



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:52 PM BST

PDB ID : 3J8K  
EMDB ID: : EMD-6181  
Title : Tilted state of actin, T2  
Authors : Galkin, V.E.; Orlova, A.; Vos, M.R.; Schroder, G.F.; Egelman, E.H.  
Deposited on : 2014-11-07  
Resolution : 12.00 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : unknown  
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

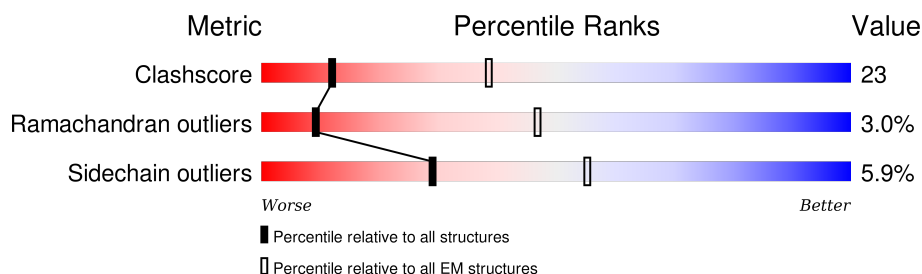
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 12.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	377	58% 37% . .
1	B	377	63% 33% . .
1	C	377	60% 36% . .
1	D	377	51% 43% 5% .
1	E	377	55% 41% . .
1	F	377	54% 40% 5% . .
1	G	377	57% 38% . .
1	H	377	55% 40% . .
1	I	377	51% 46% . .

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Mol	Chain	Length	Quality of chain
1	J	377	<div><div></div><div>50%</div><div>46%</div><div>..</div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 29330 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.

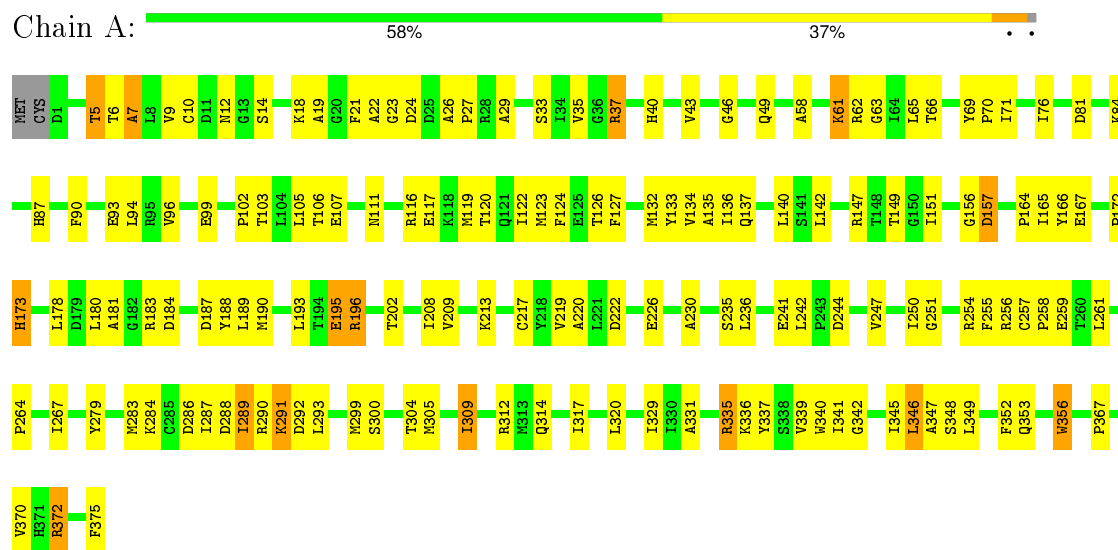
- Molecule 1 is a protein called Actin, alpha skeletal muscle.

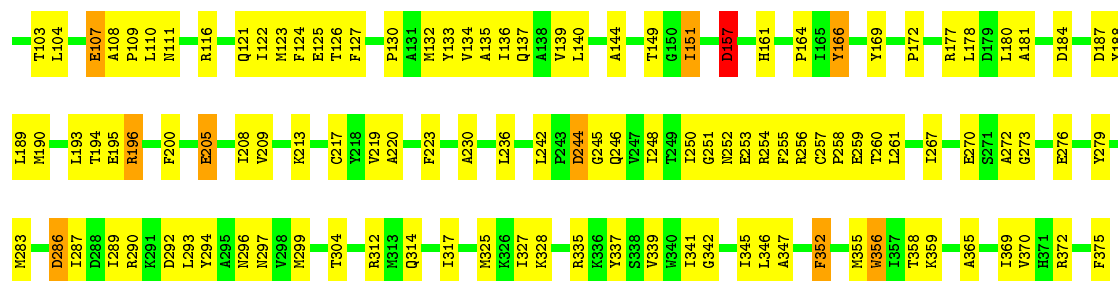
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	B	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	C	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	D	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	E	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	F	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	G	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	H	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	I	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	J	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

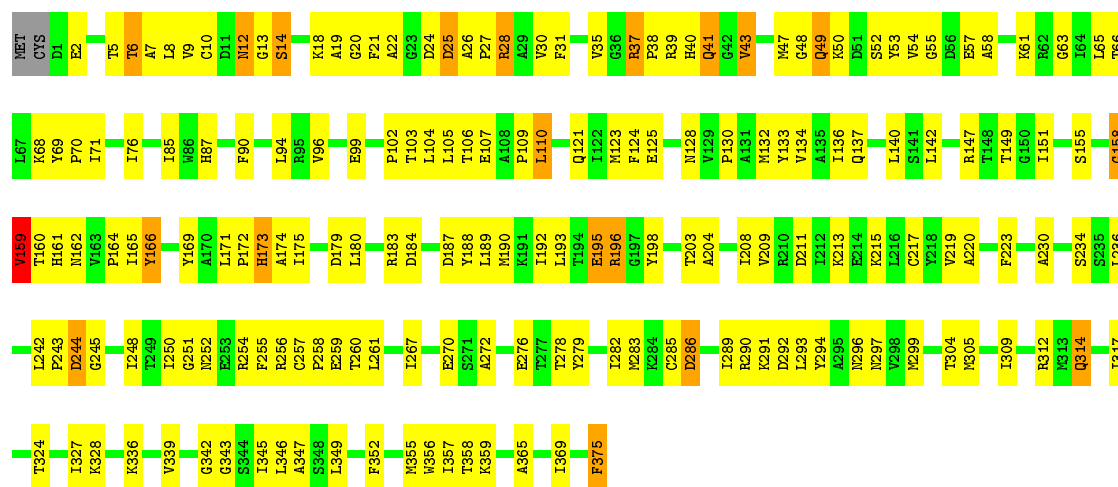
- Molecule 1: Actin, alpha skeletal muscle





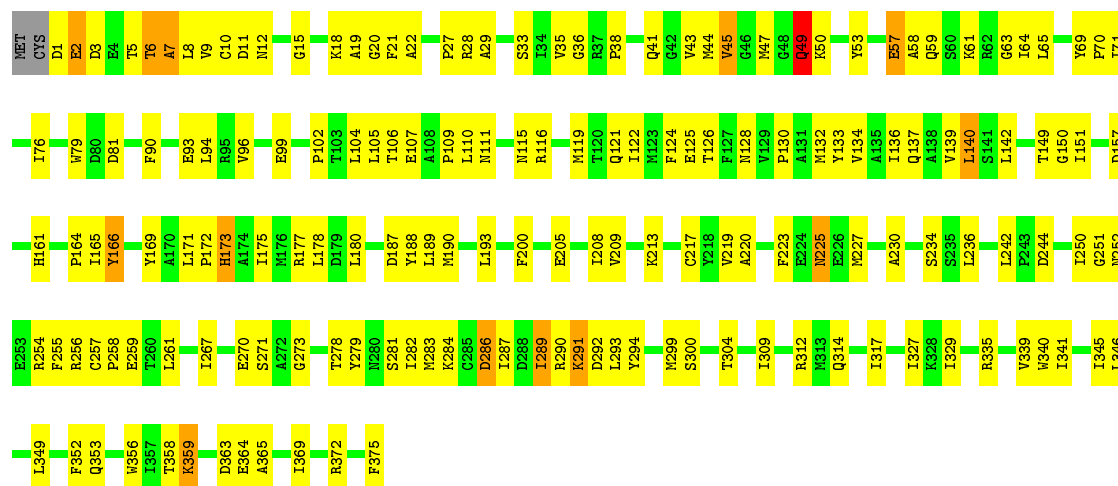
- Molecule 1: Actin, alpha skeletal muscle

Chain D: 51% 43% 5% •



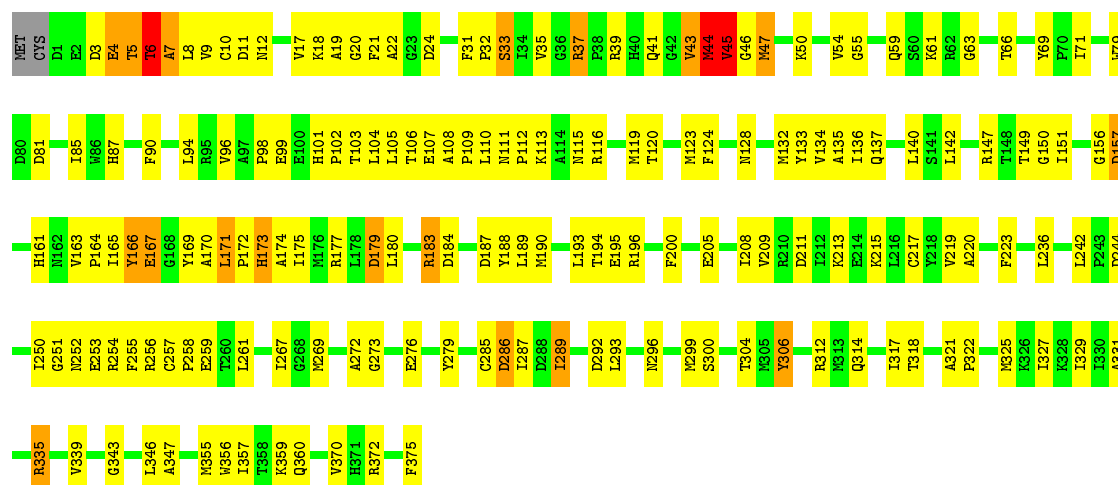
- Molecule 1: Actin, alpha skeletal muscle

Chain E: 55% 41% • •



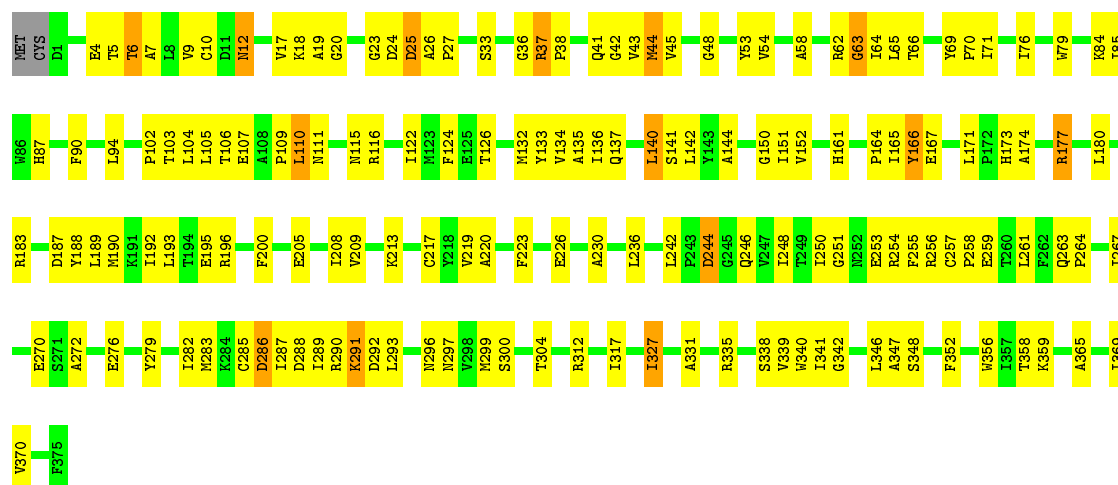
- Molecule 1: Actin, alpha skeletal muscle

Chain F: 54% 40% 5% • •



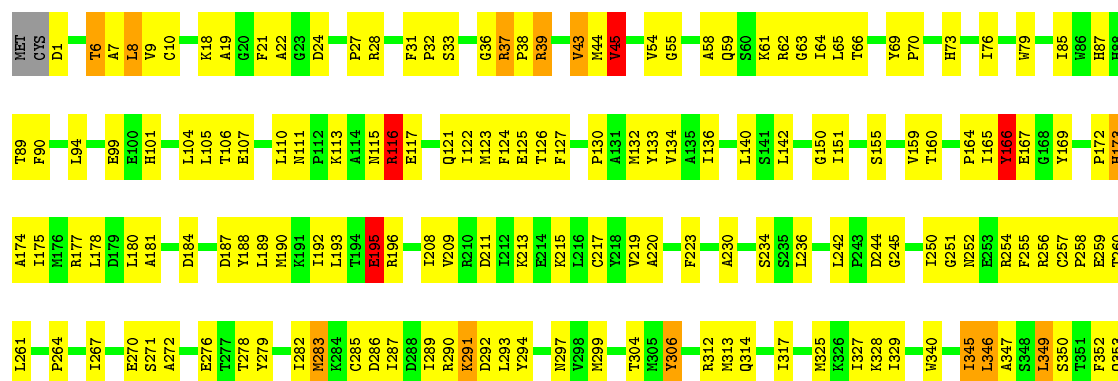
- Molecule 1: Actin, alpha skeletal muscle

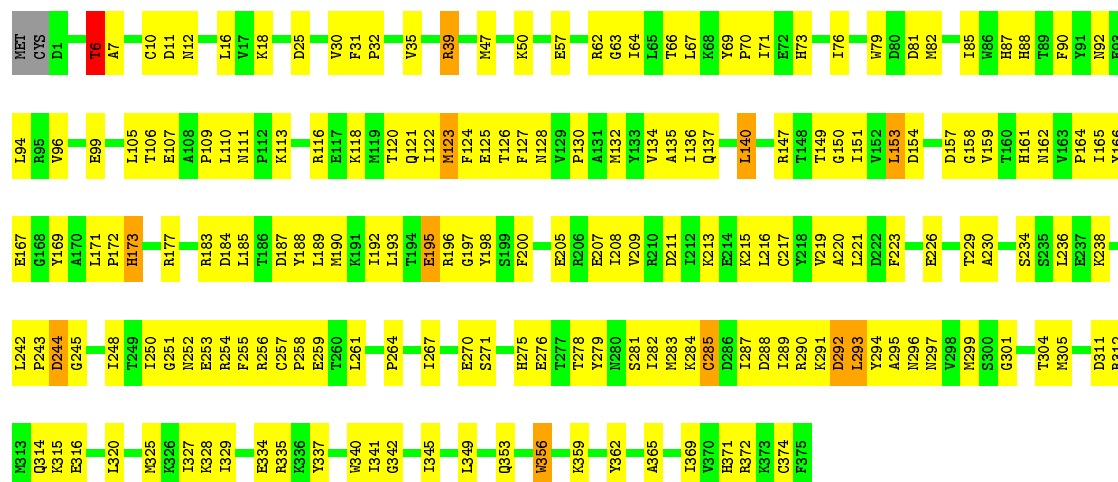
Chain G: 57% 38%



- Molecule 1: Actin, alpha skeletal muscle

Chain H: 55% 40%







## 4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	FSC and comparison with atomic model	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	Depositor
Image detector	KODAK SO-163 FILM	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
1	A	0.41	0/2996	0.63	0/4058
1	B	0.42	0/2996	0.66	1/4058 (0.0%)
1	C	0.41	0/2996	0.64	0/4058
1	D	0.42	0/2996	0.66	0/4058
1	E	0.40	0/2996	0.65	0/4058
1	F	0.41	0/2996	0.64	0/4058
1	G	0.43	0/2996	0.66	0/4058
1	H	0.44	0/2996	0.68	1/4058 (0.0%)
1	I	0.40	0/2996	0.60	0/4058
1	J	0.38	0/2996	0.58	0/4058
All	All	0.41	0/29960	0.64	2/40580 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	116	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	B	362	TYR	CB-CG-CD1	-5.20	117.88	121.00

There are no chirality outliers.

There are no planarity outliers.

### 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	2933	0	2894	117	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2933	0	2894	113	0
1	C	2933	0	2894	121	0
1	D	2933	0	2894	149	0
1	E	2933	0	2894	126	0
1	F	2933	0	2894	140	0
1	G	2933	0	2894	140	0
1	H	2933	0	2894	150	0
1	I	2933	0	2894	148	0
1	J	2933	0	2894	164	0
All	All	29330	0	28940	1317	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 23.

All (1317) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLY:HA3	1:C:287:ILE:HG21	1.34	1.06
1:B:7:ALA:HB1	1:B:104:LEU:HB2	1.40	1.00
1:G:58:ALA:HB1	1:G:65:LEU:HD21	1.46	0.97
1:C:58:ALA:HB1	1:C:65:LEU:HD21	1.47	0.95
1:H:151:ILE:HB	1:H:293:LEU:HD22	1.48	0.95
1:A:6:THR:HG22	1:A:22:ALA:HB3	1.45	0.95
1:C:180:LEU:HD21	1:C:261:LEU:HA	1.45	0.94
1:J:151:ILE:HB	1:J:293:LEU:HD13	1.49	0.94
1:I:144:ALA:HB2	1:I:342:GLY:HA2	1.47	0.94
1:I:151:ILE:HB	1:I:293:LEU:HD22	1.50	0.91
1:H:58:ALA:HB1	1:H:65:LEU:HD21	1.48	0.91
1:B:140:LEU:HG	1:B:346:LEU:HD11	1.53	0.90
1:H:289:ILE:HG22	1:H:293:LEU:HG	1.52	0.89
1:H:299:MET:HB3	1:H:304:THR:HG21	1.53	0.87
1:C:64:ILE:HD11	1:E:286:ASP:HB2	1.56	0.87
1:E:6:THR:HG22	1:E:22:ALA:HB3	1.58	0.86
1:H:188:TYR:CE1	1:H:267:ILE:HG22	2.10	0.86
1:B:9:VAL:HG22	1:B:104:LEU:HD23	1.57	0.85
1:D:43:VAL:HG21	1:F:171:LEU:HD11	1.58	0.84
1:A:90:PHE:HA	1:A:94:LEU:HD12	1.59	0.84
1:A:58:ALA:HB1	1:A:65:LEU:HD21	1.60	0.83
1:E:58:ALA:HB1	1:E:65:LEU:HD21	1.61	0.83
1:D:136:ILE:O	1:D:140:LEU:HD13	1.79	0.83
1:G:63:GLY:HA3	1:I:287:ILE:HG21	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:286:ASP:HB3	1:I:289:ILE:HD12	1.59	0.82
1:I:289:ILE:HG22	1:I:293:LEU:HG	1.62	0.82
1:D:188:TYR:CE1	1:D:267:ILE:HG22	2.13	0.82
1:D:5:THR:O	1:D:102:PRO:HG3	1.79	0.82
1:E:90:PHE:HA	1:E:94:LEU:HD12	1.60	0.81
1:E:151:ILE:HB	1:E:293:LEU:HD22	1.61	0.81
1:B:90:PHE:HA	1:B:94:LEU:HD12	1.62	0.81
1:C:286:ASP:HB2	1:C:289:ILE:HD12	1.63	0.81
1:E:180:LEU:HD21	1:E:261:LEU:HA	1.60	0.80
1:D:47:MET:HG2	1:D:50:LYS:O	1.81	0.80
1:G:116:ARG:HG2	1:G:370:VAL:HG11	1.63	0.80
1:C:149:THR:HG21	1:C:292:ASP:HB2	1.61	0.80
1:D:124:PHE:CE1	1:D:132:MET:HG2	2.17	0.80
1:A:107:GLU:HB2	1:A:134:VAL:HG22	1.63	0.80
1:F:164:PRO:HB3	1:F:285:CYS:SG	2.22	0.80
1:I:250:ILE:HD12	1:I:254:ARG:HG2	1.64	0.79
1:I:122:ILE:O	1:I:126:THR:HB	1.83	0.79
1:F:7:ALA:O	1:F:22:ALA:HB2	1.83	0.79
1:F:111:ASN:HB3	1:F:116:ARG:NH1	1.99	0.78
1:F:180:LEU:HD21	1:F:261:LEU:HA	1.63	0.78
1:F:250:ILE:HD12	1:F:254:ARG:HG2	1.65	0.78
1:C:299:MET:HB3	1:C:304:THR:HG21	1.66	0.78
1:C:188:TYR:CE1	1:C:267:ILE:HG22	2.19	0.77
1:J:99:GLU:HA	1:J:128:ASN:O	1.84	0.77
1:J:287:ILE:HD13	1:J:290:ARG:HH12	1.48	0.77
1:B:137:GLN:HG3	1:B:339:VAL:HG13	1.67	0.77
1:F:9:VAL:O	1:F:19:ALA:HA	1.84	0.77
1:J:236:LEU:O	1:J:251:GLY:HA2	1.85	0.77
1:B:58:ALA:HB1	1:B:65:LEU:HD21	1.66	0.77
1:I:230:ALA:HA	1:I:236:LEU:HD22	1.67	0.77
1:C:151:ILE:HG12	1:C:293:LEU:HD22	1.67	0.76
1:B:261:LEU:HD11	1:B:303:THR:HG22	1.65	0.76
1:H:43:VAL:HG12	1:H:44:MET:H	1.48	0.76
1:H:187:ASP:O	1:H:190:MET:HG2	1.85	0.76
1:H:236:LEU:O	1:H:251:GLY:HA2	1.85	0.76
1:I:236:LEU:O	1:I:251:GLY:HA2	1.85	0.76
1:H:54:VAL:HG21	1:H:85:ILE:HA	1.67	0.76
1:D:174:ALA:HB1	1:D:285:CYS:SG	2.25	0.76
1:F:44:MET:O	1:F:45:VAL:HB	1.86	0.76
1:H:136:ILE:O	1:H:140:LEU:HD13	1.86	0.75
1:H:250:ILE:HD12	1:H:254:ARG:HG2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ILE:O	1:C:140:LEU:HD13	1.86	0.75
1:A:286:ASP:HB3	1:A:289:ILE:HD12	1.69	0.75
1:J:230:ALA:HA	1:J:236:LEU:HD22	1.67	0.75
1:A:136:ILE:O	1:A:140:LEU:HD13	1.86	0.75
1:F:103:THR:O	1:F:132:MET:HB2	1.85	0.75
1:A:187:ASP:O	1:A:190:MET:HG2	1.86	0.75
1:D:164:PRO:HB3	1:D:285:CYS:SG	2.27	0.75
1:G:187:ASP:O	1:G:190:MET:HG2	1.86	0.75
1:H:180:LEU:HD21	1:H:261:LEU:HA	1.68	0.75
1:I:107:GLU:HB2	1:I:134:VAL:HG22	1.67	0.75
1:C:219:VAL:HG22	1:C:258:PRO:HB3	1.69	0.75
1:C:137:GLN:HG3	1:C:339:VAL:HG13	1.68	0.75
1:F:136:ILE:O	1:F:140:LEU:HD13	1.86	0.74
1:C:250:ILE:HD12	1:C:254:ARG:HG2	1.69	0.74
1:G:180:LEU:HD21	1:G:261:LEU:HA	1.69	0.74
1:H:63:GLY:HA3	1:J:288:ASP:H	1.52	0.74
1:H:150:GLY:O	1:H:165:ILE:HG21	1.87	0.74
1:C:194:THR:HG21	1:D:171:LEU:HD13	1.68	0.74
1:E:150:GLY:O	1:E:165:ILE:HB	1.88	0.74
1:H:286:ASP:HB2	1:H:289:ILE:HD12	1.69	0.74
1:E:133:TYR:CD1	1:E:356:TRP:HA	2.22	0.74
1:E:187:ASP:O	1:E:190:MET:HG2	1.88	0.74
1:I:135:ALA:HB1	1:I:140:LEU:HD11	1.69	0.74
1:H:136:ILE:HD13	1:H:375:PHE:CD1	2.22	0.74
1:E:164:PRO:HD2	1:E:175:ILE:HG22	1.70	0.73
1:J:287:ILE:HA	1:J:290:ARG:NH1	2.02	0.73
1:B:124:PHE:CE1	1:B:132:MET:HG2	2.23	0.73
1:B:289:ILE:HG22	1:B:293:LEU:HD11	1.70	0.73
1:B:346:LEU:HD13	1:B:352:PHE:CE1	2.23	0.73
1:G:26:ALA:HB1	1:G:27:PRO:HD2	1.71	0.73
1:E:27:PRO:HD3	1:E:340:TRP:CZ2	2.24	0.73
1:B:122:ILE:O	1:B:126:THR:HB	1.89	0.73
1:B:99:GLU:HG3	1:B:127:PHE:O	1.89	0.73
1:H:208:ILE:HG21	1:H:242:LEU:HD11	1.70	0.73
1:D:187:ASP:O	1:D:190:MET:HG2	1.88	0.72
1:E:299:MET:HB3	1:E:304:THR:HG21	1.70	0.72
1:H:164:PRO:HB3	1:H:285:CYS:SG	2.28	0.72
1:E:289:ILE:HG22	1:E:293:LEU:HG	1.71	0.72
1:C:136:ILE:HD13	1:C:375:PHE:CE1	2.25	0.72
1:D:137:GLN:HG3	1:D:339:VAL:HG13	1.71	0.72
1:I:188:TYR:HD2	1:I:257:CYS:HG	1.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:187:ASP:O	1:I:190:MET:HG2	1.89	0.72
1:A:236:LEU:O	1:A:251:GLY:HA2	1.90	0.72
1:H:164:PRO:HD2	1:H:175:ILE:HG22	1.72	0.71
1:F:120:THR:HA	1:F:132:MET:CE	2.19	0.71
1:F:90:PHE:HA	1:F:94:LEU:HD12	1.71	0.71
1:H:116:ARG:HH11	1:H:116:ARG:CG	2.04	0.71
1:F:150:GLY:O	1:F:165:ILE:HB	1.88	0.71
1:I:289:ILE:HG22	1:I:293:LEU:CG	2.20	0.71
1:F:151:ILE:HB	1:F:293:LEU:HD22	1.72	0.71
1:D:236:LEU:O	1:D:251:GLY:HA2	1.91	0.71
1:D:365:ALA:HB3	1:D:369:ILE:HD13	1.72	0.71
1:G:111:ASN:HB3	1:G:116:ARG:NH1	2.06	0.71
1:D:21:PHE:HB2	1:D:24:ASP:OD2	1.91	0.71
1:G:110:LEU:HD21	1:G:177:ARG:HD3	1.71	0.71
1:H:104:LEU:HD22	1:H:347:ALA:HB2	1.72	0.71
1:H:289:ILE:HG22	1:H:293:LEU:CG	2.19	0.70
1:F:285:CYS:O	1:F:286:ASP:HB2	1.90	0.70
1:C:116:ARG:HB3	1:C:370:VAL:HG21	1.73	0.70
1:F:10:CYS:HA	1:F:18:LYS:O	1.91	0.70
1:H:124:PHE:CE1	1:H:132:MET:HG2	2.26	0.70
1:G:27:PRO:HD3	1:G:340:TRP:CZ3	2.27	0.70
1:B:142:LEU:HD22	1:B:165:ILE:HG12	1.73	0.70
1:C:124:PHE:CE1	1:C:132:MET:HG2	2.27	0.70
1:F:3:ASP:O	1:F:4:GLU:HB2	1.90	0.70
1:A:122:ILE:O	1:A:126:THR:HB	1.90	0.70
1:G:133:TYR:CD1	1:G:356:TRP:HA	2.26	0.70
1:F:200:PHE:HA	1:F:205:GLU:OE2	1.92	0.70
1:F:137:GLN:HG3	1:F:339:VAL:HG11	1.74	0.70
1:A:140:LEU:HG	1:A:346:LEU:CD1	2.22	0.70
1:G:286:ASP:HB3	1:G:289:ILE:HD12	1.74	0.70
1:F:213:LYS:O	1:F:217:CYS:HB2	1.92	0.70
1:G:124:PHE:CE1	1:G:132:MET:HG2	2.27	0.70
1:D:314:GLN:OE1	1:D:328:LYS:HA	1.92	0.70
1:G:109:PRO:O	1:G:110:LEU:HD13	1.92	0.69
1:B:140:LEU:CG	1:B:346:LEU:HD11	2.20	0.69
1:J:250:ILE:HD12	1:J:254:ARG:HG2	1.73	0.69
1:D:213:LYS:O	1:D:217:CYS:HB2	1.93	0.69
1:C:99:GLU:HG3	1:C:127:PHE:O	1.93	0.69
1:G:338:SER:HA	1:G:341:ILE:HG22	1.75	0.69
1:A:166:TYR:CD1	1:A:289:ILE:HG23	2.27	0.69
1:B:116:ARG:HG2	1:B:370:VAL:HG21	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:289:ILE:HG22	1:J:293:LEU:HD23	1.73	0.69
1:J:107:GLU:HB2	1:J:134:VAL:HG22	1.73	0.69
1:E:124:PHE:CE1	1:E:132:MET:HG2	2.28	0.69
1:G:136:ILE:O	1:G:140:LEU:HD13	1.91	0.69
1:E:208:ILE:HG21	1:E:242:LEU:HD11	1.75	0.69
1:G:289:ILE:HG22	1:G:293:LEU:HG	1.75	0.69
1:C:213:LYS:O	1:C:217:CYS:HB2	1.93	0.69
1:J:122:ILE:O	1:J:126:THR:HB	1.92	0.69
1:F:236:LEU:O	1:F:251:GLY:HA2	1.93	0.69
1:E:279:TYR:OH	1:E:317:ILE:HA	1.92	0.69
1:C:289:ILE:HG22	1:C:293:LEU:HG	1.74	0.69
1:C:208:ILE:HG21	1:C:242:LEU:HD11	1.75	0.69
1:A:99:GLU:HG2	1:A:127:PHE:O	1.93	0.68
1:H:10:CYS:HA	1:H:18:LYS:O	1.93	0.68
1:F:187:ASP:O	1:F:190:MET:HG2	1.92	0.68
1:E:137:GLN:HG3	1:E:339:VAL:HG13	1.74	0.68
1:A:242:LEU:HD23	1:A:244:ASP:H	1.58	0.68
1:A:287:ILE:HD13	1:A:290:ARG:HH12	1.58	0.68
1:A:111:ASN:HB3	1:A:116:ARG:NH1	2.09	0.68
1:A:136:ILE:HD13	1:A:375:PHE:HE1	1.57	0.68
1:D:40:HIS:O	1:D:41:GLN:HG2	1.92	0.68
1:G:236:LEU:O	1:G:251:GLY:HA2	1.94	0.68
1:G:188:TYR:CE1	1:G:267:ILE:HG22	2.29	0.68
1:B:208:ILE:HG21	1:B:242:LEU:HD11	1.74	0.68
1:D:35:VAL:O	1:D:68:LYS:HB3	1.94	0.68
1:B:187:ASP:O	1:B:190:MET:HG2	1.93	0.68
1:J:151:ILE:CB	1:J:293:LEU:HD13	2.23	0.67
1:B:166:TYR:CE1	1:B:289:ILE:HG12	2.30	0.67
1:I:39:ARG:HG3	1:I:64:ILE:O	1.93	0.67
1:I:197:GLY:HA2	1:J:113:LYS:CB	2.23	0.67
1:H:213:LYS:O	1:H:217:CYS:HB2	1.94	0.67
1:E:8:LEU:HG	1:E:20:GLY:O	1.94	0.67
1:E:353:GLN:HA	1:E:356:TRP:CZ2	2.28	0.67
1:A:149:THR:HG23	1:A:166:TYR:HA	1.77	0.67
1:C:124:PHE:CZ	1:C:132:MET:HG2	2.29	0.67
1:H:107:GLU:HB2	1:H:134:VAL:HG22	1.75	0.67
1:I:219:VAL:HG22	1:I:258:PRO:HB3	1.75	0.67
1:E:236:LEU:O	1:E:251:GLY:HA2	1.93	0.67
1:B:250:ILE:HD12	1:B:254:ARG:HG2	1.77	0.67
1:H:27:PRO:HD3	1:H:340:TRP:CH2	2.30	0.67
1:C:90:PHE:HA	1:C:94:LEU:HD12	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:327:ILE:HD12	1:G:327:ILE:N	2.09	0.67
1:A:287:ILE:HA	1:A:290:ARG:NH1	2.08	0.67
1:J:337:TYR:O	1:J:341:ILE:HG12	1.95	0.67
1:I:142:LEU:HD22	1:I:165:ILE:HG21	1.77	0.67
1:I:170:ALA:O	1:I:375:PHE:HB3	1.96	0.67
1:J:50:LYS:HG3	1:J:57:GLU:OE1	1.94	0.66
1:G:213:LYS:O	1:G:217:CYS:HB2	1.94	0.66
1:J:187:ASP:O	1:J:190:MET:HG2	1.93	0.66
1:B:71:ILE:HG12	1:B:76:ILE:HG12	1.77	0.66
1:I:220:ALA:O	1:I:312:ARG:HD2	1.95	0.66
1:C:187:ASP:O	1:C:190:MET:HG2	1.95	0.66
1:D:219:VAL:HG22	1:D:258:PRO:HB3	1.77	0.66
1:H:116:ARG:HD3	1:H:370:VAL:HG11	1.77	0.66
1:C:41:GLN:HG2	1:C:43:VAL:H	1.59	0.66
1:E:7:ALA:O	1:E:22:ALA:HB2	1.96	0.66
1:G:188:TYR:CD1	1:G:267:ILE:HG22	2.30	0.66
1:H:270:GLU:HG3	1:H:271:SER:N	2.11	0.65
1:F:37:ARG:O	1:F:66:THR:HG23	1.96	0.65
1:F:188:TYR:CD1	1:F:267:ILE:HG22	2.31	0.65
1:C:188:TYR:CD1	1:C:267:ILE:HG22	2.31	0.65
1:F:120:THR:HA	1:F:132:MET:HE2	1.78	0.65
1:D:282:ILE:CG2	1:D:290:ARG:HG2	2.26	0.65
1:H:63:GLY:CA	1:J:288:ASP:H	2.10	0.65
1:F:140:LEU:HG	1:F:346:LEU:HD12	1.79	0.65
1:C:236:LEU:O	1:C:251:GLY:HA2	1.96	0.65
1:H:314:GLN:HE21	1:H:329:ILE:HG12	1.62	0.65
1:A:250:ILE:HD12	1:A:254:ARG:HG2	1.77	0.65
1:A:10:CYS:HA	1:A:18:LYS:O	1.97	0.65
1:E:111:ASN:HB3	1:E:116:ARG:NH1	2.11	0.65
1:B:236:LEU:O	1:B:251:GLY:HA2	1.95	0.65
1:I:70:PRO:O	1:I:76:ILE:HA	1.96	0.65
1:B:188:TYR:CE1	1:B:267:ILE:HG22	2.31	0.65
1:A:149:THR:HG21	1:A:292:ASP:OD2	1.97	0.65
1:J:25:ASP:O	1:J:341:ILE:HD12	1.97	0.64
1:C:289:ILE:HG22	1:C:293:LEU:CG	2.27	0.64
1:H:1:ASP:HB3	1:H:101:HIS:CE1	2.33	0.64
1:C:149:THR:HG22	1:C:296:ASN:HD22	1.62	0.64
1:D:124:PHE:CE2	1:D:359:LYS:HB2	2.33	0.64
1:A:213:LYS:O	1:A:217:CYS:HB2	1.96	0.64
1:D:90:PHE:HA	1:D:94:LEU:HD12	1.77	0.64
1:D:142:LEU:HD22	1:D:165:ILE:HG23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:112:PRO:HG2	1:F:115:ASN:OD1	1.97	0.64
1:I:136:ILE:O	1:I:140:LEU:HD13	1.97	0.64
1:H:314:GLN:NE2	1:H:329:ILE:HG12	2.12	0.64
1:G:107:GLU:HB2	1:G:134:VAL:HG22	1.78	0.64
1:C:50:LYS:HG3	1:C:52:SER:O	1.98	0.64
1:E:188:TYR:CE1	1:E:267:ILE:HG22	2.33	0.64
1:B:7:ALA:CB	1:B:104:LEU:HB2	2.24	0.64
1:G:166:TYR:CZ	1:G:289:ILE:HG12	2.32	0.64
1:B:151:ILE:HD12	1:B:164:PRO:HA	1.79	0.64
1:D:289:ILE:O	1:D:293:LEU:HG	1.96	0.64
1:E:63:GLY:HA3	1:G:287:ILE:HG21	1.78	0.64
1:E:12:ASN:HD21	1:E:71:ILE:HD11	1.62	0.63
1:D:99:GLU:HA	1:D:128:ASN:O	1.97	0.63
1:C:149:THR:CG2	1:C:292:ASP:HB2	2.28	0.63
1:E:142:LEU:HD22	1:E:165:ILE:CG2	2.28	0.63
1:F:194:THR:HG21	1:G:171:LEU:HD11	1.79	0.63
1:J:276:GLU:HA	1:J:279:TYR:CD1	2.34	0.63
1:G:250:ILE:HA	1:G:253:GLU:OE2	1.98	0.63
1:J:220:ALA:O	1:J:312:ARG:HD2	1.99	0.63
1:C:289:ILE:O	1:C:293:LEU:HG	1.97	0.63
1:F:136:ILE:HG21	1:F:375:PHE:CZ	2.34	0.63
1:H:122:ILE:O	1:H:126:THR:HB	1.98	0.63
1:D:43:VAL:HG21	1:F:171:LEU:CD1	2.29	0.62
1:H:164:PRO:HG3	1:H:174:ALA:HB3	1.81	0.62
1:D:142:LEU:HD22	1:D:165:ILE:CG2	2.29	0.62
1:B:107:GLU:HB2	1:B:134:VAL:HG22	1.81	0.62
1:B:29:ALA:HB2	1:B:93:GLU:HB2	1.82	0.62
1:G:299:MET:HB3	1:G:304:THR:HG21	1.80	0.62
1:I:285:CYS:O	1:I:286:ASP:HB2	1.99	0.62
1:G:151:ILE:HB	1:G:293:LEU:HD22	1.81	0.62
1:E:200:PHE:HA	1:E:205:GLU:OE2	2.00	0.62
1:I:286:ASP:HB3	1:I:289:ILE:CD1	2.28	0.62
1:G:116:ARG:HB3	1:G:370:VAL:HG21	1.80	0.62
1:G:250:ILE:HD12	1:G:254:ARG:HG2	1.80	0.62
1:I:50:LYS:HG3	1:I:57:GLU:OE1	2.00	0.62
1:J:151:ILE:HG22	1:J:297:ASN:HD22	1.65	0.62
1:G:248:ILE:HG22	1:G:250:ILE:HG23	1.82	0.62
1:E:107:GLU:HB2	1:E:134:VAL:HG22	1.81	0.62
1:H:36:GLY:HA3	1:H:65:LEU:HG	1.82	0.62
1:E:213:LYS:O	1:E:217:CYS:HB2	2.00	0.62
1:J:294:TYR:HB3	1:J:327:ILE:HD13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:166:TYR:CD2	1:I:289:ILE:HG12	2.35	0.61
1:E:250:ILE:HD12	1:E:254:ARG:HG2	1.80	0.61
1:F:286:ASP:HB3	1:F:289:ILE:HG13	1.82	0.61
1:C:116:ARG:CB	1:C:370:VAL:HG21	2.30	0.61
1:C:111:ASN:HB3	1:C:116:ARG:NH1	2.15	0.61
1:B:111:ASN:HB3	1:B:116:ARG:NH1	2.15	0.61
1:B:136:ILE:HD11	1:B:374:CYS:HB2	1.81	0.61
1:I:166:TYR:CE2	1:I:289:ILE:HG12	2.35	0.61
1:B:213:LYS:O	1:B:217:CYS:HB2	2.00	0.61
1:F:189:LEU:O	1:F:193:LEU:HD13	2.01	0.61
1:F:318:THR:HG22	1:F:327:ILE:HD12	1.83	0.61
1:A:7:ALA:O	1:A:22:ALA:HB2	2.00	0.61
1:H:45:VAL:HG21	1:J:169:TYR:H	1.66	0.61
1:J:353:GLN:HG3	1:J:356:TRP:CZ2	2.36	0.61
1:D:53:TYR:HB2	1:D:65:LEU:HD21	1.82	0.61
1:F:223:PHE:CD1	1:F:259:GLU:HG2	2.35	0.61
1:J:213:LYS:O	1:J:217:CYS:HB2	2.00	0.61
1:H:9:VAL:HG13	1:H:104:LEU:HD23	1.83	0.61
1:H:133:TYR:CD1	1:H:356:TRP:HA	2.36	0.61
1:H:8:LEU:HD21	1:H:90:PHE:CE1	2.36	0.61
1:G:20:GLY:HA2	1:G:94:LEU:HD21	1.82	0.61
1:J:283:MET:HA	1:J:290:ARG:NH2	2.15	0.61
1:F:6:THR:HG22	1:F:22:ALA:HB3	1.83	0.61
1:D:188:TYR:CD1	1:D:267:ILE:HG22	2.36	0.60
1:B:8:LEU:HD21	1:B:90:PHE:HE1	1.66	0.60
1:D:166:TYR:CE2	1:D:289:ILE:HG12	2.37	0.60
1:H:111:ASN:HB3	1:H:116:ARG:NH1	2.16	0.60
1:A:305:MET:SD	1:A:336:LYS:HB2	2.40	0.60
1:J:90:PHE:HA	1:J:94:LEU:HD12	1.82	0.60
1:B:156:GLY:O	1:B:157:ASP:HB2	2.00	0.60
1:H:195:GLU:HG3	1:H:196:ARG:N	2.16	0.60
1:D:345:ILE:O	1:D:349:LEU:HG	2.02	0.60
1:I:34:ILE:HD12	1:I:67:LEU:HD22	1.83	0.60
1:B:21:PHE:HB2	1:B:24:ASP:OD1	2.02	0.60
1:C:9:VAL:O	1:C:19:ALA:HA	2.02	0.60
1:G:208:ILE:HG21	1:G:242:LEU:HD11	1.83	0.60
1:E:124:PHE:CZ	1:E:132:MET:HG2	2.37	0.60
1:H:63:GLY:HA2	1:J:287:ILE:H	1.67	0.60
1:H:223:PHE:HB2	1:H:259:GLU:CD	2.22	0.60
1:B:189:LEU:O	1:B:193:LEU:HD13	2.02	0.60
1:I:144:ALA:HB2	1:I:342:GLY:CA	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4:GLU:HG3	1:G:5:THR:H	1.67	0.60
1:I:183:ARG:HG3	1:I:184:ASP:N	2.15	0.60
1:I:279:TYR:OH	1:I:317:ILE:HA	2.01	0.60
1:F:11:ASP:OD1	1:F:106:THR:HG21	2.01	0.60
1:F:321:ALA:HB1	1:F:322:PRO:HD2	1.84	0.60
1:J:136:ILE:O	1:J:140:LEU:HD13	2.01	0.60
1:D:250:ILE:HD12	1:D:254:ARG:HG2	1.82	0.60
1:G:142:LEU:HD22	1:G:165:ILE:HG12	1.83	0.60
1:E:5:THR:O	1:E:102:PRO:HG2	2.02	0.60
1:F:331:ALA:HB1	1:F:335:ARG:HH11	1.65	0.60
1:J:164:PRO:HB3	1:J:285:CYS:SG	2.42	0.59
1:C:116:ARG:HG2	1:C:370:VAL:HG11	1.83	0.59
1:I:201:VAL:HG21	1:J:110:LEU:HD13	1.83	0.59
1:A:71:ILE:HD13	1:A:76:ILE:HG12	1.83	0.59
1:H:219:VAL:HG12	1:H:312:ARG:HD2	1.84	0.59
1:F:289:ILE:HG22	1:F:293:LEU:HG	1.84	0.59
1:H:286:ASP:HB2	1:H:289:ILE:CD1	2.32	0.59
1:A:220:ALA:HB1	1:A:226:GLU:OE2	2.02	0.59
1:C:7:ALA:HB1	1:C:104:LEU:HB2	1.83	0.59
1:B:140:LEU:CD1	1:B:346:LEU:HD11	2.32	0.59
1:F:107:GLU:HB2	1:F:134:VAL:HG22	1.83	0.59
1:D:223:PHE:HB2	1:D:259:GLU:CD	2.23	0.59
1:D:10:CYS:HA	1:D:18:LYS:O	2.02	0.59
1:F:5:THR:HB	1:F:102:PRO:HG2	1.85	0.59
1:F:124:PHE:CE1	1:F:132:MET:HG2	2.38	0.59
1:F:136:ILE:HD13	1:F:375:PHE:CE1	2.38	0.59
1:G:289:ILE:HG22	1:G:293:LEU:CG	2.32	0.59
1:H:39:ARG:HB2	1:H:66:THR:HG22	1.85	0.59
1:A:133:TYR:CD1	1:A:356:TRP:HA	2.38	0.59
1:H:61:LYS:HB3	1:J:288:ASP:HB2	1.83	0.59
1:H:195:GLU:HG3	1:H:196:ARG:H	1.68	0.59
1:E:9:VAL:O	1:E:19:ALA:HA	2.02	0.59
1:B:7:ALA:O	1:B:22:ALA:HB2	2.01	0.59
1:H:136:ILE:HD12	1:H:169:TYR:CD2	2.38	0.59
1:C:144:ALA:HB2	1:C:342:GLY:HA2	1.85	0.59
1:D:18:LYS:HG2	1:D:30:VAL:HG12	1.84	0.59
1:H:276:GLU:HA	1:H:279:TYR:CD1	2.38	0.59
1:D:13:GLY:O	1:D:14:SER:HB2	2.03	0.59
1:H:189:LEU:O	1:H:193:LEU:HD13	2.03	0.58
1:G:110:LEU:HD21	1:G:177:ARG:CD	2.32	0.58
1:G:327:ILE:HD12	1:G:327:ILE:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:GLY:HA3	1:E:287:ILE:HG21	1.85	0.58
1:H:62:ARG:O	1:J:288:ASP:HB3	2.03	0.58
1:H:63:GLY:HA2	1:J:287:ILE:N	2.18	0.58
1:G:116:ARG:CG	1:G:370:VAL:HG11	2.34	0.58
1:F:286:ASP:HB3	1:F:289:ILE:CG1	2.33	0.58
1:I:136:ILE:HG21	1:I:375:PHE:CZ	2.39	0.58
1:E:70:PRO:O	1:E:76:ILE:HG12	2.04	0.58
1:F:279:TYR:OH	1:F:317:ILE:HA	2.03	0.58
1:F:223:PHE:HB2	1:F:259:GLU:CD	2.24	0.58
1:H:279:TYR:OH	1:H:317:ILE:HA	2.03	0.58
1:D:26:ALA:HB1	1:D:27:PRO:HD2	1.85	0.58
1:B:261:LEU:HD21	1:B:303:THR:HG21	1.84	0.58
1:D:58:ALA:HB1	1:D:65:LEU:HD11	1.84	0.58
1:J:94:LEU:HB3	1:J:96:VAL:HG22	1.85	0.58
1:A:220:ALA:O	1:A:312:ARG:HD2	2.04	0.58
1:I:99:GLU:HG3	1:I:127:PHE:O	2.03	0.58
1:J:71:ILE:HG12	1:J:76:ILE:HG12	1.86	0.58
1:D:22:ALA:CB	1:D:347:ALA:HB1	2.34	0.58
1:F:164:PRO:HG3	1:F:174:ALA:HB3	1.86	0.58
1:H:188:TYR:CD1	1:H:267:ILE:HG22	2.39	0.58
1:D:180:LEU:HD21	1:D:261:LEU:HA	1.85	0.58
1:D:171:LEU:HA	1:D:375:PHE:HB2	1.85	0.58
1:G:62:ARG:HG2	1:G:63:GLY:H	1.69	0.58
1:A:173:HIS:O	1:A:284:LYS:HD3	2.03	0.58
1:G:122:ILE:O	1:G:126:THR:HB	2.03	0.58
1:I:94:LEU:HB3	1:I:96:VAL:HG22	1.85	0.58
1:A:279:TYR:CE1	1:A:320:LEU:HB2	2.38	0.58
1:H:257:CYS:HB3	1:H:258:PRO:HD3	1.86	0.58
1:H:99:GLU:O	1:H:130:PRO:HD3	2.03	0.58
1:B:140:LEU:HG	1:B:346:LEU:CD1	2.31	0.58
1:F:105:LEU:HD13	1:F:119:MET:SD	2.44	0.58
1:J:219:VAL:HG22	1:J:258:PRO:HB3	1.85	0.58
1:B:261:LEU:HD11	1:B:303:THR:CG2	2.34	0.57
1:C:257:CYS:HB3	1:C:258:PRO:HD3	1.86	0.57
1:E:189:LEU:O	1:E:193:LEU:HD13	2.04	0.57
1:E:64:ILE:HD11	1:G:286:ASP:OD1	2.04	0.57
1:B:42:GLY:O	1:B:43:VAL:HB	2.03	0.57
1:C:178:LEU:HG	1:C:180:LEU:H	1.69	0.57
1:I:201:VAL:HG11	1:J:177:ARG:HB3	1.86	0.57
1:A:142:LEU:HD22	1:A:165:ILE:HG12	1.86	0.57
1:B:8:LEU:HD21	1:B:90:PHE:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:230:ALA:HA	1:H:236:LEU:HD22	1.87	0.57
1:A:289:ILE:HG22	1:A:293:LEU:HD11	1.87	0.57
1:F:257:CYS:HB3	1:F:258:PRO:HD3	1.87	0.57
1:A:136:ILE:HD13	1:A:375:PHE:CE1	2.38	0.57
1:D:189:LEU:O	1:D:193:LEU:HD13	2.04	0.57
1:I:242:LEU:HD23	1:I:244:ASP:H	1.70	0.57
1:J:172:PRO:O	1:J:173:HIS:HB2	2.04	0.57
1:J:362:TYR:HA	1:J:369:ILE:HG21	1.86	0.57
1:I:192:ILE:O	1:I:195:GLU:HG3	2.04	0.57
1:J:282:ILE:CG2	1:J:290:ARG:HG2	2.35	0.57
1:G:291:LYS:HG2	1:G:292:ASP:N	2.19	0.57
1:G:144:ALA:HB2	1:G:342:GLY:HA2	1.85	0.57
1:A:21:PHE:HB2	1:A:24:ASP:OD2	2.03	0.57
1:I:109:PRO:HB2	1:I:161:HIS:CE1	2.40	0.57
1:B:136:ILE:O	1:B:140:LEU:HD13	2.04	0.57
1:D:286:ASP:HB3	1:D:289:ILE:HD12	1.85	0.57
1:E:223:PHE:HB2	1:E:259:GLU:CD	2.25	0.57
1:F:43:VAL:HG13	1:F:44:MET:N	2.20	0.57
1:F:99:GLU:HA	1:F:128:ASN:O	2.04	0.57
1:A:37:ARG:O	1:A:66:THR:HG23	2.04	0.57
1:D:28:ARG:HG2	1:D:94:LEU:HD23	1.87	0.57
1:G:189:LEU:O	1:G:193:LEU:HD13	2.04	0.57
1:I:25:ASP:O	1:I:340:TRP:HZ3	1.87	0.56
1:G:104:LEU:CD2	1:G:347:ALA:HB2	2.35	0.56
1:E:353:GLN:HA	1:E:356:TRP:CE2	2.40	0.56
1:B:8:LEU:HB3	1:B:102:PRO:O	2.05	0.56
1:I:230:ALA:HA	1:I:236:LEU:CD2	2.35	0.56
1:I:252:ASN:HA	1:I:255:PHE:CE2	2.41	0.56
1:A:142:LEU:HG	1:A:147:ARG:O	2.05	0.56
1:G:23:GLY:HA2	1:G:348:SER:HB3	1.87	0.56
1:I:35:VAL:HG21	1:I:81:ASP:HB2	1.86	0.56
1:G:282:ILE:CG2	1:G:290:ARG:HG2	2.35	0.56
1:F:54:VAL:HG21	1:F:85:ILE:HA	1.87	0.56
1:J:282:ILE:HA	1:J:285:CYS:SG	2.45	0.56
1:D:136:ILE:HG21	1:D:375:PHE:CZ	2.40	0.56
1:D:151:ILE:HG22	1:D:297:ASN:HD22	1.69	0.56
1:G:110:LEU:O	1:G:110:LEU:HD22	2.05	0.56
1:C:136:ILE:HD12	1:C:169:TYR:CD2	2.40	0.56
1:G:4:GLU:HG3	1:G:5:THR:N	2.20	0.56
1:J:295:ALA:O	1:J:328:LYS:HB3	2.06	0.56
1:D:230:ALA:HA	1:D:236:LEU:HD22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ASP:OD2	1:A:183:ARG:HB3	2.06	0.56
1:I:362:TYR:CD1	1:I:369:ILE:HG21	2.40	0.56
1:F:142:LEU:HD22	1:F:165:ILE:CG2	2.35	0.56
1:G:285:CYS:O	1:G:286:ASP:HB2	2.06	0.56
1:A:142:LEU:HD22	1:A:165:ILE:HG21	1.88	0.56
1:C:21:PHE:HB2	1:C:24:ASP:OD2	2.06	0.56
1:F:124:PHE:CD2	1:F:359:LYS:HD3	2.41	0.56
1:G:151:ILE:CG2	1:G:297:ASN:HD22	2.19	0.56
1:E:137:GLN:HG3	1:E:339:VAL:CG1	2.35	0.56
1:A:151:ILE:HD12	1:A:164:PRO:HA	1.88	0.56
1:G:257:CYS:HB3	1:G:258:PRO:HD3	1.87	0.56
1:C:54:VAL:HG21	1:C:85:ILE:HA	1.88	0.56
1:I:357:ILE:CD1	1:I:373:LYS:HG3	2.36	0.56
1:H:264:PRO:HG2	1:H:272:ALA:C	2.27	0.56
1:I:189:LEU:O	1:I:193:LEU:HD13	2.06	0.56
1:E:219:VAL:HG22	1:E:258:PRO:HB3	1.88	0.56
1:C:279:TYR:OH	1:C:317:ILE:HA	2.06	0.56
1:H:124:PHE:CD2	1:H:359:LYS:HB2	2.41	0.55
1:A:299:MET:HB3	1:A:304:THR:HG21	1.87	0.55
1:A:178:LEU:HG	1:A:180:LEU:H	1.71	0.55
1:G:327:ILE:CD1	1:G:327:ILE:N	2.69	0.55
1:I:121:GLN:HG3	1:I:125:GLU:OE1	2.06	0.55
1:E:171:LEU:HA	1:E:375:PHE:CB	2.36	0.55
1:E:111:ASN:HB3	1:E:116:ARG:HH12	1.71	0.55
1:A:12:ASN:HD21	1:A:71:ILE:HD11	1.71	0.55
1:C:279:TYR:O	1:C:283:MET:HG2	2.07	0.55
1:H:345:ILE:HG22	1:H:345:ILE:O	2.06	0.55
1:E:220:ALA:O	1:E:312:ARG:HD2	2.06	0.55
1:E:5:THR:HG21	1:E:356:TRP:CZ2	2.42	0.55
1:J:147:ARG:HH21	1:J:296:ASN:HD21	1.53	0.55
1:F:219:VAL:HG12	1:F:312:ARG:HD2	1.89	0.55
1:E:172:PRO:HD3	1:E:375:PHE:HB2	1.87	0.55
1:J:6:THR:HG22	1:J:7:ALA:H	1.69	0.55
1:E:49:GLN:O	1:E:50:LYS:HG2	2.07	0.55
1:E:99:GLU:O	1:E:130:PRO:HD3	2.07	0.55
1:D:37:ARG:O	1:D:66:THR:HG23	2.06	0.55
1:J:213:LYS:HA	1:J:217:CYS:SG	2.47	0.55
1:I:73:HIS:CE1	1:I:183:ARG:HE	2.24	0.55
1:J:73:HIS:HA	1:J:159:VAL:HG13	1.88	0.55
1:H:136:ILE:HD13	1:H:375:PHE:CE1	2.42	0.55
1:E:105:LEU:HD13	1:E:119:MET:SD	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:HD23	1:A:209:VAL:HG13	1.87	0.55
1:B:185:LEU:HB3	1:B:257:CYS:SG	2.46	0.55
1:F:242:LEU:HD23	1:F:244:ASP:H	1.71	0.55
1:G:110:LEU:HD11	1:G:161:HIS:NE2	2.22	0.55
1:D:213:LYS:HA	1:D:217:CYS:SG	2.46	0.55
1:D:211:ASP:O	1:D:215:LYS:HG2	2.07	0.55
1:D:289:ILE:HG22	1:D:293:LEU:CG	2.37	0.55
1:G:135:ALA:HB1	1:G:140:LEU:HD11	1.88	0.55
1:I:8:LEU:O	1:I:104:LEU:HB3	2.07	0.55
1:H:294:TYR:HB3	1:H:327:ILE:HD13	1.89	0.55
1:H:167:GLU:O	1:H:167:GLU:HG2	2.07	0.55
1:J:287:ILE:HD13	1:J:290:ARG:NH1	2.20	0.54
1:I:151:ILE:CD1	1:I:164:PRO:HA	2.37	0.54
1:F:32:PRO:HG3	1:F:59:GLN:OE1	2.07	0.54
1:D:279:TYR:OH	1:D:317:ILE:HA	2.06	0.54
1:I:142:LEU:HD22	1:I:165:ILE:CG2	2.37	0.54
1:A:189:LEU:O	1:A:193:LEU:HD13	2.07	0.54
1:D:220:ALA:O	1:D:312:ARG:HD2	2.08	0.54
1:J:185:LEU:HD11	1:J:261:LEU:HD11	1.90	0.54
1:I:197:GLY:HA2	1:J:113:LYS:HB2	1.89	0.54
1:I:337:TYR:O	1:I:341:ILE:HG12	2.08	0.54
1:J:183:ARG:HG3	1:J:184:ASP:N	2.22	0.54
1:H:73:HIS:HA	1:H:159:VAL:HG23	1.88	0.54
1:I:61:LYS:O	1:I:65:LEU:HD13	2.08	0.54
1:H:7:ALA:O	1:H:22:ALA:HB2	2.07	0.54
1:F:164:PRO:HG3	1:F:174:ALA:CB	2.37	0.54
1:G:286:ASP:CB	1:G:289:ILE:HD12	2.38	0.54
1:G:90:PHE:HA	1:G:94:LEU:HD12	1.89	0.54
1:G:104:LEU:HD22	1:G:347:ALA:HB2	1.90	0.54
1:G:9:VAL:O	1:G:19:ALA:HA	2.06	0.54
1:A:117:GLU:OE1	1:A:367:PRO:HA	2.07	0.54
1:C:144:ALA:HA	1:C:345:ILE:HD12	1.88	0.54
1:I:31:PHE:HE2	1:I:85:ILE:HG23	1.73	0.54
1:B:27:PRO:HD3	1:B:340:TRP:CH2	2.43	0.54
1:C:136:ILE:HD12	1:C:169:TYR:HD2	1.72	0.54
1:H:116:ARG:HD3	1:H:370:VAL:CG1	2.37	0.54
1:J:12:ASN:H	1:J:106:THR:HG22	1.71	0.54
1:E:188:TYR:CD1	1:E:267:ILE:HG22	2.41	0.54
1:J:90:PHE:O	1:J:94:LEU:HB2	2.08	0.54
1:A:133:TYR:CE1	1:A:356:TRP:HA	2.43	0.54
1:A:26:ALA:HB1	1:A:27:PRO:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:TYR:CE1	1:B:356:TRP:HA	2.43	0.54
1:C:180:LEU:HD21	1:C:261:LEU:CA	2.30	0.54
1:D:140:LEU:HB3	1:D:342:GLY:HA3	1.90	0.54
1:D:285:CYS:O	1:D:286:ASP:HB2	2.07	0.54
1:D:71:ILE:HG12	1:D:76:ILE:HG12	1.89	0.54
1:H:8:LEU:HD21	1:H:90:PHE:HE1	1.71	0.54
1:J:365:ALA:HB3	1:J:369:ILE:HD13	1.90	0.54
1:D:276:GLU:HA	1:D:279:TYR:CD1	2.42	0.54
1:J:165:ILE:HG12	1:J:167:GLU:H	1.73	0.54
1:D:48:GLY:O	1:D:49:GLN:HB2	2.08	0.54
1:I:124:PHE:CE1	1:I:132:MET:HG2	2.43	0.54
1:B:6:THR:O	1:B:7:ALA:HB2	2.07	0.54
1:D:47:MET:HG3	1:D:48:GLY:N	2.23	0.54
1:E:171:LEU:HA	1:E:375:PHE:HB2	1.90	0.54
1:H:116:ARG:HH11	1:H:116:ARG:HG3	1.71	0.54
1:I:90:PHE:HA	1:I:94:LEU:HD12	1.90	0.54
1:I:151:ILE:CG2	1:I:297:ASN:HD22	2.21	0.53
1:E:340:TRP:CE3	1:E:341:ILE:HD13	2.43	0.53
1:E:64:ILE:HD12	1:G:288:ASP:HB2	1.89	0.53
1:J:124:PHE:CE1	1:J:132:MET:HG2	2.43	0.53
1:D:158:GLY:O	1:D:159:VAL:HG13	2.08	0.53
1:F:39:ARG:HD2	1:F:63:GLY:O	2.08	0.53
1:J:287:ILE:HA	1:J:290:ARG:HH11	1.73	0.53
1:J:230:ALA:HA	1:J:236:LEU:CD2	2.35	0.53
1:E:230:ALA:HA	1:E:236:LEU:HD22	1.91	0.53
1:C:110:LEU:HD12	1:C:177:ARG:HG3	1.89	0.53
1:I:200:PHE:HB3	1:I:205:GLU:HG3	1.89	0.53
1:J:121:GLN:HG3	1:J:125:GLU:OE1	2.09	0.53
1:F:137:GLN:HG3	1:F:339:VAL:CG1	2.38	0.53
1:G:164:PRO:HG3	1:G:174:ALA:CB	2.38	0.53
1:D:9:VAL:O	1:D:19:ALA:HA	2.07	0.53
1:D:208:ILE:HG21	1:D:242:LEU:HD11	1.89	0.53
1:J:289:ILE:O	1:J:293:LEU:HB3	2.09	0.53
1:H:136:ILE:HD12	1:H:169:TYR:HD2	1.73	0.53
1:G:109:PRO:C	1:G:110:LEU:HD13	2.28	0.53
1:H:104:LEU:HD22	1:H:347:ALA:CB	2.37	0.53
1:I:220:ALA:HB1	1:I:226:GLU:OE2	2.09	0.53
1:F:276:GLU:HA	1:F:279:TYR:CD1	2.44	0.53
1:C:276:GLU:HA	1:C:279:TYR:CD1	2.44	0.53
1:G:223:PHE:CD1	1:G:259:GLU:HG2	2.44	0.53
1:D:121:GLN:HG3	1:D:125:GLU:OE1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:178:LEU:HG	1:E:180:LEU:H	1.73	0.53
1:C:109:PRO:HB2	1:C:161:HIS:CE1	2.44	0.53
1:G:63:GLY:HA3	1:I:287:ILE:CG2	2.33	0.53
1:A:172:PRO:O	1:A:173:HIS:HB2	2.08	0.53
1:H:346:LEU:HD22	1:H:352:PHE:CD1	2.44	0.53
1:H:189:LEU:HD23	1:H:209:VAL:HG13	1.91	0.53
1:J:257:CYS:HB3	1:J:258:PRO:HD3	1.89	0.53
1:G:223:PHE:HB2	1:G:259:GLU:CD	2.30	0.53
1:C:103:THR:O	1:C:132:MET:HA	2.09	0.53
1:C:8:LEU:HD12	1:C:20:GLY:O	2.08	0.53
1:G:133:TYR:CE1	1:G:356:TRP:HA	2.44	0.53
1:G:151:ILE:HG22	1:G:297:ASN:HD22	1.74	0.53
1:D:252:ASN:HA	1:D:255:PHE:CE2	2.44	0.53
1:F:189:LEU:HD23	1:F:209:VAL:HG13	1.89	0.53
1:H:21:PHE:HB2	1:H:24:ASP:OD2	2.09	0.53
1:E:6:THR:CG2	1:E:22:ALA:HB3	2.37	0.53
1:F:20:GLY:HA2	1:F:94:LEU:HD21	1.91	0.53
1:D:70:PRO:O	1:D:76:ILE:HA	2.09	0.53
1:B:279:TYR:OH	1:B:317:ILE:HA	2.08	0.53
1:G:276:GLU:HA	1:G:279:TYR:CD1	2.43	0.53
1:B:37:ARG:HG3	1:B:38:PRO:HD2	1.91	0.53
1:I:172:PRO:O	1:I:173:HIS:HB2	2.09	0.53
1:I:189:LEU:HD23	1:I:209:VAL:HG13	1.91	0.52
1:B:257:CYS:HB3	1:B:258:PRO:HD3	1.91	0.52
1:I:110:LEU:HD12	1:I:177:ARG:HB2	1.90	0.52
1:I:12:ASN:H	1:I:106:THR:HG22	1.74	0.52
1:A:257:CYS:HB3	1:A:258:PRO:HD3	1.90	0.52
1:G:272:ALA:HB3	1:G:276:GLU:HB2	1.90	0.52
1:J:284:LYS:HZ2	1:J:284:LYS:HB2	1.75	0.52
1:F:5:THR:C	1:F:102:PRO:HG2	2.29	0.52
1:E:291:LYS:HG2	1:E:292:ASP:N	2.24	0.52
1:I:236:LEU:HA	1:I:254:ARG:HH21	1.74	0.52
1:D:289:ILE:HG22	1:D:293:LEU:HG	1.91	0.52
1:I:213:LYS:O	1:I:217:CYS:HB2	2.10	0.52
1:H:111:ASN:HB3	1:H:116:ARG:HH12	1.74	0.52
1:J:220:ALA:HB1	1:J:226:GLU:OE2	2.10	0.52
1:A:256:ARG:O	1:A:259:GLU:HB3	2.09	0.52
1:G:180:LEU:CD2	1:G:261:LEU:HA	2.37	0.52
1:G:140:LEU:HG	1:G:346:LEU:HD12	1.92	0.52
1:J:11:ASP:HB3	1:J:18:LYS:HB2	1.91	0.52
1:G:255:PHE:C	1:G:258:PRO:HD2	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:164:PRO:HG3	1:J:285:CYS:SG	2.49	0.52
1:F:6:THR:O	1:F:7:ALA:HB2	2.10	0.52
1:I:188:TYR:HD2	1:I:257:CYS:SG	2.33	0.52
1:G:327:ILE:CD1	1:G:327:ILE:H	2.22	0.52
1:A:255:PHE:C	1:A:258:PRO:HD2	2.30	0.52
1:J:281:SER:HA	1:J:284:LYS:NZ	2.24	0.52
1:F:171:LEU:H	1:F:171:LEU:HD12	1.74	0.52
1:I:219:VAL:HG23	1:I:306:TYR:HB2	1.91	0.52
1:H:116:ARG:HB3	1:H:370:VAL:HG21	1.92	0.52
1:E:283:MET:HG2	1:E:290:ARG:NH2	2.25	0.52
1:H:110:LEU:HD13	1:H:177:ARG:HB2	1.92	0.52
1:A:287:ILE:HD13	1:A:290:ARG:NH1	2.24	0.52
1:I:202:THR:HG23	1:J:177:ARG:NH2	2.25	0.52
1:J:293:LEU:HD12	1:J:293:LEU:C	2.30	0.52
1:H:299:MET:HB3	1:H:304:THR:CG2	2.35	0.52
1:D:140:LEU:HD23	1:D:343:GLY:HA2	1.91	0.52
1:F:116:ARG:HG2	1:F:370:VAL:HG11	1.91	0.52
1:A:103:THR:O	1:A:132:MET:HA	2.10	0.52
1:B:286:ASP:HB3	1:B:289:ILE:HD12	1.92	0.52
1:F:12:ASN:HB3	1:F:71:ILE:HD13	1.92	0.52
1:G:167:GLU:O	1:G:167:GLU:HG2	2.10	0.52
1:H:230:ALA:HA	1:H:236:LEU:CD2	2.41	0.51
1:I:357:ILE:HD11	1:I:373:LYS:HG3	1.91	0.51
1:F:169:TYR:HE1	1:F:355:MET:SD	2.32	0.51
1:J:283:MET:HA	1:J:290:ARG:HH21	1.74	0.51
1:B:342:GLY:O	1:B:346:LEU:HG	2.11	0.51
1:F:5:THR:HB	1:F:102:PRO:CG	2.41	0.51
1:G:289:ILE:O	1:G:293:LEU:HG	2.11	0.51
1:E:9:VAL:HG22	1:E:104:LEU:HB3	1.93	0.51
1:B:243:PRO:O	1:B:244:ASP:HB2	2.09	0.51
1:I:167:GLU:HG2	1:I:167:GLU:O	2.11	0.51
1:I:8:LEU:HD23	1:I:102:PRO:O	2.11	0.51
1:C:365:ALA:HB3	1:C:369:ILE:HD13	1.93	0.51
1:H:63:GLY:N	1:J:287:ILE:HB	2.26	0.51
1:B:163:VAL:HG11	1:B:375:PHE:CZ	2.46	0.51
1:C:172:PRO:HD3	1:C:375:PHE:HB2	1.93	0.51
1:D:22:ALA:HB1	1:D:347:ALA:HB1	1.92	0.51
1:B:41:GLN:C	1:B:43:VAL:H	2.13	0.51
1:H:270:GLU:HG3	1:H:271:SER:H	1.75	0.51
1:I:242:LEU:HD22	1:I:244:ASP:HB3	1.92	0.51
1:H:294:TYR:HB3	1:H:327:ILE:CD1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:PRO:HB2	1:F:161:HIS:CE1	2.45	0.51
1:I:178:LEU:HG	1:I:180:LEU:H	1.75	0.51
1:H:61:LYS:NZ	1:H:61:LYS:HB2	2.26	0.51
1:F:94:LEU:HB3	1:F:96:VAL:HG22	1.92	0.51
1:H:314:GLN:HE22	1:H:328:LYS:HA	1.75	0.51
1:A:180:LEU:HD21	1:A:261:LEU:HA	1.92	0.51
1:A:181:ALA:O	1:A:184:ASP:HB2	2.10	0.51
1:D:286:ASP:HB3	1:D:289:ILE:CD1	2.41	0.51
1:C:223:PHE:HB2	1:C:259:GLU:CD	2.30	0.51
1:H:252:ASN:HA	1:H:255:PHE:CE2	2.46	0.51
1:H:116:ARG:HG2	1:H:116:ARG:HH11	1.76	0.51
1:C:151:ILE:CG1	1:C:293:LEU:HD22	2.41	0.50
1:F:43:VAL:HG22	1:F:44:MET:H	1.77	0.50
1:A:105:LEU:HD13	1:A:119:MET:SD	2.50	0.50
1:E:71:ILE:HD13	1:E:76:ILE:HG12	1.93	0.50
1:D:248:ILE:HG22	1:D:250:ILE:HG23	1.92	0.50
1:F:219:VAL:HG22	1:F:258:PRO:HB3	1.92	0.50
1:G:54:VAL:HG23	1:G:85:ILE:HD13	1.92	0.50
1:J:193:LEU:HB3	1:J:198:TYR:O	2.11	0.50
1:I:289:ILE:O	1:I:293:LEU:HG	2.11	0.50
1:D:8:LEU:HD12	1:D:20:GLY:O	2.11	0.50
1:J:236:LEU:HA	1:J:254:ARG:HH21	1.77	0.50
1:C:140:LEU:HG	1:C:346:LEU:HD12	1.92	0.50
1:J:252:ASN:HA	1:J:255:PHE:CE2	2.46	0.50
1:C:161:HIS:NE2	1:C:177:ARG:HG2	2.25	0.50
1:F:166:TYR:CE1	1:F:289:ILE:HD13	2.47	0.50
1:H:213:LYS:HA	1:H:217:CYS:SG	2.50	0.50
1:H:61:LYS:HA	1:J:291:LYS:HD2	1.94	0.50
1:D:140:LEU:HD23	1:D:343:GLY:CA	2.41	0.50
1:D:189:LEU:HD23	1:D:209:VAL:HG13	1.92	0.50
1:A:58:ALA:HB1	1:A:65:LEU:CD2	2.37	0.50
1:B:124:PHE:CZ	1:B:359:LYS:HB2	2.47	0.50
1:B:180:LEU:HD11	1:B:267:ILE:CD1	2.41	0.50
1:J:189:LEU:O	1:J:193:LEU:HD13	2.11	0.50
1:I:71:ILE:HG12	1:I:76:ILE:HG12	1.94	0.50
1:J:314:GLN:OE1	1:J:329:ILE:HG12	2.12	0.50
1:E:139:VAL:HG11	1:E:169:TYR:CE2	2.47	0.50
1:J:150:GLY:HA2	1:J:293:LEU:HA	1.93	0.50
1:H:178:LEU:HG	1:H:180:LEU:H	1.76	0.50
1:I:198:TYR:CZ	1:I:248:ILE:HA	2.47	0.50
1:F:63:GLY:HA3	1:H:287:ILE:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:306:TYR:H	1:H:306:TYR:HD1	1.60	0.50
1:D:103:THR:O	1:D:132:MET:HB2	2.11	0.50
1:C:144:ALA:HA	1:C:345:ILE:CD1	2.42	0.50
1:A:287:ILE:HA	1:A:290:ARG:HH12	1.74	0.50
1:E:136:ILE:O	1:E:140:LEU:HD13	2.12	0.50
1:E:110:LEU:HD21	1:E:175:ILE:HD11	1.94	0.50
1:I:213:LYS:HD2	1:I:306:TYR:OH	2.12	0.50
1:B:236:LEU:HA	1:B:254:ARG:HH21	1.76	0.50
1:B:189:LEU:HD23	1:B:209:VAL:HG13	1.94	0.50
1:D:223:PHE:CD1	1:D:259:GLU:HG2	2.46	0.50
1:A:123:MET:SD	1:A:132:MET:SD	3.10	0.50
1:D:299:MET:HB3	1:D:304:THR:HG21	1.93	0.50
1:D:149:THR:HB	1:D:292:ASP:OD1	2.11	0.50
1:C:358:THR:HG22	1:C:359:LYS:H	1.76	0.50
1:B:136:ILE:HD11	1:B:374:CYS:CB	2.42	0.49
1:D:107:GLU:HB2	1:D:134:VAL:HG22	1.94	0.49
1:A:337:TYR:O	1:A:341:ILE:HG13	2.12	0.49
1:C:196:ARG:O	1:C:196:ARG:HD3	2.12	0.49
1:C:14:SER:HB2	1:C:157:ASP:HB3	1.94	0.49
1:C:135:ALA:HB1	1:C:140:LEU:HD11	1.94	0.49
1:D:283:MET:HG2	1:D:290:ARG:NH2	2.27	0.49
1:J:35:VAL:HG21	1:J:81:ASP:HB2	1.94	0.49
1:B:255:PHE:C	1:B:258:PRO:HD2	2.32	0.49
1:J:281:SER:HA	1:J:284:LYS:HZ2	1.78	0.49
1:A:291:LYS:H	1:A:291:LYS:HD2	1.77	0.49
1:B:180:LEU:HD11	1:B:267:ILE:HD13	1.94	0.49
1:J:279:TYR:CE1	1:J:320:LEU:HB2	2.47	0.49
1:H:346:LEU:HD13	1:H:352:PHE:CE1	2.48	0.49
1:E:109:PRO:HB2	1:E:161:HIS:CE1	2.48	0.49
1:B:223:PHE:HB2	1:B:259:GLU:CD	2.33	0.49
1:I:164:PRO:HD2	1:I:175:ILE:HG22	1.95	0.49
1:J:221:LEU:HD11	1:J:315:LYS:HD3	1.95	0.49
1:E:140:LEU:CD1	1:E:346:LEU:HD11	2.42	0.49
1:J:216:LEU:HD22	1:J:238:LYS:HD2	1.93	0.49
1:B:172:PRO:O	1:B:173:HIS:HB2	2.12	0.49
1:I:188:TYR:CE1	1:I:267:ILE:HG22	2.47	0.49
1:A:111:ASN:HB3	1:A:116:ARG:HH12	1.76	0.49
1:F:104:LEU:HD22	1:F:347:ALA:HB2	1.93	0.49
1:H:155:SER:OG	1:H:160:THR:HA	2.13	0.49
1:D:147:ARG:HH21	1:D:296:ASN:HD21	1.61	0.49
1:G:220:ALA:O	1:G:312:ARG:HD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:63:GLY:HA2	1:I:287:ILE:HD13	1.95	0.49
1:C:213:LYS:HA	1:C:217:CYS:SG	2.53	0.49
1:C:230:ALA:HA	1:C:236:LEU:HD22	1.95	0.49
1:E:47:MET:HA	1:G:166:TYR:CE2	2.48	0.49
1:F:213:LYS:HA	1:F:217:CYS:SG	2.52	0.49
1:J:255:PHE:C	1:J:258:PRO:HD2	2.33	0.49
1:B:286:ASP:HB3	1:B:289:ILE:CD1	2.43	0.49
1:B:286:ASP:O	1:B:289:ILE:HB	2.12	0.49
1:A:63:GLY:CA	1:C:287:ILE:HG21	2.24	0.49
1:E:8:LEU:HB3	1:E:102:PRO:O	2.12	0.49
1:E:140:LEU:HG	1:E:346:LEU:HD11	1.94	0.49
1:F:133:TYR:HD1	1:F:357:ILE:H	1.60	0.49
1:I:144:ALA:HA	1:I:345:ILE:HG13	1.95	0.48
1:C:8:LEU:HB3	1:C:103:THR:HA	1.95	0.48
1:D:219:VAL:HG22	1:D:258:PRO:CB	2.42	0.48
1:D:149:THR:OG1	1:D:292:ASP:HB2	2.13	0.48
1:F:179:ASP:OD2	1:F:269:MET:HE1	2.13	0.48
1:A:120:THR:HG23	1:A:124:PHE:CE1	2.48	0.48
1:E:38:PRO:HG3	1:E:44:MET:SD	2.53	0.48
1:G:17:VAL:HG23	1:G:33:SER:HB2	1.94	0.48
1:G:331:ALA:HB1	1:G:335:ARG:HH11	1.79	0.48
1:A:140:LEU:HG	1:A:346:LEU:HD11	1.95	0.48
1:F:188:TYR:CE1	1:F:267:ILE:HG22	2.48	0.48
1:B:260:THR:HG23	1:B:267:ILE:HG21	1.95	0.48
1:B:151:ILE:HD12	1:B:164:PRO:CA	2.43	0.48
1:A:353:GLN:HA	1:A:356:TRP:CE2	2.48	0.48
1:E:270:GLU:HG2	1:E:271:SER:N	2.28	0.48
1:C:70:PRO:O	1:C:76:ILE:HG23	2.12	0.48
1:F:314:GLN:OE1	1:F:329:ILE:HG12	2.13	0.48
1:I:151:ILE:HD12	1:I:164:PRO:HA	1.95	0.48
1:I:197:GLY:HA2	1:J:113:LYS:CG	2.42	0.48
1:J:39:ARG:HD2	1:J:63:GLY:O	2.13	0.48
1:J:372:ARG:HA	1:J:372:ARG:CZ	2.44	0.48
1:J:278:THR:HG22	1:J:282:ILE:HD12	1.96	0.48
1:C:236:LEU:HA	1:C:254:ARG:HH21	1.77	0.48
1:E:172:PRO:O	1:E:173:HIS:HB2	2.13	0.48
1:H:353:GLN:HG3	1:H:356:TRP:CZ2	2.48	0.48
1:C:41:GLN:HG2	1:C:43:VAL:N	2.28	0.48
1:A:10:CYS:HB3	1:A:105:LEU:HD23	1.95	0.48
1:I:157:ASP:OD2	1:I:183:ARG:HB3	2.14	0.48
1:I:193:LEU:HB3	1:I:198:TYR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:TYR:CE1	1:C:356:TRP:HA	2.48	0.48
1:A:14:SER:CB	1:A:157:ASP:HB3	2.44	0.48
1:F:172:PRO:O	1:F:173:HIS:CB	2.62	0.48
1:G:10:CYS:HA	1:G:18:LYS:O	2.13	0.48
1:H:31:PHE:HZ	1:H:89:THR:HG1	1.59	0.48
1:E:28:ARG:HB2	1:E:94:LEU:HD23	1.96	0.48
1:C:136:ILE:HD13	1:C:375:PHE:HE1	1.75	0.48
1:B:142:LEU:HD22	1:B:165:ILE:HG21	1.96	0.48
1:G:23:GLY:HA2	1:G:348:SER:CB	2.44	0.48
1:F:183:ARG:HB2	1:F:183:ARG:HH11	1.79	0.48
1:I:223:PHE:HB2	1:I:259:GLU:CD	2.34	0.48
1:H:172:PRO:O	1:H:173:HIS:HB2	2.14	0.48
1:J:151:ILE:CG2	1:J:293:LEU:HD13	2.44	0.48
1:G:213:LYS:HA	1:G:217:CYS:SG	2.54	0.48
1:B:260:THR:CG2	1:B:267:ILE:HG21	2.44	0.48
1:B:252:ASN:HA	1:B:255:PHE:CE2	2.49	0.48
1:C:189:LEU:O	1:C:193:LEU:HD13	2.13	0.48
1:F:211:ASP:O	1:F:215:LYS:HG2	2.13	0.48
1:I:304:THR:O	1:I:309:ILE:HG21	2.14	0.48
1:G:166:TYR:CE1	1:G:289:ILE:HG12	2.48	0.48
1:J:301:GLY:O	1:J:305:MET:HG2	2.14	0.48
1:F:147:ARG:HE	1:F:296:ASN:ND2	2.12	0.48
1:I:155:SER:O	1:I:301:GLY:HA3	2.14	0.48
1:D:243:PRO:O	1:D:244:ASP:HB2	2.13	0.48
1:J:290:ARG:HA	1:J:293:LEU:CD2	2.43	0.48
1:E:171:LEU:HA	1:E:375:PHE:CG	2.49	0.48
1:I:219:VAL:HG22	1:I:258:PRO:CB	2.43	0.48
1:B:178:LEU:HG	1:B:180:LEU:H	1.79	0.48
1:G:20:GLY:HA2	1:G:94:LEU:CD2	2.43	0.48
1:I:305:MET:SD	1:I:336:LYS:HB2	2.54	0.48
1:J:192:ILE:HG21	1:J:256:ARG:HD2	1.95	0.48
1:H:61:LYS:HB3	1:J:288:ASP:CB	2.44	0.47
1:D:272:ALA:HB3	1:D:276:GLU:HB2	1.95	0.47
1:D:305:MET:HE3	1:D:336:LYS:HD2	1.96	0.47
1:J:345:ILE:O	1:J:349:LEU:HG	2.14	0.47
1:J:113:LYS:HA	1:J:116:ARG:HD3	1.96	0.47
1:B:267:ILE:HG13	1:B:268:GLY:N	2.29	0.47
1:H:345:ILE:HG23	1:H:349:LEU:HD12	1.96	0.47
1:D:61:LYS:HB2	1:D:61:LYS:NZ	2.29	0.47
1:D:183:ARG:HG3	1:D:184:ASP:N	2.29	0.47
1:B:166:TYR:CG	1:B:167:GLU:N	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:133:TYR:CD2	1:H:352:PHE:HZ	2.32	0.47
1:I:282:ILE:CG2	1:I:290:ARG:HG2	2.44	0.47
1:H:61:LYS:O	1:J:288:ASP:HA	2.14	0.47
1:C:139:VAL:HG21	1:C:169:TYR:CD2	2.49	0.47
1:C:248:ILE:HG22	1:C:250:ILE:HG23	1.96	0.47
1:E:213:LYS:HA	1:E:217:CYS:SG	2.54	0.47
1:G:279:TYR:OH	1:G:317:ILE:HA	2.14	0.47
1:D:294:TYR:HB3	1:D:327:ILE:HD13	1.95	0.47
1:G:37:ARG:O	1:G:66:THR:HG23	2.13	0.47
1:J:88:HIS:O	1:J:92:ASN:HB2	2.15	0.47
1:D:8:LEU:CB	1:D:102:PRO:O	2.63	0.47
1:I:255:PHE:C	1:I:258:PRO:HD2	2.35	0.47
1:G:151:ILE:CD1	1:G:164:PRO:HA	2.44	0.47
1:D:39:ARG:HG3	1:D:40:HIS:H	1.80	0.47
1:C:220:ALA:O	1:C:312:ARG:HD2	2.15	0.47
1:E:122:ILE:O	1:E:126:THR:HB	2.14	0.47
1:J:279:TYR:O	1:J:283:MET:HG2	2.13	0.47
1:H:192:ILE:HG21	1:H:256:ARG:HD2	1.95	0.47
1:A:135:ALA:HB1	1:A:140:LEU:HD11	1.97	0.47
1:A:172:PRO:HD3	1:A:375:PHE:HB2	1.97	0.47
1:I:218:TYR:O	1:I:258:PRO:HG2	2.15	0.47
1:I:36:GLY:HA2	1:I:66:THR:O	2.14	0.47
1:E:236:LEU:HA	1:E:254:ARG:HH21	1.80	0.47
1:F:300:SER:HA	1:F:335:ARG:HB2	1.96	0.47
1:A:314:GLN:OE1	1:A:329:ILE:HG12	2.14	0.47
1:J:219:VAL:HG22	1:J:258:PRO:CB	2.44	0.47
1:F:220:ALA:O	1:F:312:ARG:HD2	2.15	0.47
1:A:304:THR:HG22	1:A:309:ILE:HD12	1.97	0.47
1:J:211:ASP:O	1:J:215:LYS:HG2	2.14	0.47
1:H:38:PRO:HA	1:H:64:ILE:HG23	1.97	0.47
1:D:289:ILE:HG22	1:D:293:LEU:HD11	1.96	0.47
1:F:252:ASN:HA	1:F:255:PHE:CE2	2.49	0.47
1:A:345:ILE:O	1:A:349:LEU:HG	2.15	0.47
1:B:289:ILE:HG22	1:B:293:LEU:CD1	2.40	0.47
1:G:230:ALA:HA	1:G:236:LEU:HD22	1.96	0.47
1:G:150:GLY:O	1:G:165:ILE:HG21	2.15	0.47
1:B:27:PRO:HD3	1:B:340:TRP:CZ2	2.50	0.47
1:D:192:ILE:HG21	1:D:256:ARG:HD2	1.96	0.47
1:B:110:LEU:HD12	1:B:161:HIS:CD2	2.50	0.47
1:F:299:MET:HB3	1:F:304:THR:HG21	1.96	0.47
1:F:167:GLU:O	1:F:167:GLU:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:174:ALA:HB1	1:I:285:CYS:HA	1.96	0.47
1:C:200:PHE:HZ	1:C:248:ILE:HD11	1.79	0.47
1:B:289:ILE:CG2	1:B:293:LEU:HD11	2.41	0.47
1:F:8:LEU:HD23	1:F:21:PHE:HA	1.97	0.47
1:J:135:ALA:HB1	1:J:140:LEU:HD11	1.97	0.47
1:F:61:LYS:HG2	1:H:291:LYS:CE	2.45	0.47
1:B:166:TYR:CD1	1:B:289:ILE:HG12	2.49	0.46
1:H:10:CYS:O	1:H:105:LEU:HA	2.15	0.46
1:B:213:LYS:HA	1:B:217:CYS:SG	2.55	0.46
1:C:272:ALA:HB3	1:C:276:GLU:HB2	1.97	0.46
1:A:124:PHE:CE1	1:A:132:MET:HB3	2.50	0.46
1:D:57:GLU:HG2	1:D:61:LYS:HE3	1.97	0.46
1:G:246:GLN:NE2	1:H:113:LYS:HE3	2.29	0.46
1:J:278:THR:HG22	1:J:282:ILE:CD1	2.45	0.46
1:H:257:CYS:O	1:H:260:THR:HB	2.15	0.46
1:A:230:ALA:HA	1:A:236:LEU:HD22	1.97	0.46
1:D:53:TYR:HB2	1:D:65:LEU:CD2	2.44	0.46
1:I:270:GLU:HG2	1:I:271:SER:N	2.30	0.46
1:D:123:MET:HB2	1:D:132:MET:SD	2.55	0.46
1:A:286:ASP:HB3	1:A:289:ILE:CD1	2.42	0.46
1:A:180:LEU:CD2	1:A:261:LEU:HA	2.46	0.46
1:C:121:GLN:HG3	1:C:125:GLU:OE1	2.16	0.46
1:A:9:VAL:O	1:A:19:ALA:HA	2.15	0.46
1:J:153:LEU:HG	1:J:162:ASN:ND2	2.30	0.46
1:E:225:ASN:C	1:E:225:ASN:HD22	2.19	0.46
1:B:6:THR:O	1:B:7:ALA:CB	2.62	0.46
1:F:111:ASN:HB3	1:F:116:ARG:HH12	1.77	0.46
1:B:99:GLU:O	1:B:130:PRO:HD3	2.15	0.46
1:E:346:LEU:HD13	1:E:352:PHE:CZ	2.50	0.46
1:B:10:CYS:HA	1:B:18:LYS:O	2.16	0.46
1:G:7:ALA:HB2	1:G:102:PRO:HB2	1.96	0.46
1:J:371:HIS:HA	1:J:374:CYS:O	2.16	0.46
1:E:180:LEU:CD2	1:E:261:LEU:HA	2.39	0.46
1:F:289:ILE:O	1:F:293:LEU:HG	2.16	0.46
1:D:151:ILE:CG2	1:D:297:ASN:HD22	2.27	0.46
1:C:169:TYR:HE1	1:C:355:MET:SD	2.39	0.46
1:C:283:MET:SD	1:C:290:ARG:NH2	2.89	0.46
1:H:306:TYR:CD1	1:H:306:TYR:N	2.84	0.46
1:A:23:GLY:HA2	1:A:348:SER:OG	2.15	0.46
1:I:216:LEU:HD22	1:I:238:LYS:HD2	1.96	0.46
1:G:253:GLU:HA	1:G:256:ARG:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:221:LEU:HD13	1:J:311:ASP:OD1	2.16	0.46
1:J:62:ARG:HE	1:J:207:GLU:CB	2.28	0.46
1:G:24:ASP:O	1:G:25:ASP:HB3	2.16	0.46
1:J:123:MET:O	1:J:127:PHE:O	2.34	0.46
1:F:170:ALA:O	1:F:375:PHE:CD1	2.69	0.46
1:F:8:LEU:CD2	1:F:21:PHE:HA	2.46	0.46
1:F:21:PHE:HB2	1:F:24:ASP:OD2	2.16	0.46
1:B:300:SER:HA	1:B:335:ARG:HB2	1.98	0.46
1:G:141:SER:OG	1:G:152:VAL:HG11	2.15	0.46
1:B:12:ASN:H	1:B:106:THR:HG22	1.80	0.46
1:F:163:VAL:HA	1:F:175:ILE:HG22	1.97	0.46
1:E:142:LEU:HD22	1:E:165:ILE:HG23	1.98	0.46
1:E:110:LEU:HD12	1:E:177:ARG:HB2	1.97	0.46
1:E:189:LEU:HD23	1:E:209:VAL:HG13	1.97	0.46
1:C:223:PHE:CD1	1:C:259:GLU:HG2	2.51	0.46
1:C:337:TYR:O	1:C:341:ILE:HG12	2.15	0.46
1:D:155:SER:OG	1:D:160:THR:HA	2.15	0.46
1:F:171:LEU:O	1:F:171:LEU:HD13	2.15	0.46
1:H:124:PHE:CE2	1:H:359:LYS:HB2	2.51	0.46
1:E:223:PHE:CD1	1:E:259:GLU:HG2	2.51	0.46
1:C:260:THR:CG2	1:C:267:ILE:HG21	2.46	0.46
1:D:172:PRO:O	1:D:173:HIS:HB3	2.16	0.46
1:I:257:CYS:HB3	1:I:258:PRO:HD3	1.97	0.46
1:H:313:MET:HB2	1:H:329:ILE:HG13	1.98	0.46
1:D:10:CYS:HB3	1:D:105:LEU:CD2	2.46	0.46
1:G:137:GLN:HG3	1:G:339:VAL:HG13	1.98	0.46
1:D:7:ALA:HB1	1:D:104:LEU:HB2	1.98	0.46
1:E:35:VAL:HA	1:E:53:TYR:O	2.16	0.46
1:D:47:MET:HG3	1:D:48:GLY:H	1.80	0.45
1:I:39:ARG:HB3	1:I:66:THR:CG2	2.47	0.45
1:A:219:VAL:HG22	1:A:258:PRO:HB3	1.97	0.45
1:E:9:VAL:HG22	1:E:104:LEU:HD23	1.98	0.45
1:F:63:GLY:HA2	1:H:287:ILE:CD1	2.46	0.45
1:E:365:ALA:HB3	1:E:369:ILE:HD13	1.98	0.45
1:C:11:ASP:O	1:C:17:VAL:HG13	2.16	0.45
1:C:260:THR:HG23	1:C:267:ILE:CG2	2.47	0.45
1:G:103:THR:O	1:G:132:MET:HA	2.15	0.45
1:G:192:ILE:HG21	1:G:256:ARG:HD2	1.98	0.45
1:I:90:PHE:O	1:I:94:LEU:HB2	2.16	0.45
1:E:255:PHE:C	1:E:258:PRO:HD2	2.36	0.45
1:H:110:LEU:CD1	1:H:177:ARG:HB2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:183:ARG:HG3	1:F:184:ASP:N	2.30	0.45
1:D:109:PRO:HB2	1:D:161:HIS:CE1	2.52	0.45
1:E:79:TRP:HZ2	1:E:115:ASN:ND2	2.14	0.45
1:H:151:ILE:HG22	1:H:297:ASN:HD22	1.82	0.45
1:D:171:LEU:CA	1:D:375:PHE:HB2	2.47	0.45
1:C:172:PRO:HG3	1:C:375:PHE:HB2	1.98	0.45
1:A:230:ALA:HA	1:A:236:LEU:CD2	2.47	0.45
1:B:116:ARG:CG	1:B:370:VAL:HG21	2.43	0.45
1:D:304:THR:O	1:D:309:ILE:HG21	2.16	0.45
1:E:29:ALA:HB2	1:E:93:GLU:HG2	1.97	0.45
1:F:110:LEU:CD1	1:F:177:ARG:HB2	2.46	0.45
1:J:208:ILE:HG21	1:J:242:LEU:HD11	1.99	0.45
1:G:79:TRP:HZ2	1:G:115:ASN:ND2	2.14	0.45
1:E:6:THR:O	1:E:7:ALA:HB3	2.16	0.45
1:H:9:VAL:HA	1:H:104:LEU:HB3	1.97	0.45
1:A:208:ILE:HG21	1:A:242:LEU:HD11	1.98	0.45
1:J:226:GLU:O	1:J:229:THR:HB	2.16	0.45
1:I:99:GLU:O	1:I:130:PRO:HD3	2.16	0.45
1:I:346:LEU:HD21	1:I:352:PHE:CD1	2.52	0.45
1:E:28:ARG:HB2	1:E:94:LEU:CD2	2.47	0.45
1:D:151:ILE:HB	1:D:293:LEU:HD22	1.97	0.45
1:J:189:LEU:HD23	1:J:209:VAL:HG13	1.99	0.45
1:B:9:VAL:O	1:B:19:ALA:HA	2.17	0.45
1:H:151:ILE:CG2	1:H:297:ASN:HD22	2.29	0.45
1:F:250:ILE:HD12	1:F:254:ARG:CG	2.42	0.45
1:B:154:ASP:OD2	1:B:339:VAL:HG22	2.17	0.45
1:D:164:PRO:HD2	1:D:175:ILE:HG22	1.98	0.45
1:C:252:ASN:HA	1:C:255:PHE:CE2	2.52	0.45
1:G:286:ASP:HB3	1:G:289:ILE:CD1	2.44	0.45
1:G:250:ILE:HG13	1:G:250:ILE:O	2.16	0.45
1:B:29:ALA:HB2	1:B:93:GLU:CB	2.47	0.45
1:J:39:ARG:HG3	1:J:64:ILE:O	2.16	0.45
1:H:63:GLY:H	1:J:287:ILE:HB	1.81	0.45
1:A:94:LEU:HB3	1:A:96:VAL:HG22	1.99	0.45
1:E:110:LEU:CD1	1:E:177:ARG:HB2	2.47	0.45
1:J:111:ASN:HB3	1:J:116:ARG:HH12	1.81	0.45
1:I:352:PHE:CE2	1:I:356:TRP:HE3	2.35	0.45
1:J:299:MET:HB3	1:J:304:THR:HG21	1.97	0.45
1:D:169:TYR:HE1	1:D:355:MET:SD	2.40	0.45
1:A:5:THR:HA	1:A:102:PRO:HG2	1.99	0.45
1:E:5:THR:O	1:E:7:ALA:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:63:GLY:CA	1:I:287:ILE:HG21	2.38	0.45
1:A:289:ILE:HG22	1:A:293:LEU:CD1	2.46	0.45
1:E:340:TRP:HE3	1:E:341:ILE:HD13	1.81	0.45
1:H:346:LEU:HD23	1:H:346:LEU:HA	1.81	0.45
1:G:164:PRO:HG3	1:G:174:ALA:HB1	1.98	0.45
1:F:12:ASN:H	1:F:106:THR:HG22	1.82	0.45
1:I:200:PHE:CB	1:I:205:GLU:HG3	2.47	0.45
1:G:64:ILE:HD11	1:I:288:ASP:OD2	2.17	0.45
1:D:124:PHE:CZ	1:D:132:MET:HG2	2.49	0.45
1:J:99:GLU:OE2	1:J:127:PHE:HB3	2.17	0.45
1:G:137:GLN:CG	1:G:339:VAL:HG13	2.47	0.45
1:F:306:TYR:N	1:F:306:TYR:CD1	2.85	0.45
1:A:84:LYS:O	1:A:87:HIS:HB3	2.16	0.45
1:I:279:TYR:O	1:I:283:MET:HG2	2.16	0.44
1:A:156:GLY:O	1:A:157:ASP:HB2	2.16	0.44
1:J:66:THR:O	1:J:67:LEU:HB2	2.17	0.44
1:A:372:ARG:CZ	1:A:372:ARG:HA	2.47	0.44
1:E:33:SER:O	1:E:70:PRO:HD2	2.18	0.44
1:B:43:VAL:CG1	1:B:44:MET:N	2.80	0.44
1:J:120:THR:HG23	1:J:124:PHE:CD1	2.51	0.44
1:G:37:ARG:HG3	1:G:38:PRO:HD2	1.97	0.44
1:E:121:GLN:HG3	1:E:125:GLU:OE1	2.18	0.44
1:B:147:ARG:HE	1:B:296:ASN:ND2	2.15	0.44
1:E:57:GLU:HG2	1:E:61:LYS:HE2	1.99	0.44
1:D:37:ARG:HG3	1:D:38:PRO:CD	2.47	0.44
1:H:181:ALA:O	1:H:184:ASP:HB2	2.18	0.44
1:B:270:GLU:HG2	1:B:271:SER:N	2.32	0.44
1:J:166:TYR:CE2	1:J:289:ILE:HG12	2.52	0.44
1:E:166:TYR:CD1	1:E:289:ILE:HD13	2.52	0.44
1:F:108:ALA:O	1:F:111:ASN:HB2	2.17	0.44
1:C:111:ASN:HB3	1:C:116:ARG:HH12	1.82	0.44
1:G:288:ASP:O	1:G:291:LYS:HD2	2.18	0.44
1:J:10:CYS:HA	1:J:18:LYS:O	2.18	0.44
1:F:317:ILE:HG22	1:F:327:ILE:HD13	1.98	0.44
1:E:99:GLU:HA	1:E:128:ASN:O	2.18	0.44
1:F:63:GLY:HA2	1:H:287:ILE:HD12	2.00	0.44
1:C:189:LEU:HD23	1:C:209:VAL:HG13	1.99	0.44
1:F:31:PHE:CD2	1:F:55:GLY:HA2	2.52	0.44
1:G:44:MET:HG2	1:G:44:MET:O	2.17	0.44
1:H:289:ILE:O	1:H:293:LEU:HG	2.17	0.44
1:C:107:GLU:HB2	1:C:134:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:THR:HA	1:A:309:ILE:HG21	2.00	0.44
1:D:37:ARG:HG3	1:D:38:PRO:HD2	1.99	0.44
1:D:149:THR:CB	1:D:292:ASP:HB2	2.47	0.44
1:B:109:PRO:HB2	1:B:161:HIS:CE1	2.53	0.44
1:J:243:PRO:O	1:J:244:ASP:HB2	2.18	0.44
1:I:260:THR:CG2	1:I:267:ILE:HG23	2.48	0.44
1:D:24:ASP:O	1:D:25:ASP:HB3	2.18	0.44
1:H:306:TYR:N	1:H:306:TYR:HD1	2.14	0.44
1:C:195:GLU:HG3	1:C:196:ARG:N	2.33	0.44
1:J:253:GLU:HA	1:J:256:ARG:HB3	1.99	0.44
1:D:305:MET:HE3	1:D:336:LYS:HB2	1.99	0.44
1:I:111:ASN:HB3	1:I:116:ARG:HH12	1.82	0.44
1:J:137:GLN:HG3	1:J:154:ASP:OD2	2.18	0.44
1:C:107:GLU:CD	1:C:116:ARG:HH12	2.20	0.44
1:J:110:LEU:HD12	1:J:177:ARG:HB2	2.00	0.44
1:D:31:PHE:CD2	1:D:55:GLY:HA2	2.52	0.44
1:B:140:LEU:HB3	1:B:342:GLY:HA3	1.98	0.44
1:D:8:LEU:HB2	1:D:102:PRO:O	2.17	0.44
1:F:135:ALA:HB1	1:F:140:LEU:HD11	1.99	0.44
1:H:347:ALA:HA	1:H:352:PHE:CD2	2.53	0.44
1:F:79:TRP:HZ2	1:F:115:ASN:ND2	2.15	0.44
1:J:31:PHE:HE2	1:J:85:ILE:HG23	1.83	0.44
1:F:156:GLY:O	1:F:157:ASP:HB3	2.18	0.44
1:H:188:TYR:OH	1:H:192:ILE:HD11	2.18	0.44
1:D:124:PHE:CG	1:D:359:LYS:HD3	2.53	0.44
1:H:43:VAL:HG23	1:J:171:LEU:CD2	2.48	0.44
1:G:219:VAL:HG22	1:G:258:PRO:HB3	1.99	0.44
1:I:154:ASP:OD1	1:I:339:VAL:HG22	2.18	0.44
1:G:36:GLY:HA3	1:G:53:TYR:HB2	2.00	0.43
1:F:171:LEU:H	1:F:171:LEU:CD1	2.31	0.43
1:F:7:ALA:HA	1:F:102:PRO:HB2	2.00	0.43
1:F:140:LEU:HD23	1:F:343:GLY:CA	2.48	0.43
1:F:208:ILE:HG21	1:F:242:LEU:HD11	2.00	0.43
1:H:6:THR:HG23	1:H:7:ALA:N	2.33	0.43
1:G:70:PRO:O	1:G:76:ILE:HG23	2.18	0.43
1:I:9:VAL:HG21	1:I:344:SER:HA	1.99	0.43
1:E:36:GLY:HA3	1:E:65:LEU:HG	1.99	0.43
1:H:272:ALA:HB3	1:H:276:GLU:HB2	1.99	0.43
1:G:84:LYS:O	1:G:87:HIS:HB3	2.17	0.43
1:J:16:LEU:HD23	1:J:32:PRO:HA	1.99	0.43
1:C:35:VAL:HA	1:C:53:TYR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:36:GLY:HA3	1:G:65:LEU:HG	2.00	0.43
1:J:294:TYR:HB3	1:J:327:ILE:CD1	2.49	0.43
1:A:90:PHE:O	1:A:94:LEU:HB2	2.17	0.43
1:I:257:CYS:CB	1:I:258:PRO:HD3	2.48	0.43
1:C:99:GLU:O	1:C:130:PRO:HD3	2.17	0.43
1:D:99:GLU:O	1:D:130:PRO:HD3	2.19	0.43
1:B:109:PRO:HB2	1:B:161:HIS:ND1	2.33	0.43
1:I:10:CYS:HA	1:I:18:LYS:O	2.18	0.43
1:D:12:ASN:H	1:D:106:THR:HG22	1.82	0.43
1:A:288:ASP:O	1:A:289:ILE:HG13	2.18	0.43
1:J:158:GLY:HA2	1:J:183:ARG:HD3	1.99	0.43
1:I:124:PHE:O	1:I:128:ASN:HA	2.18	0.43
1:J:124:PHE:CZ	1:J:132:MET:HG2	2.54	0.43
1:C:181:ALA:O	1:C:184:ASP:HB2	2.17	0.43
1:I:286:ASP:CB	1:I:289:ILE:HD12	2.41	0.43
1:H:43:VAL:HG23	1:J:171:LEU:HD21	2.00	0.43
1:J:171:LEU:HD12	1:J:171:LEU:C	2.38	0.43
1:F:43:VAL:HG13	1:F:44:MET:H	1.83	0.43
1:G:264:PRO:HG2	1:G:272:ALA:C	2.38	0.43
1:J:62:ARG:HE	1:J:207:GLU:HB3	1.83	0.43
1:J:109:PRO:HB2	1:J:161:HIS:CD2	2.53	0.43
1:H:283:MET:HA	1:H:290:ARG:HH21	1.82	0.43
1:A:7:ALA:HA	1:A:102:PRO:HB2	1.99	0.43
1:E:289:ILE:O	1:E:293:LEU:HG	2.18	0.43
1:C:137:GLN:HG3	1:C:339:VAL:CG1	2.42	0.43
1:E:304:THR:O	1:E:309:ILE:HG21	2.19	0.43
1:B:111:ASN:HB3	1:B:116:ARG:HH12	1.84	0.43
1:J:118:LYS:NZ	1:J:122:ILE:HD11	2.33	0.43
1:J:11:ASP:OD2	1:J:106:THR:HG21	2.19	0.43
1:B:71:ILE:HG12	1:B:76:ILE:CG1	2.45	0.43
1:A:188:TYR:CE2	1:A:257:CYS:HA	2.53	0.43
1:A:133:TYR:HB2	1:A:356:TRP:HB2	1.99	0.43
1:A:29:ALA:HB2	1:A:93:GLU:HB2	2.01	0.43
1:J:264:PRO:HG2	1:J:271:SER:O	2.19	0.43
1:I:163:VAL:HA	1:I:175:ILE:HG22	2.01	0.43
1:D:50:LYS:HB3	1:D:52:SER:O	2.18	0.43
1:D:124:PHE:CD2	1:D:359:LYS:HB2	2.53	0.43
1:D:286:ASP:CB	1:D:289:ILE:HD12	2.48	0.43
1:I:213:LYS:HA	1:I:217:CYS:SG	2.59	0.43
1:F:90:PHE:O	1:F:94:LEU:HB2	2.19	0.43
1:F:272:ALA:HB3	1:F:276:GLU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:124:PHE:HD2	1:J:359:LYS:CD	2.31	0.43
1:J:299:MET:HB3	1:J:304:THR:CG2	2.49	0.43
1:A:137:GLN:HG3	1:A:339:VAL:HG13	2.01	0.43
1:F:6:THR:CG2	1:F:22:ALA:HB3	2.48	0.43
1:B:137:GLN:HG2	1:B:154:ASP:OD2	2.18	0.43
1:J:248:ILE:HG22	1:J:250:ILE:HG23	2.01	0.43
1:G:338:SER:HA	1:G:341:ILE:CG2	2.47	0.43
1:J:70:PRO:HB2	1:J:82:MET:SD	2.59	0.43
1:G:6:THR:O	1:G:7:ALA:HB3	2.18	0.43
1:I:111:ASN:HB3	1:I:116:ARG:NH1	2.33	0.43
1:C:289:ILE:HG22	1:C:293:LEU:CD1	2.49	0.43
1:H:116:ARG:CG	1:H:116:ARG:NH1	2.72	0.43
1:H:9:VAL:O	1:H:19:ALA:HA	2.18	0.43
1:E:124:PHE:CD2	1:E:359:LYS:HB2	2.54	0.43
1:G:365:ALA:HB3	1:G:369:ILE:HD13	2.01	0.43
1:H:32:PRO:HG3	1:H:59:GLN:HB2	2.01	0.43
1:I:284:LYS:NZ	1:I:284:LYS:HB2	2.34	0.43
1:C:205:GLU:HG2	1:C:205:GLU:H	1.65	0.43
1:C:16:LEU:HD23	1:C:16:LEU:N	2.34	0.43
1:E:21:PHE:HZ	1:E:96:VAL:HG11	1.82	0.43
1:A:61:LYS:O	1:A:63:GLY:N	2.50	0.43
1:J:290:ARG:HB3	1:J:294:TYR:CE2	2.54	0.43
1:D:140:LEU:HG	1:D:346:LEU:HD12	2.01	0.43
1:D:230:ALA:HA	1:D:236:LEU:CD2	2.48	0.43
1:E:109:PRO:HD3	1:E:137:GLN:NE2	2.34	0.43
1:E:256:ARG:O	1:E:259:GLU:HB3	2.19	0.43
1:H:24:ASP:HB3	1:H:28:ARG:HH12	1.83	0.43
1:B:196:ARG:NH1	1:B:196:ARG:HB3	2.34	0.43
1:H:70:PRO:O	1:H:76:ILE:HG12	2.19	0.43
1:H:63:GLY:HA3	1:J:288:ASP:OD2	2.19	0.42
1:J:291:LYS:HA	1:J:325:MET:HG3	2.01	0.42
1:A:279:TYR:OH	1:A:317:ILE:HA	2.19	0.42
1:G:189:LEU:HD23	1:G:209:VAL:HG13	1.99	0.42
1:F:35:VAL:HG11	1:F:81:ASP:HB2	1.99	0.42
1:D:94:LEU:HB3	1:D:96:VAL:HG22	2.01	0.42
1:G:111:ASN:HB3	1:G:116:ARG:CZ	2.49	0.42
1:F:101:HIS:HA	1:F:102:PRO:HD3	1.88	0.42
1:H:142:LEU:HD22	1:H:165:ILE:HG12	2.01	0.42
1:E:172:PRO:HA	1:E:175:ILE:HG12	2.01	0.42
1:G:346:LEU:HB3	1:G:352:PHE:CD1	2.54	0.42
1:J:221:LEU:HA	1:J:312:ARG:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:ASN:HA	1:E:255:PHE:CE2	2.55	0.42
1:F:149:THR:HG21	1:F:292:ASP:OD2	2.19	0.42
1:C:294:TYR:HA	1:C:297:ASN:OD1	2.19	0.42
1:F:6:THR:HG22	1:F:22:ALA:CB	2.47	0.42
1:H:164:PRO:HG3	1:H:174:ALA:CB	2.47	0.42
1:D:53:TYR:CB	1:D:65:LEU:HD21	2.47	0.42
1:G:150:GLY:CA	1:G:296:ASN:HB2	2.49	0.42
1:E:294:TYR:HB3	1:E:327:ILE:HD13	2.01	0.42
1:G:200:PHE:HA	1:G:205:GLU:OE2	2.19	0.42
1:I:218:TYR:HA	1:I:307:PRO:HD2	2.01	0.42
1:D:71:ILE:HG12	1:D:76:ILE:CG1	2.48	0.42
1:B:54:VAL:HG21	1:B:85:ILE:HA	2.02	0.42
1:A:195:GLU:HG3	1:A:196:ARG:N	2.34	0.42
1:I:260:THR:HG21	1:I:267:ILE:HG23	2.02	0.42
1:G:7:ALA:CB	1:G:102:PRO:HB2	2.49	0.42
1:A:264:PRO:O	1:A:267:ILE:HG12	2.19	0.42
1:F:47:MET:HG2	1:F:50:LYS:O	2.20	0.42
1:A:33:SER:O	1:A:70:PRO:HD2	2.20	0.42
1:I:21:PHE:HB2	1:I:24:ASP:OD2	2.20	0.42
1:A:166:TYR:CG	1:A:167:GLU:N	2.87	0.42
1:F:90:PHE:CB	1:F:98:PRO:HG3	2.50	0.42
1:G:177:ARG:HB3	1:G:177:ARG:HH11	1.84	0.42
1:E:124:PHE:CE2	1:E:359:LYS:HB2	2.53	0.42
1:G:282:ILE:HG22	1:G:290:ARG:HG2	2.02	0.42
1:I:299:MET:HB3	1:I:304:THR:CG2	2.49	0.42
1:J:200:PHE:CB	1:J:205:GLU:HG3	2.50	0.42
1:C:314:GLN:OE1	1:C:328:LYS:HA	2.19	0.42
1:E:10:CYS:HA	1:E:18:LYS:O	2.19	0.42
1:J:223:PHE:HB2	1:J:259:GLU:CD	2.40	0.42
1:J:282:ILE:HG21	1:J:290:ARG:HG2	2.00	0.42
1:E:61:LYS:HG2	1:G:291:LYS:CE	2.50	0.42
1:B:133:TYR:CD1	1:B:356:TRP:HA	2.54	0.42
1:E:314:GLN:HG3	1:E:329:ILE:HG12	2.01	0.42
1:B:136:ILE:HG21	1:B:375:PHE:CZ	2.55	0.42
1:D:289:ILE:HG22	1:D:293:LEU:CD1	2.49	0.42
1:D:142:LEU:HD22	1:D:165:ILE:HG21	2.02	0.42
1:B:21:PHE:HE1	1:B:96:VAL:HG21	1.84	0.42
1:G:300:SER:HA	1:G:335:ARG:HB2	2.01	0.42
1:D:8:LEU:HD21	1:D:90:PHE:CE1	2.54	0.42
1:C:151:ILE:CD1	1:C:164:PRO:HA	2.50	0.42
1:J:99:GLU:O	1:J:130:PRO:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:105:LEU:O	1:I:134:VAL:HA	2.20	0.42
1:I:258:PRO:HG3	1:I:306:TYR:CD2	2.54	0.42
1:D:255:PHE:C	1:D:258:PRO:HD2	2.40	0.42
1:G:142:LEU:HD22	1:G:165:ILE:CG1	2.48	0.42
1:D:180:LEU:CD2	1:D:261:LEU:HA	2.50	0.42
1:A:331:ALA:HB1	1:A:335:ARG:HH11	1.85	0.42
1:I:313:MET:HB2	1:I:329:ILE:HG13	2.01	0.42
1:E:1:ASP:C	1:E:2:GLU:HG2	2.39	0.42
1:E:47:MET:HA	1:G:166:TYR:HE2	1.82	0.42
1:H:220:ALA:O	1:H:312:ARG:HD2	2.19	0.42
1:B:304:THR:HB	1:B:309:ILE:HG21	2.00	0.42
1:D:195:GLU:HG3	1:D:196:ARG:N	2.35	0.42
1:C:253:GLU:HA	1:C:256:ARG:HB3	2.02	0.42
1:D:133:TYR:HD1	1:D:357:ILE:H	1.66	0.42
1:D:136:ILE:HD13	1:D:375:PHE:CE2	2.55	0.41
1:D:166:TYR:HD1	1:D:166:TYR:HA	1.74	0.41
1:E:208:ILE:HG21	1:E:242:LEU:CD1	2.47	0.41
1:H:166:TYR:CD2	1:H:289:ILE:HD11	2.54	0.41
1:H:260:THR:HG23	1:H:267:ILE:CG2	2.51	0.41
1:H:260:THR:HG23	1:H:267:ILE:HG23	2.02	0.41
1:C:151:ILE:HG12	1:C:293:LEU:CD2	2.45	0.41
1:I:118:LYS:NZ	1:I:122:ILE:HD11	2.35	0.41
1:D:172:PRO:HA	1:D:175:ILE:HG12	2.02	0.41
1:A:346:LEU:HB2	1:A:352:PHE:CD1	2.55	0.41
1:I:188:TYR:CD1	1:I:267:ILE:HG22	2.56	0.41
1:A:283:MET:HA	1:A:290:ARG:HH21	1.84	0.41
1:D:35:VAL:HG22	1:D:54:VAL:HG23	2.01	0.41
1:A:12:ASN:H	1:A:106:THR:HG22	1.85	0.41
1:F:105:LEU:O	1:F:134:VAL:HA	2.20	0.41
1:A:353:GLN:HG3	1:A:356:TRP:CZ2	2.55	0.41
1:D:305:MET:CE	1:D:336:LYS:HD2	2.50	0.41
1:I:314:GLN:OE1	1:I:328:LYS:HA	2.20	0.41
1:D:54:VAL:HG21	1:D:85:ILE:HA	2.01	0.41
1:B:43:VAL:HG12	1:B:44:MET:N	2.35	0.41
1:C:272:ALA:HB3	1:C:276:GLU:CB	2.49	0.41
1:C:358:THR:HG22	1:C:359:LYS:N	2.35	0.41
1:F:104:LEU:CD2	1:F:347:ALA:HB2	2.49	0.41
1:A:300:SER:HA	1:A:335:ARG:HB2	2.02	0.41
1:D:196:ARG:HD2	1:D:198:TYR:CE2	2.56	0.41
1:H:123:MET:O	1:H:127:PHE:O	2.38	0.41
1:F:171:LEU:N	1:F:171:LEU:HD12	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:276:GLU:HA	1:I:279:TYR:CD1	2.56	0.41
1:J:140:LEU:HB3	1:J:342:GLY:HA3	2.03	0.41
1:H:37:ARG:O	1:H:66:THR:HG23	2.21	0.41
1:G:283:MET:HG2	1:G:290:ARG:NH2	2.35	0.41
1:J:275:HIS:CD2	1:J:316:GLU:HB3	2.56	0.41
1:E:299:MET:HB3	1:E:304:THR:CG2	2.47	0.41
1:J:18:LYS:HA	1:J:30:VAL:HG12	2.02	0.41
1:J:79:TRP:O	1:J:82:MET:HB2	2.21	0.41
1:I:7:ALA:C	1:I:8:LEU:HD22	2.41	0.41
1:A:27:PRO:HD3	1:A:340:TRP:CH2	2.56	0.41
1:I:124:PHE:CE2	1:I:359:LYS:HD3	2.55	0.41
1:J:192:ILE:O	1:J:195:GLU:HG3	2.20	0.41
1:E:35:VAL:HG11	1:E:81:ASP:HB2	2.01	0.41
1:C:294:TYR:HB3	1:C:327:ILE:HD13	2.03	0.41
1:I:151:ILE:HB	1:I:293:LEU:CD2	2.35	0.41
1:I:281:SER:O	1:I:285:CYS:SG	2.78	0.41
1:C:46:GLY:HA3	1:E:166:TYR:CD2	2.55	0.41
1:C:250:ILE:HD12	1:C:254:ARG:CG	2.45	0.41
1:F:272:ALA:HB3	1:F:276:GLU:CB	2.51	0.41
1:H:90:PHE:HA	1:H:94:LEU:HD12	2.02	0.41
1:J:70:PRO:O	1:J:76:ILE:HA	2.20	0.41
1:B:42:GLY:O	1:B:43:VAL:CB	2.69	0.41
1:I:305:MET:SD	1:I:335:ARG:HG2	2.61	0.41
1:E:284:LYS:HB2	1:E:284:LYS:HZ2	1.85	0.41
1:A:46:GLY:HA3	1:C:166:TYR:HB3	2.02	0.41
1:H:79:TRP:HZ2	1:H:115:ASN:HD22	1.68	0.41
1:D:70:PRO:HG3	1:D:85:ILE:HD11	2.03	0.41
1:G:105:LEU:O	1:G:134:VAL:HA	2.21	0.41
1:C:104:LEU:HD23	1:C:347:ALA:HB2	2.03	0.41
1:J:188:TYR:CE1	1:J:267:ILE:HG22	2.55	0.41
1:J:151:ILE:HD12	1:J:164:PRO:HA	2.02	0.41
1:J:250:ILE:HD12	1:J:254:ARG:CG	2.47	0.41
1:E:61:LYS:HG2	1:G:291:LYS:NZ	2.36	0.41
1:J:105:LEU:O	1:J:134:VAL:HA	2.20	0.41
1:I:197:GLY:HA2	1:J:113:LYS:HG3	2.02	0.41
1:D:278:THR:HG22	1:D:282:ILE:CD1	2.51	0.41
1:A:317:ILE:HD12	1:A:329:ILE:HD11	2.02	0.41
1:H:31:PHE:HB2	1:H:55:GLY:HA2	2.03	0.41
1:G:12:ASN:HB2	1:G:71:ILE:HD11	2.02	0.41
1:F:164:PRO:HD2	1:F:175:ILE:HG22	2.03	0.41
1:C:140:LEU:O	1:C:342:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:PHE:C	1:C:258:PRO:HD2	2.41	0.41
1:C:108:ALA:O	1:C:111:ASN:HB2	2.21	0.41
1:B:142:LEU:HG	1:B:147:ARG:O	2.21	0.41
1:B:149:THR:O	1:B:296:ASN:HB2	2.20	0.41
1:I:133:TYR:CE1	1:I:357:ILE:HG12	2.56	0.41
1:I:104:LEU:HD12	1:I:133:TYR:O	2.20	0.41
1:G:220:ALA:HB1	1:G:226:GLU:OE2	2.21	0.41
1:G:70:PRO:O	1:G:76:ILE:HG12	2.21	0.41
1:F:253:GLU:HA	1:F:256:ARG:HB3	2.03	0.41
1:H:278:THR:HG22	1:H:282:ILE:CD1	2.51	0.41
1:H:211:ASP:O	1:H:215:LYS:HG2	2.20	0.41
1:C:122:ILE:O	1:C:126:THR:HB	2.20	0.41
1:A:35:VAL:HG11	1:A:81:ASP:HB2	2.03	0.41
1:B:124:PHE:CE2	1:B:359:LYS:HB2	2.56	0.41
1:F:8:LEU:HA	1:F:20:GLY:O	2.21	0.41
1:G:124:PHE:CE2	1:G:359:LYS:HB2	2.56	0.41
1:B:242:LEU:C	1:B:242:LEU:HD23	2.41	0.41
1:D:35:VAL:HA	1:D:53:TYR:O	2.21	0.41
1:J:340:TRP:HE3	1:J:341:ILE:HD13	1.86	0.41
1:I:31:PHE:CE2	1:I:85:ILE:HG23	2.55	0.41
1:E:278:THR:O	1:E:282:ILE:HG13	2.20	0.41
1:A:241:GLU:OE1	1:A:247:VAL:HG12	2.21	0.41
1:F:17:VAL:CG2	1:F:33:SER:HB3	2.51	0.41
1:D:286:ASP:HB3	1:D:289:ILE:CG1	2.50	0.40
1:B:164:PRO:HG3	1:B:174:ALA:HB1	2.03	0.40
1:E:281:SER:HA	1:E:284:LYS:HZ2	1.85	0.40
1:H:325:MET:SD	1:H:325:MET:N	2.95	0.40
1:J:289:ILE:HG22	1:J:293:LEU:CD2	2.46	0.40
1:G:62:ARG:HG2	1:G:63:GLY:N	2.36	0.40
1:D:47:MET:C	1:D:49:GLN:H	2.25	0.40
1:F:4:GLU:HB3	1:F:5:THR:H	1.72	0.40
1:A:116:ARG:CB	1:A:370:VAL:HG21	2.51	0.40
1:I:226:GLU:O	1:I:229:THR:HB	2.20	0.40
1:B:21:PHE:CE1	1:B:96:VAL:HG21	2.56	0.40
1:D:110:LEU:HA	1:D:110:LEU:HD22	1.79	0.40
1:J:287:ILE:HA	1:J:290:ARG:HH12	1.80	0.40
1:I:175:ILE:HG13	1:I:175:ILE:O	2.20	0.40
1:J:70:PRO:HB3	1:J:81:ASP:OD2	2.21	0.40
1:F:219:VAL:HG22	1:F:258:PRO:CB	2.51	0.40
1:I:192:ILE:CG2	1:I:256:ARG:HD2	2.51	0.40
1:I:193:LEU:HB3	1:I:198:TYR:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:291:LYS:HG3	1:H:292:ASP:N	2.36	0.40
1:E:345:ILE:HG22	1:E:349:LEU:CD1	2.51	0.40
1:B:203:THR:HA	1:B:206:ARG:HB2	2.03	0.40
1:I:151:ILE:CB	1:I:293:LEU:HD22	2.36	0.40
1:D:260:THR:HG21	1:D:267:ILE:HG21	2.04	0.40
1:C:289:ILE:HG22	1:C:293:LEU:HD11	2.04	0.40
1:C:149:THR:HG22	1:C:296:ASN:ND2	2.33	0.40
1:J:18:LYS:HE3	1:J:337:TYR:CD1	2.56	0.40
1:B:264:PRO:O	1:B:267:ILE:HG12	2.21	0.40
1:J:149:THR:CG2	1:J:292:ASP:HB2	2.51	0.40
1:D:63:GLY:HA3	1:F:287:ILE:CG2	2.51	0.40
1:I:294:TYR:HB3	1:I:327:ILE:HD13	2.04	0.40
1:F:171:LEU:N	1:F:171:LEU:CD1	2.85	0.40
1:I:140:LEU:HD23	1:I:343:GLY:HA2	2.04	0.40
1:D:24:ASP:O	1:D:25:ASP:CB	2.69	0.40
1:G:177:ARG:NH1	1:G:177:ARG:HB3	2.37	0.40
1:A:220:ALA:HB2	1:A:255:PHE:HB2	2.03	0.40
1:A:46:GLY:HA3	1:C:166:TYR:HD2	1.87	0.40
1:H:121:GLN:HG3	1:H:125:GLU:OE1	2.21	0.40
1:E:300:SER:HA	1:E:335:ARG:HB2	2.04	0.40
1:E:11:ASP:OD2	1:E:106:THR:HG21	2.21	0.40
1:F:325:MET:N	1:F:325:MET:SD	2.95	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	373/377 (99%)	350 (94%)	14 (4%)	9 (2%)	7	47
1	B	373/377 (99%)	349 (94%)	11 (3%)	13 (4%)	4	39
1	C	373/377 (99%)	350 (94%)	14 (4%)	9 (2%)	7	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	373/377 (99%)	340 (91%)	17 (5%)	16 (4%)	3	34
1	E	373/377 (99%)	339 (91%)	18 (5%)	16 (4%)	3	34
1	F	373/377 (99%)	343 (92%)	17 (5%)	13 (4%)	4	39
1	G	373/377 (99%)	343 (92%)	19 (5%)	11 (3%)	6	43
1	H	373/377 (99%)	347 (93%)	15 (4%)	11 (3%)	6	43
1	I	373/377 (99%)	348 (93%)	18 (5%)	7 (2%)	10	52
1	J	373/377 (99%)	344 (92%)	21 (6%)	8 (2%)	9	50
All	All	3730/3770 (99%)	3453 (93%)	164 (4%)	113 (3%)	9	42

All (113) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ARG
1	B	6	THR
1	B	7	ALA
1	B	41	GLN
1	B	43	VAL
1	B	62	ARG
1	B	157	ASP
1	B	173	HIS
1	B	244	ASP
1	B	307	PRO
1	C	6	THR
1	C	157	ASP
1	D	14	SER
1	D	41	GLN
1	D	159	VAL
1	D	173	HIS
1	D	204	ALA
1	D	234	SER
1	E	6	THR
1	E	49	GLN
1	F	4	GLU
1	F	6	THR
1	F	45	VAL
1	F	286	ASP
1	G	6	THR
1	G	48	GLY
1	G	173	HIS
1	H	6	THR

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Mol	Chain	Res	Type
1	H	43	VAL
1	H	234	SER
1	H	244	ASP
1	I	286	ASP
1	J	173	HIS
1	J	234	SER
1	J	285	CYS
1	A	43	VAL
1	A	157	ASP
1	A	173	HIS
1	A	222	ASP
1	B	234	SER
1	C	43	VAL
1	C	244	ASP
1	D	25	ASP
1	D	244	ASP
1	D	352	PHE
1	E	3	ASP
1	E	7	ALA
1	E	43	VAL
1	E	57	GLU
1	E	157	ASP
1	E	173	HIS
1	E	244	ASP
1	E	286	ASP
1	E	363	ASP
1	F	7	ALA
1	F	41	GLN
1	F	43	VAL
1	F	44	MET
1	F	167	GLU
1	F	173	HIS
1	G	25	ASP
1	G	45	VAL
1	G	244	ASP
1	H	173	HIS
1	I	173	HIS
1	J	6	THR
1	J	244	ASP
1	A	342	GLY
1	B	273	GLY
1	B	308	GLY

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Mol	Chain	Res	Type
1	C	41	GLN
1	C	273	GLY
1	C	286	ASP
1	D	2	GLU
1	D	286	ASP
1	E	41	GLN
1	E	45	VAL
1	E	234	SER
1	E	273	GLY
1	F	273	GLY
1	G	41	GLN
1	G	43	VAL
1	G	286	ASP
1	H	45	VAL
1	H	166	TYR
1	I	7	ALA
1	I	197	GLY
1	I	230	ALA
1	A	347	ALA
1	D	6	THR
1	D	43	VAL
1	D	245	GLY
1	F	157	ASP
1	G	42	GLY
1	G	63	GLY
1	H	195	GLU
1	H	350	SER
1	J	197	GLY
1	A	7	ALA
1	C	352	PHE
1	D	49	GLN
1	H	245	GLY
1	J	157	ASP
1	A	289	ILE
1	C	245	GLY
1	J	245	GLY
1	I	48	GLY
1	I	273	GLY
1	B	245	GLY
1	E	15	GLY
1	F	46	GLY
1	D	158	GLY

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Mol	Chain	Res	Type
1	H	345	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	318/320 (99%)	302 (95%)	16 (5%)	30	66
1	B	318/320 (99%)	301 (95%)	17 (5%)	28	64
1	C	318/320 (99%)	297 (93%)	21 (7%)	21	57
1	D	318/320 (99%)	296 (93%)	22 (7%)	19	56
1	E	318/320 (99%)	301 (95%)	17 (5%)	28	64
1	F	318/320 (99%)	295 (93%)	23 (7%)	18	55
1	G	318/320 (99%)	300 (94%)	18 (6%)	25	62
1	H	318/320 (99%)	298 (94%)	20 (6%)	22	59
1	I	318/320 (99%)	299 (94%)	19 (6%)	24	60
1	J	318/320 (99%)	302 (95%)	16 (5%)	30	66
All	All	3180/3200 (99%)	2991 (94%)	189 (6%)	29	61

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	37	ARG
1	A	40	HIS
1	A	49	GLN
1	A	61	LYS
1	A	69	TYR
1	A	195	GLU
1	A	196	ARG
1	A	202	THR
1	A	235	SER
1	A	291	LYS
1	A	309	ILE

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Mol	Chain	Res	Type
1	A	335	ARG
1	A	346	LEU
1	A	356	TRP
1	A	372	ARG
1	B	8	LEU
1	B	33	SER
1	B	39	ARG
1	B	40	HIS
1	B	69	TYR
1	B	87	HIS
1	B	140	LEU
1	B	149	THR
1	B	155	SER
1	B	202	THR
1	B	205	GLU
1	B	227	MET
1	B	253	GLU
1	B	303	THR
1	B	320	LEU
1	B	335	ARG
1	B	356	TRP
1	C	3	ASP
1	C	6	THR
1	C	16	LEU
1	C	33	SER
1	C	69	TYR
1	C	87	HIS
1	C	107	GLU
1	C	123	MET
1	C	151	ILE
1	C	157	ASP
1	C	166	TYR
1	C	196	ARG
1	C	205	GLU
1	C	244	ASP
1	C	246	GLN
1	C	270	GLU
1	C	325	MET
1	C	335	ARG
1	C	352	PHE
1	C	356	TRP
1	C	372	ARG

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Mol	Chain	Res	Type
1	D	6	THR
1	D	12	ASN
1	D	28	ARG
1	D	37	ARG
1	D	69	TYR
1	D	87	HIS
1	D	110	LEU
1	D	159	VAL
1	D	162	ASN
1	D	166	TYR
1	D	179	ASP
1	D	195	GLU
1	D	196	ARG
1	D	203	THR
1	D	257	CYS
1	D	270	GLU
1	D	291	LYS
1	D	314	GLN
1	D	324	THR
1	D	356	TRP
1	D	358	THR
1	D	375	PHE
1	E	2	GLU
1	E	45	VAL
1	E	49	GLN
1	E	59	GLN
1	E	69	TYR
1	E	140	LEU
1	E	149	THR
1	E	166	TYR
1	E	225	ASN
1	E	227	MET
1	E	257	CYS
1	E	289	ILE
1	E	291	LYS
1	E	358	THR
1	E	359	LYS
1	E	364	GLU
1	E	372	ARG
1	F	5	THR
1	F	6	THR
1	F	33	SER

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Mol	Chain	Res	Type
1	F	37	ARG
1	F	44	MET
1	F	45	VAL
1	F	47	MET
1	F	69	TYR
1	F	87	HIS
1	F	113	LYS
1	F	123	MET
1	F	166	TYR
1	F	171	LEU
1	F	179	ASP
1	F	183	ARG
1	F	195	GLU
1	F	196	ARG
1	F	289	ILE
1	F	306	TYR
1	F	335	ARG
1	F	356	TRP
1	F	360	GLN
1	F	372	ARG
1	G	12	ASN
1	G	37	ARG
1	G	44	MET
1	G	69	TYR
1	G	106	THR
1	G	110	LEU
1	G	140	LEU
1	G	166	TYR
1	G	177	ARG
1	G	183	ARG
1	G	195	GLU
1	G	196	ARG
1	G	244	ASP
1	G	263	GLN
1	G	270	GLU
1	G	291	LYS
1	G	327	ILE
1	G	358	THR
1	H	8	LEU
1	H	33	SER
1	H	37	ARG
1	H	39	ARG

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Mol	Chain	Res	Type
1	H	45	VAL
1	H	69	TYR
1	H	87	HIS
1	H	106	THR
1	H	116	ARG
1	H	117	GLU
1	H	166	TYR
1	H	195	GLU
1	H	283	MET
1	H	291	LYS
1	H	306	TYR
1	H	346	LEU
1	H	349	LEU
1	H	355	MET
1	H	356	TRP
1	H	358	THR
1	I	6	THR
1	I	33	SER
1	I	39	ARG
1	I	47	MET
1	I	69	TYR
1	I	87	HIS
1	I	113	LYS
1	I	123	MET
1	I	137	GLN
1	I	166	TYR
1	I	183	ARG
1	I	196	ARG
1	I	224	GLU
1	I	257	CYS
1	I	292	ASP
1	I	315	LYS
1	I	334	GLU
1	I	356	TRP
1	I	358	THR
1	J	6	THR
1	J	39	ARG
1	J	47	MET
1	J	69	TYR
1	J	87	HIS
1	J	123	MET
1	J	140	LEU

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Mol	Chain	Res	Type
1	J	153	LEU
1	J	195	GLU
1	J	196	ARG
1	J	270	GLU
1	J	292	ASP
1	J	293	LEU
1	J	334	GLU
1	J	335	ARG
1	J	356	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	49	GLN
1	A	137	GLN
1	A	162	ASN
1	A	246	GLN
1	A	297	ASN
1	A	353	GLN
1	A	360	GLN
1	B	73	HIS
1	B	88	HIS
1	B	92	ASN
1	B	263	GLN
1	B	296	ASN
1	B	297	ASN
1	B	314	GLN
1	B	353	GLN
1	B	360	GLN
1	C	88	HIS
1	C	92	ASN
1	C	137	GLN
1	C	296	ASN
1	C	360	GLN
1	D	73	HIS
1	D	88	HIS
1	D	92	ASN
1	D	225	ASN
1	D	296	ASN
1	D	297	ASN
1	E	12	ASN

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Mol	Chain	Res	Type
1	E	40	HIS
1	E	49	GLN
1	E	88	HIS
1	E	92	ASN
1	E	137	GLN
1	E	225	ASN
1	E	296	ASN
1	E	297	ASN
1	E	314	GLN
1	E	353	GLN
1	F	40	HIS
1	F	73	HIS
1	F	88	HIS
1	F	92	ASN
1	F	296	ASN
1	F	297	ASN
1	F	353	GLN
1	G	12	ASN
1	G	41	GLN
1	G	73	HIS
1	G	88	HIS
1	G	92	ASN
1	G	246	GLN
1	G	296	ASN
1	G	297	ASN
1	H	161	HIS
1	H	246	GLN
1	H	297	ASN
1	H	314	GLN
1	H	353	GLN
1	I	121	GLN
1	I	137	GLN
1	I	297	ASN
1	I	353	GLN
1	I	354	GLN
1	J	88	HIS
1	J	92	ASN
1	J	162	ASN
1	J	246	GLN
1	J	296	ASN
1	J	297	ASN
1	J	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](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.