



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:19 PM BST

PDB ID : 5FTJ
EMDB ID: : EMD-3295
Title : Cryo-EM structure of human p97 bound to UPCDC30245 inhibitor
Authors : Banerjee, S.; Bartesaghi, A.; Merk, A.; Rao, P.; Bulfer, S.L.; Yan, Y.; Green, N.; Mroczkowski, B.; Neitz, R.J.; Wipf, P.; Falconieri, V.; Deshaies, R.J.; Milne, J.L.S.; Hury, D.; Arkin, M.; Subramaniam, S.
Deposited on : 2016-01-14
Resolution : 2.30 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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

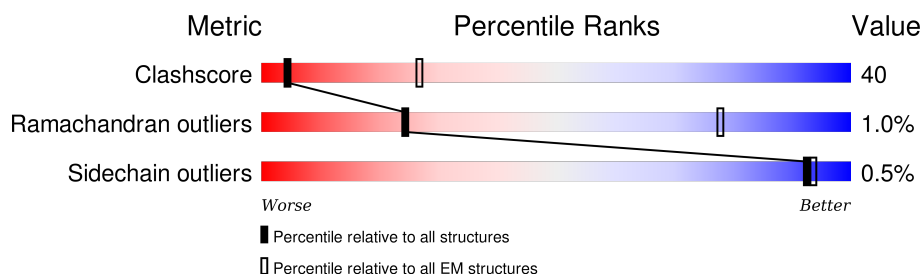
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.30 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	806	50% 39% • 10%
1	B	806	48% 40% • 10%
1	C	806	49% 39% • 10%
1	D	806	49% 40% • 10%
1	E	806	49% 40% • 10%
1	F	806	49% 39% • 10%

2 Entry composition [i](#)

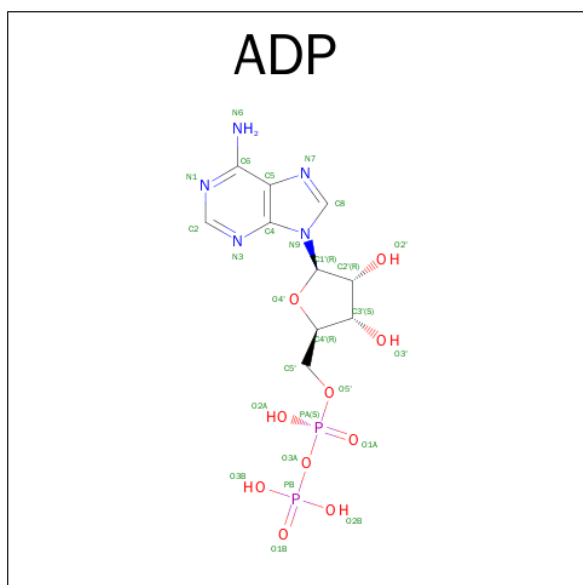
There are 4 unique types of molecules in this entry. The entry contains 34602 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE.

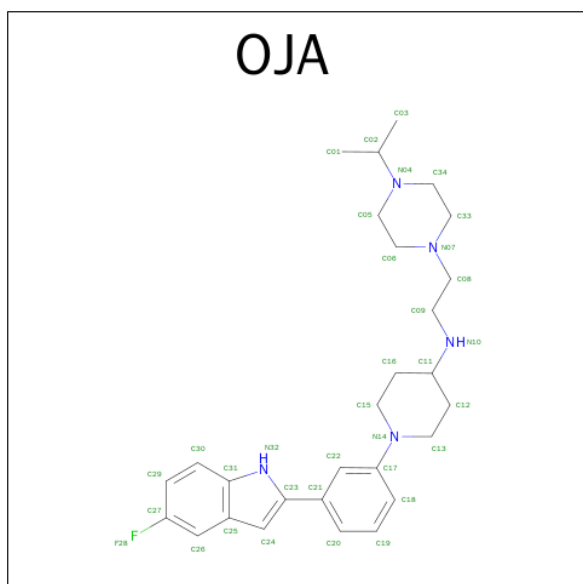
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	723	Total	C	N	O	S	0	0
			5659	3561	996	1072	30		
1	B	723	Total	C	N	O	S	0	0
			5659	3561	996	1072	30		
1	C	723	Total	C	N	O	S	0	0
			5659	3561	996	1072	30		
1	D	723	Total	C	N	O	S	0	0
			5659	3561	996	1072	30		
1	E	723	Total	C	N	O	S	0	0
			5659	3561	996	1072	30		
1	F	723	Total	C	N	O	S	0	0
			5659	3561	996	1072	30		

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	A	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	B	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	B	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	C	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	C	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	D	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	D	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	E	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	E	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	F	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	F	1	Total	C	N	O	P	0
			54	20	10	20	4	

- Molecule 3 is 1-(3-(5-FLUORO-1H-INDOL-2-YL)PHENYL)PIPERIDIN-4-YL)(2-(4-ISO
PROPYL-PIPERAZIN-1-YL)ETHYL)-CARBAMATE (three-letter code: OJA) (formula:
 $C_{28}H_{38}FN_5$).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	F	N	0
			34	28	1	5	
3	B	1	Total	C	F	N	0
			34	28	1	5	
3	C	1	Total	C	F	N	0
			34	28	1	5	
3	D	1	Total	C	F	N	0
			34	28	1	5	
3	E	1	Total	C	F	N	0
			34	28	1	5	
3	F	1	Total	C	F	N	0
			34	28	1	5	

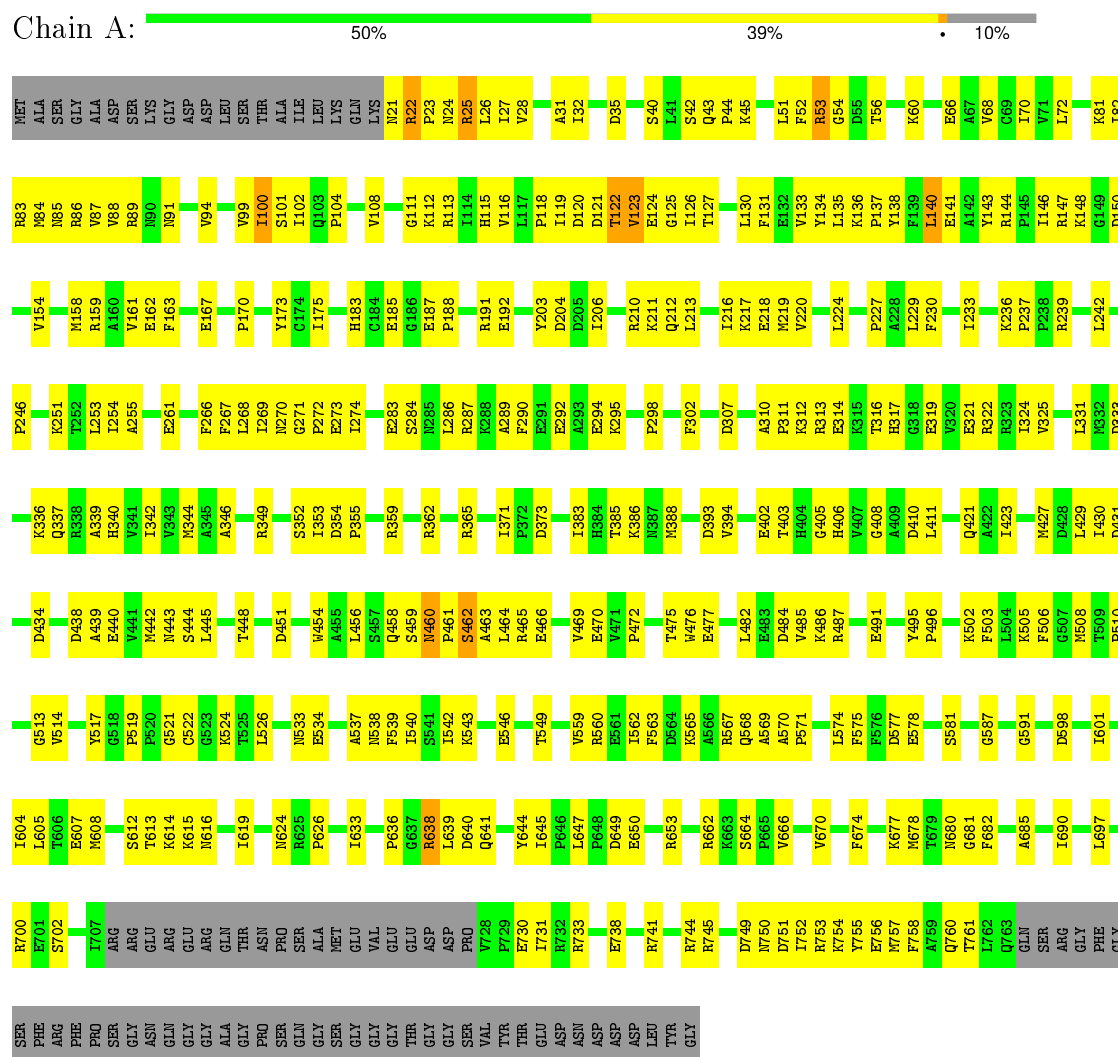
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	A	20	Total	O	0
			20	20	
4	B	20	Total	O	0
			20	20	
4	C	20	Total	O	0
			20	20	
4	D	20	Total	O	0
			20	20	
4	E	20	Total	O	0
			20	20	
4	F	20	Total	O	0
			20	20	

3 Residue-property plots

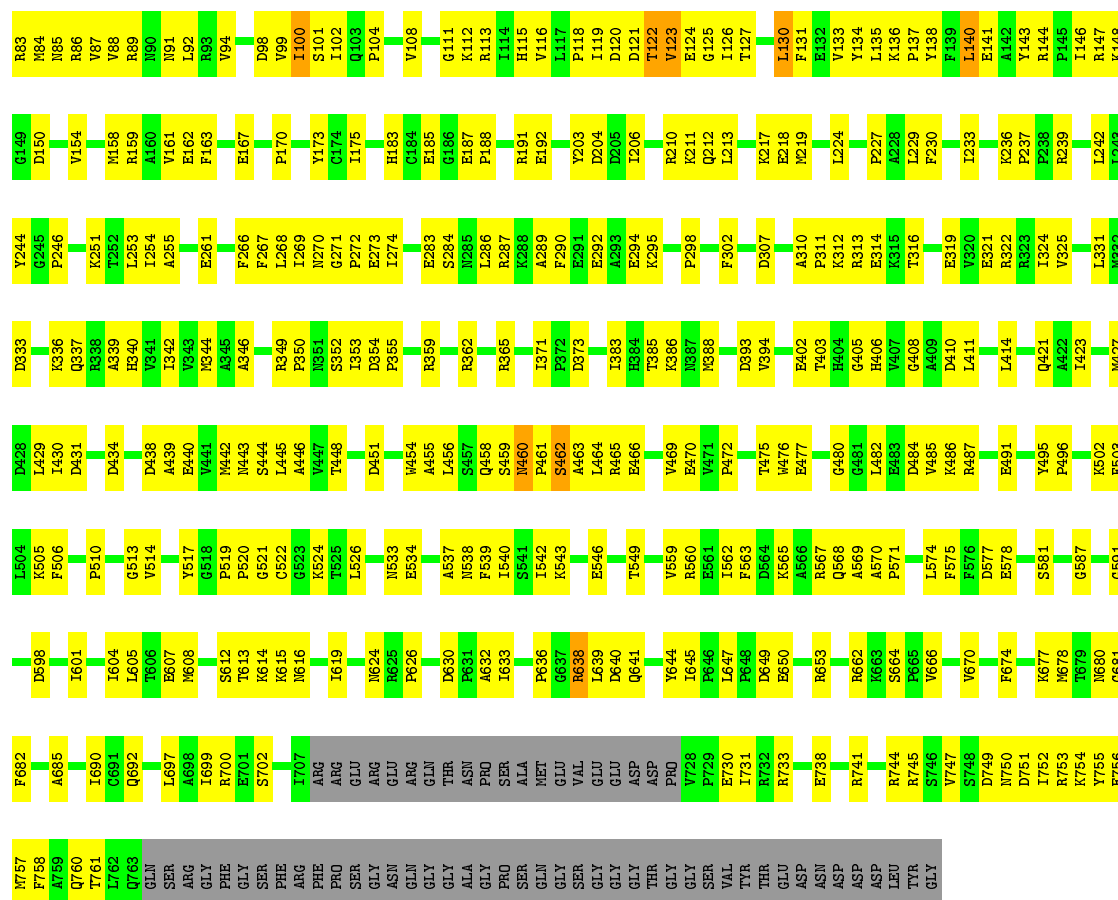
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE



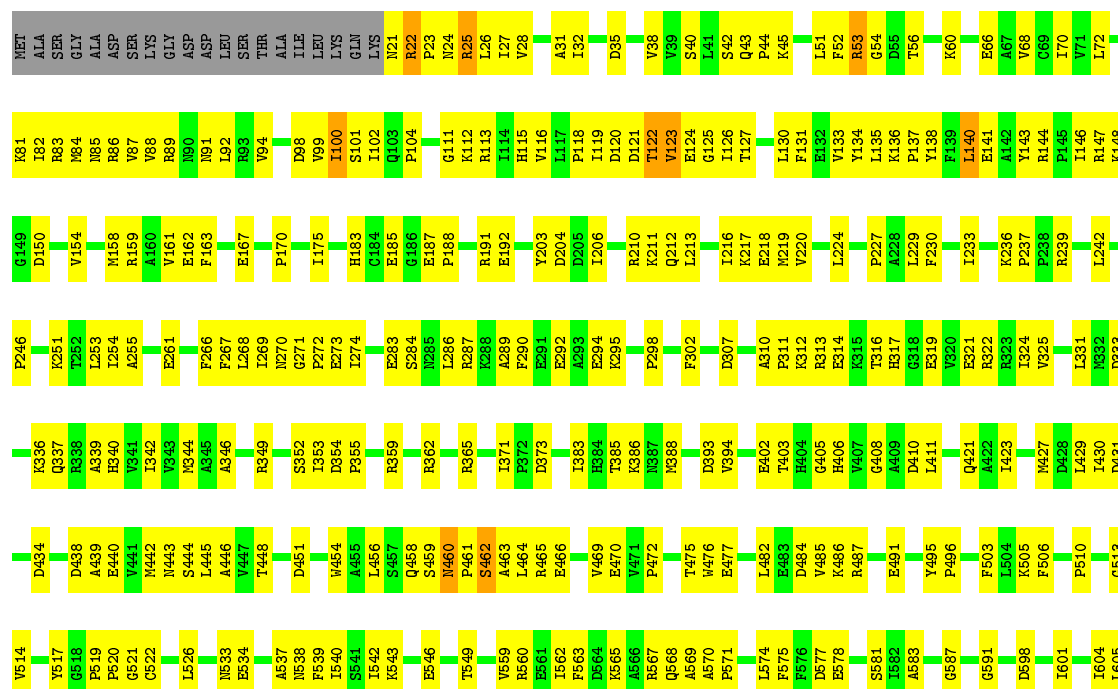
- Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE





• Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE

Chain C: 49% 39% 10%





[illegible]

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE, Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	215000	Depositor
Image detector	GATAN K2 SUMMIT (4K X 4K)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.45	0/5751	0.65	2/7767 (0.0%)
1	B	0.45	0/5751	0.65	3/7767 (0.0%)
1	C	0.45	0/5751	0.65	2/7767 (0.0%)
1	D	0.45	0/5751	0.65	2/7767 (0.0%)
1	E	0.45	0/5751	0.65	2/7767 (0.0%)
1	F	0.45	0/5751	0.65	3/7767 (0.0%)
All	All	0.45	0/34506	0.65	14/46602 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	140	LEU	CA-CB-CG	5.44	127.81	115.30
1	F	140	LEU	CA-CB-CG	5.44	127.81	115.30
1	B	140	LEU	CA-CB-CG	5.44	127.81	115.30
1	E	140	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	140	LEU	CA-CB-CG	5.42	127.78	115.30
1	D	140	LEU	CA-CB-CG	5.42	127.77	115.30
1	F	271	GLY	C-N-CD	5.17	139.25	128.40
1	D	271	GLY	C-N-CD	5.16	139.24	128.40
1	A	271	GLY	C-N-CD	5.15	139.22	128.40
1	B	271	GLY	C-N-CD	5.15	139.22	128.40
1	E	271	GLY	C-N-CD	5.14	139.19	128.40
1	C	271	GLY	C-N-CD	5.13	139.17	128.40
1	B	130	LEU	CA-CB-CG	5.00	126.80	115.30
1	F	130	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5659	0	5731	470	0
1	B	5659	0	5731	477	0
1	C	5659	0	5731	473	0
1	D	5659	0	5731	473	0
1	E	5659	0	5731	472	0
1	F	5659	0	5731	472	0
2	A	54	0	24	9	0
2	B	54	0	24	10	0
2	C	54	0	24	9	0
2	D	54	0	24	9	0
2	E	54	0	24	9	0
2	F	54	0	24	9	0
3	A	34	0	38	5	0
3	B	34	0	38	4	0
3	C	34	0	38	4	0
3	D	34	0	38	5	0
3	E	34	0	38	3	0
3	F	34	0	38	4	0
4	A	20	0	0	2	0
4	B	20	0	0	2	0
4	C	20	0	0	0	0
4	D	20	0	0	1	0
4	E	20	0	0	1	0
4	F	20	0	0	1	0
All	All	34602	0	34758	2782	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 40.

All (2782) 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:F:26:LEU:CD2	1:F:100:ILE:HD12	1.21	1.68
1:B:26:LEU:CD2	1:B:100:ILE:HD12	1.21	1.62
1:E:26:LEU:CD2	1:E:100:ILE:HD12	1.21	1.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:LEU:CD2	1:C:100:ILE:HD12	1.21	1.58
1:D:26:LEU:HD21	1:D:100:ILE:CD1	1.11	1.58
1:A:26:LEU:CD2	1:A:100:ILE:HD12	1.21	1.58
1:A:26:LEU:HD21	1:A:100:ILE:CD1	1.11	1.58
1:E:26:LEU:HD21	1:E:100:ILE:CD1	1.11	1.56
1:C:26:LEU:HD21	1:C:100:ILE:CD1	1.11	1.56
1:F:26:LEU:HD21	1:F:100:ILE:CD1	1.11	1.56
1:D:26:LEU:CD2	1:D:100:ILE:HD12	1.21	1.55
1:B:26:LEU:HD21	1:B:100:ILE:CD1	1.11	1.54
1:C:127:THR:CB	1:C:438:ASP:HA	1.39	1.53
1:D:127:THR:CB	1:D:438:ASP:HA	1.39	1.53
1:B:127:THR:CB	1:B:438:ASP:HA	1.39	1.51
1:E:127:THR:CB	1:E:438:ASP:HA	1.39	1.51
1:F:127:THR:CB	1:F:438:ASP:HA	1.39	1.49
1:A:127:THR:CB	1:A:438:ASP:HA	1.39	1.49
1:D:127:THR:HB	1:D:438:ASP:CA	1.51	1.40
1:E:127:THR:HB	1:E:438:ASP:CA	1.51	1.40
1:C:127:THR:HB	1:C:438:ASP:CA	1.51	1.39
1:A:127:THR:HB	1:A:438:ASP:CA	1.51	1.38
1:B:127:THR:HB	1:B:438:ASP:CA	1.51	1.38
1:F:127:THR:HB	1:F:438:ASP:CA	1.51	1.38
1:E:266:PHE:CD2	1:E:268:LEU:HD11	1.62	1.34
1:F:266:PHE:CD2	1:F:268:LEU:HD11	1.62	1.34
1:C:267:PHE:C	1:C:268:LEU:HD12	1.48	1.33
1:C:266:PHE:CD2	1:C:268:LEU:HD11	1.62	1.33
1:B:267:PHE:C	1:B:268:LEU:HD12	1.48	1.33
1:B:266:PHE:CD2	1:B:268:LEU:HD11	1.62	1.32
1:D:266:PHE:CD2	1:D:268:LEU:HD11	1.62	1.32
1:A:266:PHE:CD2	1:A:268:LEU:HD11	1.62	1.32
1:F:402:GLU:HG2	1:F:456:LEU:CD2	1.60	1.31
1:B:402:GLU:HG2	1:B:456:LEU:CD2	1.60	1.31
1:A:126:ILE:HA	1:A:439:ALA:CB	1.61	1.31
1:E:267:PHE:C	1:E:268:LEU:HD12	1.48	1.30
1:D:267:PHE:C	1:D:268:LEU:HD12	1.48	1.30
1:B:126:ILE:HA	1:B:439:ALA:CB	1.61	1.30
1:F:126:ILE:HA	1:F:439:ALA:CB	1.61	1.30
1:C:267:PHE:O	1:C:268:LEU:HD12	1.32	1.30
1:F:267:PHE:C	1:F:268:LEU:HD12	1.48	1.29
1:A:267:PHE:C	1:A:268:LEU:HD12	1.48	1.29
1:C:402:GLU:HG2	1:C:456:LEU:CD2	1.60	1.29
1:A:402:GLU:HG2	1:A:456:LEU:CD2	1.60	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:ILE:HD13	1:D:130:LEU:CB	1.63	1.29
1:E:402:GLU:HG2	1:E:456:LEU:CD2	1.60	1.29
1:C:126:ILE:HA	1:C:439:ALA:CB	1.61	1.29
1:D:126:ILE:HA	1:D:439:ALA:CB	1.61	1.29
1:E:126:ILE:HA	1:E:439:ALA:CB	1.61	1.29
1:F:26:LEU:HD22	1:F:102:ILE:CG1	1.63	1.28
1:E:126:ILE:HD13	1:E:130:LEU:CB	1.63	1.28
1:A:119:ILE:HD11	1:A:191:ARG:CD	1.63	1.28
1:E:26:LEU:HD22	1:E:102:ILE:CG1	1.63	1.28
1:D:267:PHE:O	1:D:268:LEU:HD12	1.32	1.28
1:D:119:ILE:HD11	1:D:191:ARG:CD	1.63	1.28
1:D:402:GLU:HG2	1:D:456:LEU:CD2	1.61	1.28
1:B:119:ILE:HD11	1:B:191:ARG:CD	1.63	1.28
1:A:26:LEU:HD22	1:A:102:ILE:CG1	1.63	1.27
1:C:126:ILE:HD13	1:C:130:LEU:CB	1.63	1.27
1:F:119:ILE:HD11	1:F:191:ARG:CD	1.63	1.27
1:D:26:LEU:HD22	1:D:102:ILE:CG1	1.63	1.27
1:A:119:ILE:CD1	1:A:191:ARG:HD3	1.65	1.27
1:E:119:ILE:HD11	1:E:191:ARG:CD	1.63	1.27
1:F:119:ILE:CD1	1:F:191:ARG:HD3	1.65	1.27
1:B:126:ILE:HD13	1:B:130:LEU:CB	1.63	1.27
1:C:119:ILE:HD11	1:C:191:ARG:CD	1.63	1.26
1:F:126:ILE:HD13	1:F:130:LEU:CB	1.63	1.26
1:B:267:PHE:O	1:B:268:LEU:HD12	1.32	1.26
1:E:26:LEU:HD13	1:E:102:ILE:CD1	1.66	1.26
1:B:26:LEU:HD22	1:B:102:ILE:CG1	1.63	1.25
1:F:26:LEU:HD13	1:F:102:ILE:CD1	1.66	1.25
1:C:126:ILE:CA	1:C:439:ALA:HB2	1.65	1.25
1:A:126:ILE:HD13	1:A:130:LEU:CB	1.63	1.25
1:D:119:ILE:CD1	1:D:191:ARG:HD3	1.65	1.25
1:C:26:LEU:HD13	1:C:102:ILE:CD1	1.66	1.25
1:A:126:ILE:CA	1:A:439:ALA:HB2	1.65	1.25
1:D:26:LEU:HD13	1:D:102:ILE:CD1	1.66	1.25
1:B:126:ILE:CA	1:B:439:ALA:HB2	1.65	1.25
1:C:119:ILE:CD1	1:C:191:ARG:HD3	1.65	1.25
1:B:26:LEU:HD13	1:B:102:ILE:CD1	1.66	1.24
1:C:26:LEU:HD22	1:C:102:ILE:CG1	1.63	1.24
1:A:26:LEU:HD13	1:A:102:ILE:CD1	1.66	1.24
1:E:126:ILE:CA	1:E:439:ALA:HB2	1.65	1.24
1:E:119:ILE:CD1	1:E:191:ARG:HD3	1.65	1.24
1:B:119:ILE:CD1	1:B:191:ARG:HD3	1.65	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:ILE:CA	1:D:439:ALA:HB2	1.65	1.24
1:D:26:LEU:CD2	1:D:100:ILE:O	1.86	1.24
1:F:126:ILE:CA	1:F:439:ALA:HB2	1.65	1.24
1:E:267:PHE:O	1:E:268:LEU:HD12	1.32	1.23
1:B:26:LEU:CD2	1:B:100:ILE:O	1.86	1.23
1:E:26:LEU:CD2	1:E:100:ILE:O	1.86	1.23
1:D:26:LEU:HD23	1:D:100:ILE:O	1.06	1.22
1:A:26:LEU:HD23	1:A:100:ILE:O	1.06	1.22
1:F:26:LEU:CD2	1:F:100:ILE:O	1.86	1.22
1:E:26:LEU:HD23	1:E:100:ILE:O	1.06	1.22
1:E:130:LEU:CD1	1:E:131:PHE:CE1	2.23	1.22
1:B:26:LEU:HD23	1:B:100:ILE:O	1.06	1.22
1:C:26:LEU:CD2	1:C:100:ILE:O	1.86	1.22
1:D:130:LEU:CD1	1:D:131:PHE:CE1	2.23	1.21
1:C:26:LEU:HD23	1:C:100:ILE:O	1.06	1.21
1:A:130:LEU:CD1	1:A:131:PHE:CE1	2.23	1.21
1:A:267:PHE:O	1:A:268:LEU:HD12	1.32	1.21
1:F:130:LEU:CD1	1:F:131:PHE:CE1	2.23	1.21
1:F:267:PHE:O	1:F:268:LEU:HD12	1.32	1.21
1:B:130:LEU:CD1	1:B:131:PHE:CE1	2.23	1.20
1:A:26:LEU:CD2	1:A:100:ILE:O	1.86	1.20
1:F:26:LEU:HD23	1:F:100:ILE:O	1.06	1.19
1:C:130:LEU:CD1	1:C:131:PHE:CE1	2.23	1.19
1:D:461:PRO:HA	1:D:462:SER:HB3	1.25	1.16
1:F:461:PRO:HA	1:F:462:SER:HB3	1.25	1.16
1:F:130:LEU:HD12	1:F:131:PHE:CD1	1.81	1.16
1:E:461:PRO:HA	1:E:462:SER:HB3	1.26	1.16
1:B:461:PRO:HA	1:B:462:SER:HB3	1.26	1.16
1:B:26:LEU:HD21	1:B:100:ILE:CG1	1.75	1.16
1:C:130:LEU:HD12	1:C:131:PHE:CD1	1.81	1.16
1:E:130:LEU:HD12	1:E:131:PHE:CD1	1.81	1.16
1:C:26:LEU:HD21	1:C:100:ILE:CG1	1.75	1.15
1:A:26:LEU:HD21	1:A:100:ILE:CG1	1.75	1.15
1:D:26:LEU:HD21	1:D:100:ILE:CG1	1.75	1.15
1:B:130:LEU:HD12	1:B:131:PHE:CD1	1.81	1.15
1:E:26:LEU:HD21	1:E:100:ILE:CG1	1.75	1.15
1:A:461:PRO:HA	1:A:462:SER:HB3	1.26	1.15
1:C:461:PRO:HA	1:C:462:SER:HB3	1.26	1.15
1:D:224:LEU:HD22	1:D:298:PRO:HB2	1.16	1.15
1:D:130:LEU:HD12	1:D:131:PHE:CD1	1.81	1.14
1:F:224:LEU:HD22	1:F:298:PRO:HB2	1.16	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:LEU:HD12	1:A:131:PHE:CD1	1.81	1.14
1:B:224:LEU:HD22	1:B:298:PRO:HB2	1.15	1.14
1:E:224:LEU:HD22	1:E:298:PRO:HB2	1.16	1.14
1:F:26:LEU:HD21	1:F:100:ILE:CG1	1.75	1.13
1:F:126:ILE:CD1	1:F:130:LEU:HB3	1.78	1.13
1:C:224:LEU:HD22	1:C:298:PRO:HB2	1.16	1.13
1:A:224:LEU:HD22	1:A:298:PRO:HB2	1.15	1.13
1:A:126:ILE:CD1	1:A:130:LEU:HB3	1.78	1.12
1:D:126:ILE:CD1	1:D:130:LEU:HB3	1.78	1.12
1:E:126:ILE:CD1	1:E:130:LEU:HB3	1.78	1.12
1:C:126:ILE:CD1	1:C:130:LEU:HB3	1.78	1.12
1:D:402:GLU:CG	1:D:456:LEU:HD21	1.79	1.12
1:B:126:ILE:CD1	1:B:130:LEU:HB3	1.78	1.12
1:B:130:LEU:HD11	1:B:131:PHE:CE1	1.85	1.11
1:E:402:GLU:CG	1:E:456:LEU:HD21	1.79	1.11
1:D:130:LEU:HD12	1:D:131:PHE:CE1	1.85	1.11
1:A:402:GLU:CG	1:A:456:LEU:HD21	1.79	1.11
1:C:402:GLU:CG	1:C:456:LEU:HD21	1.79	1.11
1:A:130:LEU:HD11	1:A:131:PHE:CE1	1.85	1.11
1:B:402:GLU:CG	1:B:456:LEU:HD21	1.79	1.11
1:C:130:LEU:HD11	1:C:131:PHE:CE1	1.85	1.10
1:F:402:GLU:CG	1:F:456:LEU:HD21	1.79	1.10
1:F:26:LEU:CD2	1:F:102:ILE:HG13	1.82	1.10
1:F:26:LEU:HD13	1:F:102:ILE:HD12	1.10	1.10
1:E:26:LEU:CD2	1:E:102:ILE:HG13	1.82	1.10
1:D:26:LEU:CD2	1:D:102:ILE:HG13	1.82	1.10
1:F:130:LEU:HD12	1:F:131:PHE:CE1	1.85	1.10
1:A:26:LEU:CD2	1:A:102:ILE:HG13	1.82	1.09
1:F:130:LEU:HD11	1:F:131:PHE:CE1	1.85	1.09
1:C:26:LEU:CD2	1:C:102:ILE:HG13	1.82	1.09
1:C:130:LEU:HD12	1:C:131:PHE:CE1	1.85	1.09
1:A:130:LEU:HD12	1:A:131:PHE:CE1	1.85	1.09
1:C:26:LEU:HD13	1:C:102:ILE:HD12	1.10	1.09
1:D:26:LEU:HD13	1:D:102:ILE:HD12	1.10	1.09
1:B:130:LEU:HD12	1:B:131:PHE:CE1	1.85	1.09
1:B:26:LEU:CD2	1:B:102:ILE:HG13	1.82	1.08
1:D:130:LEU:HD11	1:D:131:PHE:CE1	1.85	1.08
1:E:130:LEU:HD12	1:E:131:PHE:CE1	1.85	1.08
1:F:312:LYS:CE	1:F:316:THR:HG23	1.84	1.07
1:A:26:LEU:HD13	1:A:102:ILE:HD12	1.10	1.07
1:E:130:LEU:HD11	1:E:131:PHE:CE1	1.85	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:LYS:CE	1:B:316:THR:HG23	1.84	1.07
1:E:312:LYS:CE	1:E:316:THR:HG23	1.84	1.07
1:A:312:LYS:CE	1:A:316:THR:HG23	1.84	1.06
1:C:312:LYS:CE	1:C:316:THR:HG23	1.84	1.06
1:D:312:LYS:CE	1:D:316:THR:HG23	1.84	1.06
1:F:402:GLU:HG2	1:F:456:LEU:HD21	1.33	1.06
1:E:26:LEU:HD13	1:E:102:ILE:HD12	1.10	1.06
1:D:26:LEU:HD22	1:D:100:ILE:HD12	1.36	1.05
1:B:26:LEU:HD13	1:B:102:ILE:HD12	1.10	1.05
1:A:26:LEU:HD22	1:A:100:ILE:HD12	1.36	1.05
1:C:402:GLU:HG2	1:C:456:LEU:HD21	1.33	1.04
1:C:559:VAL:HG12	1:C:607:GLU:OE1	1.58	1.04
1:F:26:LEU:HD22	1:F:100:ILE:HD12	1.36	1.04
1:E:26:LEU:HD22	1:E:100:ILE:HD12	1.36	1.04
1:A:559:VAL:HG12	1:A:607:GLU:OE1	1.58	1.03
1:E:559:VAL:HG12	1:E:607:GLU:OE1	1.57	1.03
1:F:559:VAL:HG12	1:F:607:GLU:OE1	1.58	1.03
1:E:567:ARG:NH1	1:E:568:GLN:HE21	1.56	1.03
1:A:567:ARG:NH1	1:A:568:GLN:HE21	1.56	1.03
1:B:567:ARG:NH1	1:B:568:GLN:HE21	1.56	1.02
1:D:402:GLU:HG2	1:D:456:LEU:HD21	1.33	1.02
1:C:567:ARG:NH1	1:C:568:GLN:HE21	1.56	1.02
1:D:224:LEU:HD22	1:D:298:PRO:CB	1.90	1.02
1:F:567:ARG:NH1	1:F:568:GLN:HE21	1.56	1.02
1:D:127:THR:HG21	1:D:438:ASP:OD1	1.60	1.02
1:F:127:THR:HG21	1:F:438:ASP:OD1	1.60	1.02
1:E:402:GLU:HG2	1:E:456:LEU:HD21	1.33	1.02
1:A:127:THR:HG21	1:A:438:ASP:OD1	1.60	1.01
1:F:224:LEU:HD22	1:F:298:PRO:CB	1.90	1.01
1:D:567:ARG:NH1	1:D:568:GLN:HE21	1.56	1.01
1:B:26:LEU:HD22	1:B:100:ILE:HD12	1.36	1.01
1:A:402:GLU:HG2	1:A:456:LEU:HD21	1.33	1.01
1:B:559:VAL:HG12	1:B:607:GLU:OE1	1.58	1.01
1:B:127:THR:HG21	1:B:438:ASP:OD1	1.60	1.01
1:D:559:VAL:HG12	1:D:607:GLU:OE1	1.57	1.01
1:E:127:THR:HG21	1:E:438:ASP:OD1	1.59	1.01
1:E:224:LEU:HD22	1:E:298:PRO:CB	1.90	1.01
1:C:26:LEU:HD22	1:C:100:ILE:HD12	1.36	1.01
1:A:224:LEU:HD22	1:A:298:PRO:CB	1.90	1.00
1:B:224:LEU:HD22	1:B:298:PRO:CB	1.90	1.00
1:C:130:LEU:CD1	1:C:131:PHE:HE1	1.75	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:THR:HG21	1:C:438:ASP:OD1	1.60	0.99
1:C:224:LEU:HD22	1:C:298:PRO:CB	1.90	0.99
1:F:312:LYS:HE2	1:F:321:GLU:HG2	1.44	0.99
1:E:312:LYS:HE2	1:E:321:GLU:HG2	1.44	0.99
1:C:482:LEU:O	1:C:486:LYS:HG3	1.62	0.99
1:E:482:LEU:O	1:E:486:LYS:HG3	1.62	0.99
1:B:482:LEU:O	1:B:486:LYS:HG3	1.62	0.98
1:F:482:LEU:O	1:F:486:LYS:HG3	1.62	0.98
1:A:312:LYS:HE2	1:A:321:GLU:HG2	1.44	0.97
1:C:312:LYS:HE2	1:C:321:GLU:HG2	1.44	0.97
1:B:307:ASP:O	1:B:311:PRO:HB3	1.64	0.97
1:D:130:LEU:CD1	1:D:131:PHE:HE1	1.75	0.97
1:C:307:ASP:O	1:C:311:PRO:HB3	1.64	0.97
1:D:307:ASP:O	1:D:311:PRO:HB3	1.64	0.97
1:A:224:LEU:CD2	1:A:298:PRO:HB2	1.95	0.97
1:A:307:ASP:O	1:A:311:PRO:HB3	1.64	0.97
1:E:26:LEU:CD2	1:E:100:ILE:CD1	2.03	0.97
1:B:224:LEU:CD2	1:B:298:PRO:HB2	1.95	0.97
1:D:312:LYS:HE2	1:D:321:GLU:HG2	1.44	0.97
1:D:482:LEU:O	1:D:486:LYS:HG3	1.62	0.97
1:B:402:GLU:HG2	1:B:456:LEU:HD21	1.33	0.97
1:A:482:LEU:O	1:A:486:LYS:HG3	1.62	0.97
1:F:307:ASP:O	1:F:311:PRO:HB3	1.64	0.97
1:D:224:LEU:CD2	1:D:298:PRO:HB2	1.95	0.96
1:E:224:LEU:CD2	1:E:298:PRO:HB2	1.95	0.96
1:C:266:PHE:HD2	1:C:268:LEU:HD11	1.15	0.96
1:C:224:LEU:CD2	1:C:298:PRO:HB2	1.95	0.96
1:F:402:GLU:HG2	1:F:456:LEU:HD22	1.46	0.96
1:B:402:GLU:CG	1:B:456:LEU:CD2	2.41	0.96
1:B:312:LYS:HE2	1:B:321:GLU:HG2	1.44	0.96
1:E:402:GLU:CG	1:E:456:LEU:CD2	2.41	0.95
1:E:402:GLU:HG2	1:E:456:LEU:HD22	1.46	0.95
1:E:307:ASP:O	1:E:311:PRO:HB3	1.64	0.95
1:C:647:LEU:HD11	1:C:752:ILE:HD11	1.49	0.95
1:D:266:PHE:HD2	1:D:268:LEU:HD11	1.16	0.95
1:F:224:LEU:CD2	1:F:298:PRO:HB2	1.95	0.95
1:D:267:PHE:C	1:D:268:LEU:CD1	2.35	0.95
1:D:647:LEU:HD11	1:D:752:ILE:HD11	1.49	0.95
1:D:587:GLY:HA3	1:D:591:GLY:HA2	1.49	0.95
1:A:647:LEU:HD11	1:A:752:ILE:HD11	1.49	0.95
1:B:267:PHE:C	1:B:268:LEU:CD1	2.35	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:647:LEU:HD11	1:B:752:ILE:HD11	1.49	0.95
1:A:587:GLY:HA3	1:A:591:GLY:HA2	1.49	0.95
1:C:267:PHE:C	1:C:268:LEU:CD1	2.35	0.94
1:C:26:LEU:CD2	1:C:100:ILE:CD1	2.03	0.94
1:D:127:THR:H	1:D:439:ALA:H	1.07	0.94
1:B:587:GLY:HA3	1:B:591:GLY:HA2	1.49	0.94
1:E:130:LEU:CD1	1:E:131:PHE:HE1	1.75	0.94
1:D:26:LEU:HD23	1:D:100:ILE:C	1.88	0.94
1:A:267:PHE:C	1:A:268:LEU:CD1	2.35	0.94
1:A:402:GLU:HG2	1:A:456:LEU:HD22	1.46	0.94
1:E:26:LEU:HD23	1:E:100:ILE:C	1.88	0.94
1:A:126:ILE:HD11	1:A:130:LEU:CD2	1.98	0.94
1:F:266:PHE:HD2	1:F:268:LEU:HD11	1.15	0.94
1:B:130:LEU:CD1	1:B:131:PHE:HE1	1.75	0.94
1:B:266:PHE:CD2	1:B:268:LEU:CD1	2.51	0.94
1:D:571:PRO:HA	1:D:616:ASN:HB3	1.50	0.94
1:F:26:LEU:HD23	1:F:100:ILE:C	1.88	0.94
1:C:26:LEU:HD23	1:C:100:ILE:C	1.88	0.94
1:A:266:PHE:CD2	1:A:268:LEU:CD1	2.51	0.94
1:C:266:PHE:CD2	1:C:268:LEU:CD1	2.51	0.94
1:B:26:LEU:HD23	1:B:100:ILE:C	1.88	0.93
1:E:267:PHE:C	1:E:268:LEU:CD1	2.35	0.93
1:A:402:GLU:CG	1:A:456:LEU:CD2	2.41	0.93
1:A:571:PRO:HA	1:A:616:ASN:HB3	1.50	0.93
1:A:26:LEU:HD23	1:A:100:ILE:C	1.88	0.93
1:E:587:GLY:HA3	1:E:591:GLY:HA2	1.49	0.93
1:F:267:PHE:C	1:F:268:LEU:CD1	2.35	0.93
1:E:126:ILE:HD11	1:E:130:LEU:CD2	1.98	0.93
1:E:266:PHE:HD2	1:E:268:LEU:HD11	1.15	0.93
1:F:266:PHE:CD2	1:F:268:LEU:CD1	2.51	0.93
1:B:266:PHE:HD2	1:B:268:LEU:HD11	1.15	0.93
1:B:571:PRO:HA	1:B:616:ASN:HB3	1.50	0.93
1:F:647:LEU:HD11	1:F:752:ILE:HD11	1.49	0.93
1:C:560:ARG:HA	1:C:607:GLU:OE2	1.69	0.93
1:A:560:ARG:HA	1:A:607:GLU:OE2	1.69	0.93
1:B:126:ILE:HD11	1:B:130:LEU:CD2	1.98	0.93
1:E:567:ARG:HH12	1:E:568:GLN:HE21	1.13	0.93
1:B:560:ARG:HA	1:B:607:GLU:OE2	1.69	0.93
1:E:127:THR:H	1:E:439:ALA:H	1.07	0.93
1:F:126:ILE:HD11	1:F:130:LEU:CD2	1.98	0.93
1:E:647:LEU:HD11	1:E:752:ILE:HD11	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:GLU:HG2	1:B:456:LEU:HD22	1.46	0.93
1:C:402:GLU:HG2	1:C:456:LEU:HD22	1.46	0.93
1:D:560:ARG:HA	1:D:607:GLU:OE2	1.69	0.93
1:B:127:THR:H	1:B:439:ALA:H	1.07	0.92
1:A:266:PHE:HD2	1:A:268:LEU:HD11	1.15	0.92
1:D:402:GLU:HG2	1:D:456:LEU:HD22	1.46	0.92
1:F:560:ARG:HA	1:F:607:GLU:OE2	1.69	0.92
1:C:587:GLY:HA3	1:C:591:GLY:HA2	1.49	0.92
1:F:402:GLU:CG	1:F:456:LEU:CD2	2.41	0.92
1:D:402:GLU:CG	1:D:456:LEU:CD2	2.41	0.92
1:D:126:ILE:HD11	1:D:130:LEU:CD2	1.98	0.92
1:D:266:PHE:CD2	1:D:268:LEU:CD1	2.51	0.92
1:E:571:PRO:HA	1:E:616:ASN:HB3	1.50	0.92
1:B:26:LEU:CD2	1:B:100:ILE:CD1	2.03	0.92
1:F:312:LYS:CD	1:F:316:THR:HG23	2.00	0.92
1:B:567:ARG:HH12	1:B:568:GLN:HE21	1.13	0.92
1:F:571:PRO:HA	1:F:616:ASN:HB3	1.50	0.92
1:A:26:LEU:CD2	1:A:100:ILE:CD1	2.03	0.92
1:C:571:PRO:HA	1:C:616:ASN:HB3	1.50	0.92
1:C:127:THR:H	1:C:439:ALA:H	1.07	0.92
1:A:26:LEU:CD1	1:A:102:ILE:CD1	2.48	0.92
1:C:126:ILE:HD11	1:C:130:LEU:CD2	1.98	0.92
1:D:267:PHE:HE2	1:D:289:ALA:HB1	1.34	0.91
1:F:26:LEU:CD1	1:F:102:ILE:CD1	2.48	0.91
1:E:266:PHE:CD2	1:E:268:LEU:CD1	2.51	0.91
1:E:312:LYS:CD	1:E:316:THR:HG23	2.00	0.91
1:F:567:ARG:HH12	1:F:568:GLN:HE21	1.13	0.91
1:F:269:ILE:HG23	1:F:274:ILE:CD1	2.01	0.91
1:E:267:PHE:HE2	1:E:289:ALA:HB1	1.34	0.91
1:A:312:LYS:CD	1:A:316:THR:HG23	2.00	0.91
1:C:567:ARG:HH12	1:C:568:GLN:HE21	1.13	0.91
1:F:587:GLY:HA3	1:F:591:GLY:HA2	1.49	0.91
1:B:26:LEU:CD1	1:B:102:ILE:CD1	2.48	0.91
1:C:269:ILE:HG23	1:C:274:ILE:CD1	2.01	0.91
1:E:560:ARG:HA	1:E:607:GLU:OE2	1.69	0.91
1:E:26:LEU:CD1	1:E:102:ILE:CD1	2.48	0.91
1:A:127:THR:H	1:A:439:ALA:H	1.07	0.91
1:B:269:ILE:HG23	1:B:274:ILE:CD1	2.01	0.91
1:C:402:GLU:CG	1:C:456:LEU:CD2	2.41	0.91
1:D:567:ARG:HH12	1:D:568:GLN:HE21	1.13	0.91
1:F:266:PHE:CE2	1:F:268:LEU:HD11	2.06	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:LYS:CD	1:C:316:THR:HG23	2.00	0.91
1:D:312:LYS:CD	1:D:316:THR:HG23	2.00	0.91
1:D:312:LYS:HE2	1:D:321:GLU:CG	2.01	0.91
1:D:26:LEU:CD1	1:D:102:ILE:CD1	2.48	0.91
1:C:267:PHE:HE2	1:C:289:ALA:HB1	1.34	0.91
1:A:266:PHE:CE2	1:A:268:LEU:HD11	2.06	0.91
1:C:26:LEU:CD1	1:C:102:ILE:CD1	2.48	0.90
1:D:269:ILE:HG23	1:D:274:ILE:CD1	2.01	0.90
1:F:267:PHE:HE2	1:F:289:ALA:HB1	1.34	0.90
1:E:312:LYS:HE2	1:E:321:GLU:CG	2.01	0.90
1:E:269:ILE:HG23	1:E:274:ILE:CD1	2.01	0.90
1:A:130:LEU:CD1	1:A:131:PHE:HE1	1.75	0.90
1:B:312:LYS:CD	1:B:316:THR:HG23	2.00	0.90
1:E:266:PHE:CE2	1:E:268:LEU:HD11	2.06	0.90
1:B:266:PHE:CE2	1:B:268:LEU:HD11	2.07	0.90
1:A:269:ILE:HG23	1:A:274:ILE:CD1	2.01	0.90
1:A:312:LYS:HE2	1:A:321:GLU:CG	2.01	0.90
1:A:567:ARG:HH12	1:A:568:GLN:HE21	1.13	0.90
1:C:266:PHE:CE2	1:C:268:LEU:HD11	2.06	0.90
1:A:267:PHE:HE2	1:A:289:ALA:HB1	1.34	0.90
1:C:312:LYS:HE2	1:C:321:GLU:CG	2.01	0.90
1:F:127:THR:H	1:F:439:ALA:H	1.07	0.90
1:D:266:PHE:CE2	1:D:268:LEU:HD11	2.06	0.90
1:B:26:LEU:HD22	1:B:102:ILE:HG13	0.90	0.89
1:C:461:PRO:HA	1:C:462:SER:CB	2.02	0.89
1:B:312:LYS:HE2	1:B:321:GLU:CG	2.01	0.89
1:B:267:PHE:HE2	1:B:289:ALA:HB1	1.34	0.89
1:F:130:LEU:CD1	1:F:131:PHE:HE1	1.75	0.89
1:D:26:LEU:CD2	1:D:100:ILE:CD1	2.03	0.89
1:F:312:LYS:HE2	1:F:321:GLU:CG	2.01	0.89
1:C:560:ARG:CA	1:C:607:GLU:OE2	2.21	0.89
1:C:26:LEU:HD22	1:C:102:ILE:HG13	0.90	0.89
1:B:560:ARG:CA	1:B:607:GLU:OE2	2.21	0.89
1:D:560:ARG:CA	1:D:607:GLU:OE2	2.21	0.89
1:D:127:THR:HB	1:D:438:ASP:CB	2.03	0.89
1:B:461:PRO:HA	1:B:462:SER:CB	2.02	0.89
1:F:560:ARG:CA	1:F:607:GLU:OE2	2.21	0.89
1:B:127:THR:HB	1:B:438:ASP:CB	2.03	0.88
1:A:406:HIS:HE1	1:A:459:SER:HB3	1.38	0.88
1:D:406:HIS:HE1	1:D:459:SER:HB3	1.38	0.88
1:C:406:HIS:HE1	1:C:459:SER:HB3	1.38	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:LYS:HE3	1:A:316:THR:HG23	1.56	0.88
1:E:461:PRO:HA	1:E:462:SER:CB	2.02	0.88
1:A:461:PRO:HA	1:A:462:SER:CB	2.02	0.88
1:C:127:THR:HB	1:C:438:ASP:CB	2.03	0.88
1:D:461:PRO:HA	1:D:462:SER:CB	2.02	0.88
1:F:461:PRO:HA	1:F:462:SER:CB	2.02	0.88
1:E:560:ARG:CA	1:E:607:GLU:OE2	2.21	0.88
1:D:26:LEU:HD22	1:D:102:ILE:HG13	0.90	0.87
1:E:312:LYS:HE3	1:E:316:THR:HG23	1.56	0.87
1:A:560:ARG:CA	1:A:607:GLU:OE2	2.21	0.87
1:B:312:LYS:HE3	1:B:316:THR:HG23	1.56	0.87
1:E:127:THR:HB	1:E:438:ASP:CB	2.03	0.87
1:E:26:LEU:HD22	1:E:102:ILE:HG13	0.90	0.87
1:B:406:HIS:HE1	1:B:459:SER:HB3	1.38	0.87
1:F:127:THR:HB	1:F:438:ASP:CB	2.03	0.87
1:A:127:THR:HB	1:A:438:ASP:CB	2.03	0.87
1:E:406:HIS:HE1	1:E:459:SER:HB3	1.38	0.87
1:D:312:LYS:HE3	1:D:316:THR:HG23	1.56	0.87
1:A:130:LEU:HD11	1:A:131:PHE:HE1	1.29	0.87
1:F:406:HIS:HE1	1:F:459:SER:HB3	1.38	0.86
1:F:26:LEU:HD22	1:F:102:ILE:HG13	0.90	0.86
1:E:312:LYS:HD2	1:E:316:THR:HG23	1.58	0.86
1:F:403:THR:HG21	1:F:411:LEU:HD21	1.58	0.86
1:F:406:HIS:HE1	1:F:459:SER:CB	1.89	0.86
1:C:312:LYS:HE3	1:C:316:THR:HG23	1.56	0.86
1:B:130:LEU:HD11	1:B:131:PHE:HE1	1.30	0.86
1:A:26:LEU:HD22	1:A:102:ILE:HG13	0.90	0.85
1:A:406:HIS:HE1	1:A:459:SER:CB	1.89	0.85
1:E:26:LEU:CD1	1:E:102:ILE:HD12	2.04	0.85
1:B:636:PRO:HA	1:B:640:ASP:OD2	1.77	0.85
1:C:636:PRO:HA	1:C:640:ASP:OD2	1.76	0.85
1:F:26:LEU:CD2	1:F:100:ILE:CD1	2.03	0.85
1:F:312:LYS:HE3	1:F:316:THR:HG23	1.56	0.85
1:A:636:PRO:HA	1:A:640:ASP:OD2	1.77	0.85
1:A:403:THR:HG21	1:A:411:LEU:HD21	1.58	0.85
1:D:636:PRO:HA	1:D:640:ASP:OD2	1.77	0.85
1:E:403:THR:HG21	1:E:411:LEU:HD21	1.58	0.85
1:D:406:HIS:HE1	1:D:459:SER:CB	1.89	0.85
1:B:406:HIS:HE1	1:B:459:SER:CB	1.89	0.85
1:C:312:LYS:HD2	1:C:316:THR:HG23	1.58	0.85
1:F:636:PRO:HA	1:F:640:ASP:OD2	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:HIS:HE1	1:C:459:SER:CB	1.89	0.85
1:D:312:LYS:HD2	1:D:316:THR:HG23	1.58	0.85
1:B:312:LYS:HD2	1:B:316:THR:HG23	1.58	0.84
1:E:210:ARG:HG3	1:E:212:GLN:HG2	1.59	0.84
1:A:210:ARG:HG3	1:A:212:GLN:HG2	1.59	0.84
1:E:406:HIS:HE1	1:E:459:SER:CB	1.89	0.84
1:B:403:THR:HG21	1:B:411:LEU:HD21	1.58	0.84
1:F:210:ARG:HG3	1:F:212:GLN:HG2	1.59	0.84
1:D:403:THR:HG21	1:D:411:LEU:HD21	1.58	0.84
1:F:312:LYS:HD2	1:F:316:THR:HG23	1.58	0.84
1:A:312:LYS:HD2	1:A:316:THR:HG23	1.58	0.83
1:D:210:ARG:HG3	1:D:212:GLN:HG2	1.59	0.83
1:C:403:THR:HG21	1:C:411:LEU:HD21	1.58	0.83
1:B:210:ARG:HG3	1:B:212:GLN:HG2	1.60	0.83
1:E:319:GLU:HG3	1:E:322:ARG:HH21	1.43	0.83
1:D:26:LEU:CD1	1:D:102:ILE:HD12	2.03	0.83
1:D:127:THR:OG1	1:D:438:ASP:HA	1.79	0.83
1:A:116:VAL:HG13	1:A:163:PHE:HB3	1.59	0.83
1:F:127:THR:OG1	1:F:438:ASP:HA	1.79	0.83
1:D:116:VAL:HG13	1:D:163:PHE:HB3	1.59	0.83
1:B:116:VAL:HG13	1:B:163:PHE:HB3	1.59	0.83
1:E:127:THR:OG1	1:E:438:ASP:HA	1.79	0.83
1:A:127:THR:OG1	1:A:438:ASP:HA	1.79	0.83
1:E:636:PRO:HA	1:E:640:ASP:OD2	1.77	0.83
1:F:130:LEU:HD11	1:F:131:PHE:HE1	1.29	0.83
1:E:26:LEU:HD13	1:E:102:ILE:HD11	1.61	0.82
1:C:116:VAL:HG13	1:C:163:PHE:HB3	1.59	0.82
1:D:126:ILE:HD11	1:D:130:LEU:HD23	1.61	0.82
1:E:476:TRP:CZ2	1:E:534:GLU:OE1	2.32	0.82
1:C:476:TRP:CZ2	1:C:534:GLU:OE1	2.32	0.82
1:D:125:GLY:HA3	1:D:159:ARG:NH1	1.94	0.82
1:C:125:GLY:HA3	1:C:159:ARG:NH1	1.94	0.82
1:F:116:VAL:HG13	1:F:163:PHE:HB3	1.59	0.82
1:F:319:GLU:HG3	1:F:322:ARG:HH21	1.43	0.82
1:F:476:TRP:CZ2	1:F:534:GLU:OE1	2.32	0.82
1:A:476:TRP:CZ2	1:A:534:GLU:OE1	2.32	0.82
1:B:476:TRP:CZ2	1:B:534:GLU:OE1	2.32	0.82
1:B:26:LEU:HD13	1:B:102:ILE:HD11	1.62	0.82
1:E:116:VAL:HG13	1:E:163:PHE:HB3	1.59	0.82
1:E:126:ILE:HD11	1:E:130:LEU:HD23	1.61	0.82
1:B:126:ILE:CD1	1:B:130:LEU:CD2	2.57	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:ARG:HG3	1:C:212:GLN:HG2	1.59	0.82
1:D:319:GLU:HG3	1:D:322:ARG:HH21	1.43	0.82
1:D:476:TRP:CZ2	1:D:534:GLU:OE1	2.32	0.82
1:D:26:LEU:HD13	1:D:102:ILE:HD11	1.62	0.82
1:C:126:ILE:CD1	1:C:130:LEU:CD2	2.57	0.82
1:C:127:THR:OG1	1:C:438:ASP:HA	1.79	0.82
1:F:126:ILE:HD11	1:F:130:LEU:HD23	1.61	0.82
1:C:26:LEU:HD13	1:C:102:ILE:HD11	1.62	0.82
1:F:126:ILE:CD1	1:F:130:LEU:CD2	2.57	0.82
1:A:126:ILE:CD1	1:A:130:LEU:CD2	2.57	0.82
1:E:125:GLY:HA3	1:E:159:ARG:NH1	1.94	0.82
1:D:126:ILE:CD1	1:D:130:LEU:CD2	2.57	0.82
1:F:125:GLY:HA3	1:F:159:ARG:NH1	1.94	0.82
1:E:126:ILE:CD1	1:E:130:LEU:CD2	2.57	0.81
1:A:319:GLU:HG3	1:A:322:ARG:HH21	1.43	0.81
1:C:319:GLU:HG3	1:C:322:ARG:HH21	1.43	0.81
1:D:127:THR:CG2	1:D:438:ASP:OD1	2.29	0.81
1:A:126:ILE:HD11	1:A:130:LEU:HD23	1.61	0.81
1:B:319:GLU:HG3	1:B:322:ARG:HH21	1.43	0.81
1:A:513:GLY:HA3	1:A:639:LEU:HD23	1.63	0.81
1:A:26:LEU:HD13	1:A:102:ILE:HD11	1.61	0.81
1:B:127:THR:CG2	1:B:438:ASP:OD1	2.29	0.81
1:B:513:GLY:HA3	1:B:639:LEU:HD23	1.63	0.81
1:B:127:THR:OG1	1:B:438:ASP:HA	1.79	0.81
1:E:127:THR:CG2	1:E:438:ASP:OD1	2.29	0.81
1:A:120:ASP:CG	1:A:121:ASP:H	1.84	0.81
1:B:125:GLY:HA3	1:B:159:ARG:NH1	1.94	0.81
1:B:120:ASP:CG	1:B:121:ASP:H	1.84	0.81
1:F:120:ASP:CG	1:F:121:ASP:H	1.84	0.81
1:F:513:GLY:HA3	1:F:639:LEU:HD23	1.62	0.81
1:C:513:GLY:HA3	1:C:639:LEU:HD23	1.62	0.81
1:F:26:LEU:HD21	1:F:100:ILE:HD11	1.56	0.81
1:A:125:GLY:HA3	1:A:159:ARG:NH1	1.94	0.81
1:F:127:THR:CG2	1:F:438:ASP:OD1	2.29	0.80
1:E:120:ASP:CG	1:E:121:ASP:H	1.84	0.80
1:D:120:ASP:CG	1:D:121:ASP:H	1.84	0.80
1:C:120:ASP:CG	1:C:121:ASP:H	1.84	0.80
1:C:127:THR:CG2	1:C:438:ASP:OD1	2.29	0.80
1:D:130:LEU:HD11	1:D:131:PHE:HE1	1.29	0.80
1:E:224:LEU:CD2	1:E:298:PRO:CB	2.58	0.80
1:C:26:LEU:CD1	1:C:102:ILE:HD12	2.03	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ASN:HB3	1:B:273:GLU:CB	2.12	0.80
1:E:130:LEU:HD11	1:E:131:PHE:HE1	1.29	0.80
1:C:126:ILE:HD11	1:C:130:LEU:HD23	1.61	0.79
1:B:126:ILE:HD11	1:B:130:LEU:HD23	1.61	0.79
1:E:270:ASN:HB3	1:E:273:GLU:CB	2.12	0.79
1:F:270:ASN:HB3	1:F:273:GLU:CB	2.12	0.79
1:A:26:LEU:HD21	1:A:100:ILE:HD11	1.56	0.79
1:E:127:THR:CB	1:E:438:ASP:CA	2.32	0.79
1:A:127:THR:CG2	1:A:438:ASP:OD1	2.29	0.79
1:F:24:ASN:O	1:F:25:ARG:CB	2.31	0.79
1:D:578:GLU:HG2	1:D:581:SER:HB3	1.65	0.79
1:A:24:ASN:O	1:A:25:ARG:CB	2.31	0.79
1:E:513:GLY:HA3	1:E:639:LEU:HD23	1.63	0.79
1:D:513:GLY:HA3	1:D:639:LEU:HD23	1.63	0.79
1:A:578:GLU:HG2	1:A:581:SER:HB3	1.65	0.79
1:D:270:ASN:HB3	1:D:273:GLU:CB	2.12	0.79
1:A:26:LEU:CD1	1:A:102:ILE:HD12	2.04	0.79
1:B:26:LEU:HD21	1:B:100:ILE:HD11	1.56	0.79
1:C:269:ILE:HG23	1:C:274:ILE:HD11	1.65	0.79
1:C:270:ASN:HB3	1:C:273:GLU:CB	2.12	0.79
1:B:269:ILE:HG23	1:B:274:ILE:HD11	1.65	0.78
1:F:267:PHE:O	1:F:268:LEU:CD1	2.26	0.78
1:B:269:ILE:HG23	1:B:274:ILE:HD13	1.65	0.78
1:E:26:LEU:HD21	1:E:100:ILE:HD11	1.56	0.78
1:C:269:ILE:HG23	1:C:274:ILE:HD13	1.65	0.78
1:A:270:ASN:HB3	1:A:273:GLU:CB	2.12	0.78
1:B:24:ASN:O	1:B:25:ARG:CB	2.31	0.78
1:E:24:ASN:O	1:E:25:ARG:CB	2.31	0.78
1:B:578:GLU:HG2	1:B:581:SER:HB3	1.65	0.78
1:C:224:LEU:CD2	1:C:298:PRO:CB	2.58	0.78
1:F:269:ILE:HG23	1:F:274:ILE:HD11	1.65	0.78
1:E:578:GLU:HG2	1:E:581:SER:HB3	1.65	0.78
1:C:578:GLU:HG2	1:C:581:SER:HB3	1.65	0.78
1:A:126:ILE:CG2	1:A:134:TYR:CE2	2.67	0.78
1:B:26:LEU:CD1	1:B:102:ILE:HD12	2.04	0.77
1:C:130:LEU:HD11	1:C:131:PHE:HE1	1.29	0.77
1:A:224:LEU:CD2	1:A:298:PRO:CB	2.58	0.77
1:E:269:ILE:HG23	1:E:274:ILE:HD11	1.65	0.77
1:A:469:VAL:HG21	1:A:565:LYS:HE3	1.66	0.77
1:C:24:ASN:O	1:C:25:ARG:CB	2.31	0.77
1:C:126:ILE:HD13	1:C:130:LEU:HB3	0.81	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:ILE:HG23	1:D:274:ILE:HD11	1.65	0.77
1:A:269:ILE:HG23	1:A:274:ILE:HD13	1.65	0.77
1:B:118:PRO:HD2	1:B:187:GLU:O	1.85	0.77
1:C:469:VAL:HG21	1:C:565:LYS:HE3	1.66	0.77
1:C:26:LEU:CD1	1:C:102:ILE:HD11	2.14	0.77
1:F:126:ILE:CG2	1:F:134:TYR:CE2	2.67	0.77
1:C:118:PRO:HD2	1:C:187:GLU:O	1.85	0.77
1:D:24:ASN:O	1:D:25:ARG:CB	2.31	0.77
1:B:126:ILE:HD11	1:B:130:LEU:HD22	1.67	0.77
1:E:126:ILE:CG2	1:E:134:TYR:CE2	2.67	0.77
1:D:269:ILE:HG23	1:D:274:ILE:HD13	1.65	0.77
1:D:126:ILE:HD13	1:D:130:LEU:HB3	0.81	0.77
1:A:513:GLY:HA3	1:A:639:LEU:CD2	2.15	0.77
1:F:578:GLU:HG2	1:F:581:SER:HB3	1.65	0.77
1:F:127:THR:CB	1:F:438:ASP:CA	2.32	0.77
1:F:469:VAL:HG21	1:F:565:LYS:HE3	1.66	0.77
1:A:118:PRO:HD2	1:A:187:GLU:O	1.85	0.77
1:C:126:ILE:HD11	1:C:130:LEU:HD22	1.67	0.77
1:C:476:TRP:HE1	1:C:534:GLU:CD	1.88	0.77
1:D:476:TRP:HE1	1:D:534:GLU:CD	1.88	0.77
1:E:513:GLY:HA3	1:E:639:LEU:CD2	2.15	0.77
1:D:513:GLY:HA3	1:D:639:LEU:CD2	2.15	0.77
1:D:753:ARG:O	1:D:757:MET:HB2	1.85	0.77
1:B:313:ARG:O	1:B:314:GLU:HB2	1.85	0.77
1:F:26:LEU:CD1	1:F:102:ILE:HD11	2.14	0.76
1:B:126:ILE:CG2	1:B:134:TYR:CE2	2.67	0.76
1:A:126:ILE:HD11	1:A:130:LEU:HD22	1.67	0.76
1:B:224:LEU:CD2	1:B:298:PRO:CB	2.58	0.76
1:A:753:ARG:O	1:A:757:MET:HB2	1.86	0.76
1:B:469:VAL:HG21	1:B:565:LYS:HE3	1.66	0.76
1:C:126:ILE:CG2	1:C:134:TYR:CE2	2.67	0.76
1:B:126:ILE:HD13	1:B:130:LEU:HB3	0.81	0.76
1:F:126:ILE:HD13	1:F:130:LEU:HB3	0.81	0.76
1:A:267:PHE:O	1:A:268:LEU:CD1	2.26	0.76
1:F:224:LEU:CD2	1:F:298:PRO:CB	2.58	0.76
1:B:476:TRP:HE1	1:B:534:GLU:CD	1.88	0.76
1:F:513:GLY:HA3	1:F:639:LEU:CD2	2.14	0.76
1:D:118:PRO:HD2	1:D:187:GLU:O	1.85	0.76
1:F:126:ILE:CD1	1:F:130:LEU:HD23	2.16	0.76
1:E:269:ILE:HG23	1:E:274:ILE:HD13	1.65	0.76
1:C:313:ARG:O	1:C:314:GLU:HB2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:LEU:HD21	1:C:100:ILE:HD11	1.56	0.76
1:D:26:LEU:CD1	1:D:102:ILE:HD11	2.14	0.76
1:D:126:ILE:CD1	1:D:130:LEU:HD23	2.16	0.76
1:D:126:ILE:CG2	1:D:134:TYR:CE2	2.67	0.76
1:A:127:THR:HB	1:A:438:ASP:HA	0.76	0.76
1:F:402:GLU:HG3	1:F:456:LEU:HD21	1.68	0.76
1:E:26:LEU:CD1	1:E:102:ILE:HD11	2.14	0.76
1:B:127:THR:HB	1:B:438:ASP:HA	0.76	0.76
1:E:753:ARG:O	1:E:757:MET:HB2	1.86	0.76
1:C:126:ILE:CD1	1:C:130:LEU:HD23	2.16	0.76
1:F:269:ILE:HG23	1:F:274:ILE:HD13	1.65	0.76
1:F:118:PRO:HD2	1:F:187:GLU:O	1.85	0.76
1:E:118:PRO:HD2	1:E:187:GLU:O	1.85	0.76
1:D:313:ARG:O	1:D:314:GLU:HB2	1.85	0.76
1:D:224:LEU:CD2	1:D:298:PRO:CB	2.58	0.76
1:A:567:ARG:NH1	1:A:568:GLN:NE2	2.34	0.76
1:F:753:ARG:O	1:F:757:MET:HB2	1.86	0.76
1:E:126:ILE:CD1	1:E:130:LEU:HD23	2.16	0.76
1:B:753:ARG:O	1:B:757:MET:HB2	1.85	0.76
1:F:126:ILE:HD11	1:F:130:LEU:HD22	1.67	0.75
1:A:126:ILE:CD1	1:A:130:LEU:HD23	2.16	0.75
1:E:267:PHE:O	1:E:268:LEU:CD1	2.26	0.75
1:C:513:GLY:HA3	1:C:639:LEU:CD2	2.14	0.75
1:D:26:LEU:HD21	1:D:100:ILE:HD11	1.56	0.75
1:C:127:THR:HB	1:C:438:ASP:HA	0.76	0.75
1:C:753:ARG:O	1:C:757:MET:HB2	1.86	0.75
1:A:269:ILE:HG23	1:A:274:ILE:HD11	1.65	0.75
1:F:476:TRP:HE1	1:F:534:GLU:CD	1.88	0.75
1:F:26:LEU:CD1	1:F:102:ILE:HD12	2.04	0.75
1:D:126:ILE:HD11	1:D:130:LEU:HD22	1.67	0.75
1:F:461:PRO:CA	1:F:462:SER:HB3	2.14	0.75
1:D:567:ARG:NH1	1:D:568:GLN:NE2	2.34	0.75
1:B:513:GLY:HA3	1:B:639:LEU:CD2	2.15	0.75
1:D:469:VAL:HG21	1:D:565:LYS:HE3	1.66	0.75
1:E:476:TRP:HE1	1:E:534:GLU:CD	1.88	0.75
1:B:26:LEU:CD1	1:B:102:ILE:HD11	2.14	0.75
1:B:402:GLU:HG3	1:B:456:LEU:HD21	1.67	0.75
1:E:266:PHE:CE2	1:E:268:LEU:CD1	2.70	0.75
1:D:267:PHE:CE2	1:D:289:ALA:HB1	2.21	0.75
1:A:571:PRO:CA	1:A:616:ASN:HB3	2.17	0.75
1:F:571:PRO:CA	1:F:616:ASN:HB3	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:571:PRO:CA	1:E:616:ASN:HB3	2.17	0.75
1:A:476:TRP:HE1	1:A:534:GLU:CD	1.88	0.75
1:E:126:ILE:HD13	1:E:130:LEU:HB3	0.81	0.75
1:C:567:ARG:NH1	1:C:568:GLN:NE2	2.34	0.75
1:F:313:ARG:O	1:F:314:GLU:HB2	1.85	0.74
1:E:469:VAL:HG21	1:E:565:LYS:HE3	1.66	0.74
1:A:21:ASN:N	1:A:23:PRO:HD3	2.02	0.74
1:D:605:LEU:HD21	1:D:633:ILE:HD13	1.69	0.74
1:B:126:ILE:CD1	1:B:130:LEU:HD23	2.16	0.74
1:C:605:LEU:HD21	1:C:633:ILE:HD13	1.69	0.74
1:E:126:ILE:HD11	1:E:130:LEU:HD22	1.67	0.74
1:D:122:THR:OG1	1:D:161:VAL:HG23	1.88	0.74
1:B:571:PRO:CA	1:B:616:ASN:HB3	2.17	0.74
1:E:313:ARG:O	1:E:314:GLU:HB2	1.85	0.74
1:E:402:GLU:HG3	1:E:456:LEU:HD21	1.68	0.74
1:E:21:ASN:N	1:E:23:PRO:HD3	2.03	0.74
1:D:21:ASN:N	1:D:23:PRO:HD3	2.02	0.74
1:A:313:ARG:O	1:A:314:GLU:HB2	1.85	0.74
1:A:605:LEU:HD21	1:A:633:ILE:HD13	1.69	0.74
1:D:266:PHE:CE2	1:D:268:LEU:CD1	2.70	0.74
1:F:122:THR:OG1	1:F:161:VAL:HG23	1.88	0.74
1:C:123:VAL:HG22	1:C:124:GLU:H	1.53	0.74
1:A:461:PRO:CA	1:A:462:SER:HB3	2.14	0.74
1:F:567:ARG:NH1	1:F:568:GLN:NE2	2.34	0.74
1:C:127:THR:CB	1:C:438:ASP:CA	2.32	0.74
1:D:127:THR:HB	1:D:438:ASP:HA	0.76	0.74
1:E:461:PRO:CA	1:E:462:SER:HB3	2.14	0.74
1:B:567:ARG:NH1	1:B:568:GLN:NE2	2.34	0.74
1:E:421:GLN:HG2	1:E:451:ASP:OD1	1.88	0.74
1:A:26:LEU:CD1	1:A:102:ILE:HD11	2.14	0.74
1:D:571:PRO:CA	1:D:616:ASN:HB3	2.17	0.74
1:F:21:ASN:N	1:F:23:PRO:HD3	2.02	0.74
1:A:402:GLU:HG3	1:A:456:LEU:HD21	1.67	0.74
1:A:266:PHE:CE2	1:A:268:LEU:CD1	2.70	0.74
1:E:246:PRO:HG3	1:E:466:GLU:OE1	1.88	0.74
1:F:246:PRO:HG3	1:F:466:GLU:OE1	1.88	0.74
1:B:21:ASN:N	1:B:23:PRO:HD3	2.02	0.74
1:D:126:ILE:CD1	1:D:130:LEU:CB	2.53	0.74
1:E:122:THR:OG1	1:E:161:VAL:HG23	1.88	0.74
1:A:246:PRO:HG3	1:A:466:GLU:OE1	1.88	0.74
1:D:127:THR:CB	1:D:438:ASP:CA	2.32	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ASN:N	1:C:23:PRO:HD3	2.02	0.73
1:B:127:THR:CB	1:B:438:ASP:CA	2.32	0.73
1:E:267:PHE:CE2	1:E:289:ALA:HB1	2.21	0.73
1:B:266:PHE:CE2	1:B:268:LEU:CD1	2.70	0.73
1:D:123:VAL:HG22	1:D:124:GLU:H	1.53	0.73
1:B:123:VAL:HG22	1:B:124:GLU:H	1.53	0.73
1:D:66:GLU:O	1:D:147:ARG:NH1	2.21	0.73
1:B:605:LEU:HD21	1:B:633:ILE:HD13	1.69	0.73
1:B:246:PRO:HG3	1:B:466:GLU:OE1	1.88	0.73
1:C:266:PHE:CE2	1:C:268:LEU:CD1	2.70	0.73
1:C:267:PHE:CE2	1:C:289:ALA:HB1	2.21	0.73
1:F:123:VAL:HG22	1:F:124:GLU:H	1.53	0.73
1:C:571:PRO:CA	1:C:616:ASN:HB3	2.17	0.73
1:A:26:LEU:CD2	1:A:100:ILE:CG1	2.57	0.73
1:F:127:THR:HB	1:F:438:ASP:HA	0.76	0.73
1:B:267:PHE:O	1:B:268:LEU:CD1	2.26	0.73
1:D:246:PRO:HG3	1:D:466:GLU:OE1	1.88	0.73
1:F:267:PHE:CE2	1:F:289:ALA:HB1	2.21	0.73
1:C:402:GLU:HG3	1:C:456:LEU:HD21	1.68	0.73
1:B:615:LYS:O	1:B:616:ASN:HB2	1.89	0.73
1:C:126:ILE:CD1	1:C:130:LEU:CB	2.53	0.73
1:E:127:THR:HB	1:E:438:ASP:HA	0.76	0.73
1:D:267:PHE:O	1:D:268:LEU:CD1	2.26	0.73
1:A:123:VAL:HG22	1:A:124:GLU:H	1.53	0.73
1:C:246:PRO:HG3	1:C:466:GLU:OE1	1.88	0.73
1:F:605:LEU:HD21	1:F:633:ILE:HD13	1.69	0.73
1:B:421:GLN:HG2	1:B:451:ASP:OD1	1.88	0.73
1:E:476:TRP:NE1	1:E:534:GLU:OE1	2.22	0.73
1:C:476:TRP:NE1	1:C:534:GLU:OE1	2.22	0.73
1:A:421:GLN:HG2	1:A:451:ASP:OD1	1.88	0.73
1:F:66:GLU:O	1:F:147:ARG:NH1	2.21	0.73
1:C:122:THR:OG1	1:C:161:VAL:HG23	1.88	0.73
1:C:66:GLU:O	1:C:147:ARG:NH1	2.21	0.73
1:B:122:THR:OG1	1:B:161:VAL:HG23	1.88	0.73
1:A:66:GLU:O	1:A:147:ARG:NH1	2.21	0.73
1:B:66:GLU:O	1:B:147:ARG:NH1	2.21	0.73
1:D:267:PHE:HE2	1:D:289:ALA:CB	2.02	0.73
1:D:615:LYS:O	1:D:616:ASN:HB2	1.89	0.73
1:F:476:TRP:NE1	1:F:534:GLU:OE1	2.22	0.73
1:E:267:PHE:HE2	1:E:289:ALA:CB	2.02	0.72
1:D:402:GLU:HG3	1:D:456:LEU:HD21	1.67	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:421:GLN:HG2	1:F:451:ASP:OD1	1.88	0.72
1:C:421:GLN:HG2	1:C:451:ASP:OD1	1.88	0.72
1:A:127:THR:CB	1:A:438:ASP:CA	2.32	0.72
1:A:647:LEU:CD1	1:A:752:ILE:HD11	2.20	0.72
1:D:476:TRP:NE1	1:D:534:GLU:OE1	2.22	0.72
1:C:647:LEU:CD1	1:C:752:ILE:HD11	2.20	0.72
1:B:647:LEU:CD1	1:B:752:ILE:HD11	2.20	0.72
1:E:756:GLU:O	1:E:760:GLN:N	2.22	0.72
1:A:122:THR:OG1	1:A:161:VAL:HG23	1.88	0.72
1:E:66:GLU:O	1:E:147:ARG:NH1	2.21	0.72
1:D:421:GLN:HG2	1:D:451:ASP:OD1	1.88	0.72
1:E:123:VAL:HG22	1:E:124:GLU:H	1.53	0.72
1:D:461:PRO:CA	1:D:462:SER:HB3	2.14	0.72
1:C:615:LYS:O	1:C:616:ASN:HB2	1.89	0.72
1:C:756:GLU:O	1:C:760:GLN:N	2.22	0.72
1:E:605:LEU:HD21	1:E:633:ILE:HD13	1.69	0.72
1:A:126:ILE:HD13	1:A:130:LEU:HB3	0.81	0.72
1:C:267:PHE:HE2	1:C:289:ALA:CB	2.02	0.72
1:A:476:TRP:NE1	1:A:534:GLU:OE1	2.22	0.72
1:F:206:ILE:HD13	1:F:254:ILE:HD13	1.72	0.72
1:D:647:LEU:CD1	1:D:752:ILE:HD11	2.20	0.72
1:D:89:ARG:HG3	1:D:94:VAL:HG13	1.71	0.72
1:C:206:ILE:HD13	1:C:254:ILE:HD13	1.72	0.72
1:E:126:ILE:CD1	1:E:130:LEU:CB	2.53	0.72
1:C:267:PHE:O	1:C:268:LEU:CD1	2.26	0.72
1:F:307:ASP:O	1:F:311:PRO:CB	2.38	0.72
1:F:26:LEU:HD13	1:F:102:ILE:HD11	1.62	0.71
1:D:26:LEU:CD2	1:D:100:ILE:CG1	2.57	0.71
1:F:267:PHE:HE2	1:F:289:ALA:CB	2.02	0.71
1:E:406:HIS:CE1	1:E:461:PRO:HD3	2.25	0.71
1:F:615:LYS:O	1:F:616:ASN:HB2	1.89	0.71
1:B:476:TRP:NE1	1:B:534:GLU:OE1	2.22	0.71
1:B:270:ASN:HB3	1:B:273:GLU:HB3	1.72	0.71
1:A:89:ARG:HG3	1:A:94:VAL:HG13	1.71	0.71
1:B:89:ARG:HG3	1:B:94:VAL:HG13	1.71	0.71
1:E:307:ASP:O	1:E:311:PRO:CB	2.38	0.71
1:D:206:ILE:HD13	1:D:254:ILE:HD13	1.72	0.71
1:F:266:PHE:CE2	1:F:268:LEU:CD1	2.70	0.71
1:A:406:HIS:CE1	1:A:461:PRO:HD3	2.25	0.71
1:A:267:PHE:CE2	1:A:289:ALA:HB1	2.21	0.71
1:B:461:PRO:CA	1:B:462:SER:HB3	2.14	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:406:HIS:CE1	1:F:461:PRO:HD3	2.25	0.71
1:B:406:HIS:CE1	1:B:461:PRO:HD3	2.25	0.71
1:E:567:ARG:NH1	1:E:568:GLN:NE2	2.34	0.71
1:F:89:ARG:HG3	1:F:94:VAL:HG13	1.71	0.71
1:A:756:GLU:O	1:A:760:GLN:N	2.22	0.71
1:C:26:LEU:HD22	1:C:102:ILE:CD1	2.21	0.71
1:B:267:PHE:CE2	1:B:289:ALA:HB1	2.21	0.71
1:B:267:PHE:HE2	1:B:289:ALA:CB	2.02	0.71
1:A:267:PHE:HE2	1:A:289:ALA:CB	2.02	0.71
1:D:406:HIS:CE1	1:D:461:PRO:HD3	2.25	0.71
1:A:615:LYS:O	1:A:616:ASN:HB2	1.89	0.71
1:A:405:GLY:O	1:A:462:SER:O	2.09	0.71
1:C:312:LYS:HD2	1:C:316:THR:CG2	2.21	0.71
1:D:312:LYS:HD2	1:D:316:THR:CG2	2.21	0.71
1:B:405:GLY:O	1:B:462:SER:O	2.09	0.71
1:A:206:ILE:HD13	1:A:254:ILE:HD13	1.72	0.71
1:F:126:ILE:CD1	1:F:130:LEU:CB	2.53	0.71
1:B:312:LYS:HD2	1:B:316:THR:CG2	2.21	0.71
1:D:560:ARG:N	1:D:607:GLU:OE2	2.24	0.71
1:E:270:ASN:HB3	1:E:273:GLU:HB3	1.72	0.71
1:B:206:ILE:HD13	1:B:254:ILE:HD13	1.72	0.71
1:B:26:LEU:HD22	1:B:102:ILE:CD1	2.20	0.71
1:D:26:LEU:HD22	1:D:102:ILE:CD1	2.21	0.71
1:C:405:GLY:O	1:C:462:SER:O	2.09	0.70
1:E:647:LEU:CD1	1:E:752:ILE:HD11	2.20	0.70
1:C:270:ASN:HB3	1:C:273:GLU:HB3	1.72	0.70
1:E:206:ILE:HD13	1:E:254:ILE:HD13	1.72	0.70
1:B:126:ILE:CD1	1:B:130:LEU:CB	2.53	0.70
1:F:405:GLY:O	1:F:462:SER:O	2.09	0.70
1:A:312:LYS:HD2	1:A:316:THR:CG2	2.21	0.70
1:D:307:ASP:O	1:D:311:PRO:CB	2.38	0.70
1:D:476:TRP:HZ2	1:D:534:GLU:OE1	1.74	0.70
1:A:270:ASN:HB3	1:A:273:GLU:HB3	1.72	0.70
1:E:615:LYS:O	1:E:616:ASN:HB2	1.89	0.70
1:F:270:ASN:HB3	1:F:273:GLU:HB3	1.72	0.70
1:C:680:ASN:OD1	1:C:681:GLY:N	2.25	0.70
1:D:27:ILE:H	1:D:82:ILE:HD13	1.56	0.70
1:D:680:ASN:OD1	1:D:681:GLY:N	2.25	0.70
1:C:560:ARG:N	1:C:607:GLU:OE2	2.24	0.70
1:A:307:ASP:O	1:A:311:PRO:CB	2.38	0.70
1:B:680:ASN:OD1	1:B:681:GLY:N	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:ILE:H	1:F:82:ILE:HD13	1.56	0.70
1:C:89:ARG:HG3	1:C:94:VAL:HG13	1.71	0.70
1:C:461:PRO:CA	1:C:462:SER:HB3	2.14	0.70
1:E:312:LYS:HD2	1:E:316:THR:CG2	2.21	0.70
1:B:27:ILE:H	1:B:82:ILE:HD13	1.57	0.70
1:E:27:ILE:H	1:E:82:ILE:HD13	1.56	0.70
1:C:26:LEU:CD2	1:C:100:ILE:CG1	2.57	0.70
1:F:560:ARG:N	1:F:607:GLU:OE2	2.24	0.70
1:B:26:LEU:CD2	1:B:100:ILE:CG1	2.57	0.70
1:E:26:LEU:HD22	1:E:102:ILE:CD1	2.20	0.70
1:D:270:ASN:HB3	1:D:273:GLU:HB3	1.72	0.70
1:E:26:LEU:CD2	1:E:100:ILE:CG1	2.57	0.70
1:C:406:HIS:NE2	1:C:461:PRO:HG3	2.07	0.70
1:A:754:LYS:HD3	1:A:757:MET:CE	2.22	0.70
1:F:754:LYS:HD3	1:F:757:MET:CE	2.22	0.70
1:C:27:ILE:H	1:C:82:ILE:HD13	1.57	0.70
1:B:754:LYS:HD3	1:B:757:MET:CE	2.22	0.70
1:C:406:HIS:CE1	1:C:461:PRO:HD3	2.25	0.70
1:B:22:ARG:N	1:B:23:PRO:HD3	2.07	0.70
1:E:680:ASN:OD1	1:E:681:GLY:N	2.25	0.70
1:A:650:GLU:HA	1:A:653:ARG:HB2	1.74	0.70
1:A:680:ASN:OD1	1:A:681:GLY:N	2.25	0.70
1:A:26:LEU:HD22	1:A:102:ILE:CD1	2.20	0.69
1:D:405:GLY:O	1:D:462:SER:O	2.09	0.69
1:F:406:HIS:NE2	1:F:461:PRO:HG3	2.07	0.69
1:B:307:ASP:O	1:B:311:PRO:CB	2.38	0.69
1:E:476:TRP:HZ2	1:E:534:GLU:OE1	1.74	0.69
1:E:89:ARG:HG3	1:E:94:VAL:HG13	1.71	0.69
1:D:406:HIS:NE2	1:D:461:PRO:HG3	2.07	0.69
1:E:405:GLY:O	1:E:462:SER:O	2.09	0.69
1:A:406:HIS:NE2	1:A:461:PRO:HG3	2.07	0.69
1:B:313:ARG:HH21	1:B:352:SER:HA	1.57	0.69
1:D:22:ARG:N	1:D:23:PRO:HD3	2.07	0.69
1:E:560:ARG:N	1:E:607:GLU:OE2	2.24	0.69
1:F:647:LEU:CD1	1:F:752:ILE:HD11	2.20	0.69
1:A:22:ARG:N	1:A:23:PRO:HD3	2.07	0.69
1:D:517:TYR:CZ	1:D:644:TYR:HB2	2.28	0.69
1:A:27:ILE:H	1:A:82:ILE:HD13	1.56	0.69
1:F:26:LEU:HD22	1:F:102:ILE:CD1	2.20	0.69
1:F:312:LYS:HD2	1:F:316:THR:CG2	2.21	0.69
1:B:560:ARG:N	1:B:607:GLU:OE2	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:ASP:O	1:C:311:PRO:CB	2.38	0.69
1:C:754:LYS:HD3	1:C:757:MET:CE	2.22	0.69
1:E:406:HIS:NE2	1:E:461:PRO:HG3	2.07	0.69
1:D:756:GLU:O	1:D:760:GLN:N	2.22	0.69
1:F:650:GLU:HA	1:F:653:ARG:HB2	1.74	0.69
1:F:680:ASN:OD1	1:F:681:GLY:N	2.25	0.69
1:E:517:TYR:CZ	1:E:644:TYR:HB2	2.28	0.69
1:A:560:ARG:N	1:A:607:GLU:OE2	2.24	0.69
1:C:313:ARG:HH21	1:C:352:SER:HA	1.57	0.69
1:E:754:LYS:HD3	1:E:757:MET:CE	2.22	0.69
1:D:313:ARG:HH21	1:D:352:SER:HA	1.57	0.69
1:F:756:GLU:O	1:F:760:GLN:N	2.22	0.69
1:C:22:ARG:N	1:C:23:PRO:HD3	2.07	0.69
1:B:650:GLU:HA	1:B:653:ARG:HB2	1.74	0.69
1:C:517:TYR:CZ	1:C:644:TYR:HB2	2.28	0.69
1:D:126:ILE:HG21	1:D:134:TYR:CE2	2.28	0.69
1:B:126:ILE:HG21	1:B:134:TYR:CE2	2.28	0.69
1:A:126:ILE:CD1	1:A:130:LEU:CB	2.53	0.69
1:B:406:HIS:NE2	1:B:461:PRO:HG3	2.07	0.69
1:F:612:SER:O	1:F:613:THR:OG1	2.09	0.69
1:F:476:TRP:HZ2	1:F:534:GLU:OE1	1.74	0.69
1:F:28:VAL:HG21	1:F:94:VAL:HG21	1.75	0.69
1:E:650:GLU:HA	1:E:653:ARG:HB2	1.75	0.69
1:A:42:SER:HB2	1:A:44:PRO:HD2	1.75	0.69
1:B:42:SER:HB2	1:B:44:PRO:HD2	1.75	0.69
1:E:126:ILE:HG21	1:E:134:TYR:CE2	2.28	0.69
1:A:127:THR:N	1:A:439:ALA:H	1.88	0.69
1:E:28:VAL:HG21	1:E:94:VAL:HG21	1.75	0.69
1:B:517:TYR:CZ	1:B:644:TYR:HB2	2.28	0.69
1:B:127:THR:N	1:B:439:ALA:H	1.88	0.68
1:A:126:ILE:HG21	1:A:134:TYR:CE2	2.28	0.68
1:E:313:ARG:HH21	1:E:352:SER:HA	1.57	0.68
1:F:22:ARG:N	1:F:23:PRO:HD3	2.07	0.68
1:F:126:ILE:HG21	1:F:134:TYR:CE2	2.28	0.68
1:F:313:ARG:HH21	1:F:352:SER:HA	1.57	0.68
1:C:650:GLU:HA	1:C:653:ARG:HB2	1.74	0.68
1:F:42:SER:HB2	1:F:44:PRO:HD2	1.75	0.68
1:F:517:TYR:CZ	1:F:644:TYR:HB2	2.28	0.68
1:B:612:SER:O	1:B:613:THR:OG1	2.09	0.68
1:C:612:SER:O	1:C:613:THR:OG1	2.09	0.68
1:A:28:VAL:HG21	1:A:94:VAL:HG21	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ARG:HH21	1:A:352:SER:HA	1.57	0.68
1:E:22:ARG:N	1:E:23:PRO:HD3	2.07	0.68
1:D:28:VAL:HG21	1:D:94:VAL:HG21	1.75	0.68
1:C:42:SER:HB2	1:C:44:PRO:HD2	1.75	0.68
1:C:126:ILE:HG21	1:C:134:TYR:CE2	2.28	0.68
1:E:612:SER:O	1:E:613:THR:OG1	2.09	0.68
1:D:650:GLU:HA	1:D:653:ARG:HB2	1.74	0.68
1:B:756:GLU:O	1:B:760:GLN:N	2.22	0.68
1:E:60:LYS:HB3	1:E:101:SER:O	1.94	0.68
1:C:127:THR:N	1:C:439:ALA:H	1.88	0.68
1:D:754:LYS:HD3	1:D:757:MET:CE	2.22	0.68
1:A:60:LYS:HB3	1:A:101:SER:O	1.94	0.68
1:A:476:TRP:HZ2	1:A:534:GLU:OE1	1.74	0.68
1:C:477:GLU:HB2	1:C:662:ARG:HH12	1.59	0.68
1:B:60:LYS:HB3	1:B:101:SER:O	1.94	0.68
1:D:60:LYS:HB3	1:D:101:SER:O	1.94	0.68
1:D:543:LYS:HA	1:D:577:ASP:HB2	1.76	0.68
1:F:60:LYS:HB3	1:F:101:SER:O	1.94	0.67
1:A:270:ASN:HB3	1:A:273:GLU:HB2	1.76	0.67
1:B:28:VAL:HG21	1:B:94:VAL:HG21	1.75	0.67
1:C:28:VAL:HG21	1:C:94:VAL:HG21	1.75	0.67
1:D:42:SER:HB2	1:D:44:PRO:HD2	1.75	0.67
1:C:60:LYS:HB3	1:C:101:SER:O	1.94	0.67
1:A:517:TYR:CZ	1:A:644:TYR:HB2	2.28	0.67
1:E:526:LEU:HD11	2:E:900:ADP:H2'	1.77	0.67
1:C:476:TRP:CE2	1:C:534:GLU:OE1	2.47	0.67
1:B:476:TRP:HZ2	1:B:534:GLU:OE1	1.74	0.67
1:F:270:ASN:HB3	1:F:273:GLU:HB2	1.76	0.67
1:D:477:GLU:HB2	1:D:662:ARG:HH12	1.59	0.67
1:C:526:LEU:HD11	2:C:900:ADP:H2'	1.77	0.67
1:E:543:LYS:HA	1:E:577:ASP:HB2	1.76	0.67
1:D:526:LEU:HD11	2:D:900:ADP:H2'	1.77	0.67
1:B:543:LYS:HA	1:B:577:ASP:HB2	1.76	0.67
1:A:476:TRP:CE2	1:A:534:GLU:OE1	2.47	0.67
1:F:476:TRP:CE2	1:F:534:GLU:OE1	2.47	0.67
1:B:270:ASN:HB3	1:B:273:GLU:HB2	1.76	0.67
1:E:42:SER:HB2	1:E:44:PRO:HD2	1.75	0.67
1:F:127:THR:N	1:F:439:ALA:H	1.88	0.67
1:B:526:LEU:HD11	2:B:900:ADP:H2'	1.77	0.67
1:C:476:TRP:HZ2	1:C:534:GLU:OE1	1.74	0.67
1:F:526:LEU:HD11	2:F:900:ADP:H2'	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:543:LYS:HA	1:F:577:ASP:HB2	1.76	0.67
1:D:476:TRP:CE2	1:D:534:GLU:OE1	2.47	0.66
1:D:24:ASN:O	1:D:25:ARG:HB2	1.95	0.66
1:A:543:LYS:HA	1:A:577:ASP:HB2	1.76	0.66
1:E:476:TRP:CE2	1:E:534:GLU:OE1	2.47	0.66
1:E:270:ASN:HB3	1:E:273:GLU:HB2	1.76	0.66
1:A:526:LEU:HD11	2:A:900:ADP:H2'	1.77	0.66
1:E:127:THR:N	1:E:439:ALA:H	1.88	0.66
1:B:476:TRP:CE2	1:B:534:GLU:OE1	2.47	0.66
1:E:24:ASN:O	1:E:25:ARG:HB2	1.95	0.66
1:C:543:LYS:HA	1:C:577:ASP:HB2	1.76	0.66
1:F:477:GLU:HB2	1:F:662:ARG:HH12	1.59	0.66
1:F:26:LEU:CD2	1:F:100:ILE:CG1	2.57	0.66
1:D:127:THR:N	1:D:439:ALA:H	1.88	0.66
1:B:754:LYS:HA	1:B:757:MET:HE3	1.76	0.66
1:D:612:SER:O	1:D:613:THR:OG1	2.09	0.66
1:E:255:ALA:HB1	1:E:266:PHE:HE1	1.61	0.66
1:A:465:ARG:HH12	1:F:607:GLU:HG2	1.61	0.66
1:A:510:PRO:HG3	1:A:614:LYS:HE3	1.77	0.66
1:A:477:GLU:HB2	1:A:662:ARG:HH12	1.59	0.66
1:B:477:GLU:HB2	1:B:662:ARG:HH12	1.59	0.66
1:D:255:ALA:HB1	1:D:266:PHE:HE1	1.61	0.65
1:E:140:LEU:HG	1:E:141:GLU:OE1	1.97	0.65
1:B:459:SER:O	1:B:460:ASN:CG	2.35	0.65
1:B:607:GLU:HG2	1:C:465:ARG:HH12	1.61	0.65
1:C:210:ARG:CG	1:C:212:GLN:HG2	2.27	0.65
1:C:754:LYS:HA	1:C:757:MET:HE3	1.77	0.65
1:F:510:PRO:HG3	1:F:614:LYS:HE3	1.77	0.65
1:D:140:LEU:HG	1:D:141:GLU:OE1	1.96	0.65
1:F:459:SER:O	1:F:460:ASN:CG	2.35	0.65
1:C:24:ASN:O	1:C:25:ARG:HB2	1.95	0.65
1:D:459:SER:O	1:D:460:ASN:CG	2.35	0.65
1:D:236:LYS:HZ1	1:D:239:ARG:HG3	1.62	0.65
1:C:510:PRO:HG3	1:C:614:LYS:HE3	1.77	0.65
1:B:127:THR:CG2	1:B:438:ASP:CG	2.65	0.65
1:E:560:ARG:CG	1:E:607:GLU:OE2	2.45	0.65
1:D:560:ARG:CG	1:D:607:GLU:OE2	2.45	0.65
1:B:210:ARG:CG	1:B:212:GLN:HG2	2.27	0.65
1:A:140:LEU:HG	1:A:141:GLU:OE1	1.96	0.65
1:E:477:GLU:HB2	1:E:662:ARG:HH12	1.59	0.65
1:C:127:THR:CG2	1:C:438:ASP:CG	2.65	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:THR:CG2	1:E:438:ASP:CG	2.65	0.65
1:F:24:ASN:O	1:F:25:ARG:HB2	1.95	0.65
1:D:270:ASN:HB3	1:D:273:GLU:HB2	1.76	0.65
1:C:140:LEU:HG	1:C:141:GLU:OE1	1.97	0.65
1:D:127:THR:CG2	1:D:438:ASP:CG	2.65	0.65
1:A:612:SER:O	1:A:613:THR:OG1	2.09	0.65
1:C:406:HIS:CE1	1:C:459:SER:HB3	2.29	0.65
1:E:607:GLU:HG2	1:F:465:ARG:HH12	1.61	0.65
1:F:560:ARG:CG	1:F:607:GLU:OE2	2.45	0.65
1:C:270:ASN:HB3	1:C:273:GLU:HB2	1.76	0.65
1:F:140:LEU:HG	1:F:141:GLU:OE1	1.97	0.65
1:A:127:THR:CG2	1:A:438:ASP:CG	2.65	0.65
1:A:560:ARG:CG	1:A:607:GLU:OE2	2.45	0.65
1:E:510:PRO:HG3	1:E:614:LYS:HE3	1.77	0.65
1:F:127:THR:CG2	1:F:438:ASP:CG	2.65	0.65
1:F:255:ALA:HB1	1:F:266:PHE:HE1	1.61	0.65
1:C:459:SER:O	1:C:460:ASN:CG	2.35	0.65
1:A:607:GLU:HG2	1:B:465:ARG:HH12	1.61	0.65
1:E:210:ARG:CG	1:E:212:GLN:HG2	2.27	0.65
1:B:140:LEU:HG	1:B:141:GLU:OE1	1.96	0.64
1:C:255:ALA:HB1	1:C:266:PHE:HE1	1.61	0.64
1:F:210:ARG:CG	1:F:212:GLN:HG2	2.27	0.64
1:E:459:SER:O	1:E:460:ASN:CG	2.35	0.64
1:A:24:ASN:O	1:A:25:ARG:HB2	1.95	0.64
1:D:510:PRO:HG3	1:D:614:LYS:HE3	1.77	0.64
1:B:510:PRO:HG3	1:B:614:LYS:HE3	1.77	0.64
1:A:459:SER:O	1:A:460:ASN:CG	2.35	0.64
1:E:312:LYS:HD2	1:E:316:THR:CB	2.28	0.64
1:D:312:LYS:HD2	1:D:316:THR:CB	2.28	0.64
1:B:24:ASN:O	1:B:25:ARG:HB2	1.95	0.64
1:B:269:ILE:CG2	1:B:274:ILE:HD13	2.28	0.64
1:B:560:ARG:CG	1:B:607:GLU:OE2	2.45	0.64
1:A:754:LYS:HA	1:A:757:MET:HE3	1.79	0.64
1:E:754:LYS:HA	1:E:757:MET:HE3	1.80	0.64
1:A:505:LYS:NZ	1:B:730:GLU:OE2	2.29	0.64
1:B:269:ILE:HD11	1:B:290:PHE:HE1	1.63	0.64
1:D:269:ILE:HD11	1:D:290:PHE:HE1	1.63	0.64
1:E:269:ILE:HD11	1:E:290:PHE:HE1	1.63	0.64
1:F:312:LYS:HD2	1:F:316:THR:CB	2.28	0.64
1:E:269:ILE:CG2	1:E:274:ILE:HD13	2.28	0.64
1:C:269:ILE:HD11	1:C:290:PHE:HE1	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:ALA:HB1	1:B:266:PHE:HE1	1.61	0.64
1:A:269:ILE:HD11	1:A:290:PHE:HE1	1.63	0.64
1:C:560:ARG:CG	1:C:607:GLU:OE2	2.45	0.64
1:F:269:ILE:CG2	1:F:274:ILE:HD13	2.28	0.64
1:F:269:ILE:HD11	1:F:290:PHE:HE1	1.63	0.63
1:C:312:LYS:HD2	1:C:316:THR:CB	2.28	0.63
1:D:210:ARG:CG	1:D:212:GLN:HG2	2.27	0.63
1:D:269:ILE:CG2	1:D:274:ILE:HD13	2.28	0.63
1:A:255:ALA:HB1	1:A:266:PHE:HE1	1.61	0.63
1:B:312:LYS:HD2	1:B:316:THR:CB	2.28	0.63
1:B:505:LYS:NZ	1:C:730:GLU:OE2	2.30	0.63
1:A:269:ILE:CG2	1:A:274:ILE:HD13	2.28	0.63
1:B:403:THR:HG22	1:B:406:HIS:HB2	1.80	0.63
1:C:607:GLU:HG2	1:D:465:ARG:HH12	1.61	0.63
1:A:210:ARG:CG	1:A:212:GLN:HG2	2.27	0.63
1:C:269:ILE:CG2	1:C:274:ILE:HD13	2.28	0.63
1:D:406:HIS:CE1	1:D:459:SER:HB3	2.29	0.63
1:D:607:GLU:HG2	1:E:465:ARG:HH12	1.62	0.63
1:D:754:LYS:HA	1:D:757:MET:HE3	1.79	0.63
1:A:403:THR:HG22	1:A:406:HIS:HB2	1.80	0.63
1:C:403:THR:HG22	1:C:406:HIS:HB2	1.80	0.63
1:B:269:ILE:CD1	1:B:290:PHE:HE1	2.12	0.63
1:A:406:HIS:CE1	1:A:459:SER:CB	2.79	0.63
1:E:269:ILE:CD1	1:E:290:PHE:HE1	2.12	0.63
1:A:269:ILE:CD1	1:A:290:PHE:HE1	2.12	0.62
1:A:120:ASP:CG	1:A:121:ASP:N	2.53	0.62
1:A:312:LYS:HD2	1:A:316:THR:CB	2.28	0.62
1:B:312:LYS:HD2	1:B:316:THR:OG1	2.00	0.62
1:A:312:LYS:HD2	1:A:316:THR:OG1	2.00	0.62
1:F:612:SER:HG	1:F:615:LYS:HD3	1.64	0.62
1:F:269:ILE:CD1	1:F:290:PHE:HE1	2.12	0.62
1:E:406:HIS:CE1	1:E:459:SER:HB3	2.29	0.62
1:C:312:LYS:HD2	1:C:316:THR:OG1	1.99	0.62
1:B:754:LYS:HD3	1:B:757:MET:HE1	1.82	0.62
1:C:119:ILE:HD11	1:C:191:ARG:HD3	0.74	0.62
1:D:403:THR:HG22	1:D:406:HIS:HB2	1.80	0.62
1:F:406:HIS:CE1	1:F:459:SER:HB3	2.29	0.62
1:A:612:SER:HG	1:A:615:LYS:HD3	1.64	0.62
1:C:269:ILE:CD1	1:C:290:PHE:HE1	2.12	0.62
1:F:312:LYS:HD2	1:F:316:THR:OG1	1.99	0.62
1:E:312:LYS:HD2	1:E:316:THR:OG1	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:505:LYS:NZ	1:D:730:GLU:OE2	2.30	0.62
1:F:120:ASP:CG	1:F:121:ASP:N	2.53	0.62
1:D:269:ILE:CD1	1:D:290:PHE:HE1	2.12	0.62
1:A:406:HIS:CE1	1:A:459:SER:HB3	2.29	0.62
1:A:25:ARG:HG3	1:A:25:ARG:O	2.00	0.62
1:C:25:ARG:O	1:C:25:ARG:HG3	2.00	0.62
1:A:268:LEU:N	1:A:268:LEU:HD12	2.14	0.61
1:B:120:ASP:CG	1:B:121:ASP:N	2.53	0.61
1:D:312:LYS:HD2	1:D:316:THR:OG1	2.00	0.61
1:B:560:ARG:HG2	1:B:607:GLU:OE2	2.00	0.61
1:B:519:PRO:HG2	1:B:522:CYS:SG	2.40	0.61
1:F:403:THR:HG22	1:F:406:HIS:HB2	1.80	0.61
1:D:365:ARG:NH1	1:E:458:GLN:O	2.32	0.61
1:E:505:LYS:NZ	1:F:730:GLU:OE2	2.29	0.61
1:C:519:PRO:HG2	1:C:522:CYS:SG	2.40	0.61
1:B:53:ARG:HD2	1:B:72:LEU:HA	1.83	0.61
1:B:219:MET:SD	1:B:365:ARG:HG2	2.41	0.61
1:A:560:ARG:HG2	1:A:607:GLU:OE2	2.00	0.61
1:F:25:ARG:HG3	1:F:25:ARG:O	2.00	0.61
1:D:505:LYS:NZ	1:E:730:GLU:OE2	2.29	0.61
1:F:86:ARG:NH1	1:F:204:ASP:OD1	2.33	0.61
1:E:120:ASP:CG	1:E:121:ASP:N	2.53	0.61
1:C:86:ARG:NH1	1:C:204:ASP:OD1	2.33	0.61
1:D:86:ARG:NH1	1:D:204:ASP:OD1	2.33	0.61
1:F:268:LEU:N	1:F:268:LEU:HD12	2.14	0.61
1:E:560:ARG:HG2	1:E:607:GLU:OE2	2.00	0.61
1:F:754:LYS:HA	1:F:757:MET:HE3	1.83	0.61
1:E:86:ARG:NH1	1:E:204:ASP:OD1	2.34	0.61
1:D:119:ILE:HD11	1:D:191:ARG:HD3	0.74	0.61
1:A:219:MET:SD	1:A:365:ARG:HG2	2.41	0.61
1:C:560:ARG:HG2	1:C:607:GLU:OE2	2.00	0.61
1:F:560:ARG:HG2	1:F:607:GLU:OE2	2.00	0.61
1:D:560:ARG:HG2	1:D:607:GLU:OE2	2.00	0.61
1:C:754:LYS:HD3	1:C:757:MET:HE1	1.82	0.61
1:D:496:PRO:HB3	1:D:510:PRO:HG3	1.83	0.61
1:B:86:ARG:NH1	1:B:204:ASP:OD1	2.33	0.61
1:C:26:LEU:CD2	1:C:102:ILE:CG1	2.59	0.61
1:E:403:THR:HG22	1:E:406:HIS:HB2	1.80	0.61
1:B:647:LEU:HD11	1:B:752:ILE:CD1	2.29	0.61
1:A:365:ARG:NH1	1:B:458:GLN:O	2.31	0.61
1:A:575:PHE:HE2	1:A:577:ASP:OD1	1.84	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:PRO:HB3	1:A:510:PRO:HG3	1.83	0.61
1:C:219:MET:SD	1:C:365:ARG:HG2	2.41	0.61
1:D:25:ARG:O	1:D:25:ARG:HG3	2.00	0.61
1:F:575:PHE:HE2	1:F:577:ASP:OD1	1.84	0.61
1:F:496:PRO:HB3	1:F:510:PRO:HG3	1.83	0.61
1:C:236:LYS:HZ1	1:C:239:ARG:HG3	1.65	0.61
1:A:730:GLU:OE2	1:F:505:LYS:NZ	2.32	0.61
1:B:119:ILE:HD11	1:B:191:ARG:CG	2.31	0.61
1:E:605:LEU:HD22	1:E:638:ARG:HE	1.66	0.61
1:E:496:PRO:HB3	1:E:510:PRO:HG3	1.83	0.61
1:C:365:ARG:NH1	1:D:458:GLN:O	2.33	0.60
1:B:406:HIS:CE1	1:B:459:SER:CB	2.79	0.60
1:F:53:ARG:HD2	1:F:72:LEU:HA	1.82	0.60
1:D:85:ASN:HD21	1:D:87:VAL:HG22	1.66	0.60
1:E:519:PRO:HG2	1:E:522:CYS:SG	2.40	0.60
1:F:519:PRO:HG2	1:F:522:CYS:SG	2.40	0.60
1:D:406:HIS:CE1	1:D:459:SER:CB	2.79	0.60
1:E:365:ARG:NH1	1:F:458:GLN:O	2.32	0.60
1:A:571:PRO:HA	1:A:616:ASN:O	2.02	0.60
1:C:53:ARG:HD2	1:C:72:LEU:HA	1.82	0.60
1:A:119:ILE:HD11	1:A:191:ARG:CG	2.31	0.60
1:D:120:ASP:CG	1:D:121:ASP:N	2.53	0.60
1:B:25:ARG:O	1:B:25:ARG:HG3	2.00	0.60
1:A:519:PRO:HG2	1:A:522:CYS:SG	2.40	0.60
1:C:475:THR:HG22	1:C:533:ASN:HD21	1.66	0.60
1:B:406:HIS:CE1	1:B:459:SER:HB3	2.29	0.60
1:B:310:ALA:N	1:B:311:PRO:HD3	2.17	0.60
1:F:571:PRO:HA	1:F:616:ASN:O	2.02	0.60
1:D:605:LEU:HD22	1:D:638:ARG:HE	1.66	0.60
1:C:496:PRO:HB3	1:C:510:PRO:HG3	1.83	0.60
1:E:219:MET:SD	1:E:365:ARG:HG2	2.41	0.60
1:B:365:ARG:NH1	1:C:458:GLN:O	2.32	0.60
1:C:406:HIS:CE1	1:C:459:SER:CB	2.79	0.60
1:B:496:PRO:HB3	1:B:510:PRO:HG3	1.83	0.60
1:A:310:ALA:N	1:A:311:PRO:HD3	2.17	0.60
1:B:571:PRO:HA	1:B:616:ASN:O	2.02	0.60
1:B:575:PHE:HE2	1:B:577:ASP:OD1	1.84	0.60
1:E:85:ASN:HD21	1:E:87:VAL:HG22	1.66	0.60
1:D:519:PRO:HG2	1:D:522:CYS:SG	2.40	0.60
1:D:469:VAL:HG22	1:D:540:ILE:HG12	1.83	0.60
1:E:53:ARG:HD2	1:E:72:LEU:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:ILE:HD11	1:C:191:ARG:CG	2.31	0.60
1:D:219:MET:SD	1:D:365:ARG:HG2	2.41	0.60
1:E:25:ARG:O	1:E:25:ARG:HG3	2.00	0.60
1:F:605:LEU:HD22	1:F:638:ARG:HE	1.66	0.60
1:A:475:THR:HG22	1:A:533:ASN:HD21	1.66	0.60
1:A:53:ARG:HD2	1:A:72:LEU:HA	1.82	0.60
1:A:86:ARG:NH1	1:A:204:ASP:OD1	2.33	0.60
1:C:130:LEU:HD12	1:C:131:PHE:HD1	1.61	0.60
1:A:130:LEU:HD12	1:A:131:PHE:HD1	1.61	0.60
1:E:571:PRO:HA	1:E:616:ASN:O	2.02	0.60
1:E:575:PHE:HE2	1:E:577:ASP:OD1	1.84	0.60
1:C:85:ASN:HD21	1:C:87:VAL:HG22	1.66	0.60
1:E:26:LEU:CD2	1:E:102:ILE:CG1	2.59	0.60
1:F:219:MET:SD	1:F:365:ARG:HG2	2.41	0.60
1:D:571:PRO:HA	1:D:616:ASN:O	2.02	0.60
1:C:571:PRO:HA	1:C:616:ASN:O	2.02	0.60
1:C:605:LEU:HD22	1:C:638:ARG:HE	1.66	0.60
1:C:310:ALA:N	1:C:311:PRO:HD3	2.17	0.59
1:B:270:ASN:OD1	1:B:272:PRO:HD2	2.02	0.59
1:E:469:VAL:HG22	1:E:540:ILE:HG12	1.83	0.59
1:B:475:THR:HG22	1:B:533:ASN:HD21	1.66	0.59
1:E:119:ILE:HD11	1:E:191:ARG:HD3	0.74	0.59
1:B:647:LEU:CD1	1:B:752:ILE:CD1	2.80	0.59
1:F:571:PRO:HB3	1:F:616:ASN:ND2	2.18	0.59
1:F:475:THR:HG22	1:F:533:ASN:HD21	1.66	0.59
1:F:85:ASN:HD21	1:F:87:VAL:HG22	1.66	0.59
1:B:130:LEU:HD12	1:B:131:PHE:HD1	1.61	0.59
1:F:119:ILE:HD11	1:F:191:ARG:CG	2.31	0.59
1:F:310:ALA:N	1:F:311:PRO:HD3	2.17	0.59
1:C:647:LEU:CD1	1:C:752:ILE:CD1	2.80	0.59
1:F:754:LYS:HD3	1:F:757:MET:HE3	1.84	0.59
1:D:575:PHE:HE2	1:D:577:ASP:OD1	1.84	0.59
1:D:53:ARG:HD2	1:D:72:LEU:HA	1.83	0.59
1:E:647:LEU:CD1	1:E:752:ILE:CD1	2.80	0.59
1:A:469:VAL:HG22	1:A:540:ILE:HG12	1.83	0.59
1:A:270:ASN:OD1	1:A:272:PRO:HD2	2.02	0.59
1:F:469:VAL:HG22	1:F:540:ILE:HG12	1.83	0.59
1:B:605:LEU:HD22	1:B:638:ARG:HE	1.66	0.59
1:B:85:ASN:HD21	1:B:87:VAL:HG22	1.66	0.59
1:E:475:THR:HG22	1:E:533:ASN:HD21	1.67	0.59
1:F:191:ARG:NH2	1:F:192:GLU:OE2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:ARG:NH2	1:C:192:GLU:OE2	2.36	0.59
1:A:647:LEU:CD1	1:A:752:ILE:CD1	2.80	0.59
1:F:647:LEU:CD1	1:F:752:ILE:CD1	2.80	0.59
1:F:21:ASN:OD1	1:F:23:PRO:HG3	2.03	0.59
1:C:575:PHE:HE2	1:C:577:ASP:OD1	1.84	0.59
1:F:26:LEU:HD21	1:F:100:ILE:HG13	1.80	0.59
1:C:120:ASP:CG	1:C:121:ASP:N	2.53	0.59
1:A:458:GLN:O	1:F:365:ARG:NH1	2.35	0.59
1:C:270:ASN:OD1	1:C:272:PRO:HD2	2.02	0.59
1:A:605:LEU:HD22	1:A:638:ARG:HE	1.66	0.59
1:A:85:ASN:HD21	1:A:87:VAL:HG22	1.66	0.59
1:E:191:ARG:NH2	1:E:192:GLU:OE2	2.36	0.59
1:D:310:ALA:N	1:D:311:PRO:HD3	2.17	0.59
1:E:647:LEU:HD11	1:E:752:ILE:CD1	2.29	0.59
1:B:21:ASN:OD1	1:B:23:PRO:HG3	2.03	0.59
1:A:191:ARG:NH2	1:A:192:GLU:OE2	2.36	0.59
1:B:191:ARG:NH2	1:B:192:GLU:OE2	2.36	0.59
1:A:571:PRO:HB3	1:A:616:ASN:ND2	2.18	0.59
1:C:612:SER:HG	1:C:615:LYS:HD3	1.67	0.59
1:E:21:ASN:OD1	1:E:23:PRO:HG3	2.03	0.59
1:C:21:ASN:OD1	1:C:23:PRO:HG3	2.03	0.59
1:E:310:ALA:N	1:E:311:PRO:HD3	2.17	0.59
1:E:571:PRO:HB3	1:E:616:ASN:ND2	2.18	0.59
1:C:469:VAL:HG22	1:C:540:ILE:HG12	1.83	0.59
1:D:647:LEU:CD1	1:D:752:ILE:CD1	2.80	0.58
1:F:210:ARG:O	1:F:211:LYS:HB2	2.04	0.58
1:D:21:ASN:OD1	1:D:23:PRO:HG3	2.03	0.58
1:B:236:LYS:HZ1	1:B:239:ARG:HG3	1.68	0.58
1:B:310:ALA:N	1:B:311:PRO:CD	2.66	0.58
1:A:753:ARG:O	1:A:757:MET:N	2.30	0.58
1:A:310:ALA:N	1:A:311:PRO:CD	2.66	0.58
1:E:612:SER:OG	1:E:615:LYS:HD3	2.04	0.58
1:C:571:PRO:HB3	1:C:616:ASN:ND2	2.18	0.58
1:A:210:ARG:O	1:A:211:LYS:HB2	2.04	0.58
1:A:21:ASN:OD1	1:A:23:PRO:HG3	2.03	0.58
1:F:406:HIS:CE1	1:F:459:SER:CB	2.79	0.58
1:B:571:PRO:HB3	1:B:616:ASN:ND2	2.18	0.58
1:A:233:ILE:HD11	1:B:158:MET:SD	2.43	0.58
1:F:255:ALA:HB2	1:F:302:PHE:CD1	2.39	0.58
1:D:119:ILE:HD11	1:D:191:ARG:CG	2.31	0.58
1:D:571:PRO:HB3	1:D:616:ASN:ND2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:ASN:OD1	1:E:272:PRO:HD2	2.02	0.58
1:D:475:THR:HG22	1:D:533:ASN:HD21	1.67	0.58
1:F:60:LYS:O	1:F:100:ILE:CG2	2.52	0.58
1:B:60:LYS:O	1:B:100:ILE:CG2	2.52	0.58
1:E:60:LYS:O	1:E:100:ILE:CG2	2.52	0.58
1:D:191:ARG:NH2	1:D:192:GLU:OE2	2.36	0.58
1:B:119:ILE:HD11	1:B:191:ARG:HD3	0.74	0.58
1:B:210:ARG:O	1:B:211:LYS:HB2	2.04	0.58
1:A:510:PRO:CG	1:A:614:LYS:HE3	2.34	0.58
1:D:270:ASN:OD1	1:D:272:PRO:HD2	2.02	0.58
1:E:406:HIS:CE1	1:E:459:SER:CB	2.79	0.58
1:B:612:SER:HG	1:B:615:LYS:HD3	1.67	0.58
1:F:612:SER:OG	1:F:615:LYS:HD3	2.04	0.58
1:E:210:ARG:O	1:E:211:LYS:HB2	2.04	0.58
1:B:469:VAL:HG22	1:B:540:ILE:HG12	1.83	0.58
1:B:510:PRO:CG	1:B:614:LYS:HE3	2.34	0.58
1:C:26:LEU:HD21	1:C:100:ILE:HG13	1.80	0.58
1:D:26:LEU:HD21	1:D:100:ILE:HG13	1.80	0.58
1:E:255:ALA:HB2	1:E:302:PHE:CD1	2.39	0.58
1:D:255:ALA:HB2	1:D:302:PHE:CD1	2.39	0.58
1:A:255:ALA:HB2	1:A:302:PHE:CD1	2.39	0.58
1:C:310:ALA:N	1:C:311:PRO:CD	2.66	0.58
1:F:310:ALA:N	1:F:311:PRO:CD	2.66	0.58
1:D:210:ARG:O	1:D:211:LYS:HB2	2.04	0.58
1:A:754:LYS:HD3	1:A:757:MET:HE1	1.85	0.58
1:F:270:ASN:OD1	1:F:272:PRO:HD2	2.02	0.57
1:D:754:LYS:HD3	1:D:757:MET:HE1	1.85	0.57
1:F:510:PRO:CG	1:F:614:LYS:HE3	2.34	0.57
1:D:612:SER:HG	1:D:615:LYS:HD3	1.69	0.57
1:E:26:LEU:HD21	1:E:100:ILE:HG13	1.80	0.57
1:C:60:LYS:O	1:C:100:ILE:CG2	2.52	0.57
1:D:60:LYS:O	1:D:100:ILE:CG2	2.52	0.57
1:B:255:ALA:HB2	1:B:302:PHE:CD1	2.39	0.57
1:A:647:LEU:HD11	1:A:752:ILE:CD1	2.29	0.57
1:F:477:GLU:N	1:F:477:GLU:OE1	2.37	0.57
1:F:333:ASP:HB2	1:F:362:ARG:HE	1.70	0.57
1:A:333:ASP:HB2	1:A:362:ARG:HE	1.70	0.57
1:C:255:ALA:HB2	1:C:302:PHE:CD1	2.39	0.57
1:D:647:LEU:HD11	1:D:752:ILE:CD1	2.29	0.57
1:D:753:ARG:O	1:D:757:MET:N	2.30	0.57
1:D:543:LYS:HG2	1:D:577:ASP:OD2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:LYS:HG2	1:A:577:ASP:OD2	2.05	0.57
1:F:130:LEU:HD12	1:F:131:PHE:HD1	1.61	0.57
1:C:290:PHE:O	1:C:294:GLU:HG2	2.05	0.57
1:D:612:SER:OG	1:D:615:LYS:HD3	2.04	0.57
1:B:612:SER:OG	1:B:615:LYS:HD3	2.04	0.57
1:C:510:PRO:CG	1:C:614:LYS:HE3	2.34	0.57
1:E:333:ASP:HB2	1:E:362:ARG:HE	1.70	0.57
1:B:333:ASP:HB2	1:B:362:ARG:HE	1.70	0.57
1:D:333:ASP:HB2	1:D:362:ARG:HE	1.70	0.57
1:A:60:LYS:O	1:A:100:ILE:CG2	2.52	0.57
1:D:126:ILE:HA	1:D:439:ALA:HB2	0.71	0.57
1:C:543:LYS:HG2	1:C:577:ASP:OD2	2.05	0.57
1:D:670:VAL:HG23	1:D:733:ARG:HD2	1.87	0.57
1:C:333:ASP:HB2	1:C:362:ARG:HE	1.70	0.57
1:D:336:LYS:O	1:D:337:GLN:HG2	2.05	0.57
1:E:119:ILE:HD11	1:E:191:ARG:CG	2.31	0.57
1:E:754:LYS:HD3	1:E:757:MET:HE1	1.86	0.57
1:E:477:GLU:OE1	1:E:477:GLU:N	2.37	0.57
1:D:310:ALA:N	1:D:311:PRO:CD	2.66	0.57
1:C:210:ARG:O	1:C:211:LYS:HB2	2.04	0.57
1:E:510:PRO:CG	1:E:614:LYS:HE3	2.34	0.57
1:B:475:THR:HG22	1:B:533:ASN:ND2	2.20	0.57
1:C:336:LYS:O	1:C:337:GLN:HG2	2.05	0.57
1:E:242:LEU:HD11	1:E:353:ILE:HD11	1.87	0.57
1:A:612:SER:OG	1:A:615:LYS:HD3	2.04	0.57
1:E:310:ALA:N	1:E:311:PRO:CD	2.66	0.57
1:E:290:PHE:O	1:E:294:GLU:HG2	2.05	0.57
1:C:670:VAL:HG23	1:C:733:ARG:HD2	1.87	0.57
1:D:290:PHE:O	1:D:294:GLU:HG2	2.05	0.57
1:E:543:LYS:HG2	1:E:577:ASP:OD2	2.05	0.57
1:D:510:PRO:CG	1:D:614:LYS:HE3	2.34	0.57
1:A:475:THR:HG22	1:A:533:ASN:ND2	2.20	0.57
1:D:242:LEU:HD11	1:D:353:ILE:HD11	1.87	0.57
1:C:266:PHE:HE2	1:C:268:LEU:HG	1.70	0.56
1:A:123:VAL:HG13	1:A:124:GLU:CG	2.35	0.56
1:A:123:VAL:HG13	1:A:124:GLU:HG3	1.87	0.56
1:F:123:VAL:HG13	1:F:124:GLU:CG	2.35	0.56
1:E:487:ARG:O	1:E:491:GLU:HG2	2.05	0.56
1:A:51:LEU:HD11	1:A:104:PRO:HB3	1.87	0.56
1:E:336:LYS:O	1:E:337:GLN:HG2	2.05	0.56
1:F:242:LEU:HD11	1:F:353:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:PHE:HE2	1:A:268:LEU:HG	1.70	0.56
1:A:290:PHE:O	1:A:294:GLU:HG2	2.05	0.56
1:A:25:ARG:HE	1:A:45:LYS:HE2	1.71	0.56
1:E:25:ARG:HE	1:E:45:LYS:HE2	1.71	0.56
1:C:242:LEU:HD11	1:C:353:ILE:HD11	1.87	0.56
1:F:51:LEU:HD11	1:F:104:PRO:HB3	1.87	0.56
1:F:487:ARG:O	1:F:491:GLU:HG2	2.06	0.56
1:F:26:LEU:CD2	1:F:102:ILE:CG1	2.59	0.56
1:E:266:PHE:CE2	1:E:268:LEU:HG	2.41	0.56
1:D:266:PHE:CE2	1:D:268:LEU:HG	2.41	0.56
1:A:119:ILE:HD11	1:A:191:ARG:HD3	0.74	0.56
1:D:123:VAL:HG13	1:D:124:GLU:CG	2.35	0.56
1:C:123:VAL:HG13	1:C:124:GLU:HG3	1.87	0.56
1:C:570:ALA:HB1	1:C:616:ASN:CB	2.36	0.56
1:C:125:GLY:HA3	1:C:159:ARG:CZ	2.35	0.56
1:A:125:GLY:HA3	1:A:159:ARG:CZ	2.35	0.56
1:F:25:ARG:HE	1:F:45:LYS:HE2	1.71	0.56
1:C:753:ARG:O	1:C:757:MET:N	2.30	0.56
1:C:475:THR:HG22	1:C:533:ASN:ND2	2.20	0.56
1:F:475:THR:HG22	1:F:533:ASN:ND2	2.20	0.56
1:E:670:VAL:HG23	1:E:733:ARG:HD2	1.87	0.56
1:B:336:LYS:O	1:B:337:GLN:HG2	2.05	0.56
1:F:236:LYS:HZ1	1:F:239:ARG:HG3	1.69	0.56
1:B:670:VAL:HG23	1:B:733:ARG:HD2	1.87	0.56
1:A:487:ARG:O	1:A:491:GLU:HG2	2.05	0.56
1:B:290:PHE:O	1:B:294:GLU:HG2	2.05	0.56
1:B:123:VAL:HG13	1:B:124:GLU:HG3	1.88	0.56
1:F:123:VAL:HG13	1:F:124:GLU:HG3	1.87	0.56
1:B:570:ALA:HB1	1:B:616:ASN:CB	2.36	0.56
1:F:125:GLY:HA3	1:F:159:ARG:CZ	2.35	0.56
1:B:125:GLY:HA3	1:B:159:ARG:CZ	2.35	0.56
1:F:543:LYS:HG2	1:F:577:ASP:OD2	2.05	0.56
1:A:336:LYS:O	1:A:337:GLN:HG2	2.05	0.56
1:F:284:SER:HA	1:F:287:ARG:NH2	2.21	0.56
1:A:126:ILE:HA	1:A:439:ALA:HB2	0.71	0.56
1:B:266:PHE:CE2	1:B:268:LEU:HG	2.41	0.56
1:A:119:ILE:HG22	1:A:162:GLU:O	2.06	0.56
1:C:123:VAL:HG13	1:C:124:GLU:CG	2.35	0.56
1:F:290:PHE:O	1:F:294:GLU:HG2	2.05	0.56
1:B:25:ARG:HE	1:B:45:LYS:HE2	1.71	0.56
1:D:25:ARG:HE	1:D:45:LYS:HE2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:475:THR:HG22	1:D:533:ASN:ND2	2.20	0.56
1:E:284:SER:HA	1:E:287:ARG:NH2	2.21	0.56
1:F:570:ALA:HB1	1:F:616:ASN:CB	2.36	0.56
1:F:126:ILE:HA	1:F:439:ALA:HB2	0.71	0.56
1:F:266:PHE:HE2	1:F:268:LEU:HG	1.70	0.56
1:A:266:PHE:CE2	1:A:268:LEU:HG	2.41	0.56
1:B:119:ILE:HG22	1:B:162:GLU:O	2.06	0.56
1:F:119:ILE:HG22	1:F:162:GLU:O	2.06	0.56
1:A:570:ALA:HB1	1:A:616:ASN:CB	2.36	0.56
1:E:560:ARG:HA	1:E:607:GLU:CD	2.26	0.56
1:D:560:ARG:HA	1:D:607:GLU:CD	2.26	0.56
1:D:477:GLU:OE1	1:D:477:GLU:N	2.37	0.56
1:D:284:SER:HA	1:D:287:ARG:NH2	2.21	0.56
1:B:26:LEU:HD21	1:B:100:ILE:HG13	1.80	0.56
1:D:266:PHE:HE2	1:D:268:LEU:HG	1.70	0.56
1:E:570:ALA:HB1	1:E:616:ASN:CB	2.36	0.56
1:C:25:ARG:HE	1:C:45:LYS:HE2	1.71	0.56
1:C:653:ARG:NH2	1:C:680:ASN:O	2.37	0.56
1:B:543:LYS:HG2	1:B:577:ASP:OD2	2.05	0.56
1:F:670:VAL:HG23	1:F:733:ARG:HD2	1.87	0.56
1:B:487:ARG:O	1:B:491:GLU:HG2	2.05	0.56
1:C:126:ILE:HG23	1:C:134:TYR:CE2	2.41	0.56
1:C:462:SER:O	1:C:463:ALA:HB3	2.06	0.56
1:D:570:ALA:HB1	1:D:616:ASN:CB	2.36	0.56
1:E:125:GLY:HA3	1:E:159:ARG:CZ	2.35	0.56
1:B:242:LEU:HD11	1:B:353:ILE:HD11	1.87	0.56
1:E:236:LYS:HZ1	1:E:239:ARG:HG3	1.71	0.56
1:F:336:LYS:O	1:F:337:GLN:HG2	2.05	0.56
1:E:612:SER:HG	1:E:615:LYS:HD3	1.70	0.56
1:C:612:SER:OG	1:C:615:LYS:HD3	2.04	0.56
1:D:233:ILE:HD11	1:E:158:MET:SD	2.46	0.56
1:D:487:ARG:O	1:D:491:GLU:HG2	2.05	0.56
1:E:126:ILE:CA	1:E:439:ALA:CB	2.51	0.55
1:B:123:VAL:HG13	1:B:124:GLU:CG	2.35	0.55
1:D:125:GLY:HA3	1:D:159:ARG:CZ	2.35	0.55
1:B:653:ARG:NH2	1:B:680:ASN:O	2.37	0.55
1:E:475:THR:HG22	1:E:533:ASN:ND2	2.20	0.55
1:C:51:LEU:HD11	1:C:104:PRO:HB3	1.87	0.55
1:C:487:ARG:O	1:C:491:GLU:HG2	2.05	0.55
1:A:236:LYS:HZ1	1:A:239:ARG:HG3	1.71	0.55
1:D:677:LYS:HE2	1:D:678:MET:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:ILE:HG23	1:D:134:TYR:CE2	2.41	0.55
1:F:266:PHE:CE2	1:F:268:LEU:HG	2.41	0.55
1:D:119:ILE:HG22	1:D:162:GLU:O	2.06	0.55
1:E:123:VAL:HG13	1:E:124:GLU:CG	2.35	0.55
1:C:123:VAL:HG22	1:C:124:GLU:N	2.22	0.55
1:E:754:LYS:HD3	1:E:757:MET:HE3	1.88	0.55
1:C:284:SER:HA	1:C:287:ARG:NH2	2.21	0.55
1:A:670:VAL:HG23	1:A:733:ARG:HD2	1.87	0.55
1:A:284:SER:HA	1:A:287:ARG:NH2	2.21	0.55
1:F:677:LYS:HE2	1:F:678:MET:HE3	1.89	0.55
1:B:51:LEU:HD11	1:B:104:PRO:HB3	1.87	0.55
1:E:126:ILE:HA	1:E:439:ALA:HB2	0.71	0.55
1:E:266:PHE:HE2	1:E:268:LEU:HG	1.70	0.55
1:F:268:LEU:CD1	1:F:268:LEU:N	2.70	0.55
1:E:123:VAL:HG13	1:E:124:GLU:HG3	1.87	0.55
1:F:560:ARG:HA	1:F:607:GLU:CD	2.26	0.55
1:A:242:LEU:HD11	1:A:353:ILE:HD11	1.87	0.55
1:D:123:VAL:HG13	1:D:124:GLU:HG3	1.88	0.55
1:B:233:ILE:HD11	1:C:158:MET:SD	2.46	0.55
1:E:233:ILE:HD11	1:F:158:MET:SD	2.46	0.55
1:F:227:PRO:HB3	1:F:340:HIS:NE2	2.22	0.55
1:A:677:LYS:HE2	1:A:678:MET:HE3	1.89	0.55
1:B:677:LYS:HE2	1:B:678:MET:HE3	1.89	0.55
1:B:126:ILE:HG23	1:B:134:TYR:CE2	2.41	0.55
1:D:51:LEU:HD11	1:D:104:PRO:HB3	1.87	0.55
1:B:284:SER:HA	1:B:287:ARG:NH2	2.21	0.55
1:E:119:ILE:HG22	1:E:162:GLU:O	2.06	0.55
1:C:119:ILE:HG22	1:C:162:GLU:O	2.06	0.55
1:D:462:SER:O	1:D:463:ALA:HB3	2.06	0.55
1:B:462:SER:O	1:B:463:ALA:HB3	2.06	0.55
1:E:510:PRO:HG2	1:E:614:LYS:HD3	1.89	0.55
1:A:85:ASN:ND2	1:A:87:VAL:HG22	2.22	0.55
1:C:233:ILE:HD11	1:D:158:MET:SD	2.47	0.55
1:C:126:ILE:HA	1:C:439:ALA:HB2	0.71	0.55
1:C:266:PHE:CE2	1:C:268:LEU:HG	2.41	0.55
1:A:266:PHE:CE2	1:A:268:LEU:CG	2.90	0.55
1:B:560:ARG:HA	1:B:607:GLU:CD	2.26	0.55
1:D:118:PRO:HB2	1:D:188:PRO:HA	1.89	0.55
1:E:118:PRO:HB2	1:E:188:PRO:HA	1.89	0.55
1:B:434:ASP:OD1	1:B:434:ASP:N	2.40	0.55
1:E:126:ILE:HG23	1:E:134:TYR:CE2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:PHE:CE2	1:B:268:LEU:CG	2.90	0.55
1:F:403:THR:CG2	1:F:411:LEU:HD21	2.35	0.55
1:C:118:PRO:HB2	1:C:188:PRO:HA	1.89	0.55
1:A:614:LYS:O	1:A:614:LYS:HG3	2.07	0.55
1:F:85:ASN:ND2	1:F:87:VAL:HG22	2.22	0.55
1:E:227:PRO:HB3	1:E:340:HIS:NE2	2.22	0.55
1:B:123:VAL:HG22	1:B:124:GLU:N	2.22	0.55
1:E:405:GLY:O	1:E:463:ALA:HB3	2.07	0.55
1:F:118:PRO:HB2	1:F:188:PRO:HA	1.89	0.55
1:C:22:ARG:N	1:C:23:PRO:CD	2.70	0.55
1:C:477:GLU:OE1	1:C:477:GLU:N	2.37	0.55
1:C:677:LYS:HE2	1:C:678:MET:HE3	1.89	0.55
1:D:227:PRO:HB3	1:D:340:HIS:NE2	2.22	0.55
1:C:60:LYS:O	1:C:100:ILE:HG22	2.07	0.55
1:D:266:PHE:CE2	1:D:268:LEU:CG	2.90	0.55
1:D:268:LEU:CD1	1:D:268:LEU:N	2.70	0.55
1:C:403:THR:CG2	1:C:411:LEU:HD21	2.35	0.55
1:D:754:LYS:HD3	1:D:757:MET:HE3	1.89	0.55
1:D:22:ARG:N	1:D:23:PRO:CD	2.70	0.55
1:A:227:PRO:HB3	1:A:340:HIS:NE2	2.22	0.55
1:E:677:LYS:HE2	1:E:678:MET:HE3	1.89	0.55
1:B:266:PHE:HE2	1:B:268:LEU:HG	1.70	0.54
1:B:118:PRO:HB2	1:B:188:PRO:HA	1.89	0.54
1:E:22:ARG:N	1:E:23:PRO:CD	2.70	0.54
1:B:421:GLN:CG	1:B:451:ASP:OD1	2.54	0.54
1:C:421:GLN:CG	1:C:451:ASP:OD1	2.55	0.54
1:B:85:ASN:ND2	1:B:87:VAL:HG22	2.22	0.54
1:A:385:THR:HG22	1:A:388:MET:HG3	1.90	0.54
1:E:138:TYR:HD2	1:E:154:VAL:HG12	1.72	0.54
1:A:138:TYR:HD2	1:A:154:VAL:HG12	1.71	0.54
1:A:26:LEU:CD2	1:A:102:ILE:CG1	2.59	0.54
1:A:126:ILE:HG23	1:A:134:TYR:CE2	2.41	0.54
1:E:266:PHE:CE2	1:E:268:LEU:CG	2.90	0.54
1:E:462:SER:O	1:E:463:ALA:HB3	2.06	0.54
1:F:307:ASP:O	1:F:311:PRO:CG	2.56	0.54
1:A:118:PRO:HB2	1:A:188:PRO:HA	1.89	0.54
1:E:421:GLN:CG	1:E:451:ASP:OD1	2.54	0.54
1:A:477:GLU:OE1	1:A:477:GLU:N	2.37	0.54
1:F:510:PRO:HG2	1:F:614:LYS:HD3	1.89	0.54
1:F:614:LYS:O	1:F:614:LYS:HG3	2.07	0.54
1:D:510:PRO:HG2	1:D:614:LYS:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:385:THR:HG22	1:E:388:MET:HG3	1.90	0.54
1:E:51:LEU:HD11	1:E:104:PRO:HB3	1.87	0.54
1:D:138:TYR:HD2	1:D:154:VAL:HG12	1.72	0.54
1:B:126:ILE:HA	1:B:439:ALA:HB2	0.71	0.54
1:B:122:THR:O	1:B:123:VAL:HB	2.08	0.54
1:A:462:SER:O	1:A:463:ALA:HB3	2.06	0.54
1:C:307:ASP:O	1:C:311:PRO:CG	2.55	0.54
1:A:307:ASP:O	1:A:311:PRO:CG	2.56	0.54
1:A:24:ASN:O	1:A:25:ARG:HB3	2.06	0.54
1:E:753:ARG:O	1:E:757:MET:N	2.30	0.54
1:A:650:GLU:OE1	1:A:650:GLU:N	2.32	0.54
1:C:614:LYS:O	1:C:614:LYS:HG3	2.07	0.54
1:E:614:LYS:O	1:E:614:LYS:HG3	2.07	0.54
1:D:574:LEU:HD23	1:D:619:ILE:HD12	1.90	0.54
1:A:60:LYS:O	1:A:100:ILE:HG22	2.07	0.54
1:F:266:PHE:CE2	1:F:268:LEU:CG	2.90	0.54
1:F:405:GLY:O	1:F:463:ALA:HB3	2.07	0.54
1:B:405:GLY:O	1:B:463:ALA:HB3	2.07	0.54
1:C:405:GLY:O	1:C:463:ALA:HB3	2.07	0.54
1:F:482:LEU:O	1:F:486:LYS:CG	2.48	0.54
1:B:753:ARG:O	1:B:757:MET:N	2.30	0.54
1:A:421:GLN:CG	1:A:451:ASP:OD1	2.54	0.54
1:B:227:PRO:HB3	1:B:340:HIS:NE2	2.22	0.54
1:C:227:PRO:HB3	1:C:340:HIS:NE2	2.22	0.54
1:C:574:LEU:HD23	1:C:619:ILE:HD12	1.90	0.54
1:F:462:SER:O	1:F:463:ALA:HB3	2.06	0.54
1:A:560:ARG:HA	1:A:607:GLU:CD	2.26	0.54
1:D:307:ASP:O	1:D:311:PRO:CG	2.56	0.54
1:F:24:ASN:O	1:F:25:ARG:HB3	2.06	0.54
1:D:24:ASN:O	1:D:25:ARG:HB3	2.06	0.54
1:D:614:LYS:O	1:D:614:LYS:HG3	2.07	0.54
1:E:85:ASN:ND2	1:E:87:VAL:HG22	2.22	0.54
1:D:405:GLY:O	1:D:463:ALA:HB3	2.07	0.54
1:A:405:GLY:O	1:A:463:ALA:HB3	2.07	0.54
1:C:560:ARG:HA	1:C:607:GLU:CD	2.26	0.54
1:C:482:LEU:O	1:C:486:LYS:CG	2.48	0.54
1:E:24:ASN:O	1:E:25:ARG:HB3	2.06	0.54
1:D:385:THR:HG22	1:D:388:MET:HG3	1.90	0.54
1:A:423:ILE:HD11	1:F:233:ILE:HD13	1.89	0.54
1:A:574:LEU:HD23	1:A:619:ILE:HD12	1.90	0.54
1:E:574:LEU:HD23	1:E:619:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:ILE:CD1	1:C:130:LEU:HD22	2.34	0.54
1:E:27:ILE:HD13	1:E:99:VAL:HG12	1.90	0.54
1:E:434:ASP:N	1:E:434:ASP:OD1	2.40	0.54
1:B:60:LYS:O	1:B:100:ILE:HG22	2.07	0.54
1:F:126:ILE:HG23	1:F:134:TYR:CE2	2.41	0.54
1:C:266:PHE:CE2	1:C:268:LEU:CG	2.90	0.54
1:A:122:THR:O	1:A:123:VAL:HB	2.08	0.54
1:E:559:VAL:HG12	1:E:607:GLU:CD	2.27	0.54
1:D:27:ILE:HD13	1:D:99:VAL:HG12	1.89	0.54
1:C:477:GLU:CB	1:C:662:ARG:HH12	2.21	0.54
1:A:477:GLU:CB	1:A:662:ARG:HH12	2.21	0.54
1:B:614:LYS:HG3	1:B:614:LYS:O	2.07	0.54
1:D:85:ASN:ND2	1:D:87:VAL:HG22	2.22	0.54
1:F:138:TYR:HD2	1:F:154:VAL:HG12	1.72	0.54
1:F:434:ASP:OD1	1:F:434:ASP:N	2.40	0.54
1:C:434:ASP:N	1:C:434:ASP:OD1	2.40	0.54
1:E:307:ASP:O	1:E:311:PRO:CG	2.56	0.54
1:D:210:ARG:HG2	1:D:212:GLN:HB2	1.90	0.54
1:D:21:ASN:C	1:D:23:PRO:HD3	2.29	0.54
1:D:421:GLN:CG	1:D:451:ASP:OD1	2.55	0.54
1:C:85:ASN:ND2	1:C:87:VAL:HG22	2.22	0.54
1:D:26:LEU:CD2	1:D:102:ILE:CD1	2.86	0.54
1:A:123:VAL:HG22	1:A:124:GLU:N	2.22	0.54
1:A:403:THR:CG2	1:A:411:LEU:HD21	2.35	0.54
1:E:210:ARG:HG2	1:E:212:GLN:HB2	1.90	0.54
1:C:210:ARG:HG2	1:C:212:GLN:HB2	1.90	0.54
1:B:21:ASN:C	1:B:23:PRO:HD3	2.29	0.54
1:E:575:PHE:CE2	1:E:577:ASP:OD1	2.61	0.54
1:E:477:GLU:CB	1:E:662:ARG:HH12	2.21	0.54
2:E:807:ADP:H8	2:E:807:ADP:C5'	2.21	0.54
1:A:26:LEU:CD2	1:A:102:ILE:CD1	2.86	0.53
1:B:403:THR:CG2	1:B:411:LEU:HD21	2.35	0.53
1:A:210:ARG:HG2	1:A:212:GLN:HB2	1.90	0.53
1:B:24:ASN:O	1:B:25:ARG:HB3	2.06	0.53
1:A:21:ASN:C	1:A:23:PRO:HD3	2.29	0.53
1:F:385:THR:HG22	1:F:388:MET:HG3	1.90	0.53
1:B:31:ALA:HB2	1:B:84:MET:N	2.23	0.53
1:B:138:TYR:HD2	1:B:154:VAL:HG12	1.72	0.53
2:D:807:ADP:H8	2:D:807:ADP:C5'	2.21	0.53
1:D:434:ASP:OD1	1:D:434:ASP:N	2.40	0.53
1:A:268:LEU:N	1:A:268:LEU:CD1	2.70	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:THR:O	1:F:123:VAL:HB	2.08	0.53
1:C:122:THR:O	1:C:123:VAL:HB	2.08	0.53
1:B:27:ILE:HD13	1:B:99:VAL:HG12	1.89	0.53
1:B:575:PHE:CE2	1:B:577:ASP:OD1	2.61	0.53
1:F:477:GLU:CB	1:F:662:ARG:HH12	2.21	0.53
1:F:574:LEU:HD23	1:F:619:ILE:HD12	1.90	0.53
1:B:210:ARG:HG2	1:B:212:GLN:HB2	1.90	0.53
1:B:22:ARG:N	1:B:23:PRO:CD	2.70	0.53
1:A:510:PRO:HG2	1:A:614:LYS:HD3	1.89	0.53
1:B:510:PRO:HG2	1:B:614:LYS:HD3	1.89	0.53
1:C:138:TYR:HD2	1:C:154:VAL:HG12	1.71	0.53
1:E:60:LYS:O	1:E:100:ILE:HG22	2.08	0.53
1:D:60:LYS:O	1:D:100:ILE:HG22	2.08	0.53
1:B:268:LEU:CD1	1:B:268:LEU:N	2.70	0.53
1:D:403:THR:O	1:D:403:THR:HG22	2.08	0.53
1:B:307:ASP:O	1:B:311:PRO:CG	2.56	0.53
1:C:647:LEU:HD11	1:C:752:ILE:CD1	2.29	0.53
1:F:570:ALA:HB1	1:F:616:ASN:HB2	1.91	0.53
1:C:24:ASN:O	1:C:25:ARG:HB3	2.06	0.53
1:F:22:ARG:N	1:F:23:PRO:CD	2.70	0.53
1:C:575:PHE:CE2	1:C:577:ASP:OD1	2.61	0.53
2:C:807:ADP:C5'	2:C:807:ADP:H8	2.21	0.53
1:C:26:LEU:CD2	1:C:102:ILE:CD1	2.86	0.53
1:F:403:THR:HG22	1:F:403:THR:O	2.08	0.53
1:E:403:THR:O	1:E:403:THR:HG22	2.08	0.53
1:A:570:ALA:HB1	1:A:616:ASN:HB2	1.91	0.53
1:F:210:ARG:HG2	1:F:212:GLN:HB2	1.90	0.53
1:A:754:LYS:HD3	1:A:757:MET:HE3	1.89	0.53
1:B:750:ASN:OD1	1:B:751:ASP:N	2.42	0.53
1:F:27:ILE:HD13	1:F:99:VAL:HG12	1.90	0.53
1:D:575:PHE:CE2	1:D:577:ASP:OD1	2.61	0.53
2:B:807:ADP:C5'	2:B:807:ADP:H8	2.21	0.53
1:F:31:ALA:HB2	1:F:84:MET:N	2.24	0.53
1:A:31:ALA:HB2	1:A:84:MET:N	2.24	0.53
1:F:119:ILE:HD11	1:F:191:ARG:HD3	0.74	0.53
1:C:403:THR:HG22	1:C:403:THR:O	2.08	0.53
1:F:421:GLN:CG	1:F:451:ASP:OD1	2.55	0.53
1:D:650:GLU:OE1	1:D:650:GLU:N	2.32	0.53
1:B:477:GLU:N	1:B:477:GLU:OE1	2.37	0.53
1:C:510:PRO:HG2	1:C:614:LYS:HD3	1.89	0.53
1:B:385:THR:HG22	1:B:388:MET:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:LYS:O	1:F:100:ILE:HG22	2.08	0.53
1:B:403:THR:HG22	1:B:403:THR:O	2.08	0.53
1:C:570:ALA:HB1	1:C:616:ASN:HB2	1.91	0.53
1:F:750:ASN:OD1	1:F:751:ASP:N	2.42	0.53
1:E:21:ASN:C	1:E:23:PRO:HD3	2.29	0.53
1:E:147:ARG:HG2	1:E:148:LYS:O	2.09	0.53
1:B:502:LYS:HZ3	1:C:702:SER:HG	1.56	0.53
1:E:122:THR:O	1:E:123:VAL:HB	2.08	0.53
1:A:563:PHE:CD1	1:A:607:GLU:OE1	2.62	0.53
1:D:482:LEU:O	1:D:486:LYS:CG	2.48	0.53
1:D:147:ARG:HG2	1:D:148:LYS:O	2.09	0.53
1:A:147:ARG:HG2	1:A:148:LYS:O	2.09	0.53
1:F:653:ARG:NH2	1:F:680:ASN:O	2.37	0.53
1:A:575:PHE:CE2	1:A:577:ASP:OD1	2.61	0.53
1:B:574:LEU:HD23	1:B:619:ILE:HD12	1.90	0.53
1:E:31:ALA:HB2	1:E:84:MET:N	2.24	0.53
1:D:26:LEU:CD2	1:D:102:ILE:CG1	2.59	0.53
1:A:403:THR:HG22	1:A:403:THR:O	2.08	0.53
1:E:563:PHE:CD1	1:E:607:GLU:OE1	2.62	0.53
1:B:563:PHE:CD1	1:B:607:GLU:OE1	2.62	0.53
1:C:571:PRO:HB3	1:C:616:ASN:HD22	1.74	0.53
1:F:21:ASN:C	1:F:23:PRO:HD3	2.29	0.53
1:F:147:ARG:HG2	1:F:148:LYS:O	2.09	0.53
1:F:575:PHE:CE2	1:F:577:ASP:OD1	2.61	0.53
1:B:477:GLU:CB	1:B:662:ARG:HH12	2.21	0.53
2:F:807:ADP:C5'	2:F:807:ADP:H8	2.21	0.53
1:F:26:LEU:CD2	1:F:102:ILE:CD1	2.86	0.53
1:C:268:LEU:N	1:C:268:LEU:CD1	2.70	0.53
1:D:571:PRO:HB3	1:D:616:ASN:HD22	1.74	0.53
1:E:571:PRO:HB3	1:E:616:ASN:HD22	1.74	0.53
1:C:27:ILE:HD13	1:C:99:VAL:HG12	1.90	0.53
1:A:27:ILE:HD13	1:A:99:VAL:HG12	1.90	0.53
1:A:614:LYS:HB2	3:A:1001:OJA:C26	2.39	0.53
1:F:614:LYS:HB2	3:F:1001:OJA:C26	2.39	0.53
1:E:614:LYS:HB2	3:E:1001:OJA:C26	2.39	0.53
1:C:31:ALA:HB2	1:C:84:MET:N	2.24	0.53
1:C:563:PHE:CD1	1:C:607:GLU:OE1	2.62	0.52
1:F:559:VAL:HG12	1:F:607:GLU:CD	2.28	0.52
1:E:269:ILE:CG2	1:E:274:ILE:CD1	2.82	0.52
1:A:750:ASN:OD1	1:A:751:ASP:N	2.42	0.52
1:E:26:LEU:CD2	1:E:102:ILE:CD1	2.86	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:126:ILE:CA	1:F:439:ALA:CB	2.51	0.52
1:A:312:LYS:HZ2	1:A:316:THR:HA	1.73	0.52
1:C:147:ARG:HG2	1:C:148:LYS:O	2.09	0.52
1:C:385:THR:HG22	1:C:388:MET:HG3	1.90	0.52
1:A:158:MET:SD	1:F:233:ILE:HD11	2.49	0.52
1:D:111:GLY:HA2	1:D:170:PRO:HG3	1.92	0.52
1:E:266:PHE:HE2	1:E:268:LEU:CG	2.22	0.52
1:A:266:PHE:HE2	1:A:268:LEU:CG	2.22	0.52
1:B:559:VAL:HG12	1:B:607:GLU:CD	2.28	0.52
1:B:570:ALA:HB1	1:B:616:ASN:HB2	1.91	0.52
1:B:571:PRO:HB3	1:B:616:ASN:HD22	1.74	0.52
1:C:750:ASN:OD1	1:C:751:ASP:N	2.42	0.52
1:C:21:ASN:C	1:C:23:PRO:HD3	2.29	0.52
1:D:614:LYS:HB2	3:D:1001:OJA:C26	2.39	0.52
1:D:31:ALA:HB2	1:D:84:MET:N	2.24	0.52
1:D:126:ILE:CD1	1:D:130:LEU:HD22	2.34	0.52
1:D:563:PHE:CD1	1:D:607:GLU:OE1	2.62	0.52
1:D:570:ALA:HB1	1:D:616:ASN:HB2	1.91	0.52
1:E:31:ALA:HA	1:E:83:ARG:HD2	1.92	0.52
1:A:26:LEU:HD21	1:A:100:ILE:HG13	1.80	0.52
1:D:134:TYR:HD2	1:D:163:PHE:HZ	1.58	0.52
1:B:126:ILE:HD13	1:B:130:LEU:CD2	2.35	0.52
1:E:134:TYR:HD2	1:E:163:PHE:HZ	1.58	0.52
1:B:266:PHE:HE2	1:B:268:LEU:CG	2.22	0.52
1:D:122:THR:O	1:D:123:VAL:HB	2.08	0.52
1:B:614:LYS:HB2	3:B:1001:OJA:C26	2.39	0.52
1:A:111:GLY:HA2	1:A:170:PRO:HG3	1.92	0.52
1:B:111:GLY:HA2	1:B:170:PRO:HG3	1.92	0.52
1:A:434:ASP:N	1:A:434:ASP:OD1	2.40	0.52
2:A:807:ADP:H8	2:A:807:ADP:C5'	2.21	0.52
1:C:134:TYR:HD2	1:C:163:PHE:HZ	1.58	0.52
1:D:126:ILE:CA	1:D:439:ALA:CB	2.51	0.52
1:E:126:ILE:CD1	1:E:130:LEU:HD22	2.34	0.52
1:D:123:VAL:HG22	1:D:124:GLU:N	2.22	0.52
1:E:123:VAL:HG22	1:E:124:GLU:N	2.22	0.52
1:D:750:ASN:OD1	1:D:751:ASP:N	2.42	0.52
1:F:754:LYS:HD3	1:F:757:MET:HE1	1.90	0.52
1:B:31:ALA:HA	1:B:83:ARG:HD2	1.92	0.52
1:A:31:ALA:HA	1:A:83:ARG:HD2	1.92	0.52
1:B:134:TYR:HD2	1:B:163:PHE:HZ	1.58	0.52
1:C:754:LYS:HD3	1:C:757:MET:HE3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:484:ASP:OD1	1:F:485:VAL:N	2.43	0.52
1:A:134:TYR:HD2	1:A:163:PHE:HZ	1.58	0.52
1:F:563:PHE:CD1	1:F:607:GLU:OE1	2.62	0.52
1:F:571:PRO:HB3	1:F:616:ASN:HD22	1.74	0.52
1:E:750:ASN:OD1	1:E:751:ASP:N	2.42	0.52
1:A:653:ARG:NH2	1:A:680:ASN:O	2.37	0.52
1:C:614:LYS:HB2	3:C:1001:OJA:C26	2.39	0.52
1:F:236:LYS:NZ	1:F:239:ARG:HG3	2.25	0.52
1:A:236:LYS:NZ	1:A:239:ARG:HG3	2.25	0.52
1:E:233:ILE:HD13	1:F:423:ILE:HD11	1.92	0.52
1:F:442:MET:O	1:F:445:LEU:HG	2.10	0.52
1:A:484:ASP:OD1	1:A:485:VAL:N	2.43	0.52
1:F:134:TYR:HD2	1:F:163:PHE:HZ	1.58	0.52
1:E:312:LYS:HZ2	1:E:316:THR:HA	1.73	0.52
1:C:559:VAL:HG12	1:C:607:GLU:CD	2.27	0.52
1:F:753:ARG:O	1:F:757:MET:N	2.30	0.52
1:B:674:PHE:HD1	1:B:677:LYS:HZ3	1.58	0.52
1:E:442:MET:O	1:E:445:LEU:HG	2.10	0.52
1:A:482:LEU:O	1:A:486:LYS:CG	2.48	0.52
1:C:233:ILE:HD13	1:D:423:ILE:HD11	1.92	0.52
1:F:31:ALA:HA	1:F:83:ARG:HD2	1.92	0.52
1:C:459:SER:HB2	1:C:461:PRO:HD3	1.92	0.51
1:B:482:LEU:O	1:B:486:LYS:CG	2.48	0.51
1:E:570:ALA:HB1	1:E:616:ASN:HB2	1.91	0.51
1:B:147:ARG:HG2	1:B:148:LYS:O	2.09	0.51
2:D:807:ADP:C8	2:D:807:ADP:C5'	2.94	0.51
2:F:807:ADP:C5'	2:F:807:ADP:C8	2.94	0.51
1:D:31:ALA:HA	1:D:83:ARG:HD2	1.92	0.51
1:F:126:ILE:CD1	1:F:130:LEU:HD22	2.34	0.51
1:C:269:ILE:CG2	1:C:274:ILE:CD1	2.82	0.51
1:B:269:ILE:CG2	1:B:274:ILE:CD1	2.82	0.51
1:D:266:PHE:HE2	1:D:268:LEU:CG	2.22	0.51
1:F:312:LYS:HZ2	1:F:316:THR:HA	1.76	0.51
2:C:807:ADP:C5'	2:C:807:ADP:C8	2.93	0.51
1:C:442:MET:O	1:C:445:LEU:HG	2.10	0.51
1:C:266:PHE:HE2	1:C:268:LEU:CG	2.22	0.51
1:B:650:GLU:OE1	1:B:650:GLU:N	2.32	0.51
1:A:624:ASN:O	1:A:755:TYR:HE1	1.94	0.51
1:D:233:ILE:HD13	1:E:423:ILE:HD11	1.92	0.51
2:E:807:ADP:C8	2:E:807:ADP:C5'	2.93	0.51
1:E:111:GLY:HA2	1:E:170:PRO:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:GLY:HA2	1:C:170:PRO:HG3	1.92	0.51
1:B:26:LEU:CD2	1:B:102:ILE:CD1	2.86	0.51
1:F:123:VAL:HG22	1:F:124:GLU:N	2.22	0.51
1:B:25:ARG:HH21	1:B:45:LYS:HE2	1.76	0.51
1:E:653:ARG:NH2	1:E:680:ASN:O	2.37	0.51
1:F:624:ASN:O	1:F:755:TYR:HE1	1.94	0.51
1:B:233:ILE:HD13	1:C:423:ILE:HD11	1.92	0.51
1:F:459:SER:HB2	1:F:461:PRO:HD3	1.92	0.51
1:B:459:SER:HB2	1:B:461:PRO:HD3	1.92	0.51
1:D:624:ASN:O	1:D:755:TYR:HE1	1.94	0.51
1:D:526:LEU:CD1	2:D:900:ADP:H2'	2.40	0.51
1:C:236:LYS:NZ	1:C:239:ARG:HG3	2.25	0.51
1:B:236:LYS:NZ	1:B:239:ARG:HG3	2.25	0.51
2:A:807:ADP:C5'	2:A:807:ADP:C8	2.94	0.51
1:B:26:LEU:HD23	1:B:100:ILE:CA	2.41	0.51
1:F:310:ALA:HA	1:F:325:VAL:HG22	1.93	0.51
1:A:22:ARG:N	1:A:23:PRO:CD	2.70	0.51
1:D:477:GLU:CB	1:D:662:ARG:HH12	2.21	0.51
1:A:143:TYR:HB3	1:A:175:ILE:HD11	1.92	0.51
1:A:442:MET:O	1:A:445:LEU:HG	2.10	0.51
1:D:312:LYS:NZ	1:D:316:THR:HG23	2.25	0.51
1:F:147:ARG:NH2	1:F:150:ASP:HB3	2.26	0.51
1:E:624:ASN:O	1:E:755:TYR:HE1	1.94	0.51
1:C:526:LEU:CD1	2:C:900:ADP:H2'	2.40	0.51
2:B:807:ADP:C5'	2:B:807:ADP:C8	2.93	0.51
1:A:702:SER:HG	1:F:502:LYS:HZ3	1.59	0.51
1:F:666:VAL:HA	1:F:731:ILE:CG2	2.41	0.51
1:B:442:MET:O	1:B:445:LEU:HG	2.10	0.51
1:D:143:TYR:HB3	1:D:175:ILE:HD11	1.93	0.51
1:B:666:VAL:HA	1:B:731:ILE:CG2	2.41	0.51
1:C:666:VAL:HA	1:C:731:ILE:CG2	2.41	0.51
1:C:26:LEU:HD23	1:C:100:ILE:CA	2.41	0.51
1:D:224:LEU:HD11	1:D:342:ILE:CG1	2.41	0.51
1:A:224:LEU:HD11	1:A:342:ILE:CG1	2.41	0.51
1:A:559:VAL:HG12	1:A:607:GLU:CD	2.27	0.51
1:C:469:VAL:CG2	1:C:565:LYS:HE3	2.40	0.51
1:E:526:LEU:CD1	2:E:900:ADP:H2'	2.40	0.51
1:C:31:ALA:HA	1:C:83:ARG:HD2	1.92	0.51
1:D:459:SER:HB2	1:D:461:PRO:HD3	1.92	0.51
1:E:459:SER:HB2	1:E:461:PRO:HD3	1.92	0.51
1:F:312:LYS:NZ	1:F:316:THR:HG23	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ALA:HA	1:A:325:VAL:HG22	1.93	0.51
1:C:650:GLU:N	1:C:650:GLU:OE1	2.32	0.51
1:E:236:LYS:NZ	1:E:239:ARG:HG3	2.25	0.51
1:F:111:GLY:HA2	1:F:170:PRO:HG3	1.92	0.51
1:F:266:PHE:HE2	1:F:268:LEU:CG	2.22	0.51
1:E:224:LEU:HD11	1:E:342:ILE:CG1	2.41	0.51
1:F:319:GLU:CG	1:F:322:ARG:HH21	2.21	0.51
1:E:25:ARG:HH21	1:E:45:LYS:HE2	1.76	0.51
1:B:754:LYS:HD3	1:B:757:MET:HE3	1.93	0.51
1:B:624:ASN:O	1:B:755:TYR:HE1	1.94	0.51
1:D:666:VAL:HA	1:D:731:ILE:CG2	2.41	0.51
1:F:224:LEU:HD11	1:F:342:ILE:CG1	2.41	0.50
1:C:224:LEU:HD11	1:C:342:ILE:CG1	2.41	0.50
1:C:312:LYS:NZ	1:C:316:THR:HG23	2.26	0.50
1:B:210:ARG:CG	1:B:212:GLN:CG	2.90	0.50
1:C:25:ARG:HH21	1:C:45:LYS:HE2	1.76	0.50
1:D:653:ARG:NH2	1:D:680:ASN:O	2.37	0.50
1:D:442:MET:O	1:D:445:LEU:HG	2.10	0.50
1:B:143:TYR:HB3	1:B:175:ILE:HD11	1.92	0.50
1:A:761:THR:O	1:B:744:ARG:NH1	2.44	0.50
1:A:26:LEU:HD23	1:A:100:ILE:CA	2.41	0.50
1:B:269:ILE:HD11	1:B:290:PHE:CE1	2.46	0.50
1:D:403:THR:CG2	1:D:411:LEU:HD21	2.35	0.50
1:A:571:PRO:HB3	1:A:616:ASN:HD22	1.74	0.50
1:B:224:LEU:HD11	1:B:342:ILE:CG1	2.41	0.50
1:E:560:ARG:HH21	1:F:465:ARG:HG3	1.77	0.50
1:C:210:ARG:CG	1:C:212:GLN:CG	2.90	0.50
1:F:25:ARG:HH21	1:F:45:LYS:HE2	1.76	0.50
1:B:147:ARG:NH2	1:B:150:ASP:HB3	2.26	0.50
1:C:624:ASN:O	1:C:755:TYR:HE1	1.94	0.50
1:E:761:THR:O	1:F:744:ARG:NH1	2.44	0.50
1:E:312:LYS:NZ	1:E:316:THR:HG23	2.26	0.50
1:E:147:ARG:NH2	1:E:150:ASP:HB3	2.26	0.50
1:D:408:GLY:HA3	2:D:807:ADP:N7	2.26	0.50
1:F:408:GLY:HA3	2:F:807:ADP:N7	2.26	0.50
1:A:502:LYS:HZ3	1:B:702:SER:HG	1.57	0.50
1:B:26:LEU:HD22	1:B:100:ILE:O	2.02	0.50
1:E:310:ALA:HA	1:E:325:VAL:HG22	1.93	0.50
1:D:210:ARG:CG	1:D:212:GLN:CG	2.90	0.50
1:C:349:ARG:O	1:C:352:SER:OG	2.26	0.50
1:A:666:VAL:HA	1:A:731:ILE:CG2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:LEU:HD23	1:D:100:ILE:CA	2.41	0.50
1:A:147:ARG:NH2	1:A:150:ASP:HB3	2.26	0.50
1:A:408:GLY:HA3	2:A:807:ADP:N7	2.26	0.50
1:E:666:VAL:HA	1:E:731:ILE:CG2	2.41	0.50
1:E:143:TYR:HB3	1:E:175:ILE:HD11	1.92	0.50
1:B:26:LEU:CD2	1:B:102:ILE:CG1	2.59	0.50
1:C:127:THR:O	1:C:440:GLU:OE1	2.30	0.50
1:A:459:SER:HB2	1:A:461:PRO:HD3	1.92	0.50
1:F:513:GLY:HA3	1:F:639:LEU:HD22	1.92	0.50
1:C:408:GLY:HA3	2:C:807:ADP:N7	2.26	0.50
1:A:126:ILE:HD13	1:A:130:LEU:CD2	2.35	0.50
1:D:269:ILE:HD11	1:D:290:PHE:CE1	2.46	0.50
1:D:560:ARG:HH21	1:E:465:ARG:HG3	1.77	0.50
1:A:513:GLY:CA	1:A:639:LEU:CD2	2.89	0.50
1:D:147:ARG:NH2	1:D:150:ASP:HB3	2.26	0.50
1:C:147:ARG:NH2	1:C:150:ASP:HB3	2.26	0.50
1:F:526:LEU:CD1	2:F:900:ADP:H2'	2.40	0.50
1:D:674:PHE:HD1	1:D:677:LYS:HZ3	1.56	0.50
1:A:427:MET:O	1:A:429:LEU:N	2.45	0.50
1:A:744:ARG:NH1	1:F:761:THR:O	2.45	0.50
1:F:26:LEU:HD23	1:F:100:ILE:CA	2.41	0.50
1:E:26:LEU:HD23	1:E:100:ILE:CA	2.41	0.50
1:D:127:THR:O	1:D:440:GLU:OE1	2.30	0.50
1:E:302:PHE:HA	1:E:344:MET:O	2.12	0.50
1:C:269:ILE:HD11	1:C:290:PHE:CE1	2.46	0.50
1:C:310:ALA:HA	1:C:325:VAL:HG22	1.93	0.50
1:D:310:ALA:HA	1:D:325:VAL:HG22	1.93	0.50
1:E:408:GLY:HA3	2:E:807:ADP:N7	2.26	0.50
1:C:560:ARG:HH21	1:D:465:ARG:HG3	1.77	0.50
1:D:27:ILE:H	1:D:82:ILE:CD1	2.25	0.50
1:A:43:GLN:CD	1:A:44:PRO:HD3	2.33	0.50
1:A:233:ILE:HD13	1:B:423:ILE:HD11	1.93	0.50
1:C:359:ARG:HG2	1:C:362:ARG:HG3	1.94	0.50
1:F:674:PHE:HD1	1:F:677:LYS:HZ3	1.58	0.50
1:B:427:MET:O	1:B:429:LEU:N	2.45	0.50
1:B:319:GLU:CG	1:B:322:ARG:HH21	2.21	0.49
1:A:25:ARG:HH21	1:A:45:LYS:HE2	1.76	0.49
1:F:43:GLN:CD	1:F:44:PRO:HD3	2.33	0.49
1:A:85:ASN:OD1	1:A:88:VAL:HG23	2.13	0.49
1:B:408:GLY:HA3	2:B:807:ADP:N7	2.26	0.49
1:C:143:TYR:HB3	1:C:175:ILE:HD11	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:PHE:HA	1:C:344:MET:O	2.12	0.49
1:B:302:PHE:HA	1:B:344:MET:O	2.12	0.49
1:B:560:ARG:HH21	1:C:465:ARG:HG3	1.77	0.49
1:B:513:GLY:HA3	1:B:639:LEU:HD22	1.93	0.49
1:F:513:GLY:CA	1:F:639:LEU:CD2	2.89	0.49
1:B:526:LEU:CD1	2:B:900:ADP:H2'	2.40	0.49
1:F:143:TYR:HB3	1:F:175:ILE:HD11	1.92	0.49
1:B:126:ILE:CA	1:B:439:ALA:CB	2.51	0.49
1:A:127:THR:O	1:A:440:GLU:OE1	2.30	0.49
1:A:674:PHE:HD1	1:A:677:LYS:HZ3	1.59	0.49
1:F:427:MET:O	1:F:429:LEU:N	2.45	0.49
1:F:54:GLY:HA2	1:F:70:ILE:HG23	1.94	0.49
1:C:255:ALA:CB	1:C:302:PHE:CD1	2.95	0.49
1:E:210:ARG:CG	1:E:212:GLN:CG	2.90	0.49
1:D:111:GLY:CA	1:D:170:PRO:HG3	2.43	0.49
1:D:427:MET:O	1:D:429:LEU:N	2.45	0.49
1:C:54:GLY:HA2	1:C:70:ILE:HG23	1.94	0.49
1:B:127:THR:O	1:B:440:GLU:OE1	2.30	0.49
1:D:302:PHE:HA	1:D:344:MET:O	2.12	0.49
1:A:560:ARG:HH21	1:B:465:ARG:HG3	1.77	0.49
1:A:469:VAL:CG2	1:A:565:LYS:HE3	2.40	0.49
1:B:81:LYS:HA	1:B:82:ILE:HD12	1.94	0.49
1:A:526:LEU:CD1	2:A:900:ADP:H2'	2.40	0.49
1:D:85:ASN:OD1	1:D:88:VAL:HG23	2.13	0.49
1:B:359:ARG:HG2	1:B:362:ARG:HG3	1.95	0.49
1:D:359:ARG:HG2	1:D:362:ARG:HG3	1.94	0.49
1:D:54:GLY:HA2	1:D:70:ILE:HG23	1.94	0.49
1:C:427:MET:O	1:C:429:LEU:N	2.45	0.49
1:C:183:HIS:NE2	1:C:185:GLU:OE2	2.46	0.49
1:F:127:THR:O	1:F:440:GLU:OE1	2.30	0.49
1:A:183:HIS:NE2	1:A:185:GLU:OE2	2.46	0.49
1:F:469:VAL:CG2	1:F:565:LYS:HE3	2.40	0.49
1:E:469:VAL:CG2	1:E:565:LYS:HE3	2.40	0.49
1:C:43:GLN:CD	1:C:44:PRO:HD3	2.33	0.49
1:E:85:ASN:OD1	1:E:88:VAL:HG23	2.13	0.49
1:F:85:ASN:OD1	1:F:88:VAL:HG23	2.12	0.49
1:B:85:ASN:OD1	1:B:88:VAL:HG23	2.13	0.49
1:B:32:ILE:HG22	1:B:83:ARG:HH12	1.78	0.49
1:C:111:GLY:CA	1:C:170:PRO:HG3	2.43	0.49
1:A:218:GLU:OE1	1:B:454:TRP:HZ2	1.96	0.49
1:F:255:ALA:CB	1:F:302:PHE:CD1	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:LYS:NZ	1:B:316:THR:HG23	2.26	0.49
1:E:513:GLY:HA3	1:E:639:LEU:HD22	1.93	0.49
1:E:43:GLN:CD	1:E:44:PRO:HD3	2.33	0.49
1:D:236:LYS:NZ	1:D:239:ARG:HG3	2.25	0.49
1:A:491:GLU:OE1	1:A:495:TYR:HE2	1.96	0.49
2:C:807:ADP:H5'2	2:C:807:ADP:H8	1.78	0.49
1:B:183:HIS:NE2	1:B:185:GLU:OE2	2.46	0.49
1:E:183:HIS:NE2	1:E:185:GLU:OE2	2.46	0.49
1:F:183:HIS:NE2	1:F:185:GLU:OE2	2.46	0.49
1:A:126:ILE:CD1	1:A:130:LEU:HD22	2.34	0.49
1:F:302:PHE:HA	1:F:344:MET:O	2.12	0.49
1:D:255:ALA:CB	1:D:302:PHE:CD1	2.95	0.49
1:A:255:ALA:CB	1:A:302:PHE:CD1	2.95	0.49
1:A:465:ARG:HG3	1:F:560:ARG:HH21	1.78	0.49
1:D:559:VAL:HG12	1:D:607:GLU:CD	2.27	0.49
1:C:81:LYS:HA	1:C:82:ILE:HD12	1.95	0.49
1:A:624:ASN:O	1:A:626:PRO:HD3	2.13	0.49
1:E:491:GLU:OE1	1:E:495:TYR:HE2	1.96	0.49
1:E:674:PHE:HD1	1:E:677:LYS:HZ3	1.58	0.49
1:C:32:ILE:HG22	1:C:83:ARG:HH12	1.78	0.49
2:A:807:ADP:H8	2:A:807:ADP:H5'2	1.78	0.49
1:E:502:LYS:NZ	1:F:702:SER:OG	2.42	0.49
1:A:443:ASN:OD1	1:A:444:SER:N	2.46	0.49
1:A:54:GLY:HA2	1:A:70:ILE:HG23	1.94	0.49
1:E:283:GLU:OE2	1:E:324:ILE:HD13	2.13	0.49
1:B:255:ALA:CB	1:B:302:PHE:CD1	2.95	0.49
1:D:517:TYR:HB2	1:D:626:PRO:HG3	1.95	0.49
1:D:43:GLN:CD	1:D:44:PRO:HD3	2.33	0.49
1:F:136:LYS:O	1:F:140:LEU:HB2	2.13	0.49
1:F:359:ARG:HG2	1:F:362:ARG:HG3	1.94	0.49
1:A:506:PHE:O	1:B:664:SER:HB3	2.13	0.49
1:C:283:GLU:OE2	1:C:324:ILE:HD13	2.13	0.49
1:D:183:HIS:NE2	1:D:185:GLU:OE2	2.46	0.49
1:E:127:THR:O	1:E:440:GLU:OE1	2.30	0.49
1:A:302:PHE:HA	1:A:344:MET:O	2.12	0.49
1:B:310:ALA:HA	1:B:325:VAL:HG22	1.93	0.49
1:D:25:ARG:HH21	1:D:45:LYS:HE2	1.76	0.49
1:A:27:ILE:H	1:A:82:ILE:CD1	2.25	0.49
1:B:136:LYS:O	1:B:140:LEU:HB2	2.13	0.49
1:F:491:GLU:OE1	1:F:495:TYR:HE2	1.96	0.49
1:E:54:GLY:HA2	1:E:70:ILE:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:ARG:NH2	1:A:749:ASP:OD1	2.46	0.49
1:B:283:GLU:OE2	1:B:324:ILE:HD13	2.13	0.49
1:E:269:ILE:HD11	1:E:290:PHE:CE1	2.46	0.48
1:F:210:ARG:CG	1:F:212:GLN:CG	2.90	0.48
1:E:213:LEU:HD12	1:E:254:ILE:HD12	1.95	0.48
1:E:517:TYR:HB2	1:E:626:PRO:HG3	1.95	0.48
1:B:43:GLN:CD	1:B:44:PRO:HD3	2.33	0.48
1:F:517:TYR:HB2	1:F:626:PRO:HG3	1.95	0.48
1:E:136:LYS:O	1:E:140:LEU:HB2	2.13	0.48
1:D:136:LYS:O	1:D:140:LEU:HB2	2.13	0.48
1:A:136:LYS:O	1:A:140:LEU:HB2	2.13	0.48
1:C:136:LYS:O	1:C:140:LEU:HB2	2.13	0.48
1:D:537:ALA:HB2	3:D:1001:OJA:H18	1.95	0.48
2:E:807:ADP:H8	2:E:807:ADP:H5'2	1.78	0.48
1:A:32:ILE:HG22	1:A:83:ARG:HH12	1.78	0.48
1:D:745:ARG:NH2	1:D:749:ASP:OD1	2.46	0.48
1:C:598:ASP:OD1	1:C:598:ASP:N	2.46	0.48
1:B:134:TYR:CD2	1:B:163:PHE:HZ	2.32	0.48
1:C:406:HIS:ND1	1:C:410:ASP:HB3	2.29	0.48
1:B:111:GLY:CA	1:B:170:PRO:HG3	2.43	0.48
1:E:111:GLY:CA	1:E:170:PRO:HG3	2.43	0.48
1:F:283:GLU:OE2	1:F:324:ILE:HD13	2.13	0.48
1:B:443:ASN:OD1	1:B:444:SER:N	2.46	0.48
1:C:443:ASN:OD1	1:C:444:SER:N	2.46	0.48
1:C:131:PHE:CG	1:C:135:LEU:HD12	2.49	0.48
1:F:406:HIS:ND1	1:F:410:ASP:HB3	2.29	0.48
1:D:213:LEU:HD12	1:D:254:ILE:HD12	1.95	0.48
1:C:649:ASP:O	1:C:653:ARG:N	2.47	0.48
1:B:624:ASN:O	1:B:626:PRO:HD3	2.13	0.48
1:C:537:ALA:HB2	3:C:1001:OJA:H18	1.96	0.48
1:C:491:GLU:OE1	1:C:495:TYR:HE2	1.96	0.48
1:F:443:ASN:OD1	1:F:444:SER:N	2.46	0.48
1:E:131:PHE:CG	1:E:135:LEU:HD12	2.49	0.48
1:E:268:LEU:CD1	1:E:268:LEU:N	2.70	0.48
1:A:406:HIS:ND1	1:A:410:ASP:HB3	2.29	0.48
1:A:210:ARG:CG	1:A:212:GLN:CG	2.90	0.48
1:A:513:GLY:HA3	1:A:639:LEU:HD22	1.93	0.48
1:B:213:LEU:HD12	1:B:254:ILE:HD12	1.95	0.48
1:F:81:LYS:HA	1:F:82:ILE:HD12	1.95	0.48
1:C:484:ASP:OD1	1:C:485:VAL:N	2.43	0.48
1:E:427:MET:O	1:E:429:LEU:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:LEU:CD2	1:C:100:ILE:HG13	2.42	0.48
1:C:134:TYR:CD2	1:C:163:PHE:HZ	2.32	0.48
1:D:131:PHE:CG	1:D:135:LEU:HD12	2.49	0.48
1:F:126:ILE:HD13	1:F:130:LEU:CD2	2.35	0.48
1:A:134:TYR:CD2	1:A:163:PHE:HZ	2.31	0.48
1:E:255:ALA:CB	1:E:302:PHE:CD1	2.95	0.48
1:B:406:HIS:ND1	1:B:410:ASP:HB3	2.29	0.48
1:D:319:GLU:CG	1:D:322:ARG:HH21	2.21	0.48
1:B:371:ILE:HD11	1:B:466:GLU:HB3	1.96	0.48
1:B:649:ASP:O	1:B:653:ARG:N	2.46	0.48
1:E:484:ASP:OD1	1:E:485:VAL:N	2.43	0.48
1:D:283:GLU:OE2	1:D:324:ILE:HD13	2.13	0.48
1:D:443:ASN:OD1	1:D:444:SER:N	2.46	0.48
1:D:126:ILE:HD13	1:D:130:LEU:CD2	2.35	0.48
1:B:131:PHE:CG	1:B:135:LEU:HD12	2.49	0.48
1:D:406:HIS:ND1	1:D:410:ASP:HB3	2.29	0.48
1:C:513:GLY:HA3	1:C:639:LEU:HD22	1.92	0.48
1:F:213:LEU:HD12	1:F:254:ILE:HD12	1.95	0.48
1:A:213:LEU:HD12	1:A:254:ILE:HD12	1.95	0.48
1:E:81:LYS:HA	1:E:82:ILE:HD12	1.95	0.48
1:A:517:TYR:HB2	1:A:626:PRO:HG3	1.95	0.48
1:C:85:ASN:OD1	1:C:88:VAL:HG23	2.13	0.48
1:B:491:GLU:OE1	1:B:495:TYR:HE2	1.96	0.48
2:F:807:ADP:H5'2	2:F:807:ADP:H8	1.78	0.48
1:D:32:ILE:HG22	1:D:83:ARG:HH12	1.78	0.48
1:A:111:GLY:CA	1:A:170:PRO:HG3	2.43	0.48
1:D:761:THR:O	1:E:744:ARG:NH1	2.45	0.48
1:B:598:ASP:N	1:B:598:ASP:OD1	2.46	0.48
1:B:761:THR:O	1:C:744:ARG:NH1	2.45	0.48
1:C:745:ARG:NH2	1:C:749:ASP:OD1	2.46	0.48
1:F:134:TYR:CD2	1:F:163:PHE:HZ	2.31	0.48
1:E:513:GLY:CA	1:E:639:LEU:CD2	2.89	0.48
1:B:469:VAL:CG2	1:B:565:LYS:HE3	2.40	0.48
1:E:624:ASN:O	1:E:626:PRO:HD3	2.13	0.48
1:C:517:TYR:HB2	1:C:626:PRO:HG3	1.95	0.48
1:F:624:ASN:O	1:F:626:PRO:HD3	2.13	0.48
1:D:491:GLU:OE1	1:D:495:TYR:HE2	1.96	0.48
2:D:807:ADP:H5'2	2:D:807:ADP:H8	1.78	0.48
1:E:32:ILE:HG22	1:E:83:ARG:HH12	1.78	0.48
1:E:745:ARG:NH2	1:E:749:ASP:OD1	2.46	0.48
1:F:745:ARG:NH2	1:F:749:ASP:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:469:VAL:CG2	1:D:565:LYS:HE3	2.40	0.48
1:E:537:ALA:HB2	3:E:1001:OJA:H18	1.95	0.48
1:F:32:ILE:HG22	1:F:83:ARG:HH12	1.78	0.48
1:E:443:ASN:OD1	1:E:444:SER:N	2.46	0.48
1:C:383:ILE:HD12	1:C:386:LYS:HE3	1.96	0.48
1:C:127:THR:H	1:C:439:ALA:N	1.92	0.48
1:E:130:LEU:HD12	1:E:131:PHE:HD1	1.61	0.48
1:F:131:PHE:CG	1:F:135:LEU:HD12	2.49	0.48
1:A:312:LYS:NZ	1:A:316:THR:HG23	2.26	0.48
1:C:213:LEU:HD12	1:C:254:ILE:HD12	1.95	0.48
1:E:136:LYS:HB3	1:E:137:PRO:HD3	1.96	0.48
1:B:136:LYS:HB3	1:B:137:PRO:HD3	1.96	0.48
1:E:359:ARG:HG2	1:E:362:ARG:HG3	1.95	0.48
1:F:111:GLY:CA	1:F:170:PRO:HG3	2.43	0.48
1:D:427:MET:O	1:D:430:ILE:HG12	2.14	0.48
1:E:427:MET:O	1:E:430:ILE:HG12	2.14	0.48
1:B:484:ASP:OD1	1:B:485:VAL:N	2.43	0.48
1:C:126:ILE:CA	1:C:439:ALA:CB	2.51	0.48
1:C:126:ILE:HG22	1:C:439:ALA:CB	2.44	0.48
1:D:134:TYR:CD2	1:D:163:PHE:HZ	2.31	0.48
1:B:126:ILE:HG22	1:B:439:ALA:CB	2.44	0.48
1:A:131:PHE:CG	1:A:135:LEU:HD12	2.49	0.48
1:E:406:HIS:ND1	1:E:410:ASP:HB3	2.29	0.48
1:A:371:ILE:HD11	1:A:466:GLU:HB3	1.96	0.48
1:D:649:ASP:O	1:D:653:ARG:N	2.46	0.48
1:D:624:ASN:O	1:D:626:PRO:HD3	2.13	0.48
1:A:359:ARG:HG2	1:A:362:ARG:HG3	1.95	0.48
1:A:283:GLU:OE2	1:A:324:ILE:HD13	2.13	0.48
1:D:598:ASP:N	1:D:598:ASP:OD1	2.46	0.48
1:D:269:ILE:CG2	1:D:274:ILE:CD1	2.82	0.47
1:A:267:PHE:HE2	1:A:289:ALA:CA	2.27	0.47
1:C:371:ILE:HD11	1:C:466:GLU:HB3	1.96	0.47
1:A:81:LYS:HA	1:A:82:ILE:HD12	1.95	0.47
1:C:624:ASN:O	1:C:626:PRO:HD3	2.13	0.47
1:B:537:ALA:HB2	3:B:1001:OJA:H18	1.96	0.47
1:F:427:MET:O	1:F:430:ILE:HG12	2.14	0.47
1:B:54:GLY:HA2	1:B:70:ILE:HG23	1.94	0.47
1:A:604:ILE:O	1:A:608:MET:HG3	2.14	0.47
1:D:484:ASP:OD1	1:D:485:VAL:N	2.43	0.47
1:F:598:ASP:OD1	1:F:598:ASP:N	2.46	0.47
2:B:807:ADP:H8	2:B:807:ADP:H5'2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:430:ILE:HG13	1:F:431:ASP:N	2.30	0.47
1:C:267:PHE:HE2	1:C:289:ALA:CA	2.27	0.47
1:A:365:ARG:NH1	1:B:460:ASN:HD22	2.13	0.47
1:F:647:LEU:HD11	1:F:752:ILE:CD1	2.29	0.47
1:B:517:TYR:HB2	1:B:626:PRO:HG3	1.95	0.47
1:B:430:ILE:HG13	1:B:431:ASP:N	2.30	0.47
1:C:427:MET:O	1:C:430:ILE:HG12	2.14	0.47
1:B:604:ILE:O	1:B:608:MET:HG3	2.14	0.47
1:B:745:ARG:NH2	1:B:749:ASP:OD1	2.46	0.47
1:D:126:ILE:HG22	1:D:439:ALA:CB	2.44	0.47
1:E:286:LEU:O	1:E:289:ALA:HB3	2.15	0.47
1:C:136:LYS:HB3	1:C:137:PRO:HD3	1.96	0.47
1:C:430:ILE:HG13	1:C:431:ASP:N	2.30	0.47
1:E:134:TYR:CD2	1:E:163:PHE:HZ	2.32	0.47
1:E:267:PHE:HE2	1:E:289:ALA:CA	2.28	0.47
1:D:267:PHE:HE2	1:D:289:ALA:CA	2.27	0.47
1:B:312:LYS:CE	1:B:321:GLU:CG	2.87	0.47
1:B:513:GLY:CA	1:B:639:LEU:CD2	2.89	0.47
1:F:371:ILE:HD11	1:F:466:GLU:HB3	1.96	0.47
1:B:27:ILE:H	1:B:82:ILE:CD1	2.25	0.47
1:A:649:ASP:O	1:A:653:ARG:N	2.46	0.47
1:A:430:ILE:HG13	1:A:431:ASP:N	2.30	0.47
1:A:598:ASP:N	1:A:598:ASP:OD1	2.46	0.47
1:C:126:ILE:HD13	1:C:130:LEU:CD2	2.35	0.47
1:D:130:LEU:HD12	1:D:131:PHE:HD1	1.61	0.47
1:E:126:ILE:HD13	1:E:130:LEU:CD2	2.35	0.47
1:F:286:LEU:O	1:F:289:ALA:HB3	2.15	0.47
1:D:286:LEU:O	1:D:289:ALA:HB3	2.15	0.47
1:D:81:LYS:HA	1:D:82:ILE:HD12	1.94	0.47
1:A:537:ALA:HB2	3:A:1001:OJA:H18	1.96	0.47
1:D:158:MET:HG2	1:D:388:MET:SD	2.55	0.47
1:E:604:ILE:O	1:E:608:MET:HG3	2.14	0.47
1:B:383:ILE:HD12	1:B:386:LYS:HE3	1.96	0.47
1:F:126:ILE:HG22	1:F:439:ALA:CB	2.44	0.47
1:A:126:ILE:HG22	1:A:439:ALA:CB	2.44	0.47
1:C:286:LEU:O	1:C:289:ALA:HB3	2.15	0.47
1:F:269:ILE:CG2	1:F:274:ILE:CD1	2.82	0.47
1:C:513:GLY:CA	1:C:639:LEU:HD22	2.45	0.47
1:E:650:GLU:OE1	1:E:650:GLU:N	2.32	0.47
1:F:537:ALA:HB2	3:F:1001:OJA:H18	1.96	0.47
1:F:136:LYS:HB3	1:F:137:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:158:MET:HG2	1:E:388:MET:SD	2.55	0.47
1:A:158:MET:HG2	1:A:388:MET:SD	2.55	0.47
1:A:32:ILE:HG22	1:A:83:ARG:NH1	2.30	0.47
1:A:427:MET:O	1:A:430:ILE:HG12	2.14	0.47
1:B:427:MET:O	1:B:430:ILE:HG12	2.14	0.47
1:E:430:ILE:HG13	1:E:431:ASP:N	2.30	0.47
1:C:604:ILE:O	1:C:608:MET:HG3	2.14	0.47
1:A:383:ILE:HD12	1:A:386:LYS:HE3	1.96	0.47
1:A:26:LEU:HD22	1:A:100:ILE:O	2.03	0.47
1:D:130:LEU:HA	1:D:133:VAL:HG12	1.97	0.47
1:D:406:HIS:CE1	1:D:461:PRO:CD	2.98	0.47
1:B:513:GLY:HA3	1:B:639:LEU:HA	1.97	0.47
1:D:371:ILE:HD11	1:D:466:GLU:HB3	1.96	0.47
1:F:359:ARG:HD3	1:F:362:ARG:CZ	2.45	0.47
1:F:158:MET:HG2	1:F:388:MET:SD	2.55	0.47
1:F:32:ILE:HG22	1:F:83:ARG:NH1	2.30	0.47
1:D:604:ILE:O	1:D:608:MET:HG3	2.14	0.47
1:F:26:LEU:CD2	1:F:100:ILE:HG13	2.42	0.47
1:F:130:LEU:HA	1:F:133:VAL:HG12	1.97	0.47
1:F:513:GLY:CA	1:F:639:LEU:HD22	2.45	0.47
1:E:649:ASP:O	1:E:653:ARG:N	2.46	0.47
1:E:359:ARG:HD3	1:E:362:ARG:CZ	2.45	0.47
1:B:32:ILE:HG22	1:B:83:ARG:NH1	2.30	0.47
1:D:393:ASP:OD1	1:D:394:VAL:N	2.47	0.47
1:B:267:PHE:HE2	1:B:289:ALA:CA	2.27	0.47
1:A:286:LEU:O	1:A:289:ALA:HB3	2.15	0.47
1:B:349:ARG:O	1:B:352:SER:OG	2.26	0.47
1:D:136:LYS:HB3	1:D:137:PRO:HD3	1.96	0.47
1:B:52:PHE:O	1:B:53:ARG:HB2	2.15	0.47
1:D:52:PHE:O	1:D:53:ARG:HB2	2.15	0.47
1:E:506:PHE:O	1:F:664:SER:HB3	2.15	0.47
1:F:267:PHE:HE2	1:F:289:ALA:CA	2.27	0.46
1:C:607:GLU:HG2	1:D:465:ARG:NH1	2.30	0.46
1:A:319:GLU:CG	1:A:322:ARG:HH21	2.21	0.46
1:C:513:GLY:HA3	1:C:639:LEU:HA	1.97	0.46
1:E:513:GLY:CA	1:E:639:LEU:HD22	2.45	0.46
1:E:371:ILE:HD11	1:E:466:GLU:HB3	1.96	0.46
1:A:136:LYS:HB3	1:A:137:PRO:HD3	1.96	0.46
1:A:359:ARG:HD3	1:A:362:ARG:CZ	2.45	0.46
1:C:359:ARG:HD3	1:C:362:ARG:CZ	2.45	0.46
1:D:682:PHE:HE2	1:D:690:ILE:HD11	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:PHE:HE2	1:D:183:HIS:O	1.98	0.46
1:B:131:PHE:HE2	1:B:183:HIS:O	1.98	0.46
1:E:126:ILE:HG22	1:E:439:ALA:CB	2.44	0.46
1:A:127:THR:H	1:A:439:ALA:N	1.92	0.46
1:A:131:PHE:HE2	1:A:183:HIS:O	1.98	0.46
1:A:130:LEU:HA	1:A:133:VAL:HG12	1.97	0.46
1:F:161:VAL:HG22	1:F:162:GLU:H	1.81	0.46
1:C:27:ILE:O	1:C:82:ILE:HD13	2.16	0.46
1:A:52:PHE:O	1:A:53:ARG:HB2	2.15	0.46
1:D:359:ARG:HD3	1:D:362:ARG:CZ	2.45	0.46
1:D:32:ILE:HG22	1:D:83:ARG:NH1	2.30	0.46
1:D:430:ILE:HG13	1:D:431:ASP:N	2.30	0.46
1:C:761:THR:O	1:D:744:ARG:NH1	2.45	0.46
1:F:383:ILE:HD12	1:F:386:LYS:HE3	1.96	0.46
1:C:514:VAL:HG22	1:C:641:GLN:HB2	1.97	0.46
1:C:130:LEU:HA	1:C:133:VAL:HG12	1.97	0.46
1:E:131:PHE:HE2	1:E:183:HIS:O	1.98	0.46
1:A:126:ILE:CA	1:A:439:ALA:CB	2.51	0.46
1:B:267:PHE:CE2	1:B:289:ALA:CB	2.91	0.46
1:A:513:GLY:HA3	1:A:639:LEU:HA	1.97	0.46
1:D:513:GLY:CA	1:D:639:LEU:CD2	2.89	0.46
1:F:649:ASP:O	1:F:653:ARG:N	2.47	0.46
1:D:383:ILE:HD12	1:D:386:LYS:HE3	1.96	0.46
1:B:393:ASP:OD1	1:B:394:VAL:N	2.47	0.46
1:B:286:LEU:O	1:B:289:ALA:HB3	2.15	0.46
1:E:403:THR:CG2	1:E:411:LEU:HD21	2.35	0.46
1:A:513:GLY:CA	1:A:639:LEU:HD22	2.45	0.46
1:D:27:ILE:O	1:D:82:ILE:HD13	2.16	0.46
1:F:27:ILE:O	1:F:82:ILE:HD13	2.16	0.46
1:E:52:PHE:O	1:E:53:ARG:HB2	2.15	0.46
1:B:56:THR:HG23	1:B:68:VAL:CG1	2.46	0.46
1:F:26:LEU:HD11	1:F:100:ILE:HD11	1.98	0.46
1:D:134:TYR:HD2	1:D:163:PHE:CZ	2.33	0.46
1:A:460:ASN:HD22	1:F:365:ARG:NH1	2.13	0.46
1:C:513:GLY:CA	1:C:639:LEU:CD2	2.89	0.46
1:F:27:ILE:H	1:F:82:ILE:CD1	2.25	0.46
1:E:27:ILE:O	1:E:82:ILE:HD13	2.15	0.46
1:B:682:PHE:HE2	1:B:690:ILE:HD11	1.81	0.46
1:A:56:THR:HG23	1:A:68:VAL:CG1	2.46	0.46
1:E:598:ASP:N	1:E:598:ASP:OD1	2.46	0.46
1:B:127:THR:H	1:B:439:ALA:N	1.92	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:25:ARG:NE	1:F:45:LYS:HE2	2.31	0.46
1:A:25:ARG:NE	1:A:45:LYS:HE2	2.31	0.46
1:A:27:ILE:O	1:A:82:ILE:HD13	2.15	0.46
1:B:359:ARG:HD3	1:B:362:ARG:CZ	2.45	0.46
1:E:32:ILE:HG22	1:E:83:ARG:NH1	2.30	0.46
1:C:32:ILE:HG22	1:C:83:ARG:NH1	2.30	0.46
1:E:383:ILE:HD12	1:E:386:LYS:HE3	1.96	0.46
1:C:56:THR:HG23	1:C:68:VAL:CG1	2.46	0.46
1:A:682:PHE:HE2	1:A:690:ILE:HD11	1.81	0.46
1:C:131:PHE:HE2	1:C:183:HIS:O	1.98	0.46
1:A:161:VAL:HG22	1:A:162:GLU:H	1.81	0.46
1:C:161:VAL:HG22	1:C:162:GLU:H	1.81	0.46
1:E:91:ASN:ND2	1:E:150:ASP:HB2	2.31	0.46
1:A:206:ILE:HG12	1:A:253:LEU:HD13	1.98	0.46
1:B:206:ILE:HG12	1:B:253:LEU:HD13	1.98	0.46
1:B:158:MET:HG2	1:B:388:MET:SD	2.55	0.46
1:C:158:MET:HG2	1:C:388:MET:SD	2.55	0.46
1:B:56:THR:HG23	1:B:68:VAL:HG13	1.98	0.46
1:F:292:GLU:HA	1:F:295:LYS:NZ	2.31	0.46
1:A:292:GLU:HA	1:A:295:LYS:NZ	2.31	0.46
1:B:514:VAL:HG22	1:B:641:GLN:HB2	1.97	0.46
1:F:35:ASP:OD1	1:F:35:ASP:N	2.49	0.46
1:B:126:ILE:CG2	1:B:134:TYR:CZ	2.99	0.46
1:E:130:LEU:HA	1:E:133:VAL:HG12	1.97	0.46
1:B:513:GLY:CA	1:B:639:LEU:HD22	2.45	0.46
1:E:25:ARG:NE	1:E:45:LYS:HE2	2.31	0.46
1:F:206:ILE:HG12	1:F:253:LEU:HD13	1.98	0.46
1:F:82:ILE:HD12	1:F:82:ILE:N	2.31	0.46
1:B:27:ILE:O	1:B:82:ILE:HD13	2.16	0.46
1:A:485:VAL:HG11	1:A:645:ILE:HD11	1.98	0.46
1:D:506:PHE:O	1:E:664:SER:HB3	2.15	0.46
1:F:682:PHE:HE2	1:F:690:ILE:HD11	1.81	0.46
1:E:26:LEU:HD11	1:E:100:ILE:HD11	1.98	0.46
1:D:312:LYS:HZ3	1:D:316:THR:HA	1.81	0.46
1:B:570:ALA:HB1	1:B:616:ASN:HB3	1.98	0.46
1:D:25:ARG:NE	1:D:45:LYS:HE2	2.31	0.46
1:D:477:GLU:CB	1:D:662:ARG:NH1	2.79	0.46
1:B:506:PHE:O	1:C:664:SER:HB3	2.16	0.46
1:F:514:VAL:HG22	1:F:641:GLN:HB2	1.97	0.46
1:B:292:GLU:HA	1:B:295:LYS:NZ	2.31	0.46
1:C:134:TYR:HD2	1:C:163:PHE:CZ	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:127:THR:H	1:F:439:ALA:N	1.92	0.46
1:D:161:VAL:HG22	1:D:162:GLU:H	1.80	0.46
1:B:365:ARG:NH1	1:C:460:ASN:HD22	2.14	0.46
1:C:319:GLU:CG	1:C:322:ARG:HH21	2.21	0.46
1:C:25:ARG:NE	1:C:45:LYS:HE2	2.31	0.46
1:F:91:ASN:ND2	1:F:150:ASP:HB2	2.31	0.46
1:E:27:ILE:H	1:E:82:ILE:CD1	2.25	0.46
1:E:82:ILE:N	1:E:82:ILE:HD12	2.31	0.46
1:B:477:GLU:CB	1:B:662:ARG:NH1	2.79	0.46
1:C:52:PHE:O	1:C:53:ARG:HB2	2.15	0.46
1:A:56:THR:HG23	1:A:68:VAL:HG13	1.98	0.46
1:C:682:PHE:HE2	1:C:690:ILE:HD11	1.81	0.46
1:A:514:VAL:HG22	1:A:641:GLN:HB2	1.97	0.46
1:A:26:LEU:HD11	1:A:100:ILE:HD11	1.98	0.45
1:B:130:LEU:HA	1:B:133:VAL:HG12	1.97	0.45
1:B:161:VAL:HG22	1:B:162:GLU:H	1.81	0.45
1:A:570:ALA:HB1	1:A:616:ASN:HB3	1.98	0.45
1:D:513:GLY:CA	1:D:639:LEU:HD22	2.45	0.45
1:D:513:GLY:HA3	1:D:639:LEU:HA	1.97	0.45
1:A:82:ILE:N	1:A:82:ILE:HD12	2.31	0.45
1:C:477:GLU:CB	1:C:662:ARG:NH1	2.79	0.45
1:B:227:PRO:HB3	1:B:340:HIS:CD2	2.51	0.45
1:D:514:VAL:HG22	1:D:641:GLN:HB2	1.97	0.45
1:C:738:GLU:OE2	1:C:741:ARG:NH1	2.49	0.45
1:D:56:THR:HG23	1:D:68:VAL:CG1	2.46	0.45
1:C:365:ARG:NH1	1:D:460:ASN:HD22	2.14	0.45
1:C:312:LYS:HZ2	1:C:316:THR:HA	1.81	0.45
1:D:82:ILE:N	1:D:82:ILE:HD12	2.31	0.45
1:D:738:GLU:OE2	1:D:741:ARG:NH1	2.49	0.45
1:D:218:GLU:OE1	1:E:454:TRP:HZ2	1.99	0.45
1:E:738:GLU:OE2	1:E:741:ARG:NH1	2.49	0.45
1:E:514:VAL:HG22	1:E:641:GLN:HB2	1.97	0.45
1:F:604:ILE:O	1:F:608:MET:HG3	2.14	0.45
1:D:26:LEU:HD11	1:D:100:ILE:HD11	1.98	0.45
1:C:126:ILE:CG2	1:C:134:TYR:CZ	2.99	0.45
1:F:131:PHE:HE2	1:F:183:HIS:O	1.98	0.45
1:D:224:LEU:CD2	1:D:298:PRO:HB3	2.46	0.45
1:F:224:LEU:CD2	1:F:298:PRO:HB3	2.46	0.45
1:C:91:ASN:ND2	1:C:150:ASP:HB2	2.31	0.45
1:F:650:GLU:OE1	1:F:650:GLU:N	2.32	0.45
1:F:227:PRO:HB3	1:F:340:HIS:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:THR:HG23	1:C:68:VAL:HG13	1.98	0.45
1:E:542:ILE:HD12	1:E:562:ILE:HD13	1.98	0.45
1:B:35:ASP:OD1	1:B:35:ASP:N	2.49	0.45
1:B:26:LEU:CD2	1:B:100:ILE:HG13	2.42	0.45
1:B:134:TYR:HD2	1:B:163:PHE:CZ	2.34	0.45
1:E:126:ILE:CG2	1:E:134:TYR:CZ	2.99	0.45
1:F:126:ILE:CG2	1:F:134:TYR:CZ	2.99	0.45
1:E:206:ILE:HG12	1:E:253:LEU:HD13	1.98	0.45
1:F:477:GLU:CB	1:F:662:ARG:NH1	2.79	0.45
1:B:485:VAL:HG11	1:B:645:ILE:HD11	1.98	0.45
1:E:292:GLU:HA	1:E:295:LYS:NZ	2.31	0.45
1:A:538:ASN:ND2	1:A:569:ALA:O	2.50	0.45
1:E:682:PHE:HE2	1:E:690:ILE:HD11	1.81	0.45
1:C:542:ILE:HD12	1:C:562:ILE:HD13	1.98	0.45
1:D:126:ILE:CG2	1:D:134:TYR:CZ	2.99	0.45
1:B:126:ILE:CD1	1:B:130:LEU:HD22	2.34	0.45
1:E:161:VAL:HG22	1:E:162:GLU:H	1.81	0.45
1:F:406:HIS:CE1	1:F:461:PRO:CD	2.98	0.45
1:D:513:GLY:HA3	1:D:639:LEU:HD22	1.93	0.45
1:E:477:GLU:CB	1:E:662:ARG:NH1	2.79	0.45
1:F:52:PHE:O	1:F:53:ARG:HB2	2.15	0.45
1:E:227:PRO:HB3	1:E:340:HIS:CD2	2.51	0.45
1:A:227:PRO:HB3	1:A:340:HIS:CD2	2.51	0.45
1:D:292:GLU:HA	1:D:295:LYS:NZ	2.31	0.45
1:F:738:GLU:OE2	1:F:741:ARG:NH1	2.49	0.45
1:F:56:THR:HG23	1:F:68:VAL:CG1	2.46	0.45
1:B:26:LEU:HD11	1:B:100:ILE:HD11	1.98	0.45
1:C:26:LEU:HD11	1:C:100:ILE:HD11	1.98	0.45
1:A:134:TYR:HD2	1:A:163:PHE:CZ	2.33	0.45
1:C:570:ALA:HB1	1:C:616:ASN:HB3	1.98	0.45
1:D:91:ASN:ND2	1:D:150:ASP:HB2	2.31	0.45
1:F:485:VAL:HG11	1:F:645:ILE:HD11	1.98	0.45
1:E:393:ASP:OD1	1:E:394:VAL:N	2.47	0.45
1:E:56:THR:HG23	1:E:68:VAL:CG1	2.46	0.45
1:E:56:THR:HG23	1:E:68:VAL:HG13	1.98	0.45
1:A:738:GLU:OE2	1:A:741:ARG:NH1	2.49	0.45
1:A:126:ILE:CG2	1:A:134:TYR:CZ	2.99	0.45
1:F:406:HIS:HE1	1:F:459:SER:HB2	1.78	0.45
1:B:312:LYS:HZ2	1:B:316:THR:HA	1.81	0.45
1:B:607:GLU:HG2	1:C:465:ARG:NH1	2.30	0.45
1:E:513:GLY:HA3	1:E:639:LEU:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:ILE:N	1:C:82:ILE:HD12	2.31	0.45
1:C:674:PHE:HD1	1:C:677:LYS:HZ3	1.60	0.45
1:D:227:PRO:HB3	1:D:340:HIS:CD2	2.51	0.45
1:C:506:PHE:O	1:D:664:SER:HB3	2.16	0.45
1:B:738:GLU:OE2	1:B:741:ARG:NH1	2.49	0.45
1:C:35:ASP:OD1	1:C:35:ASP:N	2.49	0.45
1:C:292:GLU:HA	1:C:295:LYS:NZ	2.31	0.45
1:F:134:TYR:HD2	1:F:163:PHE:CZ	2.33	0.45
1:A:406:HIS:HE1	1:A:459:SER:HB2	1.78	0.45
1:F:513:GLY:HA3	1:F:639:LEU:HA	1.97	0.45
1:B:218:GLU:OE1	1:C:454:TRP:HZ2	1.99	0.45
1:D:538:ASN:ND2	1:D:569:ALA:O	2.50	0.45
1:B:405:GLY:HA3	1:B:464:LEU:HD23	1.99	0.45
1:D:485:VAL:HG11	1:D:645:ILE:HD11	1.98	0.45
1:A:393:ASP:OD1	1:A:394:VAL:N	2.47	0.45
1:B:542:ILE:HD12	1:B:562:ILE:HD13	1.98	0.45
1:C:567:ARG:HH11	1:C:568:GLN:NE2	2.14	0.45
1:C:206:ILE:HG12	1:C:253:LEU:HD13	1.98	0.45
1:F:542:ILE:HD12	1:F:562:ILE:HD13	1.98	0.45
1:A:35:ASP:N	1:A:35:ASP:OD1	2.49	0.45
1:A:269:ILE:HD11	1:A:290:PHE:CE1	2.46	0.44
1:F:119:ILE:HG13	1:F:191:ARG:HB2	1.99	0.44
1:C:312:LYS:CE	1:C:321:GLU:CG	2.87	0.44
1:F:570:ALA:HB1	1:F:616:ASN:HB3	1.98	0.44
1:A:91:ASN:ND2	1:A:150:ASP:HB2	2.31	0.44
1:B:82:ILE:N	1:B:82:ILE:HD12	2.31	0.44
1:C:485:VAL:HG11	1:C:645:ILE:HD11	1.98	0.44
1:E:546:GLU:HA	1:E:549:THR:HG22	2.00	0.44
1:E:538:ASN:ND2	1:E:569:ALA:O	2.50	0.44
1:E:365:ARG:NH1	1:F:460:ASN:HD22	2.14	0.44
1:B:406:HIS:CE1	1:B:461:PRO:CD	2.98	0.44
1:C:405:GLY:HA3	1:C:464:LEU:HD23	1.99	0.44
1:D:570:ALA:HB1	1:D:616:ASN:HB3	1.98	0.44
1:F:448:THR:O	1:F:451:ASP:HB2	2.17	0.44
1:C:27:ILE:H	1:C:82:ILE:CD1	2.25	0.44
1:D:56:THR:HG23	1:D:68:VAL:HG13	1.98	0.44
1:E:134:TYR:HD2	1:E:163:PHE:CZ	2.33	0.44
1:F:406:HIS:CD2	1:F:461:PRO:HG3	2.53	0.44
1:F:269:ILE:HD11	1:F:290:PHE:CE1	2.46	0.44
1:B:91:ASN:ND2	1:B:150:ASP:HB2	2.31	0.44
1:C:227:PRO:HB3	1:C:340:HIS:CD2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:697:LEU:O	1:F:700:ARG:HB3	2.18	0.44
1:C:697:LEU:O	1:C:700:ARG:HB3	2.18	0.44
1:D:35:ASP:N	1:D:35:ASP:OD1	2.49	0.44
1:B:131:PHE:HB3	1:B:135:LEU:HD12	2.00	0.44
1:E:119:ILE:HG13	1:E:191:ARG:HB2	1.99	0.44
1:A:567:ARG:HH11	1:A:568:GLN:NE2	2.14	0.44
1:B:567:ARG:HH11	1:B:568:GLN:NE2	2.14	0.44
1:C:448:THR:O	1:C:451:ASP:HB2	2.17	0.44
1:A:477:GLU:CB	1:A:662:ARG:NH1	2.79	0.44
1:F:56:THR:HG23	1:F:68:VAL:HG13	1.98	0.44
1:E:218:GLU:OE1	1:F:454:TRP:HZ2	1.99	0.44
1:E:35:ASP:OD1	1:E:35:ASP:N	2.49	0.44
1:E:131:PHE:HB3	1:E:135:LEU:HD12	2.00	0.44
1:E:405:GLY:HA3	1:E:464:LEU:HD23	1.99	0.44
1:B:406:HIS:HE1	1:B:459:SER:HB2	1.78	0.44
1:A:406:HIS:CD2	1:A:461:PRO:HG3	2.53	0.44
1:F:224:LEU:HD23	1:F:298:PRO:HB3	2.00	0.44
1:C:224:LEU:HD23	1:C:298:PRO:HB3	2.00	0.44
1:A:224:LEU:HD23	1:A:298:PRO:HB3	2.00	0.44
1:D:601:ILE:CG2	1:D:633:ILE:HD11	2.48	0.44
1:C:601:ILE:CG2	1:C:633:ILE:HD11	2.48	0.44
1:B:448:THR:O	1:B:451:ASP:HB2	2.17	0.44
1:A:448:THR:O	1:A:451:ASP:HB2	2.17	0.44
1:E:601:ILE:CG2	1:E:633:ILE:HD11	2.48	0.44
1:D:206:ILE:HG12	1:D:253:LEU:HD13	1.98	0.44
1:D:697:LEU:O	1:D:700:ARG:HB3	2.18	0.44
1:A:119:ILE:HG13	1:A:191:ARG:HB2	1.99	0.44
1:D:365:ARG:NH1	1:E:460:ASN:HD22	2.15	0.44
1:E:224:LEU:HD23	1:E:298:PRO:HB3	2.00	0.44
1:E:319:GLU:CG	1:E:322:ARG:HH21	2.21	0.44
1:E:448:THR:O	1:E:451:ASP:HB2	2.17	0.44
3:B:1001:OJA:H031	3:B:1001:OJA:H052	1.82	0.44
1:A:697:LEU:O	1:A:700:ARG:HB3	2.18	0.44
1:C:373:ASP:HB2	1:C:470:GLU:CD	2.38	0.44
1:A:542:ILE:HD12	1:A:562:ILE:HD13	1.98	0.44
1:F:393:ASP:OD1	1:F:394:VAL:N	2.47	0.44
1:E:406:HIS:CD2	1:E:461:PRO:HG3	2.53	0.44
1:B:406:HIS:CD2	1:B:461:PRO:HG3	2.53	0.44
1:A:405:GLY:HA3	1:A:464:LEU:HD23	1.99	0.44
1:E:570:ALA:HB1	1:E:616:ASN:HB3	1.98	0.44
1:F:601:ILE:CG2	1:F:633:ILE:HD11	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:448:THR:O	1:D:451:ASP:HB2	2.17	0.44
1:E:485:VAL:HG11	1:E:645:ILE:HD11	1.98	0.44
1:E:697:LEU:O	1:E:700:ARG:HB3	2.18	0.44
1:B:538:ASN:ND2	1:B:569:ALA:O	2.50	0.44
1:B:25:ARG:NE	1:B:45:LYS:HE2	2.31	0.44
1:D:373:ASP:HB2	1:D:470:GLU:CD	2.38	0.44
1:B:697:LEU:O	1:B:700:ARG:HB3	2.18	0.44
1:D:546:GLU:HA	1:D:549:THR:HG22	2.00	0.44
1:F:405:GLY:HA3	1:F:464:LEU:HD23	1.99	0.44
1:C:406:HIS:CD2	1:C:461:PRO:HG3	2.53	0.44
1:D:224:LEU:HD23	1:D:298:PRO:HB3	2.00	0.44
1:B:224:LEU:HD23	1:B:298:PRO:HB3	2.00	0.44
1:E:307:ASP:O	1:E:311:PRO:HG3	2.18	0.44
1:C:685:ALA:HB2	2:C:900:ADP:H5'1	2.00	0.44
1:E:354:ASP:OD1	1:E:355:PRO:HD2	2.18	0.44
1:D:354:ASP:OD1	1:D:355:PRO:HD2	2.18	0.44
1:D:542:ILE:HD12	1:D:562:ILE:HD13	1.98	0.44
1:C:218:GLU:OE1	1:D:454:TRP:HZ2	2.00	0.44
1:E:100:ILE:CD1	1:E:102:ILE:HD11	2.48	0.43
1:C:131:PHE:N	1:C:131:PHE:CD1	2.85	0.43
1:A:127:THR:HG22	1:A:438:ASP:CG	2.39	0.43
1:A:131:PHE:HB3	1:A:135:LEU:HD12	2.00	0.43
1:B:119:ILE:HG13	1:B:191:ARG:HB2	1.99	0.43
1:D:612:SER:C	1:D:613:THR:HG1	2.10	0.43
1:C:25:ARG:NH2	1:C:45:LYS:HE2	2.33	0.43
1:D:98:ASP:OD1	1:D:99:VAL:N	2.49	0.43
1:E:685:ALA:HB2	2:E:900:ADP:H5'1	2.00	0.43
1:D:685:ALA:HB2	2:D:900:ADP:H5'1	2.00	0.43
1:E:510:PRO:HG2	1:E:614:LYS:CD	2.48	0.43
1:F:546:GLU:HA	1:F:549:THR:HG22	2.00	0.43
1:E:373:ASP:HB2	1:E:470:GLU:CD	2.38	0.43
1:E:472:PRO:HD3	1:E:539:PHE:HB2	2.00	0.43
1:C:100:ILE:H	1:C:100:ILE:HG13	1.73	0.43
1:D:131:PHE:HB3	1:D:135:LEU:HD12	2.00	0.43
1:E:406:HIS:HE1	1:E:459:SER:HB2	1.78	0.43
1:E:224:LEU:O	1:E:298:PRO:HG3	2.18	0.43
1:F:307:ASP:O	1:F:311:PRO:HG3	2.18	0.43
1:D:25:ARG:NH2	1:D:45:LYS:HE2	2.33	0.43
1:D:27:ILE:HB	1:D:81:LYS:HG2	2.01	0.43
1:C:27:ILE:HB	1:C:81:LYS:HG2	2.00	0.43
1:A:27:ILE:HB	1:A:81:LYS:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:510:PRO:HG2	1:F:614:LYS:CD	2.48	0.43
1:C:40:SER:HA	1:C:72:LEU:O	2.19	0.43
1:D:40:SER:HA	1:D:72:LEU:O	2.19	0.43
1:B:373:ASP:HB2	1:B:470:GLU:CD	2.38	0.43
1:D:119:ILE:HG13	1:D:191:ARG:HB2	1.99	0.43
1:D:751:ASP:O	1:D:754:LYS:N	2.52	0.43
3:A:1001:OJA:H341	3:A:1001:OJA:H011	1.81	0.43
1:D:112:LYS:HB3	1:D:113:ARG:HG2	2.00	0.43
1:C:354:ASP:OD1	1:C:355:PRO:HD2	2.18	0.43
1:F:100:ILE:CD1	1:F:102:ILE:HD11	2.48	0.43
1:C:100:ILE:CD1	1:C:102:ILE:HD11	2.48	0.43
1:B:127:THR:HG22	1:B:438:ASP:CG	2.39	0.43
1:E:406:HIS:CE1	1:E:461:PRO:CD	2.98	0.43
1:A:406:HIS:CE1	1:A:461:PRO:CD	2.98	0.43
1:D:567:ARG:HH11	1:D:568:GLN:NE2	2.14	0.43
1:B:601:ILE:CG2	1:B:633:ILE:HD11	2.48	0.43
1:B:27:ILE:HB	1:B:81:LYS:HG2	2.01	0.43
1:B:472:PRO:HD3	1:B:539:PHE:HB2	2.00	0.43
1:C:472:PRO:HD3	1:C:539:PHE:HB2	2.00	0.43
1:A:100:ILE:CD1	1:A:102:ILE:HD11	2.48	0.43
1:B:25:ARG:NH2	1:B:45:LYS:HE2	2.33	0.43
1:F:27:ILE:HB	1:F:81:LYS:HG2	2.00	0.43
1:E:27:ILE:HB	1:E:81:LYS:HG2	2.01	0.43
1:A:510:PRO:HG2	1:A:614:LYS:CD	2.48	0.43
1:C:614:LYS:HB2	3:C:1001:OJA:C27	2.49	0.43
1:B:40:SER:HA	1:B:72:LEU:O	2.19	0.43
1:E:546:GLU:O	1:E:549:THR:HG22	2.19	0.43
1:F:472:PRO:HD3	1:F:539:PHE:HB2	2.00	0.43
1:F:354:ASP:OD1	1:F:355:PRO:HD2	2.18	0.43
1:E:112:LYS:HB3	1:E:113:ARG:HG2	2.00	0.43
1:E:26:LEU:CD2	1:E:100:ILE:HG13	2.42	0.43
1:D:127:THR:HB	1:D:438:ASP:CG	2.39	0.43
1:D:406:HIS:CD2	1:D:461:PRO:HG3	2.53	0.43
1:D:224:LEU:O	1:D:298:PRO:HG3	2.18	0.43
1:F:224:LEU:O	1:F:298:PRO:HG3	2.18	0.43
1:C:224:LEU:O	1:C:298:PRO:HG3	2.18	0.43
1:E:607:GLU:HG2	1:F:465:ARG:NH1	2.30	0.43
1:E:25:ARG:NH2	1:E:45:LYS:HE2	2.33	0.43
1:D:89:ARG:NH2	1:D:203:TYR:HE1	2.17	0.43
1:C:89:ARG:NH2	1:C:203:TYR:HE1	2.17	0.43
1:C:510:PRO:HG2	1:C:614:LYS:CD	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:SER:HA	1:A:72:LEU:O	2.19	0.43
1:D:100:ILE:CD1	1:D:102:ILE:HD11	2.48	0.43
1:C:131:PHE:HB3	1:C:135:LEU:HD12	2.00	0.43
1:E:127:THR:HB	1:E:438:ASP:CG	2.39	0.43
1:A:123:VAL:HG13	1:A:124:GLU:HG2	2.01	0.43
1:A:224:LEU:CD2	1:A:298:PRO:HB3	2.46	0.43
1:A:224:LEU:O	1:A:298:PRO:HG3	2.18	0.43
1:D:307:ASP:O	1:D:311:PRO:HG3	2.18	0.43
1:B:685:ALA:HB2	2:B:900:ADP:H5'1	2.00	0.43
1:D:510:PRO:HG2	1:D:614:LYS:CD	2.48	0.43
1:F:546:GLU:O	1:F:549:THR:HG22	2.19	0.43
1:A:115:HIS:HB3	1:A:167:GLU:O	2.19	0.43
1:A:546:GLU:O	1:A:549:THR:HG22	2.19	0.43
1:B:546:GLU:O	1:B:549:THR:HG22	2.19	0.43
1:B:100:ILE:CD1	1:B:102:ILE:HD11	2.48	0.43
1:E:131:PHE:N	1:E:131:PHE:CD1	2.85	0.43
1:C:119:ILE:HG13	1:C:191:ARG:HB2	1.99	0.43
1:D:224:LEU:HD23	1:D:298:PRO:CB	2.48	0.43
1:E:751:ASP:O	1:E:754:LYS:N	2.52	0.43
1:B:751:ASP:O	1:B:754:LYS:N	2.52	0.43
1:A:349:ARG:O	1:A:352:SER:OG	2.26	0.43
1:B:614:LYS:HB2	3:B:1001:OJA:C27	2.49	0.43
1:B:510:PRO:HG2	1:B:614:LYS:CD	2.48	0.43
1:A:546:GLU:HA	1:A:549:THR:HG22	2.00	0.43
1:B:546:GLU:HA	1:B:549:THR:HG22	2.00	0.43
1:A:354:ASP:OD1	1:A:355:PRO:HD2	2.18	0.43
1:A:472:PRO:HD3	1:A:539:PHE:HB2	2.00	0.43
1:F:131:PHE:HB3	1:F:135:LEU:HD12	2.00	0.43
1:A:601:ILE:CG2	1:A:633:ILE:HD11	2.48	0.43
1:C:98:ASP:OD1	1:C:99:VAL:N	2.49	0.43
1:B:517:TYR:CE2	1:B:758:PHE:CD2	3.07	0.43
1:A:503:PHE:CD2	1:B:699:ILE:HD13	2.54	0.43
1:E:40:SER:HA	1:E:72:LEU:O	2.19	0.43
1:F:373:ASP:HB2	1:F:470:GLU:CD	2.38	0.43
1:B:354:ASP:OD1	1:B:355:PRO:HD2	2.18	0.43
1:D:144:ARG:O	1:D:146:ILE:HG12	2.19	0.43
1:F:144:ARG:O	1:F:146:ILE:HG12	2.19	0.43
1:E:144:ARG:O	1:E:146:ILE:HG12	2.19	0.43
1:C:127:THR:HG22	1:C:438:ASP:CG	2.39	0.43
1:A:307:ASP:O	1:A:311:PRO:HG3	2.18	0.43
1:C:210:ARG:HG3	1:C:212:GLN:CG	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:25:ARG:NH2	1:F:45:LYS:HE2	2.33	0.43
1:D:349:ARG:O	1:D:352:SER:OG	2.26	0.43
1:C:751:ASP:O	1:C:754:LYS:N	2.52	0.43
1:F:685:ALA:HB2	2:F:900:ADP:H5'1	2.00	0.43
1:D:546:GLU:O	1:D:549:THR:HG22	2.19	0.43
1:B:217:LYS:HE2	1:B:261:GLU:OE2	2.19	0.43
1:F:112:LYS:HB3	1:F:113:ARG:HG2	2.00	0.43
1:C:217:LYS:HE2	1:C:261:GLU:OE2	2.19	0.43
1:A:112:LYS:HB3	1:A:113:ARG:HG2	2.00	0.43
1:B:127:THR:HB	1:B:438:ASP:CG	2.39	0.42
1:B:131:PHE:CD1	1:B:131:PHE:N	2.85	0.42
1:F:131:PHE:N	1:F:131:PHE:CD1	2.85	0.42
1:A:127:THR:HB	1:A:438:ASP:CG	2.39	0.42
1:F:119:ILE:O	1:F:120:ASP:HB3	2.19	0.42
1:F:123:VAL:HG13	1:F:124:GLU:HG2	2.01	0.42
1:C:406:HIS:CE1	1:C:461:PRO:CD	2.98	0.42
1:A:751:ASP:O	1:A:754:LYS:N	2.52	0.42
1:F:751:ASP:O	1:F:754:LYS:N	2.52	0.42
1:B:89:ARG:NH2	1:B:203:TYR:HE1	2.17	0.42
1:E:89:ARG:NH2	1:E:203:TYR:HE1	2.17	0.42
1:A:517:TYR:CE2	1:A:758:PHE:CD2	3.07	0.42
1:F:519:PRO:O	4:F:2006:HOH:O	2.22	0.42
2:E:807:ADP:C8	2:E:807:ADP:H5'1	2.54	0.42
1:A:230:PHE:CE2	1:A:237:PRO:HB3	2.54	0.42
1:B:230:PHE:CE2	1:B:237:PRO:HB3	2.54	0.42
1:F:538:ASN:ND2	1:F:569:ALA:O	2.50	0.42
1:A:373:ASP:HB2	1:A:470:GLU:CD	2.38	0.42
1:A:664:SER:HB3	1:F:506:PHE:O	2.18	0.42
1:F:127:THR:HB	1:F:438:ASP:CG	2.39	0.42
1:B:286:LEU:HD23	1:B:331:LEU:CD1	2.49	0.42
1:E:119:ILE:CD1	1:E:191:ARG:HB2	2.50	0.42
1:D:405:GLY:HA3	1:D:464:LEU:HD23	1.99	0.42
1:C:406:HIS:HE1	1:C:459:SER:HB2	1.78	0.42
1:B:224:LEU:O	1:B:298:PRO:HG3	2.18	0.42
1:A:607:GLU:HG2	1:B:465:ARG:NH1	2.31	0.42
1:A:25:ARG:NH2	1:A:45:LYS:HE2	2.33	0.42
1:A:685:ALA:HB2	2:A:900:ADP:H5'1	2.00	0.42
2:C:807:ADP:C8	2:C:807:ADP:H5'1	2.54	0.42
1:A:502:LYS:NZ	1:B:702:SER:OG	2.37	0.42
1:D:115:HIS:HB3	1:D:167:GLU:O	2.19	0.42
1:F:115:HIS:HB3	1:F:167:GLU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:THR:HB	1:C:438:ASP:CG	2.39	0.42
1:D:127:THR:HG22	1:D:438:ASP:CG	2.39	0.42
1:A:131:PHE:N	1:A:131:PHE:CD1	2.85	0.42
1:A:269:ILE:CG2	1:A:274:ILE:CD1	2.82	0.42
1:C:402:GLU:CG	1:C:456:LEU:HD22	2.32	0.42
1:A:119:ILE:CD1	1:A:191:ARG:HB2	2.50	0.42
1:B:119:ILE:CD1	1:B:191:ARG:HB2	2.49	0.42
1:E:312:LYS:CE	1:E:321:GLU:CG	2.87	0.42
1:C:307:ASP:O	1:C:311:PRO:HG3	2.18	0.42
1:A:147:ARG:CZ	1:A:150:ASP:HB3	2.50	0.42
1:B:147:ARG:CZ	1:B:150:ASP:HB3	2.49	0.42
1:A:89:ARG:NH2	1:A:203:TYR:HE1	2.17	0.42
1:F:89:ARG:NH2	1:F:203:TYR:HE1	2.17	0.42
1:E:98:ASP:OD1	1:E:99:VAL:N	2.49	0.42
3:F:1001:OJA:H052	3:F:1001:OJA:H031	1.83	0.42
1:E:229:LEU:O	1:E:233:ILE:HG22	2.20	0.42
2:D:807:ADP:C8	2:D:807:ADP:H5'1	2.54	0.42
1:B:144:ARG:O	1:B:146:ILE:HG12	2.19	0.42
1:D:217:LYS:HE2	1:D:261:GLU:OE2	2.19	0.42
1:C:230:PHE:CE2	1:C:237:PRO:HB3	2.54	0.42
1:A:26:LEU:CD2	1:A:100:ILE:HG13	2.42	0.42
1:A:465:ARG:NH1	1:F:607:GLU:HG2	2.30	0.42
1:C:229:LEU:O	1:C:233:ILE:HG22	2.19	0.42
2:F:807:ADP:H5'1	2:F:807:ADP:C8	2.54	0.42
1:A:144:ARG:O	1:A:146:ILE:HG12	2.19	0.42
1:D:472:PRO:HD3	1:D:539:PHE:HB2	2.00	0.42
1:C:144:ARG:O	1:C:146:ILE:HG12	2.19	0.42
1:B:115:HIS:HB3	1:B:167:GLU:O	2.19	0.42
1:C:546:GLU:HA	1:C:549:THR:HG22	2.00	0.42
1:C:538:ASN:ND2	1:C:569:ALA:O	2.50	0.42
1:A:120:ASP:HA	1:A:191:ARG:H	1.85	0.42
1:C:517:TYR:CE2	1:C:758:PHE:CD2	3.07	0.42
1:A:614:LYS:HB2	3:A:1001:OJA:C27	2.49	0.42
1:B:519:PRO:O	4:B:2006:HOH:O	2.22	0.42
1:F:40:SER:HA	1:F:72:LEU:O	2.19	0.42
1:D:229:LEU:O	1:D:233:ILE:HG22	2.20	0.42
1:C:286:LEU:HD23	1:C:331:LEU:CD1	2.49	0.42
1:E:123:VAL:HG13	1:E:124:GLU:HG2	2.01	0.42
1:D:406:HIS:HE1	1:D:459:SER:HB2	1.78	0.42
1:E:406:HIS:CE1	1:E:461:PRO:HG3	2.55	0.42
1:E:482:LEU:O	1:E:486:LYS:CG	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:ASP:O	1:B:311:PRO:HG3	2.18	0.42
1:D:614:LYS:HB2	3:D:1001:OJA:C27	2.49	0.42
1:B:229:LEU:O	1:B:233:ILE:HG22	2.20	0.42
1:C:112:LYS:HB3	1:C:113:ARG:HG2	2.00	0.42
1:A:217:LYS:HE2	1:A:261:GLU:OE2	2.19	0.42
1:F:230:PHE:CE2	1:F:237:PRO:HB3	2.54	0.42
1:E:286:LEU:HD23	1:E:331:LEU:CD1	2.49	0.42
1:A:286:LEU:HD23	1:A:331:LEU:CD1	2.49	0.42
1:A:119:ILE:O	1:A:120:ASP:HB3	2.19	0.42
1:F:120:ASP:HA	1:F:191:ARG:H	1.85	0.42
1:F:119:ILE:CD1	1:F:191:ARG:HB2	2.49	0.42
1:C:120:ASP:HA	1:C:191:ARG:H	1.85	0.42
1:D:406:HIS:CE1	1:D:461:PRO:HG3	2.54	0.42
1:F:406:HIS:CE1	1:F:461:PRO:HG3	2.55	0.42
1:D:560:ARG:HE	1:E:465:ARG:NH1	2.18	0.42
1:D:601:ILE:HG23	1:D:633:ILE:HD11	2.02	0.42
1:F:147:ARG:CZ	1:F:150:ASP:HB3	2.49	0.42
1:F:100:ILE:HG13	1:F:100:ILE:H	1.73	0.42
1:D:286:LEU:HD23	1:D:331:LEU:CD1	2.49	0.42
1:D:123:VAL:HG13	1:D:124:GLU:HG2	2.01	0.42
1:E:120:ASP:HA	1:E:191:ARG:H	1.85	0.42
1:E:224:LEU:HD11	1:E:342:ILE:HG12	2.02	0.42
1:F:312:LYS:CE	1:F:321:GLU:CG	2.87	0.42
1:E:754:LYS:HA	1:E:757:MET:CE	2.49	0.42
1:E:517:TYR:CE2	1:E:758:PHE:CD2	3.07	0.42
1:F:229:LEU:O	1:F:233:ILE:HG22	2.20	0.42
1:C:546:GLU:O	1:C:549:THR:HG22	2.19	0.42
1:A:508:MET:HG3	1:B:692:GLN:HE22	1.84	0.42
1:F:267:PHE:CE2	1:F:289:ALA:CB	2.91	0.42
1:D:517:TYR:CE2	1:D:758:PHE:CD2	3.07	0.42
3:C:1001:OJA:H341	3:C:1001:OJA:H011	1.81	0.42
1:D:230:PHE:CE2	1:D:237:PRO:HB3	2.54	0.42
1:E:216:ILE:O	1:E:220:VAL:HG22	2.20	0.42
1:A:454:TRP:HZ2	1:F:218:GLU:OE1	2.03	0.42
1:A:100:ILE:H	1:A:100:ILE:HG13	1.73	0.42
1:A:267:PHE:CE2	1:A:289:ALA:CB	2.91	0.42
1:D:119:ILE:O	1:D:120:ASP:HB3	2.20	0.42
1:B:120:ASP:HA	1:B:191:ARG:H	1.85	0.42
1:A:612:SER:HB3	1:B:464:LEU:CD2	2.50	0.42
1:C:601:ILE:HG23	1:C:633:ILE:HD11	2.02	0.42
1:D:477:GLU:HB3	1:D:662:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:614:LYS:HB2	3:F:1001:OJA:C27	2.49	0.42
1:B:670:VAL:HG23	1:B:733:ARG:CD	2.50	0.42
2:B:807:ADP:C8	2:B:807:ADP:H5'1	2.54	0.42
1:C:393:ASP:OD1	1:C:394:VAL:N	2.47	0.42
1:C:115:HIS:HB3	1:C:167:GLU:O	2.19	0.42
1:E:230:PHE:CE2	1:E:237:PRO:HB3	2.54	0.42
1:F:26:LEU:HD22	1:F:100:ILE:O	2.02	0.41
1:E:119:ILE:O	1:E:120:ASP:HB3	2.20	0.41
1:D:607:GLU:HG2	1:E:465:ARG:NH1	2.30	0.41
1:A:754:LYS:HA	1:A:757:MET:CE	2.49	0.41
1:F:517:TYR:CE2	1:F:758:PHE:CD2	3.07	0.41
1:E:477:GLU:HB3	1:E:662:ARG:NH1	2.35	0.41
1:E:614:LYS:HB2	3:E:1001:OJA:C27	2.49	0.41
1:A:519:PRO:O	4:A:2006:HOH:O	2.22	0.41
1:A:670:VAL:HG23	1:A:733:ARG:CD	2.50	0.41
1:C:386:LYS:HE2	1:C:386:LYS:HB3	1.83	0.41
1:B:119:ILE:O	1:B:120:ASP:HB3	2.20	0.41
1:C:119:ILE:CD1	1:C:191:ARG:HB2	2.50	0.41
1:C:119:ILE:O	1:C:120:ASP:HB3	2.20	0.41
1:B:406:HIS:CE1	1:B:461:PRO:HG3	2.55	0.41
1:D:224:LEU:HD11	1:D:342:ILE:HG12	2.02	0.41
1:C:312:LYS:NZ	1:C:317:HIS:O	2.53	0.41
1:C:560:ARG:HE	1:D:465:ARG:NH1	2.18	0.41
1:C:477:GLU:HB3	1:C:662:ARG:NH1	2.35	0.41
1:D:503:PHE:CD2	1:E:699:ILE:HD13	2.55	0.41
1:F:217:LYS:HE2	1:F:261:GLU:OE2	2.19	0.41
1:E:503:PHE:CD2	1:F:699:ILE:HD13	2.55	0.41
1:B:112:LYS:HB3	1:B:113:ARG:HG2	2.00	0.41
1:F:286:LEU:HD23	1:F:331:LEU:CD1	2.49	0.41
1:C:286:LEU:CD2	1:C:331:LEU:CD1	2.99	0.41
1:C:670:VAL:HG23	1:C:733:ARG:CD	2.50	0.41
1:F:670:VAL:HG23	1:F:733:ARG:CD	2.50	0.41
1:E:217:LYS:HE2	1:E:261:GLU:OE2	2.19	0.41
1:B:126:ILE:HG22	1:B:439:ALA:HB1	2.03	0.41
1:F:126:ILE:HG22	1:F:439:ALA:HB1	2.03	0.41
1:D:119:ILE:CD1	1:D:191:ARG:HB2	2.50	0.41
1:F:224:LEU:HD11	1:F:342:ILE:HG12	2.02	0.41
1:A:312:LYS:NZ	1:A:317:HIS:O	2.53	0.41
1:F:349:ARG:O	1:F:352:SER:OG	2.26	0.41
1:D:446:ALA:O	1:D:448:THR:HG23	2.21	0.41
1:C:81:LYS:C	1:C:82:ILE:HD12	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:807:ADP:H5'1	2:A:807:ADP:C8	2.54	0.41
1:B:520:PRO:HD2	1:B:747:VAL:HG22	2.02	0.41
1:D:131:PHE:N	1:D:131:PHE:CD1	2.85	0.41
1:A:126:ILE:HD13	1:A:130:LEU:CG	2.42	0.41
1:C:406:HIS:CE1	1:C:461:PRO:HG3	2.55	0.41
1:C:147:ARG:CZ	1:C:150:ASP:HB3	2.49	0.41
1:D:81:LYS:C	1:D:82:ILE:HD12	2.41	0.41
1:B:477:GLU:HB3	1:B:662:ARG:NH1	2.35	0.41
1:D:670:VAL:HG23	1:D:733:ARG:CD	2.50	0.41
1:E:670:VAL:HG23	1:E:733:ARG:CD	2.50	0.41
1:D:520:PRO:HD2	1:D:747:VAL:HG22	2.02	0.41
1:F:216:ILE:O	1:F:220:VAL:HG22	2.20	0.41
1:C:126:ILE:HG22	1:C:439:ALA:HB1	2.03	0.41
1:E:126:ILE:HG22	1:E:439:ALA:HB1	2.03	0.41
1:D:255:ALA:HB1	1:D:266:PHE:CE1	2.50	0.41
1:E:753:ARG:HG3	1:E:753:ARG:H	1.73	0.41
1:F:754:LYS:HA	1:F:757:MET:CE	2.49	0.41
1:A:229:LEU:O	1:A:233:ILE:HG22	2.20	0.41
1:E:115:HIS:HB3	1:E:167:GLU:O	2.19	0.41
1:D:100:ILE:HG13	1:D:100:ILE:H	1.73	0.41
1:B:126:ILE:HD13	1:B:130:LEU:CG	2.42	0.41
1:F:286:LEU:CD2	1:F:331:LEU:CD1	2.99	0.41
1:E:601:ILE:HG23	1:E:633:ILE:HD11	2.02	0.41
1:E:519:PRO:O	4:E:2006:HOH:O	2.22	0.41
1:D:216:ILE:O	1:D:220:VAL:HG22	2.20	0.41
1:B:414:LEU:HD12	1:B:455:ALA:HB1	2.03	0.41
1:E:127:THR:H	1:E:439:ALA:N	1.92	0.41
1:E:255:ALA:HB1	1:E:266:PHE:CE1	2.50	0.41
1:D:120:ASP:HA	1:D:191:ARG:H	1.85	0.41
1:C:123:VAL:HG13	1:C:124:GLU:HG2	2.01	0.41
1:A:224:LEU:HD11	1:A:342:ILE:HG12	2.02	0.41
1:E:560:ARG:HE	1:F:465:ARG:NH1	2.18	0.41
1:F:567:ARG:HH11	1:F:568:GLN:NE2	2.14	0.41
1:A:601:ILE:HG23	1:A:633:ILE:HD11	2.02	0.41
1:B:81:LYS:C	1:B:82:ILE:HD12	2.41	0.41
1:B:98:ASP:OD1	1:B:99:VAL:N	2.49	0.41
3:D:1001:OJA:H011	3:D:1001:OJA:H341	1.81	0.41
1:C:52:PHE:O	1:C:53:ARG:CB	2.69	0.41
1:B:491:GLU:OE1	1:B:495:TYR:CE2	2.74	0.41
1:D:126:ILE:HG22	1:D:439:ALA:HB1	2.03	0.41
1:E:127:THR:HG22	1:E:438:ASP:CG	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ILE:HG22	1:A:439:ALA:HB1	2.03	0.41
1:C:286:LEU:HD23	1:C:331:LEU:HD13	2.03	0.41
1:D:286:LEU:HD23	1:D:331:LEU:HD13	2.03	0.41
1:A:286:LEU:CD2	1:A:331:LEU:CD1	2.99	0.41
1:D:365:ARG:HD3	1:D:365:ARG:HA	1.92	0.41
1:B:560:ARG:HE	1:C:465:ARG:NH1	2.18	0.41
1:E:446:ALA:O	1:E:448:THR:HG23	2.21	0.41
1:F:601:ILE:HG23	1:F:633:ILE:HD11	2.02	0.41
1:C:446:ALA:O	1:C:448:THR:HG23	2.21	0.41
1:E:147:ARG:CZ	1:E:150:ASP:HB3	2.50	0.41
1:F:92:LEU:HB2	1:F:94:VAL:HG12	2.03	0.41
1:E:81:LYS:C	1:E:82:ILE:HD12	2.41	0.41
1:D:521:GLY:O	2:D:900:ADP:H8	2.04	0.41
1:A:521:GLY:O	2:A:900:ADP:H8	2.04	0.41
1:C:503:PHE:CD2	1:D:699:ILE:HD13	2.56	0.41
1:B:524:LYS:HE2	4:B:2006:HOH:O	2.21	0.41
1:A:524:LYS:HE2	4:A:2006:HOH:O	2.21	0.41
1:D:52:PHE:O	1:D:53:ARG:CB	2.69	0.41
1:C:445:LEU:HD12	1:C:445:LEU:O	2.21	0.41
1:C:520:PRO:HD2	1:C:747:VAL:HG22	2.02	0.41
1:C:251:LYS:HD2	1:C:346:ALA:HB1	2.03	0.41
1:B:503:PHE:CD2	1:C:699:ILE:HD13	2.56	0.41
1:B:108:VAL:HA	1:B:173:TYR:HE1	1.86	0.41
1:B:251:LYS:HD2	1:B:346:ALA:HB1	2.03	0.41
1:B:123:VAL:HG13	1:B:124:GLU:HG2	2.01	0.41
1:A:406:HIS:CE1	1:A:461:PRO:HG3	2.54	0.41
1:C:224:LEU:HD11	1:C:342:ILE:HG12	2.02	0.41
1:E:312:LYS:NZ	1:E:317:HIS:O	2.53	0.41
1:E:567:ARG:HH11	1:E:568:GLN:NE2	2.14	0.41
1:D:560:ARG:NH2	1:E:465:ARG:HG3	2.36	0.41
1:D:147:ARG:CZ	1:D:150:ASP:HB3	2.49	0.41
1:A:477:GLU:HB3	1:A:662:ARG:NH1	2.35	0.41
1:E:445:LEU:HD12	1:E:445:LEU:O	2.21	0.41
1:D:251:LYS:HD2	1:D:346:ALA:HB1	2.03	0.41
1:E:286:LEU:CD2	1:E:331:LEU:CD1	2.99	0.40
1:E:286:LEU:HD23	1:E:331:LEU:HD13	2.03	0.40
1:F:459:SER:CB	1:F:461:PRO:HD3	2.52	0.40
1:F:312:LYS:CE	1:F:321:GLU:HB3	2.51	0.40
1:D:312:LYS:CE	1:D:321:GLU:HB3	2.51	0.40
1:E:560:ARG:NH2	1:F:465:ARG:HG3	2.36	0.40
1:D:92:LEU:HB2	1:D:94:VAL:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ARG:HH22	1:A:203:TYR:HE1	1.70	0.40
1:F:81:LYS:C	1:F:82:ILE:HD12	2.41	0.40
1:F:98:ASP:OD1	1:F:99:VAL:N	2.49	0.40
1:B:480:GLY:N	2:B:900:ADP:N1	2.67	0.40
1:F:521:GLY:O	2:F:900:ADP:H8	2.04	0.40
1:F:477:GLU:HB3	1:F:662:ARG:NH1	2.35	0.40
1:C:35:ASP:OD2	1:C:38:VAL:HB	2.21	0.40
1:D:108:VAL:HA	1:D:173:TYR:HE1	1.86	0.40
1:F:108:VAL:HA	1:F:173:TYR:HE1	1.86	0.40
1:A:251:LYS:HD2	1:A:346:ALA:HB1	2.03	0.40
1:A:108:VAL:HA	1:A:173:TYR:HE1	1.86	0.40
1:D:414:LEU:HD12	1:D:455:ALA:HB1	2.03	0.40
1:D:26:LEU:CD2	1:D:100:ILE:HG13	2.42	0.40
1:B:459:SER:HB2	1:B:461:PRO:CD	2.52	0.40
1:E:312:LYS:CE	1:E:321:GLU:HB3	2.51	0.40
1:B:92:LEU:HB2	1:B:94:VAL:HG12	2.03	0.40
1:E:758:PHE:CE2	1:E:762:LEU:HD11	2.57	0.40
3:A:1001:OJA:H052	3:A:1001:OJA:H031	1.82	0.40
1:F:52:PHE:O	1:F:53:ARG:CB	2.69	0.40
1:C:491:GLU:OE1	1:C:495:TYR:CE2	2.74	0.40
1:F:445:LEU:HD12	1:F:445:LEU:O	2.21	0.40
1:E:108:VAL:HA	1:E:173:TYR:HE1	1.86	0.40
1:F:520:PRO:HD2	1:F:747:VAL:HG22	2.02	0.40
1:B:126:ILE:HG22	1:B:133:VAL:HG11	2.04	0.40
1:B:267:PHE:CE2	1:B:289:ALA:CA	3.05	0.40
1:B:286:LEU:CD2	1:B:331:LEU:CD1	2.99	0.40
1:B:286:LEU:HD23	1:B:331:LEU:HD13	2.03	0.40
1:D:286:LEU:CD2	1:D:331:LEU:CD1	2.99	0.40
1:A:290:PHE:CE2	1:A:331:LEU:HB3	2.57	0.40
1:B:753:ARG:HG3	1:B:753:ARG:H	1.73	0.40
1:B:89:ARG:HH22	1:B:203:TYR:HE1	1.70	0.40
1:C:92:LEU:HB2	1:C:94:VAL:HG12	2.03	0.40
1:C:496:PRO:HA	1:C:503:PHE:CE1	2.57	0.40
3:D:1001:OJA:H052	3:D:1001:OJA:H031	1.82	0.40
1:E:52:PHE:O	1:E:53:ARG:CB	2.69	0.40
1:A:491:GLU:OE1	1:A:495:TYR:CE2	2.74	0.40
1:F:102:ILE:HG22	1:F:103:GLN:N	2.37	0.40
1:D:26:LEU:HD22	1:D:100:ILE:O	2.02	0.40
1:D:290:PHE:CE2	1:D:331:LEU:HB3	2.57	0.40
1:C:459:SER:HB2	1:C:461:PRO:CD	2.52	0.40
1:B:560:ARG:NH2	1:C:465:ARG:HG3	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:LEU:HB2	1:E:94:VAL:HG12	2.03	0.40
1:D:758:PHE:CE2	1:D:762:LEU:HD11	2.56	0.40
1:E:521:GLY:O	2:E:900:ADP:H8	2.04	0.40
1:A:496:PRO:HA	1:A:503:PHE:CE1	2.57	0.40
1:B:52:PHE:O	1:B:53:ARG:CB	2.69	0.40
1:D:519:PRO:O	4:D:2006:HOH:O	2.22	0.40
1:F:491:GLU:OE1	1:F:495:TYR:CE2	2.74	0.40
1:A:445:LEU:O	1:A:445:LEU:HD12	2.21	0.40
1:F:251:LYS:HD2	1:F:346:ALA:HB1	2.03	0.40
1:E:520:PRO:HD2	1:E:747:VAL:HG22	2.02	0.40
1:D:583:ALA:HB3	1:D:628:ILE:HD12	2.04	0.40
1:A:216:ILE:O	1:A:220:VAL:HG22	2.20	0.40
1:B:630:ASP:OD2	1:B:632:ALA:HB3	2.22	0.40
1:E:251:LYS:HD2	1:E:346:ALA:HB1	2.03	0.40
1:C:290:PHE:CD2	1:C:331:LEU:HB3	2.57	0.40
1:B:290:PHE:CD2	1:B:331:LEU:HB3	2.57	0.40
1:D:459:SER:CB	1:D:461:PRO:HD3	2.52	0.40
1:C:560:ARG:NH2	1:D:465:ARG:HG3	2.37	0.40
1:B:446:ALA:O	1:B:448:THR:HG23	2.21	0.40
1:F:89:ARG:HH22	1:F:203:TYR:HE1	1.70	0.40
1:A:81:LYS:C	1:A:82:ILE:HD12	2.41	0.40
1:A:517:TYR:OH	1:A:644:TYR:HB2	2.22	0.40
1:C:521:GLY:O	2:C:900:ADP:H8	2.04	0.40
1:B:521:GLY:O	2:B:900:ADP:H8	2.04	0.40
1:F:496:PRO:HA	1:F:503:PHE:CE1	2.57	0.40
1:E:697:LEU:HD23	1:E:697:LEU:HA	1.89	0.40
1:E:630:ASP:OD2	1:E:632:ALA:HB3	2.22	0.40
1:E:414:LEU:HD12	1:E:455:ALA:HB1	2.03	0.40
1:F:630:ASP:OD2	1:F:632:ALA:HB3	2.22	0.40
1:C:216:ILE:O	1:C:220:VAL:HG22	2.20	0.40
1:B:244:TYR:CD2	1:B:350:PRO:HD3	2.57	0.40
1:C:583:ALA:HB3	1:C:628:ILE:HD12	2.04	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	719/806 (89%)	671 (93%)	41 (6%)	7 (1%)	19	21
1	B	719/806 (89%)	671 (93%)	41 (6%)	7 (1%)	19	21
1	C	719/806 (89%)	671 (93%)	41 (6%)	7 (1%)	19	21
1	D	719/806 (89%)	671 (93%)	41 (6%)	7 (1%)	19	21
1	E	719/806 (89%)	671 (93%)	41 (6%)	7 (1%)	19	21
1	F	719/806 (89%)	671 (93%)	41 (6%)	7 (1%)	19	21
All	All	4314/4836 (89%)	4026 (93%)	246 (6%)	42 (1%)	24	21

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
1	A	53	ARG
1	A	123	VAL
1	B	25	ARG
1	B	53	ARG
1	B	123	VAL
1	C	25	ARG
1	C	53	ARG
1	C	123	VAL
1	D	25	ARG
1	D	53	ARG
1	D	123	VAL
1	E	25	ARG
1	E	53	ARG
1	E	123	VAL
1	F	25	ARG
1	F	53	ARG
1	F	123	VAL
1	A	462	SER
1	B	462	SER
1	C	462	SER
1	D	462	SER
1	E	462	SER
1	F	462	SER
1	A	339	ALA
1	A	460	ASN

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Mol	Chain	Res	Type
1	B	339	ALA
1	B	460	ASN
1	C	339	ALA
1	C	460	ASN
1	D	339	ALA
1	D	460	ASN
1	E	339	ALA
1	E	460	ASN
1	F	339	ALA
1	F	460	ASN
1	A	22	ARG
1	B	22	ARG
1	C	22	ARG
1	D	22	ARG
1	E	22	ARG
1	F	22	ARG

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	615/678 (91%)	612 (100%)	3 (0%)	92	97
1	B	615/678 (91%)	612 (100%)	3 (0%)	92	97
1	C	615/678 (91%)	612 (100%)	3 (0%)	92	97
1	D	615/678 (91%)	612 (100%)	3 (0%)	92	97
1	E	615/678 (91%)	612 (100%)	3 (0%)	92	97
1	F	615/678 (91%)	612 (100%)	3 (0%)	92	97
All	All	3690/4068 (91%)	3672 (100%)	18 (0%)	92	97

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ILE
1	A	122	THR

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Mol	Chain	Res	Type
1	A	638	ARG
1	B	100	ILE
1	B	122	THR
1	B	638	ARG
1	C	100	ILE
1	C	122	THR
1	C	638	ARG
1	D	100	ILE
1	D	122	THR
1	D	638	ARG
1	E	100	ILE
1	E	122	THR
1	E	638	ARG
1	F	100	ILE
1	F	122	THR
1	F	638	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	HIS
1	A	226	HIS
1	A	406	HIS
1	A	421	GLN
1	A	460	ASN
1	A	533	ASN
1	A	536	GLN
1	A	568	GLN
1	A	616	ASN
1	A	692	GLN
1	A	763	GLN
1	B	115	HIS
1	B	226	HIS
1	B	406	HIS
1	B	421	GLN
1	B	460	ASN
1	B	533	ASN
1	B	536	GLN
1	B	568	GLN
1	B	616	ASN
1	B	692	GLN
1	B	763	GLN

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Mol	Chain	Res	Type
1	C	115	HIS
1	C	226	HIS
1	C	406	HIS
1	C	421	GLN
1	C	460	ASN
1	C	533	ASN
1	C	536	GLN
1	C	568	GLN
1	C	616	ASN
1	C	692	GLN
1	C	763	GLN
1	D	115	HIS
1	D	226	HIS
1	D	406	HIS
1	D	421	GLN
1	D	460	ASN
1	D	533	ASN
1	D	536	GLN
1	D	568	GLN
1	D	616	ASN
1	D	692	GLN
1	D	763	GLN
1	E	115	HIS
1	E	226	HIS
1	E	406	HIS
1	E	421	GLN
1	E	460	ASN
1	E	533	ASN
1	E	536	GLN
1	E	568	GLN
1	E	616	ASN
1	E	692	GLN
1	E	763	GLN
1	F	115	HIS
1	F	226	HIS
1	F	406	HIS
1	F	421	GLN
1	F	533	ASN
1	F	536	GLN
1	F	568	GLN
1	F	616	ASN
1	F	692	GLN

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Mol	Chain	Res	Type
1	F	763	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OJA	A	1001	-	37,38,38	0.94	3 (8%)	46,53,53	1.68	9 (19%)
2	ADP	A	807	-	24,29,29	0.96	1 (4%)	23,45,45	1.72	1 (4%)
2	ADP	A	900	-	24,29,29	0.97	1 (4%)	23,45,45	1.78	2 (8%)
3	OJA	B	1001	-	37,38,38	0.93	3 (8%)	46,53,53	1.67	10 (21%)
2	ADP	B	807	-	24,29,29	0.96	1 (4%)	23,45,45	1.72	1 (4%)
2	ADP	B	900	-	24,29,29	0.97	1 (4%)	23,45,45	1.77	2 (8%)
3	OJA	C	1001	-	37,38,38	0.94	3 (8%)	46,53,53	1.69	8 (17%)
2	ADP	C	807	-	24,29,29	0.95	1 (4%)	23,45,45	1.73	1 (4%)
2	ADP	C	900	-	24,29,29	0.97	1 (4%)	23,45,45	1.79	2 (8%)
3	OJA	D	1001	-	37,38,38	0.94	3 (8%)	46,53,53	1.68	9 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	D	807	-	24,29,29	0.96	1 (4%)	23,45,45	1.71	1 (4%)
2	ADP	D	900	-	24,29,29	0.97	1 (4%)	23,45,45	1.78	2 (8%)
3	OJA	E	1001	-	37,38,38	0.94	3 (8%)	46,53,53	1.68	10 (21%)
2	ADP	E	807	-	24,29,29	0.96	1 (4%)	23,45,45	1.71	1 (4%)
2	ADP	E	900	-	24,29,29	0.97	1 (4%)	23,45,45	1.79	3 (13%)
3	OJA	F	1001	-	37,38,38	0.94	3 (8%)	46,53,53	1.68	9 (19%)
2	ADP	F	807	-	24,29,29	0.97	1 (4%)	23,45,45	1.71	1 (4%)
2	ADP	F	900	-	24,29,29	0.97	1 (4%)	23,45,45	1.78	2 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OJA	A	1001	-	-	0/18/38/38	0/5/5/5
2	ADP	A	807	-	-	0/12/32/32	0/3/3/3
2	ADP	A	900	-	-	0/12/32/32	0/3/3/3
3	OJA	B	1001	-	-	0/18/38/38	0/5/5/5
2	ADP	B	807	-	-	0/12/32/32	0/3/3/3
2	ADP	B	900	-	-	0/12/32/32	0/3/3/3
3	OJA	C	1001	-	-	0/18/38/38	0/5/5/5
2	ADP	C	807	-	-	0/12/32/32	0/3/3/3
2	ADP	C	900	-	-	0/12/32/32	0/3/3/3
3	OJA	D	1001	-	-	0/18/38/38	0/5/5/5
2	ADP	D	807	-	-	0/12/32/32	0/3/3/3
2	ADP	D	900	-	-	0/12/32/32	0/3/3/3
3	OJA	E	1001	-	-	0/18/38/38	0/5/5/5
2	ADP	E	807	-	-	0/12/32/32	0/3/3/3
2	ADP	E	900	-	-	0/12/32/32	0/3/3/3
3	OJA	F	1001	-	-	0/18/38/38	0/5/5/5
2	ADP	F	807	-	-	0/12/32/32	0/3/3/3
2	ADP	F	900	-	-	0/12/32/32	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1001	OJA	C21-C23	-2.28	1.45	1.48
3	E	1001	OJA	C21-C23	-2.27	1.45	1.48
3	C	1001	OJA	C21-C23	-2.26	1.45	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1001	OJA	C21-C23	-2.26	1.45	1.48
3	A	1001	OJA	C21-C23	-2.26	1.45	1.48
3	B	1001	OJA	C21-C23	-2.20	1.45	1.48
3	E	1001	OJA	F28-C27	-2.20	1.31	1.36
3	D	1001	OJA	F28-C27	-2.18	1.31	1.36
3	A	1001	OJA	F28-C27	-2.18	1.31	1.36
3	B	1001	OJA	F28-C27	-2.17	1.31	1.36
3	C	1001	OJA	F28-C27	-2.17	1.31	1.36
3	F	1001	OJA	F28-C27	-2.16	1.31	1.36
3	F	1001	OJA	C02-N04	2.16	1.52	1.48
3	E	1001	OJA	C02-N04	2.17	1.52	1.48
3	B	1001	OJA	C02-N04	2.17	1.52	1.48
3	A	1001	OJA	C02-N04	2.17	1.52	1.48
3	D	1001	OJA	C02-N04	2.18	1.52	1.48
3	C	1001	OJA	C02-N04	2.20	1.52	1.48
2	F	900	ADP	C5-C4	2.97	1.47	1.40
2	B	900	ADP	C5-C4	2.98	1.47	1.40
2	A	900	ADP	C5-C4	2.98	1.47	1.40
2	D	900	ADP	C5-C4	2.99	1.47	1.40
2	C	807	ADP	C5-C4	3.00	1.47	1.40
2	E	807	ADP	C5-C4	3.00	1.47	1.40
2	B	807	ADP	C5-C4	3.00	1.47	1.40
2	C	900	ADP	C5-C4	3.01	1.47	1.40
2	E	900	ADP	C5-C4	3.02	1.47	1.40
2	A	807	ADP	C5-C4	3.03	1.47	1.40
2	F	807	ADP	C5-C4	3.03	1.47	1.40
2	D	807	ADP	C5-C4	3.03	1.47	1.40

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	807	ADP	N3-C2-N1	-6.76	123.56	128.87
2	A	807	ADP	N3-C2-N1	-6.72	123.59	128.87
2	F	807	ADP	N3-C2-N1	-6.71	123.60	128.87
2	B	807	ADP	N3-C2-N1	-6.70	123.61	128.87
2	D	807	ADP	N3-C2-N1	-6.70	123.61	128.87
2	E	807	ADP	N3-C2-N1	-6.67	123.63	128.87
2	E	900	ADP	N3-C2-N1	-6.57	123.71	128.87
2	C	900	ADP	N3-C2-N1	-6.53	123.74	128.87
2	F	900	ADP	N3-C2-N1	-6.50	123.77	128.87
2	A	900	ADP	N3-C2-N1	-6.50	123.77	128.87
2	D	900	ADP	N3-C2-N1	-6.48	123.78	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	ADP	N3-C2-N1	-6.46	123.80	128.87
3	F	1001	OJA	C09-C08-N07	-3.45	104.61	112.88
3	C	1001	OJA	C09-C08-N07	-3.45	104.62	112.88
3	A	1001	OJA	C09-C08-N07	-3.45	104.63	112.88
3	E	1001	OJA	C09-C08-N07	-3.44	104.64	112.88
3	D	1001	OJA	C09-C08-N07	-3.44	104.65	112.88
3	B	1001	OJA	C09-C08-N07	-3.43	104.67	112.88
3	B	1001	OJA	C22-C17-N14	-2.64	118.28	121.35
3	C	1001	OJA	C22-C17-N14	-2.64	118.29	121.35
3	F	1001	OJA	C22-C17-N14	-2.62	118.31	121.35
3	A	1001	OJA	C22-C17-N14	-2.61	118.32	121.35
3	E	1001	OJA	C22-C17-N14	-2.59	118.34	121.35
3	D	1001	OJA	C22-C17-N14	-2.59	118.34	121.35
3	E	1001	OJA	C08-N07-C33	-2.41	105.99	111.25
3	F	1001	OJA	C08-N07-C33	-2.41	106.01	111.25
3	C	1001	OJA	C08-N07-C33	-2.40	106.02	111.25
3	A	1001	OJA	C08-N07-C33	-2.40	106.03	111.25
3	B	1001	OJA	C08-N07-C33	-2.39	106.03	111.25
3	D	1001	OJA	C08-N07-C33	-2.38	106.06	111.25
3	B	1001	OJA	C03-C02-N04	-2.38	107.03	112.19
3	C	1001	OJA	C03-C02-N04	-2.38	107.03	112.19
3	F	1001	OJA	C03-C02-N04	-2.38	107.03	112.19
3	E	1001	OJA	C03-C02-N04	-2.38	107.03	112.19
3	A	1001	OJA	C03-C02-N04	-2.38	107.03	112.19
3	D	1001	OJA	C03-C02-N04	-2.37	107.05	112.19
2	C	900	ADP	C2'-C1'-N9	-2.14	107.74	113.47
2	B	900	ADP	C2'-C1'-N9	-2.13	107.76	113.47
2	E	900	ADP	C2'-C1'-N9	-2.13	107.77	113.47
2	A	900	ADP	C2'-C1'-N9	-2.13	107.77	113.47
2	F	900	ADP	C2'-C1'-N9	-2.12	107.79	113.47
2	D	900	ADP	C2'-C1'-N9	-2.12	107.80	113.47
3	F	1001	OJA	C05-C06-N07	-2.02	106.72	110.65
3	E	1001	OJA	C05-C06-N07	-2.01	106.74	110.65
3	D	1001	OJA	C05-C06-N07	-2.00	106.74	110.65
3	B	1001	OJA	C05-C06-N07	-2.00	106.75	110.65
3	B	1001	OJA	C23-C24-C25	2.00	109.05	106.55
3	A	1001	OJA	C23-C24-C25	2.01	109.07	106.55
3	E	1001	OJA	C23-C24-C25	2.04	109.10	106.55
2	E	900	ADP	C4'-O4'-C1'	2.04	111.81	109.64
3	D	1001	OJA	C33-C34-N04	2.18	115.41	110.65
3	C	1001	OJA	C33-C34-N04	2.20	115.45	110.65
3	F	1001	OJA	C33-C34-N04	2.20	115.45	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	OJA	C33-C34-N04	2.20	115.45	110.65
3	A	1001	OJA	C33-C34-N04	2.20	115.46	110.65
3	E	1001	OJA	C33-C34-N04	2.21	115.47	110.65
3	B	1001	OJA	C22-C21-C23	2.74	124.02	120.57
3	D	1001	OJA	C22-C21-C23	2.78	124.07	120.57
3	E	1001	OJA	C22-C21-C23	2.79	124.09	120.57
3	A	1001	OJA	C22-C21-C23	2.79	124.09	120.57
3	C	1001	OJA	C22-C21-C23	2.80	124.11	120.57
3	F	1001	OJA	C22-C21-C23	2.80	124.11	120.57
3	B	1001	OJA	C18-C17-N14	3.61	126.38	121.39
3	D	1001	OJA	C18-C17-N14	3.62	126.39	121.39
3	A	1001	OJA	C18-C17-N14	3.63	126.40	121.39
3	E	1001	OJA	C18-C17-N14	3.63	126.41	121.39
3	F	1001	OJA	C18-C17-N14	3.65	126.43	121.39
3	C	1001	OJA	C18-C17-N14	3.67	126.47	121.39
3	B	1001	OJA	C21-C22-C17	4.47	125.59	120.72
3	D	1001	OJA	C21-C22-C17	4.54	125.67	120.72
3	A	1001	OJA	C21-C22-C17	4.55	125.67	120.72
3	E	1001	OJA	C21-C22-C17	4.56	125.68	120.72
3	C	1001	OJA	C21-C22-C17	4.56	125.69	120.72
3	F	1001	OJA	C21-C22-C17	4.56	125.69	120.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	OJA	5	0
2	A	807	ADP	5	0
2	A	900	ADP	4	0
3	B	1001	OJA	4	0
2	B	807	ADP	5	0
2	B	900	ADP	5	0
3	C	1001	OJA	4	0
2	C	807	ADP	5	0
2	C	900	ADP	4	0
3	D	1001	OJA	5	0
2	D	807	ADP	5	0
2	D	900	ADP	4	0
3	E	1001	OJA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	807	ADP	5	0
2	E	900	ADP	4	0
3	F	1001	OJA	4	0
2	F	807	ADP	5	0
2	F	900	ADP	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.