1.55	0.71
2:D:258:PRO:O	2:D:261:LEU:HD13	1.90	0.71
2:C:38:PRO:HB3	2:C:64:ILE:HD11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:157:ASP:H	4:C:401:ADP:PB	2.14	0.71
2:C:61:LYS:CE	2:C:64:ILE:HG21	2.20	0.71
2:C:39:ARG:HG2	2:C:66:THR:HB	1.72	0.71
2:C:104:LEU:HD21	2:C:347:ALA:CB	2.20	0.71
2:D:18:LYS:H	2:D:18:LYS:HD2	1.54	0.71
2:B:164:PRO:HB3	2:B:293:LEU:CD2	2.21	0.71
2:B:131:ALA:HB1	2:B:357:ILE:O	1.91	0.71
2:B:20:GLY:HA2	2:B:28:ARG:HD2	1.72	0.71
2:C:121:GLN:HG3	2:C:122:ILE:N	2.02	0.71
1:A:196:TYR:HA	1:A:252:TYR:O	1.90	0.71
1:A:155:TRP:CH2	2:B:117:GLU:HB2	2.26	0.71
2:C:71:ILE:H	2:C:71:ILE:HD12	1.56	0.71
2:D:134:VAL:HG23	2:D:370:VAL:CG2	2.20	0.70
2:D:32:PRO:HB3	2:D:34:ILE:HD11	1.74	0.70
2:B:157:ASP:H	4:B:401:ADP:PB	2.14	0.70
2:D:143:TYR:CE1	2:D:345:ILE:HG21	2.25	0.70
2:C:321:ALA:HB1	2:C:322:PRO:HD2	1.72	0.70
2:C:50:LYS:HB3	2:C:53:TYR:CE1	2.26	0.70
2:B:164:PRO:HB3	2:B:293:LEU:HD21	1.72	0.70
2:B:282:ILE:HD12	2:B:290:ARG:HB3	1.71	0.70
2:B:34:ILE:HG22	2:B:68:LYS:O	1.92	0.70
2:D:196:ARG:HH22	2:D:250:ILE:HA	1.57	0.70
2:C:97:ALA:HB1	2:C:99:GLU:OE1	1.91	0.70
2:B:104:LEU:HD22	2:B:104:LEU:N	2.07	0.70
2:B:242:LEU:CD1	2:B:243:PRO:HD2	2.22	0.70
1:A:150:TYR:O	1:A:254:ILE:HG23	1.91	0.70
2:B:61:LYS:CD	2:B:64:ILE:HG21	2.15	0.70
2:D:216:LEU:HD11	2:D:250:ILE:CG2	2.21	0.70
2:C:41:GLN:HG3	2:C:42:GLY:H	1.56	0.70
2:B:180:LEU:CD1	2:B:184:ASP:HB2	2.22	0.70
1:A:156:GLU:HB3	1:A:160:ILE:HG23	1.74	0.69
2:D:185:LEU:HD11	2:D:258:PRO:HA	1.73	0.69
2:D:137:GLN:HB3	2:D:339:VAL:HG11	1.72	0.69
1:A:155:TRP:HE3	1:A:250:TRP:CB	2.04	0.69
1:A:156:GLU:HG3	1:A:253:PHE:CE1	2.28	0.69
2:C:157:ASP:O	2:C:182:GLY:HA3	1.91	0.69
2:B:242:LEU:CG	2:B:243:PRO:HD2	2.21	0.69
2:D:142:LEU:O	2:D:142:LEU:HD12	1.91	0.69
2:B:192:ILE:HD13	2:B:192:ILE:H	1.56	0.69
2:C:192:ILE:HD12	2:C:193:LEU:H	1.57	0.69
1:A:181:MET:HE1	1:A:242:LEU:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:ALA:CB	2:B:104:LEU:HD21	2.18	0.69
2:C:189:LEU:HA	2:C:192:ILE:HD11	1.75	0.69
1:A:162:LYS:O	1:A:166:LEU:HG	1.91	0.69
2:D:216:LEU:CD2	2:D:254:ARG:HG2	2.21	0.69
2:D:107:GLU:OE2	2:D:111:ASN:HB3	1.92	0.69
2:C:158:GLY:HA3	2:C:183:ARG:NH2	2.08	0.69
2:B:39:ARG:NH2	2:B:66:THR:HA	2.08	0.69
1:A:236:TYR:CE2	1:A:245:ASP:HB2	2.28	0.69
2:D:131:ALA:HB1	2:D:357:ILE:O	1.92	0.69
2:B:171:LEU:HD23	2:B:174:ALA:HB2	1.75	0.69
2:B:251:GLY:CA	2:B:254:ARG:HG3	2.22	0.69
2:B:372:ARG:NE	2:B:372:ARG:HA	2.08	0.69
1:A:157:MET:O	1:A:160:ILE:HG22	1.93	0.69
2:C:166:TYR:HD2	2:C:167:GLU:HG2	1.57	0.69
2:C:194:THR:HA	2:C:198:TYR:O	1.91	0.69
2:B:149:THR:CG2	2:B:167:GLU:H	2.06	0.69
2:D:221:LEU:H	2:D:221:LEU:HD22	1.57	0.69
2:B:206:ARG:CZ	2:B:206:ARG:HB2	2.21	0.69
2:B:216:LEU:CD1	2:B:250:ILE:HG21	2.23	0.69
2:D:194:THR:HA	2:D:198:TYR:O	1.92	0.69
2:D:149:THR:HA	2:D:165:ILE:O	1.92	0.69
2:B:193:LEU:CD2	2:B:253:GLU:HG3	2.23	0.69
2:B:357:ILE:HD11	2:B:375:PHE:O	1.93	0.69
2:D:35:VAL:HA	2:D:54:VAL:HG21	1.73	0.69
2:D:361:GLU:HG3	2:D:369:ILE:HG21	1.75	0.69
2:C:68:LYS:C	2:C:68:LYS:HD3	2.13	0.69
2:C:104:LEU:HD13	2:C:133:TYR:HB3	1.73	0.69
2:C:132:MET:O	2:C:357:ILE:HB	1.93	0.69
2:B:294:TYR:HD1	2:B:327:ILE:CD1	2.03	0.69
2:C:176:LEU:HD21	2:C:277:THR:HG23	1.75	0.69
1:A:187:ILE:O	1:A:190:LEU:HB3	1.93	0.68
2:C:15:GLY:O	2:C:32:PRO:HA	1.93	0.68
2:B:120:THR:CG2	2:B:367:PRO:HB3	2.23	0.68
2:B:104:LEU:HD21	2:B:347:ALA:CB	2.22	0.68
2:D:34:ILE:HG22	2:D:68:LYS:O	1.93	0.68
2:D:35:VAL:HG12	2:D:68:LYS:HB2	1.75	0.68
1:A:184:ILE:H	1:A:184:ILE:CD1	2.07	0.68
2:C:191:LYS:CA	2:C:191:LYS:HE3	2.16	0.68
2:C:157:ASP:N	4:C:401:ADP:O3A	2.27	0.68
2:C:299:LEU:CD2	2:C:309:ILE:HG13	2.23	0.68
2:D:148:THR:O	2:D:165:ILE:HG22	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:208:ILE:HG21	2:B:242:LEU:HD11	1.74	0.68
2:B:216:LEU:HD11	2:B:250:ILE:CG1	2.18	0.68
2:B:140:LEU:HD23	2:B:343:GLY:HA3	1.75	0.68
2:D:158:GLY:HA3	2:D:183:ARG:NH2	2.08	0.68
2:B:145:SER:HB3	2:B:147:ARG:HG2	1.75	0.68
2:B:174:ALA:CA	2:B:284:LYS:HD2	2.22	0.68
1:A:200:VAL:HA	1:A:210:PHE:O	1.93	0.68
2:B:290:ARG:HA	2:B:293:LEU:HD13	1.76	0.68
2:C:11:ASP:OD1	2:C:106:THR:HG21	1.94	0.68
2:B:261:LEU:HB3	2:B:274:ILE:HD11	1.75	0.68
2:B:208:ILE:HG21	2:B:242:LEU:CD1	2.24	0.68
2:D:208:ILE:HG21	2:D:242:LEU:HD12	1.76	0.67
2:B:216:LEU:HD11	2:B:250:ILE:CG2	2.23	0.67
2:D:187:ASP:O	2:D:191:LYS:HG2	1.95	0.67
2:C:10:VAL:HG23	2:C:105:LEU:HA	1.75	0.67
2:C:90:PHE:CG	2:C:98:PRO:HG3	2.29	0.67
2:B:99:GLU:HG2	2:B:100:GLU:OE1	1.93	0.67
2:B:7:ALA:HB1	2:B:356:TRP:HH2	1.57	0.67
2:B:54:VAL:HG12	2:B:55:GLY:N	2.10	0.67
2:D:39:ARG:HE	2:D:66:THR:HA	1.59	0.67
1:A:142:ILE:HD13	1:A:149:TYR:O	1.95	0.67
2:B:65:LEU:HD11	2:B:67:LEU:HD21	1.76	0.67
2:B:122:ILE:O	2:B:126:THR:HG22	1.94	0.67
2:B:332:PRO:HG2	2:B:335:ARG:NH2	2.05	0.67
2:D:282:ILE:HD13	2:D:293:LEU:HD22	1.75	0.67
2:B:34:ILE:HA	2:B:68:LYS:O	1.93	0.67
2:B:71:ILE:HD11	2:B:85:ILE:CD1	2.25	0.67
2:B:261:LEU:HB3	2:B:274:ILE:CD1	2.24	0.67
2:D:313:MET:HB3	2:D:329:ILE:HD13	1.76	0.67
1:A:190:LEU:HD11	1:A:194:ASN:ND2	2.08	0.67
1:A:155:TRP:HH2	2:B:117:GLU:HB2	1.60	0.67
2:C:34:ILE:O	2:C:54:VAL:HG21	1.95	0.67
2:D:149:THR:HG22	2:D:166:TYR:HA	1.75	0.67
2:D:306:TYR:HB2	2:D:309:ILE:CG2	2.25	0.67
2:B:50:LYS:N	2:B:50:LYS:HD3	2.09	0.67
1:A:157:MET:HG3	1:A:160:ILE:H	1.59	0.67
2:C:104:LEU:N	2:C:104:LEU:HD22	2.10	0.67
2:B:157:ASP:N	4:B:401:ADP:O3A	2.27	0.67
2:B:300:SER:HA	2:B:335:ARG:HD3	1.76	0.67
2:B:43:VAL:HG22	2:B:44:MET:H	1.57	0.67
1:A:184:ILE:HD12	1:A:184:ILE:N	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:242:LEU:HB3	2:D:244:ASP:OD1	1.95	0.67
2:C:68:LYS:O	2:C:70:PRO:HD3	1.94	0.67
2:D:107:GLU:O	2:D:137:GLN:HG3	1.95	0.67
2:C:73:HIC:CD2	2:C:183:ARG:HH12	2.03	0.67
2:B:9:VAL:HG22	2:B:104:LEU:CD2	2.24	0.67
2:C:190:MET:HE2	2:C:206:ARG:HA	1.76	0.67
2:C:120:THR:HA	2:C:132:MET:SD	2.35	0.67
2:C:133:TYR:HD1	2:C:357:ILE:HD12	1.58	0.67
2:D:285:CYS:HB3	2:D:289:ILE:CD1	2.18	0.67
2:B:152:VAL:CG2	2:B:298:VAL:HG12	2.22	0.67
2:D:157:ASP:N	4:D:401:ADP:O3A	2.27	0.67
2:C:35:VAL:CG1	2:C:68:LYS:HB3	2.12	0.67
2:B:42:GLY:O	2:B:43:VAL:HG12	1.95	0.67
2:C:176:LEU:HD21	2:C:277:THR:HG21	1.75	0.66
1:A:137:CYS:SG	1:A:143:GLN:HB2	2.35	0.66
2:B:34:ILE:HG12	2:B:54:VAL:HG13	1.77	0.66
2:D:294:TYR:HD1	2:D:327:ILE:CD1	2.06	0.66
2:D:299:LEU:CD2	2:D:309:ILE:HG13	2.26	0.66
2:B:35:VAL:HA	2:B:54:VAL:HG21	1.76	0.66
2:B:242:LEU:HD12	2:B:243:PRO:HD2	1.76	0.66
2:D:153:MET:HE1	2:D:274:ILE:HD13	1.77	0.66
2:C:120:THR:HG23	2:C:132:MET:SD	2.36	0.66
2:B:321:ALA:HB1	2:B:322:PRO:HD2	1.77	0.66
2:C:299:LEU:HD21	2:C:309:ILE:CG1	2.25	0.66
2:B:54:VAL:HG12	2:B:55:GLY:H	1.59	0.66
1:A:154:ARG:NH1	2:D:231:ALA:HB1	2.09	0.66
2:D:69:TYR:HB2	2:D:72:GLU:HG3	1.76	0.66
2:C:244:ASP:OD2	2:C:246:GLN:HG3	1.96	0.66
2:D:294:TYR:HD1	2:D:327:ILE:HD13	1.61	0.66
1:A:161:SER:HB2	1:A:253:PHE:CG	2.29	0.66
2:C:287:VAL:HG23	2:D:244:ASP:HB3	1.77	0.66
2:B:341:ILE:O	2:B:345:ILE:HD12	1.96	0.66
2:B:143:TYR:OH	2:B:349:LEU:HD11	1.96	0.66
2:B:195:GLU:HG2	2:C:110:LEU:HD21	1.76	0.66
2:B:32:PRO:HD2	2:B:55:GLY:HA2	1.77	0.66
1:A:157:MET:HG2	1:A:160:ILE:HG22	1.76	0.66
2:D:157:ASP:O	2:D:181:ALA:HB3	1.96	0.66
2:D:178:LEU:HD12	2:D:180:LEU:N	1.98	0.66
2:C:218:TYR:HE2	2:C:254:ARG:CZ	2.08	0.66
2:B:285:CYS:HB3	2:B:289:ILE:CD1	2.23	0.66
2:C:287:VAL:HG23	2:D:244:ASP:N	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:65:LEU:HD11	2:D:67:LEU:CD2	2.26	0.66
2:B:149:THR:HG22	2:B:166:TYR:CA	2.19	0.66
2:C:11:ASP:HA	2:C:106:THR:OG1	1.96	0.66
1:A:202:GLN:HB2	1:A:209:TRP:CH2	2.31	0.66
2:C:135:ALA:CB	2:C:140:LEU:HD11	2.10	0.66
2:D:163:VAL:CG1	2:D:175:ILE:HG13	2.26	0.66
2:B:152:VAL:CG1	2:B:163:VAL:HG23	2.25	0.66
2:C:373:LYS:O	2:C:373:LYS:HD2	1.95	0.66
2:B:136:ILE:HG22	2:B:139:VAL:HB	1.76	0.65
2:D:71:ILE:HG22	2:D:74:GLY:C	2.17	0.65
2:D:71:ILE:HG23	2:D:76:VAL:N	2.11	0.65
2:C:140:LEU:CD2	2:C:343:GLY:HA2	2.16	0.65
2:C:42:GLY:O	2:C:43:VAL:HG12	1.96	0.65
1:A:156:GLU:HB3	1:A:160:ILE:CG2	2.26	0.65
1:A:208:SER:HG	1:A:210:PHE:HE2	1.43	0.65
2:C:361:GLU:HG3	2:C:369:ILE:HG21	1.78	0.65
2:B:134:VAL:O	2:B:375:PHE:HB3	1.97	0.65
2:B:236:LEU:HD12	2:B:237:GLU:CA	2.27	0.65
2:D:190:MET:O	2:D:194:THR:HG23	1.96	0.65
2:C:190:MET:HE2	2:C:209:VAL:HG11	1.78	0.65
2:C:58:ALA:HB1	2:C:65:LEU:HD13	1.78	0.65
2:B:174:ALA:O	2:B:284:LYS:HD2	1.97	0.65
2:C:335:ARG:HB2	2:C:335:ARG:HH11	1.61	0.65
2:D:196:ARG:NH2	2:D:250:ILE:HA	2.11	0.65
2:C:7:ALA:HB1	2:C:347:ALA:HB1	1.78	0.65
2:B:174:ALA:HA	2:B:284:LYS:CD	2.27	0.65
2:B:191:LYS:HA	2:B:191:LYS:HE2	1.79	0.65
2:C:287:VAL:HG23	2:D:244:ASP:CG	2.17	0.65
2:D:36:GLY:HA2	2:D:66:THR:CG2	2.27	0.65
2:C:192:ILE:HB	2:C:256:ARG:HH21	1.61	0.65
2:C:365:SER:CB	2:C:369:ILE:HB	2.26	0.65
2:D:140:LEU:HD23	2:D:343:GLY:HA3	1.77	0.65
2:B:300:SER:HA	2:B:335:ARG:NH1	2.11	0.65
2:D:152:VAL:HG23	2:D:298:VAL:HG12	1.78	0.65
2:B:37:ARG:O	2:B:66:THR:HG22	1.95	0.65
2:D:189:LEU:HA	2:D:192:ILE:CD1	2.27	0.65
2:B:335:ARG:HB2	2:B:335:ARG:HH11	1.62	0.65
1:A:165:CYS:HB2	1:A:255:CYS:SG	2.37	0.65
2:B:97:ALA:HB3	2:B:100:GLU:OE1	1.96	0.65
2:B:21:PHE:HZ	2:B:96:VAL:HG11	1.61	0.65
1:A:243:ILE:HG22	1:A:244:SER:N	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:LEU:CD1	2:B:267:LEU:HD12	2.27	0.65
1:A:180:GLU:O	1:A:184:ILE:CD1	2.44	0.65
2:D:34:ILE:HG23	2:D:69:TYR:CE2	2.32	0.65
2:C:357:ILE:HD11	2:C:375:PHE:O	1.97	0.65
2:C:213:LYS:HA	2:C:217:CYS:SG	2.36	0.65
2:B:35:VAL:HG22	2:B:52:SER:HB2	1.78	0.64
2:D:58:ALA:CA	2:D:61:LYS:HB2	2.27	0.64
2:C:91:TYR:O	2:C:95:ARG:HA	1.96	0.64
2:D:7:ALA:HB1	2:D:356:TRP:CH2	2.31	0.64
2:B:189:LEU:HD12	2:B:189:LEU:O	1.95	0.64
1:A:151:VAL:HG22	1:A:254:ILE:CD1	2.27	0.64
2:C:250:ILE:HD11	2:C:253:GLU:HB2	1.80	0.64
2:C:107:GLU:OE2	2:C:111:ASN:HB3	1.98	0.64
2:C:112:PRO:CD	2:C:115:ASN:HD21	2.10	0.64
2:C:216:LEU:CD2	2:C:250:ILE:HG12	2.26	0.64
2:D:106:THR:HG21	2:D:140:LEU:HD22	1.80	0.64
2:B:132:MET:CE	2:B:134:VAL:HG23	2.28	0.64
2:B:194:THR:HG22	2:B:199:SER:HA	1.80	0.64
2:D:180:LEU:HD12	2:D:184:ASP:HB2	1.78	0.64
2:D:261:LEU:HD21	2:D:303:THR:HG21	1.79	0.64
2:C:133:TYR:HD1	2:C:357:ILE:CD1	2.11	0.64
2:B:73:HIC:CD2	2:B:183:ARG:HH12	2.09	0.64
2:B:112:PRO:HD2	2:B:115:ASN:HD21	1.63	0.64
2:D:335:ARG:HH11	2:D:335:ARG:HB2	1.62	0.64
2:B:132:MET:O	2:B:357:ILE:HB	1.97	0.64
2:D:37:ARG:CG	2:D:38:PRO:HD2	2.27	0.64
2:D:136:ILE:O	2:D:140:LEU:HD13	1.98	0.64
2:C:158:GLY:HA2	2:C:183:ARG:NE	2.12	0.64
2:B:194:THR:HA	2:B:198:TYR:O	1.98	0.64
2:D:109:PRO:HA	2:D:136:ILE:HD11	1.79	0.64
2:D:171:LEU:HD23	2:D:285:CYS:SG	2.37	0.64
2:C:71:ILE:HD11	2:C:85:ILE:HD11	1.80	0.64
2:B:272:CYS:CB	2:B:276:GLU:HB3	2.27	0.64
2:B:104:LEU:HD22	2:B:104:LEU:H	1.63	0.64
2:B:34:ILE:HG13	2:B:67:LEU:CD2	2.14	0.64
2:D:105:LEU:HD11	2:D:123:MET:HE1	1.78	0.64
2:D:120:THR:HA	2:D:132:MET:CE	2.28	0.64
2:D:156:GLY:O	2:D:181:ALA:HB1	1.97	0.64
2:B:158:GLY:HA2	2:B:183:ARG:NE	2.13	0.64
2:C:300:SER:HA	2:C:335:ARG:HD3	1.79	0.64
2:C:27:PRO:HG3	2:C:340:TRP:CG	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:235:SER:O	2:D:238:LYS:HE3	1.98	0.64
1:A:155:TRP:HB3	1:A:250:TRP:HB3	1.79	0.64
2:C:254:ARG:HG2	2:C:254:ARG:HH11	1.63	0.63
2:B:238:LYS:HE3	2:B:254:ARG:HH22	1.63	0.63
2:B:300:SER:H	2:B:304:THR:HG21	1.63	0.63
2:C:298:VAL:HA	2:C:330:ILE:O	1.98	0.63
2:D:91:TYR:O	2:D:95:ARG:HG2	1.98	0.63
2:D:104:LEU:HD22	2:D:104:LEU:N	2.12	0.63
2:C:288:ASP:OD1	2:D:243:PRO:HG2	1.99	0.63
2:C:250:ILE:CD1	2:C:253:GLU:HB2	2.28	0.63
2:C:164:PRO:HB3	2:C:293:LEU:HD23	1.79	0.63
2:D:64:ILE:HG23	2:D:65:LEU:N	2.14	0.63
2:C:104:LEU:HD22	2:C:356:TRP:HH2	1.62	0.63
2:C:54:VAL:HG12	2:C:55:GLY:N	2.14	0.63
2:C:139:VAL:CG1	2:C:140:LEU:HD12	2.28	0.63
2:B:201:THR:HG22	2:B:202:THR:HG23	1.79	0.63
2:D:321:ALA:HB1	2:D:322:PRO:HD2	1.81	0.63
2:D:294:TYR:CE2	2:D:325:MET:HE1	2.34	0.63
2:D:236:LEU:HD12	2:D:237:GLU:N	2.14	0.63
2:B:140:LEU:HD23	2:B:343:GLY:HA2	1.78	0.63
2:C:290:ARG:HA	2:C:293:LEU:HD12	1.80	0.63
2:D:65:LEU:HD11	2:D:67:LEU:HD21	1.81	0.63
2:B:289:ILE:HD12	2:B:293:LEU:HD11	1.81	0.63
2:C:202:THR:HG23	2:C:205:GLU:OE1	1.99	0.63
2:B:12:ASN:HD21	2:B:105:LEU:CD1	2.11	0.63
2:B:82:MET:HE3	2:B:82:MET:CA	2.27	0.63
2:B:111:ASN:OD1	2:B:112:PRO:HD2	1.99	0.63
2:B:186:THR:HG22	2:B:213:LYS:HZ2	1.64	0.63
2:B:7:ALA:HB3	2:B:347:ALA:HB1	1.80	0.63
2:C:288:ASP:HA	2:D:243:PRO:HB2	1.81	0.63
2:B:58:ALA:HB1	2:B:65:LEU:HD13	1.81	0.62
2:D:250:ILE:HG13	2:D:253:GLU:HG3	1.80	0.62
2:D:253:GLU:CA	2:D:256:ARG:HG3	2.28	0.62
2:D:97:ALA:HB1	2:D:99:GLU:CD	2.19	0.62
2:C:65:LEU:HD11	2:C:67:LEU:HD21	1.81	0.62
2:C:358:SER:O	2:C:361:GLU:HG2	1.99	0.62
2:B:21:PHE:HZ	2:B:96:VAL:CG1	2.12	0.62
2:C:153:MET:HG3	2:C:299:LEU:HB3	1.81	0.62
2:C:334:GLU:HA	2:C:334:GLU:OE1	1.99	0.62
2:C:250:ILE:HG13	2:C:251:GLY:N	2.14	0.62
2:B:370:VAL:HG13	2:B:371:HIS:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:GLN:HB3	1:A:211:TRP:CE3	2.34	0.62
2:D:140:LEU:CD2	2:D:343:GLY:HA2	2.27	0.62
2:C:131:ALA:HB1	2:C:357:ILE:O	2.00	0.62
2:D:165:ILE:HG23	2:D:168:GLY:O	1.98	0.62
2:D:152:VAL:CG2	2:D:298:VAL:HB	2.27	0.62
2:C:185:LEU:HD21	2:C:261:LEU:HD11	1.82	0.62
2:B:220:ALA:CB	2:B:226:GLU:HG3	2.23	0.62
2:D:7:ALA:HB2	2:D:356:TRP:CZ2	2.35	0.62
2:B:176:LEU:C	2:B:176:LEU:HD22	2.20	0.62
2:C:71:ILE:N	2:C:71:ILE:HD12	2.14	0.62
2:B:272:CYS:HB3	2:B:276:GLU:HG3	1.81	0.62
1:A:162:LYS:HZ2	1:A:166:LEU:HD21	1.64	0.62
2:C:226:GLU:HA	2:C:226:GLU:OE1	1.98	0.62
2:D:35:VAL:HG12	2:D:68:LYS:HB3	1.79	0.62
2:C:10:VAL:HG22	2:C:104:LEU:O	2.00	0.62
2:D:9:VAL:O	2:D:19:ALA:HA	1.99	0.62
2:C:211:ASP:O	2:C:214:GLU:HG2	2.00	0.62
1:A:209:TRP:CE2	1:A:223:PRO:HG2	2.35	0.62
2:D:120:THR:HG23	2:D:132:MET:CE	2.25	0.62
2:D:192:ILE:HG12	2:D:193:LEU:N	2.13	0.62
2:C:191:LYS:CE	2:C:191:LYS:HA	2.17	0.62
2:B:268:GLY:HA3	2:C:173:HIS:CE1	2.34	0.62
2:D:280:ASN:O	2:D:284:LYS:HG3	1.99	0.61
2:B:161:HIS:CD2	2:B:175:ILE:HD11	2.35	0.61
2:B:43:VAL:HG13	2:B:44:MET:N	2.15	0.61
2:C:294:TYR:CD2	2:C:325:MET:HE1	2.34	0.61
2:D:209:VAL:HA	2:D:212:ILE:HD12	1.82	0.61
2:D:54:VAL:HG13	2:D:58:ALA:CB	2.29	0.61
2:C:208:ILE:O	2:C:212:ILE:HD12	2.00	0.61
1:A:173:PHE:CE2	1:A:237:LEU:HD12	2.35	0.61
2:D:120:THR:HB	2:D:367:PRO:HB3	1.82	0.61
2:D:8:LEU:HD12	2:D:90:PHE:CE1	2.35	0.61
2:C:250:ILE:HD11	2:C:253:GLU:CB	2.30	0.61
2:C:157:ASP:O	2:C:181:ALA:HB3	2.00	0.61
2:C:124:PHE:O	2:C:128:ASN:HA	2.00	0.61
2:D:11:ASP:HA	2:D:106:THR:OG1	2.00	0.61
2:D:299:LEU:HD13	2:D:330:ILE:O	2.00	0.61
2:B:357:ILE:HA	2:B:361:GLU:OE2	2.00	0.61
2:C:165:ILE:CD1	2:C:170:ALA:HA	2.31	0.61
2:D:104:LEU:HD11	2:D:347:ALA:HA	1.81	0.61
2:C:287:VAL:HG23	2:D:244:ASP:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:ILE:HD12	2:B:71:ILE:N	2.14	0.61
2:C:180:LEU:HA	2:C:184:ASP:OD2	1.99	0.61
1:A:162:LYS:NZ	1:A:166:LEU:HD11	2.16	0.61
2:B:150:GLY:HA2	2:B:296:ASN:HB2	1.82	0.61
2:D:295:ALA:O	2:D:328:LYS:HB3	2.00	0.61
2:D:299:LEU:HD23	2:D:309:ILE:HG13	1.83	0.61
2:D:58:ALA:CB	2:D:65:LEU:HD13	2.30	0.61
2:D:71:ILE:HG22	2:D:75:ILE:N	2.16	0.61
2:C:9:VAL:HG11	2:C:343:GLY:HA3	1.81	0.61
2:B:250:ILE:HG13	2:B:254:ARG:HG2	1.80	0.61
2:D:218:TYR:CE1	2:D:255:PHE:HB3	2.35	0.61
2:D:106:THR:HG22	2:D:140:LEU:HD22	1.81	0.61
2:D:50:LYS:HG2	2:D:53:TYR:CE2	2.35	0.61
2:C:92:ASN:O	2:C:95:ARG:HD2	2.01	0.61
1:A:173:PHE:CE1	1:A:198:VAL:HG12	2.35	0.61
1:A:180:GLU:O	1:A:184:ILE:HD12	2.01	0.61
1:A:197:TRP:CZ2	1:A:251:LYS:HB2	2.35	0.61
2:D:120:THR:HA	2:D:132:MET:HE1	1.83	0.61
2:D:369:ILE:O	2:D:369:ILE:HD13	2.01	0.61
2:C:216:LEU:HD21	2:C:250:ILE:CG1	2.30	0.61
2:D:163:VAL:HG12	2:D:175:ILE:HG13	1.82	0.61
2:B:71:ILE:O	2:B:72:GLU:C	2.39	0.61
2:C:351:THR:HG1	2:C:352:PHE:HD1	1.47	0.61
2:C:90:PHE:CD1	2:C:98:PRO:HG3	2.36	0.61
2:C:220:ALA:CB	2:C:226:GLU:HG3	2.31	0.61
2:B:70:PRO:HB3	2:B:78:ASN:ND2	2.15	0.61
2:B:357:ILE:HG23	2:B:361:GLU:CG	2.31	0.61
2:C:166:TYR:CD2	2:C:167:GLU:HG2	2.35	0.61
2:D:191:LYS:HA	2:D:191:LYS:HE3	1.83	0.61
2:B:39:ARG:HH22	2:B:203:THR:HG21	1.64	0.60
2:B:216:LEU:HD21	2:B:250:ILE:CG1	2.31	0.60
2:C:34:ILE:HB	2:C:68:LYS:H	1.65	0.60
2:C:357:ILE:HG23	2:C:361:GLU:OE1	2.00	0.60
2:C:352:PHE:CE2	2:D:45:VAL:HG23	2.36	0.60
2:B:216:LEU:HD21	2:B:250:ILE:HG12	1.82	0.60
2:B:123:MET:O	2:B:127:PHE:HB2	2.01	0.60
2:C:26:ALA:HB1	2:C:27:PRO:HD2	1.82	0.60
2:C:71:ILE:O	2:C:71:ILE:HG22	2.01	0.60
2:C:291:LYS:HA	2:C:325:MET:SD	2.42	0.60
2:B:345:ILE:HG22	2:B:349:LEU:CD1	2.32	0.60
2:B:159:VAL:HG22	2:B:160:THR:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:178:LEU:HD13	2:C:179:ASP:N	2.16	0.60
2:C:17:CYS:HB3	2:C:31:PHE:CE1	2.36	0.60
2:C:314:GLN:HB3	2:C:329:ILE:HD13	1.83	0.60
2:D:308:GLY:HA2	2:D:311:ASP:OD1	2.00	0.60
2:D:82:MET:CE	2:D:85:ILE:HB	2.31	0.60
2:B:71:ILE:O	2:B:71:ILE:HG22	2.01	0.60
2:B:160:THR:HB	2:B:178:LEU:HB3	1.83	0.60
2:C:329:ILE:N	2:C:329:ILE:HD12	2.15	0.60
2:D:216:LEU:HD23	2:D:254:ARG:HG2	1.82	0.60
2:B:317:ILE:CD1	2:B:329:ILE:HD11	2.32	0.60
2:B:155:SER:HB3	2:B:303:THR:HB	1.84	0.60
2:D:189:LEU:HA	2:D:192:ILE:HD11	1.82	0.60
2:D:20:GLY:HA2	2:D:28:ARG:HD3	1.84	0.60
2:D:242:LEU:CG	2:D:243:PRO:HD2	2.31	0.60
2:D:257:CYS:CB	2:D:258:PRO:HD3	2.30	0.60
2:D:39:ARG:NE	2:D:66:THR:HA	2.16	0.60
2:D:304:THR:O	2:D:309:ILE:HD12	2.02	0.60
2:B:124:PHE:O	2:B:128:ASN:HA	2.02	0.60
2:C:155:SER:HB3	2:C:303:THR:HB	1.84	0.60
2:B:103:VAL:C	2:B:356:TRP:HZ3	2.04	0.60
2:C:12:ASN:ND2	2:C:105:LEU:HD12	2.17	0.60
2:D:293:LEU:N	2:D:293:LEU:HD12	2.17	0.60
2:D:133:TYR:HD1	2:D:357:ILE:CD1	2.15	0.60
2:C:167:GLU:OE2	2:D:64:ILE:HG12	2.02	0.60
2:B:317:ILE:HD11	2:B:327:ILE:CG2	2.32	0.60
2:C:178:LEU:HD12	2:C:180:LEU:N	2.16	0.60
2:C:261:LEU:HB3	2:C:274:ILE:HD11	1.83	0.60
2:D:153:MET:CE	2:D:274:ILE:HG21	2.31	0.59
2:B:192:ILE:HG13	2:B:256:ARG:NE	2.16	0.59
2:B:121:GLN:C	2:B:121:GLN:HE21	2.05	0.59
2:D:194:THR:HG22	2:D:200:PHE:H	1.67	0.59
2:D:73:HIC:HA	2:D:183:ARG:HH12	1.67	0.59
2:C:345:ILE:O	2:C:349:LEU:HD12	2.02	0.59
1:A:181:MET:HA	1:A:184:ILE:HD11	1.83	0.59
1:A:190:LEU:HD11	1:A:194:ASN:HD22	1.66	0.59
2:D:332:PRO:HG2	2:D:335:ARG:HH21	1.67	0.59
1:A:156:GLU:HG3	1:A:253:PHE:HE1	1.66	0.59
1:A:195:LYS:CG	1:A:238:LYS:HD2	2.33	0.59
2:D:31:PHE:HB2	2:D:32:PRO:HD2	1.84	0.59
2:C:41:GLN:CG	2:C:42:GLY:H	2.16	0.59
2:C:295:ALA:O	2:C:328:LYS:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:314:GLN:HA	2:C:329:ILE:HD11	1.84	0.59
2:D:264:PRO:CB	2:D:269:MET:HB2	2.32	0.59
2:B:349:LEU:HD22	2:B:352:PHE:CE1	2.37	0.59
2:C:220:ALA:HB2	2:C:226:GLU:HG3	1.85	0.59
2:C:73:HIC:CD2	2:C:183:ARG:NH1	2.45	0.59
2:B:238:LYS:HE3	2:B:254:ARG:NH2	2.18	0.59
2:B:49:GLN:HG2	2:B:50:LYS:H	1.68	0.59
2:D:34:ILE:HG23	2:D:69:TYR:CD2	2.37	0.59
2:D:136:ILE:HG23	2:D:139:VAL:H	1.68	0.59
2:D:18:LYS:N	2:D:18:LYS:HD2	2.17	0.59
2:B:34:ILE:CG1	2:B:54:VAL:HG11	2.29	0.59
1:A:210:PHE:HB3	1:A:214:GLY:HA2	1.83	0.59
1:A:236:TYR:HE2	1:A:245:ASP:HB2	1.64	0.59
2:B:194:THR:HG22	2:B:200:PHE:H	1.67	0.59
2:B:357:ILE:HG13	2:B:361:GLU:OE1	2.03	0.59
1:A:181:MET:CE	1:A:242:LEU:HD12	2.33	0.59
2:D:357:ILE:HG23	2:D:361:GLU:CD	2.22	0.59
2:D:43:VAL:HG22	2:D:44:MET:N	2.14	0.59
2:D:5:ILE:HD13	2:D:5:ILE:N	2.18	0.59
2:D:251:GLY:O	2:D:254:ARG:HG3	2.02	0.59
2:D:97:ALA:HB1	2:D:99:GLU:OE2	2.03	0.59
2:C:104:LEU:CD1	2:C:133:TYR:HB3	2.32	0.59
2:C:71:ILE:O	2:C:72:GLU:C	2.40	0.59
2:B:8:LEU:HB2	2:B:103:VAL:HG13	1.85	0.59
2:D:218:TYR:HE2	2:D:254:ARG:CZ	2.15	0.59
2:C:225:GLN:HA	2:C:225:GLN:OE1	2.02	0.59
2:B:49:GLN:HG2	2:B:50:LYS:N	2.18	0.58
2:D:28:ARG:CZ	2:D:28:ARG:HB3	2.32	0.58
2:C:104:LEU:CD2	2:C:356:TRP:HH2	2.15	0.58
2:B:154:ASP:CG	2:B:300:SER:HB3	2.24	0.58
2:C:176:LEU:CD1	2:C:277:THR:HG23	2.30	0.58
2:D:272:CYS:HB3	2:D:276:GLU:HB3	1.84	0.58
2:B:218:TYR:HD1	2:B:219:VAL:O	1.85	0.58
2:B:32:PRO:HG2	2:B:55:GLY:O	2.02	0.58
2:C:357:ILE:HG23	2:C:361:GLU:CG	2.33	0.58
2:C:357:ILE:HA	2:C:361:GLU:OE1	2.03	0.58
2:B:174:ALA:C	2:B:284:LYS:HD2	2.23	0.58
2:B:189:LEU:HD12	2:B:189:LEU:C	2.24	0.58
2:D:189:LEU:O	2:D:189:LEU:HD13	2.04	0.58
2:D:134:VAL:O	2:D:375:PHE:HB3	2.03	0.58
2:D:97:ALA:HB1	2:D:99:GLU:OE1	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ILE:N	1:A:175:ILE:HD12	2.19	0.58
2:D:26:ALA:HB1	2:D:27:PRO:HD2	1.84	0.58
2:D:261:LEU:H	2:D:261:LEU:HD12	1.68	0.58
2:D:70:PRO:HB3	2:D:78:ASN:HD21	1.66	0.58
2:B:28:ARG:HD3	2:B:94:LEU:CD2	2.33	0.58
2:B:16:MET:CG	2:B:30:VAL:HG22	2.32	0.58
1:A:201:PHE:HD1	1:A:234:CYS:HB3	1.67	0.58
2:C:324:THR:HG23	2:C:325:MET:N	2.19	0.58
2:C:372:ARG:NE	2:C:372:ARG:HA	2.19	0.58
2:D:16:MET:HG2	2:D:30:VAL:HG22	1.84	0.58
2:B:39:ARG:CZ	2:B:66:THR:HA	2.34	0.58
2:C:281:SER:HA	2:C:284:LYS:CD	2.31	0.58
2:C:39:ARG:NH2	2:C:66:THR:HA	2.18	0.58
2:D:106:THR:CG2	2:D:135:ALA:HB3	2.25	0.58
2:B:107:GLU:HG3	2:B:111:ASN:ND2	2.19	0.58
2:C:357:ILE:HG23	2:C:361:GLU:HG3	1.85	0.58
2:B:22:ALA:HB1	2:B:348:SER:HB3	1.86	0.58
2:D:50:LYS:HG3	2:D:53:TYR:CZ	2.38	0.58
2:B:263:GLN:HB2	2:B:266:PHE:CE1	2.38	0.58
2:D:216:LEU:HD23	2:D:254:ARG:CG	2.34	0.58
2:C:11:ASP:CB	2:C:18:LYS:HG2	2.26	0.58
2:D:282:ILE:CG2	2:D:290:ARG:HD3	2.28	0.58
2:B:28:ARG:HH11	2:B:28:ARG:HG2	1.66	0.58
2:C:116:ARG:HD2	2:C:371:HIS:ND1	2.18	0.58
2:B:264:PRO:HB2	2:B:269:MET:HB3	1.86	0.58
2:B:39:ARG:NH2	2:B:203:THR:HG21	2.19	0.57
2:D:362:TYR:CE1	2:D:367:PRO:HG3	2.38	0.57
2:B:269:MET:HG3	2:B:271:SER:OG	2.04	0.57
2:D:316:GLU:OE2	2:D:316:GLU:HA	2.03	0.57
2:B:120:THR:HG22	2:B:362:TYR:CE1	2.39	0.57
2:B:251:GLY:HA2	2:B:254:ARG:CG	2.34	0.57
2:B:255:PHE:O	2:B:258:PRO:HD2	2.03	0.57
1:A:195:LYS:HD2	2:B:118:LYS:HZ1	1.68	0.57
2:C:314:GLN:HG3	2:C:315:LYS:N	2.19	0.57
2:D:330:ILE:HG22	2:D:332:PRO:HD3	1.87	0.57
2:C:164:PRO:HG3	2:C:281:SER:OG	2.04	0.57
2:D:7:ALA:HB2	2:D:356:TRP:HZ2	1.68	0.57
2:C:39:ARG:HH22	2:C:203:THR:CG2	2.09	0.57
2:B:170:ALA:O	2:B:172:PRO:HD3	2.04	0.57
2:C:86:TRP:CZ3	2:C:122:ILE:HG21	2.39	0.57
2:B:250:ILE:HG13	2:B:254:ARG:CG	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:371:HIS:CD2	2:B:372:ARG:HH21	2.22	0.57
2:B:32:PRO:HD2	2:B:55:GLY:CA	2.34	0.57
2:D:250:ILE:O	2:D:250:ILE:HG23	2.04	0.57
2:D:261:LEU:N	2:D:261:LEU:HD12	2.19	0.57
2:B:104:LEU:CD2	2:B:356:TRP:HH2	2.17	0.57
2:B:157:ASP:O	2:B:183:ARG:HG2	2.05	0.57
2:B:300:SER:HA	2:B:335:ARG:HH11	1.69	0.57
2:B:306:TYR:O	2:B:309:ILE:HG23	2.05	0.57
2:C:174:ALA:O	2:C:284:LYS:HD3	2.04	0.57
2:D:236:LEU:HD13	2:D:251:GLY:HA3	1.87	0.57
2:C:34:ILE:HG23	2:C:69:TYR:CE2	2.39	0.57
2:C:139:VAL:HG13	2:C:140:LEU:HD12	1.84	0.57
2:C:314:GLN:HE21	2:C:315:LYS:HA	1.68	0.57
2:B:103:VAL:O	2:B:356:TRP:HZ3	1.87	0.57
2:B:34:ILE:C	2:B:54:VAL:HG21	2.25	0.57
2:C:316:GLU:HA	2:C:316:GLU:OE2	2.05	0.57
2:B:11:ASP:HB3	2:B:18:LYS:HG2	1.86	0.57
2:C:208:ILE:HD11	2:C:243:PRO:CG	2.35	0.57
2:B:335:ARG:NH1	2:B:335:ARG:HB2	2.20	0.57
2:C:270:GLU:HA	2:C:270:GLU:OE1	2.04	0.57
2:B:357:ILE:HG23	2:B:361:GLU:HG3	1.87	0.57
2:B:34:ILE:HG23	2:B:69:TYR:CE2	2.40	0.57
2:D:180:LEU:HD11	2:D:185:LEU:HD23	1.85	0.57
2:D:54:VAL:CA	2:D:58:ALA:HB2	2.31	0.57
1:A:162:LYS:HZ2	1:A:166:LEU:HD11	1.69	0.57
1:A:199:GLY:HA3	1:A:211:TRP:HE3	1.68	0.56
1:A:233:ILE:HG12	1:A:247:CYS:H	1.70	0.56
2:D:104:LEU:CD2	2:D:356:TRP:HH2	2.18	0.56
2:D:282:ILE:HG22	2:D:283:MET:N	2.21	0.56
2:D:335:ARG:NH1	2:D:335:ARG:HB2	2.20	0.56
2:B:12:ASN:ND2	2:B:105:LEU:HD12	2.19	0.56
2:C:16:MET:SD	2:C:30:VAL:HG22	2.45	0.56
2:B:65:LEU:HD11	2:B:67:LEU:HD23	1.86	0.56
2:B:39:ARG:HG2	2:B:66:THR:HB	1.86	0.56
2:D:37:ARG:N	2:D:66:THR:HG22	2.15	0.56
2:D:70:PRO:CB	2:D:78:ASN:HD21	2.18	0.56
2:D:41:GLN:HG3	2:D:42:GLY:N	2.13	0.56
2:D:35:VAL:HA	2:D:54:VAL:CG2	2.35	0.56
2:C:10:VAL:HG21	2:C:105:LEU:HD13	1.86	0.56
2:D:139:VAL:CG1	2:D:140:LEU:HD12	2.27	0.56
2:B:208:ILE:HD13	2:B:242:LEU:CD1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:122:ILE:HG23	2:C:126:THR:CG2	2.36	0.56
2:C:308:GLY:HA2	2:C:311:ASP:OD1	2.05	0.56
1:A:205:ILE:HG23	1:A:206:SER:H	1.70	0.56
2:C:5:ILE:N	2:C:5:ILE:HD13	2.20	0.56
1:A:181:MET:CA	1:A:184:ILE:CD1	2.74	0.56
2:D:61:LYS:HB3	2:D:65:LEU:CD2	2.29	0.56
2:B:192:ILE:N	2:B:192:ILE:HD13	2.19	0.56
2:B:256:ARG:HG3	2:B:257:CYS:N	2.19	0.56
2:C:112:PRO:HD2	2:C:115:ASN:HD21	1.71	0.56
2:B:180:LEU:HD12	2:B:184:ASP:CB	2.35	0.56
2:B:373:LYS:O	2:B:373:LYS:HD2	2.04	0.56
2:D:176:LEU:CD2	2:D:277:THR:HG23	2.19	0.56
2:B:253:GLU:CA	2:B:256:ARG:HG2	2.21	0.56
2:B:32:PRO:HD2	2:B:55:GLY:C	2.26	0.56
2:D:32:PRO:HG2	2:D:55:GLY:O	2.06	0.56
2:C:54:VAL:HG12	2:C:55:GLY:H	1.69	0.56
2:B:150:GLY:CA	2:B:296:ASN:HB2	2.35	0.56
2:B:68:LYS:HD2	2:B:69:TYR:H	1.68	0.56
2:C:254:ARG:HG2	2:C:254:ARG:NH1	2.19	0.56
2:C:335:ARG:HB2	2:C:335:ARG:NH1	2.20	0.56
2:C:176:LEU:HD22	2:C:176:LEU:C	2.26	0.56
2:C:216:LEU:HD21	2:C:250:ILE:HG12	1.88	0.56
2:B:161:HIS:HD2	2:B:175:ILE:HD11	1.71	0.56
2:B:32:PRO:HB2	2:B:34:ILE:CD1	2.36	0.56
1:A:187:ILE:HD11	1:A:254:ILE:CD1	2.36	0.56
2:D:185:LEU:CD1	2:D:258:PRO:HA	2.35	0.56
2:D:233:SER:CB	2:D:236:LEU:HG	2.34	0.56
2:D:11:ASP:OD2	2:D:340:TRP:HA	2.06	0.56
2:C:300:SER:HA	2:C:335:ARG:NH1	2.21	0.56
2:D:300:SER:HB3	2:D:335:ARG:NH1	2.20	0.55
2:B:192:ILE:H	2:B:192:ILE:CD1	2.18	0.55
1:A:175:ILE:HA	1:A:180:GLU:OE1	2.06	0.55
2:C:313:MET:O	2:C:317:ILE:HG12	2.05	0.55
2:D:103:VAL:O	2:D:132:MET:HA	2.06	0.55
2:D:209:VAL:HG12	2:D:210:ARG:N	2.21	0.55
2:C:259:GLU:OE1	2:C:259:GLU:HA	2.04	0.55
2:B:261:LEU:HD21	2:B:303:THR:CG2	2.36	0.55
2:B:28:ARG:HH11	2:B:28:ARG:CG	2.20	0.55
2:D:122:ILE:HG23	2:D:126:THR:HG22	1.89	0.55
2:D:357:ILE:HD12	2:D:357:ILE:N	2.21	0.55
2:C:357:ILE:HD13	2:C:370:VAL:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:PRO:HB3	2:B:78:ASN:HD21	1.71	0.55
2:B:27:PRO:HG3	2:B:340:TRP:CD2	2.41	0.55
2:B:362:TYR:CE1	2:B:367:PRO:HG3	2.42	0.55
1:A:151:VAL:HG22	1:A:187:ILE:HD11	1.88	0.55
2:D:76:VAL:HG11	2:D:79:TRP:CZ3	2.42	0.55
2:D:81:ASP:O	2:D:84:LYS:HB2	2.07	0.55
2:C:163:VAL:CG1	2:C:175:ILE:HG13	2.14	0.55
2:B:37:ARG:HG3	2:B:38:PRO:CD	2.31	0.55
2:B:97:ALA:HB1	2:B:99:GLU:OE1	2.07	0.55
1:A:195:LYS:HE2	1:A:236:TYR:CE1	2.41	0.55
2:D:185:LEU:HD21	2:D:261:LEU:HD11	1.88	0.55
2:D:220:ALA:HB1	2:D:226:GLU:CG	2.34	0.55
2:D:176:LEU:O	2:D:176:LEU:HD22	2.06	0.55
1:A:184:ILE:O	1:A:187:ILE:N	2.32	0.55
2:D:158:GLY:HA3	2:D:183:ARG:CZ	2.37	0.55
2:B:151:ILE:HB	2:B:293:LEU:HD23	1.89	0.55
1:A:190:LEU:HD13	1:A:190:LEU:C	2.27	0.55
2:D:133:TYR:HA	2:D:357:ILE:HD13	1.88	0.55
2:B:317:ILE:HD11	2:B:327:ILE:HG21	1.88	0.55
2:B:317:ILE:HD12	2:B:327:ILE:CG1	2.35	0.55
1:A:218:LEU:CD1	1:A:221:LEU:HD22	2.37	0.55
2:C:43:VAL:HG13	2:C:44:MET:N	2.14	0.55
2:C:314:GLN:NE2	2:C:315:LYS:HA	2.21	0.55
2:C:222:ASP:HB2	2:C:225:GLN:HB3	1.89	0.55
2:B:29:ALA:HB1	2:B:93:GLU:OE1	2.07	0.55
2:C:41:GLN:HG3	2:C:42:GLY:N	2.22	0.55
2:B:196:ARG:HH21	2:B:250:ILE:HA	1.71	0.55
2:D:216:LEU:HD22	2:D:250:ILE:HD13	1.89	0.55
1:A:170:ALA:HB1	1:A:255:CYS:HB3	1.89	0.55
2:B:251:GLY:HA2	2:B:254:ARG:HG3	1.89	0.54
1:A:195:LYS:HD3	1:A:251:LYS:HE2	1.88	0.54
1:A:222:LEU:HB3	1:A:223:PRO:HD2	1.89	0.54
2:B:110:LEU:CD2	2:D:195:GLU:HA	2.36	0.54
2:D:357:ILE:HG23	2:D:361:GLU:CG	2.37	0.54
2:D:151:ILE:HG23	2:D:297:THR:HG22	1.89	0.54
2:D:28:ARG:HB3	2:D:28:ARG:HH11	1.70	0.54
2:C:304:THR:O	2:C:309:ILE:HD12	2.07	0.54
2:C:108:ALA:O	2:C:111:ASN:HB2	2.07	0.54
2:C:314:GLN:HE21	2:C:315:LYS:CA	2.19	0.54
2:D:287:VAL:HG13	2:D:288:ASP:N	2.22	0.54
2:D:274:ILE:O	2:D:278:THR:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:314:GLN:HG3	2:D:315:LYS:N	2.22	0.54
2:B:79:TRP:CE2	2:B:118:LYS:HG3	2.43	0.54
2:D:123:MET:HB2	2:D:132:MET:SD	2.47	0.54
2:D:57:GLU:O	2:D:61:LYS:HB2	2.07	0.54
2:C:353:GLN:HA	2:C:356:TRP:HD1	1.72	0.54
2:D:82:MET:HE3	2:D:85:ILE:HB	1.89	0.54
2:B:104:LEU:HD22	2:B:356:TRP:HH2	1.72	0.54
2:B:358:SER:H	2:B:361:GLU:CD	2.10	0.54
2:C:104:LEU:HD11	2:C:347:ALA:HA	1.89	0.54
2:C:306:TYR:O	2:C:309:ILE:HG23	2.07	0.54
2:C:108:ALA:HB1	2:C:109:PRO:HD2	1.89	0.54
1:A:196:TYR:O	1:A:236:TYR:HB2	2.07	0.54
2:D:118:LYS:O	2:D:121:GLN:HG3	2.08	0.54
2:D:35:VAL:CG1	2:D:68:LYS:HB2	2.37	0.54
2:C:38:PRO:HB3	2:C:64:ILE:CD1	2.37	0.54
2:C:370:VAL:HG13	2:C:371:HIS:N	2.23	0.54
2:D:139:VAL:HG12	2:D:140:LEU:N	2.22	0.54
2:B:241:GLU:HA	2:B:247:VAL:HA	1.89	0.54
2:B:35:VAL:HG12	2:B:68:LYS:HB3	1.88	0.54
2:D:86:TRP:CD2	2:D:123:MET:HE3	2.43	0.54
2:C:34:ILE:C	2:C:54:VAL:HG21	2.28	0.54
2:C:120:THR:HG22	2:C:362:TYR:CD1	2.42	0.54
2:C:43:VAL:CG1	2:C:44:MET:H	2.09	0.54
2:C:174:ALA:HA	2:C:284:LYS:HD3	1.90	0.54
2:D:121:GLN:HE21	2:D:122:ILE:N	2.06	0.54
2:D:106:THR:HA	2:D:135:ALA:HB3	1.89	0.54
1:A:135:SER:HB2	1:A:136:PRO:CD	2.37	0.54
2:D:151:ILE:O	2:D:151:ILE:HG23	2.06	0.54
2:D:367:PRO:O	2:D:370:VAL:HG12	2.07	0.54
2:C:318:THR:HG22	2:C:327:ILE:HG13	1.89	0.54
1:A:178:LYS:HG3	1:A:179:GLU:N	2.23	0.54
2:D:293:LEU:CD1	2:D:293:LEU:H	2.20	0.54
2:B:238:LYS:O	2:B:250:ILE:HG23	2.08	0.54
2:D:7:ALA:HB1	2:D:347:ALA:HB1	1.87	0.54
2:D:104:LEU:HD13	2:D:356:TRP:CZ3	2.43	0.54
2:B:208:ILE:CD1	2:B:243:PRO:HG2	2.35	0.54
2:C:94:LEU:O	2:C:96:VAL:HG13	2.08	0.54
2:D:8:LEU:HB2	2:D:103:VAL:CG2	2.22	0.54
2:B:250:ILE:HG12	2:B:254:ARG:HG2	1.90	0.53
2:D:180:LEU:HD12	2:D:181:ALA:H	1.72	0.53
2:D:8:LEU:CG	2:D:103:VAL:HG22	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:38:PRO:HD3	2:C:49:GLN:OE1	2.08	0.53
2:B:299:LEU:HD22	2:B:331:ALA:HB2	1.90	0.53
2:C:335:ARG:CZ	2:C:335:ARG:HB3	2.34	0.53
2:B:345:ILE:HG22	2:B:349:LEU:HD12	1.90	0.53
2:C:349:LEU:HD23	2:C:352:PHE:CD1	2.43	0.53
2:C:321:ALA:HB1	2:C:322:PRO:CD	2.38	0.53
1:A:181:MET:HE1	1:A:237:LEU:HD21	1.89	0.53
2:D:210:ARG:HD2	2:D:214:GLU:OE1	2.08	0.53
2:D:39:ARG:HE	2:D:66:THR:CA	2.21	0.53
2:B:162:THR:O	2:B:175:ILE:HG13	2.07	0.53
2:B:192:ILE:HB	2:B:256:ARG:NH2	2.22	0.53
1:A:200:VAL:CG2	1:A:209:TRP:HB3	2.38	0.53
2:D:192:ILE:HG21	2:D:256:ARG:CD	2.39	0.53
2:B:155:SER:OG	2:B:160:THR:HG23	2.08	0.53
2:C:39:ARG:CZ	2:C:66:THR:HA	2.38	0.53
2:C:151:ILE:O	2:C:151:ILE:HG23	2.08	0.53
2:B:105:LEU:O	2:B:134:VAL:HA	2.09	0.53
2:D:6:ALA:O	2:D:102:PRO:HD2	2.09	0.53
2:D:230:ALA:HA	2:D:233:SER:OG	2.08	0.53
2:C:190:MET:HG3	2:C:209:VAL:HG21	1.90	0.53
2:C:172:PRO:O	2:C:175:ILE:HG22	2.09	0.53
1:A:152:PHE:HD2	1:A:154:ARG:H	1.55	0.53
1:A:154:ARG:NE	2:D:231:ALA:HB1	2.24	0.53
2:D:54:VAL:O	2:D:57:GLU:HG2	2.09	0.53
2:D:50:LYS:HB3	2:D:53:TYR:CE1	2.43	0.53
2:B:217:CYS:HB3	2:B:258:PRO:HG3	1.89	0.53
2:B:104:LEU:CD2	2:B:356:TRP:CH2	2.92	0.53
2:B:195:GLU:CA	2:C:110:LEU:HD11	2.25	0.53
2:C:133:TYR:HA	2:C:357:ILE:CD1	2.39	0.53
2:B:335:ARG:CZ	2:B:335:ARG:HB3	2.35	0.53
2:B:107:GLU:HG3	2:B:111:ASN:HD22	1.73	0.53
2:B:7:ALA:CB	2:B:356:TRP:CZ2	2.92	0.53
2:D:157:ASP:O	2:D:183:ARG:HB2	2.09	0.53
2:C:238:LYS:HE2	2:C:254:ARG:NH1	2.23	0.53
2:C:357:ILE:CD1	2:C:370:VAL:HG23	2.39	0.53
2:D:140:LEU:HB3	2:D:343:GLY:N	2.24	0.53
2:D:360:GLN:OE1	2:D:360:GLN:HA	2.07	0.53
2:B:108:ALA:HB1	2:B:109:PRO:HD2	1.91	0.53
2:B:120:THR:HG22	2:B:367:PRO:HB3	1.90	0.53
2:B:217:CYS:HB2	2:B:306:TYR:HE2	1.73	0.53
1:A:157:MET:HG2	1:A:160:ILE:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LYS:HG2	1:A:238:LYS:HD2	1.91	0.53
2:C:287:VAL:CG2	2:D:244:ASP:H	2.22	0.53
2:D:45:VAL:O	2:D:45:VAL:HG13	2.09	0.53
2:D:274:ILE:O	2:D:277:THR:HB	2.09	0.53
2:B:109:PRO:HA	2:B:136:ILE:HD11	1.90	0.53
2:B:126:THR:HG23	2:B:127:PHE:CD2	2.43	0.53
1:A:154:ARG:CD	2:D:231:ALA:HA	2.39	0.53
2:C:223:PHE:O	2:C:227:MET:HG2	2.09	0.53
2:C:38:PRO:HG2	2:C:49:GLN:HE22	1.73	0.53
2:C:10:VAL:O	2:C:10:VAL:HG23	2.07	0.53
1:A:227:GLN:O	1:A:228:ARG:HB2	2.09	0.53
2:B:104:LEU:HD11	2:B:347:ALA:HA	1.91	0.52
2:D:104:LEU:CD1	2:D:356:TRP:CH2	2.92	0.52
2:C:38:PRO:CG	2:C:49:GLN:HE22	2.22	0.52
2:C:369:ILE:C	2:C:369:ILE:HD13	2.29	0.52
2:C:9:VAL:HG11	2:C:343:GLY:CA	2.39	0.52
2:B:293:LEU:HD12	2:B:293:LEU:N	2.23	0.52
2:B:216:LEU:CD2	2:B:250:ILE:HD11	2.39	0.52
2:C:287:VAL:O	2:C:290:ARG:HG3	2.09	0.52
2:D:158:GLY:HA2	2:D:183:ARG:NE	2.24	0.52
2:D:75:ILE:O	2:D:77:THR:N	2.41	0.52
2:C:49:GLN:HG2	2:C:50:LYS:N	2.24	0.52
2:C:158:GLY:HA2	2:C:183:ARG:HE	1.73	0.52
1:A:238:LYS:HB3	1:A:243:ILE:CD1	2.36	0.52
2:C:34:ILE:HA	2:C:68:LYS:O	2.09	0.52
2:C:21:PHE:HZ	2:C:96:VAL:HG11	1.75	0.52
2:D:373:LYS:HD2	2:D:373:LYS:O	2.08	0.52
2:D:278:THR:HG21	2:D:313:MET:HE2	1.90	0.52
2:D:278:THR:CG2	2:D:313:MET:HE1	2.35	0.52
2:B:219:VAL:HG13	2:B:220:ALA:N	2.23	0.52
1:A:184:ILE:O	1:A:187:ILE:HB	2.10	0.52
2:D:242:LEU:HD12	2:D:243:PRO:CD	2.40	0.52
2:D:365:SER:OG	2:D:369:ILE:HB	2.10	0.52
2:C:7:ALA:HB3	2:C:22:ALA:CB	2.38	0.52
2:D:291:LYS:HA	2:D:325:MET:SD	2.49	0.52
2:B:136:ILE:HG22	2:B:139:VAL:CG1	2.40	0.52
2:B:118:LYS:HD2	2:B:122:ILE:CD1	2.39	0.52
2:D:180:LEU:HD13	2:D:267:LEU:HD11	1.92	0.52
2:D:99:GLU:O	2:D:130:PRO:HG3	2.09	0.52
2:C:104:LEU:CD1	2:C:356:TRP:CH2	2.93	0.52
2:B:176:LEU:N	2:B:176:LEU:HD13	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:VAL:HA	2:B:290:ARG:CG	2.39	0.52
2:C:213:LYS:HD3	2:C:214:GLU:N	2.24	0.52
2:B:259:GLU:OE1	2:B:259:GLU:HA	2.09	0.52
2:B:104:LEU:CD1	2:B:356:TRP:CH2	2.92	0.52
2:C:287:VAL:HA	2:D:244:ASP:HB3	1.92	0.52
2:D:57:GLU:H	2:D:57:GLU:CD	2.12	0.52
2:B:151:ILE:HG23	2:B:151:ILE:O	2.10	0.52
2:B:236:LEU:HD12	2:B:237:GLU:HA	1.91	0.52
2:B:216:LEU:HD21	2:B:250:ILE:HD11	1.92	0.52
2:C:10:VAL:HA	2:C:19:ALA:HB2	1.90	0.52
2:C:361:GLU:OE1	2:C:369:ILE:HD12	2.10	0.52
2:C:99:GLU:O	2:C:130:PRO:HD3	2.09	0.52
2:C:311:ASP:O	2:C:314:GLN:HG3	2.10	0.52
2:D:263:GLN:HB2	2:D:266:PHE:CE1	2.44	0.52
1:A:198:VAL:HG23	1:A:200:VAL:HG12	1.91	0.52
2:C:287:VAL:HG23	2:D:244:ASP:CA	2.39	0.52
2:D:155:SER:HB3	2:D:303:THR:HB	1.91	0.52
2:D:86:TRP:CE2	2:D:123:MET:HE1	2.44	0.52
2:D:49:GLN:HG2	2:D:50:LYS:N	2.25	0.52
2:B:70:PRO:HG3	2:B:81:ASP:CB	2.39	0.52
2:D:104:LEU:CD2	2:D:356:TRP:CH2	2.93	0.51
2:B:11:ASP:CB	2:B:18:LYS:HG2	2.39	0.51
2:B:357:ILE:HA	2:B:361:GLU:CD	2.30	0.51
1:A:152:PHE:CD1	1:A:253:PHE:CZ	2.98	0.51
2:D:118:LYS:HE3	2:D:122:ILE:HD11	1.92	0.51
2:D:253:GLU:H	2:D:253:GLU:CD	2.13	0.51
2:D:71:ILE:CG2	2:D:75:ILE:N	2.73	0.51
2:D:86:TRP:CH2	2:D:123:MET:HE1	2.45	0.51
2:C:361:GLU:HA	2:C:364:GLU:HG2	1.92	0.51
2:C:365:SER:HB2	2:C:369:ILE:HB	1.92	0.51
2:C:90:PHE:O	2:C:94:LEU:HB2	2.10	0.51
2:C:81:ASP:HA	2:C:84:LYS:HD3	1.92	0.51
2:B:6:ALA:O	2:B:102:PRO:HD2	2.09	0.51
2:D:105:LEU:HD11	2:D:123:MET:HE2	1.88	0.51
2:D:250:ILE:CG1	2:D:253:GLU:HG2	2.35	0.51
2:D:166:TYR:HD2	2:D:167:GLU:CG	2.14	0.51
2:B:189:LEU:O	2:B:192:ILE:HD13	2.10	0.51
2:C:104:LEU:CD2	2:C:356:TRP:CH2	2.93	0.51
2:D:26:ALA:HB1	2:D:27:PRO:CD	2.41	0.51
2:D:171:LEU:HD12	2:D:172:PRO:HD2	1.93	0.51
2:B:358:SER:N	2:B:361:GLU:HG2	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:MET:N	1:A:160:ILE:HG22	2.25	0.51
1:A:151:VAL:CG2	1:A:187:ILE:HD11	2.41	0.51
1:A:202:GLN:HE22	1:A:232:GLN:HG3	1.75	0.51
2:C:212:ILE:HG23	2:C:216:LEU:HD13	1.92	0.51
2:C:216:LEU:HD21	2:C:250:ILE:HG13	1.91	0.51
2:B:261:LEU:HD23	2:B:274:ILE:HD11	1.91	0.51
2:B:3:ASP:CG	2:B:4:ASP:H	2.14	0.51
2:D:314:GLN:CA	2:D:329:ILE:HD11	2.40	0.51
2:B:34:ILE:CG2	2:B:69:TYR:CZ	2.94	0.51
2:D:259:GLU:OE1	2:D:262:PHE:HB2	2.10	0.51
2:C:189:LEU:HD13	2:C:189:LEU:O	2.11	0.51
2:C:176:LEU:HD11	2:C:277:THR:HG22	1.92	0.51
2:C:186:THR:O	2:C:189:LEU:HB3	2.10	0.51
2:B:289:ILE:HG13	2:B:290:ARG:N	2.26	0.51
2:B:317:ILE:CD1	2:B:327:ILE:HG12	2.35	0.51
2:C:79:TRP:CG	2:C:118:LYS:HE2	2.45	0.51
2:B:361:GLU:O	2:B:365:SER:HB2	2.11	0.51
2:C:165:ILE:HD12	2:C:170:ALA:HA	1.93	0.51
2:D:213:LYS:NZ	4:D:401:ADP:O2'	2.36	0.51
2:D:167:GLU:C	2:D:169:TYR:H	2.13	0.51
2:C:40:HIS:O	2:C:41:GLN:HB3	2.10	0.51
2:B:263:GLN:HB2	2:B:266:PHE:CD1	2.46	0.51
2:B:113:LYS:HG2	2:B:371:HIS:CE1	2.46	0.51
2:B:190:MET:HE3	2:B:206:ARG:HB2	1.92	0.51
2:B:24:ASP:HB2	2:B:340:TRP:HH2	1.75	0.51
1:A:151:VAL:HG13	1:A:196:TYR:CE2	2.46	0.51
2:D:217:CYS:HA	2:D:254:ARG:HB3	1.92	0.51
2:C:34:ILE:CG2	2:C:69:TYR:CZ	2.94	0.51
2:B:152:VAL:HG23	2:B:298:VAL:O	2.11	0.51
2:B:282:ILE:HG13	2:B:294:TYR:CE2	2.46	0.51
2:C:332:PRO:HG2	2:C:335:ARG:NH2	2.10	0.51
2:B:180:LEU:HD13	2:B:267:LEU:CD1	2.39	0.51
2:B:192:ILE:HB	2:B:256:ARG:CZ	2.40	0.50
2:B:37:ARG:HB2	2:B:51:ASP:O	2.11	0.50
1:A:155:TRP:CD1	1:A:252:TYR:CZ	2.99	0.50
2:D:242:LEU:HD12	2:D:243:PRO:HD3	1.92	0.50
2:D:7:ALA:CB	2:D:356:TRP:CZ2	2.94	0.50
2:C:238:LYS:HE2	2:C:254:ARG:NH2	2.26	0.50
2:B:176:LEU:CD2	2:B:277:THR:CG2	2.86	0.50
2:B:317:ILE:HD11	2:B:329:ILE:CD1	2.38	0.50
2:C:14:SER:HA	2:C:71:ILE:CG2	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:143:TYR:CE2	2:D:45:VAL:HG21	2.37	0.50
2:B:88:HIS:NE2	2:B:93:GLU:HG3	2.26	0.50
2:D:34:ILE:CG2	2:D:69:TYR:CZ	2.94	0.50
2:B:167:GLU:O	2:B:167:GLU:HG3	2.11	0.50
2:C:176:LEU:CG	2:C:277:THR:HG23	2.42	0.50
2:C:5:ILE:H	2:C:5:ILE:HD13	1.76	0.50
1:A:154:ARG:HD3	2:D:231:ALA:C	2.32	0.50
1:A:187:ILE:HD11	1:A:254:ILE:HD11	1.92	0.50
2:B:126:THR:HG23	2:B:127:PHE:N	2.27	0.50
2:D:104:LEU:HD22	2:D:356:TRP:HH2	1.77	0.50
2:D:54:VAL:HG12	2:D:55:GLY:N	2.26	0.50
2:B:158:GLY:HA2	2:B:183:ARG:CD	2.42	0.50
2:C:332:PRO:CG	2:C:335:ARG:HH21	2.12	0.50
2:C:122:ILE:O	2:C:126:THR:HG22	2.10	0.50
2:C:328:LYS:C	2:C:329:ILE:HD12	2.31	0.50
2:B:223:PHE:CD1	2:B:259:GLU:HG2	2.46	0.50
1:A:155:TRP:CH2	2:B:117:GLU:CB	2.95	0.50
2:B:123:MET:HA	2:B:127:PHE:HD2	1.76	0.50
2:C:149:THR:HG22	2:C:166:TYR:HA	1.94	0.50
2:D:7:ALA:CB	2:D:356:TRP:CH2	2.93	0.50
2:D:70:PRO:CB	2:D:78:ASN:ND2	2.73	0.50
2:C:34:ILE:CG2	2:C:69:TYR:CE2	2.95	0.50
2:C:34:ILE:HG12	2:C:54:VAL:HG13	1.91	0.50
2:B:300:SER:CA	2:B:335:ARG:HD3	2.40	0.50
2:D:314:GLN:N	2:D:329:ILE:HD11	2.26	0.50
2:B:236:LEU:CD1	2:B:237:GLU:HG2	2.41	0.50
2:B:36:GLY:HA2	2:B:66:THR:HG23	1.94	0.50
1:A:233:ILE:HG12	1:A:246:LYS:C	2.32	0.50
2:D:53:TYR:HD1	2:D:53:TYR:N	2.09	0.50
2:D:43:VAL:O	2:D:44:MET:HB3	2.10	0.50
2:B:45:VAL:HG13	2:B:45:VAL:O	2.11	0.50
2:B:11:ASP:OD2	2:B:340:TRP:HA	2.12	0.50
1:A:195:LYS:HG3	1:A:238:LYS:HD2	1.92	0.50
2:D:50:LYS:HG2	2:D:53:TYR:CD2	2.47	0.50
1:A:163:LYS:O	1:A:166:LEU:HB2	2.11	0.50
2:D:16:MET:CG	2:D:30:VAL:HG22	2.41	0.50
2:D:317:ILE:CD1	2:D:327:ILE:HG21	2.42	0.50
2:B:216:LEU:CD2	2:B:254:ARG:HA	2.41	0.50
2:B:133:TYR:CE1	2:B:355:MET:CG	2.94	0.50
2:D:180:LEU:HG	2:D:181:ALA:N	2.27	0.50
2:D:261:LEU:H	2:D:261:LEU:CD1	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:134:VAL:CG2	2:D:370:VAL:HG21	2.32	0.50
2:D:65:LEU:HD12	2:D:66:THR:O	2.12	0.50
1:A:226:ARG:HG3	1:A:227:GLN:H	1.76	0.50
2:B:37:ARG:H	2:B:66:THR:CG2	2.24	0.50
2:D:193:LEU:HD13	2:D:200:PHE:CE1	2.47	0.50
2:D:218:TYR:CE2	2:D:254:ARG:CZ	2.95	0.50
2:D:305:MET:HG3	4:D:401:ADP:C5	2.45	0.50
2:D:34:ILE:CG2	2:D:69:TYR:CE1	2.95	0.50
2:C:107:GLU:O	2:C:137:GLN:HG3	2.11	0.50
2:C:176:LEU:CD2	2:C:277:THR:HG23	2.41	0.50
2:C:79:TRP:CD2	2:C:118:LYS:HG2	2.46	0.50
2:D:176:LEU:C	2:D:176:LEU:HD22	2.32	0.50
2:D:34:ILE:HA	2:D:68:LYS:O	2.12	0.50
2:D:107:GLU:CD	2:D:111:ASN:HB3	2.32	0.50
2:B:305:MET:HG3	4:B:401:ADP:C5	2.45	0.50
2:B:236:LEU:C	2:B:236:LEU:HD12	2.32	0.49
1:A:195:LYS:HG2	1:A:238:LYS:CD	2.42	0.49
2:D:104:LEU:HG	2:D:347:ALA:HB2	1.94	0.49
2:D:216:LEU:HD21	2:D:254:ARG:HG2	1.92	0.49
2:C:54:VAL:O	2:C:57:GLU:HG2	2.11	0.49
2:B:332:PRO:HD2	2:B:335:ARG:NE	2.27	0.49
2:C:180:LEU:HD12	2:C:184:ASP:HB2	1.94	0.49
2:C:3:ASP:HB3	2:C:4:ASP:OD1	2.12	0.49
2:D:335:ARG:HB3	2:D:335:ARG:CZ	2.35	0.49
2:C:58:ALA:O	2:C:61:LYS:HB3	2.11	0.49
2:C:120:THR:CG2	2:C:362:TYR:CD1	2.95	0.49
2:D:148:THR:HG22	2:D:149:THR:HG23	1.94	0.49
2:B:265:SER:HA	2:B:269:MET:O	2.12	0.49
2:B:249:THR:HG22	2:B:250:ILE:N	2.26	0.49
1:A:195:LYS:CG	1:A:236:TYR:CE1	2.96	0.49
2:D:190:MET:HE3	2:D:209:VAL:HG11	1.93	0.49
2:D:70:PRO:HB3	2:D:78:ASN:CG	2.33	0.49
2:C:190:MET:HE2	2:C:209:VAL:CG1	2.41	0.49
2:B:242:LEU:HD12	2:B:243:PRO:CD	2.41	0.49
2:B:223:PHE:CE1	2:B:259:GLU:HG2	2.47	0.49
2:D:88:HIS:O	2:D:92:ASN:HB2	2.12	0.49
2:D:313:MET:O	2:D:317:ILE:HG12	2.12	0.49
2:B:358:SER:O	2:B:361:GLU:HG2	2.11	0.49
1:A:154:ARG:CD	2:D:231:ALA:CA	2.91	0.49
2:C:192:ILE:O	2:C:195:GLU:HG3	2.13	0.49
2:D:140:LEU:N	2:D:140:LEU:HD12	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:305:MET:HG3	4:C:401:ADP:N6	2.26	0.49
2:B:92:ASN:N	2:B:92:ASN:HD22	2.10	0.49
2:B:120:THR:HG22	2:B:362:TYR:HE1	1.77	0.49
2:B:190:MET:HE1	2:B:209:VAL:HG12	1.94	0.49
2:D:40:HIS:O	2:D:41:GLN:HB3	2.12	0.49
2:D:152:VAL:HG23	2:D:298:VAL:C	2.33	0.49
2:D:50:LYS:CG	2:D:53:TYR:CZ	2.95	0.49
2:B:54:VAL:HA	2:B:58:ALA:CB	2.41	0.49
1:A:245:ASP:CG	1:A:246:LYS:H	2.15	0.49
2:D:34:ILE:HG21	2:D:69:TYR:CZ	2.47	0.49
2:D:70:PRO:O	2:D:77:THR:N	2.42	0.49
2:C:349:LEU:CD2	2:C:352:PHE:CD1	2.95	0.49
2:B:41:GLN:CG	2:B:42:GLY:H	2.25	0.49
2:B:190:MET:HE1	2:B:209:VAL:CG1	2.42	0.49
2:B:216:LEU:CD2	2:B:250:ILE:HG12	2.42	0.49
2:B:7:ALA:HB2	2:B:356:TRP:CZ2	2.47	0.49
2:B:94:LEU:HB3	2:B:96:VAL:HG13	1.94	0.49
2:C:282:ILE:HD12	2:C:290:ARG:HD3	1.95	0.49
2:B:299:LEU:HD12	2:B:299:LEU:N	2.28	0.49
2:C:341:ILE:HG22	2:C:345:ILE:CD1	2.43	0.49
2:B:214:GLU:HG2	2:B:215:LYS:N	2.27	0.49
2:B:259:GLU:HG3	2:B:266:PHE:CZ	2.47	0.49
2:B:104:LEU:CD2	2:B:347:ALA:CB	2.91	0.49
2:B:369:ILE:C	2:B:369:ILE:HD13	2.33	0.49
1:A:155:TRP:NE1	1:A:252:TYR:CZ	2.81	0.49
2:D:8:LEU:N	2:D:8:LEU:HD23	2.28	0.49
2:D:92:ASN:HD22	2:D:92:ASN:N	2.10	0.49
2:B:28:ARG:NH1	2:B:28:ARG:HB3	2.28	0.49
2:B:35:VAL:N	2:B:54:VAL:HG21	2.27	0.49
1:A:150:TYR:CE2	1:A:152:PHE:HA	2.47	0.49
2:C:192:ILE:HB	2:C:256:ARG:CZ	2.43	0.49
2:C:104:LEU:HD13	2:C:356:TRP:CH2	2.47	0.49
2:B:14:SER:HA	2:B:71:ILE:CG2	2.39	0.49
1:A:173:PHE:HD1	1:A:254:ILE:O	1.96	0.49
2:B:117:GLU:CD	2:B:368:SER:HB3	2.33	0.49
2:C:169:TYR:OH	2:D:40:HIS:HB3	2.12	0.49
2:B:71:ILE:CD1	2:B:71:ILE:H	2.23	0.49
2:B:41:GLN:HG3	2:B:42:GLY:N	2.28	0.49
2:B:44:MET:HG3	2:B:45:VAL:N	2.27	0.49
2:B:32:PRO:HB2	2:B:34:ILE:HD13	1.94	0.48
1:A:218:LEU:CD1	1:A:220:ASP:H	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:305:MET:HG3	4:C:401:ADP:C5	2.45	0.48
2:C:9:VAL:CG2	2:C:104:LEU:HD23	2.08	0.48
2:B:148:THR:HG23	2:B:167:GLU:HA	1.94	0.48
2:B:184:ASP:HB3	2:B:267:LEU:HD13	1.94	0.48
2:B:357:ILE:HG23	2:B:361:GLU:CD	2.34	0.48
2:C:285:CYS:HB3	2:C:289:ILE:CG1	2.43	0.48
2:C:286:ASP:O	2:C:289:ILE:HG12	2.12	0.48
2:D:133:TYR:CD1	2:D:357:ILE:CD1	2.95	0.48
2:C:196:ARG:HH22	2:C:250:ILE:CA	2.22	0.48
2:B:329:ILE:N	2:B:329:ILE:HD12	2.28	0.48
1:A:171:SER:O	1:A:255:CYS:HA	2.13	0.48
2:D:162:THR:HG23	2:D:277:THR:HG21	1.94	0.48
2:B:129:THR:HG23	2:B:131:ALA:N	2.29	0.48
2:B:190:MET:HE2	2:B:209:VAL:HG11	1.95	0.48
2:B:190:MET:SD	2:B:206:ARG:HA	2.52	0.48
2:D:180:LEU:HD12	2:D:181:ALA:N	2.28	0.48
2:D:34:ILE:HG21	2:D:69:TYR:CE1	2.49	0.48
2:C:353:GLN:HA	2:C:356:TRP:CD1	2.48	0.48
2:D:152:VAL:CG2	2:D:298:VAL:HG12	2.44	0.48
2:B:264:PRO:HG2	2:B:271:SER:O	2.13	0.48
2:B:17:CYS:HB3	2:B:31:PHE:CE1	2.49	0.48
2:B:104:LEU:CD2	2:B:347:ALA:HB2	2.43	0.48
2:D:120:THR:CG2	2:D:132:MET:HE2	2.29	0.48
2:C:208:ILE:HG22	2:C:212:ILE:CD1	2.43	0.48
2:C:11:ASP:HB3	2:C:18:LYS:CE	2.31	0.48
2:C:351:THR:OG1	2:C:352:PHE:HD1	1.96	0.48
2:D:264:PRO:HG2	2:D:271:SER:O	2.13	0.48
2:B:133:TYR:CE1	2:B:355:MET:HG2	2.48	0.48
2:B:53:TYR:HD1	2:B:53:TYR:N	2.12	0.48
2:D:279:PHE:CZ	2:D:283:MET:CE	2.97	0.48
2:B:21:PHE:N	2:B:21:PHE:CD1	2.82	0.48
2:B:216:LEU:HD21	2:B:250:ILE:CD1	2.43	0.48
2:C:289:ILE:O	2:C:293:LEU:HD12	2.14	0.48
2:D:105:LEU:HD21	2:D:123:MET:HE2	1.96	0.48
2:C:104:LEU:HD13	2:C:133:TYR:CB	2.43	0.48
2:C:8:LEU:H	2:C:103:VAL:HA	1.79	0.48
2:D:163:VAL:O	2:D:163:VAL:HG23	2.14	0.48
2:B:163:VAL:CG1	2:B:175:ILE:HD12	2.43	0.48
2:D:43:VAL:HG13	2:D:44:MET:N	2.29	0.48
2:B:129:THR:HG23	2:B:131:ALA:H	1.77	0.48
1:A:156:GLU:CG	1:A:253:PHE:CE1	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:148:THR:HG22	2:B:149:THR:N	2.26	0.48
2:B:362:TYR:CD1	2:B:367:PRO:HA	2.49	0.48
2:D:120:THR:HA	2:D:132:MET:SD	2.54	0.48
2:D:189:LEU:HA	2:D:192:ILE:HD13	1.95	0.48
2:C:193:LEU:HD13	2:C:200:PHE:CE1	2.48	0.48
2:C:65:LEU:HD23	2:C:65:LEU:C	2.33	0.48
2:C:332:PRO:HD2	2:C:335:ARG:NE	2.28	0.48
2:C:349:LEU:HB3	2:C:352:PHE:HB2	1.95	0.48
2:B:240:TYR:O	2:B:247:VAL:HG23	2.14	0.48
2:D:153:MET:HE3	2:D:274:ILE:HG21	1.94	0.48
2:D:180:LEU:HD11	2:D:185:LEU:HD22	1.93	0.48
2:C:299:LEU:HD12	2:C:299:LEU:N	2.28	0.48
2:B:211:ASP:O	2:B:215:LYS:HG3	2.13	0.48
2:B:136:ILE:HG22	2:B:139:VAL:CB	2.44	0.47
2:B:35:VAL:CG1	2:B:68:LYS:HB2	2.31	0.47
2:C:294:TYR:CG	2:C:325:MET:CE	2.97	0.47
2:D:86:TRP:CE3	2:D:122:ILE:HG21	2.48	0.47
2:D:126:THR:HG23	2:D:127:PHE:CD2	2.49	0.47
2:D:244:ASP:OD2	2:D:246:GLN:HG3	2.14	0.47
2:D:185:LEU:HD21	2:D:261:LEU:CD1	2.44	0.47
2:D:305:MET:HG3	4:D:401:ADP:N6	2.26	0.47
2:C:198:TYR:CE1	2:C:248:ILE:HG22	2.49	0.47
2:C:27:PRO:HG3	2:C:340:TRP:CB	2.43	0.47
2:D:148:THR:HG22	2:D:167:GLU:HA	1.90	0.47
2:B:121:GLN:HE21	2:B:122:ILE:N	2.12	0.47
2:B:103:VAL:O	2:B:132:MET:HA	2.13	0.47
2:B:39:ARG:HH22	2:B:203:THR:CG2	2.26	0.47
2:B:190:MET:CE	2:B:209:VAL:HG11	2.44	0.47
1:A:198:VAL:HG22	1:A:235:GLY:C	2.34	0.47
2:D:137:GLN:HB3	2:D:339:VAL:CG1	2.40	0.47
2:C:335:ARG:CB	2:C:335:ARG:CZ	2.91	0.47
2:C:176:LEU:N	2:C:176:LEU:HD13	2.29	0.47
2:C:81:ASP:O	2:C:84:LYS:HB2	2.13	0.47
2:B:365:SER:CB	2:B:369:ILE:HB	2.44	0.47
1:A:173:PHE:CE2	1:A:237:LEU:CD1	2.96	0.47
2:D:211:ASP:OD1	2:D:215:LYS:HD2	2.14	0.47
2:D:8:LEU:O	2:D:104:LEU:HD23	2.14	0.47
2:C:34:ILE:HG22	2:C:69:TYR:CG	2.49	0.47
2:C:358:SER:H	2:C:361:GLU:HG2	1.78	0.47
2:D:163:VAL:HG12	2:D:175:ILE:CG1	2.43	0.47
2:C:153:MET:O	2:C:299:LEU:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:309:ILE:HG12	2:B:310:ALA:N	2.30	0.47
2:B:31:PHE:N	2:B:31:PHE:CD1	2.82	0.47
2:B:61:LYS:HB3	2:B:64:ILE:HG22	1.97	0.47
2:B:69:TYR:CD1	2:B:69:TYR:N	2.83	0.47
2:C:148:THR:HG22	2:C:167:GLU:HA	1.97	0.47
2:D:122:ILE:HG22	2:D:123:MET:N	2.28	0.47
2:B:159:VAL:HG22	2:B:160:THR:H	1.77	0.47
2:B:181:ALA:O	2:B:185:LEU:HD23	2.15	0.47
2:B:212:ILE:HG23	2:B:216:LEU:HD13	1.96	0.47
2:B:26:ALA:HB1	2:B:27:PRO:HD2	1.97	0.47
2:B:34:ILE:N	2:B:34:ILE:HD13	2.30	0.47
2:B:369:ILE:HG23	2:B:370:VAL:N	2.29	0.47
2:D:104:LEU:CD2	2:D:347:ALA:CB	2.92	0.47
2:C:362:TYR:CE1	2:C:367:PRO:HG3	2.50	0.47
2:D:152:VAL:HA	2:D:298:VAL:H	1.78	0.47
2:D:53:TYR:N	2:D:53:TYR:CD1	2.81	0.47
2:D:263:GLN:O	2:D:266:PHE:HD1	1.96	0.47
2:C:73:HIC:HA	2:C:183:ARG:HH12	1.78	0.47
2:B:39:ARG:HH21	2:B:66:THR:HA	1.79	0.47
2:B:209:VAL:O	2:B:212:ILE:HB	2.14	0.47
2:B:104:LEU:HD13	2:B:356:TRP:CZ3	2.50	0.47
1:A:195:LYS:HG2	1:A:236:TYR:CE1	2.50	0.47
2:D:65:LEU:CD1	2:D:67:LEU:HD23	2.44	0.47
2:B:305:MET:HG3	4:B:401:ADP:N6	2.26	0.47
2:B:163:VAL:HG12	2:B:175:ILE:HD12	1.95	0.47
2:B:287:VAL:HG13	2:B:288:ASP:N	2.28	0.47
2:C:94:LEU:O	2:C:95:ARG:HB2	2.14	0.47
2:C:303:THR:HG22	2:C:303:THR:O	2.15	0.47
2:C:359:LYS:HE2	2:C:359:LYS:HB2	1.50	0.47
2:B:120:THR:HA	2:B:132:MET:SD	2.55	0.47
2:B:16:MET:HG3	2:B:31:PHE:O	2.14	0.47
2:D:120:THR:HG22	2:D:124:PHE:CD2	2.50	0.47
2:C:104:LEU:HG	2:C:347:ALA:HB2	1.96	0.47
2:C:345:ILE:HG22	2:C:349:LEU:CD1	2.44	0.47
2:C:264:PRO:HG2	2:C:271:SER:O	2.15	0.47
2:B:104:LEU:CG	2:B:347:ALA:HB2	2.42	0.47
2:B:53:TYR:CD1	2:B:53:TYR:N	2.83	0.47
1:A:231:GLY:O	1:A:232:GLN:HB3	2.15	0.47
2:C:164:PRO:HB3	2:C:293:LEU:HD21	1.95	0.47
2:D:303:THR:O	2:D:303:THR:HG22	2.15	0.47
2:C:206:ARG:HG3	2:C:207:GLU:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:8:LEU:HD23	2:C:101:HIS:HB3	1.96	0.47
2:C:163:VAL:O	2:C:163:VAL:HG23	2.15	0.47
2:B:176:LEU:HD23	2:B:177:ARG:O	2.14	0.47
2:C:13:GLY:HA3	2:C:18:LYS:NZ	2.29	0.47
2:B:264:PRO:CB	2:B:269:MET:HB3	2.45	0.47
2:B:120:THR:HG21	2:B:367:PRO:HB3	1.96	0.47
1:A:197:TRP:CE2	1:A:251:LYS:CB	2.94	0.47
2:B:152:VAL:HG23	2:B:298:VAL:C	2.35	0.47
2:B:190:MET:O	2:B:194:THR:HG23	2.15	0.46
1:A:195:LYS:HD2	1:A:251:LYS:HE3	1.93	0.46
2:D:79:TRP:CE2	2:D:118:LYS:HG2	2.50	0.46
2:D:192:ILE:O	2:D:195:GLU:HG3	2.15	0.46
2:D:166:TYR:O	2:D:167:GLU:HG3	2.15	0.46
2:C:176:LEU:H	2:C:176:LEU:HD13	1.79	0.46
2:C:129:THR:OG1	2:C:130:PRO:HD2	2.15	0.46
2:D:264:PRO:HB2	2:D:269:MET:HB2	1.96	0.46
1:A:158:TRP:CG	1:A:234:CYS:SG	3.06	0.46
1:A:195:LYS:HG2	1:A:236:TYR:HE1	1.81	0.46
1:A:218:LEU:HD12	1:A:221:LEU:HD22	1.96	0.46
1:A:238:LYS:HB2	1:A:243:ILE:HD12	1.97	0.46
1:A:156:GLU:CG	1:A:253:PHE:HE1	2.29	0.46
2:D:190:MET:HG2	2:D:209:VAL:HG21	1.96	0.46
2:D:94:LEU:HB3	2:D:96:VAL:HG13	1.98	0.46
2:B:152:VAL:HA	2:B:298:VAL:O	2.16	0.46
2:C:184:ASP:HB3	2:C:267:LEU:CD1	2.46	0.46
2:C:242:LEU:HD12	2:C:242:LEU:HA	1.72	0.46
2:C:219:VAL:HG22	2:C:220:ALA:N	2.30	0.46
2:D:282:ILE:HG23	2:D:290:ARG:CD	2.34	0.46
2:D:294:TYR:CD1	2:D:327:ILE:CD1	2.94	0.46
2:B:206:ARG:HG3	2:B:206:ARG:HH11	1.81	0.46
2:B:370:VAL:HG13	2:B:371:HIS:H	1.81	0.46
2:B:79:TRP:CD2	2:B:118:LYS:HG3	2.49	0.46
2:C:280:ASN:O	2:C:284:LYS:HG3	2.16	0.46
2:D:122:ILE:O	2:D:126:THR:HG22	2.16	0.46
2:D:160:THR:HB	2:D:178:LEU:HB3	1.98	0.46
2:D:205:GLU:HA	2:D:208:ILE:HG13	1.97	0.46
2:B:149:THR:HG22	2:B:167:GLU:H	1.80	0.46
2:B:133:TYR:HE2	2:B:135:ALA:HB2	1.81	0.46
2:B:216:LEU:CD2	2:B:254:ARG:HG2	2.20	0.46
2:B:36:GLY:H	2:B:52:SER:CB	2.15	0.46
2:C:58:ALA:HB1	2:C:65:LEU:HD12	1.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:LEU:HD11	2:B:329:ILE:HG23	1.96	0.46
2:D:290:ARG:CA	2:D:293:LEU:HD13	2.44	0.46
2:D:133:TYR:HD1	2:D:357:ILE:HD13	1.81	0.46
2:D:242:LEU:CD1	2:D:243:PRO:HD2	2.45	0.46
2:C:113:LYS:CG	2:C:371:HIS:CD2	2.97	0.46
2:B:184:ASP:HB3	2:B:267:LEU:CD1	2.45	0.46
2:D:113:LYS:HB2	2:D:371:HIS:CD2	2.51	0.46
2:D:272:CYS:HB3	2:D:276:GLU:CB	2.46	0.46
2:B:8:LEU:HD23	2:B:101:HIS:HB2	1.98	0.46
2:C:287:VAL:CG2	2:D:244:ASP:N	2.76	0.46
2:C:120:THR:HG22	2:C:362:TYR:CE1	2.50	0.46
2:B:152:VAL:CG1	2:B:163:VAL:CG2	2.94	0.46
2:C:18:LYS:N	2:C:18:LYS:HD3	2.30	0.46
2:B:82:MET:CE	2:B:82:MET:HA	2.33	0.46
2:C:152:VAL:HG23	2:C:298:VAL:HB	1.97	0.46
2:D:158:GLY:CA	2:D:183:ARG:CZ	2.94	0.46
2:D:185:LEU:HD11	2:D:261:LEU:CD1	2.46	0.46
2:D:78:ASN:ND2	2:D:81:ASP:OD2	2.49	0.46
2:C:362:TYR:HE1	2:C:367:PRO:CG	2.29	0.46
2:B:176:LEU:HD21	2:B:277:THR:HG23	1.95	0.46
2:D:5:ILE:H	2:D:5:ILE:HD13	1.78	0.46
2:B:194:THR:O	2:C:110:LEU:HD13	2.16	0.46
2:B:216:LEU:CD2	2:B:250:ILE:CD1	2.94	0.46
2:B:53:TYR:O	2:B:54:VAL:HB	2.16	0.46
2:B:148:THR:O	2:B:165:ILE:HG22	2.16	0.46
2:D:321:ALA:HB1	2:D:322:PRO:CD	2.45	0.46
2:B:70:PRO:HG3	2:B:81:ASP:HB2	1.97	0.46
2:C:73:HIC:C	2:C:75:ILE:H	2.28	0.46
2:B:7:ALA:HB2	2:B:356:TRP:HZ2	1.81	0.46
1:A:156:GLU:HB2	1:A:161:SER:HB3	1.98	0.46
1:A:174:GLN:C	1:A:175:ILE:HD12	2.36	0.46
1:A:202:GLN:HG2	1:A:207:GLY:HA2	1.98	0.46
2:C:361:GLU:CG	2:C:369:ILE:HG21	2.44	0.46
2:B:140:LEU:CD2	2:B:343:GLY:HA2	2.46	0.46
1:A:199:GLY:HA3	1:A:211:TRP:CE3	2.49	0.46
2:B:117:GLU:OE2	2:B:368:SER:HB3	2.16	0.46
2:D:180:LEU:CD2	2:D:261:LEU:HA	2.46	0.46
2:C:247:VAL:HG13	2:C:248:ILE:N	2.30	0.46
2:D:136:ILE:CG2	2:D:139:VAL:HB	2.39	0.46
2:D:349:LEU:HD22	2:D:352:PHE:CE1	2.48	0.46
2:B:107:GLU:OE1	2:B:116:ARG:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:VAL:HG12	2:B:140:LEU:HD12	1.97	0.45
2:B:50:LYS:HG2	2:B:53:TYR:CZ	2.51	0.45
2:B:8:LEU:CD1	2:B:94:LEU:CD1	2.89	0.45
2:D:118:LYS:HD2	2:D:121:GLN:CG	2.46	0.45
2:D:129:THR:OG1	2:D:130:PRO:HD2	2.16	0.45
2:D:185:LEU:HD11	2:D:261:LEU:HD11	1.98	0.45
2:D:58:ALA:HB1	2:D:65:LEU:HD11	1.96	0.45
2:C:253:GLU:HA	2:C:256:ARG:HG2	1.97	0.45
2:B:328:LYS:C	2:B:329:ILE:HD12	2.37	0.45
2:D:143:TYR:HE1	2:D:345:ILE:HG21	1.79	0.45
2:B:303:THR:O	2:B:303:THR:HG22	2.15	0.45
2:C:314:GLN:CB	2:C:329:ILE:CD1	2.95	0.45
2:D:299:LEU:CD2	2:D:309:ILE:CG1	2.95	0.45
2:C:286:ASP:H	2:C:289:ILE:HD11	1.81	0.45
2:C:104:LEU:CD2	2:C:347:ALA:CB	2.91	0.45
2:C:10:VAL:HG21	2:C:105:LEU:CD1	2.46	0.45
2:B:335:ARG:CB	2:B:335:ARG:CZ	2.91	0.45
2:B:81:ASP:O	2:B:84:LYS:HB2	2.15	0.45
2:B:31:PHE:HB2	2:B:32:PRO:HD2	1.97	0.45
2:D:126:THR:HG23	2:D:127:PHE:N	2.32	0.45
2:D:186:THR:CG2	2:D:213:LYS:HZ1	2.29	0.45
2:D:11:ASP:CB	2:D:18:LYS:HD3	2.21	0.45
2:D:314:GLN:HA	2:D:329:ILE:HD11	1.99	0.45
1:A:152:PHE:CG	1:A:253:PHE:CE1	3.04	0.45
2:C:317:ILE:O	2:C:320:LEU:HB2	2.16	0.45
2:D:120:THR:OG1	2:D:370:VAL:HG11	2.16	0.45
2:B:313:MET:O	2:B:317:ILE:HG12	2.16	0.45
2:C:299:LEU:N	2:C:299:LEU:CD1	2.80	0.45
1:A:162:LYS:HD3	1:A:166:LEU:HD21	1.98	0.45
2:B:257:CYS:HB3	2:B:258:PRO:CD	2.37	0.45
1:A:202:GLN:HE22	1:A:232:GLN:HE21	1.64	0.45
1:A:195:LYS:CD	1:A:236:TYR:CE1	2.99	0.45
2:C:190:MET:O	2:C:194:THR:HG23	2.17	0.45
2:C:50:LYS:HG2	2:C:53:TYR:CZ	2.52	0.45
2:B:293:LEU:H	2:B:293:LEU:CD1	2.27	0.45
2:B:173:HIS:CE1	2:D:268:GLY:HA3	2.52	0.45
2:D:162:THR:CG2	2:D:277:THR:CG2	2.95	0.45
2:D:329:ILE:C	2:D:330:ILE:HG13	2.36	0.45
2:B:238:LYS:HD2	2:B:254:ARG:NH1	2.32	0.45
2:C:290:ARG:CA	2:C:293:LEU:HD12	2.45	0.45
2:D:34:ILE:HG13	2:D:67:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:223:PHE:CD1	2:C:259:GLU:HG3	2.51	0.45
2:C:218:TYR:O	2:C:255:PHE:HA	2.17	0.45
2:C:362:TYR:HE1	2:C:367:PRO:CB	2.28	0.45
2:D:144:ALA:HB2	2:D:341:ILE:HG22	1.99	0.45
2:C:13:GLY:HA3	2:C:16:MET:O	2.17	0.45
2:C:341:ILE:HG22	2:C:345:ILE:HD11	1.97	0.45
2:B:41:GLN:HG3	2:B:42:GLY:H	1.81	0.45
2:D:335:ARG:CB	2:D:335:ARG:CZ	2.91	0.45
2:B:189:LEU:CD1	2:B:193:LEU:CD1	2.95	0.45
2:B:28:ARG:CD	2:B:94:LEU:CD2	2.94	0.45
1:A:195:LYS:CG	1:A:238:LYS:CD	2.94	0.45
1:A:156:GLU:CD	1:A:253:PHE:CE1	2.90	0.45
2:D:113:LYS:HB2	2:D:371:HIS:CG	2.52	0.45
2:B:201:THR:CG2	2:B:202:THR:CG2	2.95	0.45
2:D:335:ARG:O	2:D:338:SER:HB3	2.17	0.45
2:B:133:TYR:CE1	2:B:355:MET:HG3	2.52	0.45
1:A:158:TRP:HD1	1:A:197:TRP:HB3	1.81	0.45
1:A:202:GLN:NE2	1:A:232:GLN:HG3	2.32	0.45
1:A:218:LEU:CD1	1:A:221:LEU:CD2	2.95	0.45
1:A:198:VAL:HG11	1:A:237:LEU:HG	1.98	0.45
1:A:153:GLU:CD	2:D:236:LEU:HD11	2.36	0.45
2:C:104:LEU:N	2:C:104:LEU:CD2	2.80	0.45
2:C:107:GLU:CG	2:C:111:ASN:HD22	2.30	0.45
2:B:321:ALA:HB1	2:B:322:PRO:CD	2.44	0.45
2:D:151:ILE:O	2:D:297:THR:HA	2.16	0.45
2:B:236:LEU:HD12	2:B:237:GLU:HG2	1.99	0.45
1:A:152:PHE:CE2	1:A:154:ARG:HB2	2.52	0.45
1:A:232:GLN:O	1:A:233:ILE:HG23	2.16	0.45
1:A:238:LYS:CB	1:A:243:ILE:CD1	2.95	0.45
1:A:155:TRP:CZ3	2:B:117:GLU:OE1	2.69	0.45
2:D:203:THR:HA	2:D:206:ARG:HG3	1.99	0.45
2:D:54:VAL:CG1	2:D:58:ALA:CB	2.94	0.45
2:C:133:TYR:CD1	2:C:357:ILE:CD1	2.95	0.45
2:D:106:THR:CG2	2:D:140:LEU:CD2	2.93	0.45
2:D:3:ASP:CG	2:D:4:ASP:H	2.20	0.45
2:B:124:PHE:CE2	2:B:132:MET:HG2	2.52	0.45
2:B:7:ALA:HB1	2:B:356:TRP:CZ2	2.51	0.45
1:A:200:VAL:HG22	1:A:209:TRP:HE3	1.82	0.45
1:A:197:TRP:NE1	1:A:251:LYS:HB2	2.30	0.45
2:D:103:VAL:CG1	2:D:105:LEU:CD2	2.95	0.45
2:D:193:LEU:HA	2:D:193:LEU:HD23	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:104:LEU:HD22	2:C:356:TRP:CH2	2.48	0.45
2:D:371:HIS:HD2	2:D:372:ARG:NE	2.15	0.45
2:C:5:ILE:HG13	2:C:102:PRO:HG2	1.99	0.45
2:C:359:LYS:HG3	2:C:360:GLN:N	2.31	0.45
2:D:332:PRO:HA	2:D:333:PRO:HD3	1.51	0.44
2:D:86:TRP:CE2	2:D:123:MET:CE	2.99	0.44
2:D:155:SER:CB	2:D:303:THR:HB	2.47	0.44
2:B:175:ILE:HG23	2:B:175:ILE:O	2.16	0.44
2:C:154:ASP:HA	2:C:300:SER:HB2	1.98	0.44
2:B:13:GLY:O	2:B:71:ILE:HG21	2.17	0.44
2:C:79:TRP:CD1	2:C:118:LYS:HE2	2.51	0.44
2:C:178:LEU:HD21	2:C:271:SER:OG	2.17	0.44
2:C:99:GLU:HA	2:C:128:ASN:O	2.17	0.44
2:C:29:ALA:HB1	2:C:93:GLU:HG2	1.99	0.44
2:B:189:LEU:HD11	2:B:193:LEU:CD1	2.47	0.44
2:B:94:LEU:HD23	2:B:94:LEU:HA	1.66	0.44
1:A:218:LEU:CD1	1:A:220:ASP:CB	2.95	0.44
1:A:237:LEU:HA	1:A:237:LEU:HD23	1.64	0.44
2:B:110:LEU:CD2	2:D:195:GLU:CA	2.95	0.44
2:D:21:PHE:HD1	2:D:28:ARG:NE	2.15	0.44
2:C:249:THR:HG22	2:C:250:ILE:N	2.32	0.44
2:C:13:GLY:O	2:C:71:ILE:HG21	2.17	0.44
2:C:71:ILE:CD1	2:C:85:ILE:HD11	2.46	0.44
2:B:180:LEU:CD1	2:B:267:LEU:CD1	2.93	0.44
2:B:37:ARG:H	2:B:66:THR:HG22	1.81	0.44
2:D:223:PHE:HB2	2:D:259:GLU:OE2	2.17	0.44
2:C:218:TYR:CE2	2:C:254:ARG:CZ	2.94	0.44
2:C:53:TYR:CD1	2:C:53:TYR:N	2.85	0.44
2:C:61:LYS:HE3	2:C:64:ILE:CG2	2.41	0.44
2:C:64:ILE:HD13	2:C:64:ILE:O	2.18	0.44
2:D:247:VAL:HG13	2:D:247:VAL:O	2.16	0.44
2:B:190:MET:CE	2:B:209:VAL:CG1	2.96	0.44
2:B:32:PRO:HB2	2:B:34:ILE:HD11	2.00	0.44
2:D:216:LEU:HD22	2:D:250:ILE:CD1	2.47	0.44
2:D:349:LEU:HB3	2:D:352:PHE:HB2	1.99	0.44
2:D:221:LEU:N	2:D:221:LEU:HD22	2.27	0.44
2:D:264:PRO:HB3	2:D:269:MET:HB2	1.99	0.44
2:D:290:ARG:O	2:D:294:TYR:HD2	2.00	0.44
2:D:306:TYR:O	2:D:309:ILE:HD13	2.18	0.44
2:B:135:ALA:HB1	2:B:140:LEU:HD11	1.95	0.44
2:B:58:ALA:HB1	2:B:65:LEU:CD1	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:8:LEU:HG	2:D:103:VAL:HG22	1.99	0.44
2:D:120:THR:HG22	2:D:124:PHE:CE2	2.53	0.44
2:D:362:TYR:HE1	2:D:367:PRO:HG3	1.78	0.44
2:D:72:GLU:C	2:D:74:GLY:H	2.21	0.44
2:C:193:LEU:HD23	2:C:193:LEU:HA	1.67	0.44
2:D:151:ILE:CG2	2:D:297:THR:HG22	2.47	0.44
2:D:306:TYR:HB2	2:D:309:ILE:HG23	1.99	0.44
2:D:68:LYS:HD3	2:D:69:TYR:N	2.32	0.44
2:C:218:TYR:O	2:C:258:PRO:HG2	2.17	0.44
2:C:305:MET:CG	4:C:401:ADP:C6	2.83	0.44
2:C:26:ALA:HB1	2:C:27:PRO:CD	2.47	0.44
2:B:20:GLY:HA2	2:B:28:ARG:CD	2.46	0.44
1:A:195:LYS:HE2	1:A:236:TYR:OH	2.16	0.44
1:A:158:TRP:CD1	1:A:234:CYS:SG	3.09	0.44
2:B:110:LEU:CD2	2:D:195:GLU:HB2	2.43	0.44
2:C:169:TYR:CZ	2:D:40:HIS:HB3	2.52	0.44
2:C:358:SER:H	2:C:361:GLU:CD	2.21	0.44
2:C:86:TRP:CE3	2:C:122:ILE:HG21	2.51	0.44
2:C:151:ILE:O	2:C:297:THR:HA	2.17	0.44
2:D:294:TYR:CD1	2:D:327:ILE:HD11	2.53	0.44
2:B:104:LEU:HD13	2:B:356:TRP:CH2	2.52	0.44
2:B:251:GLY:C	2:B:254:ARG:HG3	2.38	0.44
2:B:36:GLY:HA2	2:B:66:THR:O	2.18	0.44
1:A:150:TYR:HE2	1:A:152:PHE:HA	1.83	0.44
1:A:152:PHE:HE2	1:A:154:ARG:HB2	1.82	0.44
1:A:157:MET:H	1:A:160:ILE:CG2	2.30	0.44
2:D:357:ILE:HA	2:D:361:GLU:OE2	2.18	0.44
2:D:364:GLU:CG	2:D:365:SER:N	2.81	0.44
2:D:36:GLY:N	2:D:54:VAL:CG2	2.81	0.44
2:D:143:TYR:OH	2:D:349:LEU:HD11	2.17	0.44
2:C:121:GLN:HG3	2:C:122:ILE:H	1.78	0.44
2:B:99:GLU:O	2:B:130:PRO:HG3	2.18	0.44
1:A:155:TRP:N	1:A:155:TRP:CD1	2.85	0.44
1:A:151:VAL:HG21	1:A:187:ILE:CD1	2.47	0.44
1:A:200:VAL:HG23	1:A:210:PHE:O	2.17	0.44
2:D:99:GLU:HG3	2:D:128:ASN:OD1	2.17	0.44
2:D:2:ASP:HB3	2:D:3:ASP:H	1.44	0.44
2:D:317:ILE:CD1	2:D:327:ILE:CG2	2.96	0.43
2:B:7:ALA:CB	2:B:356:TRP:CH2	2.98	0.43
2:D:103:VAL:HG12	2:D:105:LEU:HD23	2.00	0.43
2:D:305:MET:HE2	4:D:401:ADP:N6	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:VAL:HA	2:B:290:ARG:HG3	2.00	0.43
2:C:220:ALA:HB1	2:C:226:GLU:CG	2.48	0.43
1:A:226:ARG:HG3	1:A:227:GLN:N	2.33	0.43
2:D:153:MET:HE1	2:D:274:ILE:HG21	1.98	0.43
2:D:191:LYS:HA	2:D:191:LYS:CE	2.49	0.43
2:D:62:ARG:O	2:D:65:LEU:HD23	2.18	0.43
2:C:236:LEU:HD12	2:C:237:GLU:CA	2.48	0.43
2:C:362:TYR:HE1	2:C:367:PRO:HG3	1.83	0.43
2:C:113:LYS:CG	2:C:371:HIS:NE2	2.81	0.43
2:B:152:VAL:HG23	2:B:298:VAL:CB	2.49	0.43
2:B:345:ILE:HG22	2:B:349:LEU:HD11	1.99	0.43
2:B:43:VAL:O	2:B:44:MET:HB3	2.18	0.43
2:B:194:THR:CG2	2:B:200:PHE:H	2.30	0.43
2:B:357:ILE:N	2:B:357:ILE:HD12	2.32	0.43
2:C:112:PRO:CG	2:C:115:ASN:HD21	2.31	0.43
2:C:34:ILE:HG21	2:C:69:TYR:CZ	2.54	0.43
2:C:358:SER:H	2:C:361:GLU:CG	2.31	0.43
2:D:107:GLU:HG2	2:D:111:ASN:HB2	2.00	0.43
2:B:149:THR:HG23	2:B:167:GLU:H	1.80	0.43
2:B:176:LEU:CD2	2:B:277:THR:HG21	2.33	0.43
2:B:279:PHE:O	2:B:282:ILE:HG22	2.19	0.43
2:D:346:LEU:HA	2:D:349:LEU:CD1	2.41	0.43
1:A:170:ALA:HA	1:A:257:LYS:HG2	2.00	0.43
2:C:297:THR:HG1	2:C:329:ILE:HA	1.83	0.43
2:D:161:HIS:NE2	2:D:177:ARG:CD	2.81	0.43
2:B:36:GLY:N	2:B:54:VAL:CG2	2.81	0.43
2:D:208:ILE:HD13	2:D:243:PRO:CD	2.48	0.43
2:D:39:ARG:HE	2:D:66:THR:CB	2.32	0.43
2:C:7:ALA:HB2	2:C:356:TRP:HZ2	1.83	0.43
2:B:311:ASP:O	2:B:314:GLN:HG3	2.18	0.43
1:A:165:CYS:HA	1:A:168:GLU:OE1	2.17	0.43
2:D:324:THR:CG2	2:D:325:MET:N	2.82	0.43
2:D:299:LEU:C	2:D:335:ARG:HD3	2.39	0.43
2:B:104:LEU:HD13	2:B:133:TYR:HB3	1.99	0.43
2:B:50:LYS:HG2	2:B:53:TYR:CE2	2.53	0.43
2:B:64:ILE:CG2	2:B:65:LEU:N	2.81	0.43
1:A:202:GLN:OE1	1:A:207:GLY:HA2	2.19	0.43
2:D:369:ILE:CG2	2:D:370:VAL:N	2.81	0.43
2:D:270:GLU:OE1	2:D:270:GLU:HA	2.18	0.43
2:D:282:ILE:HD11	2:D:293:LEU:HB2	2.01	0.43
2:D:294:TYR:CD2	2:D:325:MET:CE	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:MET:SD	2:B:30:VAL:CG2	3.07	0.43
1:A:154:ARG:CD	2:D:231:ALA:HB1	2.49	0.43
2:B:126:THR:CG2	2:B:127:PHE:CD2	3.01	0.43
2:D:190:MET:CE	2:D:206:ARG:HA	2.48	0.43
2:D:65:LEU:CD1	2:D:67:LEU:CD2	2.95	0.43
2:D:8:LEU:HD13	2:D:94:LEU:HD13	2.01	0.43
2:B:172:PRO:O	2:B:175:ILE:HG22	2.19	0.43
2:B:317:ILE:HD11	2:B:327:ILE:HG23	1.99	0.43
2:C:300:SER:HA	2:C:335:ARG:HH11	1.83	0.43
2:C:297:THR:OG1	2:C:329:ILE:HA	2.18	0.43
2:D:92:ASN:HD22	2:D:92:ASN:H	1.67	0.43
1:A:139:HIS:O	1:A:141:TRP:HD1	2.02	0.43
2:B:190:MET:HG2	2:B:209:VAL:HG11	1.99	0.43
2:C:166:TYR:O	2:C:167:GLU:HG3	2.19	0.43
2:C:54:VAL:CG1	2:C:55:GLY:H	2.30	0.43
2:C:104:LEU:H	2:C:104:LEU:HD22	1.82	0.43
2:B:285:CYS:SG	2:B:289:ILE:HD11	2.59	0.43
2:C:21:PHE:CD1	2:C:28:ARG:NE	2.86	0.43
1:A:165:CYS:SG	1:A:171:SER:HA	2.59	0.43
2:C:261:LEU:HD21	2:C:303:THR:CG2	2.49	0.43
2:C:161:HIS:NE2	2:C:177:ARG:CD	2.82	0.43
2:D:151:ILE:CG2	2:D:293:LEU:HB3	2.48	0.43
2:D:300:SER:O	2:D:304:THR:HG23	2.18	0.43
2:B:105:LEU:CB	2:B:134:VAL:HG22	2.49	0.43
2:B:50:LYS:CB	2:B:53:TYR:CE1	2.95	0.43
1:A:181:MET:CE	1:A:242:LEU:CD1	2.96	0.43
2:D:20:GLY:HA2	2:D:28:ARG:CG	2.48	0.43
2:D:21:PHE:CD1	2:D:28:ARG:NE	2.87	0.43
2:D:354:GLN:HG3	2:D:355:MET:N	2.33	0.43
2:D:81:ASP:HA	2:D:84:LYS:HD3	2.01	0.43
2:C:257:CYS:HB3	2:C:258:PRO:CD	2.38	0.43
2:C:140:LEU:HD12	2:C:140:LEU:N	2.34	0.43
2:C:370:VAL:CG1	2:C:371:HIS:N	2.82	0.43
2:C:299:LEU:O	2:C:335:ARG:HD3	2.19	0.43
2:B:315:LYS:HB2	2:B:315:LYS:HE2	1.88	0.43
2:D:300:SER:N	2:D:335:ARG:HD3	2.33	0.43
2:B:120:THR:OG1	2:B:370:VAL:HG11	2.18	0.43
1:A:236:TYR:N	1:A:236:TYR:CD2	2.81	0.43
1:A:236:TYR:CG	1:A:236:TYR:O	2.71	0.43
2:D:35:VAL:CG2	2:D:52:SER:CB	2.94	0.43
2:C:64:ILE:CG2	2:C:65:LEU:N	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:5:ILE:N	2:C:5:ILE:CD1	2.82	0.43
2:D:178:LEU:HD13	2:D:179:ASP:H	1.83	0.43
2:C:10:VAL:CG2	2:C:105:LEU:HA	2.46	0.43
2:C:139:VAL:HG12	2:C:140:LEU:HD12	1.99	0.43
2:C:139:VAL:HG13	2:C:140:LEU:N	2.33	0.43
2:D:106:THR:HB	2:D:137:GLN:HG2	2.00	0.43
2:D:140:LEU:N	2:D:140:LEU:CD1	2.82	0.43
2:C:163:VAL:HG12	2:C:175:ILE:CD1	2.48	0.43
2:D:346:LEU:CA	2:D:349:LEU:HD12	2.41	0.43
2:B:332:PRO:HA	2:B:333:PRO:HD3	1.62	0.43
2:C:261:LEU:CD1	2:C:261:LEU:N	2.82	0.43
2:B:31:PHE:HB3	2:B:93:GLU:OE2	2.18	0.42
1:A:157:MET:HB2	1:A:157:MET:HE3	1.75	0.42
1:A:157:MET:CG	1:A:160:ILE:HB	2.42	0.42
2:B:122:ILE:HG23	2:B:126:THR:HG22	2.01	0.42
2:D:73:HIC:O	2:D:75:ILE:HG13	2.18	0.42
2:D:21:PHE:CZ	2:D:96:VAL:CG1	3.02	0.42
2:D:349:LEU:CB	2:D:352:PHE:HB2	2.49	0.42
2:C:11:ASP:HA	2:C:106:THR:HG1	1.81	0.42
2:D:49:GLN:HG2	2:D:50:LYS:H	1.84	0.42
2:B:188:TYR:HB2	2:B:267:LEU:HD21	1.99	0.42
2:B:41:GLN:CG	2:B:42:GLY:N	2.82	0.42
2:C:220:ALA:HB1	2:C:226:GLU:HG3	2.01	0.42
1:A:195:LYS:CB	1:A:236:TYR:CD1	2.95	0.42
2:C:282:ILE:CG2	2:C:283:MET:N	2.81	0.42
2:C:294:TYR:CE2	2:C:325:MET:HE1	2.53	0.42
2:D:180:LEU:CG	2:D:181:ALA:N	2.82	0.42
2:D:38:PRO:HB3	2:D:41:GLN:H	1.83	0.42
2:D:8:LEU:HD13	2:D:94:LEU:CD1	2.49	0.42
2:C:198:TYR:HB3	2:C:200:PHE:CE1	2.54	0.42
2:B:153:MET:O	2:B:153:MET:HG3	2.19	0.42
2:C:314:GLN:CG	2:C:315:LYS:N	2.82	0.42
2:C:76:VAL:HG22	2:C:82:MET:SD	2.59	0.42
2:C:150:GLY:HA2	2:C:296:ASN:HB2	2.01	0.42
2:D:314:GLN:HA	2:D:317:ILE:HD11	2.00	0.42
2:B:136:ILE:O	2:B:140:LEU:HD12	2.19	0.42
2:B:35:VAL:HA	2:B:54:VAL:CG2	2.45	0.42
1:A:156:GLU:HG3	1:A:253:PHE:CD1	2.53	0.42
1:A:160:ILE:CG2	1:A:161:SER:N	2.82	0.42
2:D:103:VAL:CG1	2:D:104:LEU:N	2.82	0.42
2:D:66:THR:O	2:D:67:LEU:HD23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:189:LEU:O	2:C:192:ILE:HD12	2.19	0.42
2:C:101:HIS:O	2:C:103:VAL:HG23	2.19	0.42
2:B:282:ILE:CG2	2:B:283:MET:N	2.82	0.42
2:C:345:ILE:CD1	2:C:345:ILE:N	2.82	0.42
2:C:76:VAL:CG2	2:C:82:MET:SD	3.08	0.42
2:D:282:ILE:CG1	2:D:293:LEU:HD22	2.49	0.42
2:D:299:LEU:HD21	2:D:309:ILE:HG13	2.00	0.42
2:B:189:LEU:HB2	2:B:257:CYS:SG	2.59	0.42
2:B:33:SER:O	2:B:34:ILE:HG23	2.19	0.42
2:B:370:VAL:CG1	2:B:371:HIS:N	2.83	0.42
1:A:157:MET:N	1:A:160:ILE:CG2	2.82	0.42
1:A:200:VAL:HG21	1:A:209:TRP:HB3	2.01	0.42
2:C:149:THR:HB	2:C:292:ASP:OD2	2.19	0.42
2:C:283:MET:HA	2:C:290:ARG:NH2	2.33	0.42
2:D:20:GLY:HA2	2:D:28:ARG:HG2	2.01	0.42
2:D:34:ILE:CG2	2:D:69:TYR:CE2	3.01	0.42
2:D:71:ILE:CG2	2:D:74:GLY:C	2.87	0.42
2:D:110:LEU:C	2:D:110:LEU:HD23	2.40	0.42
2:D:147:ARG:HB3	2:D:147:ARG:HE	1.72	0.42
2:D:174:ALA:O	2:D:284:LYS:HD2	2.19	0.42
1:A:195:LYS:HE2	1:A:236:TYR:HE1	1.83	0.42
2:D:189:LEU:HD12	2:D:209:VAL:HG22	2.01	0.42
2:D:362:TYR:CE1	2:D:367:PRO:CG	3.03	0.42
2:D:54:VAL:HG12	2:D:55:GLY:H	1.84	0.42
2:C:190:MET:HG3	2:C:209:VAL:HG11	2.01	0.42
2:B:345:ILE:HA	2:B:348:SER:OG	2.19	0.42
1:A:228:ARG:CG	1:A:229:SER:N	2.82	0.42
2:B:139:VAL:CG1	2:B:140:LEU:N	2.83	0.42
2:D:21:PHE:CZ	2:D:96:VAL:HG11	2.55	0.42
2:D:27:PRO:HG3	2:D:340:TRP:CG	2.54	0.42
2:B:327:ILE:O	2:B:327:ILE:HG22	2.19	0.42
2:C:107:GLU:HG3	2:C:111:ASN:HD22	1.85	0.42
2:C:16:MET:SD	2:C:30:VAL:CG2	3.07	0.42
2:B:107:GLU:HG2	2:B:111:ASN:HB2	2.01	0.42
2:C:314:GLN:HB3	2:C:329:ILE:CD1	2.47	0.42
2:C:110:LEU:O	2:C:112:PRO:HD3	2.19	0.42
1:A:194:ASN:HB2	1:A:196:TYR:CE1	2.55	0.42
2:D:102:PRO:HA	2:D:131:ALA:O	2.20	0.42
2:D:58:ALA:HA	2:D:61:LYS:CB	2.43	0.42
2:C:53:TYR:N	2:C:53:TYR:HD1	2.18	0.42
2:C:103:VAL:O	2:C:356:TRP:HZ3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:VAL:HA	2:B:298:VAL:H	1.84	0.42
2:B:298:VAL:HG12	2:B:299:LEU:O	2.20	0.42
2:B:71:ILE:HD11	2:B:85:ILE:HD13	1.98	0.42
2:D:314:GLN:N	2:D:329:ILE:CD1	2.83	0.42
2:B:105:LEU:HB2	2:B:134:VAL:HG22	2.00	0.42
2:B:17:CYS:SG	2:B:31:PHE:HE1	2.42	0.42
2:B:21:PHE:O	2:B:24:ASP:HB2	2.20	0.42
1:A:196:TYR:CD2	1:A:252:TYR:HB2	2.55	0.42
2:B:110:LEU:CD2	2:D:195:GLU:CB	2.93	0.42
2:D:256:ARG:O	2:D:259:GLU:HB3	2.20	0.42
2:C:250:ILE:CG1	2:C:251:GLY:N	2.82	0.42
2:C:39:ARG:HE	2:C:66:THR:CB	2.33	0.42
2:C:65:LEU:HD11	2:C:67:LEU:CD2	2.48	0.42
2:C:133:TYR:HA	2:C:357:ILE:HD12	2.00	0.42
2:D:163:VAL:HG13	2:D:175:ILE:HG13	1.98	0.42
2:B:295:ALA:O	2:B:328:LYS:HB3	2.20	0.42
2:D:152:VAL:HA	2:D:298:VAL:O	2.19	0.42
2:C:349:LEU:CB	2:C:352:PHE:HB2	2.49	0.42
2:C:126:THR:HG23	2:C:127:PHE:CD2	2.55	0.42
2:D:220:ALA:HB2	2:D:226:GLU:HG3	1.98	0.42
2:B:223:PHE:O	2:B:227:MET:HG2	2.19	0.42
2:B:189:LEU:HG	2:B:209:VAL:HG22	2.00	0.42
2:B:362:TYR:CE1	2:B:367:PRO:CG	3.03	0.42
2:B:195:GLU:O	2:C:110:LEU:HD22	2.20	0.42
1:A:160:ILE:HG23	1:A:161:SER:N	2.34	0.42
1:A:200:VAL:N	1:A:211:TRP:CE3	2.88	0.42
2:D:261:LEU:CD2	2:D:303:THR:CG2	2.94	0.42
2:D:31:PHE:N	2:D:31:PHE:CD1	2.87	0.42
2:C:188:TYR:CZ	2:C:192:ILE:HG21	2.55	0.42
2:C:49:GLN:CG	2:C:50:LYS:N	2.82	0.42
2:D:107:GLU:CG	2:D:111:ASN:CB	2.98	0.42
2:C:107:GLU:HG3	2:C:111:ASN:HB2	2.01	0.42
2:D:50:LYS:CG	2:D:53:TYR:CE2	3.01	0.42
2:C:219:VAL:CG2	2:C:220:ALA:N	2.83	0.42
2:C:314:GLN:CB	2:C:329:ILE:HD13	2.47	0.42
2:B:193:LEU:HD23	2:B:193:LEU:HA	1.78	0.42
2:B:250:ILE:HG13	2:B:251:GLY:H	1.80	0.42
1:A:222:LEU:HB3	1:A:223:PRO:CD	2.50	0.42
2:D:187:ASP:HA	2:D:190:MET:HG3	2.01	0.42
2:D:104:LEU:HD13	2:D:356:TRP:CH2	2.53	0.42
2:C:34:ILE:HG22	2:C:69:TYR:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:22:ALA:HB1	2:C:348:SER:HB3	2.00	0.42
2:C:362:TYR:CD1	2:C:367:PRO:HA	2.55	0.42
2:B:164:PRO:HG2	2:B:174:ALA:HB3	1.98	0.42
2:C:71:ILE:H	2:C:71:ILE:CD1	2.25	0.42
2:B:71:ILE:HG23	2:B:74:GLY:O	2.20	0.42
2:D:47:MET:HB2	2:D:48:GLY:H	1.38	0.42
2:B:357:ILE:CG2	2:B:358:SER:N	2.83	0.41
2:B:50:LYS:CB	2:B:53:TYR:CD1	2.98	0.41
1:A:161:SER:HB2	1:A:253:PHE:CD2	2.55	0.41
1:A:218:LEU:HD13	1:A:220:ASP:H	1.84	0.41
2:C:282:ILE:HG13	2:C:294:TYR:HE2	1.75	0.41
2:D:178:LEU:CD1	2:D:179:ASP:N	2.83	0.41
2:B:110:LEU:HD11	2:D:195:GLU:HA	1.94	0.41
2:D:180:LEU:HD21	2:D:261:LEU:HG	2.01	0.41
2:D:133:TYR:CE1	2:D:355:MET:CG	3.03	0.41
2:D:357:ILE:N	2:D:357:ILE:CD1	2.83	0.41
2:D:97:ALA:HA	2:D:98:PRO:HD3	1.76	0.41
2:B:166:TYR:HE1	2:B:292:ASP:OD2	2.03	0.41
2:C:43:VAL:CG1	2:C:44:MET:N	2.80	0.41
2:C:118:LYS:HD2	2:C:121:GLN:CG	2.45	0.41
1:A:161:SER:CB	1:A:253:PHE:CG	3.00	0.41
2:D:218:TYR:O	2:D:255:PHE:HA	2.19	0.41
2:D:32:PRO:CB	2:D:34:ILE:HD11	2.44	0.41
2:D:37:ARG:O	2:D:65:LEU:HA	2.21	0.41
2:C:361:GLU:HB2	2:C:369:ILE:HG21	2.01	0.41
2:D:265:SER:C	2:D:268:GLY:H	2.23	0.41
1:A:201:PHE:CG	1:A:202:GLN:N	2.89	0.41
2:D:118:LYS:O	2:D:122:ILE:HD13	2.19	0.41
2:C:190:MET:HE3	2:C:209:VAL:HG11	2.01	0.41
2:C:143:TYR:C	2:C:143:TYR:CD1	2.94	0.41
2:B:201:THR:HG22	2:B:202:THR:CG2	2.48	0.41
2:B:247:VAL:HG13	2:B:247:VAL:O	2.20	0.41
2:B:101:HIS:HA	2:B:102:PRO:HD3	1.86	0.41
2:B:39:ARG:NE	2:B:66:THR:HA	2.34	0.41
1:A:233:ILE:HG13	1:A:245:ASP:C	2.39	0.41
2:B:122:ILE:HG23	2:B:126:THR:CG2	2.51	0.41
2:B:126:THR:CG2	2:B:127:PHE:N	2.82	0.41
2:C:169:TYR:CE1	2:D:42:GLY:O	2.73	0.41
2:C:165:ILE:HD13	2:C:170:ALA:HA	2.03	0.41
2:D:188:TYR:CZ	2:D:192:ILE:CG2	3.03	0.41
2:C:38:PRO:HA	2:C:64:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:53:TYR:O	2:C:54:VAL:HB	2.19	0.41
2:C:362:TYR:CE1	2:C:367:PRO:CG	3.03	0.41
2:B:176:LEU:HB3	2:B:284:LYS:HZ1	1.84	0.41
2:D:144:ALA:HB1	2:D:341:ILE:HG21	2.02	0.41
1:A:163:LYS:HD3	1:A:166:LEU:HD12	2.02	0.41
2:B:218:TYR:HE2	2:B:254:ARG:HE	1.68	0.41
2:D:213:LYS:HA	2:D:217:CYS:SG	2.61	0.41
2:C:216:LEU:HD22	2:C:250:ILE:HG12	2.00	0.41
2:D:18:LYS:N	2:D:18:LYS:CD	2.82	0.41
1:A:142:ILE:HD11	1:A:149:TYR:CB	2.25	0.41
2:B:176:LEU:CD1	2:B:277:THR:CG2	2.92	0.41
2:B:159:VAL:CG2	2:B:160:THR:N	2.83	0.41
2:B:155:SER:CB	2:B:303:THR:HB	2.49	0.41
2:C:122:ILE:HG23	2:C:126:THR:HG21	2.02	0.41
2:B:306:TYR:O	2:B:309:ILE:HD12	2.20	0.41
1:A:201:PHE:O	1:A:209:TRP:HA	2.21	0.41
2:D:104:LEU:HD22	2:D:356:TRP:CH2	2.55	0.41
2:D:191:LYS:HE3	2:D:191:LYS:CA	2.43	0.41
2:C:54:VAL:CA	2:C:58:ALA:HB2	2.37	0.41
2:B:267:LEU:HA	2:B:267:LEU:HD23	1.86	0.41
2:C:329:ILE:N	2:C:329:ILE:CD1	2.82	0.41
1:A:216:SER:HA	1:A:217:PRO:HD3	1.86	0.41
2:B:249:THR:CG2	2:B:250:ILE:N	2.84	0.41
2:B:18:LYS:HA	2:B:30:VAL:HG23	2.02	0.41
2:B:8:LEU:HD11	2:B:94:LEU:HD12	1.95	0.41
2:D:133:TYR:CE1	2:D:355:MET:HG2	2.56	0.41
2:D:31:PHE:CE1	2:D:93:GLU:OE1	2.73	0.41
2:B:305:MET:HE2	4:B:401:ADP:N6	2.36	0.41
2:B:317:ILE:CD1	2:B:327:ILE:CG2	2.99	0.41
1:A:228:ARG:HG3	1:A:229:SER:H	1.85	0.41
2:C:158:GLY:HA3	2:C:183:ARG:HH21	1.80	0.41
2:B:361:GLU:HG3	2:B:369:ILE:HG21	2.03	0.41
2:D:190:MET:HE2	2:D:209:VAL:HB	2.03	0.41
2:C:10:VAL:HG13	2:C:10:VAL:H	1.38	0.41
2:B:332:PRO:CD	2:B:335:ARG:HE	2.33	0.41
2:C:340:TRP:CH2	2:C:344:SER:HB3	2.55	0.41
2:B:345:ILE:CG2	2:B:349:LEU:HD11	2.51	0.41
2:C:155:SER:CB	2:C:303:THR:HB	2.49	0.41
2:C:3:ASP:CG	2:C:4:ASP:H	2.24	0.41
2:D:164:PRO:HB3	2:D:293:LEU:HD21	2.03	0.41
2:D:314:GLN:O	2:D:318:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:PHE:CE1	2:B:359:LYS:HA	2.56	0.41
2:B:54:VAL:CG1	2:B:55:GLY:N	2.78	0.41
2:B:129:THR:OG1	2:B:130:PRO:HD2	2.20	0.41
2:B:359:LYS:O	2:B:362:TYR:HB3	2.20	0.41
2:B:34:ILE:CG2	2:B:69:TYR:CE1	3.04	0.41
2:B:34:ILE:HG21	2:B:69:TYR:CZ	2.56	0.41
1:A:153:GLU:O	1:A:252:TYR:HE2	2.04	0.41
2:C:279:PHE:HB2	2:C:320:LEU:HD12	2.01	0.41
2:D:104:LEU:CD2	2:D:104:LEU:N	2.81	0.41
2:D:190:MET:CE	2:D:209:VAL:HG11	2.51	0.41
2:D:361:GLU:CG	2:D:369:ILE:HG21	2.48	0.41
2:D:64:ILE:CG2	2:D:65:LEU:N	2.83	0.41
1:A:154:ARG:HD2	2:D:231:ALA:CA	2.41	0.41
2:D:116:ARG:NH1	2:D:134:VAL:HG12	2.35	0.41
2:D:208:ILE:HD13	2:D:243:PRO:HD2	2.03	0.41
2:D:34:ILE:C	2:D:54:VAL:HG21	2.41	0.41
2:D:21:PHE:HZ	2:D:96:VAL:CG1	2.34	0.41
2:B:82:MET:HE3	2:B:85:ILE:HD12	2.02	0.41
2:B:180:LEU:CD1	2:B:184:ASP:CB	2.96	0.41
2:C:327:ILE:CG2	2:C:328:LYS:N	2.84	0.41
2:B:19:ALA:O	2:B:28:ARG:HG3	2.21	0.41
2:B:365:SER:HB2	2:B:369:ILE:HB	2.03	0.41
1:A:175:ILE:HG21	1:A:181:MET:HB2	2.02	0.41
2:D:124:PHE:O	2:D:128:ASN:HA	2.20	0.41
2:B:152:VAL:HG13	2:B:152:VAL:O	2.20	0.41
2:B:71:ILE:CD1	2:B:85:ILE:CD1	2.96	0.41
2:C:41:GLN:CG	2:C:42:GLY:N	2.81	0.41
2:B:259:GLU:HG3	2:B:266:PHE:CE1	2.55	0.41
2:B:320:LEU:HA	2:B:320:LEU:HD23	1.87	0.41
2:B:353:GLN:O	2:B:356:TRP:HD1	2.04	0.40
2:D:120:THR:CA	2:D:132:MET:HE1	2.49	0.40
2:D:34:ILE:CG2	2:D:69:TYR:CD1	3.04	0.40
2:D:305:MET:CG	4:D:401:ADP:C6	2.83	0.40
2:D:73:HIC:HD2	2:D:183:ARG:NH1	2.36	0.40
2:D:18:LYS:HG2	2:D:340:TRP:HD1	1.85	0.40
2:B:211:ASP:OD1	2:B:215:LYS:HD2	2.20	0.40
2:C:21:PHE:CD1	2:C:21:PHE:N	2.89	0.40
2:C:94:LEU:HA	2:C:94:LEU:HD23	1.87	0.40
2:D:162:THR:HG21	2:D:277:THR:CG2	2.51	0.40
2:B:124:PHE:CZ	2:B:132:MET:HG2	2.57	0.40
2:D:103:VAL:HG11	2:D:105:LEU:CD2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:208:ILE:HD13	2:D:243:PRO:HG2	2.03	0.40
2:D:358:SER:H	2:D:361:GLU:HG2	1.85	0.40
2:D:54:VAL:HG13	2:D:58:ALA:HB2	2.01	0.40
2:D:8:LEU:HD11	2:D:96:VAL:HG21	2.01	0.40
2:D:31:PHE:CD1	2:D:93:GLU:OE1	2.74	0.40
2:C:254:ARG:O	2:C:258:PRO:HD2	2.21	0.40
2:B:302:GLY:HA3	4:B:401:ADP:O5'	2.21	0.40
2:D:10:VAL:HG23	2:D:12:ASN:OD1	2.20	0.40
2:B:218:TYR:C	2:B:218:TYR:CD1	2.95	0.40
2:B:58:ALA:O	2:B:65:LEU:HD22	2.21	0.40
2:B:64:ILE:HG23	2:B:65:LEU:N	2.36	0.40
1:A:199:GLY:CA	1:A:211:TRP:HE3	2.33	0.40
2:C:294:TYR:CG	2:C:325:MET:HE1	2.57	0.40
2:D:31:PHE:HB2	2:D:32:PRO:CD	2.50	0.40
2:D:133:TYR:CD1	2:D:357:ILE:HD13	2.54	0.40
2:C:203:THR:O	2:C:206:ARG:HG2	2.21	0.40
2:C:209:VAL:CG1	2:C:210:ARG:N	2.82	0.40
2:C:68:LYS:HZ2	2:C:68:LYS:HG2	1.77	0.40
2:B:153:MET:SD	2:B:313:MET:SD	3.19	0.40
2:B:297:THR:OG1	2:B:329:ILE:HA	2.21	0.40
2:B:260:ALA:HA	2:B:263:GLN:O	2.20	0.40
2:B:47:MET:HB2	2:B:48:GLY:H	1.27	0.40
2:D:299:LEU:N	2:D:299:LEU:HD12	2.36	0.40
2:B:206:ARG:CG	2:B:206:ARG:HH11	2.35	0.40
2:B:252:ASN:HA	2:B:255:PHE:CE2	2.56	0.40
1:A:208:SER:OG	1:A:210:PHE:HE2	2.02	0.40
2:D:192:ILE:CG2	2:D:256:ARG:CZ	3.00	0.40
2:C:218:TYR:HE2	2:C:254:ARG:NH2	2.19	0.40
2:C:34:ILE:CG2	2:C:69:TYR:CE1	3.05	0.40
2:B:261:LEU:HD21	2:B:303:THR:HG21	2.01	0.40
2:C:152:VAL:HG23	2:C:298:VAL:O	2.21	0.40
2:B:10:VAL:CG2	2:B:105:LEU:CD1	2.94	0.40
2:B:209:VAL:CG1	2:B:210:ARG:N	2.82	0.40
2:B:34:ILE:HG22	2:B:68:LYS:C	2.42	0.40
2:B:374:CYS:HB2	2:B:375:PHE:H	1.75	0.40
1:A:196:TYR:O	1:A:198:VAL:HG13	2.22	0.40
2:D:117:GLU:HA	2:D:367:PRO:HB2	2.02	0.40
2:D:212:ILE:O	2:D:216:LEU:HB2	2.22	0.40
2:C:104:LEU:HD13	2:C:356:TRP:CZ3	2.56	0.40
2:C:305:MET:HE2	4:C:401:ADP:N6	2.37	0.40
2:B:349:LEU:HB3	2:B:352:PHE:HB2	2.02	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	129/131 (98%)	117 (91%)	7 (5%)	5 (4%)	4 36
2	B	371/374 (99%)	347 (94%)	16 (4%)	8 (2%)	8 49
2	C	371/374 (99%)	343 (92%)	22 (6%)	6 (2%)	12 56
2	D	371/374 (99%)	342 (92%)	23 (6%)	6 (2%)	12 56
All	All	1242/1253 (99%)	1149 (92%)	68 (6%)	25 (2%)	14 51

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	43	VAL
2	B	72	GLU
2	B	244	ASP
2	B	374	CYS
2	C	43	VAL
2	C	44	MET
2	C	72	GLU
2	C	323	SER
2	D	76	VAL
1	A	237	LEU
2	B	44	MET
2	B	54	VAL
2	B	238	LYS
2	C	54	VAL
2	C	238	LYS
2	D	4	ASP
2	D	43	VAL
2	D	167	GLU
2	D	238	LYS
1	A	228	ARG

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Mol	Chain	Res	Type
2	B	4	ASP
1	A	232	GLN
2	D	54	VAL
1	A	229	SER
1	A	233	ILE

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	115/115 (100%)	105 (91%)	10 (9%)	13 45
2	B	316/316 (100%)	244 (77%)	72 (23%)	1 8
2	C	316/316 (100%)	248 (78%)	68 (22%)	1 9
2	D	316/316 (100%)	258 (82%)	58 (18%)	2 14
All	All	1063/1063 (100%)	855 (80%)	208 (20%)	5 12

All (208) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	CYS
1	A	142	ILE
1	A	162	LYS
1	A	165	CYS
1	A	185	SER
1	A	205	ILE
1	A	206	SER
1	A	216	SER
1	A	251	LYS
1	A	264	ILE
2	B	5	ILE
2	B	8	LEU
2	B	11	ASP
2	B	17	CYS
2	B	18	LYS
2	B	28	ARG

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Mol	Chain	Res	Type
2	B	30	VAL
2	B	34	ILE
2	B	43	VAL
2	B	49	GLN
2	B	50	LYS
2	B	57	GLU
2	B	64	ILE
2	B	65	LEU
2	B	68	LYS
2	B	92	ASN
2	B	95	ARG
2	B	104	LEU
2	B	105	LEU
2	B	118	LYS
2	B	120	THR
2	B	121	GLN
2	B	145	SER
2	B	147	ARG
2	B	148	THR
2	B	163	VAL
2	B	175	ILE
2	B	176	LEU
2	B	178	LEU
2	B	189	LEU
2	B	192	ILE
2	B	195	GLU
2	B	199	SER
2	B	201	THR
2	B	203	THR
2	B	206	ARG
2	B	209	VAL
2	B	213	LYS
2	B	214	GLU
2	B	215	LYS
2	B	216	LEU
2	B	219	VAL
2	B	222	ASP
2	B	233	SER
2	B	238	LYS
2	B	250	ILE
2	B	254	ARG
2	B	256	ARG

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Mol	Chain	Res	Type
2	B	259	GLU
2	B	281	SER
2	B	282	ILE
2	B	290	ARG
2	B	291	LYS
2	B	292	ASP
2	B	300	SER
2	B	309	ILE
2	B	313	MET
2	B	314	GLN
2	B	315	LYS
2	B	325	MET
2	B	326	LYS
2	B	327	ILE
2	B	328	LYS
2	B	334	GLU
2	B	335	ARG
2	B	338	SER
2	B	344	SER
2	B	349	LEU
2	B	355	MET
2	B	359	LYS
2	B	369	ILE
2	B	374	CYS
2	C	4	ASP
2	C	5	ILE
2	C	8	LEU
2	C	16	MET
2	C	18	LYS
2	C	28	ARG
2	C	33	SER
2	C	34	ILE
2	C	44	MET
2	C	64	ILE
2	C	65	LEU
2	C	68	LYS
2	C	95	ARG
2	C	104	LEU
2	C	107	GLU
2	C	110	LEU
2	C	115	ASN
2	C	121	GLN

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Mol	Chain	Res	Type
2	C	122	ILE
2	C	123	MET
2	C	134	VAL
2	C	141	SER
2	C	145	SER
2	C	148	THR
2	C	153	MET
2	C	159	VAL
2	C	164	PRO
2	C	171	LEU
2	C	176	LEU
2	C	178	LEU
2	C	180	LEU
2	C	183	ARG
2	C	186	THR
2	C	189	LEU
2	C	190	MET
2	C	191	LYS
2	C	196	ARG
2	C	199	SER
2	C	201	THR
2	C	206	ARG
2	C	209	VAL
2	C	213	LYS
2	C	215	LYS
2	C	216	LEU
2	C	234	SER
2	C	236	LEU
2	C	238	LYS
2	C	242	LEU
2	C	254	ARG
2	C	259	GLU
2	C	261	LEU
2	C	263	GLN
2	C	276	GLU
2	C	282	ILE
2	C	287	VAL
2	C	291	LYS
2	C	299	LEU
2	C	309	ILE
2	C	313	MET
2	C	320	LEU

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Mol	Chain	Res	Type
2	C	324	THR
2	C	328	LYS
2	C	335	ARG
2	C	345	ILE
2	C	359	LYS
2	C	368	SER
2	C	369	ILE
2	C	373	LYS
2	D	5	ILE
2	D	8	LEU
2	D	17	CYS
2	D	18	LYS
2	D	28	ARG
2	D	30	VAL
2	D	33	SER
2	D	34	ILE
2	D	47	MET
2	D	61	LYS
2	D	65	LEU
2	D	85	ILE
2	D	92	ASN
2	D	104	LEU
2	D	105	LEU
2	D	113	LYS
2	D	116	ARG
2	D	119	MET
2	D	121	GLN
2	D	123	MET
2	D	139	VAL
2	D	141	SER
2	D	147	ARG
2	D	151	ILE
2	D	167	GLU
2	D	176	LEU
2	D	178	LEU
2	D	189	LEU
2	D	191	LYS
2	D	192	ILE
2	D	195	GLU
2	D	201	THR
2	D	206	ARG
2	D	209	VAL

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Mol	Chain	Res	Type
2	D	213	LYS
2	D	214	GLU
2	D	216	LEU
2	D	236	LEU
2	D	238	LYS
2	D	239	SER
2	D	253	GLU
2	D	256	ARG
2	D	282	ILE
2	D	300	SER
2	D	309	ILE
2	D	313	MET
2	D	314	GLN
2	D	316	GLU
2	D	335	ARG
2	D	344	SER
2	D	348	SER
2	D	349	LEU
2	D	354	GLN
2	D	358	SER
2	D	359	LYS
2	D	369	ILE
2	D	372	ARG
2	D	373	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	A	144	ASN
1	A	194	ASN
1	A	232	GLN
2	B	12	ASN
2	B	49	GLN
2	B	92	ASN
2	B	121	GLN
2	B	353	GLN
2	C	92	ASN
2	C	115	ASN
2	C	121	GLN
2	C	314	GLN
2	C	353	GLN

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Mol	Chain	Res	Type
2	D	49	GLN
2	D	59	GLN
2	D	87	HIS
2	D	92	ASN
2	D	111	ASN
2	D	121	GLN
2	D	137	GLN
2	D	252	ASN
2	D	353	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HIC	B	73	2	6,11,12	1.28	1 (16%)	6,14,16	0.86	0
2	HIC	C	73	2	6,11,12	1.26	1 (16%)	6,14,16	0.86	1 (16%)
2	HIC	D	73	2	6,11,12	1.27	1 (16%)	6,14,16	0.94	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HIC	B	73	2	-	0/4/6/8	0/1/1/1
2	HIC	C	73	2	-	0/4/6/8	0/1/1/1
2	HIC	D	73	2	-	0/4/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	73	HIC	CD2-NE2	-2.84	1.34	1.38
2	D	73	HIC	CD2-NE2	-2.81	1.34	1.38
2	C	73	HIC	CD2-NE2	-2.78	1.34	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	73	HIC	O-C-CA	-2.21	119.78	125.72
2	C	73	HIC	O-C-CA	-2.00	120.36	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	73	HIC	3	0
2	C	73	HIC	7	0
2	D	73	HIC	3	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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	$\#\|Z\| > 2$
4	ADP	B	401	-	24,29,29	0.99	1 (4%)	23,45,45	1.76	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	ADP	C	401	-	24,29,29	0.99	1 (4%)	23,45,45	1.77	2 (8%)
4	ADP	D	401	-	24,29,29	1.00	1 (4%)	23,45,45	1.76	1 (4%)

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
4	ADP	B	401	-	-	0/12/32/32	0/3/3/3
4	ADP	C	401	-	-	0/12/32/32	0/3/3/3
4	ADP	D	401	-	-	0/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	401	ADP	C5-C4	3.12	1.47	1.40
4	B	401	ADP	C5-C4	3.12	1.47	1.40
4	C	401	ADP	C5-C4	3.12	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	401	ADP	N3-C2-N1	-6.61	123.68	128.87
4	D	401	ADP	N3-C2-N1	-6.53	123.74	128.87
4	B	401	ADP	N3-C2-N1	-6.52	123.75	128.87
4	C	401	ADP	C4'-O4'-C1'	2.01	111.77	109.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401	ADP	7	0
4	C	401	ADP	7	0
4	D	401	ADP	8	0

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.