



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Feb 17, 2018 – 01:48 am GMT

PDB ID : 3J2P
EMDB ID: : EMD-5499
Title : CryoEM structure of Dengue virus envelope protein heterotetramer
Authors : Zhang, X.; Ge, P.; Yu, X.; Brannan, J.M.; Bi, G.; Zhang, Q.; Schein, S.; Zhou, Z.H.
Deposited on : 2012-11-30
Resolution : 3.60 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

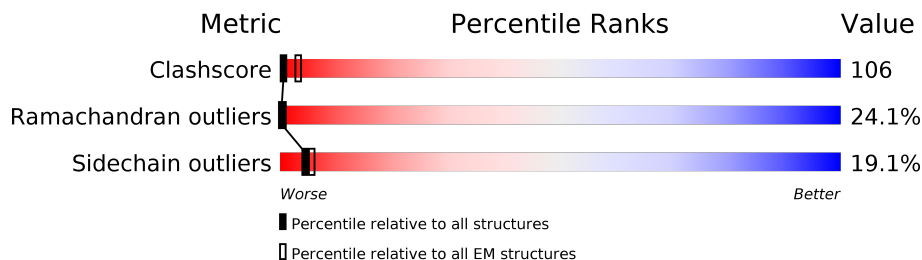
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	136279	1886
Ramachandran outliers	132675	1663
Sidechain outliers	132484	1531

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	495	<div> <div>13%</div> <div>55%</div> <div>28%</div> <div>.</div> </div>
1	C	495	<div> <div>12%</div> <div>56%</div> <div>28%</div> <div>.</div> </div>
2	B	75	<div> <div>17%</div> <div>53%</div> <div>23%</div> <div>.</div> <div>.</div> </div>
2	D	75	<div> <div>13%</div> <div>57%</div> <div>23%</div> <div>.</div> <div>.</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9890 atoms, of which 1086 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 Envelope protein E.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	495	Total	C	H	N	O	S	0	0
			4276	2410	475	648	711	32		
1	C	495	Total	C	H	N	O	S	0	0
			4276	2410	475	648	711	32		

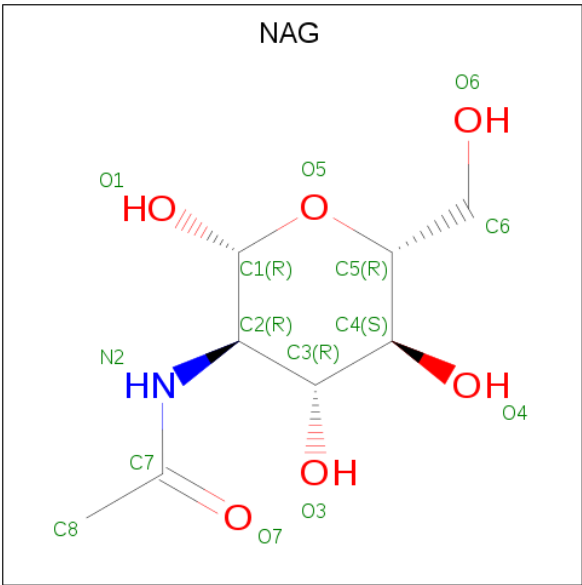
- Molecule 2 is a protein called Small envelope protein M.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	72	Total	C	H	N	O	S	0	0
			627	366	68	95	95	3		
2	D	72	Total	C	H	N	O	S	0	0
			627	366	68	95	95	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	15	ALA	ARG	SEE REMARK 999	UNP P14340
D	15	ALA	ARG	SEE REMARK 999	UNP P14340

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).

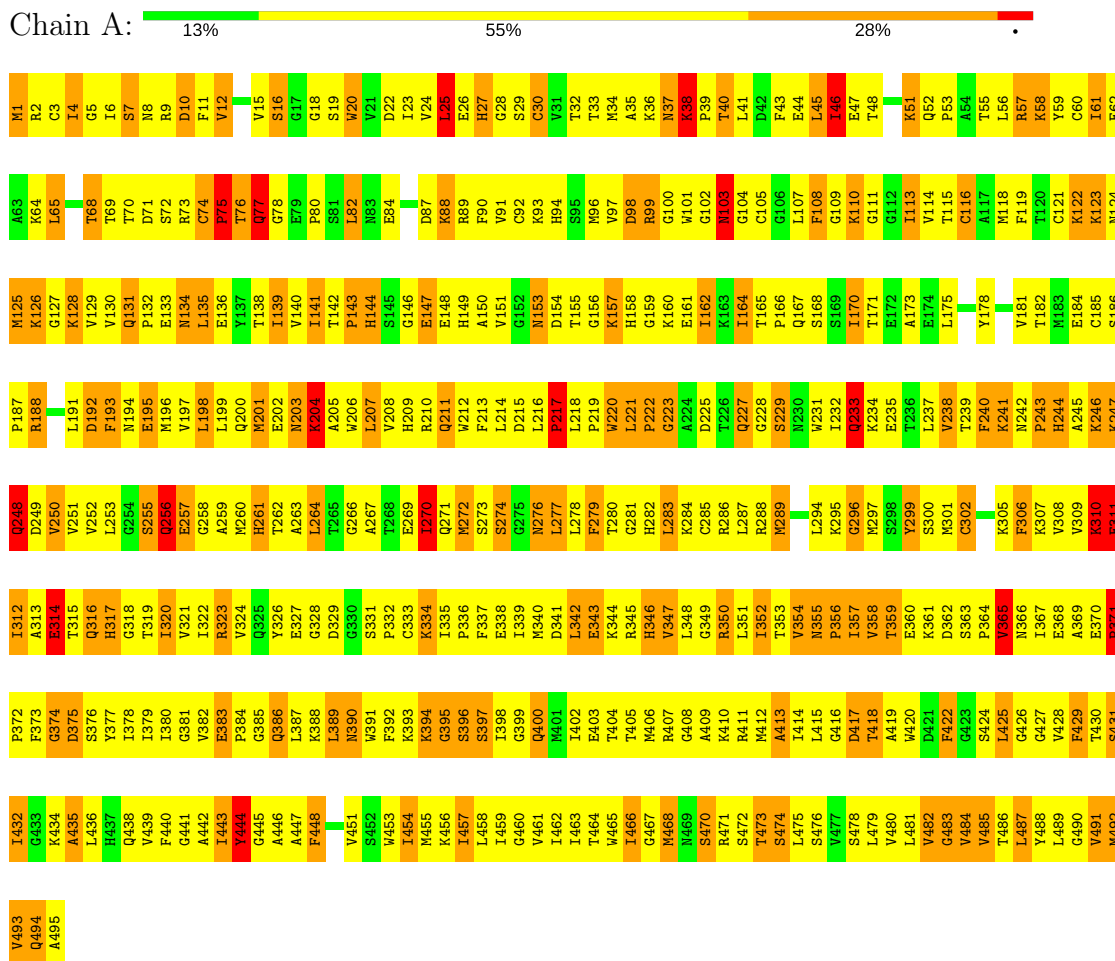


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			42	24	3	15	
3	A	1	Total	C	N	O	0
			42	24	3	15	
3	A	1	Total	C	N	O	0
			42	24	3	15	
3	C	1	Total	C	N	O	0
			42	24	3	15	
3	C	1	Total	C	N	O	0
			42	24	3	15	
3	C	1	Total	C	N	O	0
			42	24	3	15	

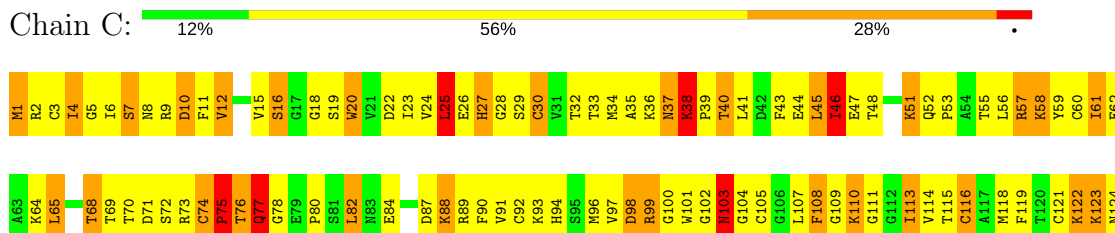
3 Residue-property plots

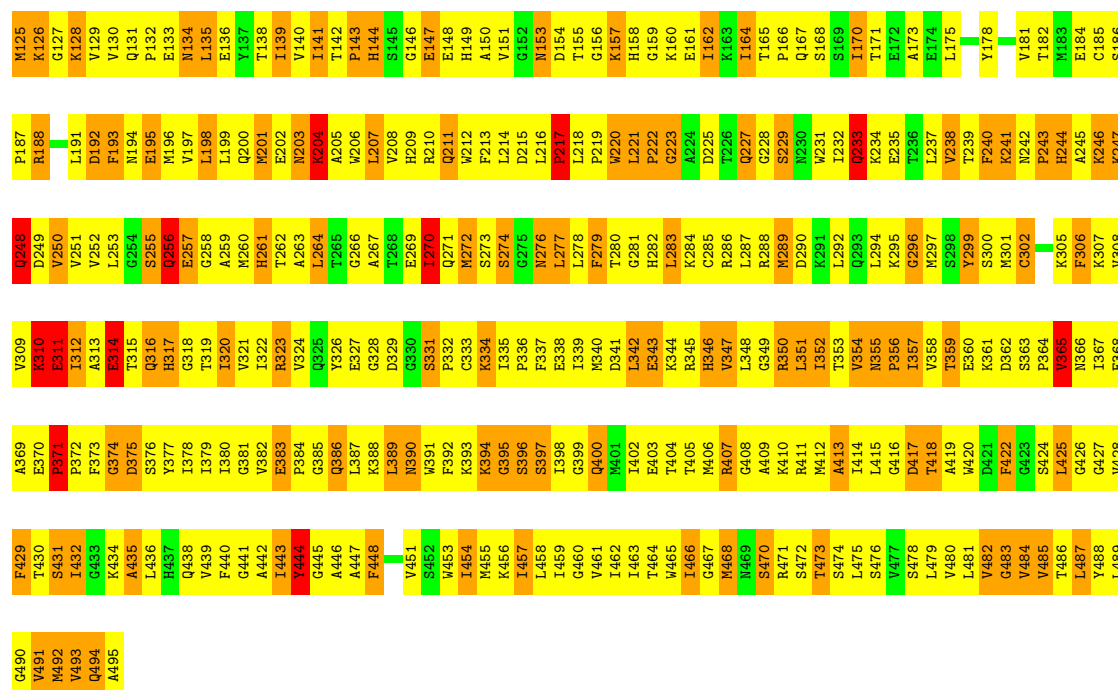
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

• Molecule 1: Envelope protein E



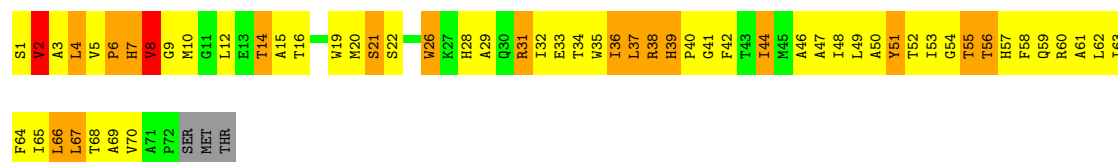
• Molecule 1: Envelope protein E





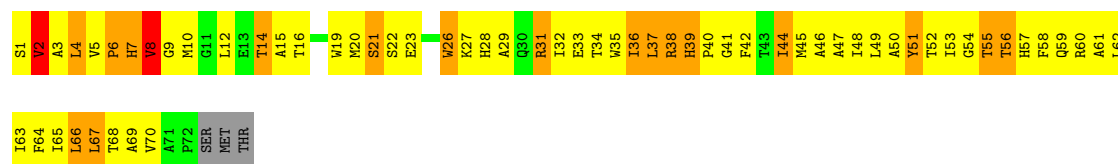
• Molecule 2: Small envelope protein M

Chain B: 17% 53% 23%



• Molecule 2: Small envelope protein M

Chain D: 13% 57% 23%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	9288	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	EMAN, per particle, with astigmatism compensation	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	57518	Depositor
Image detector	KODAK SO-163 FILM	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:
NAG

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	0.46	0/3876	0.82	1/5237 (0.0%)
1	C	0.46	0/3876	0.82	1/5237 (0.0%)
2	B	0.49	0/575	0.77	0/786
2	D	0.50	0/575	0.77	0/786
All	All	0.46	0/8902	0.82	2/12046 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	LEU	CA-CB-CG	-5.64	102.33	115.30
1	C	25	LEU	CA-CB-CG	-5.56	102.51	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3801	475	3844	838	0
1	C	3801	475	3844	820	0
2	B	559	68	569	117	0
2	D	559	68	569	119	0
3	A	42	0	38	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	42	0	38	3	0
All	All	8804	1086	8902	1831	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 106.

All (1831) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:51:TYR:HA	2:D:60:ARG:HD3	1.18	1.17
2:B:51:TYR:HA	2:B:60:ARG:HD3	1.17	1.14
2:B:55:THR:HA	2:B:60:ARG:HH11	1.01	1.14
2:B:55:THR:HA	2:B:60:ARG:NH1	1.65	1.10
2:D:55:THR:HA	2:D:60:ARG:HH11	1.01	1.08
2:D:55:THR:HA	2:D:60:ARG:NH1	1.66	1.08
1:C:464:THR:HB	1:C:482:VAL:HG11	1.33	1.07
1:A:464:THR:HB	1:A:482:VAL:HG11	1.33	1.04
1:C:463:ILE:HG23	1:C:482:VAL:HG22	1.39	1.03
2:B:56:THR:OG1	2:B:59:GLN:HB2	1.61	1.01
1:C:270:ILE:CD1	1:C:278:LEU:HA	1.90	1.01
1:A:270:ILE:CD1	1:A:278:LEU:HA	1.90	1.00
2:B:47:ALA:O	2:B:50:ALA:HB3	1.63	0.99
1:A:463:ILE:HG23	1:A:482:VAL:HG22	1.39	0.99
2:D:56:THR:OG1	2:D:59:GLN:HB2	1.60	0.99
1:A:62:GLU:HB3	1:A:122:LYS:O	1.63	0.98
1:A:99:ARG:HH11	1:A:105:CYS:HB3	1.28	0.98
1:C:101:TRP:H	1:C:108:PHE:HB3	1.28	0.98
1:C:99:ARG:HH11	1:C:105:CYS:HB3	1.29	0.98
2:D:47:ALA:O	2:D:50:ALA:HB3	1.63	0.97
1:A:166:PRO:HB3	1:A:187:PRO:HG2	1.47	0.97
1:A:173:ALA:HB3	1:A:181:VAL:HG12	1.44	0.96
1:C:173:ALA:HB3	1:C:181:VAL:HG12	1.44	0.96
1:C:62:GLU:HB3	1:C:122:LYS:O	1.64	0.96
1:A:306:PHE:HB3	1:A:326:TYR:HA	1.46	0.96
1:A:101:TRP:H	1:A:108:PHE:HB3	1.28	0.96
1:A:270:ILE:HD11	1:A:278:LEU:HA	1.47	0.95
1:C:464:THR:HA	1:C:482:VAL:HG21	1.47	0.95
1:A:65:LEU:HD21	1:A:252:VAL:HA	1.48	0.95
1:C:166:PRO:HB3	1:C:187:PRO:HG2	1.48	0.95
1:C:101:TRP:HB2	1:C:108:PHE:HD2	1.32	0.94
1:C:270:ILE:HD11	1:C:278:LEU:HA	1.46	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:PHE:HB3	1:C:326:TYR:HA	1.46	0.94
1:A:101:TRP:HB2	1:A:108:PHE:HD2	1.32	0.94
1:A:464:THR:HA	1:A:482:VAL:HG21	1.47	0.94
1:C:65:LEU:HD21	1:C:252:VAL:HA	1.48	0.94
1:A:460:GLY:O	1:A:463:ILE:HG22	1.69	0.93
1:C:206:TRP:CG	1:C:264:LEU:HD21	2.03	0.93
1:A:206:TRP:CG	1:A:264:LEU:HD21	2.02	0.93
1:A:178:TYR:HE2	1:A:295:LYS:HZ2	0.99	0.93
2:B:4:LEU:HB3	2:D:31:ARG:HH22	1.31	0.93
2:B:31:ARG:HH22	2:D:4:LEU:HB3	1.31	0.93
1:C:460:GLY:O	1:C:463:ILE:HG22	1.69	0.93
1:C:191:LEU:HD21	1:C:281:GLY:HA2	1.50	0.92
1:A:60:CYS:HA	1:A:124:ASN:HA	1.51	0.92
1:A:309:VAL:O	1:A:310:LYS:HB2	1.69	0.92
1:C:60:CYS:HA	1:C:124:ASN:HA	1.51	0.92
1:A:185:CYS:HA	1:A:285:CYS:HB3	1.50	0.92
1:A:256:GLN:HE21	1:A:256:GLN:HA	1.35	0.91
1:C:256:GLN:HA	1:C:256:GLN:HE21	1.35	0.91
1:A:191:LEU:HD21	1:A:281:GLY:HA2	1.50	0.91
1:A:311:GLU:HG2	1:A:312:ILE:H	1.33	0.91
1:C:309:VAL:O	1:C:310:LYS:HB2	1.69	0.91
1:C:311:GLU:HG2	1:C:312:ILE:H	1.33	0.91
1:C:320:ILE:HD12	1:C:320:ILE:H	1.35	0.91
1:C:185:CYS:HA	1:C:285:CYS:HB3	1.50	0.90
1:C:61:ILE:HB	1:C:256:GLN:HB2	1.53	0.90
1:A:139:ILE:HG22	1:A:162:ILE:HG23	1.54	0.90
1:A:61:ILE:HB	1:A:256:GLN:HB2	1.53	0.90
1:A:320:ILE:HD12	1:A:320:ILE:H	1.34	0.90
1:C:139:ILE:HG22	1:C:162:ILE:HG23	1.54	0.90
1:C:178:TYR:HE2	1:C:295:LYS:HZ2	0.99	0.89
1:A:92:CYS:SG	1:A:116:CYS:HB3	2.12	0.89
1:A:484:VAL:HA	1:A:488:TYR:HB2	1.55	0.89
2:B:52:THR:HG21	1:C:466:ILE:HD11	1.53	0.89
1:C:484:VAL:HA	1:C:488:TYR:HB2	1.55	0.89
1:C:92:CYS:SG	1:C:116:CYS:HB3	2.12	0.89
1:A:466:ILE:HD11	2:D:52:THR:HG21	1.53	0.89
1:C:73:ARG:O	1:C:74:CYS:HB3	1.72	0.88
1:A:101:TRP:HE1	1:C:310:LYS:NZ	1.71	0.88
1:C:296:GLY:HA2	1:C:299:TYR:HE1	1.39	0.88
1:C:410:LYS:O	1:C:414:ILE:HD13	1.74	0.87
1:A:164:ILE:HD13	1:A:164:ILE:O	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LYS:NZ	1:C:101:TRP:HE1	1.71	0.87
1:A:53:PRO:HB3	1:A:130:VAL:HG12	1.57	0.87
1:A:56:LEU:O	1:A:57:ARG:HB2	1.74	0.87
1:C:58:LYS:HD2	1:C:221:LEU:HD23	1.57	0.87
1:A:170:ILE:HG22	1:A:184:GLU:HG3	1.55	0.87
1:A:296:GLY:HA2	1:A:299:TYR:HE1	1.38	0.87
1:C:170:ILE:HG22	1:C:184:GLU:HG3	1.55	0.87
1:C:164:ILE:HD13	1:C:164:ILE:O	1.74	0.87
1:A:339:ILE:CG2	1:A:349:GLY:HA3	2.04	0.86
1:C:4:ILE:HB	1:C:151:VAL:CG1	2.06	0.86
1:A:410:LYS:O	1:A:414:ILE:HD13	1.75	0.86
1:C:339:ILE:CG2	1:C:349:GLY:HA3	2.04	0.86
1:C:53:PRO:HB3	1:C:130:VAL:HG12	1.57	0.86
1:C:282:HIS:O	1:C:282:HIS:CG	2.29	0.86
1:C:94:HIS:HA	1:C:114:VAL:HG12	1.57	0.86
1:A:282:HIS:O	1:A:282:HIS:CG	2.29	0.86
1:C:56:LEU:O	1:C:57:ARG:HB2	1.73	0.85
1:A:390:ASN:HD22	1:A:391:TRP:N	1.73	0.85
1:A:4:ILE:HB	1:A:151:VAL:CG1	2.06	0.85
1:A:73:ARG:O	1:A:74:CYS:HB3	1.73	0.85
1:C:390:ASN:HD22	1:C:391:TRP:N	1.73	0.85
1:A:320:ILE:HD13	1:A:371:PRO:HD2	1.57	0.85
1:C:305:LYS:HD2	1:C:327:GLU:HB3	1.58	0.85
1:A:94:HIS:HA	1:A:114:VAL:HG12	1.56	0.85
2:D:55:THR:CA	2:D:60:ARG:HH11	1.88	0.85
1:A:58:LYS:HD2	1:A:221:LEU:HD23	1.57	0.85
1:A:259:ALA:O	1:A:262:THR:HG22	1.77	0.85
2:B:44:ILE:O	2:B:48:ILE:HG13	1.77	0.85
1:C:339:ILE:CD1	1:C:378:ILE:HG22	2.07	0.85
1:A:306:PHE:HZ	1:A:381:GLY:HA3	1.40	0.85
1:C:233:GLN:HE21	1:C:233:GLN:HA	1.41	0.84
2:D:44:ILE:O	2:D:48:ILE:HG13	1.76	0.84
1:C:306:PHE:HZ	1:C:381:GLY:HA3	1.39	0.84
2:B:55:THR:CA	2:B:60:ARG:HH11	1.88	0.84
1:C:259:ALA:O	1:C:262:THR:HG22	1.77	0.84
1:C:270:ILE:HD12	1:C:271:GLN:N	1.93	0.83
1:A:270:ILE:HD12	1:A:271:GLN:N	1.94	0.83
1:C:320:ILE:HD13	1:C:371:PRO:HD2	1.58	0.83
1:A:233:GLN:HE21	1:A:233:GLN:HA	1.41	0.83
1:A:305:LYS:HD2	1:A:327:GLU:HB3	1.59	0.83
2:B:31:ARG:HH22	2:D:4:LEU:CB	1.91	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:63:ILE:HD12	2:D:64:PHE:N	1.93	0.83
1:A:339:ILE:CD1	1:A:378:ILE:HG22	2.08	0.83
1:C:336:PRO:HG2	1:C:381:GLY:HA2	1.60	0.83
2:B:66:LEU:HD23	2:D:66:LEU:HB3	1.61	0.83
2:B:63:ILE:HD12	2:B:64:PHE:N	1.94	0.82
2:B:4:LEU:CB	2:D:31:ARG:HH22	1.91	0.82
1:A:220:TRP:HD1	1:A:221:LEU:O	1.63	0.82
1:A:336:PRO:HG2	1:A:381:GLY:HA2	1.60	0.82
1:C:220:TRP:CD1	1:C:221:LEU:O	2.33	0.81
1:A:310:LYS:HZ2	1:C:101:TRP:HE1	0.84	0.81
1:A:220:TRP:CD1	1:A:221:LEU:O	2.33	0.81
1:A:25:LEU:HB2	1:A:45:LEU:HD12	1.61	0.81
1:C:25:LEU:HB2	1:C:45:LEU:HD12	1.61	0.81
1:A:23:ILE:HD13	1:A:25:LEU:HD21	1.62	0.81
1:C:220:TRP:HD1	1:C:221:LEU:O	1.63	0.81
1:C:23:ILE:HD13	1:C:25:LEU:HD21	1.61	0.81
2:D:1:SER:C	2:D:3:ALA:H	1.82	0.81
2:B:1:SER:C	2:B:3:ALA:H	1.82	0.80
1:A:240:PHE:HA	1:A:250:VAL:HA	1.62	0.80
1:C:311:GLU:O	1:C:312:ILE:HG23	1.82	0.80
1:C:6:ILE:HG22	1:C:6:ILE:O	1.80	0.80
1:A:320:ILE:CD1	1:A:320:ILE:H	1.94	0.80
1:C:320:ILE:CD1	1:C:320:ILE:H	1.94	0.80
1:A:61:ILE:HD13	1:A:123:LYS:O	1.81	0.80
2:B:66:LEU:HB3	2:D:66:LEU:HD23	1.62	0.80
1:C:240:PHE:HA	1:C:250:VAL:HA	1.61	0.80
1:A:320:ILE:HD12	1:A:320:ILE:N	1.96	0.80
1:C:197:VAL:CG2	1:C:210:ARG:HA	2.13	0.79
1:A:466:ILE:O	1:A:466:ILE:HD13	1.82	0.79
1:C:320:ILE:N	1:C:320:ILE:HD12	1.97	0.79
1:A:6:ILE:HG22	1:A:6:ILE:O	1.80	0.79
1:C:247:LYS:HA	1:C:247:LYS:NZ	1.97	0.79
1:A:233:GLN:NE2	1:A:233:GLN:HA	1.97	0.79
1:C:61:ILE:HD13	1:C:123:LYS:O	1.82	0.79
1:A:247:LYS:HA	1:A:247:LYS:NZ	1.97	0.79
2:B:26:TRP:HA	2:B:26:TRP:CE3	2.14	0.79
2:D:26:TRP:CE3	2:D:26:TRP:HA	2.15	0.79
1:A:311:GLU:O	1:A:312:ILE:HG23	1.81	0.79
1:C:233:GLN:NE2	1:C:233:GLN:HA	1.98	0.79
1:C:339:ILE:HB	1:C:349:GLY:HA3	1.65	0.79
1:A:74:CYS:SG	1:A:75:PRO:HD2	2.23	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:ILE:O	1:C:466:ILE:HD13	1.81	0.79
1:C:367:ILE:HG22	1:C:368:GLU:H	1.48	0.78
1:A:99:ARG:HH11	1:A:105:CYS:CB	1.96	0.78
2:D:37:LEU:HD23	2:D:38:ARG:N	1.99	0.78
1:A:380:ILE:O	1:A:380:ILE:HG13	1.83	0.78
1:C:198:LEU:HD12	1:C:272:MET:HE1	1.65	0.78
1:A:197:VAL:CG2	1:A:210:ARG:HA	2.13	0.78
1:C:443:ILE:HG13	1:C:444:TYR:H	1.48	0.78
1:C:99:ARG:HH11	1:C:105:CYS:CB	1.97	0.78
1:A:367:ILE:HG22	1:A:368:GLU:H	1.48	0.77
1:C:122:LYS:HG3	1:C:123:LYS:HD3	1.66	0.77
1:C:74:CYS:SG	1:C:75:PRO:HD2	2.24	0.77
1:C:156:GLY:C	1:C:157:LYS:HE2	2.05	0.77
1:A:135:LEU:HD21	1:A:193:PHE:HE1	1.49	0.77
1:A:270:ILE:CG1	1:A:271:GLN:H	1.97	0.77
1:A:339:ILE:HB	1:A:349:GLY:HA3	1.65	0.77
1:C:270:ILE:CG1	1:C:271:GLN:H	1.97	0.77
1:C:185:CYS:HA	1:C:285:CYS:CB	2.14	0.77
1:C:454:ILE:HD13	1:C:455:MET:N	2.00	0.77
1:A:122:LYS:HG3	1:A:123:LYS:HD3	1.67	0.76
2:B:37:LEU:HD23	2:B:38:ARG:N	1.99	0.76
1:A:156:GLY:C	1:A:157:LYS:HE2	2.05	0.76
1:C:463:ILE:HG23	1:C:482:VAL:CG2	2.15	0.76
1:A:185:CYS:HA	1:A:285:CYS:CB	2.15	0.76
1:A:383:GLU:HB3	1:A:384:PRO:CD	2.16	0.76
1:A:30:CYS:HA	1:A:43:PHE:O	1.86	0.76
2:D:51:TYR:HA	2:D:60:ARG:CD	2.09	0.76
1:A:443:ILE:HG13	1:A:444:TYR:H	1.49	0.76
1:A:488:TYR:HA	1:A:491:VAL:HG22	1.67	0.76
1:A:198:LEU:HD12	1:A:272:MET:HE1	1.67	0.76
2:B:51:TYR:HA	2:B:60:ARG:CD	2.09	0.76
1:C:1:MET:HG3	1:C:151:VAL:HA	1.67	0.76
1:C:135:LEU:HD21	1:C:193:PHE:HE1	1.49	0.76
1:A:101:TRP:HE1	1:C:310:LYS:HZ2	1.34	0.75
1:C:339:ILE:HD13	1:C:378:ILE:HG22	1.68	0.75
1:C:23:ILE:HD12	1:C:23:ILE:O	1.86	0.75
1:C:30:CYS:HA	1:C:43:PHE:O	1.86	0.75
1:C:380:ILE:O	1:C:380:ILE:HG13	1.83	0.75
1:A:201:MET:HB3	1:A:206:TRP:HZ3	1.50	0.75
2:D:55:THR:O	2:D:56:THR:HG23	1.86	0.75
1:A:47:GLU:O	1:A:138:THR:HG22	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HG3	1:A:151:VAL:HA	1.67	0.75
1:A:454:ILE:HG23	1:A:455:MET:H	1.50	0.75
1:C:454:ILE:HG23	1:C:455:MET:H	1.50	0.75
1:C:488:TYR:HA	1:C:491:VAL:HG22	1.67	0.75
1:A:385:GLY:O	1:A:387:LEU:N	2.20	0.75
1:C:270:ILE:HD12	1:C:270:ILE:C	2.07	0.75
1:A:35:ALA:HB3	1:A:37:ASN:O	1.87	0.74
1:A:463:ILE:HG23	1:A:482:VAL:CG2	2.15	0.74
1:C:327:GLU:HG2	1:C:328:GLY:H	1.52	0.74
1:C:35:ALA:HB3	1:C:37:ASN:O	1.87	0.74
1:A:206:TRP:CD2	1:A:264:LEU:HD21	2.22	0.74
1:A:454:ILE:HD13	1:A:455:MET:N	2.01	0.74
1:C:146:GLY:O	1:C:147:GLU:HG3	1.88	0.74
1:A:101:TRP:N	1:A:108:PHE:HB3	2.00	0.74
1:A:327:GLU:HG2	1:A:328:GLY:H	1.51	0.74
2:B:55:THR:O	2:B:56:THR:HG23	1.86	0.74
1:C:470:SER:HB3	1:C:475:LEU:HB3	1.70	0.74
1:A:470:SER:HB3	1:A:475:LEU:HB3	1.70	0.74
1:C:385:GLY:O	1:C:387:LEU:N	2.20	0.74
1:A:339:ILE:CB	1:A:349:GLY:HA3	2.17	0.74
1:C:47:GLU:O	1:C:138:THR:HG22	1.87	0.74
1:C:239:THR:O	1:C:251:VAL:HG22	1.87	0.74
1:C:37:ASN:C	1:C:38:LYS:HD2	2.08	0.74
1:C:383:GLU:HB3	1:C:384:PRO:CD	2.16	0.74
1:C:206:TRP:CD2	1:C:264:LEU:HD21	2.22	0.74
1:A:239:THR:O	1:A:251:VAL:HG22	1.88	0.74
1:C:20:TRP:HZ3	1:C:288:ARG:HE	1.35	0.74
1:C:101:TRP:N	1:C:108:PHE:HB3	2.01	0.74
1:C:375:ASP:HA	1:C:392:PHE:HA	1.70	0.74
1:C:4:ILE:HB	1:C:151:VAL:HG11	1.68	0.74
1:A:146:GLY:O	1:A:147:GLU:HG3	1.88	0.74
1:C:201:MET:HB3	1:C:206:TRP:HZ3	1.50	0.74
1:C:339:ILE:CB	1:C:349:GLY:HA3	2.17	0.74
1:A:4:ILE:HB	1:A:151:VAL:HG11	1.69	0.73
1:C:51:LYS:HZ1	1:C:136:GLU:HB2	1.52	0.73
1:C:387:LEU:HD22	1:C:388:LYS:H	1.54	0.73
1:A:20:TRP:HA	1:A:20:TRP:CE3	2.23	0.73
1:A:23:ILE:O	1:A:23:ILE:HD12	1.89	0.73
1:A:270:ILE:HD12	1:A:270:ILE:C	2.07	0.73
1:A:367:ILE:HD12	1:A:367:ILE:N	2.04	0.73
1:A:339:ILE:HD13	1:A:378:ILE:HG22	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ARG:HG3	1:A:10:ASP:N	2.03	0.73
1:A:37:ASN:C	1:A:38:LYS:HD2	2.08	0.73
1:A:387:LEU:HD22	1:A:388:LYS:H	1.53	0.73
1:A:270:ILE:HG13	1:A:271:GLN:H	1.54	0.73
1:C:20:TRP:HA	1:C:20:TRP:CE3	2.23	0.72
1:C:170:ILE:H	1:C:170:ILE:HD13	1.54	0.72
1:A:20:TRP:HZ3	1:A:288:ARG:HE	1.36	0.72
1:C:193:PHE:O	1:C:195:GLU:HG2	1.90	0.72
1:C:39:PRO:HD3	1:C:294:LEU:HA	1.72	0.72
1:A:193:PHE:O	1:A:195:GLU:HG2	1.89	0.72
1:A:384:PRO:HG2	1:A:386:GLN:HE21	1.55	0.72
1:A:37:ASN:O	1:A:38:LYS:HD2	1.90	0.72
1:A:488:TYR:O	1:A:489:LEU:C	2.28	0.72
1:C:44:GLU:O	1:C:140:VAL:HG22	1.88	0.72
1:C:4:ILE:HB	1:C:151:VAL:HG13	1.71	0.72
1:C:9:ARG:HG3	1:C:10:ASP:N	2.03	0.72
1:C:338:GLU:HB2	1:C:379:ILE:HG23	1.72	0.72
1:C:367:ILE:N	1:C:367:ILE:HD12	2.05	0.72
1:C:464:THR:CB	1:C:482:VAL:HG11	2.17	0.72
1:A:365:VAL:HG23	1:A:366:ASN:N	2.04	0.71
2:D:56:THR:O	2:D:58:PHE:N	2.23	0.71
1:A:219:PRO:HA	1:A:233:GLN:HB2	1.72	0.71
1:A:39:PRO:HD3	1:A:294:LEU:HA	1.72	0.71
1:A:44:GLU:O	1:A:140:VAL:HG22	1.89	0.71
2:B:14:THR:O	2:B:16:THR:N	2.23	0.71
1:A:338:GLU:HB2	1:A:379:ILE:HG23	1.72	0.71
2:D:3:ALA:HB3	2:D:4:LEU:HD22	1.73	0.71
2:B:31:ARG:HD2	2:B:32:ILE:N	2.06	0.71
2:B:3:ALA:HB3	2:B:4:LEU:HD22	1.73	0.71
1:C:302:CYS:SG	1:C:333:CYS:HB2	2.31	0.71
1:A:170:ILE:HD13	1:A:170:ILE:H	1.54	0.71
1:A:5:GLY:HA2	1:A:315:THR:HG21	1.73	0.71
2:B:56:THR:O	2:B:58:PHE:N	2.23	0.71
1:C:203:ASN:C	1:C:204:LYS:HG2	2.11	0.71
1:C:270:ILE:HG13	1:C:271:GLN:H	1.54	0.71
1:C:37:ASN:O	1:C:38:LYS:HD2	1.90	0.71
2:D:14:THR:O	2:D:16:THR:N	2.24	0.71
1:A:375:ASP:HA	1:A:392:PHE:HA	1.71	0.71
1:A:424:SER:O	1:A:425:LEU:HB2	1.90	0.71
1:C:272:MET:HA	1:C:276:ASN:HB3	1.73	0.71
1:A:414:ILE:HG22	1:A:415:LEU:HD23	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:461:VAL:O	1:C:464:THR:HG22	1.91	0.71
1:A:203:ASN:C	1:A:204:LYS:HG2	2.11	0.70
1:A:302:CYS:SG	1:A:333:CYS:HB2	2.31	0.70
1:A:413:ALA:C	1:A:414:ILE:HD12	2.11	0.70
1:A:4:ILE:HB	1:A:151:VAL:HG13	1.71	0.70
1:C:197:VAL:HG23	1:C:210:ARG:HA	1.73	0.70
1:C:397:SER:O	1:C:400:GLN:HB2	1.91	0.70
1:A:221:LEU:HG	1:A:222:PRO:HD2	1.72	0.70
1:A:397:SER:O	1:A:400:GLN:HB2	1.91	0.70
1:C:269:GLU:HG2	1:C:270:ILE:H	1.55	0.70
1:C:365:VAL:HG23	1:C:366:ASN:N	2.05	0.70
1:C:414:ILE:HG22	1:C:415:LEU:HD23	1.72	0.70
1:C:5:GLY:HA2	1:C:315:THR:HG21	1.73	0.70
1:C:413:ALA:C	1:C:414:ILE:HD12	2.11	0.70
1:C:424:SER:O	1:C:425:LEU:HB2	1.90	0.70
1:A:58:LYS:HB2	1:A:58:LYS:NZ	2.06	0.70
2:B:4:LEU:HD22	2:B:4:LEU:N	2.06	0.70
1:C:384:PRO:HG2	1:C:386:GLN:HE21	1.56	0.70
2:D:4:LEU:N	2:D:4:LEU:HD22	2.07	0.70
1:A:272:MET:HA	1:A:276:ASN:HB3	1.72	0.70
1:A:367:ILE:HG22	1:A:368:GLU:N	2.07	0.70
1:A:464:THR:CB	1:A:482:VAL:HG11	2.17	0.70
1:C:277:LEU:HD23	1:C:277:LEU:H	1.55	0.70
1:C:296:GLY:HA2	1:C:299:TYR:CE1	2.25	0.70
1:C:339:ILE:HG21	1:C:349:GLY:HA3	1.72	0.70
1:A:277:LEU:HD23	1:A:277:LEU:H	1.55	0.70
1:A:339:ILE:HG21	1:A:349:GLY:HA3	1.72	0.70
1:A:64:LYS:HB3	1:A:64:LYS:NZ	2.07	0.70
1:A:269:GLU:HG2	1:A:270:ILE:H	1.55	0.70
1:C:367:ILE:HG22	1:C:368:GLU:N	2.06	0.70
1:C:64:LYS:HB3	1:C:64:LYS:NZ	2.07	0.70
1:A:492:MET:HA	1:A:492:MET:CE	2.22	0.69
1:C:122:LYS:HZ3	1:C:122:LYS:HB2	1.57	0.69
1:C:221:LEU:HG	1:C:222:PRO:CD	2.22	0.69
1:A:387:LEU:HD22	1:A:388:LYS:N	2.07	0.69
1:A:127:GLY:O	1:A:128:LYS:HB2	1.91	0.69
1:A:221:LEU:HG	1:A:222:PRO:CD	2.22	0.69
1:C:100:GLY:O	1:C:103:ASN:HB3	1.92	0.69
1:C:34:MET:HA	1:C:40:THR:HG22	1.73	0.69
1:A:109:GLY:HA2	1:C:315:THR:HB	1.72	0.69
1:C:221:LEU:HG	1:C:222:PRO:HD2	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:TRP:NE1	1:C:310:LYS:NZ	2.39	0.69
1:C:488:TYR:O	1:C:489:LEU:C	2.28	0.69
2:D:31:ARG:HD2	2:D:32:ILE:N	2.06	0.69
1:C:57:ARG:NH2	1:C:214:LEU:HD22	2.08	0.69
1:C:387:LEU:HD22	1:C:388:LYS:N	2.08	0.69
1:A:57:ARG:NH2	1:A:214:LEU:HD22	2.08	0.69
1:A:315:THR:HB	1:C:109:GLY:HA2	1.73	0.69
1:A:100:GLY:O	1:A:103:ASN:HB3	1.92	0.69
1:C:263:ALA:HB2	2:D:2:VAL:C	2.13	0.69
1:A:197:VAL:HG23	1:A:210:ARG:HA	1.74	0.69
1:A:307:LYS:HG2	1:A:308:VAL:H	1.58	0.69
1:A:34:MET:HA	1:A:40:THR:HG22	1.73	0.69
1:A:461:VAL:O	1:A:464:THR:HG22	1.91	0.69
1:C:58:LYS:HB2	1:C:58:LYS:NZ	2.07	0.69
1:C:127:GLY:O	1:C:128:LYS:HB2	1.92	0.69
1:C:219:PRO:HA	1:C:233:GLN:HB2	1.73	0.69
1:C:9:ARG:HG3	1:C:10:ASP:H	1.58	0.68
1:A:320:ILE:CD1	1:A:371:PRO:HD2	2.23	0.68
1:A:53:PRO:HG2	1:A:128:LYS:HZ2	1.58	0.68
1:C:202:GLU:HG3	1:C:257:GLU:OE2	1.93	0.68
1:C:492:MET:CE	1:C:492:MET:HA	2.22	0.68
1:A:296:GLY:HA2	1:A:299:TYR:CE1	2.25	0.68
1:A:478:SER:O	1:A:482:VAL:HG23	1.94	0.68
1:C:307:LYS:HG2	1:C:308:VAL:H	1.58	0.68
1:A:9:ARG:HG3	1:A:10:ASP:H	1.58	0.68
1:A:263:ALA:HB2	2:B:2:VAL:C	2.14	0.68
1:C:448:PHE:HZ	1:C:456:LYS:HD3	1.59	0.68
1:C:162:ILE:HD11	1:C:171:THR:HB	1.76	0.68
1:C:27:HIS:CE1	1:C:279:PHE:HA	2.29	0.67
1:C:320:ILE:CD1	1:C:371:PRO:HD2	2.23	0.67
1:A:202:GLU:HG3	1:A:257:GLU:OE2	1.93	0.67
1:A:27:HIS:CE1	1:A:279:PHE:HA	2.29	0.67
1:A:53:PRO:HG2	1:A:128:LYS:NZ	2.09	0.67
2:B:26:TRP:HA	2:B:26:TRP:HE3	1.59	0.67
1:C:443:ILE:HG13	1:C:444:TYR:N	2.10	0.67
1:A:178:TYR:HE2	1:A:295:LYS:NZ	1.86	0.67
1:A:443:ILE:HG13	1:A:444:TYR:N	2.10	0.67
1:A:448:PHE:HZ	1:A:456:LYS:HD3	1.58	0.67
1:C:87:ASP:O	1:C:89:ARG:N	2.27	0.67
1:C:270:ILE:CG1	1:C:271:GLN:N	2.57	0.67
1:C:340:MET:SD	1:C:345:ARG:HD2	2.35	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:478:SER:O	1:C:482:VAL:HG23	1.94	0.67
1:A:383:GLU:HB3	1:A:384:PRO:HD2	1.77	0.67
1:A:453:TRP:O	1:A:456:LYS:HB3	1.95	0.67
1:A:463:ILE:HA	1:A:466:ILE:HG22	1.77	0.67
1:C:53:PRO:HG2	1:C:128:LYS:NZ	2.09	0.67
1:C:398:ILE:O	1:C:402:ILE:HG22	1.95	0.67
1:C:463:ILE:HA	1:C:466:ILE:HG22	1.77	0.67
1:A:3:CYS:HB2	1:A:30:CYS:SG	2.35	0.66
1:A:149:HIS:O	3:A:502:NAG:H83	1.94	0.66
1:C:383:GLU:HB3	1:C:384:PRO:HD2	1.77	0.66
1:A:33:THR:O	1:A:40:THR:HB	1.94	0.66
1:C:73:ARG:O	1:C:74:CYS:CB	2.42	0.66
1:A:270:ILE:CG1	1:A:271:GLN:N	2.57	0.66
1:C:453:TRP:O	1:C:456:LYS:HB3	1.95	0.66
1:A:162:ILE:HD11	1:A:171:THR:HB	1.76	0.66
1:A:257:GLU:O	1:A:260:MET:HB3	1.96	0.66
1:A:391:TRP:O	1:A:392:PHE:HB3	1.95	0.66
1:A:398:ILE:O	1:A:402:ILE:HG22	1.95	0.66
1:C:33:THR:O	1:C:40:THR:HB	1.94	0.66
1:A:87:ASP:O	1:A:89:ARG:N	2.27	0.66
1:C:133:GLU:O	1:C:134:ASN:HB2	1.96	0.66
1:C:173:ALA:HB3	1:C:181:VAL:CG1	2.24	0.66
1:A:294:LEU:HD23	1:A:295:LYS:N	2.11	0.66
1:C:283:LEU:C	1:C:283:LEU:HD12	2.16	0.66
1:C:149:HIS:O	3:C:502:NAG:H83	1.94	0.66
1:C:93:LYS:O	1:C:114:VAL:HA	1.96	0.66
1:C:53:PRO:HG2	1:C:128:LYS:HZ2	1.61	0.66
1:A:20:TRP:HA	1:A:20:TRP:HE3	1.61	0.65
1:A:283:LEU:C	1:A:283:LEU:HD12	2.16	0.65
1:A:35:ALA:C	1:A:37:ASN:H	1.99	0.65
1:A:51:LYS:NZ	1:A:136:GLU:HB2	2.11	0.65
1:A:240:PHE:HB3	1:A:250:VAL:HG13	1.77	0.65
1:C:200:GLN:CG	1:C:272:MET:HG2	2.26	0.65
1:C:3:CYS:HB2	1:C:30:CYS:SG	2.35	0.65
2:D:26:TRP:HE3	2:D:26:TRP:HA	1.60	0.65
1:A:318:GLY:N	1:A:393:LYS:HE2	2.12	0.65
1:C:357:ILE:O	1:C:357:ILE:HG23	1.96	0.65
1:A:200:GLN:CG	1:A:272:MET:HG2	2.26	0.65
1:A:357:ILE:HG23	1:A:357:ILE:O	1.96	0.65
1:C:240:PHE:HB3	1:C:250:VAL:HG13	1.77	0.65
1:A:434:LYS:O	1:A:436:LEU:N	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ARG:HH21	1:A:57:ARG:HG3	1.62	0.65
1:C:57:ARG:HG3	1:C:57:ARG:HH21	1.62	0.65
1:A:122:LYS:HZ2	1:A:122:LYS:HA	1.62	0.65
1:A:173:ALA:HB3	1:A:181:VAL:CG1	2.24	0.65
1:A:340:MET:SD	1:A:345:ARG:HD2	2.36	0.65
1:A:427:GLY:O	1:A:428:VAL:HB	1.97	0.65
1:C:434:LYS:O	1:C:436:LEU:N	2.29	0.65
2:D:62:LEU:C	2:D:62:LEU:HD13	2.17	0.65
1:A:26:GLU:HB3	1:A:282:HIS:HB2	1.78	0.65
1:C:270:ILE:CD1	1:C:271:GLN:N	2.60	0.65
1:C:352:ILE:HG22	1:C:368:GLU:HB2	1.79	0.65
1:A:182:THR:OG1	1:A:288:ARG:HB3	1.97	0.65
1:A:352:ILE:HG22	1:A:368:GLU:HB2	1.79	0.65
1:C:26:GLU:HB3	1:C:282:HIS:HB2	1.78	0.65
1:A:448:PHE:O	1:A:448:PHE:CD1	2.50	0.65
1:C:457:ILE:HD12	1:C:457:ILE:C	2.16	0.65
1:A:133:GLU:O	1:A:134:ASN:HB2	1.95	0.64
1:A:270:ILE:CD1	1:A:271:GLN:N	2.60	0.64
1:A:457:ILE:HD12	1:A:457:ILE:C	2.16	0.64
1:C:170:ILE:CG2	1:C:184:GLU:HG3	2.27	0.64
1:C:463:ILE:O	1:C:466:ILE:HG22	1.97	0.64
1:A:93:LYS:O	1:A:114:VAL:HA	1.96	0.64
1:A:319:THR:H	1:A:320:ILE:HD12	1.61	0.64
1:A:58:LYS:HB2	1:A:58:LYS:HZ3	1.63	0.64
2:B:62:LEU:C	2:B:62:LEU:HD13	2.17	0.64
1:C:294:LEU:HD23	1:C:295:LYS:N	2.11	0.64
1:C:448:PHE:O	1:C:448:PHE:CD1	2.50	0.64
1:A:141:ILE:O	1:A:159:GLY:HA3	1.98	0.64
1:A:233:GLN:HE21	1:A:233:GLN:CA	2.10	0.64
1:C:484:VAL:O	1:C:486:THR:N	2.30	0.64
1:A:428:VAL:O	1:A:432:ILE:HB	1.97	0.64
1:A:73:ARG:O	1:A:74:CYS:CB	2.43	0.64
1:C:390:ASN:HD22	1:C:391:TRP:H	1.44	0.64
1:A:393:LYS:HZ2	1:A:395:GLY:CA	2.10	0.64
1:A:463:ILE:O	1:A:466:ILE:HG22	1.96	0.64
1:C:188:ARG:HG3	1:C:188:ARG:HH21	1.62	0.64
1:C:428:VAL:O	1:C:429:PHE:O	2.16	0.64
1:A:390:ASN:HD22	1:A:391:TRP:H	1.43	0.64
1:A:428:VAL:O	1:A:429:PHE:O	2.15	0.64
1:A:9:ARG:O	1:A:10:ASP:HB3	1.97	0.64
1:C:257:GLU:O	1:C:260:MET:HB3	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:GLU:HG2	1:C:270:ILE:N	2.13	0.64
1:C:390:ASN:ND2	1:C:391:TRP:N	2.45	0.64
2:D:40:PRO:O	2:D:44:ILE:HG12	1.97	0.64
1:A:153:ASN:O	1:A:155:THR:N	2.31	0.64
1:A:188:ARG:HH21	1:A:188:ARG:HG3	1.62	0.64
1:A:390:ASN:ND2	1:A:391:TRP:N	2.45	0.64
1:C:393:LYS:HZ2	1:C:395:GLY:CA	2.11	0.64
1:C:318:GLY:N	1:C:393:LYS:HE2	2.12	0.64
1:C:427:GLY:O	1:C:428:VAL:HB	1.97	0.64
1:C:448:PHE:CZ	1:C:456:LYS:HD3	2.33	0.64
1:A:56:LEU:HG	1:A:56:LEU:O	1.98	0.64
1:C:391:TRP:O	1:C:392:PHE:HB3	1.96	0.64
1:A:205:ALA:C	1:A:206:TRP:CE3	2.72	0.64
1:A:484:VAL:O	1:A:486:THR:N	2.30	0.64
1:C:232:ILE:O	1:C:233:GLN:HG2	1.98	0.64
1:C:319:THR:H	1:C:320:ILE:HD12	1.61	0.64
2:D:3:ALA:O	2:D:4:LEU:HD13	1.98	0.64
1:A:473:THR:O	1:A:475:LEU:HD23	1.98	0.63
2:B:40:PRO:O	2:B:44:ILE:HG12	1.97	0.63
1:C:9:ARG:O	1:C:10:ASP:HB3	1.97	0.63
1:C:178:TYR:HE2	1:C:295:LYS:NZ	1.86	0.63
1:C:205:ALA:C	1:C:206:TRP:CE3	2.72	0.63
1:C:35:ALA:C	1:C:37:ASN:H	1.99	0.63
1:A:232:ILE:O	1:A:233:GLN:HG2	1.98	0.63
1:A:448:PHE:CZ	1:A:456:LYS:HD3	2.33	0.63
1:C:233:GLN:CA	1:C:233:GLN:HE21	2.11	0.63
1:C:336:PRO:CG	1:C:381:GLY:HA2	2.29	0.63
1:C:45:LEU:C	1:C:45:LEU:HD22	2.19	0.63
1:C:473:THR:O	1:C:475:LEU:HD23	1.98	0.63
1:A:393:LYS:O	1:A:394:LYS:HB2	1.98	0.63
1:C:182:THR:OG1	1:C:288:ARG:HB3	1.96	0.63
1:C:153:ASN:O	1:C:155:THR:N	2.31	0.63
1:A:269:GLU:HG2	1:A:270:ILE:N	2.13	0.63
1:C:141:ILE:O	1:C:159:GLY:HA3	1.98	0.63
1:C:320:ILE:HG12	1:C:371:PRO:HG2	1.81	0.63
1:C:428:VAL:O	1:C:432:ILE:HB	1.98	0.63
1:A:311:GLU:C	1:A:312:ILE:HD13	2.19	0.63
1:A:320:ILE:HG12	1:A:371:PRO:HG2	1.81	0.63
1:A:3:CYS:HA	1:A:6:ILE:HG13	1.79	0.63
1:A:240:PHE:HA	1:A:249:ASP:O	1.99	0.63
1:A:413:ALA:O	1:A:414:ILE:HD12	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:LYS:NZ	1:C:136:GLU:HB2	2.12	0.63
1:C:441:GLY:O	1:C:446:ALA:HB3	1.99	0.63
1:A:209:HIS:ND1	2:B:10:MET:HB3	2.14	0.63
1:C:3:CYS:HA	1:C:6:ILE:HG13	1.79	0.63
2:B:54:GLY:HA2	2:D:59:GLN:OE1	1.99	0.63
2:B:1:SER:C	2:B:3:ALA:N	2.52	0.62
2:B:3:ALA:O	2:B:4:LEU:HD13	1.98	0.62
1:C:459:ILE:HA	1:C:462:ILE:HG22	1.80	0.62
1:C:240:PHE:HA	1:C:249:ASP:O	1.99	0.62
1:A:442:ALA:O	1:A:446:ALA:O	2.18	0.62
1:A:65:LEU:HD21	1:A:252:VAL:CA	2.27	0.62
1:C:12:VAL:HG23	1:C:33:THR:OG1	1.99	0.62
1:C:311:GLU:C	1:C:312:ILE:HD13	2.19	0.62
1:A:45:LEU:C	1:A:45:LEU:HD22	2.20	0.62
1:A:53:PRO:HB3	1:A:130:VAL:CG1	2.29	0.62
1:A:233:GLN:C	1:A:235:GLU:H	2.03	0.62
1:A:305:LYS:CD	1:A:327:GLU:HB3	2.30	0.62
1:C:413:ALA:O	1:C:414:ILE:HD12	1.99	0.62
1:C:201:MET:HE2	1:C:202:GLU:HB2	1.81	0.62
1:C:200:GLN:HG3	1:C:272:MET:HG2	1.81	0.62
1:C:393:LYS:O	1:C:394:LYS:HB2	1.98	0.62
1:A:416:GLY:O	1:A:417:ASP:C	2.37	0.62
1:C:101:TRP:HB2	1:C:108:PHE:CD2	2.24	0.62
2:B:59:GLN:OE1	2:D:54:GLY:HA2	1.99	0.62
1:C:209:HIS:ND1	2:D:10:MET:HB3	2.14	0.62
1:C:20:TRP:CG	1:C:286:ARG:NH1	2.68	0.62
1:C:53:PRO:HB3	1:C:130:VAL:CG1	2.29	0.62
1:A:361:LYS:N	1:A:361:LYS:HD3	2.15	0.62
1:A:20:TRP:HB3	1:A:425:LEU:HD21	1.82	0.62
1:A:441:GLY:O	1:A:446:ALA:HB3	1.99	0.62
1:C:277:LEU:HD23	1:C:277:LEU:N	2.15	0.62
1:C:442:ALA:O	1:C:446:ALA:O	2.17	0.62
1:A:20:TRP:CG	1:A:286:ARG:NH1	2.68	0.61
1:C:416:GLY:O	1:C:417:ASP:C	2.37	0.61
1:C:20:TRP:HB3	1:C:425:LEU:HD21	1.82	0.61
1:C:443:ILE:HG23	1:C:444:TYR:N	2.15	0.61
2:D:63:ILE:HD12	2:D:63:ILE:C	2.20	0.61
1:A:19:SER:HB3	1:A:289:MET:N	2.15	0.61
1:A:459:ILE:HA	1:A:462:ILE:HG22	1.80	0.61
2:B:66:LEU:O	2:B:67:LEU:C	2.37	0.61
1:C:20:TRP:HA	1:C:20:TRP:HE3	1.61	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:SER:HB3	1:C:289:MET:N	2.15	0.61
1:C:361:LYS:N	1:C:361:LYS:HD3	2.15	0.61
1:A:99:ARG:NH1	1:A:105:CYS:HB3	2.10	0.61
1:A:200:GLN:HG3	1:A:272:MET:HG2	1.81	0.61
1:A:336:PRO:CG	1:A:381:GLY:HA2	2.29	0.61
1:A:58:LYS:HG2	1:A:58:LYS:O	2.00	0.61
1:C:205:ALA:HA	1:C:206:TRP:CE3	2.36	0.61
1:A:125:MET:O	1:A:126:LYS:HB3	2.01	0.61
1:A:277:LEU:HD23	1:A:277:LEU:N	2.15	0.61
1:A:306:PHE:CB	1:A:326:TYR:HA	2.27	0.61
2:B:63:ILE:HD12	2:B:63:ILE:C	2.20	0.61
1:C:56:LEU:O	1:C:56:LEU:HG	1.99	0.61
1:C:58:LYS:HG2	1:C:58:LYS:O	2.00	0.61
1:A:178:TYR:CE2	1:A:295:LYS:NZ	2.66	0.61
1:A:170:ILE:CG2	1:A:184:GLU:HG3	2.27	0.61
1:C:343:GLU:O	1:C:345:ARG:HD2	2.01	0.61
1:A:205:ALA:HA	1:A:206:TRP:CE3	2.35	0.61
1:A:233:GLN:O	1:A:234:LYS:HB2	2.01	0.61
1:A:153:ASN:ND2	3:A:502:NAG:C7	2.64	0.61
1:C:309:VAL:HB	1:C:323:ARG:HG2	1.82	0.61
1:A:312:ILE:N	1:A:312:ILE:HD13	2.16	0.61
1:A:378:ILE:CG1	1:A:389:LEU:HB3	2.31	0.61
1:A:99:ARG:NE	1:A:105:CYS:SG	2.74	0.61
1:C:220:TRP:CD1	1:C:220:TRP:C	2.74	0.61
1:C:233:GLN:C	1:C:235:GLU:H	2.03	0.61
1:C:378:ILE:CG1	1:C:389:LEU:HB3	2.31	0.61
1:A:220:TRP:C	1:A:220:TRP:CD1	2.75	0.61
1:C:312:ILE:HD13	1:C:312:ILE:N	2.16	0.61
1:A:443:ILE:HG23	1:A:444:TYR:N	2.15	0.61
1:C:87:ASP:C	1:C:89:ARG:H	2.04	0.61
1:A:12:VAL:HG23	1:A:33:THR:OG1	2.00	0.60
1:C:99:ARG:NH1	1:C:105:CYS:HB3	2.11	0.60
1:C:233:GLN:O	1:C:234:LYS:HB2	2.01	0.60
1:A:101:TRP:HB2	1:A:108:PHE:CD2	2.24	0.60
1:A:309:VAL:HB	1:A:323:ARG:HG2	1.82	0.60
1:C:166:PRO:C	1:C:168:SER:H	2.04	0.60
1:C:197:VAL:HG21	1:C:210:ARG:HA	1.83	0.60
1:C:463:ILE:CG2	1:C:482:VAL:HG22	2.24	0.60
1:C:342:LEU:H	1:C:342:LEU:HD12	1.66	0.60
1:A:23:ILE:HD11	1:A:285:CYS:SG	2.42	0.60
2:B:28:HIS:O	2:B:31:ARG:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:PRO:C	1:A:168:SER:H	2.04	0.60
1:A:259:ALA:HB2	1:C:259:ALA:HB2	1.83	0.60
1:A:193:PHE:CZ	1:A:278:LEU:HD11	2.37	0.60
1:C:153:ASN:ND2	3:C:502:NAG:C7	2.64	0.60
2:D:28:HIS:O	2:D:31:ARG:HG3	2.02	0.60
1:A:92:CYS:HA	1:A:115:THR:O	2.02	0.60
1:A:197:VAL:HG21	1:A:210:ARG:HA	1.83	0.60
1:A:1:MET:HE2	1:A:151:VAL:HG22	1.84	0.60
1:A:58:LYS:CD	1:A:221:LEU:HD23	2.32	0.60
1:A:312:ILE:HG13	1:A:391:TRP:CD1	2.37	0.60
1:A:463:ILE:CG2	1:A:482:VAL:HG22	2.24	0.60
2:B:5:VAL:N	2:B:6:PRO:HD3	2.17	0.60
1:C:23:ILE:HD11	1:C:285:CYS:SG	2.42	0.60
1:C:58:LYS:HB2	1:C:58:LYS:HZ3	1.66	0.60
1:C:99:ARG:NE	1:C:105:CYS:SG	2.74	0.60
2:D:66:LEU:O	2:D:67:LEU:C	2.38	0.60
1:A:315:THR:HG22	1:C:108:PHE:CE1	2.37	0.60
1:C:360:GLU:O	1:C:360:GLU:HG2	2.02	0.60
1:A:270:ILE:HD13	1:A:278:LEU:HA	1.79	0.59
1:C:94:HIS:CA	1:C:114:VAL:HG12	2.32	0.59
1:C:125:MET:O	1:C:126:LYS:HB3	2.00	0.59
1:C:193:PHE:CZ	1:C:278:LEU:HD11	2.37	0.59
1:C:305:LYS:HD3	1:C:305:LYS:C	2.22	0.59
2:D:1:SER:C	2:D:3:ALA:N	2.52	0.59
2:D:36:ILE:HD13	2:D:37:LEU:N	2.17	0.59
1:A:343:GLU:O	1:A:345:ARG:HD2	2.01	0.59
1:A:352:ILE:HB	1:A:368:GLU:O	2.02	0.59
1:C:92:CYS:HA	1:C:115:THR:O	2.02	0.59
1:A:108:PHE:CE1	1:C:315:THR:HG22	2.37	0.59
1:A:201:MET:HE2	1:A:202:GLU:HB2	1.83	0.59
1:A:222:PRO:HG2	1:A:223:GLY:H	1.67	0.59
1:A:87:ASP:C	1:A:89:ARG:H	2.05	0.59
1:C:222:PRO:HG2	1:C:223:GLY:H	1.67	0.59
2:B:36:ILE:HD13	2:B:37:LEU:N	2.17	0.59
1:C:270:ILE:HD13	1:C:278:LEU:HA	1.80	0.59
2:D:5:VAL:N	2:D:6:PRO:HD3	2.17	0.59
1:A:12:VAL:HG23	1:A:33:THR:CB	2.32	0.59
1:A:141:ILE:HD13	1:A:141:ILE:H	1.68	0.59
1:A:200:GLN:HG2	1:A:201:MET:H	1.68	0.59
1:A:383:GLU:CB	1:A:384:PRO:CD	2.80	0.59
1:C:12:VAL:HG23	1:C:33:THR:CB	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:LYS:HB2	1:C:240:PHE:CZ	2.38	0.59
1:C:270:ILE:HD11	1:C:278:LEU:CA	2.27	0.59
1:C:305:LYS:CD	1:C:327:GLU:HB3	2.29	0.59
1:C:312:ILE:HG13	1:C:391:TRP:CD1	2.37	0.59
1:C:352:ILE:HB	1:C:368:GLU:O	2.02	0.59
1:C:457:ILE:HG22	1:C:490:GLY:HA3	1.83	0.59
1:A:305:LYS:HD3	1:A:305:LYS:C	2.23	0.59
1:C:208:VAL:HG21	1:C:212:TRP:HZ3	1.68	0.59
1:A:101:TRP:CZ2	1:C:310:LYS:HG2	2.38	0.59
1:C:312:ILE:HG13	1:C:391:TRP:NE1	2.18	0.59
1:C:60:CYS:SG	1:C:219:PRO:HG2	2.42	0.59
1:C:200:GLN:HG2	1:C:201:MET:H	1.67	0.59
1:C:404:THR:HA	1:C:407:ARG:NH1	2.18	0.59
1:C:479:LEU:O	1:C:480:VAL:C	2.40	0.59
1:A:278:LEU:H	1:A:278:LEU:HD23	1.68	0.59
1:A:404:THR:HA	1:A:407:ARG:NH1	2.18	0.59
1:A:457:ILE:HG22	1:A:490:GLY:HA3	1.83	0.59
1:C:20:TRP:CZ3	1:C:288:ARG:NE	2.70	0.59
1:C:20:TRP:HZ3	1:C:288:ARG:NE	2.01	0.59
1:C:383:GLU:CB	1:C:384:PRO:CD	2.80	0.59
1:C:260:MET:HA	2:D:2:VAL:HB	1.84	0.59
1:A:121:CYS:HG	1:A:231:TRP:HZ2	1.50	0.59
1:A:93:LYS:HB2	1:A:240:PHE:CZ	2.38	0.59
2:B:48:ILE:C	2:B:50:ALA:N	2.56	0.59
1:A:133:GLU:O	1:A:134:ASN:CB	2.51	0.58
1:A:260:MET:HA	2:B:2:VAL:HB	1.84	0.58
1:A:273:SER:O	1:A:274:SER:HB3	2.03	0.58
1:A:310:LYS:HG2	1:C:101:TRP:CZ2	2.37	0.58
1:A:312:ILE:HG13	1:A:391:TRP:NE1	2.18	0.58
1:A:327:GLU:HG2	1:A:328:GLY:N	2.18	0.58
1:C:3:CYS:O	1:C:6:ILE:HG12	2.03	0.58
1:C:74:CYS:C	1:C:77:GLN:HE22	2.06	0.58
1:A:20:TRP:CZ3	1:A:288:ARG:NE	2.70	0.58
1:C:479:LEU:O	1:C:482:VAL:N	2.35	0.58
2:D:41:GLY:O	2:D:44:ILE:HB	2.03	0.58
1:A:360:GLU:HG2	1:A:360:GLU:O	2.02	0.58
1:A:279:PHE:CD2	1:A:279:PHE:N	2.72	0.58
2:B:32:ILE:HD12	2:B:33:GLU:N	2.19	0.58
2:B:3:ALA:CB	2:B:4:LEU:HD22	2.33	0.58
1:C:133:GLU:O	1:C:134:ASN:CB	2.51	0.58
1:C:191:LEU:O	1:C:192:ASP:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:LYS:HA	1:C:247:LYS:HZ2	1.66	0.58
1:C:327:GLU:HG2	1:C:328:GLY:N	2.18	0.58
1:A:20:TRP:HZ3	1:A:288:ARG:NE	2.01	0.58
1:A:393:LYS:HG2	1:A:394:LYS:N	2.18	0.58
1:A:60:CYS:SG	1:A:219:PRO:HG2	2.44	0.58
1:A:62:GLU:HG3	1:A:122:LYS:HB3	1.85	0.58
1:A:74:CYS:C	1:A:77:GLN:HE22	2.06	0.58
1:C:34:MET:HG2	1:C:40:THR:HG21	1.84	0.58
2:D:48:ILE:C	2:D:50:ALA:N	2.57	0.58
1:C:59:TYR:HD2	1:C:218:LEU:HB2	1.68	0.58
1:C:315:THR:O	1:C:316:GLN:HB2	2.04	0.58
1:A:273:SER:O	1:A:274:SER:CB	2.52	0.58
1:A:34:MET:HG2	1:A:40:THR:HG21	1.85	0.58
2:B:32:ILE:HG13	2:B:33:GLU:H	1.68	0.58
1:C:273:SER:O	1:C:274:SER:CB	2.52	0.58
1:C:393:LYS:HG2	1:C:394:LYS:N	2.18	0.58
1:C:406:MET:O	1:C:409:ALA:N	2.36	0.58
2:D:3:ALA:CB	2:D:4:LEU:HD22	2.33	0.58
1:A:255:SER:O	1:A:256:GLN:HG2	2.04	0.58
1:C:141:ILE:H	1:C:141:ILE:HD13	1.68	0.58
2:D:32:ILE:HD12	2:D:33:GLU:N	2.19	0.58
2:D:32:ILE:HG13	2:D:33:GLU:H	1.68	0.58
2:D:50:ALA:CB	2:D:63:ILE:HD11	2.34	0.58
2:D:50:ALA:HA	2:D:63:ILE:HD11	1.85	0.58
1:A:314:GLU:HA	1:A:319:THR:HB	1.85	0.58
1:A:6:ILE:CG2	1:A:6:ILE:O	2.52	0.58
2:B:38:ARG:HE	2:B:38:ARG:HA	1.69	0.58
2:B:38:ARG:NE	2:B:38:ARG:HA	2.18	0.58
1:C:211:GLN:O	1:C:214:LEU:N	2.33	0.58
1:C:229:SER:HA	1:C:231:TRP:NE1	2.19	0.58
1:C:278:LEU:HD23	1:C:278:LEU:H	1.68	0.58
1:A:208:VAL:HG12	1:A:267:ALA:HB2	1.85	0.57
1:A:342:LEU:HD12	1:A:342:LEU:H	1.67	0.57
1:A:406:MET:O	1:A:409:ALA:N	2.37	0.57
1:A:479:LEU:O	1:A:480:VAL:C	2.40	0.57
1:C:178:TYR:CE2	1:C:295:LYS:NZ	2.66	0.57
1:C:448:PHE:CG	1:C:448:PHE:O	2.57	0.57
1:A:140:VAL:O	1:A:140:VAL:HG23	2.03	0.57
1:A:208:VAL:HG21	1:A:212:TRP:HZ3	1.69	0.57
1:A:309:VAL:O	1:A:310:LYS:CB	2.50	0.57
1:A:409:ALA:O	1:A:412:MET:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:GLU:HG3	1:C:122:LYS:HB3	1.85	0.57
1:C:273:SER:O	1:C:274:SER:HB3	2.03	0.57
1:C:314:GLU:HA	1:C:319:THR:HB	1.85	0.57
1:C:490:GLY:O	1:C:492:MET:N	2.37	0.57
2:D:38:ARG:HA	2:D:38:ARG:HE	1.69	0.57
1:A:383:GLU:HG2	1:A:384:PRO:HD3	1.85	0.57
1:A:479:LEU:O	1:A:482:VAL:N	2.35	0.57
2:B:33:GLU:O	2:B:34:THR:C	2.41	0.57
2:B:41:GLY:O	2:B:44:ILE:HB	2.04	0.57
1:C:166:PRO:HB3	1:C:187:PRO:O	2.05	0.57
2:D:44:ILE:HG22	2:D:48:ILE:HD11	1.86	0.57
1:A:101:TRP:HE1	1:C:310:LYS:HZ3	1.49	0.57
1:A:270:ILE:HD11	1:A:278:LEU:CA	2.28	0.57
1:C:409:ALA:O	1:C:412:MET:HB3	2.04	0.57
2:D:38:ARG:HA	2:D:38:ARG:NE	2.18	0.57
1:A:166:PRO:HB3	1:A:187:PRO:O	2.04	0.57
1:A:199:LEU:HG	1:A:199:LEU:O	2.03	0.57
1:A:244:HIS:HD2	2:D:16:THR:HG21	1.70	0.57
2:B:50:ALA:HA	2:B:63:ILE:HD11	1.85	0.57
1:C:199:LEU:HG	1:C:199:LEU:O	2.04	0.57
1:C:407:ARG:CZ	1:C:407:ARG:HB3	2.35	0.57
1:A:229:SER:HA	1:A:231:TRP:NE1	2.19	0.57
1:A:315:THR:O	1:A:316:GLN:HB2	2.04	0.57
1:A:3:CYS:O	1:A:6:ILE:HG12	2.04	0.57
1:C:140:VAL:O	1:C:140:VAL:HG23	2.03	0.57
2:B:16:THR:HG21	1:C:244:HIS:HD2	1.70	0.57
1:A:59:TYR:HD2	1:A:218:LEU:HB2	1.68	0.57
1:A:84:GLU:HB3	1:A:90:PHE:CE1	2.40	0.57
1:C:122:LYS:O	1:C:123:LYS:HB2	2.04	0.57
1:C:255:SER:O	1:C:256:GLN:HG2	2.05	0.57
1:C:316:GLN:O	1:C:317:HIS:C	2.43	0.57
1:C:319:THR:O	1:C:321:VAL:HG22	2.05	0.57
1:C:383:GLU:HG2	1:C:384:PRO:HD3	1.86	0.57
1:A:126:LYS:HG2	1:A:127:GLY:O	2.05	0.57
1:A:490:GLY:C	1:A:492:MET:H	2.08	0.57
2:B:44:ILE:HG22	2:B:48:ILE:HD11	1.86	0.57
1:C:340:MET:SD	1:C:345:ARG:CD	2.93	0.57
1:A:299:TYR:CD1	1:A:299:TYR:N	2.71	0.57
1:C:202:GLU:O	1:C:203:ASN:CB	2.53	0.57
1:C:443:ILE:O	1:C:446:ALA:C	2.43	0.57
1:A:122:LYS:HB2	1:A:122:LYS:HZ3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LEU:O	1:A:192:ASP:HB2	2.04	0.57
1:A:211:GLN:O	1:A:214:LEU:N	2.33	0.57
1:A:310:LYS:NZ	1:C:101:TRP:NE1	2.39	0.57
1:C:58:LYS:CD	1:C:221:LEU:HD23	2.32	0.57
1:C:65:LEU:HD21	1:C:252:VAL:CA	2.27	0.57
1:A:146:GLY:HA3	1:A:366:ASN:OD1	2.05	0.56
1:A:339:ILE:HG22	1:A:339:ILE:O	2.04	0.56
1:A:340:MET:SD	1:A:345:ARG:CD	2.93	0.56
1:A:475:LEU:O	1:A:478:SER:N	2.38	0.56
1:C:340:MET:HG2	1:C:341:ASP:N	2.19	0.56
1:A:201:MET:HB3	1:A:206:TRP:CZ3	2.37	0.56
1:A:448:PHE:CG	1:A:448:PHE:O	2.57	0.56
1:A:56:LEU:O	1:A:57:ARG:CB	2.50	0.56
1:A:89:ARG:HD3	1:A:118:MET:CE	2.36	0.56
1:C:279:PHE:N	1:C:279:PHE:CD2	2.72	0.56
1:C:309:VAL:O	1:C:310:LYS:CB	2.50	0.56
2:D:3:ALA:C	2:D:4:LEU:HD22	2.26	0.56
1:A:475:LEU:HG	1:A:476:SER:N	2.21	0.56
1:A:486:THR:O	1:A:487:LEU:C	2.43	0.56
1:C:208:VAL:HG12	1:C:267:ALA:HB2	1.86	0.56
1:C:89:ARG:HD3	1:C:118:MET:CE	2.35	0.56
1:A:192:ASP:O	1:A:195:GLU:HB2	2.05	0.56
1:C:126:LYS:HG2	1:C:127:GLY:O	2.04	0.56
1:A:340:MET:HG2	1:A:341:ASP:N	2.19	0.56
1:A:378:ILE:O	1:A:378:ILE:HG13	2.04	0.56
1:A:72:SER:HA	1:A:113:ILE:HA	1.87	0.56
1:C:203:ASN:O	1:C:204:LYS:HG2	2.06	0.56
1:C:299:TYR:N	1:C:299:TYR:CD1	2.71	0.56
1:C:339:ILE:O	1:C:339:ILE:HG22	2.04	0.56
1:C:378:ILE:HD11	1:C:389:LEU:HB3	1.88	0.56
1:C:378:ILE:O	1:C:378:ILE:HG13	2.05	0.56
1:A:122:LYS:O	1:A:123:LYS:HB2	2.04	0.56
2:B:3:ALA:C	2:B:4:LEU:HD22	2.25	0.56
1:C:475:LEU:O	1:C:478:SER:N	2.38	0.56
1:A:240:PHE:HB3	1:A:250:VAL:CG1	2.36	0.56
1:A:443:ILE:O	1:A:446:ALA:C	2.44	0.56
1:C:443:ILE:HG23	1:C:444:TYR:H	1.71	0.56
1:C:80:PRO:HG3	1:C:113:ILE:N	2.20	0.56
1:C:84:GLU:HB3	1:C:90:PHE:CE1	2.41	0.56
1:A:178:TYR:N	1:A:178:TYR:CD2	2.73	0.56
1:A:490:GLY:O	1:A:492:MET:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:ALA:CB	2:B:63:ILE:HD11	2.35	0.56
1:C:121:CYS:HG	1:C:231:TRP:HZ2	1.51	0.56
1:C:475:LEU:HG	1:C:476:SER:N	2.20	0.56
1:C:60:CYS:SG	1:C:219:PRO:CG	2.94	0.56
1:A:39:PRO:HD3	1:A:294:LEU:CA	2.35	0.56
1:C:465:TRP:C	1:C:467:GLY:N	2.59	0.56
1:A:247:LYS:HA	1:A:247:LYS:HZ3	1.68	0.56
1:A:319:THR:O	1:A:321:VAL:HG22	2.06	0.56
1:A:483:GLY:O	1:A:484:VAL:C	2.44	0.56
1:A:80:PRO:HG3	1:A:113:ILE:N	2.20	0.56
1:C:490:GLY:C	1:C:492:MET:H	2.08	0.56
1:C:72:SER:HA	1:C:113:ILE:HA	1.87	0.56
1:A:316:GLN:O	1:A:317:HIS:C	2.43	0.56
1:A:407:ARG:CZ	1:A:407:ARG:HB3	2.35	0.56
1:A:7:SER:O	1:A:8:ASN:C	2.43	0.56
1:C:367:ILE:H	1:C:367:ILE:HD12	1.70	0.55
1:C:400:GLN:HE21	1:C:400:GLN:HA	1.71	0.55
1:C:486:THR:O	1:C:487:LEU:C	2.43	0.55
1:C:74:CYS:SG	1:C:75:PRO:CD	2.95	0.55
2:D:62:LEU:HD13	2:D:66:LEU:HD13	1.87	0.55
1:A:378:ILE:HD11	1:A:389:LEU:HB3	1.87	0.55
1:C:39:PRO:HD3	1:C:294:LEU:CA	2.35	0.55
1:C:340:MET:HA	1:C:347:VAL:HA	1.88	0.55
1:A:203:ASN:O	1:A:204:LYS:HG2	2.06	0.55
1:A:443:ILE:HG23	1:A:444:TYR:H	1.71	0.55
1:A:74:CYS:SG	1:A:75:PRO:CD	2.93	0.55
1:A:465:TRP:C	1:A:467:GLY:N	2.59	0.55
2:B:62:LEU:HD13	2:B:66:LEU:HD13	1.87	0.55
2:D:33:GLU:O	2:D:34:THR:C	2.42	0.55
1:A:337:PHE:CD1	1:A:337:PHE:C	2.80	0.55
1:A:487:LEU:C	1:A:487:LEU:HD13	2.26	0.55
1:A:94:HIS:CA	1:A:114:VAL:HG12	2.32	0.55
1:C:1:MET:CE	1:C:151:VAL:HG22	2.37	0.55
1:C:192:ASP:O	1:C:195:GLU:HB2	2.05	0.55
1:C:350:ARG:HB2	1:C:350:ARG:CZ	2.37	0.55
2:B:49:LEU:CD1	1:C:459:ILE:HD12	2.37	0.55
1:C:260:MET:HA	2:D:2:VAL:CG1	2.37	0.55
2:D:32:ILE:O	2:D:36:ILE:HG22	2.07	0.55
1:A:193:PHE:O	1:A:194:ASN:C	2.45	0.55
1:A:202:GLU:O	1:A:203:ASN:CB	2.53	0.55
2:B:51:TYR:CA	2:B:60:ARG:HD3	2.12	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:LEU:HD21	1:C:193:PHE:CE1	2.36	0.55
1:C:1:MET:HE2	1:C:151:VAL:HG22	1.88	0.55
1:C:178:TYR:N	1:C:178:TYR:CD2	2.73	0.55
1:C:233:GLN:O	1:C:234:LYS:CB	2.55	0.55
1:A:383:GLU:CG	1:A:384:PRO:HD3	2.37	0.55
1:C:37:ASN:O	1:C:38:LYS:HB2	2.07	0.55
1:A:247:LYS:HA	1:A:247:LYS:HZ2	1.70	0.55
1:A:350:ARG:CZ	1:A:350:ARG:HB2	2.37	0.55
1:A:37:ASN:O	1:A:38:LYS:HB2	2.07	0.55
1:C:306:PHE:CZ	1:C:381:GLY:HA3	2.31	0.55
1:A:102:GLY:C	1:A:104:GLY:N	2.60	0.55
1:A:400:GLN:HA	1:A:400:GLN:HE21	1.71	0.55
1:C:193:PHE:O	1:C:194:ASN:C	2.45	0.55
1:A:459:ILE:HD12	2:D:49:LEU:CD1	2.37	0.55
1:C:212:TRP:CD2	2:D:7:HIS:HB2	2.42	0.55
1:A:212:TRP:CD2	2:B:7:HIS:HB2	2.42	0.55
1:A:367:ILE:H	1:A:367:ILE:HD12	1.68	0.55
1:A:470:SER:CB	1:A:475:LEU:HB3	2.37	0.55
1:C:240:PHE:HB3	1:C:250:VAL:CG1	2.36	0.55
1:C:337:PHE:CD1	1:C:337:PHE:C	2.80	0.55
1:A:260:MET:HA	2:B:2:VAL:CG1	2.37	0.54
1:C:146:GLY:HA3	1:C:366:ASN:OD1	2.06	0.54
1:C:74:CYS:O	1:C:77:GLN:NE2	2.40	0.54
1:A:232:ILE:O	1:A:233:GLN:CB	2.55	0.54
1:A:340:MET:HA	1:A:347:VAL:HA	1.88	0.54
1:A:453:TRP:CG	1:A:454:ILE:N	2.76	0.54
1:C:301:MET:HA	1:C:334:LYS:HB2	1.89	0.54
1:C:20:TRP:CB	1:C:425:LEU:HD21	2.37	0.54
1:C:487:LEU:HD13	1:C:487:LEU:C	2.27	0.54
1:C:7:SER:O	1:C:8:ASN:C	2.43	0.54
1:A:311:GLU:HG2	1:A:312:ILE:N	2.14	0.54
1:C:232:ILE:O	1:C:233:GLN:CB	2.54	0.54
1:C:448:PHE:C	1:C:448:PHE:CD1	2.80	0.54
1:C:464:THR:CA	1:C:482:VAL:HG21	2.30	0.54
1:A:80:PRO:HG2	1:A:114:VAL:HG13	1.89	0.54
1:A:92:CYS:HG	1:A:116:CYS:HB3	1.73	0.54
1:A:311:GLU:HB2	1:A:312:ILE:HD13	1.90	0.54
1:A:301:MET:HA	1:A:334:LYS:HB2	1.89	0.54
1:A:74:CYS:O	1:A:77:GLN:NE2	2.40	0.54
2:B:32:ILE:O	2:B:36:ILE:HG22	2.07	0.54
1:C:247:LYS:HA	1:C:247:LYS:HZ3	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:VAL:HG23	1:C:113:ILE:HG21	1.89	0.54
1:A:60:CYS:SG	1:A:219:PRO:CG	2.96	0.54
1:A:373:PHE:CD1	1:A:374:GLY:N	2.76	0.54
1:C:56:LEU:O	1:C:57:ARG:CB	2.49	0.54
1:A:233:GLN:O	1:A:234:LYS:CB	2.55	0.54
1:A:306:PHE:CZ	1:A:381:GLY:HA3	2.32	0.54
1:A:34:MET:HA	1:A:40:THR:CG2	2.38	0.54
1:A:20:TRP:CB	1:A:425:LEU:HD21	2.37	0.54
1:C:373:PHE:CD1	1:C:374:GLY:N	2.76	0.54
1:A:108:PHE:HE2	1:C:321:VAL:HG21	1.73	0.54
1:A:75:PRO:HA	1:A:110:LYS:O	2.08	0.54
1:A:143:PRO:HB3	1:A:178:TYR:HE1	1.73	0.54
2:B:4:LEU:HB3	2:D:31:ARG:NH2	2.13	0.54
1:C:20:TRP:CD1	1:C:286:ARG:NH1	2.76	0.54
1:C:284:LYS:O	1:C:285:CYS:HB3	2.07	0.54
1:C:306:PHE:CB	1:C:326:TYR:HA	2.27	0.54
1:C:483:GLY:O	1:C:484:VAL:C	2.44	0.54
1:C:75:PRO:HA	1:C:110:LYS:O	2.08	0.54
1:A:97:VAL:HG23	1:A:113:ILE:HG21	1.89	0.54
1:A:135:LEU:HD21	1:A:193:PHE:CE1	2.36	0.54
1:C:201:MET:HB3	1:C:206:TRP:CZ3	2.37	0.54
1:C:206:TRP:CD1	1:C:264:LEU:HD11	2.43	0.54
1:C:229:SER:O	1:C:231:TRP:HD1	1.91	0.54
1:C:340:MET:CE	1:C:345:ARG:HG3	2.38	0.54
1:C:383:GLU:CG	1:C:384:PRO:HD3	2.37	0.54
1:C:80:PRO:HG2	1:C:114:VAL:HG13	1.90	0.54
1:A:229:SER:O	1:A:231:TRP:HD1	1.91	0.54
1:A:436:LEU:HD13	1:A:436:LEU:C	2.29	0.54
1:C:122:LYS:HA	1:C:122:LYS:HZ2	1.73	0.54
1:C:279:PHE:N	1:C:279:PHE:HD2	2.06	0.54
1:C:484:VAL:HA	1:C:488:TYR:CB	2.35	0.54
1:A:311:GLU:CG	1:A:312:ILE:H	2.10	0.53
1:C:294:LEU:HD23	1:C:294:LEU:C	2.27	0.53
2:D:5:VAL:N	2:D:6:PRO:CD	2.71	0.53
1:A:484:VAL:HA	1:A:488:TYR:CB	2.35	0.53
1:A:62:GLU:O	1:A:122:LYS:HB3	2.09	0.53
1:C:211:GLN:O	1:C:212:TRP:C	2.47	0.53
1:C:311:GLU:HB2	1:C:312:ILE:HD13	1.90	0.53
1:C:453:TRP:CG	1:C:454:ILE:N	2.76	0.53
1:A:20:TRP:CD1	1:A:286:ARG:NH1	2.76	0.53
1:A:448:PHE:C	1:A:448:PHE:CD1	2.81	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:LEU:O	1:C:217:PRO:O	2.26	0.53
1:A:1:MET:CE	1:A:151:VAL:HG22	2.37	0.53
2:B:48:ILE:O	2:B:50:ALA:N	2.42	0.53
1:C:234:LYS:O	1:C:238:VAL:HG12	2.08	0.53
1:C:62:GLU:O	1:C:122:LYS:HB3	2.09	0.53
1:A:294:LEU:HD23	1:A:294:LEU:C	2.27	0.53
1:A:327:GLU:CG	1:A:328:GLY:H	2.21	0.53
1:A:393:LYS:HZ2	1:A:395:GLY:HA2	1.72	0.53
1:A:87:ASP:C	1:A:89:ARG:N	2.61	0.53
1:C:208:VAL:HG12	1:C:267:ALA:CB	2.39	0.53
1:C:335:ILE:HB	1:C:356:PRO:CG	2.39	0.53
1:C:436:LEU:C	1:C:436:LEU:HD13	2.28	0.53
1:C:490:GLY:C	1:C:492:MET:N	2.62	0.53
2:D:32:ILE:CG1	2:D:33:GLU:N	2.72	0.53
1:A:211:GLN:O	1:A:212:TRP:C	2.46	0.53
1:A:340:MET:CE	1:A:345:ARG:HG3	2.39	0.53
1:A:27:HIS:H	1:A:45:LEU:HD11	1.74	0.53
1:A:482:VAL:O	1:A:483:GLY:O	2.27	0.53
1:A:206:TRP:CD1	1:A:264:LEU:HD11	2.43	0.53
1:A:314:GLU:O	1:A:315:THR:C	2.47	0.53
1:A:108:PHE:CE2	1:C:313:ALA:HB3	2.44	0.53
2:B:5:VAL:N	2:B:6:PRO:CD	2.71	0.53
1:C:153:ASN:HA	3:C:502:NAG:O7	2.09	0.53
1:C:340:MET:HE3	1:C:379:ILE:HG21	1.90	0.53
1:A:205:ALA:HB3	1:A:270:ILE:HG23	1.91	0.53
1:A:335:ILE:HB	1:A:356:PRO:CG	2.39	0.53
1:A:45:LEU:HD22	1:A:45:LEU:O	2.09	0.53
1:A:490:GLY:C	1:A:492:MET:N	2.63	0.53
1:A:51:LYS:HZ1	1:A:136:GLU:HB2	1.73	0.53
1:C:143:PRO:HB3	1:C:178:TYR:HE1	1.73	0.53
1:C:200:GLN:HG2	1:C:201:MET:N	2.24	0.53
1:C:482:VAL:O	1:C:483:GLY:O	2.27	0.53
2:D:48:ILE:O	2:D:50:ALA:N	2.42	0.53
1:A:208:VAL:HG12	1:A:267:ALA:CB	2.39	0.52
1:C:91:VAL:O	1:C:116:CYS:HA	2.09	0.52
1:A:20:TRP:CA	1:A:20:TRP:CE3	2.92	0.52
1:A:234:LYS:O	1:A:238:VAL:HG12	2.08	0.52
1:A:284:LYS:O	1:A:285:CYS:HB3	2.08	0.52
1:A:91:VAL:O	1:A:116:CYS:HA	2.09	0.52
1:C:20:TRP:CA	1:C:20:TRP:CE3	2.92	0.52
1:C:240:PHE:CA	1:C:249:ASP:O	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:ASP:O	1:C:419:ALA:N	2.42	0.52
1:C:427:GLY:N	1:C:431:SER:OG	2.42	0.52
1:C:432:ILE:HD13	1:C:435:ALA:HB3	1.91	0.52
1:C:97:VAL:HG13	1:C:246:LYS:HA	1.91	0.52
1:A:313:ALA:HB3	1:C:108:PHE:CE2	2.43	0.52
1:A:432:ILE:HD13	1:A:435:ALA:HB3	1.92	0.52
1:C:241:LYS:HD2	1:C:241:LYS:O	2.09	0.52
1:A:153:ASN:HA	3:A:502:NAG:O7	2.10	0.52
1:A:128:LYS:HB3	1:A:198:LEU:HB3	1.92	0.52
1:A:221:LEU:HD22	1:A:231:TRP:CZ2	2.45	0.52
1:C:43:PHE:CE2	1:C:141:ILE:HG21	2.45	0.52
1:C:205:ALA:HB3	1:C:270:ILE:HG23	1.91	0.52
1:C:473:THR:C	1:C:475:LEU:HD23	2.30	0.52
2:B:31:ARG:NH2	2:D:4:LEU:HB3	2.13	0.52
1:A:242:ASN:HB2	1:A:248:GLN:HG2	1.90	0.52
1:A:257:GLU:HA	1:A:257:GLU:OE1	2.10	0.52
1:A:406:MET:O	1:A:407:ARG:C	2.48	0.52
1:A:417:ASP:O	1:A:419:ALA:N	2.42	0.52
1:C:307:LYS:HG2	1:C:308:VAL:N	2.24	0.52
1:C:87:ASP:C	1:C:89:ARG:N	2.61	0.52
1:A:215:ASP:O	1:A:216:LEU:C	2.48	0.52
1:A:270:ILE:HG23	1:A:271:GLN:N	2.24	0.52
1:A:335:ILE:HB	1:A:356:PRO:HG2	1.92	0.52
1:A:427:GLY:N	1:A:431:SER:OG	2.42	0.52
1:A:478:SER:O	1:A:481:LEU:HB3	2.10	0.52
1:A:64:LYS:HZ2	1:A:64:LYS:HB3	1.74	0.52
1:C:128:LYS:HB3	1:C:198:LEU:HB3	1.92	0.52
1:C:270:ILE:CD1	1:C:270:ILE:C	2.77	0.52
1:A:279:PHE:N	1:A:279:PHE:HD2	2.06	0.52
1:A:340:MET:HE3	1:A:379:ILE:HG21	1.90	0.52
1:A:390:ASN:C	1:A:390:ASN:HD22	2.12	0.52
1:A:43:PHE:CE2	1:A:141:ILE:HG21	2.44	0.52
1:A:9:ARG:CG	1:A:10:ASP:N	2.73	0.52
1:C:141:ILE:HD13	1:C:141:ILE:O	2.09	0.52
1:C:165:THR:C	1:C:167:GLN:H	2.12	0.52
1:C:221:LEU:HD22	1:C:231:TRP:CZ2	2.45	0.52
1:C:327:GLU:CG	1:C:328:GLY:H	2.20	0.52
1:A:165:THR:C	1:A:167:GLN:H	2.12	0.52
1:C:242:ASN:HB2	1:C:248:GLN:HG2	1.90	0.52
1:A:240:PHE:CA	1:A:249:ASP:O	2.58	0.52
1:A:20:TRP:HD1	1:A:425:LEU:HD11	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:SER:OG	2:B:2:VAL:N	2.43	0.52
1:C:19:SER:HB3	1:C:289:MET:H	1.75	0.52
1:C:237:LEU:O	1:C:238:VAL:O	2.28	0.52
1:C:270:ILE:HG23	1:C:271:GLN:N	2.25	0.52
1:A:141:ILE:HD13	1:A:141:ILE:O	2.10	0.52
1:A:216:LEU:O	1:A:217:PRO:O	2.27	0.52
1:A:241:LYS:O	1:A:241:LYS:HD2	2.10	0.52
1:A:321:VAL:HG21	1:C:108:PHE:HE2	1.74	0.52
1:C:27:HIS:H	1:C:45:LEU:HD11	1.74	0.52
1:C:45:LEU:HD22	1:C:45:LEU:O	2.09	0.52
1:A:19:SER:HB3	1:A:289:MET:H	1.74	0.51
1:A:97:VAL:HG13	1:A:246:LYS:HA	1.91	0.51
1:C:257:GLU:HA	1:C:257:GLU:OE1	2.09	0.51
1:C:459:ILE:HA	1:C:462:ILE:CG2	2.40	0.51
1:C:406:MET:O	1:C:407:ARG:C	2.48	0.51
1:A:459:ILE:HA	1:A:462:ILE:CG2	2.39	0.51
1:C:416:GLY:O	1:C:418:THR:N	2.44	0.51
1:C:481:LEU:HD13	1:C:481:LEU:O	2.11	0.51
2:D:32:ILE:HG13	2:D:33:GLU:N	2.26	0.51
1:A:102:GLY:O	1:A:104:GLY:N	2.43	0.51
1:A:200:GLN:HG2	1:A:201:MET:N	2.24	0.51
1:A:277:LEU:HD12	1:A:279:PHE:HE2	1.76	0.51
1:A:416:GLY:O	1:A:418:THR:N	2.44	0.51
1:A:88:LYS:O	1:A:88:LYS:HG2	2.11	0.51
2:B:32:ILE:CG1	2:B:33:GLU:N	2.72	0.51
1:C:215:ASP:O	1:C:216:LEU:C	2.48	0.51
1:C:277:LEU:HD12	1:C:279:PHE:HE2	1.75	0.51
1:A:202:GLU:O	1:A:203:ASN:HB3	2.10	0.51
1:A:378:ILE:HG13	1:A:389:LEU:HB3	1.92	0.51
2:B:32:ILE:HG13	2:B:33:GLU:N	2.26	0.51
1:C:302:CYS:SG	1:C:333:CYS:CB	2.99	0.51
1:C:20:TRP:HD1	1:C:425:LEU:HD11	1.75	0.51
1:A:237:LEU:O	1:A:238:VAL:O	2.29	0.51
1:A:340:MET:HG2	1:A:341:ASP:H	1.76	0.51
1:A:484:VAL:HG12	1:A:485:VAL:H	1.75	0.51
2:B:19:TRP:O	2:B:20:MET:SD	2.69	0.51
2:B:29:ALA:O	2:B:32:ILE:HG13	2.11	0.51
1:C:102:GLY:O	1:C:104:GLY:N	2.43	0.51
1:C:335:ILE:HB	1:C:356:PRO:HG2	1.92	0.51
1:C:9:ARG:CG	1:C:10:ASP:N	2.73	0.51
2:D:60:ARG:O	2:D:61:ALA:C	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:ARG:O	1:A:472:SER:HB2	2.11	0.51
1:C:102:GLY:C	1:C:104:GLY:N	2.60	0.51
1:C:378:ILE:HG13	1:C:389:LEU:HB3	1.92	0.51
1:C:394:LYS:C	1:C:396:SER:H	2.13	0.51
1:C:470:SER:CB	1:C:475:LEU:HB3	2.37	0.51
1:C:484:VAL:HG12	1:C:485:VAL:H	1.75	0.51
1:A:165:THR:C	1:A:167:GLN:N	2.64	0.51
1:A:302:CYS:SG	1:A:333:CYS:CB	2.98	0.51
1:A:464:THR:CA	1:A:482:VAL:HG21	2.30	0.51
1:C:356:PRO:O	1:C:357:ILE:CB	2.59	0.51
2:D:66:LEU:C	2:D:70:VAL:HG23	2.31	0.51
1:A:238:VAL:HG13	1:A:238:VAL:O	2.11	0.51
1:A:270:ILE:HG12	1:A:278:LEU:HB3	1.93	0.51
1:C:323:ARG:HD2	1:C:364:PRO:O	2.11	0.51
1:C:352:ILE:CG2	1:C:368:GLU:HB2	2.40	0.51
1:C:393:LYS:HZ2	1:C:395:GLY:HA2	1.74	0.51
1:A:345:ARG:CD	1:A:345:ARG:H	2.24	0.51
1:A:394:LYS:C	1:A:396:SER:H	2.13	0.51
1:C:198:LEU:HD21	1:C:278:LEU:HD13	1.93	0.51
1:C:322:ILE:O	1:C:366:ASN:HA	2.10	0.51
2:D:29:ALA:O	2:D:32:ILE:HG13	2.11	0.51
1:A:19:SER:HA	1:A:289:MET:HB2	1.93	0.50
1:A:456:LYS:NZ	1:A:493:VAL:HG11	2.27	0.50
1:A:486:THR:O	1:A:488:TYR:N	2.44	0.50
1:C:270:ILE:HG12	1:C:278:LEU:HB3	1.93	0.50
1:C:339:ILE:HB	1:C:349:GLY:CA	2.39	0.50
1:C:345:ARG:CD	1:C:345:ARG:H	2.24	0.50
1:C:34:MET:HA	1:C:40:THR:CG2	2.38	0.50
1:A:15:VAL:HG13	1:A:35:ALA:CB	2.41	0.50
1:A:270:ILE:CD1	1:A:270:ILE:C	2.77	0.50
1:A:84:GLU:HB3	1:A:90:PHE:CD1	2.46	0.50
1:C:165:THR:C	1:C:167:GLN:N	2.64	0.50
1:C:232:ILE:O	1:C:233:GLN:HB2	2.11	0.50
1:C:471:ARG:O	1:C:472:SER:HB2	2.11	0.50
1:A:454:ILE:HG23	1:A:455:MET:N	2.23	0.50
1:A:473:THR:C	1:A:475:LEU:HD23	2.30	0.50
1:A:76:THR:O	1:A:78:GLY:N	2.44	0.50
1:C:125:MET:HE3	1:C:260:MET:HE1	1.93	0.50
1:C:19:SER:HA	1:C:289:MET:HB2	1.93	0.50
1:A:237:LEU:O	1:A:238:VAL:C	2.50	0.50
1:C:197:VAL:HG11	1:C:213:PHE:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:PHE:HD1	1:C:250:VAL:CG1	2.24	0.50
1:C:312:ILE:CG2	1:C:322:ILE:HG12	2.42	0.50
1:C:478:SER:O	1:C:481:LEU:HB3	2.10	0.50
2:D:19:TRP:O	2:D:20:MET:SD	2.70	0.50
1:A:232:ILE:O	1:A:233:GLN:HB2	2.12	0.50
1:A:264:LEU:C	1:A:264:LEU:HD12	2.31	0.50
1:A:309:VAL:O	1:A:323:ARG:HB3	2.12	0.50
1:A:322:ILE:O	1:A:366:ASN:HA	2.10	0.50
1:A:481:LEU:HD13	1:A:481:LEU:O	2.11	0.50
1:C:97:VAL:CG2	1:C:113:ILE:HG21	2.42	0.50
1:C:157:LYS:HE2	1:C:157:LYS:N	2.26	0.50
1:C:202:GLU:O	1:C:203:ASN:HB3	2.10	0.50
1:A:68:THR:HA	1:A:116:CYS:O	2.12	0.50
1:C:9:ARG:CG	1:C:10:ASP:H	2.24	0.50
1:C:146:GLY:O	1:C:147:GLU:CG	2.59	0.50
1:C:319:THR:N	1:C:320:ILE:HD12	2.26	0.50
1:A:323:ARG:HD2	1:A:364:PRO:O	2.12	0.50
1:A:342:LEU:HD12	1:A:342:LEU:N	2.27	0.50
2:B:66:LEU:C	2:B:70:VAL:HG23	2.31	0.50
1:C:283:LEU:O	1:C:283:LEU:HD12	2.12	0.50
1:C:342:LEU:N	1:C:342:LEU:HD12	2.27	0.50
1:C:486:THR:O	1:C:488:TYR:N	2.44	0.50
1:A:146:GLY:O	1:A:147:GLU:CG	2.59	0.50
1:A:312:ILE:CG2	1:A:322:ILE:HG12	2.42	0.50
1:A:475:LEU:O	1:A:476:SER:C	2.49	0.50
1:C:24:VAL:C	1:C:25:LEU:HD23	2.32	0.50
1:C:264:LEU:C	1:C:264:LEU:HD12	2.32	0.50
1:C:314:GLU:O	1:C:315:THR:C	2.47	0.50
2:D:1:SER:OG	2:D:2:VAL:N	2.44	0.50
1:A:24:VAL:C	1:A:25:LEU:HD23	2.31	0.50
1:A:29:SER:O	1:A:30:CYS:SG	2.68	0.50
1:A:370:GLU:O	1:A:370:GLU:HG2	2.12	0.50
2:B:60:ARG:O	2:B:61:ALA:C	2.49	0.50
1:C:237:LEU:O	1:C:238:VAL:C	2.50	0.50
1:A:240:PHE:HD1	1:A:250:VAL:CG1	2.24	0.49
1:A:282:HIS:ND1	1:A:282:HIS:O	2.44	0.49
1:A:315:THR:O	1:A:316:GLN:CB	2.60	0.49
1:A:393:LYS:HG2	1:A:394:LYS:H	1.77	0.49
1:C:340:MET:HG2	1:C:341:ASP:H	1.75	0.49
1:C:88:LYS:O	1:C:88:LYS:HG2	2.11	0.49
1:A:205:ALA:CA	1:A:206:TRP:CE3	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:LEU:CD1	1:A:267:ALA:HB3	2.41	0.49
1:A:339:ILE:HB	1:A:349:GLY:CA	2.39	0.49
1:C:311:GLU:HG2	1:C:312:ILE:N	2.15	0.49
1:C:356:PRO:O	1:C:357:ILE:HB	2.13	0.49
1:C:68:THR:HA	1:C:116:CYS:O	2.12	0.49
1:C:76:THR:O	1:C:78:GLY:N	2.44	0.49
1:A:9:ARG:CG	1:A:10:ASP:H	2.24	0.49
1:A:122:LYS:HB2	1:A:122:LYS:NZ	2.27	0.49
1:A:196:MET:CE	1:A:196:MET:HA	2.43	0.49
1:A:283:LEU:HD12	1:A:283:LEU:O	2.12	0.49
1:C:282:HIS:O	1:C:282:HIS:ND1	2.45	0.49
1:C:315:THR:O	1:C:316:GLN:CB	2.60	0.49
1:C:332:PRO:HB3	1:C:359:THR:HA	1.94	0.49
1:C:370:GLU:HG2	1:C:370:GLU:O	2.12	0.49
1:C:475:LEU:O	1:C:476:SER:C	2.49	0.49
1:C:89:ARG:HD3	1:C:118:MET:HE1	1.93	0.49
1:A:11:PHE:CD1	1:A:11:PHE:N	2.81	0.49
1:A:121:CYS:SG	1:A:231:TRP:CZ2	3.06	0.49
1:A:264:LEU:HD11	1:A:267:ALA:HB3	1.95	0.49
1:A:26:GLU:HB3	1:A:282:HIS:CB	2.43	0.49
1:A:484:VAL:O	1:A:485:VAL:C	2.51	0.49
1:A:8:ASN:O	1:A:9:ARG:HB2	2.13	0.49
1:C:84:GLU:HB3	1:C:90:PHE:CD1	2.47	0.49
1:C:263:ALA:HB2	2:D:2:VAL:O	2.13	0.49
1:A:332:PRO:HB3	1:A:359:THR:HA	1.93	0.49
1:A:352:ILE:CG2	1:A:368:GLU:HB2	2.40	0.49
1:C:11:PHE:CD1	1:C:11:PHE:N	2.80	0.49
1:C:15:VAL:HG13	1:C:35:ALA:CB	2.42	0.49
1:C:205:ALA:CA	1:C:206:TRP:CE3	2.95	0.49
1:A:57:ARG:NH2	1:A:214:LEU:CD2	2.76	0.49
1:C:29:SER:O	1:C:30:CYS:SG	2.68	0.49
1:C:144:HIS:HB3	1:C:353:THR:HG23	1.95	0.49
1:C:388:LYS:NZ	1:C:388:LYS:HB3	2.28	0.49
1:C:456:LYS:NZ	1:C:493:VAL:HG11	2.27	0.49
1:A:135:LEU:HA	1:A:135:LEU:HD22	1.62	0.49
1:A:157:LYS:N	1:A:157:LYS:HE2	2.26	0.49
1:A:263:ALA:HB2	2:B:2:VAL:O	2.13	0.49
1:A:356:PRO:O	1:A:357:ILE:CB	2.60	0.49
1:C:100:GLY:HA2	1:C:108:PHE:CB	2.42	0.49
1:C:264:LEU:CD1	1:C:267:ALA:HB3	2.42	0.49
1:C:64:LYS:HB3	1:C:64:LYS:HZ2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ARG:O	1:A:10:ASP:CB	2.61	0.49
1:C:121:CYS:SG	1:C:231:TRP:CZ2	3.06	0.49
1:C:1:MET:HG2	1:C:150:ALA:O	2.13	0.49
1:C:341:ASP:O	1:C:342:LEU:C	2.51	0.49
1:A:197:VAL:HG11	1:A:213:PHE:CD2	2.48	0.49
1:A:388:LYS:NZ	1:A:388:LYS:HB3	2.28	0.49
1:C:170:ILE:H	1:C:170:ILE:CD1	2.25	0.49
1:C:196:MET:CE	1:C:196:MET:HA	2.43	0.49
1:C:26:GLU:HB3	1:C:282:HIS:CB	2.43	0.49
1:C:309:VAL:O	1:C:323:ARG:HB3	2.12	0.49
1:C:308:VAL:HA	1:C:324:VAL:HA	1.95	0.49
1:C:411:ARG:HD2	1:C:422:PHE:CD1	2.48	0.49
1:C:443:ILE:O	1:C:446:ALA:N	2.45	0.49
1:C:454:ILE:C	1:C:454:ILE:HD13	2.34	0.49
1:A:283:LEU:C	1:A:283:LEU:CD1	2.81	0.49
1:A:57:ARG:O	1:A:58:LYS:HB2	2.13	0.49
1:C:187:PRO:HG2	1:C:187:PRO:O	2.13	0.49
1:C:57:ARG:O	1:C:58:LYS:HB2	2.13	0.49
1:A:1:MET:HG2	1:A:150:ALA:O	2.12	0.48
1:A:307:LYS:HG2	1:A:308:VAL:N	2.24	0.48
1:A:407:ARG:HH21	1:A:407:ARG:HG2	1.78	0.48
1:C:125:MET:HB2	1:C:201:MET:SD	2.52	0.48
1:C:191:LEU:HB3	1:C:193:PHE:CE2	2.48	0.48
1:C:238:VAL:HG13	1:C:238:VAL:O	2.12	0.48
1:C:270:ILE:HG12	1:C:278:LEU:CB	2.43	0.48
1:C:367:ILE:CD1	1:C:367:ILE:N	2.75	0.48
1:C:74:CYS:HB2	1:C:99:ARG:NH1	2.28	0.48
1:C:8:ASN:O	1:C:9:ARG:HB2	2.13	0.48
1:A:383:GLU:C	1:A:385:GLY:H	2.16	0.48
1:A:411:ARG:HD2	1:A:422:PHE:CD1	2.48	0.48
1:C:160:LYS:HG3	1:C:161:GLU:H	1.78	0.48
1:C:200:GLN:HB2	1:C:272:MET:CE	2.43	0.48
1:C:393:LYS:NZ	1:C:395:GLY:HA2	2.28	0.48
1:A:125:MET:HB2	1:A:201:MET:SD	2.53	0.48
1:A:157:LYS:HG2	1:A:157:LYS:O	2.13	0.48
1:A:356:PRO:O	1:A:357:ILE:HB	2.13	0.48
1:A:443:ILE:O	1:A:446:ALA:N	2.45	0.48
1:C:213:PHE:CG	1:C:213:PHE:O	2.66	0.48
1:C:264:LEU:HD11	1:C:267:ALA:HB3	1.95	0.48
1:A:100:GLY:HA2	1:A:108:PHE:CB	2.42	0.48
1:A:454:ILE:C	1:A:454:ILE:HD13	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:CYS:HB2	1:A:99:ARG:NH1	2.29	0.48
1:A:160:LYS:HG3	1:A:161:GLU:H	1.78	0.48
1:A:213:PHE:CG	1:A:213:PHE:O	2.67	0.48
1:A:390:ASN:C	1:A:390:ASN:ND2	2.66	0.48
1:C:141:ILE:H	1:C:141:ILE:CD1	2.26	0.48
1:C:125:MET:HB2	1:C:201:MET:HE3	1.94	0.48
1:A:187:PRO:O	1:A:187:PRO:HG2	2.13	0.48
1:A:191:LEU:HB3	1:A:193:PHE:CE2	2.48	0.48
1:A:45:LEU:H	1:A:45:LEU:HD13	1.79	0.48
1:C:27:HIS:HE1	1:C:279:PHE:HA	1.76	0.48
1:A:125:MET:HE3	1:A:260:MET:HE1	1.94	0.48
1:A:141:ILE:CD1	1:A:141:ILE:H	2.26	0.48
1:A:181:VAL:CG2	1:A:287:LEU:HD11	2.43	0.48
1:A:319:THR:N	1:A:320:ILE:HD12	2.26	0.48
1:A:144:HIS:HB3	1:A:353:THR:HG23	1.95	0.48
2:B:48:ILE:O	2:B:49:LEU:C	2.52	0.48
1:C:311:GLU:CG	1:C:312:ILE:H	2.10	0.48
1:C:400:GLN:NE2	1:C:400:GLN:HA	2.28	0.48
2:D:49:LEU:O	2:D:53:ILE:HG22	2.14	0.48
1:A:205:ALA:C	1:A:206:TRP:CD2	2.87	0.48
1:A:341:ASP:O	1:A:342:LEU:C	2.51	0.48
1:C:390:ASN:C	1:C:390:ASN:ND2	2.66	0.48
2:D:50:ALA:O	2:D:52:THR:N	2.47	0.48
1:A:97:VAL:CG2	1:A:113:ILE:HG21	2.42	0.48
1:A:256:GLN:HE21	1:A:256:GLN:CA	2.16	0.48
1:A:270:ILE:HG12	1:A:278:LEU:CB	2.43	0.48
1:A:360:GLU:C	1:A:362:ASP:N	2.68	0.48
2:B:6:PRO:O	2:B:7:HIS:C	2.52	0.48
1:C:122:LYS:NZ	1:C:122:LYS:HB2	2.27	0.48
1:C:256:GLN:HA	1:C:256:GLN:NE2	2.17	0.48
1:C:373:PHE:HA	1:C:395:GLY:CA	2.44	0.48
1:C:484:VAL:O	1:C:485:VAL:C	2.51	0.48
2:D:6:PRO:O	2:D:7:HIS:C	2.52	0.48
1:A:1:MET:O	1:A:3:CYS:N	2.47	0.48
1:C:157:LYS:HG2	1:C:157:LYS:O	2.13	0.48
1:C:88:LYS:O	1:C:234:LYS:NZ	2.47	0.48
1:A:308:VAL:HA	1:A:324:VAL:HA	1.95	0.47
1:A:350:ARG:NE	1:A:350:ARG:HA	2.29	0.47
1:C:205:ALA:C	1:C:206:TRP:CD2	2.87	0.47
1:C:248:GLN:O	1:C:248:GLN:NE2	2.46	0.47
1:C:181:VAL:CG2	1:C:287:LEU:HD11	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:GLU:O	1:A:285:CYS:HB2	2.14	0.47
1:A:400:GLN:HA	1:A:400:GLN:NE2	2.29	0.47
2:B:49:LEU:O	2:B:53:ILE:HG22	2.14	0.47
2:B:66:LEU:O	2:B:68:THR:N	2.46	0.47
1:A:102:GLY:HA3	1:C:151:VAL:O	2.13	0.47
1:C:1:MET:O	1:C:3:CYS:N	2.47	0.47
1:C:25:LEU:HG	1:C:25:LEU:H	1.52	0.47
1:C:356:PRO:O	1:C:357:ILE:HG22	2.14	0.47
1:C:378:ILE:CD1	1:C:389:LEU:HB3	2.44	0.47
1:A:125:MET:HE2	1:A:260:MET:HE3	1.96	0.47
1:A:200:GLN:HB2	1:A:272:MET:CE	2.44	0.47
1:A:245:ALA:O	1:A:246:LYS:O	2.32	0.47
1:A:252:VAL:O	1:A:253:LEU:CB	2.63	0.47
1:A:378:ILE:CD1	1:A:389:LEU:HB3	2.44	0.47
1:C:283:LEU:C	1:C:283:LEU:CD1	2.81	0.47
2:D:66:LEU:O	2:D:68:THR:N	2.47	0.47
1:A:94:HIS:ND1	1:A:114:VAL:CG1	2.77	0.47
1:A:210:ARG:NH2	1:A:210:ARG:HG3	2.29	0.47
1:A:88:LYS:O	1:A:234:LYS:NZ	2.47	0.47
1:A:89:ARG:HD3	1:A:118:MET:HE2	1.95	0.47
1:C:188:ARG:HG2	1:C:188:ARG:O	2.15	0.47
1:C:242:ASN:O	1:C:243:PRO:O	2.33	0.47
1:C:350:ARG:NE	1:C:350:ARG:HA	2.29	0.47
2:D:4:LEU:N	2:D:4:LEU:CD2	2.77	0.47
1:C:245:ALA:O	1:C:246:LYS:O	2.32	0.47
1:C:360:GLU:C	1:C:362:ASP:N	2.68	0.47
1:C:383:GLU:C	1:C:385:GLY:H	2.16	0.47
2:D:62:LEU:O	2:D:65:ILE:HG22	2.15	0.47
1:A:198:LEU:HD21	1:A:278:LEU:HD13	1.94	0.47
1:A:393:LYS:NZ	1:A:395:GLY:HA2	2.28	0.47
1:C:407:ARG:HH21	1:C:407:ARG:HG2	1.78	0.47
2:D:31:ARG:O	2:D:32:ILE:C	2.50	0.47
1:A:191:LEU:HD13	1:A:193:PHE:CZ	2.50	0.47
1:C:184:GLU:O	1:C:285:CYS:HB2	2.14	0.47
1:C:393:LYS:HG2	1:C:394:LYS:H	1.78	0.47
1:C:402:ILE:HG23	1:C:403:GLU:H	1.80	0.47
1:A:373:PHE:HA	1:A:395:GLY:CA	2.44	0.47
1:A:402:ILE:HG23	1:A:403:GLU:H	1.80	0.47
1:A:61:ILE:H	1:A:61:ILE:HD13	1.80	0.47
1:C:94:HIS:ND1	1:C:114:VAL:CG1	2.77	0.47
1:C:232:ILE:O	1:C:233:GLN:CG	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:MET:O	1:C:261:HIS:C	2.53	0.47
1:C:326:TYR:HE2	1:C:329:ASP:O	1.98	0.47
1:C:57:ARG:NH2	1:C:214:LEU:CD2	2.75	0.47
2:D:3:ALA:HB3	2:D:4:LEU:CD2	2.44	0.47
2:D:48:ILE:O	2:D:49:LEU:C	2.52	0.47
1:A:193:PHE:C	1:A:195:GLU:N	2.66	0.47
1:A:326:TYR:HE2	1:A:329:ASP:O	1.98	0.47
1:A:367:ILE:CG2	1:A:368:GLU:H	2.23	0.47
2:B:50:ALA:O	2:B:52:THR:N	2.47	0.47
1:C:162:ILE:O	1:C:162:ILE:HG12	2.14	0.47
1:C:261:HIS:O	1:C:264:LEU:N	2.48	0.47
1:C:410:LYS:O	1:C:412:MET:N	2.48	0.47
1:C:482:VAL:C	1:C:483:GLY:O	2.53	0.47
1:A:233:GLN:NE2	1:A:233:GLN:CA	2.69	0.47
1:A:457:ILE:CD1	1:A:457:ILE:C	2.82	0.47
1:A:310:LYS:HG2	1:C:101:TRP:CE2	2.49	0.47
1:C:125:MET:HE2	1:C:260:MET:HE3	1.96	0.47
1:C:191:LEU:HD13	1:C:193:PHE:CZ	2.50	0.47
1:C:196:MET:HE2	1:C:196:MET:HA	1.96	0.47
1:C:454:ILE:HG23	1:C:455:MET:N	2.23	0.47
1:C:479:LEU:C	1:C:479:LEU:HD23	2.35	0.47
1:C:61:ILE:H	1:C:61:ILE:HD13	1.80	0.47
1:A:151:VAL:O	1:C:102:GLY:HA3	2.14	0.47
1:A:232:ILE:O	1:A:233:GLN:CG	2.61	0.47
1:A:261:HIS:O	1:A:264:LEU:N	2.48	0.47
1:A:434:LYS:O	1:A:435:ALA:C	2.53	0.47
1:C:188:ARG:HG3	1:C:188:ARG:NH2	2.28	0.47
2:D:50:ALA:O	2:D:51:TYR:C	2.53	0.47
1:A:399:GLY:O	1:A:402:ILE:HG23	2.15	0.46
2:B:31:ARG:O	2:B:32:ILE:C	2.50	0.46
2:B:62:LEU:O	2:B:65:ILE:HG22	2.15	0.46
1:C:32:THR:HA	1:C:41:LEU:O	2.15	0.46
1:A:255:SER:OG	1:A:256:GLN:N	2.48	0.46
1:A:260:MET:O	1:A:261:HIS:C	2.53	0.46
1:A:27:HIS:HE1	1:A:279:PHE:HA	1.77	0.46
1:A:356:PRO:O	1:A:357:ILE:HG22	2.15	0.46
1:A:395:GLY:O	1:A:397:SER:N	2.48	0.46
1:A:485:VAL:O	1:A:489:LEU:HG	2.15	0.46
1:C:142:THR:OG1	1:C:143:PRO:HD2	2.16	0.46
1:C:354:VAL:O	1:C:355:ASN:O	2.33	0.46
1:C:393:LYS:CG	1:C:394:LYS:N	2.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:VAL:O	1:C:489:LEU:HG	2.15	0.46
1:C:443:ILE:O	1:C:444:TYR:C	2.54	0.46
1:A:115:THR:HB	1:A:248:GLN:HE22	1.80	0.46
1:A:35:ALA:C	1:A:37:ASN:N	2.68	0.46
1:C:122:LYS:CB	1:C:122:LYS:NZ	2.78	0.46
1:C:205:ALA:C	1:C:270:ILE:HG22	2.36	0.46
1:A:94:HIS:ND1	1:A:114:VAL:HG11	2.30	0.46
1:A:15:VAL:HG23	1:A:16:SER:N	2.31	0.46
1:A:260:MET:HA	2:B:2:VAL:CB	2.46	0.46
1:A:366:ASN:OD1	1:A:366:ASN:N	2.49	0.46
1:A:404:THR:O	1:A:405:THR:C	2.53	0.46
1:A:440:PHE:C	1:A:443:ILE:HG22	2.36	0.46
1:C:94:HIS:ND1	1:C:114:VAL:HG11	2.30	0.46
1:C:20:TRP:O	1:C:424:SER:HB3	2.16	0.46
1:C:434:LYS:O	1:C:435:ALA:C	2.54	0.46
1:C:45:LEU:HD13	1:C:45:LEU:H	1.79	0.46
1:A:101:TRP:CE2	1:C:310:LYS:HG2	2.50	0.46
1:A:205:ALA:C	1:A:270:ILE:HG22	2.36	0.46
1:A:242:ASN:O	1:A:243:PRO:O	2.33	0.46
1:A:90:PHE:HE2	1:A:118:MET:CE	2.28	0.46
1:C:15:VAL:HG23	1:C:16:SER:N	2.31	0.46
1:C:193:PHE:C	1:C:195:GLU:N	2.66	0.46
1:C:90:PHE:HE2	1:C:118:MET:CE	2.29	0.46
2:D:62:LEU:O	2:D:66:LEU:HD13	2.16	0.46
2:D:7:HIS:C	2:D:7:HIS:CD2	2.88	0.46
1:A:147:GLU:HB3	1:A:148:GLU:H	1.59	0.46
1:A:162:ILE:HG12	1:A:162:ILE:O	2.14	0.46
1:A:188:ARG:HG2	1:A:188:ARG:O	2.15	0.46
1:A:356:PRO:C	1:A:357:ILE:HG22	2.36	0.46
1:C:356:PRO:C	1:C:357:ILE:HG22	2.36	0.46
1:A:122:LYS:CB	1:A:122:LYS:NZ	2.79	0.46
1:A:354:VAL:O	1:A:355:ASN:O	2.33	0.46
1:A:350:ARG:HB3	1:A:370:GLU:HB3	1.98	0.46
1:A:1:MET:C	1:A:3:CYS:H	2.19	0.46
1:A:70:THR:OG1	1:A:115:THR:HA	2.16	0.46
1:A:89:ARG:HD3	1:A:118:MET:HE1	1.98	0.46
1:C:166:PRO:CB	1:C:187:PRO:HG2	2.34	0.46
1:C:395:GLY:O	1:C:397:SER:N	2.48	0.46
1:C:440:PHE:C	1:C:443:ILE:HG22	2.36	0.46
1:A:51:LYS:HZ2	1:A:136:GLU:HB2	1.79	0.46
1:A:313:ALA:O	1:A:314:GLU:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:LEU:C	1:A:479:LEU:HD23	2.35	0.46
1:A:20:TRP:O	1:A:424:SER:HB3	2.16	0.46
1:A:248:GLN:O	1:A:248:GLN:NE2	2.46	0.46
1:A:256:GLN:NE2	1:A:256:GLN:HA	2.17	0.46
1:A:384:PRO:HG2	1:A:386:GLN:NE2	2.27	0.46
1:C:210:ARG:NH2	1:C:210:ARG:HG3	2.29	0.46
1:C:115:THR:HB	1:C:248:GLN:HE22	1.80	0.46
1:C:252:VAL:O	1:C:253:LEU:CB	2.63	0.46
1:C:384:PRO:CG	1:C:386:GLN:HE21	2.27	0.46
1:C:461:VAL:HA	1:C:464:THR:HG22	1.97	0.46
2:D:51:TYR:CA	2:D:60:ARG:HD3	2.13	0.46
1:A:165:THR:HG22	1:A:167:GLN:H	1.81	0.45
1:A:270:ILE:HG23	1:A:271:GLN:H	1.80	0.45
1:A:32:THR:HA	1:A:41:LEU:O	2.15	0.45
1:A:443:ILE:O	1:A:444:TYR:C	2.53	0.45
1:A:57:ARG:HG3	1:A:57:ARG:NH2	2.29	0.45
1:C:196:MET:HE1	2:D:12:LEU:HD21	1.96	0.45
1:C:207:LEU:O	1:C:267:ALA:HB1	2.16	0.45
1:C:313:ALA:O	1:C:314:GLU:HB3	2.16	0.45
1:A:142:THR:OG1	1:A:143:PRO:HD2	2.16	0.45
1:A:166:PRO:CB	1:A:187:PRO:HG2	2.33	0.45
1:A:318:GLY:N	1:A:393:LYS:CE	2.78	0.45
1:A:410:LYS:O	1:A:412:MET:N	2.49	0.45
2:B:50:ALA:O	2:B:51:TYR:C	2.53	0.45
1:C:399:GLY:O	1:C:402:ILE:HG23	2.16	0.45
1:C:457:ILE:CD1	1:C:457:ILE:C	2.81	0.45
1:C:60:CYS:SG	1:C:219:PRO:HG3	2.56	0.45
1:C:6:ILE:O	1:C:6:ILE:CG2	2.52	0.45
2:B:3:ALA:HB3	2:B:4:LEU:CD2	2.44	0.45
2:B:4:LEU:N	2:B:4:LEU:CD2	2.77	0.45
1:C:283:LEU:HD13	1:C:284:LYS:O	2.16	0.45
1:A:461:VAL:HA	1:A:464:THR:HG22	1.97	0.45
2:B:7:HIS:CD2	2:B:7:HIS:C	2.88	0.45
1:C:100:GLY:HA2	1:C:108:PHE:HB2	1.99	0.45
1:C:260:MET:HA	2:D:2:VAL:CB	2.46	0.45
1:C:35:ALA:C	1:C:37:ASN:N	2.68	0.45
1:C:1:MET:C	1:C:3:CYS:H	2.19	0.45
1:A:221:LEU:CG	1:A:222:PRO:CD	2.94	0.45
2:B:32:ILE:CD1	2:B:33:GLU:N	2.79	0.45
1:A:209:HIS:H	2:B:7:HIS:CE1	2.35	0.45
1:C:351:LEU:HA	1:C:351:LEU:HD23	1.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:MET:O	1:C:408:GLY:N	2.49	0.45
1:C:465:TRP:C	1:C:467:GLY:H	2.19	0.45
1:C:58:LYS:O	1:C:59:TYR:C	2.54	0.45
1:A:306:PHE:CD1	1:A:306:PHE:N	2.84	0.45
1:A:387:LEU:C	1:A:387:LEU:HD13	2.36	0.45
1:A:489:LEU:O	1:A:493:VAL:HG13	2.16	0.45
1:A:58:LYS:O	1:A:59:TYR:C	2.54	0.45
2:B:34:THR:O	2:B:37:LEU:HD22	2.16	0.45
1:C:165:THR:O	1:C:167:GLN:N	2.50	0.45
1:C:165:THR:HG22	1:C:167:GLN:H	1.81	0.45
1:C:306:PHE:CD1	1:C:306:PHE:N	2.84	0.45
1:C:69:THR:HG22	1:C:70:THR:H	1.81	0.45
1:C:366:ASN:OD1	1:C:366:ASN:N	2.49	0.45
1:A:15:VAL:HG13	1:A:35:ALA:HB1	1.99	0.45
1:A:188:ARG:HG3	1:A:188:ARG:NH2	2.28	0.45
1:A:221:LEU:HD22	1:A:231:TRP:CH2	2.51	0.45
1:A:283:LEU:HD13	1:A:284:LYS:O	2.16	0.45
1:A:320:ILE:CG1	1:A:371:PRO:HD2	2.47	0.45
1:A:377:TYR:HD1	1:A:388:LYS:HD2	1.81	0.45
2:B:62:LEU:O	2:B:66:LEU:HD13	2.16	0.45
1:C:193:PHE:O	1:C:195:GLU:N	2.50	0.45
1:C:233:GLN:C	1:C:235:GLU:N	2.70	0.45
1:C:258:GLY:O	1:C:259:ALA:C	2.55	0.45
1:C:480:VAL:O	1:C:481:LEU:C	2.55	0.45
1:C:57:ARG:HG3	1:C:57:ARG:NH2	2.29	0.45
1:A:119:PHE:CD2	1:A:119:PHE:O	2.70	0.45
2:B:50:ALA:CA	2:B:63:ILE:HD11	2.46	0.45
1:C:200:GLN:O	1:C:201:MET:HB2	2.17	0.45
1:C:221:LEU:HD22	1:C:231:TRP:CH2	2.52	0.45
1:C:23:ILE:HD12	1:C:23:ILE:C	2.37	0.45
1:C:270:ILE:HG23	1:C:271:GLN:H	1.81	0.45
1:C:320:ILE:CG1	1:C:371:PRO:HD2	2.47	0.45
1:C:489:LEU:O	1:C:493:VAL:HG13	2.17	0.45
2:D:34:THR:O	2:D:37:LEU:HD22	2.16	0.45
1:A:165:THR:O	1:A:167:GLN:N	2.49	0.45
1:C:70:THR:OG1	1:C:115:THR:HA	2.16	0.45
1:C:9:ARG:O	1:C:10:ASP:CB	2.61	0.45
1:A:193:PHE:O	1:A:195:GLU:N	2.50	0.44
1:A:258:GLY:O	1:A:259:ALA:C	2.55	0.44
1:A:337:PHE:C	1:A:337:PHE:HD1	2.20	0.44
1:A:393:LYS:CG	1:A:394:LYS:N	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:TRP:C	1:A:467:GLY:H	2.19	0.44
1:A:480:VAL:O	1:A:481:LEU:C	2.54	0.44
1:A:494:GLN:O	1:A:494:GLN:HG3	2.17	0.44
2:B:32:ILE:O	2:B:35:TRP:HB3	2.17	0.44
1:C:387:LEU:C	1:C:387:LEU:HD13	2.37	0.44
1:C:404:THR:O	1:C:405:THR:C	2.54	0.44
1:C:209:HIS:H	2:D:7:HIS:CE1	2.35	0.44
1:A:60:CYS:SG	1:A:219:PRO:HG3	2.58	0.44
1:C:205:ALA:O	1:C:270:ILE:HG22	2.18	0.44
1:C:350:ARG:HB3	1:C:370:GLU:HB3	1.98	0.44
1:C:377:TYR:HD1	1:C:388:LYS:HD2	1.81	0.44
1:C:62:GLU:O	1:C:62:GLU:HG3	2.17	0.44
1:A:99:ARG:HG2	1:A:103:ASN:OD1	2.18	0.44
1:A:170:ILE:CD1	1:A:170:ILE:H	2.25	0.44
1:A:396:SER:O	1:A:397:SER:C	2.56	0.44
1:A:458:LEU:HD13	1:A:458:LEU:C	2.38	0.44
1:A:482:VAL:C	1:A:483:GLY:O	2.52	0.44
1:A:489:LEU:C	1:A:493:VAL:HG13	2.38	0.44
1:A:69:THR:HG22	1:A:70:THR:H	1.81	0.44
1:C:402:ILE:O	1:C:403:GLU:C	2.55	0.44
1:C:411:ARG:CD	1:C:422:PHE:CE1	3.01	0.44
1:C:493:VAL:HG23	1:C:494:GLN:N	2.33	0.44
1:C:89:ARG:HH21	1:C:89:ARG:HG2	1.82	0.44
1:A:100:GLY:HA2	1:A:108:PHE:HB2	1.99	0.44
1:A:200:GLN:O	1:A:201:MET:HB2	2.17	0.44
1:A:222:PRO:HG2	1:A:223:GLY:N	2.31	0.44
1:A:406:MET:O	1:A:408:GLY:N	2.50	0.44
1:A:493:VAL:HG23	1:A:494:GLN:N	2.33	0.44
2:B:6:PRO:O	2:B:8:VAL:N	2.51	0.44
1:C:119:PHE:CD2	1:C:119:PHE:O	2.70	0.44
1:C:355:ASN:OD1	1:C:355:ASN:O	2.36	0.44
1:C:458:LEU:C	1:C:458:LEU:HD13	2.38	0.44
1:A:20:TRP:HB3	1:A:425:LEU:CD2	2.47	0.44
1:A:229:SER:O	1:A:231:TRP:CD1	2.71	0.44
1:A:411:ARG:NE	1:A:422:PHE:CE1	2.86	0.44
1:A:420:TRP:CD1	1:A:434:LYS:HA	2.53	0.44
1:A:56:LEU:CG	1:A:56:LEU:O	2.63	0.44
1:C:164:ILE:HD13	1:C:164:ILE:C	2.38	0.44
1:A:396:SER:O	1:A:398:ILE:N	2.51	0.44
1:A:89:ARG:HG2	1:A:89:ARG:HH21	1.82	0.44
2:B:32:ILE:O	2:B:33:GLU:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:ARG:HD3	1:C:118:MET:HE2	1.99	0.44
1:C:319:THR:O	1:C:321:VAL:N	2.50	0.44
2:D:32:ILE:CD1	2:D:33:GLU:N	2.80	0.44
2:D:50:ALA:CA	2:D:63:ILE:HD11	2.46	0.44
1:A:181:VAL:HG22	1:A:287:LEU:HD11	1.99	0.44
1:A:207:LEU:O	1:A:267:ALA:HB1	2.17	0.44
1:A:411:ARG:CD	1:A:422:PHE:CE1	3.00	0.44
1:A:62:GLU:O	1:A:62:GLU:HG3	2.18	0.44
1:A:97:VAL:HG12	1:A:98:ASP:N	2.33	0.44
1:C:15:VAL:HG13	1:C:35:ALA:HB1	1.99	0.44
1:C:27:HIS:CE1	1:C:279:PHE:CA	2.99	0.44
1:C:460:GLY:O	1:C:482:VAL:HG13	2.18	0.44
1:A:140:VAL:O	1:A:140:VAL:CG2	2.66	0.44
1:C:410:LYS:O	1:C:411:ARG:C	2.56	0.44
1:C:420:TRP:CD1	1:C:434:LYS:HA	2.53	0.44
1:C:439:VAL:O	1:C:443:ILE:HG22	2.18	0.44
2:D:32:ILE:O	2:D:33:GLU:C	2.55	0.44
1:A:200:GLN:HB2	1:A:272:MET:HE3	2.00	0.44
1:A:125:MET:HB2	1:A:201:MET:HE3	2.00	0.44
1:A:311:GLU:CG	1:A:312:ILE:N	2.79	0.44
1:A:320:ILE:HD13	1:A:369:ALA:O	2.18	0.44
1:A:460:GLY:O	1:A:482:VAL:HG13	2.18	0.44
1:C:204:LYS:HE3	1:C:204:LYS:HB3	1.74	0.44
1:C:318:GLY:N	1:C:393:LYS:CE	2.79	0.44
1:C:494:GLN:HG3	1:C:494:GLN:O	2.17	0.44
1:C:97:VAL:HG12	1:C:98:ASP:N	2.33	0.44
2:D:39:HIS:C	2:D:41:GLY:N	2.71	0.44
1:A:482:VAL:O	1:A:483:GLY:C	2.57	0.43
1:A:196:MET:HE1	2:B:12:LEU:HD11	2.00	0.43
1:C:181:VAL:HG22	1:C:287:LEU:HD11	1.99	0.43
1:C:221:LEU:HA	1:C:221:LEU:HD12	1.77	0.43
1:A:319:THR:O	1:A:321:VAL:N	2.51	0.43
1:A:327:GLU:CG	1:A:328:GLY:N	2.81	0.43
2:B:65:ILE:HD12	2:B:65:ILE:HA	1.93	0.43
1:A:313:ALA:HB3	1:C:108:PHE:CZ	2.53	0.43
1:C:320:ILE:HD13	1:C:369:ALA:O	2.18	0.43
1:C:489:LEU:C	1:C:493:VAL:HG13	2.38	0.43
1:A:11:PHE:O	1:A:12:VAL:HG13	2.18	0.43
1:A:256:GLN:O	1:A:257:GLU:C	2.56	0.43
1:C:256:GLN:O	1:C:257:GLU:C	2.56	0.43
1:C:51:LYS:N	1:C:51:LYS:HD3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:GLY:C	1:A:104:GLY:H	2.22	0.43
1:A:164:ILE:C	1:A:164:ILE:HD13	2.38	0.43
1:A:205:ALA:O	1:A:270:ILE:HG22	2.18	0.43
1:A:337:PHE:CE2	1:A:367:ILE:HG21	2.53	0.43
1:A:80:PRO:HG3	1:A:113:ILE:CA	2.49	0.43
1:C:140:VAL:CG2	1:C:140:VAL:O	2.66	0.43
1:C:16:SER:HB2	1:C:425:LEU:HD23	2.01	0.43
1:C:59:TYR:CD2	1:C:218:LEU:HB2	2.52	0.43
2:D:35:TRP:HH2	2:D:42:PHE:HD2	1.66	0.43
2:D:6:PRO:HG2	2:D:6:PRO:O	2.19	0.43
1:A:27:HIS:CE1	1:A:279:PHE:CA	3.00	0.43
1:A:410:LYS:C	1:A:412:MET:N	2.71	0.43
1:A:51:LYS:HD3	1:A:51:LYS:N	2.33	0.43
1:A:196:MET:HE1	2:B:12:LEU:HD21	2.00	0.43
2:B:37:LEU:HD23	2:B:37:LEU:C	2.38	0.43
1:C:221:LEU:CG	1:C:222:PRO:CD	2.94	0.43
1:C:222:PRO:HG2	1:C:223:GLY:N	2.31	0.43
1:C:464:THR:O	1:C:468:MET:HB2	2.18	0.43
2:D:66:LEU:O	2:D:70:VAL:HG23	2.19	0.43
1:A:108:PHE:CZ	1:C:313:ALA:HB3	2.53	0.43
1:A:23:ILE:C	1:A:23:ILE:HD12	2.38	0.43
1:A:355:ASN:OD1	1:A:355:ASN:O	2.35	0.43
1:A:402:ILE:O	1:A:403:GLU:C	2.56	0.43
1:A:464:THR:O	1:A:468:MET:HB2	2.19	0.43
1:A:467:GLY:O	1:A:470:SER:N	2.52	0.43
1:C:229:SER:O	1:C:231:TRP:CD1	2.71	0.43
1:C:247:LYS:O	1:C:248:GLN:CB	2.67	0.43
1:A:61:ILE:CD1	1:A:123:LYS:O	2.61	0.43
1:A:37:ASN:O	1:A:38:LYS:CB	2.66	0.43
1:A:454:ILE:CD1	1:A:455:MET:N	2.79	0.43
1:A:489:LEU:HD23	1:A:489:LEU:HA	1.79	0.43
2:B:35:TRP:HH2	2:B:42:PHE:HD2	1.66	0.43
1:C:337:PHE:HE1	1:C:339:ILE:HG12	1.83	0.43
1:C:396:SER:O	1:C:397:SER:C	2.56	0.43
1:C:64:LYS:HZ3	1:C:64:LYS:HB3	1.79	0.43
1:C:74:CYS:HB2	1:C:99:ARG:CZ	2.49	0.43
2:D:32:ILE:O	2:D:35:TRP:HB3	2.17	0.43
1:A:337:PHE:HE1	1:A:339:ILE:HG12	1.84	0.43
1:A:74:CYS:HB2	1:A:99:ARG:CZ	2.49	0.43
1:C:37:ASN:O	1:C:38:LYS:CB	2.66	0.43
1:C:396:SER:O	1:C:398:ILE:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:TRP:CE3	2:D:36:ILE:N	2.87	0.43
2:D:66:LEU:O	2:D:69:ALA:N	2.52	0.43
2:D:6:PRO:O	2:D:8:VAL:N	2.51	0.43
1:A:233:GLN:C	1:A:235:GLU:N	2.70	0.43
1:A:58:LYS:CG	1:A:58:LYS:O	2.67	0.43
1:C:102:GLY:C	1:C:104:GLY:H	2.22	0.43
1:C:11:PHE:HA	1:C:32:THR:O	2.19	0.43
1:C:410:LYS:C	1:C:412:MET:N	2.70	0.43
1:C:411:ARG:NE	1:C:422:PHE:CE1	2.86	0.43
2:D:19:TRP:CD1	2:D:20:MET:SD	3.12	0.43
2:D:37:LEU:HD23	2:D:37:LEU:C	2.38	0.43
1:A:439:VAL:O	1:A:443:ILE:HG22	2.18	0.43
2:B:58:PHE:O	2:B:59:GLN:C	2.57	0.43
2:B:65:ILE:CG2	2:B:66:LEU:N	2.82	0.43
1:C:99:ARG:HG2	1:C:103:ASN:OD1	2.18	0.43
1:C:157:LYS:CG	1:C:157:LYS:O	2.67	0.43
1:C:229:SER:HA	1:C:231:TRP:CD1	2.53	0.43
1:C:454:ILE:HD13	1:C:455:MET:CA	2.48	0.43
1:A:101:TRP:CB	1:A:108:PHE:HD2	2.18	0.42
1:A:199:LEU:CD1	1:A:200:GLN:O	2.67	0.42
1:A:376:SER:C	1:A:377:TYR:HD2	2.23	0.42
1:A:494:GLN:O	1:A:495:ALA:C	2.57	0.42
1:C:11:PHE:O	1:C:12:VAL:HG13	2.19	0.42
1:C:144:HIS:C	1:C:146:GLY:H	2.22	0.42
1:C:196:MET:HB3	1:C:207:LEU:CD1	2.49	0.42
1:C:337:PHE:CE2	1:C:367:ILE:HG21	2.54	0.42
1:C:467:GLY:O	1:C:470:SER:N	2.52	0.42
1:C:482:VAL:O	1:C:483:GLY:C	2.57	0.42
1:C:80:PRO:HG3	1:C:113:ILE:CA	2.48	0.42
1:A:185:CYS:C	1:A:187:PRO:HD3	2.40	0.42
1:A:208:VAL:O	1:A:208:VAL:HG23	2.19	0.42
1:A:360:GLU:O	1:A:362:ASP:N	2.52	0.42
1:A:426:GLY:HA3	1:A:431:SER:HB3	2.01	0.42
2:B:36:ILE:C	2:B:36:ILE:HD13	2.40	0.42
2:B:35:TRP:CE3	2:B:36:ILE:N	2.87	0.42
2:B:8:VAL:HG23	2:B:9:GLY:H	1.83	0.42
1:A:229:SER:HA	1:A:231:TRP:CD1	2.53	0.42
2:D:65:ILE:CG2	2:D:66:LEU:N	2.82	0.42
1:A:294:LEU:HD22	1:A:297:MET:HG2	2.02	0.42
1:A:345:ARG:N	1:A:345:ARG:HD2	2.35	0.42
1:A:414:ILE:N	1:A:414:ILE:HD12	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:VAL:O	1:A:462:ILE:C	2.57	0.42
2:B:19:TRP:CD1	2:B:20:MET:SD	3.12	0.42
1:C:185:CYS:C	1:C:187:PRO:HD3	2.40	0.42
1:C:294:LEU:HD22	1:C:297:MET:HG2	2.01	0.42
1:C:360:GLU:O	1:C:362:ASP:N	2.52	0.42
1:C:461:VAL:O	1:C:462:ILE:C	2.57	0.42
1:C:480:VAL:HG12	1:C:481:LEU:N	2.35	0.42
2:D:62:LEU:CD1	2:D:62:LEU:C	2.87	0.42
1:A:196:MET:HB3	1:A:207:LEU:CD1	2.49	0.42
1:A:270:ILE:HD12	1:A:271:GLN:HG2	2.00	0.42
1:A:309:VAL:HB	1:A:323:ARG:CG	2.48	0.42
1:A:313:ALA:O	1:A:314:GLU:CB	2.66	0.42
1:A:454:ILE:HD13	1:A:455:MET:CA	2.48	0.42
1:C:337:PHE:HD1	1:C:337:PHE:C	2.20	0.42
1:C:376:SER:C	1:C:377:TYR:HD2	2.22	0.42
1:A:444:TYR:O	1:A:446:ALA:N	2.52	0.42
1:A:487:LEU:O	1:A:487:LEU:HD13	2.19	0.42
2:B:66:LEU:O	2:B:69:ALA:N	2.52	0.42
1:C:20:TRP:HB3	1:C:425:LEU:CD2	2.47	0.42
1:C:311:GLU:O	1:C:312:ILE:CG2	2.59	0.42
2:D:20:MET:O	2:D:21:SER:C	2.58	0.42
2:D:8:VAL:HG23	2:D:9:GLY:H	1.84	0.42
1:A:103:ASN:ND2	1:A:103:ASN:O	2.52	0.42
1:A:125:MET:HG3	1:A:199:LEU:HD11	2.02	0.42
1:A:261:HIS:O	1:A:262:THR:C	2.58	0.42
1:A:29:SER:O	1:A:30:CYS:O	2.38	0.42
1:A:463:ILE:CG2	1:A:482:VAL:HG13	2.50	0.42
2:B:20:MET:O	2:B:21:SER:C	2.58	0.42
2:B:33:GLU:HA	2:B:36:ILE:CG2	2.50	0.42
1:C:103:ASN:O	1:C:103:ASN:ND2	2.52	0.42
1:C:125:MET:HG3	1:C:199:LEU:HD11	2.02	0.42
1:C:130:VAL:HG23	1:C:130:VAL:O	2.20	0.42
1:C:345:ARG:N	1:C:345:ARG:HD2	2.35	0.42
1:C:346:HIS:O	1:C:347:VAL:O	2.37	0.42
1:C:284:LYS:CE	1:C:418:THR:HB	2.50	0.42
1:C:426:GLY:HA3	1:C:431:SER:HB3	2.01	0.42
1:C:494:GLN:O	1:C:495:ALA:C	2.57	0.42
2:D:58:PHE:O	2:D:59:GLN:C	2.57	0.42
2:D:65:ILE:CG2	2:D:66:LEU:HD12	2.50	0.42
1:A:122:LYS:HZ2	1:A:122:LYS:CA	2.30	0.42
1:A:271:GLN:OE1	1:A:271:GLN:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:HIS:H	1:A:45:LEU:CD1	2.32	0.42
1:A:294:LEU:HD23	1:A:296:GLY:N	2.34	0.42
1:A:384:PRO:CG	1:A:386:GLN:HE21	2.27	0.42
1:A:463:ILE:CA	1:A:466:ILE:HG22	2.49	0.42
2:B:6:PRO:O	2:B:6:PRO:HG2	2.18	0.42
1:C:208:VAL:HG23	1:C:208:VAL:O	2.19	0.42
1:C:210:ARG:HH21	1:C:210:ARG:HG3	1.85	0.42
1:C:240:PHE:CD1	1:C:250:VAL:CG1	3.03	0.42
1:C:255:SER:OG	1:C:256:GLN:N	2.48	0.42
1:C:277:LEU:HD12	1:C:279:PHE:CE2	2.53	0.42
1:C:463:ILE:CG2	1:C:482:VAL:HG13	2.50	0.42
1:A:142:THR:HA	1:A:143:PRO:HD3	1.72	0.42
1:A:210:ARG:HH21	1:A:210:ARG:HG3	1.85	0.42
1:A:221:LEU:HG	1:A:222:PRO:HD3	2.00	0.42
1:A:25:LEU:H	1:A:25:LEU:HG	1.51	0.42
1:A:346:HIS:O	1:A:347:VAL:O	2.37	0.42
1:A:360:GLU:C	1:A:362:ASP:H	2.23	0.42
1:C:124:ASN:C	1:C:124:ASN:OD1	2.58	0.42
1:C:185:CYS:CB	1:C:187:PRO:HD3	2.50	0.42
1:C:295:LYS:HB2	1:C:295:LYS:NZ	2.35	0.42
1:C:294:LEU:HD23	1:C:296:GLY:N	2.34	0.42
1:C:384:PRO:HG2	1:C:386:GLN:NE2	2.28	0.42
2:D:36:ILE:C	2:D:36:ILE:HD13	2.40	0.42
1:A:144:HIS:C	1:A:146:GLY:H	2.22	0.42
1:A:157:LYS:CG	1:A:157:LYS:O	2.67	0.42
1:A:240:PHE:CD1	1:A:250:VAL:CG1	3.02	0.42
1:A:247:LYS:O	1:A:248:GLN:CB	2.67	0.42
1:A:11:PHE:HA	1:A:32:THR:O	2.19	0.42
1:A:350:ARG:NH2	1:A:350:ARG:HB2	2.35	0.42
1:A:410:LYS:O	1:A:411:ARG:C	2.56	0.42
1:A:284:LYS:CE	1:A:418:THR:HB	2.50	0.42
1:A:41:LEU:CB	1:A:43:PHE:HE1	2.32	0.42
1:A:458:LEU:O	1:A:458:LEU:HD13	2.20	0.42
1:C:29:SER:O	1:C:30:CYS:O	2.37	0.42
1:A:16:SER:HB2	1:A:425:LEU:HD23	2.02	0.41
1:A:367:ILE:O	1:A:368:GLU:HG2	2.20	0.41
1:A:39:PRO:O	1:A:40:THR:C	2.58	0.41
2:B:62:LEU:CD1	2:B:62:LEU:C	2.87	0.41
2:B:65:ILE:CG2	2:B:66:LEU:HD12	2.50	0.41
2:B:66:LEU:O	2:B:70:VAL:HG23	2.20	0.41
1:C:271:GLN:OE1	1:C:271:GLN:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:SER:HA	1:C:332:PRO:HD3	1.92	0.41
1:C:39:PRO:O	1:C:40:THR:C	2.58	0.41
1:C:444:TYR:O	1:C:446:ALA:N	2.53	0.41
1:A:99:ARG:NH1	1:A:105:CYS:CB	2.76	0.41
1:A:311:GLU:O	1:A:312:ILE:CG2	2.58	0.41
1:A:43:PHE:CE2	1:A:141:ILE:CG2	3.03	0.41
1:A:487:LEU:O	1:A:491:VAL:HG13	2.20	0.41
1:A:74:CYS:SG	1:A:75:PRO:N	2.93	0.41
1:C:422:PHE:HA	1:C:422:PHE:HD2	1.67	0.41
1:C:22:ASP:HB2	1:C:424:SER:HA	2.02	0.41
1:C:41:LEU:CB	1:C:43:PHE:HE1	2.32	0.41
1:C:458:LEU:O	1:C:458:LEU:HD13	2.20	0.41
1:C:475:LEU:HG	1:C:476:SER:H	1.85	0.41
1:A:41:LEU:CD2	1:A:143:PRO:HA	2.51	0.41
1:A:23:ILE:CD1	1:A:285:CYS:SG	3.08	0.41
1:A:295:LYS:HB2	1:A:295:LYS:NZ	2.35	0.41
1:A:384:PRO:CG	1:A:386:GLN:NE2	2.83	0.41
1:A:51:LYS:O	1:A:52:GLN:HB2	2.20	0.41
2:B:38:ARG:CG	2:B:39:HIS:CE1	3.04	0.41
1:C:102:GLY:O	1:C:103:ASN:C	2.59	0.41
1:C:132:PRO:O	1:C:135:LEU:HB2	2.20	0.41
1:C:1:MET:C	1:C:3:CYS:N	2.73	0.41
1:C:261:HIS:O	1:C:262:THR:C	2.58	0.41
1:C:350:ARG:CZ	1:C:350:ARG:CB	2.98	0.41
1:C:74:CYS:SG	1:C:77:GLN:NE2	2.93	0.41
2:D:33:GLU:HA	2:D:36:ILE:CG2	2.50	0.41
1:A:124:ASN:C	1:A:124:ASN:OD1	2.58	0.41
2:B:35:TRP:O	2:B:38:ARG:N	2.53	0.41
1:C:100:GLY:O	1:C:103:ASN:CB	2.65	0.41
1:C:394:LYS:O	1:C:396:SER:N	2.51	0.41
1:A:178:TYR:N	1:A:178:TYR:HD2	2.17	0.41
1:A:284:LYS:HG3	1:A:285:CYS:N	2.35	0.41
1:C:135:LEU:HA	1:C:135:LEU:HD22	1.62	0.41
1:C:23:ILE:CD1	1:C:285:CYS:SG	3.08	0.41
1:C:75:PRO:HG3	1:C:110:LYS:O	2.20	0.41
2:D:35:TRP:O	2:D:38:ARG:N	2.54	0.41
1:A:101:TRP:HZ3	1:C:321:VAL:HB	1.85	0.41
1:A:102:GLY:O	1:A:103:ASN:C	2.59	0.41
1:A:142:THR:OG1	1:A:143:PRO:CD	2.69	0.41
1:A:186:SER:O	1:A:188:ARG:N	2.53	0.41
1:A:1:MET:C	1:A:3:CYS:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:MET:HB3	1:A:207:LEU:HD11	2.03	0.41
1:A:277:LEU:HD12	1:A:279:PHE:CE2	2.54	0.41
1:A:74:CYS:SG	1:A:77:GLN:NE2	2.93	0.41
2:B:63:ILE:CD1	2:B:63:ILE:C	2.87	0.41
1:C:309:VAL:HB	1:C:323:ARG:CG	2.49	0.41
1:C:384:PRO:CG	1:C:386:GLN:NE2	2.83	0.41
1:C:489:LEU:HD23	1:C:489:LEU:HA	1.80	0.41
1:A:130:VAL:O	1:A:130:VAL:HG23	2.20	0.41
1:A:221:LEU:HA	1:A:221:LEU:HD12	1.77	0.41
1:A:321:VAL:HG23	1:A:321:VAL:O	2.21	0.41
1:A:320:ILE:O	1:A:368:GLU:HA	2.20	0.41
1:C:142:THR:OG1	1:C:143:PRO:CD	2.69	0.41
1:C:270:ILE:HD12	1:C:271:GLN:HG2	2.01	0.41
1:C:270:ILE:HD11	1:C:277:LEU:C	2.41	0.41
1:C:27:HIS:H	1:C:45:LEU:CD1	2.33	0.41
1:C:315:THR:HG23	1:C:315:THR:O	2.19	0.41
1:C:320:ILE:O	1:C:368:GLU:HA	2.21	0.41
1:C:345:ARG:CD	1:C:345:ARG:N	2.82	0.41
1:C:360:GLU:C	1:C:362:ASP:H	2.23	0.41
1:C:414:ILE:HD12	1:C:414:ILE:N	2.35	0.41
1:C:43:PHE:CE2	1:C:141:ILE:CG2	3.03	0.41
1:C:487:LEU:O	1:C:491:VAL:HG13	2.21	0.41
1:C:96:MET:HA	1:C:111:GLY:O	2.20	0.41
2:D:54:GLY:O	2:D:55:THR:HB	2.20	0.41
1:A:71:ASP:O	1:A:113:ILE:HG13	2.21	0.41
1:A:204:LYS:HE3	1:A:204:LYS:HB3	1.73	0.41
1:A:313:ALA:C	1:A:314:GLU:HG3	2.41	0.41
1:A:386:GLN:HA	1:A:386:GLN:NE2	2.36	0.41
1:A:45:LEU:CD1	1:A:45:LEU:H	2.34	0.41
1:A:480:VAL:HG12	1:A:481:LEU:N	2.35	0.41
1:A:82:LEU:HD12	1:A:82:LEU:H	1.86	0.41
2:B:54:GLY:O	2:B:55:THR:HB	2.20	0.41
1:C:41:LEU:CD2	1:C:143:PRO:HA	2.51	0.41
1:C:1:MET:CG	1:C:151:VAL:HA	2.45	0.41
1:C:253:LEU:CD2	1:C:253:LEU:O	2.69	0.41
1:C:350:ARG:NH2	1:C:350:ARG:HB2	2.35	0.41
1:C:386:GLN:NE2	1:C:386:GLN:HA	2.36	0.41
1:A:1:MET:CG	1:A:151:VAL:HA	2.45	0.41
1:A:301:MET:O	1:A:302:CYS:O	2.39	0.41
1:A:391:TRP:O	1:A:392:PHE:CB	2.66	0.41
1:A:317:HIS:HB3	1:A:393:LYS:NZ	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:PRO:HG3	1:A:110:LYS:O	2.20	0.41
1:C:178:TYR:N	1:C:178:TYR:HD2	2.17	0.41
1:C:186:SER:O	1:C:188:ARG:N	2.53	0.41
1:C:402:ILE:O	1:C:405:THR:N	2.53	0.41
1:C:487:LEU:HD13	1:C:487:LEU:O	2.21	0.41
2:D:35:TRP:HH2	2:D:42:PHE:CD2	2.39	0.41
1:A:227:GLN:CD	1:A:227:GLN:O	2.59	0.41
1:A:253:LEU:O	1:A:253:LEU:CD2	2.69	0.41
1:A:367:ILE:CD1	1:A:367:ILE:N	2.74	0.41
1:A:82:LEU:N	1:A:82:LEU:HD12	2.36	0.41
1:A:96:MET:HA	1:A:111:GLY:O	2.20	0.41
1:C:199:LEU:CD1	1:C:200:GLN:O	2.68	0.41
1:C:284:LYS:HG3	1:C:285:CYS:N	2.36	0.41
1:C:367:ILE:O	1:C:368:GLU:HG2	2.20	0.41
1:C:471:ARG:HE	1:C:471:ARG:HB3	1.69	0.41
2:D:48:ILE:O	2:D:51:TYR:N	2.54	0.41
2:D:59:GLN:O	2:D:60:ARG:C	2.58	0.41
2:D:50:ALA:HB1	2:D:63:ILE:HD11	2.03	0.41
1:A:125:MET:HB2	1:A:201:MET:CE	2.51	0.41
1:A:53:PRO:HB2	1:A:129:VAL:O	2.21	0.41
1:A:306:PHE:HZ	1:A:381:GLY:CA	2.22	0.41
1:A:353:THR:O	1:A:353:THR:HG22	2.20	0.41
1:A:357:ILE:O	1:A:357:ILE:CG2	2.65	0.41
1:A:402:ILE:O	1:A:405:THR:N	2.54	0.41
1:A:411:ARG:CZ	1:A:411:ARG:HB2	2.51	0.41
1:C:53:PRO:HB2	1:C:129:VAL:O	2.21	0.41
1:C:196:MET:HB3	1:C:207:LEU:HD11	2.03	0.41
1:C:290:ASP:C	1:C:292:LEU:N	2.74	0.41
1:C:353:THR:O	1:C:353:THR:HG22	2.21	0.41
1:C:411:ARG:HB2	1:C:411:ARG:CZ	2.51	0.41
1:C:82:LEU:HD12	1:C:82:LEU:N	2.36	0.41
2:D:37:LEU:HD21	2:D:38:ARG:CZ	2.51	0.41
1:A:132:PRO:O	1:A:135:LEU:HB2	2.21	0.40
1:A:270:ILE:HD11	1:A:277:LEU:C	2.41	0.40
1:A:41:LEU:HD23	1:A:41:LEU:HA	1.80	0.40
1:A:22:ASP:CB	1:A:424:SER:HA	2.51	0.40
1:A:472:SER:O	1:A:474:SER:N	2.54	0.40
1:A:57:ARG:HD3	1:A:57:ARG:HA	1.83	0.40
1:A:310:LYS:HG2	1:C:101:TRP:NE1	2.36	0.40
1:C:125:MET:HB2	1:C:201:MET:CE	2.51	0.40
1:C:367:ILE:CG2	1:C:368:GLU:H	2.23	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:ARG:HA	1:C:57:ARG:HD3	1.83	0.40
1:A:101:TRP:NE1	1:C:310:LYS:HG2	2.36	0.40
1:A:185:CYS:CB	1:A:187:PRO:HD3	2.51	0.40
1:A:22:ASP:HB2	1:A:424:SER:HA	2.02	0.40
1:A:284:LYS:HE3	1:A:418:THR:HB	2.03	0.40
2:B:39:HIS:C	2:B:41:GLY:N	2.71	0.40
2:B:48:ILE:O	2:B:51:TYR:N	2.54	0.40
1:C:61:ILE:CD1	1:C:123:LYS:O	2.62	0.40
1:C:259:ALA:O	1:C:260:MET:C	2.59	0.40
1:C:313:ALA:O	1:C:314:GLU:CB	2.66	0.40
1:C:335:ILE:HG22	1:C:335:ILE:O	2.18	0.40
1:C:45:LEU:H	1:C:45:LEU:CD1	2.34	0.40
1:C:196:MET:HE1	2:D:12:LEU:HD11	2.03	0.40
1:A:131:GLN:H	1:A:131:GLN:NE2	2.20	0.40
1:A:315:THR:O	1:A:315:THR:HG23	2.20	0.40
1:A:425:LEU:HD22	1:A:425:LEU:N	2.37	0.40
1:A:440:PHE:HA	1:A:443:ILE:HG22	2.04	0.40
1:A:46:ILE:HD11	1:A:140:VAL:HG11	2.03	0.40
2:B:50:ALA:HA	2:B:63:ILE:CD1	2.52	0.40
1:C:147:GLU:HB3	1:C:148:GLU:H	1.59	0.40
1:C:340:MET:HE1	1:C:345:ARG:HG3	2.03	0.40
1:C:440:PHE:HA	1:C:443:ILE:HG22	2.04	0.40
1:C:51:LYS:O	1:C:52:GLN:HB2	2.20	0.40
1:C:71:ASP:O	1:C:113:ILE:HG13	2.21	0.40
1:A:373:PHE:HA	1:A:395:GLY:HA3	2.04	0.40
1:A:8:ASN:CB	1:A:28:GLY:O	2.70	0.40
2:B:37:LEU:HD21	2:B:38:ARG:CZ	2.51	0.40
1:C:227:GLN:O	1:C:227:GLN:CD	2.60	0.40
1:C:8:ASN:CB	1:C:28:GLY:O	2.70	0.40
1:C:317:HIS:HB3	1:C:393:LYS:NZ	2.36	0.40
2:D:23:GLU:O	2:D:27:LYS:HB2	2.22	0.40
2:D:38:ARG:CG	2:D:39:HIS:CE1	3.04	0.40
1:A:333:CYS:H	1:A:358:VAL:HG23	1.87	0.40
1:A:396:SER:O	1:A:399:GLY:N	2.54	0.40
1:C:46:ILE:HB	1:C:47:GLU:H	1.66	0.40
2:D:45:MET:HA	2:D:48: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	493/495 (100%)	228 (46%)	144 (29%)	121 (24%)	0	0
1	C	493/495 (100%)	227 (46%)	144 (29%)	122 (25%)	0	0
2	B	70/75 (93%)	33 (47%)	23 (33%)	14 (20%)	0	2
2	D	70/75 (93%)	33 (47%)	23 (33%)	14 (20%)	0	2
All	All	1126/1140 (99%)	521 (46%)	334 (30%)	271 (24%)	0	0

All (271) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	30	CYS
1	A	57	ARG
1	A	74	CYS
1	A	77	GLN
1	A	88	LYS
1	A	134	ASN
1	A	147	GLU
1	A	154	ASP
1	A	188	ARG
1	A	203	ASN
1	A	217	PRO
1	A	222	PRO
1	A	225	ASP
1	A	233	GLN
1	A	238	VAL
1	A	243	PRO
1	A	246	LYS
1	A	255	SER
1	A	257	GLU
1	A	270	ILE
1	A	272	MET

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Mol	Chain	Res	Type
1	A	274	SER
1	A	279	PHE
1	A	300	SER
1	A	302	CYS
1	A	310	LYS
1	A	314	GLU
1	A	342	LEU
1	A	344	LYS
1	A	346	HIS
1	A	347	VAL
1	A	355	ASN
1	A	357	ILE
1	A	383	GLU
1	A	386	GLN
1	A	394	LYS
1	A	396	SER
1	A	397	SER
1	A	417	ASP
1	A	429	PHE
1	A	435	ALA
1	A	444	TYR
1	A	468	MET
1	A	493	VAL
1	A	494	GLN
2	B	15	ALA
2	B	21	SER
2	B	56	THR
2	B	57	HIS
1	C	16	SER
1	C	30	CYS
1	C	57	ARG
1	C	74	CYS
1	C	77	GLN
1	C	88	LYS
1	C	134	ASN
1	C	147	GLU
1	C	154	ASP
1	C	188	ARG
1	C	203	ASN
1	C	217	PRO
1	C	222	PRO
1	C	225	ASP

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Mol	Chain	Res	Type
1	C	233	GLN
1	C	238	VAL
1	C	243	PRO
1	C	246	LYS
1	C	255	SER
1	C	257	GLU
1	C	270	ILE
1	C	272	MET
1	C	274	SER
1	C	279	PHE
1	C	300	SER
1	C	302	CYS
1	C	310	LYS
1	C	314	GLU
1	C	342	LEU
1	C	344	LYS
1	C	346	HIS
1	C	347	VAL
1	C	355	ASN
1	C	357	ILE
1	C	383	GLU
1	C	386	GLN
1	C	394	LYS
1	C	396	SER
1	C	397	SER
1	C	417	ASP
1	C	429	PHE
1	C	435	ALA
1	C	444	TYR
1	C	468	MET
1	C	493	VAL
1	C	494	GLN
2	D	15	ALA
2	D	21	SER
2	D	56	THR
2	D	57	HIS
1	A	2	ARG
1	A	10	ASP
1	A	40	THR
1	A	46	ILE
1	A	58	LYS
1	A	68	THR

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Mol	Chain	Res	Type
1	A	99	ARG
1	A	110	LYS
1	A	128	LYS
1	A	143	PRO
1	A	193	PHE
1	A	211	GLN
1	A	276	ASN
1	A	296	GLY
1	A	317	HIS
1	A	356	PRO
1	A	372	PRO
1	A	374	GLY
1	A	418	THR
1	A	443	ILE
1	A	447	ALA
1	A	473	THR
1	A	483	GLY
1	A	484	VAL
1	A	485	VAL
2	B	7	HIS
2	B	22	SER
1	C	2	ARG
1	C	10	ASP
1	C	40	THR
1	C	46	ILE
1	C	58	LYS
1	C	68	THR
1	C	99	ARG
1	C	110	LYS
1	C	128	LYS
1	C	143	PRO
1	C	193	PHE
1	C	211	GLN
1	C	276	ASN
1	C	296	GLY
1	C	317	HIS
1	C	356	PRO
1	C	372	PRO
1	C	374	GLY
1	C	418	THR
1	C	443	ILE
1	C	447	ALA

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Mol	Chain	Res	Type
1	C	473	THR
1	C	483	GLY
1	C	484	VAL
1	C	485	VAL
2	D	7	HIS
2	D	22	SER
1	A	27	HIS
1	A	37	ASN
1	A	103	ASN
1	A	108	PHE
1	A	192	ASP
1	A	204	LYS
1	A	221	LEU
1	A	256	GLN
1	A	261	HIS
1	A	331	SER
1	A	334	LYS
1	A	371	PRO
1	A	413	ALA
1	A	430	THR
1	A	470	SER
1	A	474	SER
2	B	51	TYR
2	B	66	LEU
1	C	4	ILE
1	C	27	HIS
1	C	37	ASN
1	C	103	ASN
1	C	108	PHE
1	C	192	ASP
1	C	204	LYS
1	C	221	LEU
1	C	256	GLN
1	C	261	HIS
1	C	331	SER
1	C	334	LYS
1	C	371	PRO
1	C	413	ALA
1	C	430	THR
1	C	470	SER
1	C	474	SER
1	C	491	VAL

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Mol	Chain	Res	Type
2	D	51	TYR
1	A	4	ILE
1	A	18	GLY
1	A	38	LYS
1	A	76	THR
1	A	201	MET
1	A	229	SER
1	A	289	MET
1	A	316	GLN
1	A	354	VAL
1	A	363	SER
1	A	425	LEU
1	A	491	VAL
2	B	2	VAL
2	B	46	ALA
1	C	18	GLY
1	C	38	LYS
1	C	76	THR
1	C	201	MET
1	C	229	SER
1	C	289	MET
1	C	316	GLN
1	C	354	VAL
1	C	363	SER
1	C	425	LEU
2	D	2	VAL
2	D	46	ALA
2	D	66	LEU
1	A	7	SER
1	A	75	PRO
1	A	123	LYS
1	A	126	LYS
1	A	144	HIS
1	A	195	GLU
1	A	227	GLN
1	A	228	GLY
1	A	311	GLU
1	A	343	GLU
1	A	365	VAL
1	A	445	GLY
2	B	44	ILE
2	B	67	LEU

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Mol	Chain	Res	Type
1	C	7	SER
1	C	75	PRO
1	C	123	LYS
1	C	126	LYS
1	C	144	HIS
1	C	195	GLU
1	C	227	GLN
1	C	228	GLY
1	C	311	GLU
1	C	343	GLU
1	C	365	VAL
1	C	445	GLY
2	D	44	ILE
1	A	36	LYS
1	A	248	GLN
1	A	487	LEU
2	B	55	THR
1	C	36	LYS
1	C	248	GLN
1	C	407	ARG
1	C	487	LEU
2	D	55	THR
2	D	67	LEU
1	A	320	ILE
2	B	8	VAL
1	C	320	ILE
2	D	8	VAL
1	A	395	GLY
1	C	395	GLY
1	A	382	VAL
1	C	382	VAL
1	A	223	GLY
1	C	223	GLY
1	A	12	VAL
1	A	266	GLY
1	A	482	VAL
1	C	12	VAL
1	C	266	GLY
1	C	482	VAL

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	420/420 (100%)	340 (81%)	80 (19%)	1	11
1	C	420/420 (100%)	340 (81%)	80 (19%)	1	11
2	B	57/60 (95%)	46 (81%)	11 (19%)	1	10
2	D	57/60 (95%)	46 (81%)	11 (19%)	1	10
All	All	954/960 (99%)	772 (81%)	182 (19%)	4	10

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	20	TRP
1	A	25	LEU
1	A	38	LYS
1	A	45	LEU
1	A	46	ILE
1	A	48	THR
1	A	51	LYS
1	A	55	THR
1	A	61	ILE
1	A	65	LEU
1	A	75	PRO
1	A	77	GLN
1	A	82	LEU
1	A	98	ASP
1	A	103	ASN
1	A	107	LEU
1	A	113	ILE
1	A	116	CYS
1	A	122	LYS
1	A	125	MET
1	A	131	GLN
1	A	135	LEU
1	A	139	ILE

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Mol	Chain	Res	Type
1	A	141	ILE
1	A	153	ASN
1	A	157	LYS
1	A	158	HIS
1	A	162	ILE
1	A	164	ILE
1	A	170	ILE
1	A	175	LEU
1	A	198	LEU
1	A	204	LYS
1	A	207	LEU
1	A	217	PRO
1	A	220	TRP
1	A	233	GLN
1	A	240	PHE
1	A	241	LYS
1	A	244	HIS
1	A	247	LYS
1	A	248	GLN
1	A	250	VAL
1	A	256	GLN
1	A	264	LEU
1	A	270	ILE
1	A	277	LEU
1	A	280	THR
1	A	283	LEU
1	A	299	TYR
1	A	306	PHE
1	A	310	LYS
1	A	311	GLU
1	A	312	ILE
1	A	314	GLU
1	A	323	ARG
1	A	348	LEU
1	A	350	ARG
1	A	351	LEU
1	A	352	ILE
1	A	358	VAL
1	A	359	THR
1	A	365	VAL
1	A	371	PRO
1	A	375	ASP

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Mol	Chain	Res	Type
1	A	389	LEU
1	A	390	ASN
1	A	400	GLN
1	A	422	PHE
1	A	431	SER
1	A	432	ILE
1	A	438	GLN
1	A	444	TYR
1	A	448	PHE
1	A	451	VAL
1	A	454	ILE
1	A	457	ILE
1	A	466	ILE
1	A	492	MET
2	B	2	VAL
2	B	4	LEU
2	B	6	PRO
2	B	8	VAL
2	B	14	THR
2	B	26	TRP
2	B	31	ARG
2	B	36	ILE
2	B	37	LEU
2	B	38	ARG
2	B	39	HIS
1	C	1	MET
1	C	20	TRP
1	C	25	LEU
1	C	38	LYS
1	C	45	LEU
1	C	46	ILE
1	C	48	THR
1	C	51	LYS
1	C	55	THR
1	C	61	ILE
1	C	65	LEU
1	C	75	PRO
1	C	77	GLN
1	C	82	LEU
1	C	98	ASP
1	C	103	ASN
1	C	107	LEU

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Mol	Chain	Res	Type
1	C	113	ILE
1	C	116	CYS
1	C	122	LYS
1	C	125	MET
1	C	131	GLN
1	C	135	LEU
1	C	139	ILE
1	C	141	ILE
1	C	153	ASN
1	C	157	LYS
1	C	158	HIS
1	C	162	ILE
1	C	164	ILE
1	C	170	ILE
1	C	175	LEU
1	C	198	LEU
1	C	204	LYS
1	C	207	LEU
1	C	217	PRO
1	C	220	TRP
1	C	233	GLN
1	C	240	PHE
1	C	241	LYS
1	C	244	HIS
1	C	247	LYS
1	C	248	GLN
1	C	250	VAL
1	C	256	GLN
1	C	264	LEU
1	C	270	ILE
1	C	277	LEU
1	C	280	THR
1	C	283	LEU
1	C	299	TYR
1	C	306	PHE
1	C	310	LYS
1	C	311	GLU
1	C	312	ILE
1	C	314	GLU
1	C	323	ARG
1	C	348	LEU
1	C	350	ARG

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Mol	Chain	Res	Type
1	C	351	LEU
1	C	352	ILE
1	C	358	VAL
1	C	359	THR
1	C	365	VAL
1	C	371	PRO
1	C	375	ASP
1	C	389	LEU
1	C	390	ASN
1	C	400	GLN
1	C	422	PHE
1	C	431	SER
1	C	432	ILE
1	C	438	GLN
1	C	444	TYR
1	C	448	PHE
1	C	451	VAL
1	C	454	ILE
1	C	457	ILE
1	C	466	ILE
1	C	492	MET
2	D	2	VAL
2	D	4	LEU
2	D	6	PRO
2	D	8	VAL
2	D	14	THR
2	D	26	TRP
2	D	31	ARG
2	D	36	ILE
2	D	37	LEU
2	D	38	ARG
2	D	39	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	77	GLN
1	A	83	ASN
1	A	131	GLN
1	A	167	GLN
1	A	200	GLN

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Mol	Chain	Res	Type
1	A	230	ASN
1	A	233	GLN
1	A	248	GLN
1	A	256	GLN
1	A	386	GLN
1	A	390	ASN
1	A	400	GLN
2	B	7	HIS
1	C	27	HIS
1	C	77	GLN
1	C	83	ASN
1	C	131	GLN
1	C	167	GLN
1	C	200	GLN
1	C	230	ASN
1	C	233	GLN
1	C	242	ASN
1	C	248	GLN
1	C	256	GLN
1	C	386	GLN
1	C	390	ASN
1	C	400	GLN
2	D	7	HIS

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 ⓘ

6 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	NAG	A	501	1	14,14,15	0.51	0	17,19,21	0.84	1 (5%)
3	NAG	A	502	1,3	14,14,15	0.56	0	17,19,21	0.78	0
3	NAG	A	503	3	14,14,15	0.58	0	17,19,21	0.81	1 (5%)
3	NAG	C	501	1	14,14,15	0.51	0	17,19,21	0.85	1 (5%)
3	NAG	C	502	1,3	14,14,15	0.57	0	17,19,21	0.77	0
3	NAG	C	503	3	14,14,15	0.57	0	17,19,21	0.79	1 (5%)

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	NAG	A	501	1	-	0/6/23/26	0/1/1/1
3	NAG	A	502	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	503	3	-	0/6/23/26	0/1/1/1
3	NAG	C	501	1	-	0/6/23/26	0/1/1/1
3	NAG	C	502	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	503	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	NAG	C2-N2-C7	-2.59	119.17	122.94
3	A	501	NAG	C2-N2-C7	-2.54	119.23	122.94
3	A	503	NAG	C2-N2-C7	-2.11	119.86	122.94
3	C	503	NAG	C2-N2-C7	-2.09	119.90	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	NAG	3	0
3	C	502	NAG	3	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.