



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:57 PM BST

PDB ID : 4BZJ  
EMDB ID: : EMD-2430  
Title : The structure of the COPII coat assembled on membranes  
Authors : Zanetti, G.; Prinz, S.; Daum, S.; Meister, A.; Schekman, R.; Bacia, K.; Briggs, J.A.G.  
Deposited on : 2013-07-26  
Resolution : 40.00 Å(reported)  
Based on PDB ID : 2PM6, 2PM9

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

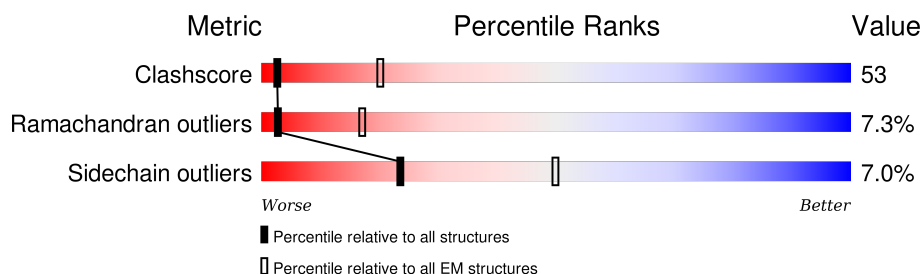
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 40.00 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	1273	
1	C	1273	
2	B	291	
3	F	291	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15423 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 PROTEIN TRANSPORT PROTEIN SEC31.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	691	Total	C	N	O	S	0	0
			5410	3406	908	1084	12		
1	C	693	Total	C	N	O	S	0	0
			5427	3417	911	1087	12		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	367	SER	THR	CONFLICT	UNP P38968
C	367	SER	THR	CONFLICT	UNP P38968

- Molecule 2 is a protein called PROTEIN TRANSPORT PROTEIN SEC13.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	279	Total	C	N	O	S	0	0
			2196	1403	375	415	3		

- Molecule 3 is a protein called PROTEIN TRANSPORT PROTEIN SEC13.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	280	Total	C	N	O	S	0	0
			2205	1402	376	418	9		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	11	MET	LEU	CONFLICT	UNP Q04491
F	17	MET	LEU	CONFLICT	UNP Q04491
F	24	MET	LEU	CONFLICT	UNP Q04491
F	80	MET	LEU	CONFLICT	UNP Q04491
F	115	MET	LEU	CONFLICT	UNP Q04491
F	222	MET	LEU	CONFLICT	UNP Q04491

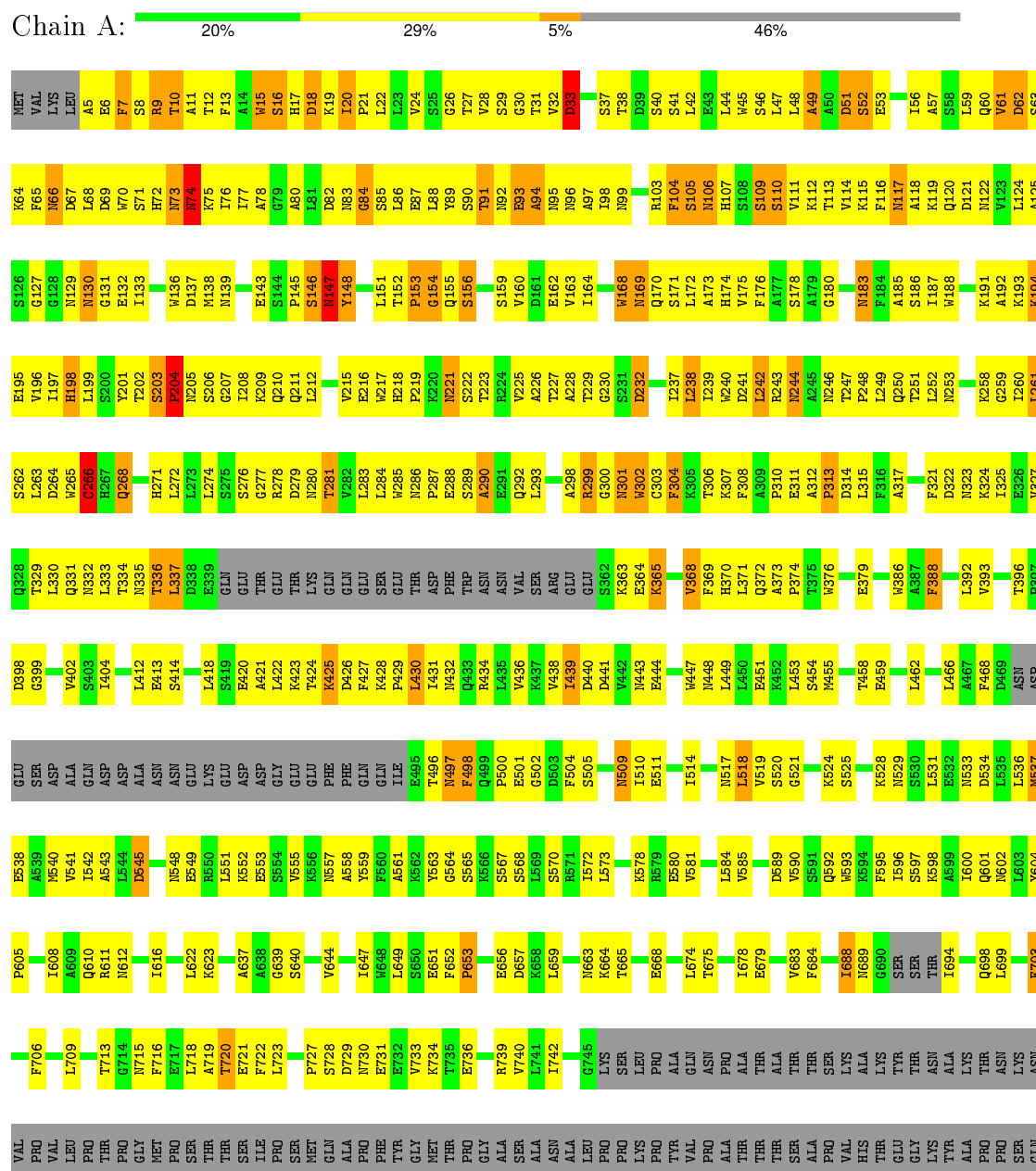
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	A	45	Total 45	O 45	0
4	B	61	Total 61	O 61	0
4	C	68	Total 68	O 68	0
4	F	11	Total 11	O 11	0

### 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: PROTEIN TRANSPORT PROTEIN SEC31



- Molecule 1: PROTEIN TRANSPORT PROTEIN SEC31








## 4 Experimental information

Property	Value	Source
Reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH TILTED IMAGE WITHIN TOMOGRAM	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	80	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	19500	Depositor
Image detector	2K X 2K MULTISCAN CHARGE-COUPLED DEVICE CAMERA	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	0/5516	0.70	2/7479 (0.0%)
1	C	0.44	0/5533	0.71	2/7502 (0.0%)
2	B	0.40	0/2256	0.68	0/3079
3	F	0.41	0/2265	0.67	0/3085
All	All	0.42	0/15570	0.69	4/21145 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	154	GLY	N-CA-C	5.10	125.85	113.10
1	A	156	SER	N-CA-C	5.10	124.76	111.00
1	A	154	GLY	N-CA-C	5.09	125.83	113.10
1	C	156	SER	N-CA-C	5.09	124.73	111.00

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	5410	0	5272	605	0
1	C	5427	0	5289	609	0
2	B	2196	0	2138	189	0
3	F	2205	0	2131	304	0
4	A	45	0	0	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	61	0	0	26	0
4	C	68	0	0	25	0
4	F	11	0	0	4	0
All	All	15423	0	14830	1582	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 53.

All (1582) 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:C:739:ARG:HA	3:F:20:TYR:CE1	1.28	1.64
1:C:664:LYS:C	3:F:285:LEU:HD21	1.30	1.47
1:C:739:ARG:CA	3:F:20:TYR:HE1	1.28	1.45
1:A:314:ASP:OD2	1:A:376:TRP:CD2	1.64	1.44
1:A:314:ASP:OD2	1:A:376:TRP:CE2	1.76	1.38
1:C:665:THR:N	3:F:285:LEU:HD21	1.38	1.38
1:C:665:THR:HA	3:F:285:LEU:CD2	1.58	1.33
1:A:313:PRO:HG3	4:A:2118:HOH:O	1.14	1.30
1:C:313:PRO:HG3	4:C:1545:HOH:O	1.32	1.29
1:C:663:ASN:C	3:F:285:LEU:HD11	1.53	1.26
1:C:268:GLN:HB3	1:C:374:PRO:O	1.29	1.26
1:A:268:GLN:HB3	1:A:374:PRO:O	1.15	1.25
1:C:331:GLN:NE2	4:C:1544:HOH:O	1.74	1.21
1:A:268:GLN:HG3	4:A:2118:HOH:O	1.32	1.21
1:A:268:GLN:CB	1:A:374:PRO:O	1.87	1.21
1:C:665:THR:CA	3:F:285:LEU:CD2	2.19	1.20
1:C:314:ASP:OD2	1:C:376:TRP:CD2	1.95	1.20
1:C:663:ASN:C	3:F:285:LEU:CD1	2.13	1.16
1:C:314:ASP:OD1	4:C:1411:HOH:O	1.63	1.13
1:A:314:ASP:CG	1:A:376:TRP:CE2	2.22	1.13
1:C:664:LYS:N	3:F:285:LEU:HD11	1.65	1.12
1:C:314:ASP:OD2	1:C:376:TRP:CE2	2.01	1.11
1:C:665:THR:N	3:F:285:LEU:CD2	2.14	1.09
1:C:22:LEU:HD11	1:C:94:ALA:HB1	1.30	1.08
1:C:313:PRO:CG	4:C:1545:HOH:O	1.86	1.08
1:C:665:THR:CA	3:F:285:LEU:HD23	1.81	1.08
1:A:268:GLN:CG	4:A:2118:HOH:O	1.91	1.08
1:A:93:GLU:HB2	1:A:96:ASN:HD22	1.16	1.07
3:F:256:VAL:HG12	3:F:257:LEU:H	1.11	1.07
1:A:314:ASP:OD2	1:A:376:TRP:CE3	2.06	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:GLU:HB2	1:C:96:ASN:HD22	1.16	1.07
1:C:665:THR:HA	3:F:285:LEU:HD23	1.09	1.07
1:A:22:LEU:HD11	1:A:94:ALA:HB1	1.30	1.06
1:C:664:LYS:C	3:F:285:LEU:CD2	2.24	1.05
1:C:665:THR:CA	3:F:285:LEU:HD21	1.83	1.05
1:C:268:GLN:HA	1:C:373:ALA:HB1	1.34	1.05
1:C:408:LYS:HD3	1:C:408:LYS:H	1.22	1.05
1:C:268:GLN:NE2	4:C:1546:HOH:O	1.87	1.04
1:C:425:LYS:HE2	1:C:686:ASN:HD21	1.21	1.04
3:F:24:MET:HG2	3:F:25:ALA:H	1.18	1.03
1:A:268:GLN:HE21	1:A:313:PRO:HD3	1.19	1.03
3:F:46:ILE:HG22	3:F:47:ASP:H	1.20	1.02
1:C:739:ARG:CA	3:F:20:TYR:CE1	2.15	1.02
1:C:268:GLN:HE21	1:C:313:PRO:HD3	1.19	1.02
1:C:663:ASN:O	3:F:285:LEU:CD1	2.08	1.02
1:C:664:LYS:O	3:F:285:LEU:HD21	1.58	1.02
2:B:11:LEU:O	2:B:28:SER:HB2	1.61	1.01
1:C:688:ILE:HG13	1:C:689:ASN:H	1.20	1.01
1:A:304:PHE:HD1	1:A:304:PHE:H	1.03	1.01
2:B:128:VAL:HG22	2:B:138:PRO:HB3	1.43	1.00
1:C:154:GLY:O	1:C:155:GLN:HG2	1.61	1.00
1:A:431:ILE:HD11	1:A:683:VAL:HG11	1.42	0.99
1:C:623:LYS:HE3	1:C:647:ILE:HD12	1.44	0.99
3:F:69:ILE:HD11	3:F:83:LYS:HE2	1.43	0.99
1:A:154:GLY:O	1:A:155:GLN:HG2	1.61	0.99
3:F:80:MET:HG2	3:F:94:VAL:HG23	1.43	0.99
1:C:304:PHE:HD1	1:C:304:PHE:H	1.03	0.99
1:A:268:GLN:HA	1:A:373:ALA:HB1	1.45	0.98
3:F:69:ILE:HG12	3:F:83:LYS:HG2	1.45	0.97
1:C:377:TYR:CE2	3:F:75:TYR:HE1	1.80	0.97
1:C:268:GLN:CB	1:C:374:PRO:O	2.13	0.97
1:C:314:ASP:CG	4:C:1411:HOH:O	2.01	0.97
1:C:535:LEU:HB3	1:C:538:GLU:HG3	1.48	0.95
1:A:93:GLU:HB2	1:A:96:ASN:ND2	1.81	0.95
1:A:438:VAL:HG23	1:A:443:ASN:HD22	1.28	0.95
1:C:268:GLN:HA	1:C:373:ALA:CB	1.95	0.95
1:C:407:PRO:HD2	4:C:1614:HOH:O	1.67	0.94
1:A:720:THR:HA	1:A:723:LEU:HD12	1.46	0.94
1:A:299:ARG:HE	1:A:323:ASN:HB2	1.32	0.94
1:C:93:GLU:HB2	1:C:96:ASN:ND2	1.81	0.94
1:A:370:HIS:CE1	2:B:75:TYR:CE2	2.56	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:THR:HG23	1:A:28:VAL:HG12	1.50	0.93
1:C:16:SER:O	1:C:310:PRO:HG3	1.69	0.93
1:A:370:HIS:CE1	2:B:75:TYR:HE2	1.86	0.93
1:A:16:SER:O	1:A:310:PRO:HG3	1.69	0.93
1:A:72:HIS:CE1	1:A:118:ALA:HA	2.04	0.93
1:A:364:GLU:O	1:A:365:LYS:HB2	1.66	0.93
1:C:22:LEU:CD1	1:C:94:ALA:HB1	1.99	0.93
1:C:72:HIS:CE1	1:C:118:ALA:HA	2.04	0.92
1:A:268:GLN:HG3	4:A:2079:HOH:O	1.67	0.92
1:C:202:THR:C	1:C:204:PRO:HD2	1.90	0.92
1:C:10:THR:HG23	1:C:28:VAL:HG12	1.50	0.92
1:C:125:ALA:HB2	1:C:168:TRP:CH2	2.05	0.92
1:C:368:VAL:O	1:C:370:HIS:N	2.02	0.91
1:C:377:TYR:CE2	3:F:75:TYR:CE1	2.58	0.91
1:A:639:GLY:HA2	1:A:688:ILE:HD11	1.51	0.91
1:A:22:LEU:CD1	1:A:94:ALA:HB1	1.99	0.91
1:C:739:ARG:CB	3:F:20:TYR:HE1	1.83	0.91
1:C:420:GLU:O	1:C:423:LYS:HG2	1.70	0.91
1:A:368:VAL:O	1:A:370:HIS:N	2.02	0.91
3:F:233:ILE:H	3:F:233:ILE:HD12	1.33	0.91
1:A:125:ALA:HB2	1:A:168:TRP:CH2	2.05	0.91
1:A:202:THR:C	1:A:204:PRO:HD2	1.89	0.91
1:C:31:THR:HG22	1:C:32:VAL:H	1.33	0.91
1:C:664:LYS:CA	3:F:285:LEU:HD11	2.00	0.90
1:C:364:GLU:O	1:C:365:LYS:HB2	1.66	0.90
1:C:299:ARG:HE	1:C:323:ASN:HB2	1.33	0.90
1:C:244:ASN:HD21	1:C:246:ASN:ND2	1.70	0.90
1:A:314:ASP:N	1:A:376:TRP:HE1	1.69	0.90
1:A:31:THR:HG22	1:A:32:VAL:H	1.33	0.89
1:A:428:LYS:HB2	1:A:429:PRO:HD3	1.54	0.89
1:A:244:ASN:HD21	1:A:246:ASN:ND2	1.70	0.89
1:A:370:HIS:HE1	2:B:75:TYR:CE2	1.90	0.88
3:F:249:LYS:HE3	3:F:251:GLU:HB2	1.54	0.88
1:A:496:THR:HG23	1:C:557:ASN:HB3	1.54	0.88
1:A:202:THR:O	1:A:204:PRO:HD2	1.74	0.88
1:C:649:LEU:HD22	1:C:698:GLN:HG2	1.55	0.88
2:B:81:ILE:HB	4:B:1320:HOH:O	1.73	0.88
1:C:739:ARG:HA	3:F:20:TYR:CD1	2.08	0.87
1:A:268:GLN:HE21	1:A:313:PRO:CD	1.87	0.87
1:C:313:PRO:HG3	4:C:1480:HOH:O	1.73	0.87
2:B:81:ILE:HD13	2:B:93:ALA:HB3	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:TYR:HB3	3:F:57:TRP:CH2	2.10	0.87
1:A:314:ASP:OD2	1:A:376:TRP:CZ2	2.28	0.86
1:C:268:GLN:HE21	1:C:313:PRO:CD	1.87	0.86
1:A:592:GLN:HE21	1:C:506:LEU:HD12	1.40	0.86
1:C:425:LYS:O	1:C:425:LYS:HD3	1.75	0.86
1:C:202:THR:O	1:C:204:PRO:HD2	1.74	0.86
1:A:106:ASN:HD22	1:A:106:ASN:N	1.70	0.86
1:A:75:LYS:NZ	1:A:94:ALA:H	1.74	0.86
1:C:106:ASN:N	1:C:106:ASN:HD22	1.70	0.86
1:C:663:ASN:O	3:F:285:LEU:HD11	1.69	0.85
1:C:10:THR:CG2	1:C:28:VAL:HG12	2.06	0.85
4:A:2245:HOH:O	1:C:602:ASN:HB3	1.75	0.85
1:C:377:TYR:HB3	3:F:57:TRP:CZ2	2.11	0.85
3:F:73:CYS:HB3	3:F:79:VAL:HG12	1.59	0.85
1:A:313:PRO:C	1:A:376:TRP:HE1	1.79	0.85
1:A:10:THR:CG2	1:A:28:VAL:HG12	2.06	0.85
1:C:314:ASP:OD2	1:C:376:TRP:CE3	2.30	0.85
1:C:663:ASN:O	3:F:285:LEU:HD12	1.74	0.84
3:F:180:ASN:N	3:F:180:ASN:HD22	1.72	0.84
1:C:75:LYS:NZ	1:C:94:ALA:H	1.74	0.84
2:B:257:LEU:HD13	2:B:271:LEU:HD21	1.59	0.84
1:A:412:LEU:HD21	1:A:713:THR:HG22	1.57	0.84
1:C:73:ASN:O	1:C:75:LYS:N	2.11	0.84
2:B:12:ILE:HA	2:B:28:SER:HB3	1.59	0.84
1:C:117:ASN:HD22	1:C:118:ALA:N	1.75	0.84
2:B:83:LYS:O	2:B:89:TRP:HA	1.76	0.84
1:C:314:ASP:CG	1:C:376:TRP:CE2	2.50	0.84
3:F:24:MET:CG	3:F:25:ALA:H	1.90	0.84
1:A:73:ASN:O	1:A:75:LYS:N	2.11	0.83
3:F:69:ILE:CD1	3:F:83:LYS:HE2	2.07	0.83
1:C:494:ILE:HG13	1:C:495:GLU:H	1.42	0.83
1:A:117:ASN:HD22	1:A:118:ALA:N	1.75	0.83
1:C:119:LYS:HB2	1:C:173:ALA:HB2	1.59	0.83
1:C:703:PHE:O	1:C:707:ILE:HG12	1.78	0.83
3:F:79:VAL:HG23	3:F:95:HIS:HB3	1.60	0.83
1:C:524:LYS:HG3	1:C:525:SER:H	1.43	0.83
1:A:119:LYS:HB2	1:A:173:ALA:HB2	1.59	0.82
1:C:75:LYS:HZ1	1:C:94:ALA:H	1.22	0.82
1:C:74:ASN:HD22	1:C:74:ASN:N	1.77	0.82
1:A:268:GLN:NE2	1:A:313:PRO:HD3	1.94	0.82
1:C:380:PRO:HG3	3:F:11:MET:CE	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:ALA:HB1	4:F:1302:HOH:O	1.80	0.82
3:F:150:SER:OG	3:F:209:ASP:HA	1.79	0.82
3:F:46:ILE:HG22	3:F:47:ASP:N	1.95	0.82
1:C:268:GLN:NE2	1:C:313:PRO:HD3	1.94	0.82
1:A:336:THR:HB	2:B:96:ALA:O	1.80	0.82
1:C:30:GLY:HA3	1:C:321:PHE:HE2	1.44	0.81
1:C:665:THR:HG22	3:F:285:LEU:HA	1.61	0.81
1:A:314:ASP:CG	1:A:376:TRP:CD2	2.48	0.81
3:F:256:VAL:HG12	3:F:257:LEU:N	1.92	0.81
1:C:427:PHE:O	1:C:431:ILE:HG12	1.81	0.81
1:A:30:GLY:HA3	1:A:321:PHE:HE2	1.44	0.81
1:A:221:ASN:HD22	1:A:222:SER:N	1.79	0.81
1:A:370:HIS:CG	1:A:371:LEU:H	1.99	0.81
1:C:31:THR:HG22	1:C:32:VAL:N	1.95	0.81
1:A:314:ASP:N	1:A:376:TRP:NE1	2.29	0.80
1:A:74:ASN:N	1:A:74:ASN:HD22	1.77	0.80
3:F:83:LYS:HG3	3:F:92:ILE:HD13	1.62	0.80
1:A:31:THR:HG22	1:A:32:VAL:N	1.95	0.80
1:C:133:ILE:HD11	1:C:163:VAL:HG21	1.62	0.80
1:C:221:ASN:HD22	1:C:222:SER:N	1.78	0.80
1:C:314:ASP:H	1:C:376:TRP:HZ2	1.30	0.80
1:C:74:ASN:HD22	1:C:74:ASN:H	1.30	0.80
1:C:370:HIS:CG	1:C:371:LEU:H	1.99	0.80
1:A:133:ILE:HD11	1:A:163:VAL:HG21	1.62	0.80
1:A:505:SER:HB3	1:C:589:ASP:HB2	1.62	0.79
1:A:315:LEU:HD11	2:B:146:ILE:HD12	1.65	0.79
1:A:292:GLN:O	1:A:368:VAL:HG23	1.81	0.79
3:F:24:MET:HG2	3:F:25:ALA:N	1.96	0.79
1:A:74:ASN:H	1:A:74:ASN:HD22	1.30	0.79
1:C:300:GLY:O	1:C:301:ASN:HB2	1.81	0.79
1:C:439:ILE:HG21	1:C:659:LEU:HD21	1.63	0.79
1:A:518:LEU:HB3	1:C:576:ILE:HD13	1.63	0.79
1:C:292:GLN:O	1:C:368:VAL:HG23	1.82	0.79
1:A:80:ALA:HB1	1:A:111:VAL:HG12	1.65	0.79
1:A:300:GLY:O	1:A:301:ASN:HB2	1.81	0.79
1:A:19:LYS:O	1:A:21:PRO:HD3	1.82	0.79
1:C:56:ILE:HD13	1:C:95:ASN:HA	1.65	0.79
1:A:250:GLN:NE2	1:A:251:THR:H	1.81	0.79
1:C:250:GLN:NE2	1:C:251:THR:H	1.81	0.79
1:A:420:GLU:HA	1:A:423:LYS:HE2	1.63	0.79
1:A:268:GLN:HG3	1:A:313:PRO:HG3	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ILE:HD13	1:A:95:ASN:HA	1.65	0.78
1:C:19:LYS:O	1:C:21:PRO:HD3	1.82	0.78
1:A:590:VAL:HG13	1:A:622:LEU:HD23	1.65	0.78
1:C:93:GLU:CB	1:C:96:ASN:HD22	1.97	0.78
1:C:652:PHE:HB3	1:C:653:PRO:HD3	1.64	0.78
1:C:513:THR:HB	4:C:1602:HOH:O	1.84	0.78
3:F:37:GLU:HG2	3:F:46:ILE:HD11	1.65	0.78
1:C:664:LYS:O	3:F:285:LEU:CD2	2.31	0.78
1:C:80:ALA:HB1	1:C:111:VAL:HG12	1.65	0.77
1:C:72:HIS:O	1:C:74:ASN:ND2	2.16	0.77
1:A:93:GLU:CB	1:A:96:ASN:HD22	1.97	0.77
1:C:739:ARG:HG3	3:F:20:TYR:CE1	2.20	0.77
1:A:72:HIS:O	1:A:74:ASN:ND2	2.16	0.77
1:A:304:PHE:N	1:A:304:PHE:CD1	2.52	0.77
3:F:71:ALA:HB2	3:F:81:ILE:HG22	1.67	0.77
1:C:196:VAL:HG23	1:C:197:ILE:HG13	1.66	0.77
1:C:268:GLN:HG3	1:C:313:PRO:HG3	1.65	0.76
1:A:75:LYS:HZ1	1:A:94:ALA:H	1.31	0.76
1:C:80:ALA:HB2	1:C:114:VAL:HG23	1.67	0.76
1:A:174:HIS:NE2	1:A:191:LYS:HB2	2.00	0.76
1:A:589:ASP:HB2	1:C:505:SER:HB3	1.67	0.76
1:A:80:ALA:HB2	1:A:114:VAL:HG23	1.67	0.76
1:C:174:HIS:NE2	1:C:191:LYS:HB2	1.99	0.76
1:C:372:GLN:O	1:C:372:GLN:HG3	1.86	0.76
1:A:372:GLN:O	1:A:372:GLN:HG3	1.86	0.76
1:C:304:PHE:N	1:C:304:PHE:CD1	2.52	0.76
1:C:151:LEU:HD12	1:C:152:THR:H	1.50	0.76
1:A:196:VAL:HG23	1:A:197:ILE:HG13	1.66	0.76
1:A:393:VAL:HG22	1:A:404:ILE:HG13	1.67	0.76
3:F:65:LYS:HD3	3:F:110:HIS:HB2	1.68	0.75
3:F:256:VAL:CG1	3:F:257:LEU:H	1.94	0.75
1:C:202:THR:C	1:C:204:PRO:CD	2.55	0.75
1:C:524:LYS:HG3	1:C:525:SER:N	2.01	0.75
1:A:151:LEU:HD12	1:A:152:THR:H	1.51	0.75
1:A:719:ALA:O	1:A:723:LEU:HG	1.87	0.75
1:A:202:THR:C	1:A:204:PRO:CD	2.55	0.75
2:B:10:GLU:HB2	4:B:1336:HOH:O	1.86	0.75
3:F:154:ALA:HB2	3:F:212:TRP:CZ3	2.21	0.75
3:F:33:ILE:HB	3:F:49:LEU:HD12	1.68	0.74
1:C:428:LYS:HB2	1:C:429:PRO:HD3	1.69	0.74
1:A:652:PHE:HB3	1:A:653:PRO:HD3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:592:GLN:HG3	1:C:595:PHE:HB3	1.69	0.74
1:C:688:ILE:HG13	1:C:689:ASN:N	1.98	0.74
1:C:133:ILE:CD1	1:C:163:VAL:HG21	2.17	0.74
1:A:723:LEU:HD11	1:A:740:VAL:HG21	1.69	0.74
1:C:739:ARG:CB	3:F:20:TYR:CE1	2.64	0.74
1:C:313:PRO:CD	4:C:1546:HOH:O	2.35	0.73
3:F:83:LYS:HG3	3:F:92:ILE:HG21	1.68	0.73
1:A:393:VAL:HG21	2:B:17:LEU:HG	1.69	0.73
3:F:282:LYS:HA	4:F:1298:HOH:O	1.87	0.73
1:C:548:ASN:O	1:C:552:LYS:HB2	1.89	0.73
3:F:117:LEU:HD23	3:F:151:ALA:O	1.86	0.73
2:B:117:LEU:HA	4:B:1340:HOH:O	1.86	0.73
1:A:78:ALA:CB	1:A:114:VAL:HG11	2.19	0.73
1:A:31:THR:CG2	1:A:32:VAL:H	2.02	0.73
1:A:10:THR:HG23	1:A:28:VAL:CG1	2.18	0.73
1:C:377:TYR:CZ	3:F:75:TYR:HE1	2.06	0.73
1:A:85:SER:HB2	1:A:104:PHE:O	1.88	0.73
1:C:31:THR:CG2	1:C:32:VAL:H	2.02	0.73
1:A:276:SER:OG	1:A:303:CYS:HB2	1.88	0.73
1:C:85:SER:HB2	1:C:104:PHE:O	1.88	0.73
1:C:408:LYS:N	1:C:408:LYS:HD3	1.97	0.73
1:A:578:LYS:O	1:A:580:GLU:HG3	1.88	0.73
1:C:10:THR:HG23	1:C:28:VAL:CG1	2.18	0.72
1:A:133:ILE:CD1	1:A:163:VAL:HG21	2.17	0.72
3:F:225:VAL:HG22	3:F:257:LEU:HD13	1.72	0.72
1:C:314:ASP:OD2	1:C:376:TRP:CZ2	2.42	0.72
1:C:93:GLU:CB	1:C:96:ASN:ND2	2.52	0.72
3:F:225:VAL:HG22	3:F:257:LEU:HB3	1.70	0.72
1:C:276:SER:OG	1:C:303:CYS:HB2	1.88	0.72
1:A:93:GLU:CB	1:A:96:ASN:ND2	2.52	0.72
1:A:73:ASN:C	1:A:75:LYS:H	1.92	0.71
1:A:420:GLU:HG3	1:A:423:LYS:HE2	1.72	0.71
1:A:171:SER:O	1:A:172:LEU:HD23	1.90	0.71
1:C:73:ASN:C	1:C:75:LYS:H	1.92	0.71
3:F:16:VAL:HG12	3:F:61:TRP:HD1	1.54	0.71
1:A:69:ASP:OD2	1:A:116:PHE:HB2	1.90	0.71
2:B:255:ASP:OD2	2:B:274:GLY:HA3	1.89	0.71
1:C:78:ALA:CB	1:C:114:VAL:HG11	2.19	0.71
3:F:73:CYS:CB	3:F:79:VAL:HG12	2.20	0.71
1:A:202:THR:OG1	1:A:209:LYS:HD3	1.90	0.71
1:A:496:THR:O	1:A:497:ASN:HB2	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:510:ILE:HD12	1:C:510:ILE:H	1.55	0.71
3:F:196:LEU:HD11	3:F:198:SER:O	1.90	0.71
3:F:46:ILE:N	3:F:46:ILE:HD12	2.04	0.71
1:A:331:GLN:OE1	1:A:333:LEU:HD21	1.91	0.71
1:A:388:PHE:HB2	1:A:739:ARG:HH21	1.56	0.71
1:C:202:THR:OG1	1:C:209:LYS:HD3	1.90	0.71
1:C:171:SER:O	1:C:172:LEU:HD23	1.90	0.71
3:F:224:SER:HB2	3:F:234:TRP:HE1	1.53	0.70
3:F:154:ALA:HB2	3:F:212:TRP:CE3	2.26	0.70
2:B:74:SER:HB3	2:B:76:ASP:OD1	1.91	0.70
1:A:665:THR:OG1	1:A:668:GLU:HG3	1.91	0.70
3:F:82:TRP:O	3:F:89:TRP:HZ3	1.74	0.70
1:A:431:ILE:HD13	1:A:447:TRP:HZ3	1.55	0.70
1:C:331:GLN:OE1	1:C:333:LEU:HD21	1.91	0.70
1:A:164:ILE:HG12	1:A:180:GLY:HA2	1.74	0.70
1:A:94:ALA:O	1:A:95:ASN:HB2	1.92	0.70
1:A:518:LEU:HD13	1:C:576:ILE:HD12	1.73	0.70
1:C:212:LEU:HD13	1:C:227:THR:HG21	1.74	0.70
1:C:314:ASP:CB	4:C:1411:HOH:O	2.34	0.69
1:C:69:ASP:OD2	1:C:116:PHE:HB2	1.90	0.69
1:C:109:SER:O	1:C:110:SER:HB2	1.91	0.69
1:C:164:ILE:HG12	1:C:180:GLY:HA2	1.74	0.69
2:B:105:VAL:HG23	2:B:118:VAL:HG22	1.73	0.69
1:A:289:SER:OG	1:A:290:ALA:N	2.24	0.69
1:A:336:THR:CB	2:B:96:ALA:O	2.40	0.69
1:C:425:LYS:HE2	1:C:686:ASN:ND2	2.02	0.69
1:A:203:SER:O	1:A:205:ASN:N	2.26	0.69
1:A:595:PHE:CZ	1:C:515:SER:HB2	2.28	0.69
2:B:144:HIS:CE1	2:B:183:LYS:HD2	2.28	0.69
1:A:314:ASP:CG	1:A:376:TRP:NE1	2.46	0.69
1:A:212:LEU:HD13	1:A:227:THR:HG21	1.74	0.69
1:C:203:SER:O	1:C:205:ASN:N	2.26	0.69
2:B:53:GLU:HG3	4:B:1337:HOH:O	1.93	0.69
1:C:567:SER:HB3	1:C:570:SER:HB2	1.73	0.69
1:C:94:ALA:O	1:C:95:ASN:HB2	1.92	0.69
1:A:28:VAL:HG22	1:A:29:SER:H	1.58	0.69
1:A:428:LYS:NZ	1:A:455:MET:HG2	2.06	0.69
1:C:444:GLU:HG2	1:C:448:ASN:ND2	2.08	0.69
3:F:29:SER:C	3:F:31:LYS:H	1.95	0.68
1:A:185:ALA:HB3	1:A:199:LEU:HB2	1.75	0.68
1:C:28:VAL:HG22	1:C:29:SER:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:233:ILE:N	3:F:233:ILE:HD12	2.05	0.68
1:C:19:LYS:HD2	3:F:206:TRP:HE1	1.58	0.68
3:F:16:VAL:HG12	3:F:61:TRP:CD1	2.29	0.68
1:C:185:ALA:HB3	1:C:199:LEU:HB2	1.75	0.68
1:C:314:ASP:HB3	4:C:1411:HOH:O	1.93	0.68
1:A:75:LYS:NZ	1:A:94:ALA:HB2	2.08	0.68
1:A:402:VAL:HG11	2:B:24:LEU:HD21	1.76	0.68
1:C:86:LEU:CD2	1:C:104:PHE:HB2	2.24	0.68
3:F:105:VAL:HG22	3:F:116:LEU:HD11	1.75	0.68
1:C:75:LYS:NZ	1:C:94:ALA:HB2	2.08	0.68
1:A:109:SER:O	1:A:110:SER:HB2	1.91	0.68
1:A:333:LEU:HD23	4:B:1298:HOH:O	1.59	0.68
3:F:227:GLN:HA	3:F:256:VAL:HG13	1.75	0.68
1:A:736:GLU:O	1:A:740:VAL:HG23	1.93	0.68
1:C:289:SER:OG	1:C:290:ALA:N	2.24	0.68
1:C:107:HIS:ND1	1:C:111:VAL:HG22	2.09	0.67
1:A:107:HIS:ND1	1:A:111:VAL:HG22	2.09	0.67
1:C:117:ASN:HD22	1:C:118:ALA:H	1.40	0.67
1:A:427:PHE:O	1:A:431:ILE:HG12	1.94	0.67
1:A:590:VAL:HG13	1:A:622:LEU:CD2	2.23	0.67
1:A:314:ASP:OD2	1:A:376:TRP:CZ3	2.46	0.67
1:A:528:LYS:HG3	1:C:493:GLN:HE22	1.58	0.67
1:A:86:LEU:CD2	1:A:104:PHE:HB2	2.24	0.67
1:A:249:LEU:HD23	1:A:249:LEU:O	1.94	0.67
1:C:377:TYR:CB	3:F:57:TRP:CZ2	2.78	0.67
1:A:557:ASN:HB3	1:C:496:THR:HG23	1.77	0.67
3:F:144:HIS:HB2	3:F:147:GLY:O	1.95	0.67
1:A:314:ASP:H	1:A:376:TRP:HZ2	1.38	0.67
1:A:124:LEU:HG	1:A:125:ALA:N	2.10	0.67
3:F:75:TYR:CD1	3:F:101:SER:HB2	2.31	0.66
1:C:30:GLY:HA3	1:C:321:PHE:CE2	2.30	0.66
1:C:106:ASN:ND2	1:C:106:ASN:N	2.42	0.66
1:C:439:ILE:HG13	1:C:440:ASP:H	1.60	0.66
1:C:249:LEU:HD23	1:C:249:LEU:O	1.94	0.66
1:A:117:ASN:HD22	1:A:118:ALA:H	1.39	0.66
2:B:24:LEU:HB3	2:B:36:PHE:HB2	1.76	0.66
3:F:153:TRP:O	3:F:212:TRP:HB3	1.95	0.66
3:F:200:LEU:HB3	3:F:234:TRP:CZ3	2.30	0.66
1:C:535:LEU:HB3	1:C:538:GLU:CG	2.23	0.66
1:A:639:GLY:CA	1:A:688:ILE:HD11	2.25	0.66
2:B:233:ILE:HD11	2:B:248:LEU:HD13	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:LYS:NZ	1:C:94:ALA:N	2.44	0.66
2:B:157:THR:OG1	2:B:170:SER:HB2	1.95	0.66
1:C:124:LEU:HG	1:C:125:ALA:N	2.10	0.66
1:A:414:SER:OG	1:A:715:ASN:HB2	1.96	0.66
1:A:304:PHE:N	1:A:304:PHE:HD1	1.87	0.66
1:A:536:LEU:O	1:A:540:MET:HG3	1.96	0.66
3:F:225:VAL:CG2	3:F:257:LEU:HB3	2.26	0.65
3:F:69:ILE:HD11	3:F:83:LYS:CE	2.25	0.65
1:C:647:ILE:O	1:C:651:GLU:HG3	1.96	0.65
1:C:250:GLN:HE21	1:C:251:THR:H	1.45	0.65
1:C:509:ASN:HD22	1:C:509:ASN:N	1.92	0.65
1:C:400:LYS:O	3:F:7:ALA:N	2.29	0.65
1:C:325:ILE:HD12	1:C:325:ILE:N	2.12	0.65
1:A:498:PHE:HB2	1:C:561:ALA:HA	1.77	0.65
2:B:102:VAL:CG2	4:B:1353:HOH:O	2.45	0.65
1:C:590:VAL:HG13	1:C:622:LEU:CD2	2.25	0.65
1:C:125:ALA:HB2	1:C:168:TRP:HH2	1.62	0.65
1:A:325:ILE:HD12	1:A:325:ILE:N	2.12	0.65
1:A:75:LYS:NZ	1:A:94:ALA:N	2.44	0.65
1:C:408:LYS:CD	1:C:408:LYS:H	2.05	0.65
2:B:238:ASN:HD22	2:B:240:GLN:H	1.45	0.65
1:C:124:LEU:HG	1:C:125:ALA:H	1.62	0.65
1:A:557:ASN:HB3	1:C:496:THR:CG2	2.27	0.65
3:F:2:VAL:HG13	3:F:41:GLU:HA	1.79	0.65
3:F:207:VAL:HA	3:F:226:SER:HB2	1.78	0.65
1:C:416:THR:HG22	1:C:420:GLU:OE2	1.96	0.65
1:C:304:PHE:N	1:C:304:PHE:HD1	1.87	0.65
1:A:124:LEU:HG	1:A:125:ALA:H	1.62	0.64
1:A:96:ASN:HB2	4:A:1420:HOH:O	1.96	0.64
1:A:427:PHE:CD2	1:A:683:VAL:HG22	2.31	0.64
1:A:438:VAL:HG23	1:A:443:ASN:ND2	2.07	0.64
1:A:337:LEU:HD21	2:B:97:VAL:CG1	2.26	0.64
1:A:20:ILE:O	1:A:20:ILE:HG13	1.97	0.64
1:C:268:GLN:CA	1:C:373:ALA:HB1	2.21	0.64
3:F:52:HIS:N	4:F:1307:HOH:O	2.29	0.64
1:A:592:GLN:HG3	1:A:595:PHE:HB3	1.80	0.64
2:B:40:GLY:N	4:B:1335:HOH:O	2.30	0.64
1:A:608:ILE:HB	1:A:611:ARG:HH12	1.62	0.64
1:C:96:ASN:HB2	4:C:2420:HOH:O	1.96	0.64
3:F:184:ILE:HD11	3:F:222:MET:CE	2.28	0.64
1:C:20:ILE:HG13	1:C:20:ILE:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ASN:HD22	1:A:221:ASN:C	2.01	0.64
1:C:212:LEU:HD22	1:C:227:THR:CG2	2.28	0.64
1:A:519:VAL:HG13	1:C:599:ALA:HA	1.79	0.64
1:A:78:ALA:HB3	1:A:114:VAL:HG11	1.80	0.64
3:F:49:LEU:HD22	3:F:82:TRP:CD2	2.32	0.64
3:F:224:SER:CB	3:F:234:TRP:HE1	2.11	0.64
1:A:212:LEU:HD22	1:A:227:THR:CG2	2.28	0.64
1:A:608:ILE:HD13	1:A:611:ARG:HH11	1.62	0.64
1:A:727:PRO:C	1:A:729:ASP:H	2.01	0.64
1:A:458:THR:HG23	1:A:459:GLU:N	2.14	0.64
1:C:193:LYS:O	1:C:194:LYS:HB3	1.99	0.63
1:A:241:ASP:C	1:A:243:ARG:H	2.02	0.63
1:A:250:GLN:HE21	1:A:251:THR:H	1.44	0.63
1:C:395:ILE:HD13	3:F:12:ILE:O	1.98	0.63
1:C:206:SER:O	1:C:208:ILE:HG13	1.98	0.63
3:F:225:VAL:CG2	3:F:257:LEU:HD13	2.28	0.63
1:A:592:GLN:HG3	1:A:592:GLN:O	1.99	0.63
1:A:280:ASN:C	1:A:298:ALA:HB3	2.19	0.63
2:B:18:ASP:HB2	4:B:1317:HOH:O	1.98	0.63
1:C:78:ALA:HB3	1:C:114:VAL:HG11	1.80	0.63
1:C:739:ARG:CG	3:F:20:TYR:CE1	2.82	0.63
1:A:106:ASN:HD22	1:A:106:ASN:H	1.46	0.63
1:C:280:ASN:C	1:C:298:ALA:HB3	2.19	0.63
1:A:206:SER:O	1:A:208:ILE:HG13	1.98	0.62
1:C:639:GLY:HA2	1:C:688:ILE:HD11	1.81	0.62
2:B:33:ILE:HD11	2:B:56:VAL:HG11	1.80	0.62
3:F:105:VAL:CG2	3:F:116:LEU:HD11	2.28	0.62
1:A:30:GLY:HA3	1:A:321:PHE:CE2	2.30	0.62
1:A:51:ASP:O	1:A:53:GLU:HG3	1.99	0.62
1:C:192:ALA:O	1:C:194:LYS:HG2	2.00	0.62
3:F:249:LYS:CE	3:F:251:GLU:HB2	2.28	0.62
1:A:239:ILE:HB	1:A:250:GLN:HB3	1.81	0.62
1:C:377:TYR:CB	3:F:57:TRP:CH2	2.82	0.62
2:B:157:THR:O	2:B:157:THR:HG22	2.00	0.62
1:C:239:ILE:HB	1:C:250:GLN:HB3	1.81	0.62
3:F:118:VAL:O	3:F:125:VAL:HG13	2.00	0.62
3:F:233:ILE:HD11	3:F:248:LEU:HD13	1.82	0.62
2:B:23:ARG:NH1	2:B:68:THR:HG21	2.14	0.62
1:A:514:ILE:HA	1:A:517:ASN:HD22	1.65	0.62
1:A:268:GLN:OE1	1:A:374:PRO:HD2	1.99	0.62
1:A:314:ASP:OD1	1:A:376:TRP:CD1	2.52	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:274:GLY:C	2:B:276:ASN:H	2.00	0.62
1:C:153:PRO:HB2	1:C:188:TRP:CZ3	2.35	0.62
1:A:192:ALA:O	1:A:194:LYS:HG2	2.00	0.61
1:A:392:LEU:HD13	4:A:2219:HOH:O	2.00	0.61
1:C:51:ASP:O	1:C:53:GLU:HG3	1.99	0.61
3:F:147:GLY:N	3:F:178:ALA:HB3	2.15	0.61
2:B:66:PHE:HE1	2:B:114:PRO:HD3	1.65	0.61
1:A:193:LYS:O	1:A:194:LYS:HB3	1.99	0.61
1:A:517:ASN:ND2	1:A:529:ASN:HD22	1.98	0.61
3:F:274:GLY:C	3:F:276:ASN:H	2.03	0.61
3:F:27:CYS:HB2	3:F:56:VAL:HG11	1.82	0.61
1:A:703:PHE:HA	4:A:2200:HOH:O	2.00	0.61
1:A:596:ILE:O	1:A:600:ILE:HG12	2.00	0.61
3:F:115:MET:HG2	3:F:129:GLU:HB2	1.82	0.61
2:B:52:HIS:HA	4:B:1337:HOH:O	2.01	0.61
1:C:314:ASP:N	1:C:376:TRP:CZ2	2.68	0.61
1:A:370:HIS:HE1	2:B:75:TYR:CD2	2.18	0.61
1:C:519:VAL:C	1:C:521:GLY:H	2.02	0.61
1:C:458:THR:HG23	1:C:459:GLU:H	1.65	0.61
1:C:739:ARG:HG3	3:F:20:TYR:CD1	2.35	0.61
3:F:23:ARG:HA	3:F:36:PHE:O	2.01	0.61
1:A:241:ASP:OD1	1:A:243:ARG:HB2	2.00	0.61
1:C:241:ASP:C	1:C:243:ARG:H	2.02	0.61
1:C:510:ILE:HA	4:C:1602:HOH:O	1.99	0.61
2:B:155:PRO:HG3	2:B:214:PRO:HA	1.83	0.61
1:C:313:PRO:HG2	1:C:376:TRP:CE2	2.36	0.61
1:C:641:LEU:HD13	1:C:688:ILE:HG21	1.82	0.61
1:C:106:ASN:HD22	1:C:106:ASN:H	1.45	0.61
3:F:172:LYS:HA	3:F:185:TRP:O	2.01	0.61
1:A:75:LYS:HZ1	1:A:94:ALA:HB2	1.66	0.61
3:F:81:ILE:HD13	3:F:81:ILE:H	1.66	0.61
2:B:30:ASP:OD1	2:B:32:THR:N	2.34	0.61
1:A:559:TYR:CD2	1:C:541:VAL:HG21	2.35	0.61
1:A:370:HIS:CG	1:A:371:LEU:N	2.68	0.61
2:B:102:VAL:HG23	4:B:1353:HOH:O	2.00	0.61
1:A:153:PRO:HB2	1:A:188:TRP:CZ3	2.35	0.60
1:A:396:THR:HG23	4:A:2251:HOH:O	2.01	0.60
1:A:675:THR:O	1:A:679:GLU:HG3	2.01	0.60
1:A:187:ILE:HG22	1:A:196:VAL:HG22	1.83	0.60
2:B:37:GLU:HG2	2:B:46:ILE:HG13	1.82	0.60
1:A:268:GLN:CA	1:A:373:ALA:HB1	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:553:GLU:HG2	1:C:557:ASN:HD21	1.67	0.60
1:C:221:ASN:C	1:C:221:ASN:HD22	2.01	0.60
2:B:3:VAL:C	2:B:4:ILE:HD12	2.21	0.60
3:F:169:GLU:HG2	3:F:187:TYR:HD2	1.67	0.60
1:A:742:ILE:HB	2:B:20:TYR:CD2	2.36	0.60
1:A:202:THR:HG22	1:A:202:THR:O	2.01	0.60
1:A:709:LEU:O	1:A:713:THR:HG23	2.02	0.60
1:A:608:ILE:CD1	1:A:611:ARG:HH11	2.14	0.60
3:F:196:LEU:HD12	3:F:197:GLU:H	1.66	0.60
1:A:537:MET:O	1:A:541:VAL:HG23	2.02	0.60
1:C:399:GLY:O	3:F:12:ILE:HG13	2.01	0.60
2:B:257:LEU:CD1	2:B:271:LEU:HD21	2.30	0.60
1:C:377:TYR:HB3	4:C:1513:HOH:O	2.02	0.60
1:A:92:ASN:O	1:A:93:GLU:HB2	2.02	0.60
1:A:227:THR:O	1:A:227:THR:HG22	2.02	0.60
1:C:667:TYR:CE2	3:F:266:GLY:HA2	2.37	0.60
1:C:604:TYR:CE1	1:C:610:GLN:HG2	2.36	0.60
2:B:12:ILE:HA	2:B:28:SER:CB	2.30	0.60
1:C:241:ASP:OD1	1:C:243:ARG:HB2	2.01	0.60
3:F:106:GLN:O	3:F:116:LEU:HD12	2.01	0.60
1:C:75:LYS:HZ1	1:C:94:ALA:N	1.98	0.60
3:F:28:SER:OG	3:F:29:SER:N	2.35	0.60
2:B:200:LEU:HB3	2:B:234:TRP:CZ3	2.36	0.60
3:F:14:ASP:OD2	3:F:59:VAL:HG22	2.01	0.60
1:C:202:THR:O	1:C:202:THR:HG22	2.01	0.60
2:B:4:ILE:HG13	2:B:43:HIS:ND1	2.16	0.60
1:C:665:THR:HG22	3:F:285:LEU:CA	2.30	0.59
1:C:78:ALA:HB1	1:C:114:VAL:HG11	1.83	0.59
1:C:71:SER:O	1:C:73:ASN:N	2.34	0.59
1:A:272:LEU:HD22	1:A:284:LEU:HD11	1.83	0.59
1:C:272:LEU:HD22	1:C:284:LEU:HD11	1.83	0.59
3:F:81:ILE:HD13	3:F:81:ILE:N	2.18	0.59
3:F:247:LEU:HD13	3:F:249:LYS:O	2.02	0.59
1:C:227:THR:O	1:C:227:THR:HG22	2.02	0.59
1:A:386:TRP:HA	4:A:2219:HOH:O	2.01	0.59
1:C:129:ASN:HA	1:C:162:GLU:HB3	1.84	0.59
1:A:146:SER:O	1:A:147:ASN:HB2	2.02	0.59
1:C:330:LEU:O	1:C:371:LEU:HD21	2.02	0.59
1:A:71:SER:O	1:A:73:ASN:N	2.34	0.59
1:A:15:TRP:HB3	1:A:310:PRO:HD3	1.85	0.59
1:C:187:ILE:HG22	1:C:196:VAL:HG22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:TRP:CZ2	3:F:280:LEU:HD22	2.37	0.59
1:A:330:LEU:O	1:A:371:LEU:HD21	2.02	0.59
2:B:225:VAL:HG13	2:B:257:LEU:HB2	1.84	0.59
1:A:388:PHE:CD1	1:A:739:ARG:CZ	2.86	0.59
1:A:519:VAL:C	1:A:521:GLY:H	2.05	0.59
1:C:217:TRP:CD2	1:C:225:VAL:HG22	2.37	0.59
1:A:217:TRP:CD2	1:A:225:VAL:HG22	2.37	0.59
3:F:219:ARG:HG3	3:F:221:TYR:CE1	2.37	0.59
2:B:180:ASN:HD22	2:B:180:ASN:N	2.00	0.59
1:A:78:ALA:HB1	1:A:114:VAL:HG11	1.84	0.59
3:F:225:VAL:HG22	3:F:257:LEU:CD1	2.32	0.59
1:A:306:THR:HA	1:A:317:ALA:O	2.03	0.59
1:C:40:SER:OG	1:C:61:VAL:HG23	2.03	0.59
3:F:249:LYS:HG2	3:F:251:GLU:OE1	2.03	0.59
1:A:289:SER:O	1:A:290:ALA:HB2	2.03	0.59
1:C:727:PRO:C	1:C:729:ASP:H	2.06	0.59
1:A:584:LEU:HD12	1:A:584:LEU:N	2.18	0.59
3:F:4:ILE:HD12	3:F:4:ILE:N	2.18	0.59
1:C:15:TRP:HB3	1:C:310:PRO:HD3	1.85	0.59
1:C:244:ASN:ND2	1:C:246:ASN:ND2	2.47	0.59
1:C:92:ASN:O	1:C:93:GLU:HB2	2.02	0.59
3:F:80:MET:CG	3:F:94:VAL:HG23	2.27	0.59
1:C:306:THR:HA	1:C:317:ALA:O	2.03	0.59
1:C:84:GLY:HA3	1:C:110:SER:H	1.68	0.59
1:A:88:LEU:HD13	1:A:138:MET:SD	2.43	0.59
1:C:268:GLN:HG3	1:C:313:PRO:CG	2.33	0.58
2:B:19:TYR:CD2	2:B:64:PRO:HG2	2.38	0.58
1:C:112:LYS:HG3	1:C:164:ILE:HG22	1.85	0.58
1:C:509:ASN:ND2	1:C:509:ASN:N	2.51	0.58
1:C:665:THR:CG2	3:F:285:LEU:HD23	2.33	0.58
1:A:370:HIS:CE1	2:B:75:TYR:CD2	2.90	0.58
1:C:592:GLN:HG3	1:C:595:PHE:CB	2.33	0.58
1:C:175:VAL:HG12	1:C:176:PHE:N	2.18	0.58
1:A:228:ALA:HB1	1:A:260:ILE:HG21	1.85	0.58
1:A:40:SER:OG	1:A:61:VAL:HG23	2.02	0.58
2:B:120:SER:HB3	2:B:122:ASP:OD1	2.03	0.58
1:A:84:GLY:HA3	1:A:110:SER:H	1.68	0.58
1:A:518:LEU:HB3	1:C:576:ILE:CD1	2.31	0.58
1:A:458:THR:HG23	1:A:459:GLU:H	1.66	0.58
1:A:509:ASN:HD22	1:A:509:ASN:N	2.01	0.58
1:A:112:LYS:HG3	1:A:164:ILE:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:ASN:ND2	1:C:74:ASN:N	2.50	0.58
1:C:438:VAL:HG23	1:C:443:ASN:HD22	1.68	0.58
1:C:670:HIS:HE1	1:C:705:GLU:OE1	1.86	0.58
3:F:187:TYR:CG	3:F:188:ASN:N	2.71	0.58
1:C:661:LYS:C	1:C:663:ASN:H	2.06	0.58
2:B:83:LYS:HB2	2:B:92:ILE:HD13	1.85	0.58
2:B:68:THR:C	2:B:69:ILE:HD12	2.23	0.58
2:B:216:VAL:HG12	2:B:216:VAL:O	2.03	0.58
1:C:280:ASN:HB3	1:C:300:GLY:C	2.24	0.58
3:F:147:GLY:H	3:F:178:ALA:HB3	1.66	0.58
1:A:314:ASP:OD2	1:A:376:TRP:CH2	2.55	0.58
1:C:88:LEU:HD13	1:C:138:MET:SD	2.43	0.58
3:F:37:GLU:HB2	3:F:44:LYS:HB3	1.85	0.58
3:F:29:SER:O	3:F:31:LYS:N	2.37	0.58
1:A:496:THR:O	1:A:497:ASN:CB	2.51	0.58
1:A:280:ASN:HB3	1:A:300:GLY:C	2.24	0.58
1:C:289:SER:O	1:C:290:ALA:HB2	2.03	0.58
1:C:146:SER:O	1:C:147:ASN:HB2	2.02	0.58
1:A:314:ASP:N	1:A:376:TRP:CE2	2.72	0.58
1:A:175:VAL:HG12	1:A:176:PHE:N	2.18	0.58
1:A:228:ALA:HB2	1:A:263:LEU:HD11	1.85	0.58
1:A:612:ASN:O	1:A:616:ILE:HG12	2.03	0.58
1:A:129:ASN:HA	1:A:162:GLU:HB3	1.84	0.58
1:A:329:THR:HB	1:A:331:GLN:O	2.04	0.58
1:A:306:THR:O	1:A:307:LYS:HD3	2.04	0.58
1:C:147:ASN:O	1:C:148:TYR:C	2.42	0.58
1:C:228:ALA:HB2	1:C:263:LEU:HD11	1.85	0.58
1:A:511:GLU:HG3	4:A:2107:HOH:O	2.03	0.58
1:A:365:LYS:HD2	1:A:365:LYS:O	2.04	0.58
1:C:306:THR:O	1:C:307:LYS:HD3	2.04	0.58
1:C:21:PRO:HB2	1:C:47:LEU:HD11	1.86	0.58
3:F:25:ALA:HB1	3:F:70:LEU:HD21	1.86	0.57
1:A:283:LEU:HD22	1:A:292:GLN:HE21	1.69	0.57
3:F:130:PHE:HA	3:F:136:THR:HG22	1.86	0.57
1:C:11:ALA:HB1	1:C:26:GLY:O	2.04	0.57
1:C:380:PRO:HG3	3:F:11:MET:SD	2.43	0.57
1:A:674:LEU:O	1:A:678:ILE:HG12	2.03	0.57
1:A:315:LEU:HD11	2:B:146:ILE:CD1	2.33	0.57
1:C:370:HIS:CG	1:C:371:LEU:N	2.68	0.57
1:A:11:ALA:HB1	1:A:26:GLY:O	2.04	0.57
1:C:656:GLU:OE2	1:C:670:HIS:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:ILE:HG13	2:B:43:HIS:CG	2.40	0.57
1:C:228:ALA:HB1	1:C:260:ILE:HG21	1.85	0.57
1:A:731:GLU:O	1:A:734:LYS:HB3	2.04	0.57
1:C:329:THR:HB	1:C:331:GLN:O	2.04	0.57
1:A:730:ASN:O	1:A:733:VAL:HB	2.03	0.57
1:A:221:ASN:ND2	1:A:223:THR:H	2.03	0.57
1:C:221:ASN:ND2	1:C:223:THR:H	2.02	0.57
1:A:423:LYS:HG3	1:A:424:THR:HG23	1.86	0.57
1:A:147:ASN:O	1:A:148:TYR:C	2.42	0.57
1:A:647:ILE:O	1:A:651:GLU:HG3	2.04	0.57
2:B:29:SER:HA	2:B:55:PRO:HB3	1.84	0.57
1:C:386:TRP:HZ2	3:F:280:LEU:HD22	1.68	0.57
1:A:72:HIS:ND1	1:A:118:ALA:HA	2.19	0.57
1:A:468:PHE:CE1	1:A:598:LYS:HE3	2.40	0.57
1:C:75:LYS:HZ1	1:C:94:ALA:HB2	1.69	0.57
3:F:180:ASN:N	3:F:180:ASN:ND2	2.46	0.57
2:B:108:ALA:HB1	2:B:109:PRO:CD	2.34	0.57
1:A:71:SER:HA	1:A:116:PHE:CG	2.40	0.57
1:C:62:ASP:CG	1:C:103:ARG:HH12	2.08	0.57
1:A:268:GLN:HB2	1:A:374:PRO:O	1.98	0.57
1:C:44:LEU:HD23	1:C:56:ILE:HB	1.87	0.57
1:A:262:SER:HB2	1:A:304:PHE:O	2.05	0.57
1:A:155:GLN:CB	1:A:195:GLU:HB3	2.35	0.57
1:C:241:ASP:O	1:C:243:ARG:N	2.38	0.57
1:C:155:GLN:CB	1:C:195:GLU:HB3	2.35	0.56
3:F:239:GLU:N	4:F:1304:HOH:O	2.38	0.56
1:A:268:GLN:HG3	1:A:313:PRO:CG	2.34	0.56
1:C:283:LEU:HD22	1:C:292:GLN:HE21	1.69	0.56
1:C:71:SER:HA	1:C:116:PHE:CG	2.40	0.56
3:F:10:GLU:HG3	3:F:30:ASP:HB3	1.87	0.56
1:A:292:GLN:O	1:A:368:VAL:CG2	2.53	0.56
1:C:72:HIS:ND1	1:C:118:ALA:HA	2.19	0.56
1:A:106:ASN:ND2	1:A:106:ASN:N	2.42	0.56
1:C:145:PRO:O	1:C:147:ASN:N	2.39	0.56
1:A:62:ASP:CG	1:A:103:ARG:HH12	2.08	0.56
3:F:79:VAL:CG2	3:F:95:HIS:HB3	2.35	0.56
1:A:431:ILE:HD13	1:A:447:TRP:CZ3	2.40	0.56
3:F:29:SER:C	3:F:31:LYS:N	2.59	0.56
1:A:496:THR:HG23	1:C:557:ASN:CB	2.32	0.56
1:A:241:ASP:O	1:A:243:ARG:N	2.38	0.56
4:C:1535:HOH:O	3:F:282:LYS:NZ	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:196:LEU:HG	3:F:197:GLU:N	2.21	0.56
2:B:222:LEU:HB2	2:B:234:TRP:HB2	1.85	0.56
1:C:365:LYS:O	1:C:365:LYS:HD2	2.04	0.56
1:C:494:ILE:HG13	1:C:495:GLU:N	2.18	0.56
1:C:113:THR:HG22	1:C:114:VAL:N	2.20	0.56
1:A:113:THR:HG22	1:A:114:VAL:N	2.20	0.56
1:A:21:PRO:HB2	1:A:47:LEU:HD11	1.86	0.56
2:B:4:ILE:HD12	2:B:4:ILE:N	2.20	0.56
2:B:56:VAL:HA	2:B:74:SER:HB2	1.87	0.56
1:C:430:LEU:HD11	1:C:679:GLU:HG2	1.86	0.56
3:F:4:ILE:O	3:F:4:ILE:HG22	2.04	0.56
2:B:24:LEU:HG	2:B:25:ALA:N	2.20	0.56
2:B:180:ASN:N	2:B:180:ASN:ND2	2.53	0.56
1:A:74:ASN:O	1:A:76:ILE:HG12	2.06	0.56
1:A:244:ASN:ND2	1:A:246:ASN:ND2	2.47	0.56
1:C:280:ASN:HB3	1:C:300:GLY:O	2.06	0.56
1:C:87:GLU:HG2	1:C:89:TYR:CE1	2.41	0.56
3:F:257:LEU:HD23	3:F:273:GLY:HA2	1.87	0.56
3:F:184:ILE:HG12	3:F:198:SER:HB2	1.88	0.56
1:A:438:VAL:HG22	1:A:439:ILE:N	2.20	0.56
1:A:74:ASN:H	1:A:74:ASN:ND2	2.02	0.56
1:A:153:PRO:HB2	1:A:188:TRP:CE3	2.41	0.56
1:A:584:LEU:HD12	1:A:584:LEU:H	1.71	0.56
1:C:260:ILE:CG2	1:C:261:LEU:N	2.69	0.56
1:C:120:GLN:HG3	1:C:122:ASN:OD1	2.06	0.56
1:A:120:GLN:HG3	1:A:122:ASN:OD1	2.06	0.56
1:C:268:GLN:HG3	4:C:1545:HOH:O	2.06	0.56
1:C:17:HIS:HB2	1:C:73:ASN:HB2	1.87	0.56
1:A:42:LEU:HD21	1:A:89:TYR:CD2	2.41	0.56
1:A:365:LYS:NZ	1:A:371:LEU:HD22	2.21	0.56
1:C:444:GLU:HG2	1:C:448:ASN:HD21	1.71	0.56
1:A:280:ASN:HB3	1:A:300:GLY:O	2.06	0.56
1:C:178:SER:HB2	1:C:186:SER:HB2	1.88	0.56
2:B:66:PHE:CE1	2:B:114:PRO:HD3	2.41	0.56
2:B:189:SER:C	2:B:191:ALA:H	2.09	0.56
1:A:80:ALA:CB	1:A:111:VAL:HG12	2.37	0.55
1:C:262:SER:HB2	1:C:304:PHE:O	2.05	0.55
1:A:74:ASN:N	1:A:74:ASN:ND2	2.50	0.55
1:C:203:SER:N	1:C:204:PRO:CD	2.69	0.55
1:C:153:PRO:HB2	1:C:188:TRP:CE3	2.41	0.55
1:C:292:GLN:O	1:C:368:VAL:CG2	2.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:LYS:NZ	1:C:371:LEU:HD22	2.21	0.55
1:C:42:LEU:HD21	1:C:89:TYR:CD2	2.41	0.55
2:B:8:HIS:ND1	2:B:30:ASP:OD2	2.39	0.55
1:A:162:GLU:O	1:A:164:ILE:HG23	2.06	0.55
1:A:616:ILE:HD11	1:A:640:SER:HB2	1.88	0.55
1:C:313:PRO:HD2	4:C:1546:HOH:O	2.00	0.55
1:A:17:HIS:HB2	1:A:73:ASN:HB2	1.87	0.55
1:A:730:ASN:HB3	1:A:733:VAL:CG2	2.36	0.55
1:C:462:LEU:HD22	1:C:637:ALA:HB2	1.87	0.55
1:A:44:LEU:HD23	1:A:56:ILE:HB	1.87	0.55
3:F:71:ALA:CB	3:F:81:ILE:HG22	2.37	0.55
1:C:535:LEU:HD22	1:C:538:GLU:HG3	1.88	0.55
1:A:106:ASN:ND2	1:A:106:ASN:H	2.05	0.55
1:A:420:GLU:HG3	1:A:423:LYS:CE	2.37	0.55
1:A:12:THR:O	1:A:12:THR:HG23	2.06	0.55
1:A:87:GLU:HG2	1:A:89:TYR:CE1	2.41	0.55
1:C:431:ILE:HD11	1:C:683:VAL:HG11	1.88	0.55
1:C:667:TYR:CD2	3:F:266:GLY:HA2	2.41	0.55
1:A:260:ILE:CG2	1:A:261:LEU:N	2.69	0.55
3:F:155:PRO:HG2	3:F:214:PRO:HA	1.88	0.55
2:B:69:ILE:HD12	2:B:69:ILE:N	2.22	0.55
1:A:199:LEU:HD13	1:A:240:TRP:CG	2.42	0.55
1:A:517:ASN:HD21	1:A:529:ASN:ND2	2.04	0.55
1:A:312:ALA:CB	1:A:315:LEU:HD12	2.36	0.55
3:F:81:ILE:HG12	3:F:92:ILE:HG13	1.88	0.55
3:F:74:SER:HB3	3:F:76:ASP:OD1	2.06	0.55
3:F:150:SER:HB2	3:F:210:VAL:HG22	1.88	0.55
3:F:2:VAL:HG12	3:F:2:VAL:O	2.07	0.55
1:A:623:LYS:HE3	1:A:647:ILE:HD12	1.89	0.55
1:A:38:THR:O	1:A:64:LYS:HE2	2.07	0.55
1:C:105:SER:C	1:C:107:HIS:H	2.09	0.55
1:A:105:SER:C	1:A:107:HIS:H	2.09	0.55
3:F:145:ALA:HB3	3:F:179:ASP:HB3	1.89	0.55
1:A:145:PRO:O	1:A:147:ASN:N	2.38	0.55
1:A:247:THR:CG2	1:A:248:PRO:HD2	2.37	0.55
1:A:41:SER:O	1:A:42:LEU:HB3	2.07	0.55
1:A:80:ALA:HB2	1:A:114:VAL:CG2	2.36	0.55
1:A:203:SER:N	1:A:204:PRO:CD	2.69	0.55
1:A:418:LEU:HD23	1:A:718:LEU:HD21	1.89	0.55
1:A:129:ASN:ND2	1:A:162:GLU:OE1	2.38	0.54
1:A:434:ARG:HG3	1:A:447:TRP:CZ2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:260:ALA:HA	3:F:271:LEU:HD12	1.89	0.54
1:C:519:VAL:HG23	1:C:520:SER:N	2.21	0.54
1:A:418:LEU:HG	1:A:718:LEU:HD11	1.87	0.54
1:C:733:VAL:O	1:C:737:LYS:HG3	2.07	0.54
1:C:312:ALA:CB	1:C:315:LEU:HD12	2.36	0.54
1:C:162:GLU:O	1:C:164:ILE:HG23	2.06	0.54
1:C:199:LEU:HD13	1:C:240:TRP:CG	2.42	0.54
1:C:12:THR:HG23	1:C:12:THR:O	2.06	0.54
1:C:59:LEU:HD22	1:C:98:ILE:HG12	1.90	0.54
1:A:46:SER:HB2	1:A:56:ILE:HD11	1.90	0.54
2:B:73:CYS:HB2	2:B:102:VAL:CG1	2.37	0.54
1:C:247:THR:CG2	1:C:248:PRO:HD2	2.37	0.54
1:C:38:THR:O	1:C:64:LYS:HE2	2.07	0.54
1:C:26:GLY:HA2	1:C:42:LEU:HA	1.89	0.54
1:A:66:ASN:N	1:A:80:ALA:O	2.39	0.54
1:C:244:ASN:HD21	1:C:246:ASN:HD22	1.49	0.54
1:A:337:LEU:CD2	2:B:97:VAL:HG12	2.36	0.54
3:F:183:LYS:HB2	3:F:185:TRP:HE1	1.72	0.54
1:A:510:ILE:HB	4:A:2107:HOH:O	2.06	0.54
3:F:208:ARG:H	3:F:226:SER:HA	1.72	0.54
3:F:92:ILE:HG13	3:F:93:ALA:H	1.72	0.54
1:C:104:PHE:N	1:C:104:PHE:CD1	2.75	0.54
1:C:590:VAL:HG13	1:C:622:LEU:HD23	1.90	0.54
1:C:696:ASN:O	1:C:700:ILE:HG13	2.08	0.54
1:C:74:ASN:O	1:C:76:ILE:HG12	2.06	0.54
1:A:244:ASN:HD21	1:A:246:ASN:HD22	1.49	0.54
1:A:178:SER:HB2	1:A:186:SER:HB2	1.88	0.54
3:F:184:ILE:CG1	3:F:198:SER:HB2	2.38	0.54
1:C:129:ASN:ND2	1:C:162:GLU:OE1	2.38	0.54
2:B:45:LEU:O	2:B:46:ILE:HD13	2.08	0.54
1:C:41:SER:O	1:C:42:LEU:HB3	2.07	0.54
1:C:402:VAL:HG11	3:F:24:MET:SD	2.47	0.54
1:C:80:ALA:HB2	1:C:114:VAL:CG2	2.36	0.54
1:C:66:ASN:N	1:C:80:ALA:O	2.39	0.54
1:A:26:GLY:HA2	1:A:42:LEU:HA	1.89	0.54
1:A:73:ASN:C	1:A:75:LYS:N	2.59	0.54
3:F:225:VAL:HG22	3:F:257:LEU:CB	2.37	0.54
3:F:283:GLU:HA	3:F:288:LYS:O	2.07	0.54
1:C:73:ASN:C	1:C:75:LYS:N	2.58	0.54
3:F:39:GLU:O	3:F:41:GLU:N	2.33	0.54
1:A:314:ASP:CG	1:A:376:TRP:CD1	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:25:ALA:HA	3:F:34:LYS:O	2.08	0.54
1:C:510:ILE:HG21	1:C:533:ASN:ND2	2.23	0.54
2:B:80:LEU:HD23	2:B:94:VAL:HG23	1.90	0.54
1:A:509:ASN:ND2	1:A:509:ASN:N	2.54	0.53
2:B:80:LEU:CD2	2:B:94:VAL:HG23	2.38	0.53
1:A:48:LEU:O	1:A:49:ALA:O	2.25	0.53
3:F:229:ARG:HG2	3:F:256:VAL:HA	1.90	0.53
1:A:154:GLY:O	1:A:155:GLN:CG	2.48	0.53
1:C:74:ASN:ND2	1:C:74:ASN:H	2.02	0.53
2:B:25:ALA:HB2	2:B:61:TRP:CZ2	2.44	0.53
3:F:155:PRO:CG	3:F:214:PRO:HA	2.37	0.53
3:F:236:GLN:HG2	3:F:237:ASP:N	2.22	0.53
1:C:48:LEU:O	1:C:49:ALA:O	2.25	0.53
1:A:528:LYS:HG3	1:C:493:GLN:NE2	2.22	0.53
1:A:551:LEU:C	1:A:553:GLU:H	2.11	0.53
1:C:259:GLY:HA3	1:C:278:ARG:HH11	1.74	0.53
1:C:46:SER:HB2	1:C:56:ILE:HD11	1.90	0.53
3:F:17:MET:C	3:F:61:TRP:CD1	2.81	0.53
1:C:707:ILE:O	1:C:710:THR:HB	2.09	0.53
1:A:110:SER:OG	1:A:129:ASN:ND2	2.41	0.53
1:A:125:ALA:HB2	1:A:168:TRP:HH2	1.62	0.53
1:A:59:LEU:HD22	1:A:98:ILE:HG12	1.90	0.53
1:C:423:LYS:CG	1:C:424:THR:N	2.71	0.53
1:A:439:ILE:HG21	1:A:659:LEU:HD21	1.90	0.53
1:A:175:VAL:HG13	1:A:188:TRP:O	2.08	0.53
2:B:39:GLU:HB2	4:B:1335:HOH:O	2.08	0.53
1:A:285:TRP:CZ3	1:A:292:GLN:HG3	2.44	0.53
1:C:604:TYR:CZ	1:C:610:GLN:HG2	2.43	0.53
3:F:215:THR:HG23	3:F:215:THR:O	2.08	0.53
1:C:665:THR:HG22	3:F:285:LEU:HD23	1.91	0.53
1:A:13:PHE:HA	1:A:24:VAL:O	2.09	0.53
3:F:46:ILE:CG2	3:F:47:ASP:H	1.99	0.53
2:B:33:ILE:CD1	2:B:56:VAL:HG11	2.39	0.53
2:B:49:LEU:HB3	2:B:82:TRP:CZ3	2.44	0.53
1:C:80:ALA:CB	1:C:111:VAL:HG12	2.37	0.53
1:C:386:TRP:NE1	3:F:270:ALA:HB2	2.24	0.53
1:C:13:PHE:HA	1:C:24:VAL:O	2.09	0.53
1:A:57:ALA:O	1:A:98:ILE:HG22	2.09	0.53
1:C:535:LEU:CB	1:C:538:GLU:HG3	2.31	0.53
1:A:723:LEU:HA	4:A:2255:HOH:O	2.08	0.53
1:A:337:LEU:HD11	2:B:97:VAL:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:PRO:C	1:C:376:TRP:HE1	2.12	0.53
1:C:408:LYS:HE2	3:F:292:ALA:O	2.09	0.53
3:F:119:ALA:HB2	3:F:151:ALA:HB2	1.91	0.53
1:C:110:SER:OG	1:C:129:ASN:ND2	2.42	0.53
1:C:199:LEU:HD13	1:C:240:TRP:CD2	2.44	0.53
1:A:451:GLU:O	1:A:454:SER:HB3	2.09	0.52
1:A:104:PHE:N	1:A:104:PHE:CD1	2.75	0.52
1:C:286:ASN:HB2	1:C:293:LEU:HD11	1.92	0.52
1:A:129:ASN:C	1:A:131:GLY:H	2.11	0.52
3:F:108:ALA:HB2	3:F:153:TRP:CZ2	2.44	0.52
3:F:184:ILE:HD11	3:F:222:MET:HE3	1.89	0.52
1:A:199:LEU:HD13	1:A:240:TRP:CD2	2.44	0.52
1:A:7:PHE:O	1:A:324:LYS:HD3	2.09	0.52
1:A:90:SER:O	1:A:91:THR:HB	2.08	0.52
2:B:128:VAL:CG2	2:B:138:PRO:HB3	2.27	0.52
3:F:52:HIS:CE1	3:F:80:MET:HE3	2.44	0.52
1:C:175:VAL:HG13	1:C:188:TRP:O	2.09	0.52
3:F:59:VAL:HG12	3:F:72:SER:HA	1.89	0.52
1:A:172:LEU:C	1:A:174:HIS:H	2.13	0.52
1:A:388:PHE:CD1	1:A:739:ARG:NH2	2.77	0.52
3:F:78:LYS:HG2	3:F:96:ALA:CB	2.40	0.52
1:C:285:TRP:CZ3	1:C:292:GLN:HG3	2.44	0.52
1:C:57:ALA:O	1:C:98:ILE:HG22	2.09	0.52
1:C:106:ASN:ND2	1:C:106:ASN:H	2.04	0.52
1:A:137:ASP:OD1	1:A:139:ASN:HB2	2.10	0.52
1:C:7:PHE:O	1:C:324:LYS:HD3	2.09	0.52
3:F:46:ILE:N	3:F:46:ILE:CD1	2.71	0.52
1:C:172:LEU:C	1:C:174:HIS:H	2.13	0.52
3:F:188:ASN:HB3	3:F:191:ALA:HB3	1.92	0.52
1:C:252:LEU:HD13	1:C:285:TRP:CG	2.45	0.52
3:F:233:ILE:H	3:F:233:ILE:CD1	2.10	0.52
1:C:145:PRO:O	1:C:146:SER:C	2.48	0.52
1:C:137:ASP:OD1	1:C:139:ASN:HB2	2.10	0.52
1:C:314:ASP:OD2	1:C:376:TRP:CZ3	2.62	0.52
2:B:238:ASN:HD22	2:B:240:GLN:N	2.07	0.52
1:A:742:ILE:H	1:A:742:ILE:HD12	1.73	0.52
1:A:531:LEU:C	1:A:533:ASN:H	2.13	0.52
1:C:268:GLN:HA	1:C:373:ALA:HB3	1.88	0.52
1:C:312:ALA:HB1	1:C:315:LEU:HD12	1.92	0.52
3:F:99:SER:O	3:F:100:ALA:CB	2.58	0.52
1:C:22:LEU:CD1	1:C:94:ALA:CB	2.82	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:SER:O	1:C:91:THR:HB	2.09	0.52
3:F:206:TRP:N	3:F:206:TRP:CD1	2.78	0.52
1:A:27:THR:HB	1:A:40:SER:CB	2.40	0.52
1:C:155:GLN:HG3	1:C:194:LYS:HB2	1.93	0.51
3:F:231:CYS:HB3	3:F:248:LEU:HD22	1.92	0.51
3:F:180:ASN:CG	3:F:205:ASP:O	2.49	0.51
2:B:117:LEU:HD12	4:B:1340:HOH:O	2.08	0.51
1:C:27:THR:HB	1:C:40:SER:CB	2.40	0.51
1:C:261:LEU:HB2	1:C:277:GLY:HA2	1.92	0.51
1:C:636:LEU:HD12	1:C:688:ILE:HD12	1.93	0.51
1:A:155:GLN:HG3	1:A:194:LYS:HB2	1.92	0.51
1:A:688:ILE:HD13	1:A:689:ASN:N	2.25	0.51
1:A:593:TRP:C	1:A:595:PHE:H	2.12	0.51
1:A:252:LEU:HD13	1:A:285:TRP:CG	2.45	0.51
1:C:129:ASN:C	1:C:131:GLY:H	2.11	0.51
1:A:519:VAL:CG1	1:C:599:ALA:HA	2.40	0.51
1:A:145:PRO:O	1:A:146:SER:C	2.48	0.51
1:A:259:GLY:HA3	1:A:278:ARG:HH11	1.74	0.51
1:A:649:LEU:HB3	1:A:698:GLN:OE1	2.09	0.51
1:A:314:ASP:N	1:A:376:TRP:CZ2	2.72	0.51
3:F:23:ARG:NH1	3:F:68:THR:CG2	2.74	0.51
1:C:674:LEU:HD21	1:C:705:GLU:HB3	1.91	0.51
3:F:123:GLY:HA2	3:F:147:GLY:HA2	1.92	0.51
1:A:261:LEU:HB2	1:A:277:GLY:HA2	1.92	0.51
1:C:70:TRP:HD1	1:C:71:SER:O	1.94	0.51
2:B:255:ASP:CG	2:B:256:VAL:H	2.14	0.51
3:F:85:GLU:O	3:F:86:ASN:HB2	2.11	0.51
2:B:69:ILE:HG22	2:B:70:LEU:N	2.25	0.51
1:C:400:LYS:O	3:F:6:ASN:HA	2.11	0.51
1:A:608:ILE:HD13	1:A:611:ARG:NH1	2.24	0.51
2:B:33:ILE:HB	2:B:49:LEU:HB2	1.92	0.51
1:C:377:TYR:HA	4:C:1513:HOH:O	2.11	0.51
3:F:94:VAL:HG13	3:F:94:VAL:O	2.11	0.51
1:A:241:ASP:C	1:A:243:ARG:N	2.65	0.51
3:F:65:LYS:CD	3:F:110:HIS:HB2	2.40	0.51
1:A:584:LEU:CD1	1:A:584:LEU:H	2.22	0.51
3:F:171:ARG:O	3:F:186:LYS:HA	2.11	0.51
1:A:283:LEU:HD13	1:A:292:GLN:NE2	2.26	0.51
1:A:286:ASN:HB2	1:A:293:LEU:HD11	1.92	0.51
1:C:117:ASN:ND2	1:C:118:ALA:N	2.54	0.51
3:F:233:ILE:HG21	3:F:289:TRP:CZ2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:677:PHE:CD2	1:C:678:ILE:HD12	2.46	0.51
2:B:105:VAL:CG2	2:B:116:LEU:HD21	2.41	0.51
3:F:259:ARG:HG3	3:F:259:ARG:HH11	1.76	0.51
1:C:283:LEU:HD13	1:C:292:GLN:NE2	2.26	0.51
1:C:333:LEU:HG	3:F:100:ALA:HA	1.93	0.51
1:C:241:ASP:C	1:C:243:ARG:N	2.65	0.51
1:C:430:LEU:O	1:C:430:LEU:HD23	2.11	0.51
1:A:524:LYS:HG3	1:A:525:SER:N	2.26	0.51
3:F:92:ILE:HG13	3:F:93:ALA:N	2.26	0.50
2:B:95:HIS:CE1	2:B:128:VAL:HG21	2.46	0.50
1:A:212:LEU:HD13	1:A:227:THR:CG2	2.41	0.50
1:A:312:ALA:HB1	1:A:315:LEU:HD12	1.92	0.50
1:A:75:LYS:HZ2	1:A:94:ALA:N	2.09	0.50
1:A:274:LEU:HG	1:A:308:PHE:CZ	2.46	0.50
2:B:259:ARG:HH11	2:B:259:ARG:HG3	1.77	0.50
1:A:268:GLN:CB	4:A:2118:HOH:O	2.46	0.50
1:C:271:HIS:O	1:C:272:LEU:HD23	2.12	0.50
3:F:24:MET:CG	3:F:25:ALA:N	2.60	0.50
3:F:27:CYS:HB2	3:F:56:VAL:CG1	2.41	0.50
2:B:4:ILE:HG22	2:B:4:ILE:O	2.11	0.50
1:A:608:ILE:HB	1:A:611:ARG:NH1	2.27	0.50
1:A:70:TRP:HD1	1:A:71:SER:O	1.94	0.50
1:C:519:VAL:C	1:C:521:GLY:N	2.62	0.50
1:A:314:ASP:CB	1:A:376:TRP:CE2	2.95	0.50
1:C:335:ASN:OD1	3:F:99:SER:HB3	2.11	0.50
1:C:124:LEU:CG	1:C:125:ALA:H	2.24	0.50
3:F:78:LYS:HG2	3:F:96:ALA:HB1	1.94	0.50
1:A:432:ASN:O	1:A:436:VAL:HG23	2.11	0.50
3:F:59:VAL:HA	3:F:71:ALA:O	2.12	0.50
1:C:31:THR:CG2	1:C:32:VAL:N	2.64	0.50
1:A:731:GLU:HA	1:A:734:LYS:HB3	1.93	0.50
3:F:286:GLU:HG3	3:F:288:LYS:HD2	1.94	0.50
1:A:663:ASN:HA	2:B:285:LEU:HD11	1.94	0.50
1:A:57:ALA:O	1:A:98:ILE:CG2	2.60	0.50
3:F:71:ALA:HB2	3:F:81:ILE:CG2	2.40	0.50
1:A:664:LYS:HA	1:A:668:GLU:OE1	2.11	0.50
2:B:200:LEU:HD13	2:B:234:TRP:CE3	2.47	0.50
1:A:567:SER:HB3	1:A:570:SER:HB2	1.93	0.50
1:C:274:LEU:HG	1:C:308:PHE:CZ	2.46	0.50
1:C:551:LEU:C	1:C:551:LEU:HD23	2.33	0.50
1:A:28:VAL:HG22	1:A:29:SER:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ALA:HB3	1:A:325:ILE:HD11	1.93	0.50
3:F:29:SER:HA	3:F:55:PRO:HB3	1.93	0.50
1:A:271:HIS:O	1:A:272:LEU:HD23	2.12	0.50
1:A:505:SER:CB	1:C:589:ASP:HB2	2.37	0.50
1:A:402:VAL:HG11	2:B:24:LEU:CD2	2.42	0.50
1:A:555:VAL:O	1:A:558:ALA:HB3	2.12	0.50
3:F:63:HIS:ND1	3:F:64:PRO:HD2	2.26	0.50
1:A:314:ASP:CG	1:A:376:TRP:CG	2.85	0.49
1:A:72:HIS:HE1	1:A:118:ALA:HA	1.72	0.49
1:A:314:ASP:OD1	1:A:376:TRP:CG	2.65	0.49
1:C:11:ALA:HB3	1:C:325:ILE:HD11	1.93	0.49
1:A:15:TRP:HB3	1:A:310:PRO:CD	2.41	0.49
1:A:117:ASN:ND2	1:A:118:ALA:N	2.54	0.49
1:A:496:THR:HG22	1:A:497:ASN:N	2.27	0.49
1:A:412:LEU:CD2	1:A:713:THR:HG22	2.38	0.49
3:F:47:ASP:OD2	3:F:89:TRP:HB2	2.12	0.49
3:F:10:GLU:CG	3:F:30:ASP:HB3	2.42	0.49
2:B:112:TYR:CZ	2:B:171:ARG:HG2	2.46	0.49
1:A:536:LEU:HD23	1:C:537:MET:HE3	1.94	0.49
1:C:601:GLN:HE22	1:C:611:ARG:HD3	1.77	0.49
1:C:28:VAL:HG22	1:C:29:SER:N	2.26	0.49
3:F:52:HIS:CG	3:F:80:MET:HE1	2.47	0.49
1:A:115:LYS:O	1:A:124:LEU:HD12	2.13	0.49
1:C:530:SER:O	1:C:533:ASN:O	2.31	0.49
1:A:196:VAL:C	1:A:197:ILE:HG13	2.32	0.49
1:A:337:LEU:CD2	2:B:97:VAL:CG1	2.90	0.49
3:F:131:LYS:HB3	3:F:132:GLU:OE2	2.12	0.49
1:C:665:THR:HG22	3:F:285:LEU:N	2.27	0.49
1:A:284:LEU:HD23	1:A:371:LEU:HD11	1.94	0.49
1:A:15:TRP:HZ3	1:A:307:LYS:O	1.96	0.49
1:C:439:ILE:CG2	1:C:659:LEU:HD21	2.39	0.49
1:C:196:VAL:C	1:C:197:ILE:HG13	2.32	0.49
1:A:665:THR:HG1	1:A:668:GLU:HG3	1.78	0.49
1:A:568:SER:HB2	1:C:511:GLU:OE1	2.13	0.49
2:B:148:VAL:O	4:B:1338:HOH:O	2.20	0.49
1:A:268:GLN:HE21	1:A:313:PRO:CG	2.25	0.49
1:C:268:GLN:HE21	1:C:313:PRO:CG	2.25	0.49
1:C:237:ILE:HB	1:C:252:LEU:HB2	1.93	0.49
2:B:95:HIS:HE1	2:B:138:PRO:HG3	1.78	0.49
1:A:237:ILE:HB	1:A:252:LEU:HB2	1.93	0.49
3:F:129:GLU:HG2	3:F:130:PHE:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:ILE:CD1	2:B:248:LEU:HD13	2.43	0.49
1:C:733:VAL:HG12	1:C:737:LYS:HE3	1.95	0.49
3:F:259:ARG:HB2	3:F:272:SER:HB2	1.95	0.49
1:C:115:LYS:O	1:C:124:LEU:HD12	2.13	0.49
1:C:29:SER:HB2	1:C:82:ASP:OD1	2.13	0.49
1:C:15:TRP:HB3	1:C:310:PRO:CD	2.41	0.49
1:C:494:ILE:HG23	1:C:495:GLU:N	2.27	0.49
1:C:212:LEU:HD13	1:C:227:THR:CG2	2.41	0.49
1:A:33:ASP:OD1	1:A:37:SER:HB3	2.13	0.49
1:C:57:ALA:O	1:C:98:ILE:CG2	2.60	0.49
1:A:187:ILE:HB	1:A:197:ILE:HB	1.95	0.49
1:A:430:LEU:HD23	1:A:430:LEU:O	2.13	0.49
1:C:115:LYS:O	1:C:168:TRP:HZ3	1.96	0.49
1:A:124:LEU:CG	1:A:125:ALA:N	2.76	0.49
1:C:130:ASN:HB3	1:C:132:GLU:HG3	1.95	0.49
2:B:63:HIS:CD2	4:B:1334:HOH:O	2.65	0.49
2:B:26:THR:O	2:B:33:ILE:HG23	2.12	0.49
2:B:29:SER:C	2:B:31:LYS:H	2.16	0.49
1:A:22:LEU:CD1	1:A:94:ALA:CB	2.82	0.48
1:A:264:ASP:HB2	1:A:307:LYS:HD3	1.94	0.48
1:A:203:SER:C	1:A:205:ASN:H	2.17	0.48
1:A:31:THR:O	1:A:32:VAL:HG23	2.13	0.48
1:A:130:ASN:HB3	1:A:132:GLU:HG3	1.95	0.48
1:C:19:LYS:HD2	3:F:206:TRP:NE1	2.27	0.48
3:F:75:TYR:C	3:F:77:GLY:H	2.17	0.48
1:C:325:ILE:CD1	1:C:325:ILE:N	2.76	0.48
1:C:75:LYS:HZ1	1:C:94:ALA:CB	2.25	0.48
1:A:115:LYS:O	1:A:168:TRP:HZ3	1.96	0.48
1:C:154:GLY:O	1:C:155:GLN:CG	2.48	0.48
3:F:52:HIS:ND1	3:F:74:SER:HB2	2.28	0.48
1:C:15:TRP:HZ3	1:C:307:LYS:O	1.96	0.48
1:A:420:GLU:CA	1:A:423:LYS:HE2	2.38	0.48
1:C:19:LYS:C	1:C:21:PRO:HD3	2.33	0.48
1:A:466:LEU:O	1:A:598:LYS:HE2	2.13	0.48
1:A:19:LYS:C	1:A:21:PRO:HD3	2.33	0.48
1:A:325:ILE:CD1	1:A:325:ILE:N	2.76	0.48
1:A:593:TRP:C	1:A:595:PHE:N	2.66	0.48
1:A:151:LEU:CD1	1:A:152:THR:H	2.25	0.48
1:A:585:VAL:HA	1:A:596:ILE:HG21	1.95	0.48
2:B:119:ALA:HB1	2:B:148:VAL:HG12	1.96	0.48
2:B:184:ILE:HD12	2:B:184:ILE:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:ASP:O	1:C:460:GLU:HB2	2.14	0.48
1:C:331:GLN:HG2	1:C:371:LEU:HD23	1.96	0.48
1:A:124:LEU:CG	1:A:125:ALA:H	2.24	0.48
1:A:331:GLN:HG2	1:A:371:LEU:HD23	1.96	0.48
1:C:264:ASP:HB2	1:C:307:LYS:HD3	1.94	0.48
1:C:203:SER:C	1:C:205:ASN:H	2.16	0.48
1:C:219:PRO:HG3	1:C:266:CYS:O	2.14	0.48
1:A:29:SER:HB2	1:A:82:ASP:OD1	2.13	0.48
1:A:75:LYS:HD2	1:A:91:THR:HG22	1.95	0.48
1:C:284:LEU:HD23	1:C:371:LEU:HD11	1.95	0.48
3:F:108:ALA:HB3	3:F:115:MET:HB2	1.96	0.48
1:A:86:LEU:HD23	1:A:104:PHE:HB2	1.96	0.48
2:B:18:ASP:OD2	2:B:23:ARG:HB3	2.14	0.48
3:F:102:VAL:HA	3:F:120:SER:HA	1.96	0.48
1:A:514:ILE:HA	1:A:517:ASN:ND2	2.28	0.48
1:C:728:SER:HB3	1:C:737:LYS:NZ	2.29	0.48
2:B:59:VAL:HA	2:B:71:ALA:O	2.14	0.48
1:C:664:LYS:N	3:F:285:LEU:CD1	2.53	0.48
3:F:95:HIS:CE1	3:F:128:VAL:HG21	2.48	0.48
1:A:365:LYS:HZ3	1:A:371:LEU:HD22	1.77	0.48
2:B:108:ALA:HA	2:B:153:TRP:CD1	2.49	0.48
2:B:37:GLU:HG2	2:B:46:ILE:CG1	2.44	0.48
1:A:644:VAL:HG11	1:A:684:PHE:CE2	2.48	0.48
1:A:42:LEU:CD2	1:A:98:ILE:HD11	2.44	0.48
1:C:31:THR:O	1:C:32:VAL:HG23	2.13	0.48
1:C:33:ASP:OD1	1:C:37:SER:HB3	2.13	0.48
2:B:57:TRP:O	2:B:58:ARG:HG2	2.13	0.48
3:F:24:MET:O	3:F:61:TRP:HZ2	1.97	0.48
3:F:205:ASP:H	3:F:228:ASP:HB3	1.78	0.48
1:A:412:LEU:C	1:A:412:LEU:HD23	2.35	0.48
1:C:187:ILE:HB	1:C:197:ILE:HB	1.95	0.48
1:C:75:LYS:HD2	1:C:91:THR:HG22	1.95	0.47
3:F:196:LEU:CG	3:F:197:GLU:N	2.77	0.47
1:C:271:HIS:CE1	1:C:288:GLU:OE2	2.67	0.47
1:C:124:LEU:CG	1:C:125:ALA:N	2.76	0.47
1:A:92:ASN:O	1:A:93:GLU:CB	2.62	0.47
1:A:75:LYS:HZ1	1:A:94:ALA:CB	2.25	0.47
3:F:82:TRP:N	3:F:82:TRP:CD1	2.82	0.47
1:C:514:ILE:HA	1:C:517:ASN:HD22	1.79	0.47
2:B:172:LYS:HA	2:B:185:TRP:O	2.13	0.47
1:C:388:PHE:CE1	1:C:739:ARG:HD3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:GLN:CA	1:C:373:ALA:CB	2.80	0.47
1:C:364:GLU:O	1:C:365:LYS:CB	2.47	0.47
1:A:10:THR:O	1:A:11:ALA:HB2	2.14	0.47
3:F:24:MET:HB3	3:F:36:PHE:HB2	1.96	0.47
1:A:426:ASP:OD1	1:A:429:PRO:HD3	2.14	0.47
2:B:15:ALA:HA	2:B:25:ALA:O	2.14	0.47
2:B:34:LYS:HB3	2:B:36:PHE:HE1	1.80	0.47
2:B:8:HIS:CE1	2:B:34:LYS:HE2	2.48	0.47
1:A:542:ILE:HD11	1:C:573:LEU:HD21	1.96	0.47
3:F:109:PRO:HD2	3:F:112:TYR:CD2	2.49	0.47
2:B:259:ARG:NH1	2:B:259:ARG:HG3	2.30	0.47
3:F:157:THR:HB	3:F:170:SER:OG	2.13	0.47
1:A:462:LEU:HD13	1:A:637:ALA:HB2	1.97	0.47
1:A:114:VAL:HA	1:A:125:ALA:O	2.14	0.47
1:C:16:SER:HB2	1:C:18:ASP:OD1	2.14	0.47
1:C:553:GLU:HG2	1:C:557:ASN:ND2	2.28	0.47
1:C:186:SER:HB3	1:C:188:TRP:NE1	2.29	0.47
2:B:212:TRP:CD2	2:B:222:LEU:HD21	2.49	0.47
1:A:7:PHE:HB2	1:A:8:SER:H	1.51	0.47
3:F:131:LYS:HD2	3:F:135:THR:O	2.14	0.47
1:A:219:PRO:HG3	1:A:266:CYS:O	2.13	0.47
1:A:542:ILE:HD11	1:C:573:LEU:CD2	2.44	0.47
1:A:42:LEU:HD23	1:A:98:ILE:HD11	1.96	0.47
3:F:23:ARG:NH1	3:F:68:THR:HG21	2.29	0.47
1:A:639:GLY:HA2	1:A:688:ILE:CD1	2.35	0.47
1:C:114:VAL:HA	1:C:125:ALA:O	2.14	0.47
1:C:42:LEU:HD23	1:C:98:ILE:HD11	1.96	0.47
1:A:91:THR:HG22	1:A:91:THR:O	2.14	0.47
1:C:424:THR:O	1:C:425:LYS:CB	2.62	0.47
3:F:31:LYS:HB3	3:F:52:HIS:O	2.15	0.47
1:A:271:HIS:CE1	1:A:288:GLU:OE2	2.67	0.47
1:A:15:TRP:CZ3	1:A:317:ALA:N	2.83	0.47
3:F:209:ASP:HB2	3:F:258:TRP:O	2.14	0.47
1:A:336:THR:OG1	2:B:96:ALA:O	2.33	0.47
1:A:186:SER:HB3	1:A:188:TRP:NE1	2.29	0.47
1:C:86:LEU:HD23	1:C:104:PHE:HB2	1.96	0.47
1:A:392:LEU:CD1	4:A:2219:HOH:O	2.61	0.47
2:B:31:LYS:O	4:B:1321:HOH:O	2.20	0.47
1:C:412:LEU:CD2	1:C:713:THR:HG22	2.45	0.47
1:C:739:ARG:CD	3:F:19:TYR:CE2	2.71	0.47
1:C:313:PRO:HG2	4:C:1545:HOH:O	1.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:LYS:HZ3	1:C:371:LEU:HD22	1.79	0.47
1:C:92:ASN:O	1:C:93:GLU:CB	2.62	0.47
1:A:364:GLU:O	1:A:365:LYS:CB	2.47	0.47
1:A:16:SER:HB2	1:A:18:ASP:OD1	2.14	0.47
2:B:69:ILE:CG2	2:B:70:LEU:N	2.77	0.47
1:A:664:LYS:HB3	1:A:668:GLU:HB2	1.96	0.47
3:F:146:ILE:HB	3:F:178:ALA:HB3	1.96	0.47
1:C:727:PRO:C	1:C:729:ASP:N	2.67	0.47
1:C:731:GLU:HA	1:C:734:LYS:HB3	1.97	0.47
3:F:124:LYS:HG2	3:F:142:ASP:OD1	2.15	0.47
1:C:42:LEU:CD2	1:C:98:ILE:HD11	2.44	0.47
1:A:202:THR:CG2	1:A:209:LYS:HD3	2.45	0.47
2:B:225:VAL:HG13	2:B:257:LEU:CB	2.43	0.47
1:C:172:LEU:C	1:C:174:HIS:N	2.69	0.47
1:A:337:LEU:HD21	2:B:140:ILE:HD11	1.97	0.47
1:A:51:ASP:O	1:A:52:SER:C	2.54	0.47
1:A:718:LEU:O	1:A:722:PHE:HD1	1.98	0.47
1:C:312:ALA:O	1:C:314:ASP:N	2.48	0.47
3:F:210:VAL:HG23	3:F:210:VAL:O	2.14	0.47
1:A:572:ILE:CD1	1:C:504:PHE:HE2	2.28	0.47
1:C:10:THR:O	1:C:11:ALA:HB2	2.14	0.46
1:C:641:LEU:HD12	1:C:684:PHE:HE2	1.80	0.46
1:C:386:TRP:HZ3	4:C:1614:HOH:O	1.98	0.46
2:B:121:SER:HA	4:B:1338:HOH:O	2.15	0.46
2:B:72:SER:O	2:B:79:VAL:HG13	2.14	0.46
1:C:314:ASP:OD2	1:C:376:TRP:CH2	2.67	0.46
1:A:252:LEU:HD13	1:A:285:TRP:CB	2.45	0.46
1:C:202:THR:CG2	1:C:209:LYS:HD3	2.46	0.46
1:C:439:ILE:HG13	1:C:440:ASP:N	2.27	0.46
1:A:172:LEU:C	1:A:174:HIS:N	2.68	0.46
2:B:109:PRO:HD2	2:B:112:TYR:CD2	2.50	0.46
1:A:739:ARG:HD2	2:B:19:TYR:CZ	2.50	0.46
2:B:124:LYS:HE2	2:B:142:ASP:OD1	2.15	0.46
1:C:252:LEU:HD13	1:C:285:TRP:CB	2.45	0.46
3:F:99:SER:O	3:F:100:ALA:HB2	2.15	0.46
2:B:27:CYS:HB2	2:B:56:VAL:CG1	2.45	0.46
3:F:118:VAL:HB	3:F:126:SER:OG	2.15	0.46
1:C:377:TYR:CA	4:C:1513:HOH:O	2.64	0.46
1:C:91:THR:HG22	1:C:91:THR:O	2.14	0.46
1:A:68:LEU:HD22	1:A:77:ILE:HG22	1.98	0.46
3:F:226:SER:OG	3:F:227:GLN:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:69:ILE:CG1	3:F:83:LYS:HG2	2.32	0.46
1:C:15:TRP:CZ3	1:C:317:ALA:N	2.83	0.46
1:C:203:SER:C	1:C:205:ASN:N	2.69	0.46
2:B:93:ALA:HB1	4:B:1344:HOH:O	2.14	0.46
2:B:119:ALA:HB1	2:B:148:VAL:CG1	2.45	0.46
3:F:152:SER:CB	3:F:211:ALA:HA	2.45	0.46
3:F:75:TYR:O	3:F:77:GLY:N	2.49	0.46
1:A:593:TRP:O	1:A:595:PHE:N	2.48	0.46
2:B:74:SER:CB	2:B:76:ASP:OD1	2.61	0.46
3:F:40:GLY:O	3:F:41:GLU:CG	2.62	0.46
2:B:29:SER:O	2:B:31:LYS:HG3	2.14	0.46
1:C:183:ASN:HA	1:C:211:GLN:HA	1.97	0.46
3:F:194:TYR:H	3:F:194:TYR:HD1	1.63	0.46
1:C:169:ASN:HB3	1:C:172:LEU:O	2.16	0.46
2:B:117:LEU:HB2	2:B:153:TRP:NE1	2.31	0.46
1:A:608:ILE:CD1	1:A:611:ARG:NH1	2.78	0.46
3:F:141:ILE:O	3:F:141:ILE:HD13	2.14	0.46
1:C:45:TRP:N	1:C:45:TRP:CD1	2.84	0.46
1:A:312:ALA:O	1:A:314:ASP:N	2.48	0.46
1:C:68:LEU:HD22	1:C:77:ILE:HG22	1.98	0.46
1:A:68:LEU:HA	1:A:78:ALA:O	2.15	0.46
3:F:37:GLU:O	3:F:43:HIS:HA	2.15	0.46
1:C:674:LEU:O	1:C:678:ILE:HD13	2.15	0.46
1:A:169:ASN:HB3	1:A:172:LEU:O	2.16	0.46
1:A:169:ASN:OD1	1:A:172:LEU:HB2	2.16	0.46
1:A:652:PHE:HB3	1:A:653:PRO:CD	2.44	0.46
1:C:458:THR:HG23	1:C:459:GLU:N	2.30	0.46
1:A:183:ASN:HA	1:A:211:GLN:HA	1.97	0.46
1:C:68:LEU:HA	1:C:78:ALA:O	2.16	0.46
1:C:204:PRO:C	1:C:206:SER:H	2.19	0.46
1:C:212:LEU:HD22	1:C:227:THR:HG22	1.98	0.46
1:C:51:ASP:O	1:C:52:SER:C	2.54	0.46
2:B:200:LEU:HB3	2:B:234:TRP:CH2	2.50	0.46
1:A:219:PRO:HD3	1:A:265:TRP:CD1	2.51	0.46
3:F:14:ASP:HB3	3:F:27:CYS:SG	2.55	0.46
1:A:663:ASN:CA	2:B:285:LEU:HD11	2.46	0.46
1:C:432:ASN:O	1:C:436:VAL:HG23	2.16	0.46
1:A:45:TRP:N	1:A:45:TRP:CD1	2.84	0.46
1:C:382:PRO:CB	3:F:278:VAL:HG23	2.46	0.46
1:A:63:SER:HB3	1:A:82:ASP:HB2	1.98	0.46
3:F:200:LEU:HD13	3:F:234:TRP:CE3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:121:SER:C	3:F:123:GLY:H	2.20	0.46
1:A:536:LEU:HD23	1:C:537:MET:CE	2.46	0.46
1:A:259:GLY:HA3	1:A:278:ARG:NH1	2.31	0.46
1:A:279:ASP:OD2	1:A:281:THR:HG22	2.16	0.46
1:C:438:VAL:HG23	1:C:443:ASN:ND2	2.30	0.45
2:B:127:VAL:HA	4:B:1340:HOH:O	2.15	0.45
3:F:216:VAL:HG12	3:F:216:VAL:O	2.15	0.45
1:C:268:GLN:HG3	1:C:313:PRO:CB	2.46	0.45
1:A:162:GLU:HG3	1:A:164:ILE:HG23	1.99	0.45
1:C:380:PRO:HG3	3:F:11:MET:HE1	1.93	0.45
1:A:127:GLY:HA2	1:A:132:GLU:O	2.16	0.45
2:B:30:ASP:C	2:B:30:ASP:OD1	2.55	0.45
1:C:212:LEU:HB3	1:C:227:THR:HG23	1.98	0.45
2:B:239:GLU:HG3	4:B:1327:HOH:O	2.16	0.45
1:A:441:ASP:HA	4:A:2212:HOH:O	2.15	0.45
1:A:371:LEU:O	1:A:372:GLN:C	2.55	0.45
3:F:120:SER:O	3:F:148:VAL:HG23	2.16	0.45
3:F:255:ASP:HB2	3:F:275:ASP:HB3	1.98	0.45
1:C:279:ASP:OD2	1:C:281:THR:HG22	2.15	0.45
3:F:284:ASN:HB3	3:F:290:GLU:CD	2.36	0.45
2:B:284:ASN:HB2	4:B:1352:HOH:O	2.16	0.45
1:C:590:VAL:CG1	1:C:590:VAL:O	2.64	0.45
1:A:337:LEU:HD21	2:B:97:VAL:HG11	1.97	0.45
1:C:260:ILE:HG23	1:C:261:LEU:N	2.31	0.45
1:C:259:GLY:HA3	1:C:278:ARG:NH1	2.31	0.45
1:A:564:GLY:HA2	1:A:570:SER:OG	2.16	0.45
1:C:219:PRO:HD3	1:C:265:TRP:CD1	2.51	0.45
1:C:596:ILE:O	1:C:600:ILE:HG13	2.16	0.45
3:F:46:ILE:CG2	3:F:47:ASP:N	2.66	0.45
1:C:15:TRP:CH2	1:C:317:ALA:HB2	2.52	0.45
1:A:221:ASN:C	1:A:221:ASN:ND2	2.69	0.45
1:A:86:LEU:HD21	1:A:104:PHE:HB2	1.99	0.45
1:C:622:LEU:O	1:C:627:HIS:HB2	2.16	0.45
1:A:559:TYR:CE2	1:C:541:VAL:HG21	2.52	0.45
1:C:641:LEU:HD12	1:C:684:PHE:CE2	2.51	0.45
1:A:15:TRP:CH2	1:A:317:ALA:HB2	2.52	0.45
3:F:271:LEU:HA	3:F:271:LEU:HD12	1.57	0.45
2:B:35:ILE:HG13	2:B:89:TRP:CE2	2.51	0.45
1:A:392:LEU:HA	4:A:2219:HOH:O	2.16	0.45
1:A:581:VAL:HG11	1:A:600:ILE:HD13	1.98	0.45
3:F:85:GLU:HG2	3:F:86:ASN:ND2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:LEU:HD23	1:C:518:LEU:CD1	2.47	0.45
1:A:504:PHE:CZ	1:C:588:LEU:HD13	2.52	0.45
1:A:155:GLN:HB2	1:A:195:GLU:HB3	1.99	0.45
1:A:688:ILE:HG12	1:A:689:ASN:H	1.82	0.45
1:A:204:PRO:C	1:A:206:SER:H	2.19	0.45
1:C:221:ASN:ND2	1:C:221:ASN:C	2.69	0.45
1:C:197:ILE:HG22	1:C:198:HIS:N	2.32	0.45
1:C:249:LEU:C	1:C:249:LEU:HD23	2.38	0.45
1:A:601:GLN:HE22	1:A:611:ARG:HD3	1.82	0.45
1:A:543:ALA:C	1:A:545:ASP:H	2.19	0.45
1:C:665:THR:CG2	3:F:285:LEU:N	2.80	0.45
1:C:438:VAL:HG21	1:C:444:GLU:HA	1.97	0.45
2:B:105:VAL:HG22	2:B:116:LEU:HD11	1.99	0.45
1:C:232:ASP:O	1:C:258:LYS:HA	2.17	0.45
1:A:75:LYS:NZ	1:A:94:ALA:CB	2.80	0.45
1:C:169:ASN:OD1	1:C:172:LEU:HB2	2.16	0.45
3:F:196:LEU:CD1	3:F:197:GLU:H	2.30	0.45
3:F:274:GLY:C	3:F:276:ASN:N	2.67	0.45
1:C:5:ALA:N	4:C:2426:HOH:O	2.49	0.45
1:C:66:ASN:HD22	1:C:66:ASN:HA	1.64	0.44
1:C:155:GLN:HB2	1:C:195:GLU:HB3	1.99	0.44
1:A:333:LEU:CD2	4:B:1298:HOH:O	2.13	0.44
3:F:179:ASP:C	3:F:180:ASN:HD22	2.20	0.44
1:C:431:ILE:HD13	1:C:447:TRP:HZ3	1.82	0.44
1:A:289:SER:O	1:A:290:ALA:CB	2.65	0.44
1:C:727:PRO:O	1:C:729:ASP:N	2.50	0.44
2:B:29:SER:C	2:B:31:LYS:N	2.70	0.44
1:A:436:VAL:HG12	1:A:436:VAL:O	2.16	0.44
1:C:72:HIS:HE1	1:C:118:ALA:HA	1.72	0.44
2:B:30:ASP:OD1	2:B:32:THR:HG23	2.17	0.44
1:A:212:LEU:HB3	1:A:227:THR:HG23	1.98	0.44
1:A:260:ILE:HG23	1:A:261:LEU:N	2.31	0.44
1:A:232:ASP:O	1:A:258:LYS:HA	2.17	0.44
1:A:5:ALA:N	4:A:1426:HOH:O	2.49	0.44
2:B:213:SER:HB2	2:B:262:TRP:CE2	2.53	0.44
1:A:75:LYS:HZ1	1:A:94:ALA:N	2.06	0.44
3:F:59:VAL:HG12	3:F:72:SER:CB	2.46	0.44
1:C:127:GLY:HA2	1:C:132:GLU:O	2.16	0.44
1:A:212:LEU:HD22	1:A:227:THR:HG22	1.98	0.44
1:C:289:SER:O	1:C:290:ALA:CB	2.65	0.44
3:F:38:VAL:HA	3:F:42:THR:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:PHE:CD1	2:B:114:PRO:HB3	2.51	0.44
1:A:584:LEU:N	1:A:584:LEU:CD1	2.81	0.44
1:A:232:ASP:HA	1:A:259:GLY:H	1.83	0.44
1:C:371:LEU:O	1:C:372:GLN:C	2.55	0.44
1:C:78:ALA:HB3	1:C:114:VAL:CG1	2.45	0.44
1:A:129:ASN:HA	1:A:162:GLU:CB	2.47	0.44
1:A:399:GLY:O	2:B:11:LEU:HD12	2.17	0.44
1:C:155:GLN:HB3	1:C:195:GLU:HB3	1.99	0.44
3:F:52:HIS:ND1	3:F:74:SER:CB	2.81	0.44
1:A:423:LYS:HG3	1:A:424:THR:N	2.33	0.44
2:B:74:SER:C	2:B:76:ASP:N	2.71	0.44
1:A:88:LEU:CD1	1:A:138:MET:SD	3.06	0.44
1:A:688:ILE:CG1	1:A:689:ASN:H	2.31	0.44
1:A:119:LYS:CB	1:A:173:ALA:HB2	2.41	0.44
2:B:4:ILE:HG21	2:B:36:PHE:CE2	2.52	0.44
3:F:184:ILE:O	3:F:196:LEU:HD12	2.18	0.44
1:C:232:ASP:HA	1:C:259:GLY:H	1.83	0.44
1:A:449:LEU:O	1:A:453:LEU:HB2	2.17	0.44
1:A:242:LEU:N	1:A:242:LEU:HD23	2.33	0.44
1:C:242:LEU:HD23	1:C:242:LEU:N	2.33	0.44
1:A:604:TYR:N	1:A:605:PRO:CD	2.81	0.44
1:C:63:SER:HB3	1:C:82:ASP:HB2	1.98	0.44
3:F:72:SER:O	3:F:79:VAL:HA	2.17	0.44
1:C:117:ASN:C	1:C:117:ASN:HD22	2.17	0.44
1:C:162:GLU:HG3	1:C:164:ILE:CG2	2.48	0.44
1:C:27:THR:O	1:C:65:PHE:HB2	2.17	0.44
1:A:511:GLU:HG2	1:C:569:LEU:HB2	1.99	0.44
3:F:63:HIS:HB3	3:F:66:PHE:CE1	2.53	0.44
2:B:85:GLU:O	2:B:86:ASN:HB2	2.18	0.44
1:C:204:PRO:HG2	1:C:208:ILE:O	2.18	0.44
1:C:86:LEU:HD21	1:C:104:PHE:HB2	1.99	0.44
2:B:274:GLY:C	2:B:276:ASN:N	2.69	0.44
1:C:116:PHE:CE1	1:C:124:LEU:HD13	2.53	0.44
1:A:496:THR:CG2	1:A:497:ASN:N	2.81	0.44
1:A:197:ILE:HG22	1:A:198:HIS:N	2.32	0.44
1:C:20:ILE:CG1	1:C:20:ILE:O	2.65	0.44
2:B:191:ALA:HB1	2:B:193:THR:HG22	1.99	0.44
1:A:379:GLU:HG2	2:B:258:TRP:CZ2	2.53	0.44
1:A:268:GLN:NE2	4:A:2118:HOH:O	2.51	0.44
1:A:105:SER:C	1:A:107:HIS:N	2.71	0.44
1:A:162:GLU:HG3	1:A:164:ILE:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:GLN:HB3	1:A:195:GLU:HB3	1.99	0.44
1:C:151:LEU:CD1	1:C:152:THR:H	2.25	0.44
2:B:63:HIS:CE1	2:B:65:LYS:HB3	2.53	0.44
1:C:162:GLU:HG3	1:C:164:ILE:HG23	1.99	0.44
1:A:537:MET:CE	1:C:536:LEU:HD23	2.48	0.44
3:F:259:ARG:NH1	3:F:259:ARG:HG3	2.33	0.44
1:A:274:LEU:HA	1:A:274:LEU:HD23	1.69	0.44
2:B:181:LEU:CD2	2:B:201:GLU:HG2	2.47	0.44
1:C:313:PRO:HD3	4:C:1546:HOH:O	2.13	0.43
1:C:42:LEU:O	1:C:42:LEU:HG	2.18	0.43
1:A:67:ASP:OD2	1:A:113:THR:HG23	2.18	0.43
1:A:24:VAL:CG2	1:A:70:TRP:CZ3	3.01	0.43
1:A:232:ASP:HA	1:A:259:GLY:N	2.33	0.43
1:C:608:ILE:HD13	1:C:611:ARG:NH1	2.33	0.43
1:C:312:ALA:N	1:C:313:PRO:CD	2.80	0.43
1:A:116:PHE:CE1	1:A:124:LEU:HD13	2.53	0.43
1:A:42:LEU:HG	1:A:42:LEU:O	2.18	0.43
1:C:639:GLY:HA2	1:C:688:ILE:CD1	2.47	0.43
3:F:233:ILE:HG21	3:F:289:TRP:HZ2	1.82	0.43
2:B:14:ASP:HB3	2:B:27:CYS:SG	2.58	0.43
1:A:20:ILE:O	1:A:20:ILE:CG1	2.65	0.43
1:A:27:THR:O	1:A:65:PHE:HB2	2.17	0.43
1:C:232:ASP:HA	1:C:259:GLY:N	2.33	0.43
3:F:240:GLN:O	3:F:241:GLY:C	2.55	0.43
1:C:313:PRO:HG2	1:C:376:TRP:NE1	2.34	0.43
3:F:26:THR:O	3:F:33:ILE:HA	2.18	0.43
1:A:438:VAL:CG2	1:A:439:ILE:N	2.81	0.43
1:C:119:LYS:CB	1:C:173:ALA:HB2	2.41	0.43
1:A:249:LEU:HD23	1:A:249:LEU:C	2.38	0.43
1:A:62:ASP:N	1:A:62:ASP:OD1	2.36	0.43
1:A:504:PHE:CE2	1:C:588:LEU:HD13	2.53	0.43
1:C:614:MET:HE2	1:C:614:MET:HA	2.01	0.43
1:C:252:LEU:HD13	1:C:285:TRP:CD2	2.53	0.43
1:C:24:VAL:CG2	1:C:70:TRP:CZ3	3.01	0.43
1:C:67:ASP:OD2	1:C:113:THR:HG23	2.18	0.43
1:A:429:PRO:HD2	4:A:2159:HOH:O	2.19	0.43
2:B:64:PRO:HD2	4:B:1334:HOH:O	2.17	0.43
2:B:238:ASN:ND2	2:B:240:GLN:H	2.15	0.43
1:A:549:GLU:HA	1:A:552:LYS:HB3	2.01	0.43
1:A:22:LEU:HD21	1:A:95:ASN:ND2	2.33	0.43
1:A:78:ALA:HB3	1:A:114:VAL:CG1	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:GLU:HA	1:C:423:LYS:HD3	2.01	0.43
1:A:204:PRO:HG2	1:A:208:ILE:O	2.18	0.43
2:B:112:TYR:N	2:B:112:TYR:CD1	2.86	0.43
2:B:255:ASP:CG	2:B:256:VAL:N	2.72	0.43
3:F:224:SER:HB2	3:F:234:TRP:NE1	2.28	0.43
2:B:102:VAL:HG22	4:B:1353:HOH:O	2.14	0.43
1:A:706:PHE:CB	4:A:2200:HOH:O	2.66	0.43
1:C:519:VAL:O	1:C:521:GLY:N	2.51	0.43
1:C:412:LEU:HD21	1:C:713:THR:HG22	2.01	0.43
2:B:281:TRP:N	2:B:281:TRP:CD1	2.87	0.43
1:C:424:THR:O	1:C:425:LYS:HB3	2.18	0.43
1:C:196:VAL:O	1:C:197:ILE:HG13	2.19	0.43
1:A:551:LEU:C	1:A:553:GLU:N	2.71	0.43
1:C:22:LEU:HD21	1:C:95:ASN:ND2	2.33	0.43
3:F:233:ILE:HD11	3:F:248:LEU:CD1	2.48	0.43
1:A:133:ILE:HD11	1:A:163:VAL:CG2	2.41	0.43
1:C:677:PHE:HD2	1:C:678:ILE:HD12	1.83	0.43
3:F:219:ARG:CG	3:F:221:TYR:CE1	3.02	0.43
1:A:120:GLN:C	1:A:122:ASN:H	2.22	0.43
1:A:422:LEU:CD2	1:A:721:GLU:HG2	2.49	0.43
1:A:201:TYR:CD2	1:A:238:LEU:HD11	2.54	0.43
1:A:312:ALA:N	1:A:313:PRO:CD	2.80	0.43
1:A:314:ASP:CB	1:A:376:TRP:CZ2	3.02	0.43
1:C:636:LEU:HD12	1:C:688:ILE:CD1	2.48	0.43
1:A:203:SER:C	1:A:205:ASN:N	2.69	0.43
2:B:25:ALA:HB2	2:B:61:TRP:HZ2	1.81	0.43
2:B:227:GLN:HA	2:B:256:VAL:HG13	2.01	0.43
2:B:46:ILE:O	2:B:46:ILE:HG22	2.19	0.43
1:C:120:GLN:C	1:C:122:ASN:H	2.22	0.43
3:F:213:SER:OG	3:F:214:PRO:HD2	2.19	0.43
2:B:107:TRP:CH2	2:B:130:PHE:HE2	2.37	0.43
1:C:78:ALA:CB	1:C:114:VAL:CG1	2.95	0.43
1:A:302:TRP:CD1	1:A:321:PHE:CD1	3.07	0.43
1:C:223:THR:O	1:C:241:ASP:HA	2.19	0.43
1:C:536:LEU:O	1:C:537:MET:C	2.57	0.43
1:A:727:PRO:C	1:A:729:ASP:N	2.69	0.43
2:B:226:SER:HB3	2:B:228:ASP:OD1	2.19	0.43
1:C:93:GLU:O	1:C:94:ALA:C	2.57	0.42
2:B:18:ASP:CG	2:B:23:ARG:HB3	2.39	0.42
3:F:39:GLU:HB2	3:F:42:THR:OG1	2.19	0.42
1:C:664:LYS:C	3:F:285:LEU:HD11	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:201:GLU:O	3:F:234:TRP:HH2	2.02	0.42
1:C:274:LEU:HA	1:C:274:LEU:HD23	1.69	0.42
1:A:211:GLN:O	1:A:229:THR:HA	2.19	0.42
1:C:201:TYR:CD2	1:C:238:LEU:HD11	2.54	0.42
3:F:3:VAL:HG12	3:F:5:ALA:N	2.34	0.42
1:C:666:ILE:HD13	1:C:666:ILE:HA	1.93	0.42
1:C:661:LYS:C	1:C:663:ASN:N	2.72	0.42
1:C:314:ASP:CG	1:C:376:TRP:CD2	2.80	0.42
1:A:125:ALA:HB2	1:A:168:TRP:CZ3	2.53	0.42
1:A:93:GLU:O	1:A:94:ALA:C	2.57	0.42
1:A:299:ARG:HD2	1:A:299:ARG:HA	1.86	0.42
1:A:204:PRO:HG3	1:A:210:GLN:HG3	2.00	0.42
1:A:196:VAL:O	1:A:197:ILE:HG13	2.19	0.42
2:B:63:HIS:CD2	2:B:110:HIS:HB3	2.54	0.42
1:C:590:VAL:HG13	1:C:622:LEU:HD22	1.99	0.42
1:A:27:THR:HB	1:A:40:SER:HB2	2.01	0.42
1:C:571:ARG:O	1:C:574:TYR:HB3	2.19	0.42
2:B:87:GLY:C	2:B:88:ARG:HG3	2.39	0.42
1:C:105:SER:C	1:C:107:HIS:N	2.71	0.42
1:C:29:SER:OG	1:C:66:ASN:ND2	2.53	0.42
1:C:88:LEU:CD1	1:C:138:MET:SD	3.06	0.42
1:C:420:GLU:HA	1:C:423:LYS:CD	2.50	0.42
1:C:129:ASN:HA	1:C:162:GLU:CB	2.47	0.42
3:F:62:ALA:HB2	3:F:107:TRP:CE2	2.55	0.42
2:B:152:SER:OG	2:B:210:VAL:O	2.33	0.42
1:C:6:GLU:OE2	1:C:324:LYS:HB2	2.20	0.42
3:F:250:GLU:C	3:F:251:GLU:OE1	2.58	0.42
1:A:497:ASN:OD1	1:A:498:PHE:N	2.53	0.42
1:A:223:THR:O	1:A:241:ASP:HA	2.19	0.42
1:C:589:ASP:C	1:C:591:SER:H	2.23	0.42
1:A:608:ILE:HA	1:A:611:ARG:NH1	2.34	0.42
1:A:268:GLN:CA	1:A:374:PRO:O	2.63	0.42
1:C:70:TRP:C	1:C:71:SER:O	2.55	0.42
1:A:70:TRP:C	1:A:71:SER:O	2.55	0.42
3:F:35:ILE:HG13	3:F:89:TRP:NE1	2.35	0.42
1:A:252:LEU:HD13	1:A:285:TRP:CD2	2.53	0.42
1:A:330:LEU:HA	1:A:330:LEU:HD12	1.87	0.42
1:A:15:TRP:HZ3	1:A:317:ALA:H	1.67	0.42
1:A:540:MET:HB2	1:C:540:MET:HE1	2.01	0.42
1:C:215:VAL:HA	1:C:226:ALA:O	2.20	0.42
1:C:272:LEU:HD23	1:C:272:LEU:HA	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:ARG:HB3	1:C:10:THR:H	1.65	0.42
1:A:399:GLY:HA3	2:B:11:LEU:CD1	2.49	0.42
1:A:420:GLU:O	1:A:423:LYS:HG2	2.20	0.42
1:C:211:GLN:O	1:C:229:THR:HA	2.19	0.42
1:A:694:ILE:HG23	1:A:699:LEU:HD23	2.02	0.42
3:F:23:ARG:HD3	3:F:61:TRP:CH2	2.54	0.42
3:F:68:THR:HG22	3:F:89:TRP:CH2	2.54	0.42
1:A:237:ILE:HD12	1:A:237:ILE:N	2.35	0.42
1:C:204:PRO:HG3	1:C:210:GLN:HG3	2.00	0.42
3:F:231:CYS:HB2	3:F:271:LEU:HD21	2.00	0.42
1:A:202:THR:CG2	1:A:202:THR:O	2.67	0.42
1:C:302:TRP:CD1	1:C:321:PHE:CD1	3.07	0.42
1:C:493:GLN:HG3	1:C:494:ILE:N	2.35	0.42
1:C:379:GLU:HB3	3:F:258:TRP:CZ2	2.54	0.42
1:C:133:ILE:HD11	1:C:163:VAL:CG2	2.41	0.42
1:A:388:PHE:CE2	1:A:716:PHE:HE2	2.37	0.42
3:F:194:TYR:N	3:F:194:TYR:CD1	2.88	0.42
3:F:262:TRP:HA	3:F:262:TRP:CE3	2.55	0.42
1:A:610:GLN:HA	1:A:610:GLN:OE1	2.20	0.42
1:A:66:ASN:HD22	1:A:66:ASN:HA	1.64	0.42
1:C:202:THR:O	1:C:202:THR:CG2	2.67	0.42
2:B:30:ASP:OD1	2:B:32:THR:OG1	2.36	0.42
1:A:519:VAL:O	1:A:521:GLY:N	2.52	0.42
1:A:261:LEU:N	1:A:277:GLY:HA2	2.35	0.42
1:C:62:ASP:OD1	1:C:62:ASP:N	2.36	0.42
3:F:213:SER:OG	3:F:215:THR:HG22	2.20	0.42
2:B:213:SER:HB2	2:B:262:TRP:CD2	2.55	0.42
1:A:500:PRO:O	1:A:501:GLU:HG2	2.20	0.42
1:C:7:PHE:HB2	1:C:8:SER:H	1.51	0.42
1:A:29:SER:OG	1:A:66:ASN:ND2	2.53	0.42
3:F:33:ILE:HD13	3:F:72:SER:HB3	2.02	0.42
1:A:447:TRP:O	1:A:451:GLU:N	2.53	0.42
1:A:431:ILE:HG21	1:A:451:GLU:HA	2.02	0.42
1:C:438:VAL:HG21	1:C:444:GLU:CA	2.50	0.42
1:A:152:THR:HA	1:A:153:PRO:HD3	1.81	0.42
3:F:232:ILE:HG21	3:F:234:TRP:CZ2	2.55	0.42
2:B:52:HIS:CD2	2:B:56:VAL:HG22	2.55	0.42
3:F:105:VAL:HG21	3:F:116:LEU:HD21	2.02	0.42
3:F:102:VAL:HG22	3:F:120:SER:HB2	2.02	0.42
1:A:706:PHE:HB2	4:A:2200:HOH:O	2.19	0.42
1:C:247:THR:HG23	1:C:248:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:PHE:N	1:C:7:PHE:CD1	2.87	0.41
1:A:125:ALA:CB	1:A:168:TRP:CH2	2.92	0.41
1:A:733:VAL:HG13	4:A:2255:HOH:O	2.19	0.41
1:C:31:THR:OG1	1:C:321:PHE:HD2	2.03	0.41
1:C:380:PRO:HG3	3:F:11:MET:HE2	1.96	0.41
1:C:447:TRP:CE3	1:C:450:LEU:HD12	2.55	0.41
1:A:598:LYS:O	1:A:602:ASN:HB2	2.20	0.41
2:B:121:SER:CA	4:B:1338:HOH:O	2.68	0.41
1:A:644:VAL:HG21	1:A:684:PHE:CZ	2.55	0.41
3:F:60:ASP:O	3:F:107:TRP:NE1	2.52	0.41
1:A:268:GLN:CD	4:A:2118:HOH:O	2.36	0.41
1:C:261:LEU:N	1:C:277:GLY:HA2	2.35	0.41
1:A:247:THR:HG23	1:A:248:PRO:HD2	2.02	0.41
1:A:538:GLU:N	1:A:538:GLU:OE1	2.43	0.41
1:C:271:HIS:HB3	1:C:286:ASN:OD1	2.21	0.41
3:F:49:LEU:HD22	3:F:82:TRP:CG	2.55	0.41
1:C:187:ILE:HD13	1:C:187:ILE:HA	1.88	0.41
3:F:120:SER:OG	3:F:121:SER:N	2.53	0.41
1:A:519:VAL:C	1:A:521:GLY:N	2.71	0.41
1:A:458:THR:CG2	1:A:459:GLU:N	2.81	0.41
1:C:252:LEU:HB3	1:C:285:TRP:CE3	2.55	0.41
1:A:404:ILE:HD12	1:A:404:ILE:N	2.34	0.41
2:B:49:LEU:HA	4:B:1355:HOH:O	2.20	0.41
2:B:233:ILE:HD12	2:B:233:ILE:N	2.35	0.41
1:C:27:THR:HB	1:C:40:SER:HB2	2.01	0.41
1:C:572:ILE:HG22	1:C:573:LEU:N	2.35	0.41
1:A:6:GLU:OE2	1:A:324:LYS:HB2	2.20	0.41
1:A:563:TYR:C	1:A:565:SER:H	2.24	0.41
1:C:331:GLN:NE2	3:F:75:TYR:CZ	2.88	0.41
2:B:225:VAL:CG2	2:B:271:LEU:HD11	2.50	0.41
1:C:214:VAL:HB	1:C:228:ALA:HB3	2.03	0.41
3:F:112:TYR:HA	3:F:171:ARG:NH2	2.36	0.41
1:A:444:GLU:HG2	1:A:448:ASN:ND2	2.36	0.41
1:A:215:VAL:HA	1:A:226:ALA:O	2.20	0.41
1:C:377:TYR:CD2	3:F:75:TYR:CE1	3.09	0.41
2:B:225:VAL:CG1	2:B:257:LEU:O	2.69	0.41
1:A:412:LEU:HD23	1:A:413:GLU:N	2.36	0.41
2:B:4:ILE:CD1	2:B:4:ILE:N	2.83	0.41
1:A:96:ASN:O	1:A:97:ALA:HB2	2.21	0.41
1:C:193:LYS:O	1:C:194:LYS:CB	2.65	0.41
1:A:578:LYS:HD3	1:A:580:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:THR:HB	1:A:398:ASP:OD2	2.21	0.41
1:A:229:THR:HG22	1:A:230:GLY:N	2.35	0.41
1:C:237:ILE:HD12	1:C:237:ILE:N	2.35	0.41
1:C:96:ASN:O	1:C:97:ALA:HB2	2.21	0.41
1:A:252:LEU:HB3	1:A:285:TRP:CE3	2.55	0.41
2:B:238:ASN:HB2	4:B:1327:HOH:O	2.20	0.41
2:B:46:ILE:O	2:B:47:ASP:HB2	2.21	0.41
1:C:497:ASN:O	1:C:497:ASN:CG	2.59	0.41
3:F:58:ARG:HE	3:F:58:ARG:HB2	1.60	0.41
1:A:268:GLN:NE2	1:A:313:PRO:CD	2.69	0.41
1:C:124:LEU:HB2	1:C:138:MET:HE3	2.03	0.41
1:C:41:SER:O	1:C:42:LEU:CB	2.67	0.41
1:C:75:LYS:HZ2	1:C:94:ALA:N	2.17	0.41
3:F:4:ILE:CD1	3:F:4:ILE:N	2.84	0.41
1:A:434:ARG:HG3	1:A:447:TRP:CH2	2.55	0.41
3:F:30:ASP:O	3:F:31:LYS:HB2	2.21	0.41
1:A:329:THR:C	1:A:331:GLN:N	2.73	0.41
1:A:271:HIS:HB3	1:A:286:ASN:OD1	2.21	0.41
1:A:31:THR:OG1	1:A:321:PHE:HD2	2.03	0.41
1:A:595:PHE:C	1:A:597:SER:N	2.72	0.41
1:A:127:GLY:HA3	1:A:163:VAL:HB	2.03	0.41
2:B:16:VAL:HG12	2:B:61:TRP:HD1	1.85	0.41
1:A:9:ARG:HA	1:A:324:LYS:HA	2.02	0.41
3:F:152:SER:O	3:F:173:PHE:HB2	2.21	0.41
2:B:282:LYS:HB3	2:B:292:ALA:HB2	2.02	0.41
1:A:502:GLY:O	1:C:587:ASN:HB3	2.21	0.41
1:C:439:ILE:CG1	1:C:440:ASP:H	2.28	0.41
1:C:129:ASN:C	1:C:131:GLY:N	2.74	0.41
1:C:217:TRP:CE3	1:C:225:VAL:HG22	2.56	0.41
1:C:15:TRP:HZ3	1:C:317:ALA:H	1.67	0.40
1:A:428:LYS:CB	1:A:429:PRO:HD3	2.37	0.40
1:A:244:ASN:HD22	1:A:244:ASN:C	2.24	0.40
1:A:592:GLN:O	1:A:595:PHE:HB3	2.21	0.40
1:C:127:GLY:HA3	1:C:163:VAL:HB	2.03	0.40
1:A:19:LYS:HD3	1:A:311:GLU:HG3	2.03	0.40
2:B:17:LEU:HD23	2:B:24:LEU:HA	2.03	0.40
1:C:229:THR:HG22	1:C:230:GLY:N	2.35	0.40
2:B:145:ALA:O	2:B:147:GLY:N	2.50	0.40
1:C:9:ARG:HA	1:C:324:LYS:HA	2.02	0.40
3:F:59:VAL:HG12	3:F:72:SER:CA	2.50	0.40
1:A:439:ILE:HG13	1:A:440:ASP:H	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LEU:HA	1:A:272:LEU:HD23	1.81	0.40
1:C:702:LYS:HA	1:C:705:GLU:HB2	2.03	0.40
1:C:289:SER:HG	1:C:291:GLU:HG3	1.87	0.40
1:A:7:PHE:CD1	1:A:7:PHE:N	2.87	0.40
1:A:421:ALA:O	1:A:425:LYS:HA	2.21	0.40
1:C:125:ALA:HB2	1:C:168:TRP:CZ3	2.53	0.40
3:F:10:GLU:HG3	3:F:30:ASP:CA	2.51	0.40
1:A:497:ASN:O	1:A:498:PHE:HB3	2.20	0.40
1:C:438:VAL:HG22	1:C:439:ILE:N	2.36	0.40
1:C:569:LEU:O	1:C:573:LEU:HG	2.21	0.40
1:C:314:ASP:N	1:C:376:TRP:HE1	2.20	0.40
1:A:83:ASN:O	1:A:84:GLY:C	2.59	0.40
2:B:78:LYS:HG2	2:B:96:ALA:CB	2.52	0.40
3:F:115:MET:HE3	3:F:153:TRP:CZ2	2.56	0.40
2:B:23:ARG:NH1	2:B:68:THR:CG2	2.83	0.40
2:B:212:TRP:HA	2:B:222:LEU:HD23	2.02	0.40
2:B:87:GLY:O	2:B:88:ARG:HG3	2.21	0.40
1:C:113:THR:CG2	1:C:114:VAL:N	2.84	0.40
1:A:84:GLY:HA2	1:A:111:VAL:HG23	2.03	0.40
1:A:116:PHE:CD1	1:A:124:LEU:HD13	2.57	0.40
3:F:4:ILE:HG13	3:F:43:HIS:HB3	2.03	0.40
3:F:247:LEU:C	3:F:249:LYS:N	2.74	0.40
1:A:218:HIS:CE1	1:A:221:ASN:H	2.40	0.40
1:C:652:PHE:CE2	1:C:702:LYS:HE2	2.56	0.40
1:A:187:ILE:HD13	1:A:187:ILE:HA	1.88	0.40
2:B:17:LEU:HB3	2:B:21:GLY:HA2	2.03	0.40
1:A:653:PRO:O	1:A:656:GLU:N	2.54	0.40
1:C:592:GLN:NE2	4:C:1629:HOH:O	2.53	0.40
2:B:69:ILE:HA	2:B:82:TRP:O	2.22	0.40
2:B:143:ALA:O	2:B:144:HIS:CG	2.75	0.40
3:F:105:VAL:HG13	3:F:105:VAL:O	2.21	0.40
1:C:400:LYS:HA	3:F:12:ILE:HG13	2.04	0.40
1:A:517:ASN:ND2	1:A:529:ASN:ND2	2.63	0.40
1:A:217:TRP:CE3	1:A:225:VAL:HG22	2.56	0.40
1:C:412:LEU:HD23	1:C:412:LEU:C	2.41	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	681/1273 (54%)	518 (76%)	107 (16%)	56 (8%)	1	18
1	C	683/1273 (54%)	532 (78%)	97 (14%)	54 (8%)	1	19
2	B	275/291 (94%)	241 (88%)	30 (11%)	4 (2%)	13	57
3	F	276/291 (95%)	214 (78%)	37 (13%)	25 (9%)	1	17
All	All	1915/3128 (61%)	1505 (79%)	271 (14%)	139 (7%)	3	21

All (139) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	49	ALA
1	A	74	ASN
1	A	110	SER
1	A	143	GLU
1	A	146	SER
1	A	147	ASN
1	A	159	SER
1	A	203	SER
1	A	242	LEU
1	A	290	ALA
1	A	301	ASN
1	A	313	PRO
1	A	335	ASN
1	A	336	THR
1	A	365	LYS
1	A	369	PHE
1	A	497	ASN
2	B	131	LYS
1	C	33	ASP
1	C	49	ALA
1	C	74	ASN

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Mol	Chain	Res	Type
1	C	110	SER
1	C	143	GLU
1	C	146	SER
1	C	147	ASN
1	C	159	SER
1	C	203	SER
1	C	242	LEU
1	C	290	ALA
1	C	301	ASN
1	C	313	PRO
1	C	335	ASN
1	C	336	THR
1	C	365	LYS
1	C	369	PHE
1	C	715	ASN
3	F	76	ASP
3	F	100	ALA
3	F	131	LYS
1	A	10	THR
1	A	84	GLY
1	A	105	SER
1	A	160	VAL
1	A	194	LYS
1	A	238	LEU
1	A	266	CYS
1	A	322	ASP
1	A	332	ASN
1	A	337	LEU
1	A	388	PHE
1	A	425	LYS
1	A	518	LEU
2	B	135	THR
1	C	10	THR
1	C	84	GLY
1	C	105	SER
1	C	160	VAL
1	C	194	LYS
1	C	238	LEU
1	C	266	CYS
1	C	322	ASP
1	C	332	ASN
1	C	337	LEU

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Mol	Chain	Res	Type
1	C	425	LYS
3	F	30	ASP
3	F	41	GLU
3	F	133	ASN
3	F	241	GLY
3	F	254	PRO
3	F	256	VAL
3	F	273	GLY
1	A	16	SER
1	A	52	SER
1	A	60	GLN
1	A	93	GLU
1	A	121	ASP
1	A	153	PRO
1	A	204	PRO
1	A	299	ARG
1	A	363	LYS
1	A	520	SER
1	A	728	SER
2	B	190	ASP
1	C	16	SER
1	C	52	SER
1	C	60	GLN
1	C	93	GLU
1	C	121	ASP
1	C	153	PRO
1	C	204	PRO
1	C	299	ARG
1	C	363	LYS
1	C	439	ILE
1	C	552	LYS
1	C	728	SER
3	F	40	GLY
3	F	47	ASP
3	F	101	SER
3	F	145	ALA
3	F	240	GLN
3	F	291	PRO
1	A	91	THR
1	A	148	TYR
1	A	302	TRP
1	A	368	VAL

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Mol	Chain	Res	Type
1	A	439	ILE
1	A	498	PHE
1	A	561	ALA
2	B	202	GLY
1	C	91	THR
1	C	148	TYR
1	C	302	TRP
1	C	368	VAL
1	C	407	PRO
3	F	46	ILE
3	F	218	LEU
3	F	267	ASN
3	F	274	GLY
1	A	9	ARG
1	A	94	ALA
1	A	109	SER
1	A	207	GLY
1	A	548	ASN
1	A	653	PRO
1	C	9	ARG
1	C	94	ALA
1	C	109	SER
1	C	207	GLY
1	C	520	SER
1	C	662	ASP
3	F	51	GLY
3	F	170	SER
3	F	187	TYR
3	F	21	GLY
3	F	287	GLY
1	A	287	PRO
1	C	287	PRO
1	C	494	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	608/1113 (55%)	562 (92%)	46 (8%)	16	53
1	C	610/1113 (55%)	562 (92%)	48 (8%)	15	51
2	B	237/247 (96%)	232 (98%)	5 (2%)	61	84
3	F	238/247 (96%)	218 (92%)	20 (8%)	14	48
All	All	1693/2720 (62%)	1574 (93%)	119 (7%)	23	56

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PHE
1	A	15	TRP
1	A	18	ASP
1	A	20	ILE
1	A	33	ASP
1	A	51	ASP
1	A	61	VAL
1	A	62	ASP
1	A	66	ASN
1	A	73	ASN
1	A	74	ASN
1	A	99	ASN
1	A	104	PHE
1	A	106	ASN
1	A	117	ASN
1	A	130	ASN
1	A	136	TRP
1	A	147	ASN
1	A	156	SER
1	A	168	TRP
1	A	169	ASN
1	A	170	GLN
1	A	183	ASN
1	A	198	HIS
1	A	204	PRO
1	A	216	GLU
1	A	221	ASN
1	A	232	ASP
1	A	244	ASN
1	A	253	ASN
1	A	261	LEU
1	A	266	CYS
1	A	268	GLN

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Mol	Chain	Res	Type
1	A	281	THR
1	A	304	PHE
1	A	327	VAL
1	A	334	THR
1	A	430	LEU
1	A	509	ASN
1	A	534	ASP
1	A	537	MET
1	A	545	ASP
1	A	657	ASP
1	A	688	ILE
1	A	703	PHE
1	A	720	THR
2	B	92	ILE
2	B	180	ASN
2	B	204	SER
2	B	225	VAL
2	B	238	ASN
1	C	7	PHE
1	C	15	TRP
1	C	18	ASP
1	C	20	ILE
1	C	33	ASP
1	C	51	ASP
1	C	61	VAL
1	C	62	ASP
1	C	66	ASN
1	C	73	ASN
1	C	74	ASN
1	C	99	ASN
1	C	104	PHE
1	C	106	ASN
1	C	117	ASN
1	C	130	ASN
1	C	136	TRP
1	C	147	ASN
1	C	156	SER
1	C	168	TRP
1	C	169	ASN
1	C	170	GLN
1	C	183	ASN
1	C	198	HIS

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Mol	Chain	Res	Type
1	C	204	PRO
1	C	216	GLU
1	C	221	ASN
1	C	232	ASP
1	C	244	ASN
1	C	253	ASN
1	C	261	LEU
1	C	266	CYS
1	C	268	GLN
1	C	281	THR
1	C	304	PHE
1	C	327	VAL
1	C	334	THR
1	C	377	TYR
1	C	381	SER
1	C	408	LYS
1	C	413	GLU
1	C	432	ASN
1	C	509	ASN
1	C	510	ILE
1	C	534	ASP
1	C	538	GLU
1	C	545	ASP
1	C	629	GLN
3	F	33	ILE
3	F	66	PHE
3	F	81	ILE
3	F	82	TRP
3	F	122	ASP
3	F	129	GLU
3	F	133	ASN
3	F	141	ILE
3	F	180	ASN
3	F	199	THR
3	F	200	LEU
3	F	205	ASP
3	F	206	TRP
3	F	225	VAL
3	F	233	ILE
3	F	237	ASP
3	F	247	LEU
3	F	255	ASP

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Mol	Chain	Res	Type
3	F	261	SER
3	F	286	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	72	HIS
1	A	73	ASN
1	A	74	ASN
1	A	95	ASN
1	A	96	ASN
1	A	99	ASN
1	A	106	ASN
1	A	117	ASN
1	A	129	ASN
1	A	130	ASN
1	A	139	ASN
1	A	147	ASN
1	A	221	ASN
1	A	244	ASN
1	A	246	ASN
1	A	250	GLN
1	A	268	GLN
1	A	292	GLN
1	A	370	HIS
1	A	433	GLN
1	A	443	ASN
1	A	448	ASN
1	A	509	ASN
1	A	517	ASN
1	A	592	GLN
1	A	601	GLN
2	B	95	HIS
2	B	103	ASN
2	B	149	ASN
2	B	180	ASN
2	B	238	ASN
2	B	240	GLN
2	B	276	ASN
1	C	66	ASN
1	C	72	HIS

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Mol	Chain	Res	Type
1	C	73	ASN
1	C	74	ASN
1	C	95	ASN
1	C	96	ASN
1	C	99	ASN
1	C	106	ASN
1	C	117	ASN
1	C	129	ASN
1	C	130	ASN
1	C	139	ASN
1	C	147	ASN
1	C	221	ASN
1	C	244	ASN
1	C	246	ASN
1	C	250	GLN
1	C	268	GLN
1	C	292	GLN
1	C	443	ASN
1	C	448	ASN
1	C	493	GLN
1	C	509	ASN
1	C	517	ASN
1	C	557	ASN
1	C	592	GLN
1	C	601	GLN
1	C	606	ASN
1	C	670	HIS
1	C	686	ASN
3	F	86	ASN
3	F	149	ASN
3	F	180	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [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.