Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 11:19 PM EST

PDB ID	:	3J27
EMDB ID	:	EMD-5520
Title	:	CryoEM structure of Dengue virus
Authors	:	Zhang, X.; Ge, P.; Yu, X.; Brannan, J.M.; Bi, G.; Zhang, Q.; Schein, S.; Zhou, Z.H.
Deposited on	:	2012-09-26
Resolution	:	3.60 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB 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.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

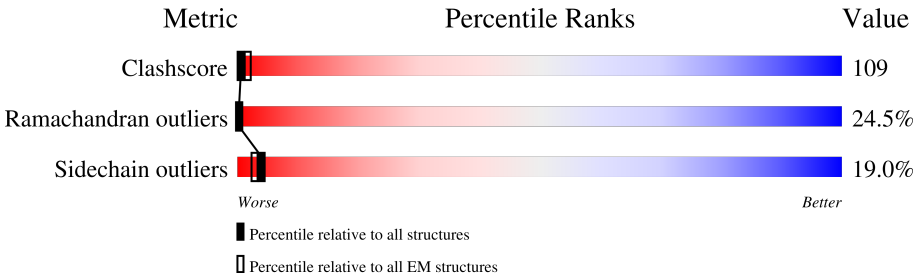
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	495	10% 56% 29% .
1	C	495	13% 55% 28% .
1	E	495	13% 51% 31% .
2	B	75	19% 51% 27% .
2	D	75	11% 48% 32% 5% .
2	F	75	8% 63% 25% .
3	G	2	100%
3	H	2	100%

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Mol	Chain	Length	Quality of chain
3	I	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	I	1	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14835 atoms, of which 1629 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		
1	E	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		
2	F	72	Total	C	H	N	O	S	0	0
			627	366	68	95	95	3		

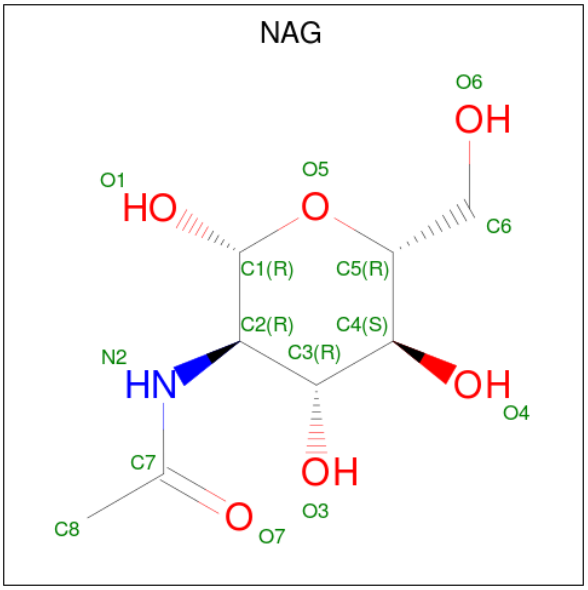
There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	AltConf	Trace
3	G	2	Total C N O 28 16 2 10	0	0
3	H	2	Total C N O 28 16 2 10	0	0
3	I	2	Total C N O 28 16 2 10	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

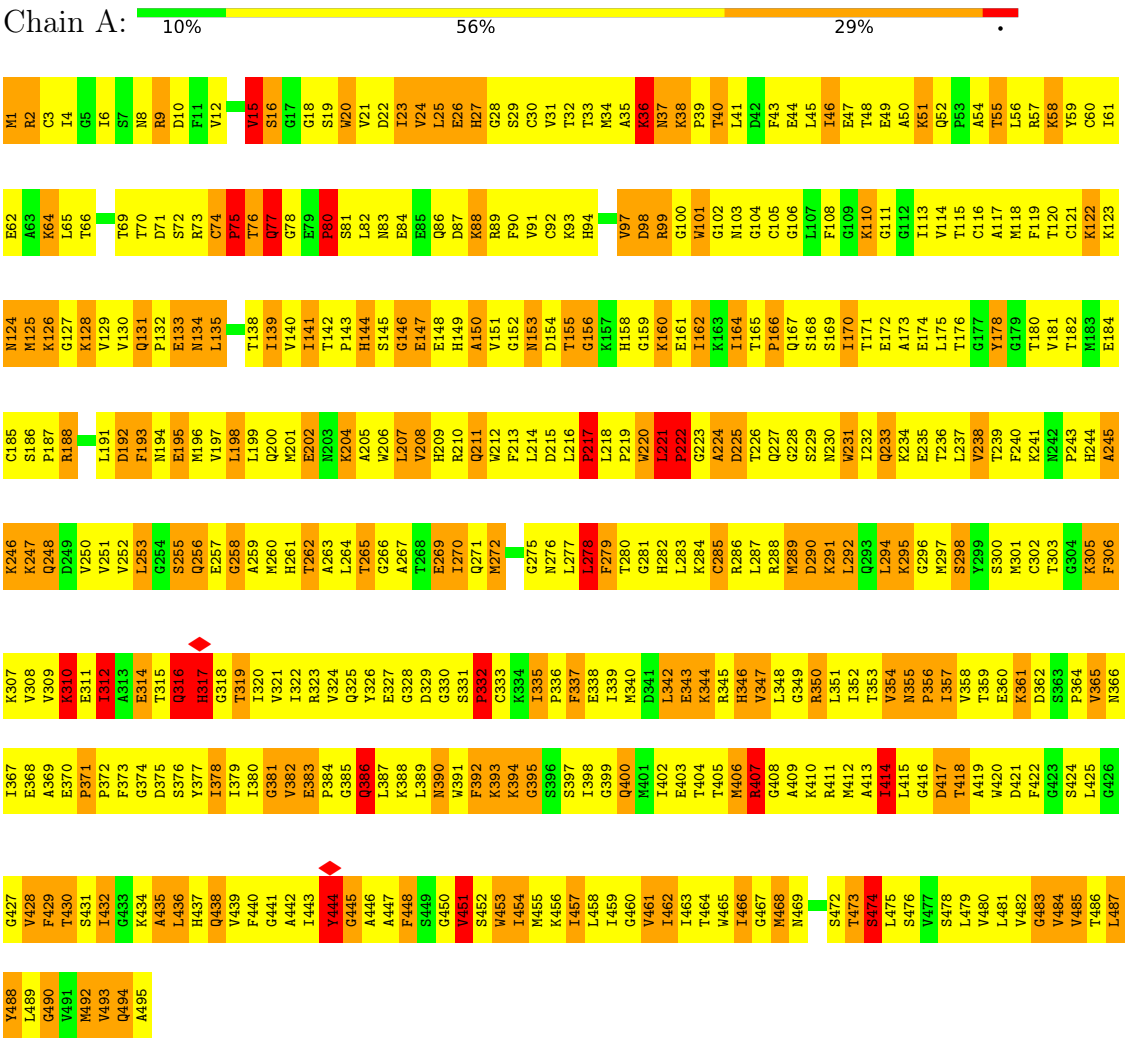


Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	E	1	Total C N O 14 8 1 5	0

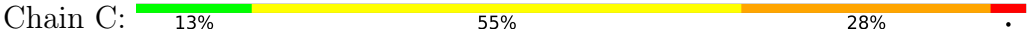
3 Residue-property plots (i)

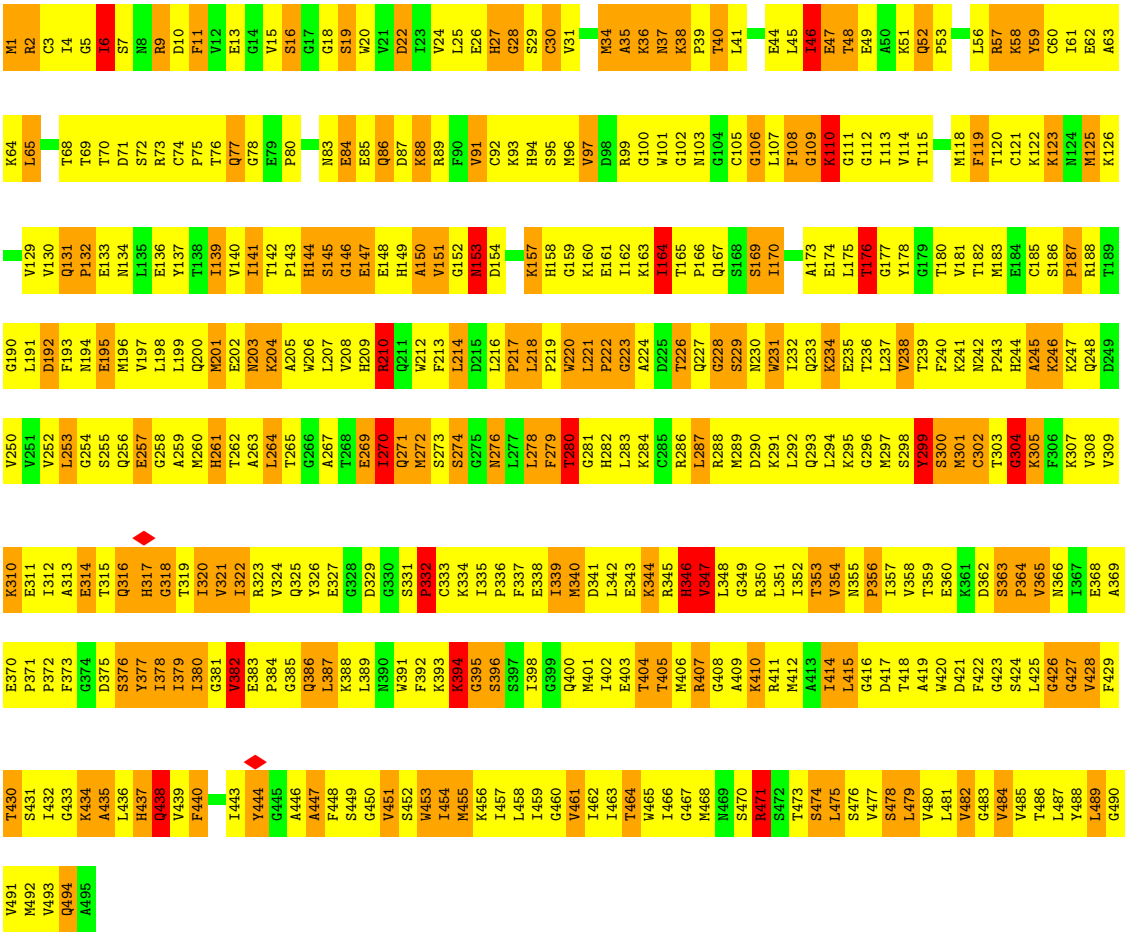
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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



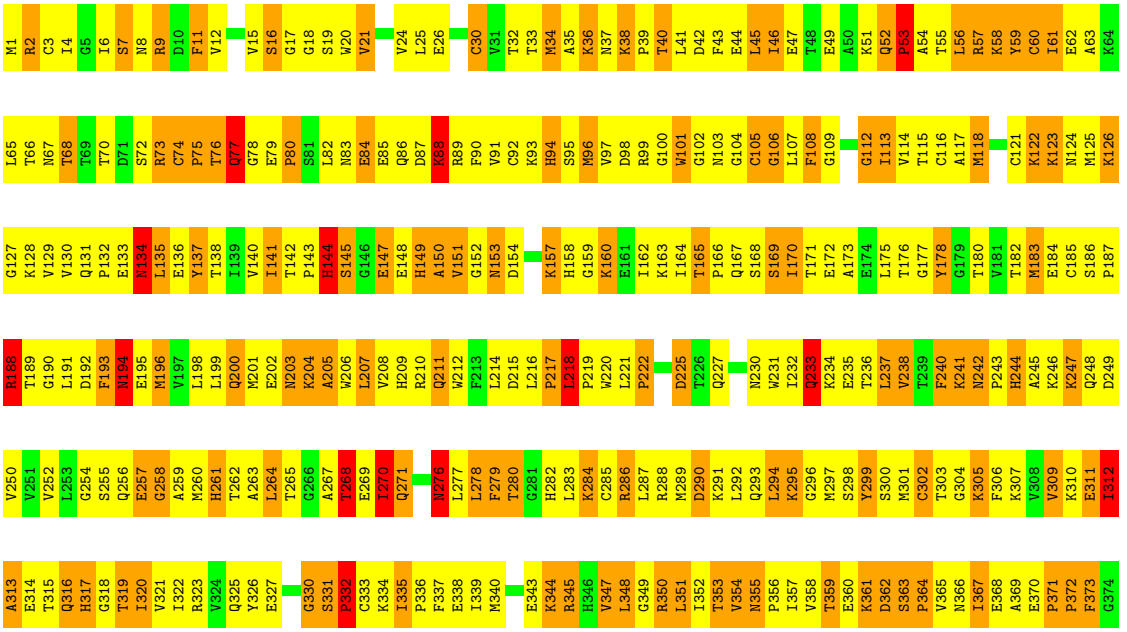
• Molecule 1: Envelope protein E

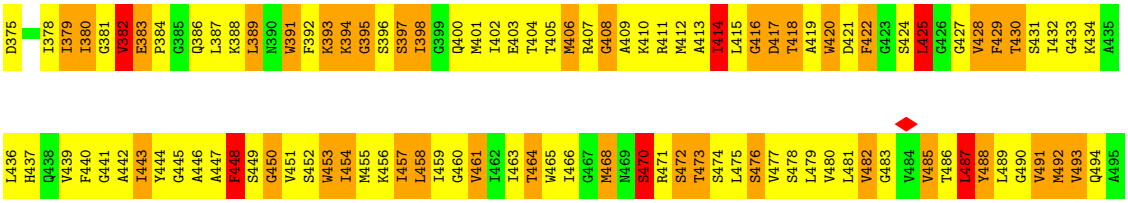




• Molecule 1: Envelope protein E

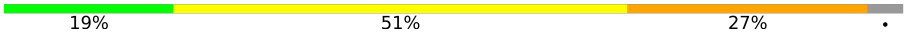
Chain E: 13% 51% 31%

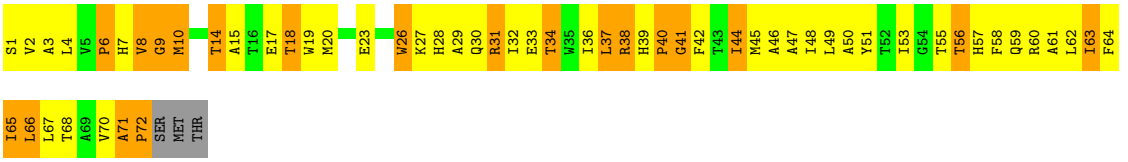




• Molecule 2: Small envelope protein M

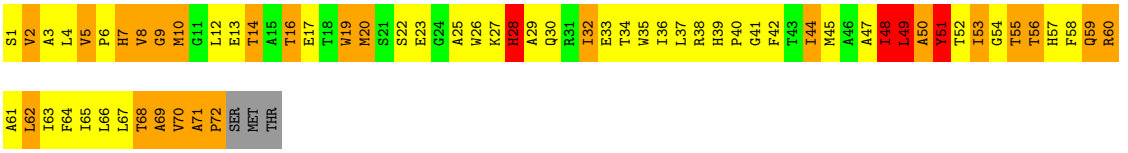
Chain B:





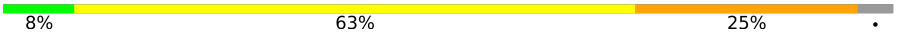
• Molecule 2: Small envelope protein M

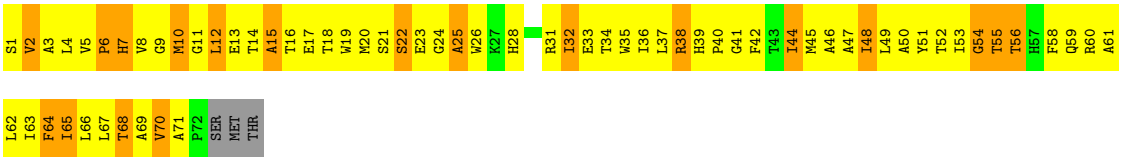
Chain D:



• Molecule 2: Small envelope protein M

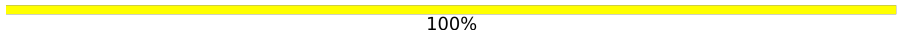
Chain F:





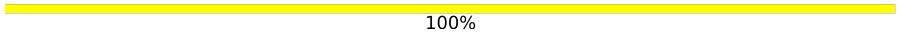
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

4 Experimental information (i)

Property	Value	Source
EM 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 ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	57518	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	1.538	Depositor
Minimum map value	-0.075	Depositor
Average map value	0.077	Depositor
Map value standard deviation	0.203	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	529.92, 529.92, 529.92	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.104, 1.104, 1.104	Depositor

5 Model quality

5.1 Standard geometry

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	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.45	0/3876	0.80	2/5237 (0.0%)
1	C	0.46	0/3876	0.82	3/5237 (0.1%)
1	E	0.46	0/3876	0.84	2/5237 (0.0%)
2	B	0.47	0/575	0.76	0/786
2	D	0.52	0/575	0.89	1/786 (0.1%)
2	F	0.50	0/575	0.73	0/786
All	All	0.46	0/13353	0.82	8/18069 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	223	GLY	N-CA-C	-6.15	97.73	113.10
2	D	56	THR	N-CA-C	-6.08	94.60	111.00
1	C	304	GLY	N-CA-C	5.63	127.17	113.10
1	A	223	GLY	N-CA-C	-5.59	99.13	113.10
1	E	470	SER	N-CA-C	5.34	125.41	111.00
1	A	378	ILE	N-CA-C	-5.15	97.11	111.00
1	C	41	LEU	CA-CB-CG	-5.14	103.48	115.30
1	E	320	ILE	N-CA-C	-5.04	97.38	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	299	TYR	Sidechain

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	3845	901	0
1	C	3801	475	3845	780	0
1	E	3801	475	3844	906	0
2	B	559	68	569	101	0
2	D	559	68	569	114	0
2	F	559	68	569	127	0
3	G	28	0	25	0	0
3	H	28	0	25	3	0
3	I	28	0	25	7	0
4	A	14	0	13	0	0
4	C	14	0	13	0	0
4	E	14	0	13	2	0
All	All	13206	1629	13355	2844	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 109.

All (2844) 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:56:THR:HG23	2:D:59:GLN:HE21	1.12	1.12
1:C:99:ARG:HB3	1:C:103:ASN:HD21	1.11	1.11
1:A:4:ILE:HB	1:A:151:VAL:HG11	1.24	1.11
1:E:221:LEU:HD11	1:E:225:ASP:HB2	1.26	1.10
1:E:381:GLY:HA3	1:E:386:GLN:HB2	1.28	1.10
1:C:312:ILE:HD13	1:C:391:TRP:HE1	1.12	1.10
1:A:20:TRP:HB3	1:A:425:LEU:HD11	1.26	1.09
1:E:1:MET:HG2	1:E:151:VAL:HA	1.21	1.09
1:A:182:THR:HB	1:A:288:ARG:HB3	1.30	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:339:ILE:HB	1:E:349:GLY:HA2	1.33	1.06
1:A:464:THR:HB	1:A:482:VAL:HG11	1.29	1.06
1:E:233:GLN:HE21	1:E:233:GLN:HA	1.21	1.06
1:E:34:MET:HB3	1:E:40:THR:HA	1.35	1.05
1:E:367:ILE:HD12	1:E:368:GLU:N	1.70	1.05
1:E:99:ARG:HA	1:E:103:ASN:ND2	1.71	1.05
1:E:149:HIS:NE2	3:I:1:NAG:H61	1.70	1.05
1:E:164:ILE:HD12	1:E:185:CYS:SG	1.97	1.05
1:E:310:LYS:HB2	1:E:323:ARG:HB3	1.39	1.05
1:E:481:LEU:O	1:E:485:VAL:HB	1.57	1.04
1:A:166:PRO:HB3	1:A:187:PRO:HG2	1.34	1.03
2:D:17:GLU:HG2	1:E:243:PRO:HA	1.40	1.03
1:C:65:LEU:HD21	1:C:252:VAL:HA	1.37	1.02
1:C:4:ILE:HG21	1:C:151:VAL:HB	1.39	1.01
1:E:373:PHE:HA	1:E:393:LYS:HD2	1.40	1.01
1:A:74:CYS:HA	1:A:99:ARG:HE	1.24	1.01
1:C:15:VAL:HG23	1:C:35:ALA:HB3	1.43	1.01
1:C:94:HIS:HA	1:C:114:VAL:HG12	1.42	1.00
1:A:380:ILE:HG23	1:A:382:VAL:HG23	1.42	0.99
1:C:89:ARG:NH2	1:C:89:ARG:HB3	1.77	0.99
1:C:45:LEU:HD13	1:C:46:ILE:N	1.76	0.99
1:E:453:TRP:HB2	1:E:494:GLN:HG3	1.44	0.98
1:C:408:GLY:HA2	1:C:411:ARG:HH22	1.26	0.98
1:A:140:VAL:HG12	1:A:161:GLU:HA	1.46	0.97
1:E:178:TYR:H	1:E:178:TYR:HD2	1.09	0.97
1:C:73:ARG:HD3	1:C:77:GLN:O	1.65	0.96
1:E:1:MET:CG	1:E:151:VAL:HA	1.94	0.96
1:C:166:PRO:HB3	1:C:187:PRO:CG	1.95	0.96
1:A:60:CYS:HA	1:A:124:ASN:HA	1.45	0.96
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.45	0.96
1:C:430:THR:HG23	1:C:431:SER:H	1.27	0.96
1:A:2:ARG:HG2	1:A:152:GLY:HA2	1.46	0.95
1:A:208:VAL:HG12	2:B:7:HIS:CE1	2.00	0.95
1:A:411:ARG:HD2	1:A:422:PHE:HE1	1.32	0.95
1:A:464:THR:HA	1:A:482:VAL:HG21	1.46	0.95
1:E:66:THR:O	1:E:118:MET:HG2	1.66	0.95
2:D:53:ILE:HG23	2:D:54:GLY:H	1.32	0.95
1:C:408:GLY:HA2	1:C:411:ARG:NH2	1.81	0.94
2:B:37:LEU:HD23	2:B:38:ARG:N	1.82	0.94
1:E:184:GLU:HB3	1:E:286:ARG:HB2	1.47	0.94
1:C:115:THR:HG21	1:C:248:GLN:HE22	1.31	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ALA:HB3	1:A:129:VAL:HG22	1.49	0.94
2:D:29:ALA:O	2:D:32:ILE:HG13	1.67	0.94
1:E:148:GLU:HG3	1:E:323:ARG:CZ	1.98	0.94
1:E:340:MET:HB3	1:E:347:VAL:HG12	1.47	0.94
1:E:25:LEU:HD13	1:E:45:LEU:HB2	1.50	0.93
1:C:166:PRO:HB3	1:C:187:PRO:HG3	1.50	0.93
1:E:57:ARG:HH22	1:E:214:LEU:HA	1.32	0.93
1:E:460:GLY:O	1:E:463:ILE:HG22	1.68	0.93
1:E:220:TRP:HB3	1:E:232:ILE:HB	1.50	0.92
1:A:246:LYS:HZ2	1:A:246:LYS:H	1.09	0.92
1:C:475:LEU:HD23	1:C:476:SER:N	1.84	0.92
1:C:305:LYS:H	1:C:386:GLN:HG2	1.33	0.92
2:D:56:THR:HG23	2:D:59:GLN:NE2	1.85	0.91
1:E:231:TRP:HB2	1:E:234:LYS:NZ	1.85	0.91
2:B:56:THR:OG1	2:B:59:GLN:HB2	1.69	0.91
1:C:456:LYS:O	1:C:459:ILE:HG22	1.71	0.91
1:C:332:PRO:HB3	1:C:358:VAL:HB	1.53	0.91
1:E:389:LEU:HD23	1:E:389:LEU:H	1.35	0.91
1:E:231:TRP:HB2	1:E:234:LYS:HZ3	1.33	0.91
1:C:89:ARG:HB3	1:C:89:ARG:HH21	1.33	0.91
1:C:197:VAL:CG2	1:C:210:ARG:HA	1.99	0.91
1:E:21:VAL:HG13	1:E:287:LEU:HB3	1.53	0.91
1:E:73:ARG:HA	1:E:73:ARG:HE	1.37	0.90
1:E:447:ALA:O	1:E:448:PHE:HB2	1.69	0.90
1:C:221:LEU:HB3	1:C:222:PRO:HD2	1.50	0.90
1:E:106:GLY:C	1:E:107:LEU:HD12	1.92	0.90
1:C:391:TRP:HZ3	1:C:393:LYS:HB2	1.36	0.90
1:A:306:PHE:HE2	1:A:326:TYR:HB2	1.36	0.89
1:C:1:MET:SD	1:C:2:ARG:HG2	2.12	0.89
2:D:67:LEU:O	2:D:70:VAL:HG22	1.72	0.89
1:A:34:MET:HA	1:A:40:THR:HG22	1.53	0.89
1:A:420:TRP:HB2	1:A:434:LYS:HG3	1.53	0.89
2:B:47:ALA:O	2:B:50:ALA:HB3	1.73	0.89
1:A:185:CYS:HA	1:A:285:CYS:HB3	1.55	0.89
1:A:19:SER:HB3	1:A:290:ASP:H	1.35	0.88
1:E:92:CYS:HB3	1:E:116:CYS:HB3	1.53	0.88
1:E:309:VAL:HG23	1:E:323:ARG:HG2	1.56	0.88
1:A:20:TRP:CB	1:A:425:LEU:HD11	2.03	0.88
1:A:359:THR:O	1:A:361:LYS:HD3	1.73	0.88
1:A:252:VAL:O	1:A:253:LEU:HB2	1.72	0.88
1:E:75:PRO:HD3	1:E:99:ARG:HG2	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:ARG:NH1	1:C:214:LEU:HD11	1.89	0.88
1:C:20:TRP:HE1	1:C:425:LEU:HB2	1.39	0.88
1:E:203:ASN:HB3	1:E:204:LYS:NZ	1.89	0.88
1:A:58:LYS:HD2	1:A:221:LEU:HD23	1.55	0.88
1:A:387:LEU:HD22	1:A:388:LYS:H	1.37	0.88
1:C:101:TRP:CD1	1:C:108:PHE:HZ	1.92	0.88
1:C:73:ARG:HH21	1:C:80:PRO:HA	1.40	0.87
1:E:314:GLU:HB2	1:E:391:TRP:CH2	2.09	0.87
1:E:420:TRP:HD1	1:E:434:LYS:HA	1.38	0.87
1:A:306:PHE:CD1	1:A:380:ILE:HG12	2.09	0.87
1:C:2:ARG:HB3	1:C:2:ARG:HH21	1.37	0.87
1:E:263:ALA:HB2	2:F:2:VAL:O	1.75	0.87
1:A:311:GLU:C	1:A:312:ILE:HD13	1.95	0.87
1:E:238:VAL:HG12	1:E:252:VAL:HA	1.56	0.87
1:A:20:TRP:HZ3	1:A:288:ARG:HE	1.19	0.87
1:A:387:LEU:HD22	1:A:388:LYS:N	1.90	0.87
1:E:325:GLN:HE22	1:E:364:PRO:HD3	1.39	0.86
1:A:4:ILE:HB	1:A:151:VAL:CG1	2.03	0.86
1:A:387:LEU:HD11	1:A:389:LEU:HG	1.58	0.86
1:C:304:GLY:H	1:C:382:VAL:HG21	1.39	0.86
1:A:411:ARG:HD2	1:A:422:PHE:CE1	2.10	0.86
1:E:138:THR:HG22	1:E:163:LYS:HD2	1.58	0.86
1:C:217:PRO:HG2	1:C:218:LEU:HD12	1.57	0.86
1:A:1:MET:HG2	1:A:150:ALA:O	1.76	0.86
1:C:99:ARG:HB3	1:C:103:ASN:ND2	1.89	0.86
1:A:224:ALA:O	1:A:226:THR:HG22	1.76	0.86
1:C:139:ILE:HG22	1:C:162:ILE:HG22	1.55	0.86
1:E:145:SER:HB3	1:E:353:THR:HG21	1.58	0.85
1:E:428:VAL:HG23	1:E:429:PHE:H	1.41	0.85
1:E:454:ILE:H	1:E:454:ILE:HD12	1.39	0.85
1:E:373:PHE:HA	1:E:393:LYS:CD	2.06	0.85
1:A:390:ASN:HD22	1:A:391:TRP:N	1.74	0.85
1:C:72:SER:HB3	1:C:113:ILE:HD13	1.58	0.85
1:E:38:LYS:HG3	1:E:292:LEU:HB3	1.55	0.85
1:C:58:LYS:HZ1	1:C:126:LYS:HG3	1.40	0.85
1:E:464:THR:HB	1:E:482:VAL:HG11	1.58	0.85
1:C:470:SER:H	1:C:475:LEU:HD12	1.41	0.85
1:E:182:THR:O	1:E:288:ARG:HB2	1.75	0.85
1:A:206:TRP:CD2	1:A:264:LEU:HD21	2.12	0.85
1:A:322:ILE:HD12	1:A:323:ARG:H	1.40	0.85
1:A:463:ILE:HG23	1:A:482:VAL:HG22	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:GLU:O	1:E:134:ASN:HB2	1.76	0.85
1:E:25:LEU:HD11	1:E:283:LEU:HD23	1.58	0.85
1:E:218:LEU:HB3	1:E:219:PRO:HD2	1.58	0.85
1:A:246:LYS:HZ2	1:A:246:LYS:N	1.73	0.84
1:E:141:ILE:HD13	1:E:141:ILE:H	1.40	0.84
1:E:270:ILE:HD13	1:E:278:LEU:HA	1.60	0.84
1:C:89:ARG:HH21	1:C:89:ARG:CB	1.88	0.84
1:C:165:THR:HG22	1:C:167:GLN:H	1.41	0.84
1:C:199:LEU:HD12	1:C:200:GLN:H	1.41	0.84
1:C:451:VAL:HG13	1:C:455:MET:HB3	1.57	0.84
2:B:28:HIS:O	2:B:31:ARG:HG3	1.76	0.84
2:B:44:ILE:HG22	2:B:48:ILE:HD11	1.58	0.84
1:A:173:ALA:HB3	1:A:181:VAL:HB	1.58	0.83
1:C:325:GLN:HB2	1:C:364:PRO:HG3	1.57	0.83
1:C:451:VAL:CG1	1:C:455:MET:HB3	2.08	0.83
1:A:448:PHE:O	1:A:451:VAL:HG13	1.76	0.83
1:A:306:PHE:CE2	1:A:326:TYR:HB2	2.12	0.83
1:E:36:LYS:HA	1:E:36:LYS:NZ	1.94	0.83
1:E:123:LYS:H	1:E:123:LYS:HD2	1.42	0.83
2:B:44:ILE:O	2:B:48:ILE:HG13	1.77	0.83
1:C:345:ARG:N	1:C:345:ARG:HD2	1.94	0.83
1:A:454:ILE:HG23	1:A:455:MET:H	1.42	0.82
1:C:237:LEU:HA	1:C:253:LEU:HD23	1.59	0.82
1:A:20:TRP:HA	1:A:20:TRP:CE3	2.12	0.82
1:A:220:TRP:CD1	1:A:221:LEU:O	2.32	0.82
1:A:350:ARG:NH1	1:A:372:PRO:HB3	1.95	0.82
1:E:411:ARG:HD2	1:E:422:PHE:CD1	2.14	0.82
1:E:463:ILE:HG23	1:E:482:VAL:HG22	1.61	0.82
1:C:53:PRO:HB3	1:C:130:VAL:HA	1.61	0.82
1:A:384:PRO:HD2	1:A:386:GLN:NE2	1.95	0.82
2:B:38:ARG:HA	2:B:38:ARG:HE	1.45	0.82
1:E:221:LEU:HD13	1:E:222:PRO:N	1.94	0.82
1:E:252:VAL:HG12	1:E:254:GLY:H	1.44	0.82
1:C:2:ARG:HB3	1:C:2:ARG:NH2	1.92	0.82
1:E:276:ASN:O	1:E:277:LEU:HD12	1.80	0.82
1:A:25:LEU:HD12	1:A:45:LEU:HB2	1.62	0.82
1:E:240:PHE:HB3	1:E:250:VAL:HA	1.60	0.82
1:C:312:ILE:HD13	1:C:391:TRP:NE1	1.93	0.82
1:E:2:ARG:NH1	1:E:154:ASP:HA	1.94	0.82
1:A:2:ARG:HH12	1:A:44:GLU:HG2	1.45	0.81
1:C:51:LYS:HB2	1:C:134:ASN:HD22	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:ILE:HD11	1:C:358:VAL:HG22	1.60	0.81
1:E:233:GLN:HA	1:E:233:GLN:NE2	1.94	0.81
1:E:265:THR:HA	2:F:19:TRP:HD1	1.45	0.81
1:A:443:ILE:HG12	1:A:444:TYR:H	1.45	0.81
1:E:240:PHE:HA	1:E:250:VAL:HA	1.61	0.81
1:E:464:THR:HA	1:E:482:VAL:HG21	1.61	0.81
1:A:322:ILE:HD12	1:A:323:ARG:N	1.96	0.81
1:E:26:GLU:O	1:E:45:LEU:HB3	1.80	0.81
1:A:309:VAL:O	1:A:310:LYS:HB2	1.79	0.81
1:A:39:PRO:HG3	1:A:178:TYR:HD1	1.44	0.81
1:A:307:LYS:HG2	1:A:308:VAL:N	1.94	0.81
1:A:323:ARG:HA	1:A:366:ASN:HA	1.63	0.81
1:C:451:VAL:HG12	1:C:452:SER:H	1.44	0.81
1:E:93:LYS:O	1:E:114:VAL:HG23	1.81	0.81
1:E:1:MET:HG2	1:E:151:VAL:CA	2.07	0.81
1:A:19:SER:HB3	1:A:290:ASP:N	1.96	0.80
1:C:99:ARG:O	1:C:108:PHE:HA	1.81	0.80
1:A:27:HIS:HB2	1:A:281:GLY:H	1.46	0.80
1:A:407:ARG:HH21	1:A:407:ARG:HB3	1.44	0.80
1:A:461:VAL:HA	1:A:464:THR:HG22	1.64	0.80
1:E:1:MET:SD	1:E:150:ALA:O	2.40	0.80
1:A:20:TRP:HA	1:A:20:TRP:HE3	1.43	0.80
1:A:265:THR:O	2:B:19:TRP:HB3	1.81	0.80
1:A:31:VAL:HB	1:A:43:PHE:HB2	1.61	0.80
2:D:16:THR:HG22	1:E:244:HIS:HB3	1.62	0.80
1:E:183:MET:HB2	1:E:285:CYS:SG	2.21	0.80
1:E:207:LEU:HD22	1:E:207:LEU:O	1.82	0.80
1:E:350:ARG:HH12	1:E:372:PRO:HD3	1.45	0.80
1:C:307:LYS:HB2	1:C:325:GLN:HB3	1.63	0.80
1:A:309:VAL:HB	1:A:323:ARG:HG2	1.63	0.79
2:D:63:ILE:HD12	2:D:64:PHE:N	1.97	0.79
2:F:32:ILE:HG13	2:F:33:GLU:H	1.47	0.79
1:C:293:GLN:C	1:C:294:LEU:HD12	2.02	0.79
1:E:145:SER:HB3	1:E:353:THR:CG2	2.12	0.79
1:A:173:ALA:CB	1:A:181:VAL:HB	2.12	0.79
1:C:375:ASP:HA	1:C:392:PHE:HA	1.64	0.79
1:C:70:THR:HG22	1:C:115:THR:HA	1.65	0.79
1:E:56:LEU:O	1:E:57:ARG:HB2	1.82	0.79
1:E:202:GLU:O	1:E:203:ASN:HB2	1.81	0.79
1:E:332:PRO:HD3	1:E:359:THR:O	1.83	0.79
1:A:383:GLU:CB	1:A:384:PRO:HD3	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:PRO:HG2	1:C:114:VAL:HG13	1.63	0.79
1:C:221:LEU:HB3	1:C:222:PRO:CD	2.11	0.79
1:E:52:GLN:HB2	1:E:134:ASN:OD1	1.83	0.79
1:A:197:VAL:HG11	1:A:213:PHE:CD2	2.18	0.79
2:B:62:LEU:HD13	2:B:63:ILE:N	1.97	0.79
1:C:142:THR:HB	1:C:159:GLY:HA3	1.65	0.79
1:E:339:ILE:HB	1:E:349:GLY:CA	2.12	0.79
2:B:1:SER:C	2:B:3:ALA:H	1.83	0.79
1:C:38:LYS:HA	1:C:294:LEU:HD11	1.64	0.79
1:E:95:SER:CB	1:E:248:GLN:HE22	1.96	0.79
1:E:343:GLU:O	1:E:345:ARG:N	2.16	0.79
2:B:26:TRP:HA	2:B:26:TRP:CE3	2.18	0.79
1:E:383:GLU:HB3	1:E:384:PRO:CD	2.12	0.79
1:E:463:ILE:O	1:E:466:ILE:HG22	1.83	0.79
1:E:19:SER:HB3	1:E:289:MET:H	1.47	0.78
1:E:74:CYS:HB3	1:E:77:GLN:HE22	1.48	0.78
1:E:221:LEU:HD11	1:E:225:ASP:CB	2.12	0.78
1:A:428:VAL:O	1:A:432:ILE:HB	1.83	0.78
1:C:294:LEU:HD12	1:C:294:LEU:N	1.99	0.78
1:A:458:LEU:O	1:A:461:VAL:HG23	1.82	0.78
1:C:377:TYR:HE2	1:C:388:LYS:HB3	1.46	0.78
1:C:76:THR:O	1:C:78:GLY:N	2.17	0.78
1:C:379:ILE:HD12	1:C:380:ILE:N	1.98	0.78
1:E:11:PHE:HA	1:E:32:THR:O	1.84	0.78
2:F:1:SER:C	2:F:3:ALA:H	1.87	0.78
1:A:94:HIS:HA	1:A:114:VAL:HG12	1.65	0.78
1:A:337:PHE:CD2	1:A:367:ILE:HD13	2.19	0.78
1:E:44:GLU:O	1:E:140:VAL:HG22	1.84	0.78
1:A:74:CYS:CA	1:A:99:ARG:HE	1.94	0.77
1:E:93:LYS:C	1:E:114:VAL:HG23	2.04	0.77
1:E:135:LEU:N	1:E:135:LEU:HD23	1.99	0.77
1:A:197:VAL:HG23	1:A:210:ARG:HA	1.65	0.77
1:C:453:TRP:N	1:C:494:GLN:HE22	1.81	0.77
2:D:48:ILE:HG22	2:D:49:LEU:N	1.98	0.77
2:D:50:ALA:O	2:D:52:THR:N	2.17	0.77
2:B:60:ARG:O	2:B:63:ILE:HD13	1.85	0.77
1:A:2:ARG:CG	1:A:152:GLY:HA2	2.13	0.77
1:A:6:ILE:HG13	1:A:30:CYS:SG	2.24	0.77
1:A:75:PRO:HD3	1:A:99:ARG:HG3	1.67	0.77
1:C:197:VAL:HG23	1:C:210:ARG:HA	1.64	0.77
1:C:220:TRP:CD1	1:C:221:LEU:O	2.37	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:GLU:HG3	1:E:92:CYS:SG	2.24	0.77
1:A:307:LYS:HG2	1:A:308:VAL:H	1.49	0.77
1:E:37:ASN:HB2	1:E:38:LYS:NZ	1.99	0.77
1:E:61:ILE:HD12	1:E:61:ILE:N	1.99	0.77
1:E:220:TRP:CD1	1:E:221:LEU:N	2.53	0.77
1:E:270:ILE:CD1	1:E:278:LEU:HA	2.14	0.77
1:E:383:GLU:HB3	1:E:384:PRO:HD3	1.66	0.77
1:A:146:GLY:O	1:A:147:GLU:HB2	1.85	0.77
1:E:11:PHE:HD2	1:E:32:THR:HB	1.50	0.77
1:A:184:GLU:O	1:A:285:CYS:HB2	1.85	0.77
1:C:192:ASP:O	1:C:195:GLU:HB3	1.85	0.77
1:E:15:VAL:HG13	1:E:16:SER:H	1.49	0.77
1:C:434:LYS:HD2	1:C:434:LYS:C	2.05	0.76
1:E:331:SER:OG	1:E:332:PRO:HD2	1.85	0.76
1:E:204:LYS:N	1:E:204:LYS:HE3	2.01	0.76
1:E:381:GLY:CA	1:E:386:GLN:HB2	2.13	0.76
1:E:51:LYS:HB2	1:E:134:ASN:ND2	2.01	0.76
1:E:97:VAL:HG13	1:E:113:ILE:HG21	1.65	0.76
1:C:191:LEU:O	1:C:193:PHE:N	2.18	0.76
1:E:320:ILE:HG12	1:E:371:PRO:HD2	1.66	0.76
1:E:320:ILE:HG13	1:E:369:ALA:O	1.85	0.76
1:E:389:LEU:HD23	1:E:389:LEU:N	2.01	0.76
1:A:233:GLN:C	1:A:235:GLU:H	1.87	0.76
1:E:420:TRP:HA	1:E:420:TRP:CE3	2.19	0.76
1:A:141:ILE:O	1:A:159:GLY:HA3	1.85	0.76
1:C:57:ARG:HH12	1:C:214:LEU:HD11	1.49	0.76
1:A:166:PRO:HB3	1:A:187:PRO:CG	2.16	0.76
1:A:339:ILE:CG2	1:A:349:GLY:HA2	2.16	0.76
1:A:391:TRP:CZ3	1:A:393:LYS:HA	2.19	0.76
1:C:51:LYS:HB2	1:C:134:ASN:ND2	2.01	0.76
1:A:224:ALA:HB2	1:C:73:ARG:NH1	2.01	0.76
2:F:8:VAL:HG13	2:F:9:GLY:H	1.51	0.76
1:A:33:THR:O	1:A:40:THR:HB	1.86	0.75
1:E:195:GLU:O	1:E:209:HIS:HB2	1.87	0.75
1:A:36:LYS:O	1:A:37:ASN:HB2	1.86	0.75
1:A:383:GLU:HB3	1:A:384:PRO:CD	2.15	0.75
1:E:170:ILE:HG12	1:E:184:GLU:HG3	1.68	0.75
1:E:340:MET:CB	1:E:347:VAL:HG12	2.15	0.75
1:E:388:LYS:NZ	1:E:388:LYS:HB3	2.01	0.75
1:E:478:SER:O	1:E:481:LEU:HB3	1.86	0.75
1:A:20:TRP:HH2	1:A:288:ARG:HH11	1.35	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:THR:HA	2:B:19:TRP:HD1	1.50	0.75
1:C:222:PRO:HG2	1:C:223:GLY:H	1.50	0.75
1:E:178:TYR:CE2	1:E:295:LYS:HD2	2.21	0.75
1:A:339:ILE:HG21	1:A:349:GLY:HA2	1.69	0.75
1:C:141:ILE:HD13	1:C:141:ILE:H	1.51	0.75
1:E:184:GLU:HB3	1:E:286:ARG:CB	2.16	0.75
1:A:331:SER:O	1:A:333:CYS:SG	2.42	0.75
1:C:91:VAL:HG11	1:C:238:VAL:HG11	1.67	0.75
1:C:415:LEU:H	1:C:415:LEU:CD2	1.99	0.75
1:E:413:ALA:HB3	1:E:414:ILE:HD13	1.69	0.75
1:C:71:ASP:O	1:C:113:ILE:HD12	1.86	0.75
1:E:61:ILE:HG22	1:E:256:GLN:H	1.52	0.75
1:A:62:GLU:HB3	1:A:122:LYS:O	1.87	0.74
1:A:460:GLY:O	1:A:463:ILE:HG22	1.87	0.74
1:C:454:ILE:HG23	1:C:455:MET:H	1.52	0.74
1:E:140:VAL:HG23	1:E:140:VAL:O	1.84	0.74
1:A:57:ARG:HH21	1:A:57:ARG:HG3	1.51	0.74
1:A:205:ALA:C	1:A:270:ILE:HG22	2.07	0.74
1:A:302:CYS:SG	1:A:333:CYS:HB3	2.26	0.74
1:C:53:PRO:HB3	1:C:129:VAL:O	1.87	0.74
1:C:451:VAL:HG12	1:C:452:SER:N	2.03	0.74
1:E:35:ALA:HB3	1:E:38:LYS:HE2	1.68	0.74
1:E:54:ALA:O	1:E:128:LYS:HA	1.87	0.74
1:A:20:TRP:HH2	1:A:288:ARG:NH1	1.84	0.74
1:C:452:SER:HA	1:C:494:GLN:NE2	2.02	0.74
1:E:417:ASP:H	1:E:437:HIS:HE1	1.35	0.74
1:C:283:LEU:HD22	1:C:284:LYS:N	2.02	0.74
1:E:263:ALA:O	2:F:6:PRO:HB2	1.86	0.74
1:A:290:ASP:HB2	1:A:291:LYS:HD2	1.67	0.74
1:E:420:TRP:HA	1:E:420:TRP:HE3	1.52	0.74
1:A:413:ALA:O	1:A:414:ILE:HG12	1.86	0.74
1:E:74:CYS:HB3	1:E:77:GLN:NE2	2.03	0.74
1:E:325:GLN:NE2	1:E:364:PRO:HD3	2.02	0.74
1:A:252:VAL:HG23	1:A:253:LEU:H	1.53	0.74
1:C:25:LEU:HB3	1:C:45:LEU:HB2	1.70	0.74
1:E:304:GLY:O	1:E:305:LYS:HB2	1.88	0.74
1:C:89:ARG:HD2	1:C:229:SER:HB2	1.70	0.74
1:C:205:ALA:HB3	1:C:270:ILE:O	1.87	0.74
1:E:37:ASN:HA	1:E:294:LEU:HD21	1.69	0.74
1:E:220:TRP:HD1	1:E:221:LEU:N	1.84	0.74
1:E:470:SER:HB2	1:E:475:LEU:HD13	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:ILE:HG22	1:A:490:GLY:HA3	1.70	0.74
1:E:375:ASP:HB3	1:E:392:PHE:CD1	2.22	0.74
1:C:491:VAL:HG23	1:C:492:MET:HE2	1.68	0.73
1:A:127:GLY:HA2	1:A:199:LEU:HA	1.69	0.73
1:A:221:LEU:HD22	1:A:231:TRP:CZ2	2.22	0.73
1:C:166:PRO:CB	1:C:187:PRO:HG3	2.17	0.73
1:E:87:ASP:O	1:E:89:ARG:N	2.20	0.73
2:F:55:THR:HG21	2:F:60:ARG:NH1	2.03	0.73
1:C:113:ILE:HD12	1:C:114:VAL:H	1.53	0.73
1:A:307:LYS:HB3	1:A:325:GLN:HB3	1.69	0.73
1:C:153:ASN:ND2	3:H:1:NAG:C7	2.50	0.73
1:C:199:LEU:HD12	1:C:200:GLN:N	2.00	0.73
1:C:236:THR:C	1:C:237:LEU:HD23	2.08	0.73
1:E:56:LEU:HD21	1:E:129:VAL:HG13	1.70	0.73
1:A:61:ILE:HD12	1:A:62:GLU:N	2.04	0.73
1:C:6:ILE:HG13	1:C:6:ILE:O	1.86	0.73
1:C:443:ILE:HA	1:C:447:ALA:HB2	1.71	0.73
1:E:411:ARG:HD2	1:E:422:PHE:HD1	1.52	0.73
1:E:320:ILE:HG12	1:E:371:PRO:CD	2.18	0.73
2:B:62:LEU:O	2:B:62:LEU:HD22	1.87	0.73
1:A:93:LYS:NZ	1:A:240:PHE:HB2	2.03	0.73
1:A:295:LYS:HD2	1:A:296:GLY:H	1.54	0.73
1:A:407:ARG:HH21	1:A:407:ARG:CB	2.01	0.73
1:E:415:LEU:H	1:E:415:LEU:HD23	1.53	0.73
1:E:463:ILE:HD12	1:E:466:ILE:HG21	1.70	0.73
1:A:86:GLN:OE1	1:C:230:ASN:HB2	1.88	0.73
1:A:282:HIS:ND1	1:A:282:HIS:O	2.22	0.73
1:C:218:LEU:HD12	1:C:218:LEU:N	2.03	0.73
1:E:203:ASN:HB3	1:E:204:LYS:HZ1	1.53	0.73
1:A:441:GLY:O	1:A:446:ALA:HB3	1.88	0.72
1:C:119:PHE:HD2	1:C:234:LYS:HD3	1.53	0.72
1:A:34:MET:HA	1:A:40:THR:CG2	2.19	0.72
1:A:74:CYS:HB3	1:A:77:GLN:NE2	2.05	0.72
1:A:270:ILE:HG23	1:A:271:GLN:N	2.02	0.72
1:A:340:MET:HG2	1:A:347:VAL:HG12	1.71	0.72
1:C:381:GLY:O	1:C:382:VAL:HG13	1.89	0.72
1:E:373:PHE:HB2	1:E:396:SER:HA	1.71	0.72
1:A:197:VAL:CG2	1:A:210:ARG:HA	2.19	0.72
1:A:373:PHE:O	1:A:393:LYS:HB3	1.89	0.72
1:C:1:MET:SD	1:C:2:ARG:N	2.62	0.72
1:E:477:VAL:O	1:E:480:VAL:HG12	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:479:LEU:HD12	1:E:480:VAL:N	2.04	0.72
1:A:386:GLN:HA	1:A:386:GLN:HE21	1.54	0.72
1:C:20:TRP:HE1	1:C:425:LEU:CB	2.03	0.72
1:C:302:CYS:HB2	1:C:334:LYS:O	1.89	0.72
1:C:391:TRP:CZ3	1:C:393:LYS:HB2	2.22	0.72
1:A:61:ILE:HG13	1:A:123:LYS:O	1.88	0.72
1:E:296:GLY:O	1:E:334:LYS:HE2	1.89	0.72
1:A:302:CYS:HB3	1:A:333:CYS:HB3	1.71	0.72
1:A:459:ILE:HA	1:A:462:ILE:HG22	1.69	0.72
2:B:27:LYS:O	2:B:30:GLN:HB3	1.89	0.72
1:C:270:ILE:HG13	1:C:278:LEU:HA	1.70	0.72
1:E:57:ARG:NH2	1:E:214:LEU:HA	2.04	0.72
2:F:59:GLN:NE2	2:F:63:ILE:HD13	2.05	0.72
1:C:236:THR:O	1:C:237:LEU:HD23	1.90	0.72
2:F:56:THR:HB	2:F:59:GLN:CB	2.19	0.72
1:A:72:SER:OG	1:A:113:ILE:HB	1.89	0.71
1:E:185:CYS:HA	1:E:285:CYS:HA	1.71	0.71
1:A:72:SER:HG	1:A:113:ILE:HB	1.55	0.71
1:C:315:THR:HG23	1:E:108:PHE:HB3	1.71	0.71
1:C:339:ILE:O	1:C:339:ILE:HD13	1.90	0.71
1:C:10:ASP:HB2	1:C:31:VAL:HG22	1.72	0.71
1:A:24:VAL:HG22	1:A:421:ASP:HB3	1.71	0.71
1:A:45:LEU:HD23	1:A:139:ILE:HG12	1.70	0.71
1:E:204:LYS:HB2	1:E:206:TRP:CH2	2.25	0.71
1:E:322:ILE:HG22	1:E:323:ARG:N	2.05	0.71
1:C:108:PHE:CD1	1:E:315:THR:OG1	2.39	0.71
2:D:53:ILE:HG23	2:D:54:GLY:N	2.05	0.71
1:E:270:ILE:HD12	1:E:271:GLN:N	2.06	0.71
1:A:144:HIS:HD2	1:A:368:GLU:HG3	1.56	0.71
1:A:230:ASN:OD1	1:C:86:GLN:HG2	1.90	0.71
1:A:238:VAL:HG12	1:A:252:VAL:HA	1.71	0.71
1:A:409:ALA:HA	1:A:412:MET:SD	2.30	0.71
1:A:47:GLU:HG3	1:A:138:THR:HB	1.73	0.71
1:C:283:LEU:HD22	1:C:284:LYS:H	1.56	0.71
1:E:1:MET:CB	1:E:151:VAL:HA	2.21	0.71
1:E:312:ILE:HG12	1:E:322:ILE:HG13	1.73	0.71
1:E:420:TRP:HD1	1:E:434:LYS:CA	2.04	0.71
1:A:164:ILE:O	1:A:164:ILE:HD13	1.91	0.71
1:C:478:SER:O	1:C:481:LEU:HB3	1.91	0.71
1:A:221:LEU:HD22	1:A:231:TRP:CH2	2.26	0.71
1:E:193:PHE:C	1:E:195:GLU:H	1.95	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:303:THR:HG22	1:E:326:TYR:OH	1.91	0.71
1:E:305:LYS:HD2	1:E:327:GLU:HB3	1.73	0.71
1:E:378:ILE:CG2	1:E:389:LEU:HG	2.21	0.71
1:E:383:GLU:CB	1:E:384:PRO:HD3	2.21	0.71
1:C:342:LEU:HA	1:C:377:TYR:HD1	1.55	0.70
2:D:70:VAL:O	2:D:72:PRO:N	2.23	0.70
1:E:375:ASP:HB3	1:E:392:PHE:HD1	1.54	0.70
1:A:74:CYS:HA	1:A:99:ARG:NE	2.04	0.70
1:A:291:LYS:HD2	1:A:291:LYS:H	1.56	0.70
1:A:473:THR:O	1:A:475:LEU:HD23	1.91	0.70
1:C:56:LEU:O	1:C:57:ARG:HB2	1.89	0.70
1:C:101:TRP:CH2	1:E:310:LYS:HD2	2.25	0.70
1:E:99:ARG:CA	1:E:103:ASN:ND2	2.52	0.70
1:A:86:GLN:O	1:C:88:LYS:HB2	1.91	0.70
1:A:220:TRP:CD1	1:A:220:TRP:C	2.65	0.70
1:A:205:ALA:C	1:A:206:TRP:CE3	2.65	0.70
1:A:269:GLU:HG2	1:A:270:ILE:H	1.57	0.70
1:E:305:LYS:HD2	1:E:327:GLU:H	1.56	0.70
1:E:312:ILE:HG23	1:E:313:ALA:H	1.55	0.70
1:A:323:ARG:HB2	1:A:323:ARG:NH2	2.06	0.70
1:E:219:PRO:HA	1:E:233:GLN:HB3	1.72	0.70
1:A:54:ALA:HB3	1:A:129:VAL:CG2	2.21	0.70
1:E:188:ARG:HA	1:E:188:ARG:CZ	2.20	0.70
1:E:240:PHE:CB	1:E:250:VAL:HA	2.22	0.70
1:E:380:ILE:H	1:E:380:ILE:HD13	1.56	0.70
1:A:185:CYS:HA	1:A:285:CYS:CB	2.21	0.70
1:A:196:MET:HE2	1:A:196:MET:HA	1.73	0.70
1:E:294:LEU:H	1:E:294:LEU:HD12	1.55	0.70
2:B:26:TRP:HA	2:B:26:TRP:HE3	1.53	0.70
1:C:353:THR:O	1:C:353:THR:HG22	1.91	0.70
1:C:427:GLY:HA3	1:C:430:THR:CG2	2.20	0.70
1:E:56:LEU:N	1:E:56:LEU:HD23	2.07	0.70
1:E:178:TYR:HD2	1:E:178:TYR:N	1.86	0.70
2:D:66:LEU:HD12	2:F:66:LEU:HD23	1.74	0.70
1:E:240:PHE:HB3	1:E:250:VAL:CA	2.21	0.70
1:E:450:GLY:HA2	2:F:9:GLY:HA3	1.73	0.70
1:A:27:HIS:HB2	1:A:281:GLY:N	2.06	0.70
1:A:71:ASP:HB2	1:A:82:LEU:CD2	2.22	0.70
1:A:259:ALA:HB1	2:B:2:VAL:O	1.92	0.70
1:C:384:PRO:HB2	1:C:386:GLN:HE22	1.56	0.70
1:C:410:LYS:HD3	1:C:410:LYS:C	2.12	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:PRO:HG2	1:E:178:TYR:CD1	2.27	0.70
1:E:414:ILE:HD13	1:E:414:ILE:N	2.07	0.70
1:E:453:TRP:HB3	1:E:454:ILE:HD12	1.73	0.70
1:A:65:LEU:HG	1:A:252:VAL:HG12	1.73	0.69
1:E:476:SER:HA	1:E:479:LEU:HG	1.73	0.69
1:A:448:PHE:CE2	1:A:451:VAL:HG11	2.27	0.69
1:C:379:ILE:HD12	1:C:379:ILE:C	2.12	0.69
2:D:19:TRP:CD1	2:D:20:MET:N	2.61	0.69
1:A:12:VAL:HB	1:A:33:THR:OG1	1.93	0.69
1:A:24:VAL:C	1:A:25:LEU:HD23	2.12	0.69
1:A:99:ARG:HD3	1:A:111:GLY:HA3	1.75	0.69
1:A:339:ILE:O	1:A:339:ILE:HG22	1.91	0.69
1:C:229:SER:HA	1:C:231:TRP:HE1	1.55	0.69
1:A:173:ALA:O	1:A:180:THR:HA	1.91	0.69
1:C:312:ILE:HD12	1:C:312:ILE:O	1.92	0.69
1:E:218:LEU:O	1:E:233:GLN:HG2	1.93	0.69
1:A:131:GLN:HE21	1:A:131:GLN:H	1.41	0.69
1:C:220:TRP:HD1	1:C:221:LEU:O	1.75	0.69
1:C:212:TRP:CZ3	1:C:216:LEU:HD11	2.26	0.69
1:E:417:ASP:H	1:E:437:HIS:CE1	2.11	0.69
1:E:475:LEU:HD23	1:E:476:SER:H	1.56	0.69
1:A:409:ALA:O	1:A:412:MET:HB2	1.93	0.69
1:A:9:ARG:HG3	1:A:10:ASP:N	2.08	0.69
1:A:15:VAL:O	1:A:16:SER:O	2.10	0.69
1:A:369:ALA:O	1:A:371:PRO:HD3	1.93	0.69
2:B:64:PHE:O	2:B:68:THR:HG23	1.92	0.69
1:C:185:CYS:HB3	1:C:283:LEU:HD11	1.75	0.69
1:C:463:ILE:HG23	1:C:482:VAL:HG22	1.74	0.69
1:E:20:TRP:CZ3	1:E:425:LEU:HB2	2.27	0.69
1:E:240:PHE:N	1:E:240:PHE:CD1	2.59	0.69
1:E:414:ILE:HG21	2:F:15:ALA:HB2	1.75	0.69
1:E:443:ILE:HG22	1:E:444:TYR:N	2.06	0.69
1:C:36:LYS:O	1:C:38:LYS:HD2	1.91	0.69
2:D:58:PHE:O	2:D:59:GLN:C	2.30	0.69
1:E:416:GLY:O	1:E:418:THR:N	2.26	0.69
1:A:19:SER:HA	1:A:289:MET:HB2	1.75	0.69
1:A:453:TRP:O	1:A:456:LYS:HB3	1.93	0.69
1:E:457:ILE:HD11	1:E:491:VAL:HG13	1.75	0.69
1:E:464:THR:CA	1:E:482:VAL:HG21	2.22	0.69
1:A:286:ARG:HH11	1:A:425:LEU:HD21	1.58	0.68
1:C:119:PHE:HD2	1:C:234:LYS:CD	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:HIS:HA	1:A:153:ASN:OD1	1.94	0.68
1:A:427:GLY:H	1:A:431:SER:HB2	1.57	0.68
1:C:415:LEU:H	1:C:415:LEU:HD23	1.57	0.68
1:C:463:ILE:HG23	1:C:482:VAL:CG2	2.22	0.68
1:E:178:TYR:HE2	1:E:295:LYS:HD2	1.55	0.68
1:A:131:GLN:H	1:A:131:GLN:NE2	1.90	0.68
1:C:299:TYR:O	1:C:333:CYS:HB3	1.92	0.68
1:E:373:PHE:H	1:E:373:PHE:HD2	1.41	0.68
1:E:386:GLN:O	1:E:387:LEU:HD22	1.94	0.68
1:C:149:HIS:CE1	1:C:150:ALA:O	2.47	0.68
1:C:377:TYR:CE2	1:C:388:LYS:HB3	2.28	0.68
1:A:342:LEU:HA	1:A:377:TYR:CZ	2.28	0.68
1:E:65:LEU:HD11	1:E:238:VAL:HB	1.75	0.68
1:C:355:ASN:O	1:C:357:ILE:N	2.26	0.68
1:E:52:GLN:NE2	1:E:134:ASN:HD21	1.92	0.68
1:E:305:LYS:CE	1:E:327:GLU:HB3	2.23	0.68
1:A:448:PHE:CD2	1:A:451:VAL:HG11	2.28	0.68
1:C:61:ILE:HG12	1:C:123:LYS:O	1.92	0.68
1:C:94:HIS:ND1	1:C:114:VAL:HG11	2.08	0.68
1:C:430:THR:HG23	1:C:431:SER:N	2.04	0.68
1:E:58:LYS:NZ	1:E:58:LYS:HB3	2.09	0.68
1:A:164:ILE:HG13	1:A:185:CYS:SG	2.34	0.68
1:A:199:LEU:C	1:A:199:LEU:HD12	2.14	0.68
1:A:323:ARG:HH21	1:A:366:ASN:HB3	1.59	0.68
1:A:333:CYS:O	1:A:358:VAL:HG22	1.94	0.68
1:A:337:PHE:CE2	1:A:367:ILE:HG21	2.28	0.68
1:C:427:GLY:HA3	1:C:430:THR:HG22	1.75	0.68
1:E:178:TYR:HA	1:E:293:GLN:O	1.93	0.68
1:C:137:TYR:HB2	1:C:164:ILE:HG23	1.76	0.68
2:D:3:ALA:HB1	2:F:3:ALA:HB1	1.76	0.68
1:E:240:PHE:CA	1:E:250:VAL:HA	2.24	0.68
2:F:21:SER:O	2:F:22:SER:HB3	1.92	0.68
1:C:39:PRO:O	1:C:40:THR:O	2.11	0.67
1:C:453:TRP:H	1:C:494:GLN:HE22	1.40	0.67
1:E:315:THR:O	1:E:317:HIS:N	2.27	0.67
1:E:415:LEU:O	1:E:418:THR:HG22	1.94	0.67
1:C:77:GLN:O	1:C:77:GLN:HG2	1.92	0.67
2:D:47:ALA:O	2:D:50:ALA:HB3	1.94	0.67
1:E:241:LYS:O	1:E:248:GLN:HB2	1.93	0.67
1:E:314:GLU:HB2	1:E:391:TRP:HH2	1.56	0.67
1:A:239:THR:O	1:A:251:VAL:HG22	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:GLN:H	1:C:194:ASN:HD21	1.43	0.67
1:C:256:GLN:OE1	1:C:256:GLN:HA	1.94	0.67
1:C:339:ILE:HD12	1:C:349:GLY:N	2.09	0.67
1:C:410:LYS:HD3	1:C:411:ARG:N	2.09	0.67
2:D:17:GLU:CG	1:E:243:PRO:HA	2.22	0.67
1:E:383:GLU:CG	1:E:384:PRO:HD3	2.24	0.67
1:E:453:TRP:HE3	1:E:454:ILE:N	1.91	0.67
1:C:25:LEU:O	1:C:282:HIS:HA	1.94	0.67
1:C:57:ARG:O	1:C:58:LYS:HB2	1.93	0.67
1:C:73:ARG:NH2	1:C:80:PRO:HA	2.10	0.67
1:E:73:ARG:HA	1:E:73:ARG:NE	2.07	0.67
1:E:396:SER:O	1:E:398:ILE:N	2.27	0.67
1:E:398:ILE:O	1:E:398:ILE:HD13	1.94	0.67
1:E:407:ARG:N	1:E:407:ARG:HD2	2.10	0.67
2:D:3:ALA:CB	2:F:3:ALA:HB1	2.24	0.67
1:E:351:LEU:O	1:E:352:ILE:HD13	1.94	0.67
1:E:380:ILE:HD13	1:E:380:ILE:N	2.10	0.67
1:E:409:ALA:C	1:E:411:ARG:H	1.98	0.67
1:C:302:CYS:SG	1:C:333:CYS:HB2	2.35	0.67
2:F:32:ILE:HG13	2:F:33:GLU:N	2.09	0.67
1:C:300:SER:HB3	1:C:333:CYS:SG	2.35	0.67
1:E:216:LEU:HD23	1:E:217:PRO:N	2.10	0.67
1:E:277:LEU:O	1:E:279:PHE:HD2	1.77	0.67
1:A:56:LEU:O	1:A:57:ARG:HB2	1.93	0.67
1:A:284:LYS:O	1:A:285:CYS:HB3	1.95	0.67
1:C:34:MET:N	1:C:34:MET:SD	2.67	0.67
1:C:346:HIS:O	1:C:347:VAL:C	2.32	0.67
1:E:75:PRO:HD3	1:E:99:ARG:CG	2.23	0.67
1:E:388:LYS:HB3	1:E:388:LYS:HZ3	1.60	0.67
1:C:282:HIS:CG	1:C:282:HIS:O	2.48	0.66
1:E:100:GLY:H	1:E:103:ASN:HD22	1.43	0.66
1:E:260:MET:HA	2:F:2:VAL:HB	1.77	0.66
1:A:19:SER:HB2	1:A:289:MET:N	2.10	0.66
1:A:166:PRO:C	1:A:168:SER:H	1.97	0.66
1:A:337:PHE:CE2	1:A:367:ILE:HD13	2.31	0.66
1:E:65:LEU:HD21	1:E:238:VAL:HG11	1.77	0.66
2:F:38:ARG:CZ	2:F:38:ARG:HA	2.25	0.66
2:B:37:LEU:HD23	2:B:38:ARG:H	1.58	0.66
1:C:59:TYR:HB2	1:C:125:MET:HB2	1.76	0.66
1:A:226:THR:HG23	1:A:226:THR:O	1.95	0.66
1:A:448:PHE:CE1	1:A:451:VAL:HG21	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:58:PHE:O	2:F:61:ALA:HB3	1.96	0.66
1:A:57:ARG:HG3	1:A:57:ARG:NH2	2.09	0.66
1:C:463:ILE:HG23	1:C:482:VAL:CG1	2.25	0.66
1:A:35:ALA:O	1:A:37:ASN:N	2.28	0.66
1:C:365:VAL:HG23	1:C:366:ASN:N	2.11	0.66
1:A:56:LEU:HD11	1:A:214:LEU:HD21	1.77	0.66
1:A:312:ILE:O	1:A:320:ILE:HD11	1.95	0.66
1:C:15:VAL:O	1:C:16:SER:O	2.13	0.66
1:C:101:TRP:CD1	1:C:108:PHE:CZ	2.80	0.66
1:C:377:TYR:CZ	1:C:388:LYS:HD2	2.30	0.66
2:D:33:GLU:HA	2:D:36:ILE:CD1	2.26	0.66
1:E:157:LYS:H	1:E:157:LYS:HD2	1.59	0.66
1:E:240:PHE:CG	1:E:250:VAL:HG12	2.31	0.66
1:E:449:SER:O	1:E:451:VAL:HG23	1.94	0.66
1:A:8:ASN:HB3	1:A:29:SER:HB2	1.77	0.66
1:E:99:ARG:HB3	1:E:109:GLY:O	1.95	0.66
1:E:218:LEU:HD23	1:E:218:LEU:N	2.10	0.66
1:C:36:LYS:HD3	1:C:37:ASN:ND2	2.10	0.65
1:A:237:LEU:O	1:A:238:VAL:O	2.14	0.65
2:B:1:SER:C	2:B:3:ALA:N	2.50	0.65
1:C:166:PRO:HB3	1:C:187:PRO:HG2	1.76	0.65
1:C:463:ILE:HG23	1:C:482:VAL:HG13	1.77	0.65
1:E:170:ILE:HA	1:E:184:GLU:HA	1.76	0.65
1:A:306:PHE:CD2	1:A:325:GLN:O	2.49	0.65
1:A:388:LYS:NZ	1:A:388:LYS:HB3	2.12	0.65
1:C:342:LEU:HD12	1:C:377:TYR:CD1	2.32	0.65
1:C:462:ILE:HG22	2:D:58:PHE:HZ	1.61	0.65
1:E:99:ARG:HA	1:E:103:ASN:HD21	1.62	0.65
1:E:420:TRP:O	1:E:422:PHE:N	2.30	0.65
1:E:457:ILE:HD11	1:E:487:LEU:HD13	1.79	0.65
1:A:27:HIS:CD2	1:A:280:THR:H	2.15	0.65
1:A:198:LEU:HD23	1:A:278:LEU:HD13	1.78	0.65
1:E:193:PHE:O	1:E:195:GLU:HG3	1.95	0.65
1:E:231:TRP:O	1:E:234:LYS:HE2	1.96	0.65
1:A:380:ILE:HG23	1:A:382:VAL:CG2	2.20	0.65
2:B:31:ARG:NH2	2:B:31:ARG:HG2	2.11	0.65
1:C:453:TRP:O	1:C:457:ILE:HG12	1.95	0.65
2:D:63:ILE:O	2:D:67:LEU:HD12	1.96	0.65
1:A:26:GLU:O	1:A:28:GLY:N	2.30	0.65
1:A:406:MET:O	1:A:409:ALA:N	2.30	0.65
1:C:97:VAL:HG23	1:C:99:ARG:HG2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:LEU:CD1	1:E:207:LEU:H	2.09	0.65
1:E:453:TRP:CB	1:E:494:GLN:HG3	2.22	0.65
2:F:1:SER:N	2:F:4:LEU:HD12	2.12	0.65
2:F:32:ILE:O	2:F:35:TRP:N	2.30	0.65
1:C:34:MET:HB3	1:C:40:THR:HA	1.79	0.65
1:C:80:PRO:HG3	1:C:113:ILE:N	2.12	0.65
1:E:46:ILE:HG12	1:E:47:GLU:H	1.60	0.65
1:A:283:LEU:HD12	1:A:284:LYS:N	2.11	0.65
1:A:66:THR:HG23	1:A:118:MET:HB3	1.79	0.65
1:A:75:PRO:HA	1:A:110:LYS:O	1.97	0.65
1:A:246:LYS:H	1:A:246:LYS:NZ	1.92	0.65
2:B:4:LEU:HD22	2:B:4:LEU:N	2.12	0.65
1:C:36:LYS:HD3	1:C:37:ASN:N	2.12	0.65
1:C:443:ILE:HG13	1:C:443:ILE:O	1.94	0.65
1:C:337:PHE:CD1	1:C:337:PHE:C	2.71	0.64
1:E:475:LEU:O	1:E:478:SER:HB2	1.96	0.64
2:F:55:THR:HG21	2:F:60:ARG:HH11	1.62	0.64
1:E:241:LYS:O	1:E:241:LYS:HD2	1.98	0.64
1:E:361:LYS:O	1:E:363:SER:N	2.30	0.64
1:E:463:ILE:HA	1:E:466:ILE:HG22	1.78	0.64
1:A:453:TRP:HE3	1:A:454:ILE:N	1.94	0.64
1:C:38:LYS:CA	1:C:294:LEU:HD11	2.27	0.64
1:E:218:LEU:CB	1:E:219:PRO:HD2	2.26	0.64
1:E:439:VAL:HG12	1:E:440:PHE:N	2.11	0.64
1:A:93:LYS:O	1:A:114:VAL:HA	1.97	0.64
1:C:449:SER:HB2	2:D:9:GLY:O	1.96	0.64
1:E:380:ILE:HD11	1:E:387:LEU:HB3	1.78	0.64
1:E:413:ALA:O	1:E:415:LEU:N	2.30	0.64
1:C:317:HIS:O	1:C:319:THR:N	2.31	0.64
1:A:269:GLU:HG2	1:A:270:ILE:N	2.11	0.64
1:C:197:VAL:HG21	1:C:210:ARG:HA	1.79	0.64
1:C:256:GLN:O	1:C:259:ALA:HB3	1.98	0.64
1:C:487:LEU:O	1:C:490:GLY:N	2.31	0.64
1:E:450:GLY:HA2	2:F:10:MET:H	1.61	0.64
1:A:262:THR:HG22	1:A:262:THR:O	1.98	0.64
1:A:411:ARG:HB3	1:A:411:ARG:HH21	1.63	0.64
1:A:427:GLY:N	1:A:431:SER:HB2	2.13	0.64
1:C:324:VAL:HG23	1:C:324:VAL:O	1.95	0.64
1:C:462:ILE:O	1:C:466:ILE:HG22	1.97	0.64
1:E:255:SER:OG	1:E:257:GLU:HG3	1.97	0.64
1:E:351:LEU:HD12	1:E:352:ILE:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:GLN:HB3	1:A:272:MET:HE3	1.80	0.64
1:A:221:LEU:HG	1:A:225:ASP:HB2	1.79	0.64
1:C:24:VAL:C	1:C:25:LEU:HD12	2.18	0.64
1:C:444:TYR:C	1:C:446:ALA:H	2.00	0.64
1:E:470:SER:OG	1:E:475:LEU:HD22	1.98	0.64
1:A:302:CYS:CB	1:A:333:CYS:HB3	2.28	0.63
1:A:323:ARG:HB2	1:A:366:ASN:HB3	1.79	0.63
1:C:97:VAL:CG1	1:C:113:ILE:HG21	2.29	0.63
1:C:107:LEU:O	1:C:108:PHE:HB2	1.98	0.63
1:C:170:ILE:O	1:C:170:ILE:HG13	1.98	0.63
1:C:208:VAL:HG12	1:C:267:ALA:HB2	1.78	0.63
1:C:481:LEU:O	1:C:485:VAL:HB	1.97	0.63
1:A:409:ALA:HA	1:A:412:MET:CG	2.28	0.63
1:C:227:GLN:O	1:C:228:GLY:C	2.36	0.63
1:C:394:LYS:HD3	1:C:394:LYS:N	2.13	0.63
1:C:464:THR:HG22	1:C:465:TRP:N	2.12	0.63
1:E:159:GLY:O	1:E:160:LYS:HB2	1.99	0.63
1:E:206:TRP:CE3	1:E:264:LEU:HD21	2.32	0.63
1:E:463:ILE:HG23	1:E:464:THR:N	2.12	0.63
1:A:282:HIS:NE2	1:A:415:LEU:HA	2.13	0.63
1:E:378:ILE:HG23	1:E:389:LEU:HG	1.80	0.63
1:A:38:LYS:HA	1:A:292:LEU:O	1.98	0.63
1:A:357:ILE:O	1:A:357:ILE:HG23	1.98	0.63
1:C:209:HIS:ND1	2:D:10:MET:HG3	2.13	0.63
1:C:240:PHE:CD1	1:C:250:VAL:HG12	2.34	0.63
1:E:232:ILE:O	1:E:233:GLN:HB2	1.98	0.63
1:A:93:LYS:HE2	1:A:240:PHE:HD1	1.64	0.63
2:B:31:ARG:HG2	2:B:31:ARG:HH21	1.64	0.63
1:C:37:ASN:O	1:C:38:LYS:HD2	1.98	0.63
2:D:22:SER:HA	2:D:25:ALA:HB3	1.81	0.63
1:E:306:PHE:CD2	1:E:326:TYR:HB2	2.33	0.63
1:A:101:TRP:HB2	1:A:108:PHE:HD2	1.61	0.63
1:A:386:GLN:HE21	1:A:386:GLN:CA	2.09	0.63
1:A:448:PHE:CD1	1:A:448:PHE:C	2.71	0.63
1:E:125:MET:O	1:E:126:LYS:HG3	1.98	0.63
1:E:381:GLY:HA3	1:E:386:GLN:CB	2.19	0.63
1:A:71:ASP:HB2	1:A:82:LEU:HD21	1.80	0.63
1:C:29:SER:O	1:C:30:CYS:HB3	1.99	0.63
1:C:357:ILE:HD12	1:C:357:ILE:O	1.99	0.63
1:C:113:ILE:HD12	1:C:114:VAL:N	2.14	0.63
1:C:199:LEU:CD1	1:C:200:GLN:O	2.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:PRO:HG2	1:C:218:LEU:CD1	2.29	0.63
1:E:9:ARG:HB2	1:E:30:CYS:O	1.99	0.63
1:E:210:ARG:C	1:E:212:TRP:H	2.01	0.63
1:A:387:LEU:HD13	1:A:387:LEU:C	2.19	0.62
1:C:212:TRP:CD2	1:C:216:LEU:HD21	2.33	0.62
1:C:378:ILE:HG22	1:C:389:LEU:HB2	1.81	0.62
2:F:6:PRO:O	2:F:8:VAL:N	2.32	0.62
1:A:444:TYR:C	1:A:446:ALA:H	2.02	0.62
1:C:339:ILE:HD13	1:C:339:ILE:C	2.20	0.62
1:E:86:GLN:OE1	1:E:86:GLN:HA	1.98	0.62
1:E:303:THR:HG23	1:E:304:GLY:N	2.15	0.62
1:A:323:ARG:NH2	1:A:366:ASN:HB3	2.13	0.62
1:A:385:GLY:O	1:A:387:LEU:N	2.32	0.62
2:B:56:THR:O	2:B:58:PHE:N	2.31	0.62
1:C:199:LEU:HD11	1:C:200:GLN:O	1.99	0.62
1:E:39:PRO:HD3	1:E:294:LEU:HA	1.80	0.62
1:E:148:GLU:HG2	1:E:148:GLU:O	2.00	0.62
1:E:367:ILE:HD12	1:E:368:GLU:CA	2.28	0.62
1:E:437:HIS:O	1:E:441:GLY:HA3	1.99	0.62
1:A:51:LYS:O	1:A:52:GLN:HB2	2.00	0.62
1:C:89:ARG:CD	1:C:229:SER:HB2	2.29	0.62
1:C:394:LYS:HD3	1:C:394:LYS:H	1.65	0.62
1:E:218:LEU:HB3	1:E:219:PRO:CD	2.29	0.62
1:E:289:MET:O	1:E:290:ASP:O	2.18	0.62
1:A:22:ASP:HB2	1:A:424:SER:HA	1.82	0.62
1:A:93:LYS:HZ1	1:A:240:PHE:HB2	1.64	0.62
1:A:191:LEU:O	1:A:192:ASP:HB2	1.98	0.62
1:A:220:TRP:HD1	1:A:221:LEU:O	1.83	0.62
1:A:330:GLY:O	1:A:331:SER:HB3	2.00	0.62
1:C:220:TRP:CZ2	1:C:232:ILE:HD11	2.34	0.62
1:E:131:GLN:C	1:E:133:GLU:H	2.02	0.62
1:A:81:SER:C	1:A:82:LEU:HD23	2.20	0.62
1:A:101:TRP:N	1:A:108:PHE:HB3	2.15	0.62
1:A:277:LEU:HG	1:A:279:PHE:HE2	1.65	0.62
1:A:484:VAL:O	1:A:485:VAL:C	2.38	0.62
1:C:115:THR:HG21	1:C:248:GLN:NE2	2.09	0.62
1:C:379:ILE:HD12	1:C:380:ILE:CA	2.29	0.62
2:D:34:THR:HG22	2:D:38:ARG:HE	1.64	0.62
1:E:305:LYS:CD	1:E:327:GLU:HB3	2.30	0.62
1:A:122:LYS:HA	1:A:122:LYS:HZ2	1.62	0.62
1:A:169:SER:HB3	1:E:388:LYS:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ARG:NH2	1:A:372:PRO:HA	2.14	0.62
1:A:352:ILE:HG22	1:A:368:GLU:O	2.00	0.62
1:E:241:LYS:HD2	1:E:241:LYS:C	2.20	0.62
1:C:218:LEU:N	1:C:236:THR:HG21	2.14	0.62
2:D:32:ILE:CD1	2:D:36:ILE:HD11	2.30	0.62
1:E:37:ASN:HB2	1:E:38:LYS:HZ3	1.64	0.62
1:E:90:PHE:HA	1:E:117:ALA:O	1.99	0.62
1:E:102:GLY:C	1:E:104:GLY:N	2.49	0.62
1:E:164:ILE:HD12	1:E:185:CYS:HG	1.65	0.62
1:A:99:ARG:HB2	1:A:99:ARG:NH2	2.15	0.62
1:A:467:GLY:O	1:A:469:ASN:N	2.33	0.62
1:C:451:VAL:HG11	1:C:456:LYS:N	2.14	0.61
2:D:48:ILE:O	2:D:52:THR:HG22	2.00	0.61
1:E:38:LYS:H	1:E:294:LEU:HG	1.64	0.61
1:A:379:ILE:HG12	1:A:381:GLY:H	1.64	0.61
1:C:141:ILE:H	1:C:141:ILE:CD1	2.13	0.61
1:C:426:GLY:O	1:C:428:VAL:N	2.32	0.61
1:E:137:TYR:HD1	1:E:283:LEU:HD22	1.65	0.61
1:A:294:LEU:O	1:A:295:LYS:O	2.18	0.61
1:C:228:GLY:O	1:C:230:ASN:N	2.32	0.61
1:E:148:GLU:HB2	1:E:364:PRO:HG2	1.82	0.61
1:A:233:GLN:C	1:A:235:GLU:N	2.53	0.61
1:E:453:TRP:HE3	1:E:454:ILE:CA	2.13	0.61
1:A:200:GLN:HB3	1:A:272:MET:CE	2.29	0.61
1:C:93:LYS:HB2	1:C:240:PHE:CZ	2.35	0.61
1:E:270:ILE:HD12	1:E:270:ILE:C	2.21	0.61
1:E:420:TRP:CD1	1:E:434:LYS:HA	2.29	0.61
1:A:252:VAL:HG23	1:A:253:LEU:N	2.15	0.61
1:A:265:THR:HG23	1:A:266:GLY:H	1.65	0.61
1:A:278:LEU:HD23	1:A:278:LEU:H	1.65	0.61
1:A:464:THR:CA	1:A:482:VAL:HG21	2.27	0.61
2:D:19:TRP:HD1	2:D:20:MET:N	1.99	0.61
1:E:221:LEU:HD13	1:E:222:PRO:CD	2.30	0.61
1:E:322:ILE:CG2	1:E:323:ARG:N	2.64	0.61
1:E:468:MET:HA	1:E:475:LEU:HD12	1.82	0.61
1:A:207:LEU:HD23	1:A:207:LEU:C	2.21	0.61
1:A:305:LYS:CG	1:A:327:GLU:HB3	2.31	0.61
1:C:46:ILE:HG23	1:C:46:ILE:O	1.99	0.61
2:F:38:ARG:HB2	2:F:38:ARG:NH2	2.16	0.61
1:A:205:ALA:HA	1:A:206:TRP:CE3	2.35	0.61
1:A:306:PHE:HZ	1:A:335:ILE:HG13	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:VAL:HG21	1:E:19:SER:HA	1.83	0.61
1:A:122:LYS:HZ3	1:A:122:LYS:HB2	1.64	0.61
1:E:170:ILE:CD1	1:E:184:GLU:HG3	2.31	0.61
1:E:487:LEU:O	1:E:491:VAL:HG22	2.01	0.61
2:F:44:ILE:O	2:F:48:ILE:HG13	2.01	0.61
2:F:56:THR:HB	2:F:59:GLN:HB3	1.82	0.61
1:A:141:ILE:O	1:A:141:ILE:HD13	2.00	0.61
1:A:323:ARG:HG3	1:A:365:VAL:O	2.00	0.61
1:A:360:GLU:C	1:A:362:ASP:H	2.04	0.61
1:A:386:GLN:NE2	1:A:386:GLN:HA	2.15	0.61
1:E:182:THR:O	1:E:288:ARG:CB	2.49	0.61
1:A:73:ARG:CB	1:A:80:PRO:HG3	2.30	0.60
1:A:166:PRO:HD3	1:A:187:PRO:CB	2.31	0.60
1:A:213:PHE:CG	1:A:213:PHE:O	2.53	0.60
1:A:350:ARG:HD2	1:A:350:ARG:N	2.15	0.60
1:A:463:ILE:O	1:A:466:ILE:HG22	2.00	0.60
2:D:4:LEU:O	2:D:5:VAL:HG13	2.00	0.60
1:E:260:MET:O	1:E:263:ALA:HB3	2.00	0.60
2:F:48:ILE:O	2:F:51:TYR:N	2.33	0.60
2:B:19:TRP:O	2:B:20:MET:SD	2.58	0.60
1:C:142:THR:OG1	1:C:143:PRO:HD2	2.01	0.60
1:E:450:GLY:HA2	2:F:10:MET:N	2.16	0.60
1:A:101:TRP:H	1:A:108:PHE:HB3	1.66	0.60
1:A:166:PRO:HD3	1:A:187:PRO:HB2	1.84	0.60
1:A:305:LYS:HG2	1:A:327:GLU:HB3	1.82	0.60
2:B:7:HIS:CE1	2:B:10:MET:HG3	2.36	0.60
1:C:110:LYS:NZ	1:C:110:LYS:HB3	2.16	0.60
1:C:402:ILE:O	1:C:405:THR:HB	2.00	0.60
1:E:19:SER:HB3	1:E:289:MET:N	2.14	0.60
2:B:33:GLU:O	2:B:34:THR:C	2.38	0.60
1:C:2:ARG:HH21	1:C:2:ARG:CB	2.09	0.60
1:C:37:ASN:C	1:C:38:LYS:HD2	2.21	0.60
1:C:149:HIS:O	1:C:150:ALA:CB	2.49	0.60
1:C:304:GLY:H	1:C:382:VAL:CG2	2.11	0.60
1:A:94:HIS:CA	1:A:114:VAL:HG12	2.31	0.60
1:A:350:ARG:HD3	1:A:370:GLU:O	2.02	0.60
1:A:399:GLY:O	1:A:402:ILE:HG23	2.01	0.60
1:A:483:GLY:O	1:A:484:VAL:C	2.37	0.60
2:B:37:LEU:HD21	2:B:38:ARG:NH1	2.16	0.60
1:C:428:VAL:HG12	1:C:429:PHE:N	2.15	0.60
2:D:48:ILE:O	2:D:50:ALA:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:217:PRO:O	1:E:218:LEU:HG	2.01	0.60
1:E:305:LYS:O	1:E:305:LYS:HD3	2.02	0.60
1:E:463:ILE:HD12	1:E:466:ILE:CG2	2.31	0.60
2:F:49:LEU:O	2:F:53:ILE:HG22	2.00	0.60
1:A:140:VAL:HG11	1:A:161:GLU:HG2	1.83	0.60
1:A:479:LEU:O	1:A:482:VAL:N	2.33	0.60
1:C:220:TRP:CE2	1:C:232:ILE:HD11	2.37	0.60
1:C:311:GLU:O	1:C:312:ILE:HG23	2.00	0.60
1:E:170:ILE:CG1	1:E:184:GLU:HG3	2.30	0.60
1:E:312:ILE:C	1:E:312:ILE:HD13	2.21	0.60
1:E:428:VAL:O	1:E:432:ILE:HG22	2.01	0.60
1:E:454:ILE:H	1:E:454:ILE:CD1	2.13	0.60
3:H:1:NAG:C6	3:H:2:NAG:H82	2.31	0.60
1:E:420:TRP:CD1	1:E:434:LYS:CA	2.84	0.60
1:E:450:GLY:CA	2:F:9:GLY:HA3	2.32	0.60
4:E:501:NAG:HN2	4:E:501:NAG:H5	1.66	0.60
1:E:84:GLU:HB3	1:E:90:PHE:HD1	1.67	0.60
1:E:299:TYR:HB2	1:E:334:LYS:CE	2.32	0.60
1:A:256:GLN:O	1:A:257:GLU:C	2.39	0.60
1:A:291:LYS:HD2	1:A:291:LYS:N	2.17	0.60
1:A:263:ALA:HB2	2:B:2:VAL:O	2.02	0.60
1:E:141:ILE:H	1:E:141:ILE:CD1	2.12	0.60
1:E:184:GLU:CB	1:E:286:ARG:HB2	2.27	0.60
1:E:321:VAL:HG13	1:E:321:VAL:O	2.02	0.60
2:F:56:THR:O	2:F:59:GLN:HB3	2.02	0.60
1:A:19:SER:CB	1:A:289:MET:HB2	2.32	0.59
1:C:2:ARG:C	1:C:4:ILE:H	2.06	0.59
1:C:231:TRP:N	1:C:231:TRP:CD1	2.69	0.59
1:C:394:LYS:H	1:C:394:LYS:CD	2.15	0.59
1:C:463:ILE:CG2	1:C:482:VAL:HG13	2.32	0.59
2:D:51:TYR:HA	2:D:60:ARG:NE	2.17	0.59
1:C:313:ALA:HB1	1:E:108:PHE:HB2	1.83	0.59
1:A:185:CYS:HB2	1:A:187:PRO:HD3	1.83	0.59
2:B:62:LEU:HD22	2:B:62:LEU:C	2.22	0.59
1:C:164:ILE:HD13	1:C:164:ILE:O	2.02	0.59
1:E:318:GLY:O	1:E:320:ILE:N	2.35	0.59
1:E:343:GLU:HG3	1:E:344:LYS:N	2.17	0.59
1:A:74:CYS:SG	1:A:75:PRO:HD2	2.42	0.59
1:A:220:TRP:O	1:A:231:TRP:HA	2.03	0.59
1:A:270:ILE:HG13	1:A:271:GLN:H	1.66	0.59
2:B:6:PRO:HG2	2:B:8:VAL:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:TYR:CD1	1:C:333:CYS:HA	2.37	0.59
2:D:33:GLU:HA	2:D:36:ILE:HD12	1.82	0.59
1:E:92:CYS:HA	1:E:115:THR:O	2.02	0.59
1:C:62:GLU:HG2	1:C:122:LYS:HD3	1.84	0.59
1:C:86:GLN:NE2	1:C:86:GLN:C	2.56	0.59
1:C:427:GLY:O	1:C:428:VAL:HB	2.01	0.59
1:E:57:ARG:NH1	1:E:214:LEU:HD22	2.18	0.59
1:E:414:ILE:CG2	2:F:15:ALA:HB2	2.31	0.59
2:F:55:THR:HA	2:F:60:ARG:HB2	1.85	0.59
1:C:194:ASN:HD22	1:C:194:ASN:N	1.99	0.59
1:C:220:TRP:CD1	1:C:220:TRP:C	2.76	0.59
1:E:9:ARG:CZ	1:E:11:PHE:HE2	2.16	0.59
1:E:113:ILE:HG23	1:E:113:ILE:O	2.01	0.59
1:A:411:ARG:HH21	1:A:411:ARG:CB	2.14	0.59
1:C:174:GLU:HA	1:C:180:THR:HG22	1.84	0.59
1:C:252:VAL:HG23	1:C:253:LEU:N	2.18	0.59
1:C:444:TYR:C	1:C:446:ALA:N	2.53	0.59
2:D:32:ILE:HD12	2:D:36:ILE:HD11	1.84	0.59
1:E:9:ARG:HH22	1:E:319:THR:HG21	1.66	0.59
1:E:348:LEU:O	1:E:350:ARG:NH2	2.35	0.59
1:E:420:TRP:CD1	1:E:434:LYS:N	2.71	0.59
1:A:226:THR:O	1:A:227:GLN:HB3	2.03	0.59
1:C:149:HIS:O	1:C:150:ALA:HB2	2.02	0.59
1:C:332:PRO:HB3	1:C:358:VAL:CB	2.28	0.59
1:E:99:ARG:HD2	1:E:103:ASN:CG	2.23	0.59
1:A:101:TRP:HE3	1:A:108:PHE:CE2	2.20	0.59
1:A:221:LEU:HD12	1:A:222:PRO:HD3	1.85	0.59
1:A:240:PHE:N	1:A:240:PHE:CD2	2.71	0.59
2:B:3:ALA:CB	2:B:4:LEU:HD22	2.32	0.59
2:B:62:LEU:HD13	2:B:62:LEU:C	2.22	0.59
1:C:22:ASP:HB3	1:C:421:ASP:O	2.03	0.59
2:D:65:ILE:CG2	2:D:66:LEU:N	2.66	0.59
1:E:123:LYS:H	1:E:123:LYS:CD	2.13	0.59
1:E:187:PRO:HG2	1:E:188:ARG:H	1.67	0.59
1:E:191:LEU:HD23	1:E:193:PHE:CZ	2.38	0.59
1:E:233:GLN:C	1:E:235:GLU:H	2.06	0.59
1:E:340:MET:HA	1:E:347:VAL:HA	1.85	0.59
1:A:19:SER:HB2	1:A:289:MET:H	1.67	0.59
1:A:27:HIS:CE1	1:A:279:PHE:HB3	2.37	0.59
1:C:207:LEU:HD13	1:C:278:LEU:HD11	1.84	0.59
1:C:349:GLY:HA3	1:C:372:PRO:HD3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LEU:HG	1:A:222:PRO:CD	2.33	0.58
1:C:51:LYS:C	1:C:53:PRO:HD3	2.23	0.58
1:C:318:GLY:N	1:C:393:LYS:HZ1	2.00	0.58
1:E:203:ASN:HB3	1:E:204:LYS:CE	2.33	0.58
2:F:32:ILE:CG1	2:F:33:GLU:N	2.65	0.58
1:A:20:TRP:CZ3	1:A:288:ARG:NE	2.68	0.58
1:A:416:GLY:O	1:A:417:ASP:C	2.40	0.58
1:C:65:LEU:HD21	1:C:252:VAL:CA	2.24	0.58
1:E:322:ILE:HD12	1:E:322:ILE:H	1.68	0.58
1:C:383:GLU:C	1:C:383:GLU:CD	2.62	0.58
1:C:451:VAL:CG1	1:C:456:LYS:N	2.65	0.58
2:F:35:TRP:HH2	2:F:42:PHE:HD2	1.52	0.58
1:A:45:LEU:HD13	1:A:45:LEU:C	2.23	0.58
1:A:73:ARG:HB2	1:A:80:PRO:HG3	1.85	0.58
1:A:208:VAL:HG11	1:A:212:TRP:CZ3	2.38	0.58
1:A:340:MET:HG2	1:A:347:VAL:CG1	2.33	0.58
1:C:46:ILE:O	1:C:47:GLU:HB2	2.02	0.58
2:D:37:LEU:O	2:D:40:PRO:HD3	2.03	0.58
1:A:139:ILE:CG2	1:A:162:ILE:HG23	2.33	0.58
1:A:219:PRO:HA	1:A:233:GLN:HB2	1.86	0.58
1:A:286:ARG:HH11	1:A:425:LEU:CD2	2.16	0.58
1:A:312:ILE:HG23	1:A:322:ILE:HB	1.86	0.58
1:A:464:THR:CB	1:A:482:VAL:HG11	2.20	0.58
2:B:65:ILE:O	2:B:68:THR:OG1	2.18	0.58
1:E:74:CYS:C	1:E:77:GLN:HE22	2.05	0.58
1:E:350:ARG:HH12	1:E:372:PRO:CD	2.13	0.58
2:F:19:TRP:CG	2:F:20:MET:N	2.71	0.58
1:A:60:CYS:SG	1:A:219:PRO:HG2	2.44	0.58
1:A:397:SER:O	1:A:400:GLN:HB2	2.03	0.58
2:B:1:SER:N	2:B:4:LEU:H	2.01	0.58
1:C:57:ARG:HH12	1:C:214:LEU:CD1	2.16	0.58
1:C:58:LYS:NZ	1:C:126:LYS:HG3	2.16	0.58
1:C:325:GLN:HB2	1:C:364:PRO:CG	2.29	0.58
1:E:52:GLN:HE21	1:E:134:ASN:HD21	1.50	0.58
1:E:490:GLY:O	1:E:492:MET:N	2.37	0.58
1:C:36:LYS:HA	1:C:36:LYS:HZ2	1.68	0.58
1:C:87:ASP:O	1:C:89:ARG:N	2.37	0.58
1:C:119:PHE:CD2	1:C:234:LYS:HD3	2.36	0.58
1:C:178:TYR:HA	1:C:293:GLN:HB2	1.84	0.58
1:C:282:HIS:O	1:C:282:HIS:ND1	2.37	0.58
2:D:50:ALA:O	2:D:53:ILE:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:SER:CB	1:E:248:GLN:NE2	2.67	0.58
1:E:143:PRO:HB3	1:E:175:LEU:HD21	1.84	0.58
1:A:119:PHE:CD2	1:A:120:THR:N	2.71	0.58
1:A:193:PHE:O	1:A:195:GLU:HG2	2.04	0.58
1:A:220:TRP:HD1	1:A:221:LEU:N	2.02	0.58
1:A:275:GLY:O	1:A:276:ASN:HB3	2.03	0.58
1:C:15:VAL:CG2	1:C:35:ALA:HB3	2.26	0.58
1:C:325:GLN:CB	1:C:364:PRO:HG3	2.33	0.58
1:C:383:GLU:C	1:C:385:GLY:H	2.07	0.58
1:C:406:MET:O	1:C:407:ARG:C	2.41	0.58
1:C:478:SER:O	1:C:482:VAL:HG23	2.02	0.58
1:E:339:ILE:CB	1:E:349:GLY:HA2	2.21	0.58
1:C:247:LYS:HA	1:C:247:LYS:HE3	1.85	0.58
1:E:61:ILE:O	1:E:255:SER:HA	2.04	0.58
1:E:132:PRO:HA	1:E:135:LEU:HD21	1.85	0.58
1:E:325:GLN:HE22	1:E:364:PRO:CD	2.15	0.58
2:F:67:LEU:O	2:F:70:VAL:HB	2.04	0.58
1:A:20:TRP:CH2	1:A:288:ARG:NH1	2.71	0.57
1:A:164:ILE:HD13	1:A:164:ILE:C	2.24	0.57
1:A:306:PHE:CD1	1:A:380:ILE:CG1	2.85	0.57
1:C:36:LYS:HA	1:C:36:LYS:NZ	2.19	0.57
1:E:210:ARG:O	1:E:212:TRP:N	2.37	0.57
1:E:299:TYR:HB2	1:E:334:LYS:HE3	1.86	0.57
1:A:232:ILE:O	1:A:233:GLN:HG2	2.04	0.57
1:C:185:CYS:O	1:C:187:PRO:HD3	2.04	0.57
1:C:320:ILE:HD12	1:C:321:VAL:N	2.19	0.57
1:E:99:ARG:HA	1:E:103:ASN:CG	2.24	0.57
1:E:304:GLY:O	1:E:305:LYS:CB	2.52	0.57
1:E:417:ASP:HA	1:E:437:HIS:CE1	2.39	0.57
1:E:442:ALA:O	1:E:446:ALA:HB2	2.05	0.57
1:E:475:LEU:HD23	1:E:476:SER:N	2.18	0.57
1:A:20:TRP:HB3	1:A:425:LEU:CD1	2.17	0.57
1:A:283:LEU:HD12	1:A:284:LYS:H	1.66	0.57
1:A:306:PHE:HD1	1:A:380:ILE:HG12	1.64	0.57
1:A:459:ILE:O	1:A:463:ILE:HG22	2.03	0.57
1:C:60:CYS:SG	1:C:219:PRO:HG2	2.44	0.57
1:E:3:CYS:HB2	1:E:42:ASP:HB3	1.86	0.57
1:E:233:GLN:HG3	1:E:236:THR:HG23	1.86	0.57
1:E:318:GLY:O	1:E:320:ILE:HG23	2.05	0.57
1:E:472:SER:O	1:E:474:SER:N	2.37	0.57
1:A:224:ALA:HB2	1:C:73:ARG:CZ	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:GLU:O	1:A:312:ILE:HG23	2.03	0.57
2:B:40:PRO:HG2	2:B:41:GLY:H	1.70	0.57
1:C:463:ILE:CG2	1:C:482:VAL:HG22	2.33	0.57
2:D:48:ILE:CG2	2:D:49:LEU:N	2.68	0.57
1:E:36:LYS:HA	1:E:36:LYS:CE	2.33	0.57
1:E:338:GLU:HB2	1:E:379:ILE:HD12	1.87	0.57
1:A:432:ILE:O	1:A:435:ALA:HB3	2.04	0.57
2:B:38:ARG:HA	2:B:38:ARG:NE	2.17	0.57
1:C:26:GLU:HB2	1:C:29:SER:OG	2.03	0.57
1:C:34:MET:CB	1:C:40:THR:HA	2.34	0.57
1:C:108:PHE:O	1:C:110:LYS:N	2.36	0.57
1:C:318:GLY:HA3	1:C:393:LYS:NZ	2.19	0.57
2:D:50:ALA:O	2:D:53:ILE:HG22	2.04	0.57
1:E:463:ILE:CG2	1:E:464:THR:N	2.67	0.57
1:C:20:TRP:HA	1:C:287:LEU:O	2.05	0.57
1:C:201:MET:O	1:C:202:GLU:HB3	2.04	0.57
1:E:19:SER:CB	1:E:289:MET:HB2	2.35	0.57
1:E:36:LYS:HA	1:E:36:LYS:HZ3	1.66	0.57
1:E:365:VAL:HG23	1:E:366:ASN:N	2.19	0.57
1:E:383:GLU:CB	1:E:384:PRO:CD	2.81	0.57
1:A:19:SER:CA	1:A:289:MET:HB2	2.34	0.57
1:A:92:CYS:HA	1:A:115:THR:O	2.04	0.57
1:A:232:ILE:O	1:A:233:GLN:CB	2.53	0.57
1:A:321:VAL:HG12	1:A:368:GLU:HA	1.87	0.57
1:A:337:PHE:CD1	1:A:337:PHE:C	2.77	0.57
1:A:486:THR:O	1:A:489:LEU:HB2	2.05	0.57
1:E:74:CYS:SG	1:E:106:GLY:HA3	2.45	0.57
1:E:188:ARG:HA	1:E:188:ARG:NH2	2.19	0.57
1:E:191:LEU:O	1:E:192:ASP:HB2	2.05	0.57
1:E:345:ARG:HB3	1:E:347:VAL:HG13	1.85	0.57
1:A:99:ARG:NH1	1:A:105:CYS:SG	2.77	0.57
1:A:159:GLY:HA2	1:A:175:LEU:HD11	1.86	0.57
1:A:323:ARG:HD2	1:A:364:PRO:HB2	1.84	0.57
1:C:62:GLU:HB3	1:C:122:LYS:O	2.05	0.57
1:C:163:LYS:HE2	1:C:163:LYS:HA	1.86	0.57
1:C:434:LYS:O	1:C:436:LEU:N	2.38	0.57
1:A:306:PHE:HD2	1:A:325:GLN:O	1.86	0.57
1:A:427:GLY:H	1:A:431:SER:CB	2.17	0.57
1:A:492:MET:HA	1:A:492:MET:CE	2.35	0.57
1:C:222:PRO:HG2	1:C:224:ALA:H	1.68	0.57
1:C:288:ARG:HB2	1:C:288:ARG:HH21	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:451:VAL:CG1	1:C:452:SER:H	2.14	0.57
1:E:258:GLY:O	1:E:261:HIS:N	2.38	0.57
1:E:277:LEU:O	1:E:279:PHE:CD2	2.56	0.57
1:E:443:ILE:C	1:E:445:GLY:H	2.06	0.57
1:E:453:TRP:HE3	1:E:454:ILE:HA	1.69	0.57
1:C:57:ARG:NH2	1:C:214:LEU:HD22	2.20	0.57
1:E:126:LYS:HB3	1:E:128:LYS:HE2	1.86	0.57
1:A:193:PHE:O	1:A:194:ASN:C	2.41	0.56
1:A:197:VAL:O	1:A:208:VAL:HG23	2.05	0.56
1:C:173:ALA:O	1:C:180:THR:HA	2.04	0.56
1:C:385:GLY:O	1:C:387:LEU:N	2.37	0.56
1:E:42:ASP:HB2	1:E:142:THR:CG2	2.34	0.56
1:E:42:ASP:O	1:E:141:ILE:HA	2.05	0.56
1:E:178:TYR:O	1:E:293:GLN:N	2.37	0.56
1:E:265:THR:HB	2:F:20:MET:HB2	1.87	0.56
1:E:409:ALA:O	1:E:411:ARG:N	2.38	0.56
1:A:74:CYS:O	1:A:77:GLN:HG3	2.06	0.56
2:B:31:ARG:HD2	2:B:32:ILE:N	2.20	0.56
1:C:19:SER:O	1:C:288:ARG:HA	2.05	0.56
1:C:35:ALA:O	1:C:36:LYS:C	2.42	0.56
1:C:141:ILE:O	1:C:142:THR:HB	2.05	0.56
1:C:166:PRO:HD3	1:C:187:PRO:HG3	1.87	0.56
1:C:332:PRO:HG2	1:C:360:GLU:CA	2.34	0.56
1:E:34:MET:O	1:E:34:MET:SD	2.63	0.56
1:A:9:ARG:HD2	1:A:10:ASP:H	1.68	0.56
1:A:56:LEU:CD2	1:A:210:ARG:HH12	2.18	0.56
1:A:70:THR:HB	1:A:115:THR:HG22	1.86	0.56
1:A:99:ARG:HG3	1:A:99:ARG:O	2.05	0.56
1:A:339:ILE:HD13	1:A:378:ILE:HA	1.86	0.56
1:A:414:ILE:HG22	1:A:415:LEU:CD2	2.36	0.56
2:B:33:GLU:HA	2:B:36:ILE:HG22	1.87	0.56
1:C:58:LYS:CE	1:C:126:LYS:HZ3	2.18	0.56
1:C:59:TYR:H	1:C:125:MET:HB3	1.69	0.56
1:C:105:CYS:SG	1:C:106:GLY:N	2.79	0.56
1:C:141:ILE:HD13	1:C:141:ILE:O	2.06	0.56
1:C:295:LYS:NZ	1:C:295:LYS:HB3	2.21	0.56
1:C:384:PRO:HB2	1:C:386:GLN:NE2	2.20	0.56
2:D:17:GLU:HG3	2:D:17:GLU:O	2.05	0.56
1:E:38:LYS:HB3	1:E:292:LEU:HD23	1.88	0.56
1:E:56:LEU:O	1:E:57:ARG:CB	2.53	0.56
1:E:125:MET:HG2	1:E:201:MET:SD	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:LYS:O	1:E:205:ALA:HB2	2.05	0.56
1:E:383:GLU:HG3	1:E:384:PRO:HD3	1.87	0.56
1:E:492:MET:HA	1:E:492:MET:CE	2.34	0.56
1:A:56:LEU:HD22	1:A:210:ARG:HH12	1.69	0.56
1:A:140:VAL:CG1	1:A:161:GLU:HG2	2.35	0.56
2:B:47:ALA:C	2:B:50:ALA:HB3	2.24	0.56
1:C:36:LYS:HD3	1:C:37:ASN:H	1.70	0.56
1:C:173:ALA:HB3	1:C:181:VAL:HG12	1.87	0.56
1:C:294:LEU:N	1:C:294:LEU:CD1	2.68	0.56
1:E:63:ALA:HA	1:E:121:CYS:HA	1.86	0.56
1:E:412:MET:HA	1:E:419:ALA:HB1	1.85	0.56
1:A:3:CYS:HA	1:A:30:CYS:SG	2.45	0.56
1:A:125:MET:HB3	1:A:201:MET:HE3	1.88	0.56
1:A:318:GLY:O	1:A:370:GLU:HA	2.05	0.56
1:A:336:PRO:HB2	1:A:381:GLY:O	2.05	0.56
1:C:110:LYS:HD2	1:C:110:LYS:O	2.05	0.56
1:C:206:TRP:NE1	2:D:19:TRP:CE3	2.73	0.56
1:C:339:ILE:O	1:C:347:VAL:HA	2.05	0.56
1:C:373:PHE:CB	1:C:396:SER:HB3	2.36	0.56
2:D:42:PHE:O	2:D:45:MET:HB3	2.04	0.56
1:E:290:ASP:O	1:E:292:LEU:N	2.39	0.56
1:A:165:THR:O	1:A:167:GLN:N	2.39	0.56
1:A:205:ALA:HB3	1:A:271:GLN:O	2.06	0.56
1:C:27:HIS:CG	1:C:45:LEU:HD12	2.40	0.56
1:C:176:THR:O	1:C:178:TYR:N	2.38	0.56
1:C:260:MET:O	1:C:263:ALA:HB3	2.05	0.56
2:D:66:LEU:O	2:D:70:VAL:HG13	2.06	0.56
1:E:20:TRP:CE3	1:E:425:LEU:HB2	2.40	0.56
1:E:207:LEU:HD11	1:E:268:THR:HG23	1.85	0.56
1:E:256:GLN:O	1:E:257:GLU:C	2.42	0.56
2:F:40:PRO:O	2:F:44:ILE:HG12	2.06	0.56
2:F:69:ALA:O	2:F:71:ALA:N	2.38	0.56
1:A:1:MET:O	1:A:3:CYS:N	2.38	0.56
1:A:383:GLU:CG	1:A:384:PRO:HD3	2.35	0.56
1:C:60:CYS:HB3	1:C:231:TRP:CZ3	2.41	0.56
1:E:73:ARG:HG2	1:E:80:PRO:HG3	1.87	0.56
1:E:260:MET:HA	1:E:263:ALA:HB2	1.88	0.56
1:E:262:THR:O	1:E:262:THR:HG22	2.06	0.56
1:E:296:GLY:C	1:E:298:SER:H	2.08	0.56
1:E:373:PHE:HB3	1:E:397:SER:H	1.70	0.56
2:F:64:PHE:O	2:F:65:ILE:C	2.42	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ALA:O	1:A:128:LYS:HA	2.06	0.56
1:A:312:ILE:HG13	1:A:391:TRP:CD1	2.41	0.56
1:A:315:THR:HG22	1:A:316:GLN:N	2.21	0.56
1:A:376:SER:O	1:A:390:ASN:ND2	2.39	0.56
1:A:435:ALA:O	1:A:438:GLN:HB3	2.06	0.56
1:C:434:LYS:HD2	1:C:435:ALA:N	2.20	0.56
1:C:479:LEU:C	1:C:479:LEU:HD12	2.26	0.56
1:E:84:GLU:C	1:E:86:GLN:H	2.09	0.56
1:E:312:ILE:HG23	1:E:313:ALA:N	2.20	0.56
1:A:2:ARG:HH22	1:A:44:GLU:HG2	1.71	0.56
1:C:20:TRP:CD2	1:C:286:ARG:NH1	2.73	0.56
1:C:210:ARG:HH21	1:C:210:ARG:CG	2.19	0.56
1:C:240:PHE:HD1	1:C:250:VAL:HG12	1.71	0.56
1:C:343:GLU:C	1:C:345:ARG:NH2	2.59	0.56
1:E:475:LEU:O	1:E:478:SER:N	2.39	0.56
1:A:2:ARG:NH1	1:A:44:GLU:HG2	2.16	0.56
1:A:9:ARG:CG	1:A:10:ASP:N	2.69	0.56
1:C:99:ARG:NH2	1:C:103:ASN:HD22	2.04	0.56
1:C:322:ILE:O	1:C:366:ASN:HA	2.06	0.56
1:C:430:THR:CG2	1:C:431:SER:H	2.10	0.56
1:C:454:ILE:HG12	1:C:455:MET:N	2.20	0.56
2:D:19:TRP:CD1	2:D:20:MET:SD	2.99	0.56
1:E:2:ARG:HB3	1:E:142:THR:HG21	1.87	0.56
1:E:107:LEU:HD12	1:E:107:LEU:N	2.21	0.56
1:E:196:MET:CE	1:E:209:HIS:HB3	2.36	0.56
1:E:420:TRP:C	1:E:422:PHE:H	2.10	0.56
2:F:38:ARG:HA	2:F:38:ARG:NE	2.20	0.56
1:A:27:HIS:CD2	1:A:280:THR:N	2.74	0.55
1:A:205:ALA:CA	1:A:206:TRP:CE3	2.89	0.55
1:A:270:ILE:HG23	1:A:271:GLN:O	2.05	0.55
1:C:233:GLN:O	1:C:235:GLU:N	2.39	0.55
1:C:342:LEU:HA	1:C:377:TYR:CD1	2.40	0.55
1:C:363:SER:O	1:C:365:VAL:N	2.39	0.55
1:C:391:TRP:HZ3	1:C:393:LYS:CB	2.15	0.55
1:C:479:LEU:HD12	1:C:480:VAL:N	2.21	0.55
1:E:61:ILE:HD12	1:E:123:LYS:O	2.05	0.55
1:E:471:ARG:O	1:E:472:SER:HB3	2.06	0.55
1:A:409:ALA:HA	1:A:412:MET:HG3	1.88	0.55
1:C:359:THR:HG22	1:C:360:GLU:HG3	1.87	0.55
1:C:434:LYS:O	1:C:438:GLN:HB2	2.06	0.55
1:E:379:ILE:HG12	1:E:380:ILE:N	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:SER:OG	1:A:30:CYS:N	2.40	0.55
1:A:280:THR:HG21	2:B:14:THR:HG21	1.87	0.55
1:A:483:GLY:O	1:A:485:VAL:N	2.39	0.55
1:C:252:VAL:HG23	1:C:253:LEU:H	1.72	0.55
2:D:59:GLN:O	2:D:60:ARG:C	2.44	0.55
1:E:246:LYS:O	1:E:247:LYS:O	2.24	0.55
2:F:11:GLY:C	2:F:12:LEU:HD22	2.26	0.55
1:A:74:CYS:O	1:A:75:PRO:C	2.44	0.55
1:C:85:GLU:HA	1:C:92:CYS:SG	2.46	0.55
1:C:178:TYR:HE2	1:C:295:LYS:NZ	2.04	0.55
1:E:12:VAL:HB	1:E:33:THR:OG1	2.07	0.55
1:E:94:HIS:ND1	1:E:114:VAL:HG21	2.20	0.55
1:E:153:ASN:CG	3:I:1:NAG:HN2	2.10	0.55
1:A:267:ALA:HB2	2:B:7:HIS:CG	2.41	0.55
1:A:318:GLY:O	1:A:369:ALA:O	2.25	0.55
1:A:321:VAL:O	1:A:321:VAL:HG23	2.06	0.55
1:A:461:VAL:O	1:A:462:ILE:C	2.43	0.55
2:B:49:LEU:O	2:B:53:ILE:HG22	2.06	0.55
1:E:9:ARG:HB2	1:E:30:CYS:H	1.72	0.55
1:E:258:GLY:O	1:E:259:ALA:C	2.44	0.55
1:E:265:THR:HA	2:F:19:TRP:CD1	2.33	0.55
1:E:276:ASN:C	1:E:277:LEU:HD12	2.26	0.55
1:E:373:PHE:CD2	1:E:373:PHE:N	2.75	0.55
1:A:58:LYS:HB2	1:A:58:LYS:NZ	2.21	0.55
1:A:76:THR:O	1:A:77:GLN:C	2.45	0.55
1:A:93:LYS:HE2	1:A:240:PHE:CD1	2.42	0.55
1:A:315:THR:O	1:A:317:HIS:N	2.39	0.55
1:A:318:GLY:N	1:A:393:LYS:HE3	2.20	0.55
1:C:237:LEU:O	1:C:238:VAL:O	2.24	0.55
1:E:25:LEU:HD12	1:E:25:LEU:O	2.05	0.55
1:E:45:LEU:HD23	1:E:45:LEU:C	2.27	0.55
1:E:88:LYS:HA	1:E:88:LYS:HZ1	1.72	0.55
1:E:428:VAL:HG23	1:E:429:PHE:N	2.19	0.55
1:A:199:LEU:HD12	1:A:200:GLN:N	2.22	0.55
1:A:479:LEU:O	1:A:480:VAL:C	2.44	0.55
2:B:3:ALA:C	2:B:4:LEU:HD22	2.27	0.55
1:C:226:THR:O	1:C:227:GLN:HB2	2.07	0.55
1:C:388:LYS:O	1:C:389:LEU:HG	2.07	0.55
1:E:137:TYR:CD1	1:E:283:LEU:HD22	2.41	0.55
1:E:305:LYS:HB3	1:E:327:GLU:O	2.06	0.55
1:E:339:ILE:HG22	1:E:339:ILE:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:420:TRP:HB2	1:E:434:LYS:HG3	1.88	0.55
1:A:232:ILE:O	1:A:233:GLN:HB2	2.06	0.55
1:A:246:LYS:NZ	1:A:246:LYS:HB2	2.21	0.55
1:A:331:SER:OG	1:A:332:PRO:HD2	2.07	0.55
1:A:353:THR:O	1:A:353:THR:HG22	2.06	0.55
1:C:309:VAL:O	1:C:310:LYS:HB2	2.07	0.55
2:D:45:MET:O	2:D:48:ILE:HB	2.06	0.55
1:E:260:MET:O	1:E:263:ALA:N	2.38	0.55
1:E:305:LYS:HD2	1:E:327:GLU:N	2.22	0.55
1:A:165:THR:C	1:A:167:GLN:H	2.10	0.55
1:A:342:LEU:H	1:A:342:LEU:HD12	1.71	0.55
1:C:15:VAL:HG23	1:C:35:ALA:CB	2.28	0.55
1:C:157:LYS:N	1:C:157:LYS:HD2	2.21	0.55
1:A:373:PHE:CD1	1:A:374:GLY:N	2.75	0.55
1:C:36:LYS:CD	1:C:37:ASN:ND2	2.70	0.55
1:C:238:VAL:O	1:C:238:VAL:HG13	2.07	0.55
1:C:317:HIS:ND1	1:C:400:GLN:HG2	2.21	0.55
1:E:12:VAL:O	1:E:34:MET:HE3	2.06	0.55
1:E:95:SER:HB2	1:E:248:GLN:NE2	2.23	0.55
1:E:142:THR:HA	1:E:159:GLY:HA3	1.89	0.55
1:E:381:GLY:O	1:E:382:VAL:HG13	2.06	0.55
1:E:458:LEU:O	1:E:459:ILE:C	2.44	0.55
1:C:132:PRO:HB2	1:C:188:ARG:CZ	2.36	0.54
1:C:332:PRO:HG2	1:C:359:THR:C	2.27	0.54
1:C:489:LEU:O	1:C:493:VAL:HG23	2.07	0.54
1:E:219:PRO:HB2	1:E:231:TRP:CE3	2.42	0.54
1:A:232:ILE:HG22	1:A:233:GLN:HE21	1.72	0.54
1:A:478:SER:O	1:A:482:VAL:HG23	2.07	0.54
1:C:131:GLN:HA	1:C:194:ASN:OD1	2.07	0.54
1:C:339:ILE:HD12	1:C:349:GLY:H	1.72	0.54
2:D:49:LEU:O	2:D:53:ILE:HB	2.07	0.54
1:E:1:MET:HA	1:E:151:VAL:CA	2.37	0.54
1:E:15:VAL:HG13	1:E:16:SER:N	2.21	0.54
1:E:359:THR:HG22	1:E:360:GLU:N	2.21	0.54
1:E:367:ILE:CD1	1:E:368:GLU:N	2.58	0.54
1:E:373:PHE:HD2	1:E:373:PHE:N	2.05	0.54
1:A:1:MET:C	1:A:3:CYS:N	2.60	0.54
1:A:316:GLN:O	1:A:317:HIS:ND1	2.39	0.54
1:A:489:LEU:O	1:A:492:MET:N	2.39	0.54
1:C:61:ILE:HD12	1:C:257:GLU:HG2	1.89	0.54
1:C:143:PRO:HB3	1:C:178:TYR:HE1	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:405:THR:HG22	1:C:406:MET:N	2.22	0.54
2:D:61:ALA:O	2:D:64:PHE:HB3	2.07	0.54
1:E:271:GLN:NE2	1:E:279:PHE:CE2	2.76	0.54
1:C:6:ILE:O	1:C:6:ILE:CG1	2.55	0.54
1:C:59:TYR:HD2	1:C:218:LEU:HB2	1.72	0.54
1:C:257:GLU:O	1:C:260:MET:HB3	2.07	0.54
1:C:282:HIS:HD2	1:C:415:LEU:HD12	1.72	0.54
1:C:353:THR:O	1:C:355:ASN:N	2.40	0.54
1:E:386:GLN:C	1:E:387:LEU:HD22	2.27	0.54
1:A:25:LEU:CD1	1:A:45:LEU:HB2	2.36	0.54
1:A:459:ILE:HA	1:A:462:ILE:CG2	2.37	0.54
1:C:327:GLU:OE1	1:C:327:GLU:HA	2.07	0.54
1:C:427:GLY:O	1:C:428:VAL:CB	2.55	0.54
1:C:452:SER:CA	1:C:494:GLN:HE22	2.20	0.54
1:E:21:VAL:HG23	1:E:424:SER:OG	2.06	0.54
1:E:168:SER:O	1:E:169:SER:CB	2.55	0.54
1:E:219:PRO:HA	1:E:233:GLN:CB	2.37	0.54
1:E:242:ASN:HB2	1:E:248:GLN:HB3	1.89	0.54
1:E:442:ALA:O	1:E:446:ALA:CB	2.56	0.54
1:A:9:ARG:HB3	1:A:316:GLN:NE2	2.22	0.54
1:C:288:ARG:HB2	1:C:288:ARG:NH2	2.22	0.54
1:C:288:ARG:HH21	1:C:288:ARG:CB	2.21	0.54
1:C:352:ILE:HG23	1:C:368:GLU:O	2.08	0.54
2:D:39:HIS:O	2:D:41:GLY:N	2.41	0.54
1:E:61:ILE:HG22	1:E:256:GLN:N	2.20	0.54
1:E:149:HIS:CD2	3:I:1:NAG:H61	2.42	0.54
1:E:311:GLU:HG2	1:E:312:ILE:N	2.23	0.54
1:E:448:PHE:CZ	1:E:459:ILE:HG21	2.42	0.54
3:H:1:NAG:H62	3:H:2:NAG:H82	1.89	0.54
1:A:267:ALA:HB2	2:B:7:HIS:CB	2.38	0.54
1:C:166:PRO:CD	1:C:187:PRO:HG3	2.38	0.54
1:C:459:ILE:O	1:C:463:ILE:HG22	2.08	0.54
2:D:66:LEU:O	2:D:69:ALA:HB3	2.07	0.54
1:E:204:LYS:N	1:E:204:LYS:CE	2.69	0.54
1:E:306:PHE:CE2	1:E:335:ILE:HD11	2.41	0.54
1:C:383:GLU:HB3	1:C:384:PRO:HD3	1.89	0.54
1:C:446:ALA:O	1:C:447:ALA:HB2	2.07	0.54
1:C:470:SER:N	1:C:475:LEU:HD12	2.17	0.54
1:A:91:VAL:CG1	1:A:117:ALA:HB3	2.38	0.54
1:A:340:MET:SD	1:A:379:ILE:HG21	2.48	0.54
1:C:20:TRP:CE2	1:C:286:ARG:NH1	2.76	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:VAL:HG12	1:C:161:GLU:HA	1.90	0.54
1:C:460:GLY:O	1:C:463:ILE:HG22	2.07	0.54
1:C:483:GLY:C	1:C:485:VAL:H	2.11	0.54
1:E:303:THR:HG23	1:E:304:GLY:H	1.73	0.54
1:E:432:ILE:HG23	1:E:433:GLY:N	2.23	0.54
1:A:269:GLU:CG	1:A:270:ILE:N	2.70	0.54
1:A:322:ILE:CD1	1:A:323:ARG:N	2.69	0.54
1:A:450:GLY:HA2	2:B:9:GLY:C	2.29	0.54
1:C:4:ILE:O	1:C:4:ILE:HG23	2.07	0.54
1:C:83:ASN:O	1:C:85:GLU:N	2.40	0.54
1:C:269:GLU:C	1:C:270:ILE:HG22	2.29	0.54
1:E:46:ILE:HG12	1:E:47:GLU:N	2.22	0.54
1:E:123:LYS:HZ3	1:E:123:LYS:N	2.04	0.54
2:F:48:ILE:O	2:F:51:TYR:HB3	2.08	0.54
1:A:92:CYS:SG	1:A:116:CYS:HA	2.48	0.53
1:A:443:ILE:HG12	1:A:444:TYR:N	2.20	0.53
1:A:465:TRP:C	1:A:467:GLY:N	2.54	0.53
1:C:200:GLN:HG2	1:C:201:MET:H	1.72	0.53
1:C:221:LEU:HG	1:C:231:TRP:CE3	2.44	0.53
1:C:233:GLN:C	1:C:235:GLU:H	2.11	0.53
1:C:352:ILE:O	1:C:352:ILE:HG13	2.07	0.53
1:C:434:LYS:HZ3	1:C:435:ALA:H	1.56	0.53
1:E:260:MET:HA	1:E:263:ALA:CB	2.38	0.53
1:E:299:TYR:N	1:E:334:LYS:HE3	2.24	0.53
1:E:306:PHE:HE2	1:E:335:ILE:HD11	1.72	0.53
1:A:36:LYS:O	1:A:37:ASN:CB	2.55	0.53
1:A:427:GLY:O	1:A:428:VAL:HB	2.08	0.53
2:B:61:ALA:O	2:B:65:ILE:HG22	2.08	0.53
1:C:379:ILE:HD12	1:C:380:ILE:HA	1.89	0.53
1:C:457:ILE:HG13	1:C:458:LEU:N	2.22	0.53
1:E:17:GLY:O	1:E:20:TRP:HB2	2.09	0.53
1:E:19:SER:O	1:E:287:LEU:O	2.26	0.53
1:E:53:PRO:HA	1:E:129:VAL:O	2.08	0.53
1:E:402:ILE:O	1:E:405:THR:N	2.41	0.53
1:E:429:PHE:O	1:E:430:THR:C	2.46	0.53
2:F:32:ILE:O	2:F:33:GLU:C	2.46	0.53
1:A:194:ASN:O	1:A:195:GLU:HG2	2.08	0.53
1:A:391:TRP:O	1:A:392:PHE:CB	2.56	0.53
1:A:481:LEU:O	1:A:481:LEU:HD13	2.08	0.53
1:C:96:MET:HB3	1:C:110:LYS:CG	2.37	0.53
1:C:164:ILE:HD13	1:C:164:ILE:C	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:ARG:HH21	1:C:210:ARG:HG2	1.71	0.53
1:C:434:LYS:NZ	1:C:434:LYS:HB3	2.23	0.53
2:D:32:ILE:O	2:D:36:ILE:HG13	2.07	0.53
1:A:220:TRP:CD1	1:A:221:LEU:N	2.75	0.53
1:A:246:LYS:O	1:A:247:LYS:C	2.47	0.53
1:A:318:GLY:C	1:A:320:ILE:H	2.12	0.53
1:A:342:LEU:HD12	1:A:342:LEU:N	2.24	0.53
1:C:204:LYS:HB3	1:C:206:TRP:CH2	2.43	0.53
1:E:380:ILE:N	1:E:380:ILE:CD1	2.72	0.53
1:E:436:LEU:O	1:E:439:VAL:N	2.40	0.53
1:A:73:ARG:N	1:A:80:PRO:HG3	2.23	0.53
1:A:76:THR:O	1:A:78:GLY:N	2.41	0.53
1:A:495:ALA:O	2:B:18:THR:HG23	2.08	0.53
2:D:32:ILE:HD12	2:D:32:ILE:C	2.29	0.53
2:D:56:THR:OG1	2:D:59:GLN:HG3	2.08	0.53
1:E:62:GLU:HB3	1:E:123:LYS:HD2	1.89	0.53
1:A:442:ALA:O	1:A:446:ALA:O	2.26	0.53
1:C:107:LEU:O	1:C:108:PHE:CB	2.56	0.53
1:E:38:LYS:HD3	1:E:38:LYS:N	2.24	0.53
1:E:125:MET:O	1:E:126:LYS:CG	2.57	0.53
1:E:311:GLU:O	1:E:312:ILE:HB	2.09	0.53
1:E:407:ARG:O	1:E:409:ALA:N	2.41	0.53
1:E:436:LEU:HD13	1:E:436:LEU:C	2.28	0.53
1:E:470:SER:CB	1:E:475:LEU:HB3	2.37	0.53
1:A:25:LEU:HD23	1:A:25:LEU:N	2.23	0.53
1:A:213:PHE:HA	1:A:216:LEU:HD22	1.90	0.53
1:A:479:LEU:HD23	1:A:479:LEU:C	2.29	0.53
1:C:200:GLN:HB2	1:C:272:MET:SD	2.49	0.53
2:D:50:ALA:O	2:D:51:TYR:C	2.47	0.53
1:E:67:ASN:HB2	1:E:118:MET:CE	2.39	0.53
1:A:144:HIS:HB2	1:A:353:THR:HG23	1.90	0.53
1:A:173:ALA:HB3	1:A:181:VAL:CB	2.33	0.53
1:A:384:PRO:HD2	1:A:386:GLN:HE22	1.70	0.53
2:B:66:LEU:O	2:B:67:LEU:C	2.48	0.53
1:C:25:LEU:HD22	1:C:139:ILE:HD11	1.90	0.53
1:C:320:ILE:HD12	1:C:320:ILE:C	2.29	0.53
1:C:340:MET:N	1:C:340:MET:SD	2.82	0.53
1:C:345:ARG:N	1:C:345:ARG:CD	2.70	0.53
2:D:38:ARG:C	2:D:40:PRO:HD3	2.29	0.53
1:E:201:MET:HB2	1:E:206:TRP:HZ3	1.74	0.53
1:E:361:LYS:HG2	1:E:362:ASP:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:463:ILE:CG2	1:E:482:VAL:HG22	2.36	0.53
1:E:485:VAL:O	1:E:486:THR:C	2.46	0.53
1:A:224:ALA:O	1:A:225:ASP:C	2.47	0.53
1:C:53:PRO:CB	1:C:130:VAL:HA	2.37	0.53
1:C:204:LYS:CB	1:C:206:TRP:CH2	2.92	0.53
1:E:133:GLU:O	1:E:134:ASN:CB	2.54	0.53
1:E:134:ASN:N	1:E:135:LEU:HD23	2.23	0.53
1:E:427:GLY:O	1:E:428:VAL:C	2.47	0.53
1:A:22:ASP:CB	1:A:424:SER:HA	2.39	0.53
1:A:277:LEU:HG	1:A:279:PHE:CE2	2.42	0.53
1:E:137:TYR:N	1:E:137:TYR:CD2	2.76	0.53
1:E:196:MET:HG2	1:E:207:LEU:HD23	1.90	0.53
1:E:351:LEU:HA	1:E:369:ALA:HB2	1.91	0.53
1:E:359:THR:HG22	1:E:360:GLU:H	1.71	0.53
1:E:439:VAL:O	1:E:442:ALA:N	2.42	0.53
2:F:1:SER:C	2:F:3:ALA:N	2.55	0.53
1:A:364:PRO:C	1:A:365:VAL:HG13	2.30	0.52
1:A:466:ILE:O	1:A:466:ILE:HD13	2.07	0.52
1:C:197:VAL:HG23	1:C:210:ARG:CA	2.38	0.52
1:C:233:GLN:C	1:C:235:GLU:N	2.62	0.52
1:C:448:PHE:CG	1:C:448:PHE:O	2.62	0.52
1:E:51:LYS:HZ2	1:E:136:GLU:HB3	1.74	0.52
1:E:60:CYS:HB3	1:E:219:PRO:HG2	1.91	0.52
1:E:339:ILE:H	1:E:349:GLY:HA3	1.73	0.52
1:E:428:VAL:HG23	1:E:429:PHE:HD1	1.75	0.52
1:A:62:GLU:HG2	1:A:122:LYS:HB3	1.90	0.52
1:A:378:ILE:C	1:A:378:ILE:HD12	2.28	0.52
1:A:475:LEU:O	1:A:476:SER:C	2.46	0.52
1:E:132:PRO:C	1:E:135:LEU:HD21	2.30	0.52
1:E:218:LEU:CB	1:E:219:PRO:CD	2.87	0.52
1:A:27:HIS:CG	1:A:280:THR:H	2.26	0.52
1:A:86:GLN:HA	1:C:230:ASN:HD22	1.73	0.52
1:A:131:GLN:O	1:A:132:PRO:C	2.47	0.52
1:A:238:VAL:O	1:A:238:VAL:HG23	2.08	0.52
1:A:340:MET:HE2	1:A:345:ARG:HG3	1.90	0.52
1:A:453:TRP:HE3	1:A:454:ILE:CA	2.22	0.52
1:A:485:VAL:O	1:A:489:LEU:HG	2.09	0.52
1:C:57:ARG:O	1:C:58:LYS:CB	2.58	0.52
1:C:209:HIS:ND1	2:D:10:MET:CG	2.72	0.52
1:C:246:LYS:HD2	1:C:246:LYS:C	2.30	0.52
1:C:341:ASP:O	1:C:342:LEU:C	2.48	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:LEU:HD23	1:C:415:LEU:N	2.24	0.52
1:E:144:HIS:O	1:E:145:SER:O	2.27	0.52
1:E:233:GLN:CG	1:E:236:THR:HG23	2.40	0.52
2:F:6:PRO:O	2:F:7:HIS:C	2.48	0.52
1:A:121:CYS:HG	1:A:231:TRP:HZ2	1.55	0.52
1:A:391:TRP:HZ3	1:A:393:LYS:HA	1.70	0.52
1:A:482:VAL:HG12	1:A:487:LEU:HD23	1.90	0.52
2:B:32:ILE:HG13	2:B:33:GLU:N	2.25	0.52
1:C:212:TRP:CE2	1:C:216:LEU:HD21	2.45	0.52
1:C:296:GLY:O	1:C:299:TYR:HB2	2.09	0.52
1:C:386:GLN:O	1:C:387:LEU:HG	2.09	0.52
1:C:420:TRP:CB	1:C:434:LYS:HB2	2.39	0.52
2:D:62:LEU:O	2:D:65:ILE:HG22	2.10	0.52
1:E:140:VAL:O	1:E:140:VAL:CG2	2.56	0.52
1:E:351:LEU:HD12	1:E:353:THR:N	2.24	0.52
1:A:37:ASN:O	1:A:38:LYS:HB2	2.09	0.52
1:A:71:ASP:HB2	1:A:82:LEU:HD22	1.89	0.52
1:A:191:LEU:O	1:A:192:ASP:CB	2.57	0.52
1:A:224:ALA:CB	1:C:73:ARG:NH1	2.72	0.52
1:A:295:LYS:HD2	1:A:296:GLY:N	2.22	0.52
1:A:411:ARG:CB	1:A:411:ARG:NH2	2.72	0.52
1:C:165:THR:C	1:C:167:GLN:N	2.62	0.52
1:C:194:ASN:N	1:C:194:ASN:ND2	2.57	0.52
1:C:411:ARG:O	1:C:415:LEU:HD23	2.09	0.52
1:E:7:SER:O	1:E:9:ARG:N	2.42	0.52
1:E:91:VAL:HG12	1:E:92:CYS:N	2.25	0.52
1:E:381:GLY:C	1:E:382:VAL:HG22	2.30	0.52
1:E:414:ILE:HG21	2:F:15:ALA:CB	2.39	0.52
2:F:60:ARG:O	2:F:61:ALA:C	2.47	0.52
1:A:390:ASN:HD22	1:A:390:ASN:C	2.08	0.52
1:A:463:ILE:HG23	1:A:464:THR:N	2.25	0.52
1:C:432:ILE:O	1:C:433:GLY:C	2.47	0.52
2:D:62:LEU:O	2:D:66:LEU:HG	2.09	0.52
1:E:168:SER:O	1:E:169:SER:HB3	2.09	0.52
1:E:209:HIS:NE2	2:F:10:MET:HB3	2.25	0.52
1:A:139:ILE:HD13	1:A:140:VAL:N	2.24	0.52
1:C:194:ASN:HD22	1:C:194:ASN:H	1.56	0.52
1:C:458:LEU:C	1:C:458:LEU:HD13	2.30	0.52
1:E:2:ARG:NE	1:E:2:ARG:HA	2.23	0.52
1:E:60:CYS:HB3	1:E:219:PRO:CG	2.39	0.52
1:E:338:GLU:HB2	1:E:379:ILE:CD1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ASP:H	1:A:424:SER:CB	2.23	0.52
1:A:356:PRO:O	1:A:357:ILE:CB	2.58	0.52
1:A:372:PRO:CG	1:A:376:SER:HB2	2.40	0.52
1:A:444:TYR:N	1:A:447:ALA:HB2	2.25	0.52
1:A:461:VAL:HA	1:A:464:THR:CG2	2.37	0.52
1:C:141:ILE:CD1	1:C:141:ILE:N	2.73	0.52
1:C:383:GLU:CB	1:C:384:PRO:HD3	2.40	0.52
1:C:448:PHE:O	1:C:448:PHE:CD2	2.63	0.52
1:E:15:VAL:O	1:E:16:SER:CB	2.58	0.52
1:E:240:PHE:HB3	1:E:250:VAL:HG12	1.91	0.52
1:E:311:GLU:HG2	1:E:312:ILE:HG22	1.92	0.52
1:A:280:THR:O	1:A:280:THR:HG22	2.10	0.52
1:C:164:ILE:HG23	1:C:164:ILE:O	2.10	0.52
1:C:323:ARG:HA	1:C:365:VAL:O	2.10	0.52
1:C:493:VAL:O	1:C:494:GLN:HB2	2.08	0.52
1:E:51:LYS:NZ	1:E:136:GLU:HB3	2.24	0.52
1:E:486:THR:OG1	1:E:487:LEU:N	2.42	0.52
1:A:9:ARG:NH2	1:A:316:GLN:OE1	2.42	0.52
1:A:39:PRO:HG3	1:A:178:TYR:CD1	2.35	0.52
1:A:192:ASP:O	1:A:195:GLU:HB2	2.09	0.52
1:A:356:PRO:O	1:A:357:ILE:HB	2.10	0.52
1:C:48:THR:HG23	1:C:137:TYR:CD1	2.45	0.52
1:C:206:TRP:CG	1:C:264:LEU:HD11	2.45	0.52
1:E:32:THR:O	1:E:33:THR:HB	2.09	0.52
1:E:74:CYS:SG	1:E:106:GLY:CA	2.98	0.52
1:A:246:LYS:O	1:A:248:GLN:N	2.43	0.51
1:A:453:TRP:CE3	1:A:454:ILE:N	2.78	0.51
1:C:318:GLY:HA3	1:C:393:LYS:HZ2	1.74	0.51
2:D:69:ALA:O	2:D:71:ALA:N	2.43	0.51
1:E:380:ILE:HD11	1:E:387:LEU:CB	2.38	0.51
2:F:38:ARG:CG	2:F:39:HIS:CE1	2.93	0.51
1:A:267:ALA:O	2:B:19:TRP:HB2	2.10	0.51
1:A:461:VAL:O	1:A:464:THR:HG22	2.11	0.51
1:A:487:LEU:HD22	1:A:487:LEU:N	2.24	0.51
1:C:3:CYS:SG	1:C:30:CYS:HB2	2.50	0.51
1:C:45:LEU:HD13	1:C:45:LEU:C	2.30	0.51
1:C:300:SER:OG	1:C:301:MET:N	2.43	0.51
1:C:353:THR:C	1:C:355:ASN:H	2.13	0.51
1:E:88:LYS:HA	1:E:88:LYS:NZ	2.24	0.51
1:E:153:ASN:CG	3:I:1:NAG:N2	2.63	0.51
1:A:295:LYS:C	1:A:297:MET:H	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:CYS:HB3	1:C:44:GLU:HG3	1.93	0.51
1:C:95:SER:O	1:C:113:ILE:HG22	2.10	0.51
1:C:434:LYS:C	1:C:436:LEU:H	2.14	0.51
1:C:482:VAL:O	1:C:486:THR:N	2.43	0.51
2:D:48:ILE:HG22	2:D:49:LEU:H	1.76	0.51
1:E:24:VAL:HG11	1:E:415:LEU:HD13	1.93	0.51
1:E:350:ARG:NH1	1:E:372:PRO:HD3	2.20	0.51
1:A:305:LYS:HG3	1:A:305:LYS:O	2.10	0.51
1:A:394:LYS:HG3	1:A:394:LYS:O	2.11	0.51
1:C:165:THR:C	1:C:167:GLN:H	2.14	0.51
2:D:28:HIS:O	2:D:32:ILE:HG23	2.11	0.51
1:A:59:TYR:HD2	1:A:218:LEU:HB2	1.76	0.51
1:A:88:LYS:O	1:A:234:LYS:NZ	2.40	0.51
1:A:302:CYS:SG	1:A:333:CYS:CB	2.98	0.51
1:A:311:GLU:CA	1:A:312:ILE:HD13	2.41	0.51
1:A:312:ILE:HD13	1:A:312:ILE:N	2.25	0.51
1:A:354:VAL:O	1:A:355:ASN:O	2.28	0.51
1:A:390:ASN:HD22	1:A:391:TRP:H	1.54	0.51
1:A:411:ARG:CD	1:A:422:PHE:CE1	2.88	0.51
1:C:178:TYR:HE2	1:C:295:LYS:HZ2	1.57	0.51
1:C:379:ILE:C	1:C:379:ILE:CD1	2.76	0.51
1:E:122:LYS:HB3	1:E:123:LYS:HD2	1.93	0.51
1:E:305:LYS:HD2	1:E:327:GLU:CB	2.40	0.51
2:F:3:ALA:C	2:F:4:LEU:HG	2.30	0.51
2:F:21:SER:O	2:F:22:SER:CB	2.59	0.51
1:A:15:VAL:HG13	1:A:35:ALA:HB2	1.91	0.51
1:A:439:VAL:O	1:A:443:ILE:HG22	2.11	0.51
2:B:45:MET:HA	2:B:48:ILE:HD12	1.91	0.51
1:C:52:GLN:N	1:C:53:PRO:HD3	2.25	0.51
1:E:34:MET:HB3	1:E:40:THR:CA	2.25	0.51
1:E:82:LEU:HD12	1:E:83:ASN:H	1.75	0.51
1:E:91:VAL:HG12	1:E:240:PHE:HZ	1.75	0.51
1:E:137:TYR:N	1:E:137:TYR:HD2	2.08	0.51
1:A:23:ILE:HD12	1:A:285:CYS:O	2.10	0.51
1:A:484:VAL:O	1:A:488:TYR:N	2.44	0.51
1:C:36:LYS:O	1:C:38:LYS:CD	2.57	0.51
1:C:210:ARG:O	1:C:213:PHE:HB3	2.11	0.51
1:C:314:GLU:HG3	1:C:315:THR:H	1.76	0.51
1:C:474:SER:O	1:C:475:LEU:C	2.49	0.51
1:E:126:LYS:HD3	1:E:128:LYS:HZ1	1.76	0.51
1:E:199:LEU:O	1:E:205:ALA:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:391:TRP:CZ3	1:E:392:PHE:O	2.64	0.51
1:A:21:VAL:HB	1:A:287:LEU:HB3	1.93	0.51
1:A:38:LYS:HG2	1:A:292:LEU:HB3	1.92	0.51
1:A:259:ALA:HB3	2:B:2:VAL:CG2	2.41	0.51
1:A:303:THR:HA	1:A:382:VAL:CG1	2.41	0.51
1:A:436:LEU:C	1:A:436:LEU:HD13	2.30	0.51
1:A:444:TYR:C	1:A:446:ALA:N	2.64	0.51
1:C:40:THR:HG21	1:C:353:THR:HA	1.92	0.51
1:C:369:ALA:C	1:C:371:PRO:HD3	2.32	0.51
1:E:170:ILE:HG23	1:E:184:GLU:HB2	1.93	0.51
2:F:53:ILE:HD12	2:F:54:GLY:H	1.76	0.51
1:A:87:ASP:C	1:A:89:ARG:H	2.13	0.51
1:A:170:ILE:O	1:A:170:ILE:HD13	2.11	0.51
1:A:173:ALA:HB3	1:A:181:VAL:N	2.26	0.51
1:A:174:GLU:O	1:A:175:LEU:HD22	2.11	0.51
1:A:191:LEU:HD13	1:A:193:PHE:CE2	2.46	0.51
1:C:141:ILE:HD13	1:C:141:ILE:N	2.23	0.51
1:C:453:TRP:O	1:C:457:ILE:HG23	2.11	0.51
1:E:150:ALA:HB3	1:E:153:ASN:OD1	2.11	0.51
1:E:193:PHE:C	1:E:195:GLU:N	2.63	0.51
1:E:242:ASN:C	1:E:242:ASN:HD22	2.12	0.51
1:E:336:PRO:O	1:E:380:ILE:HA	2.11	0.51
1:E:413:ALA:CB	1:E:414:ILE:HD13	2.41	0.51
1:A:32:THR:HA	1:A:41:LEU:O	2.10	0.51
1:A:239:THR:HG22	1:A:240:PHE:N	2.26	0.51
1:A:243:PRO:O	1:A:244:HIS:HB2	2.11	0.51
1:A:246:LYS:N	1:A:246:LYS:HD3	2.26	0.51
1:C:198:LEU:HD21	1:C:272:MET:HG3	1.93	0.51
1:C:200:GLN:HG2	1:C:201:MET:N	2.26	0.51
1:C:301:MET:O	1:C:302:CYS:O	2.29	0.51
1:C:450:GLY:HA2	2:D:9:GLY:CA	2.41	0.51
1:E:53:PRO:HB2	1:E:128:LYS:HB3	1.92	0.51
1:E:95:SER:HB2	1:E:248:GLN:HE22	1.76	0.51
1:E:99:ARG:CA	1:E:103:ASN:HD21	2.22	0.51
1:E:317:HIS:ND1	1:E:317:HIS:O	2.44	0.51
1:E:417:ASP:N	1:E:437:HIS:HE1	2.05	0.51
2:F:1:SER:H1	2:F:4:LEU:HD12	1.76	0.51
2:F:12:LEU:O	2:F:14:THR:HG23	2.12	0.51
1:A:165:THR:C	1:A:167:GLN:N	2.64	0.50
1:A:265:THR:HA	2:B:19:TRP:CD1	2.39	0.50
1:A:312:ILE:CG2	1:A:322:ILE:HB	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:TYR:CD1	1:A:388:LYS:HE2	2.46	0.50
1:A:460:GLY:O	1:A:482:VAL:HG13	2.11	0.50
1:C:355:ASN:N	1:C:356:PRO:HD3	2.26	0.50
2:D:1:SER:O	2:D:2:VAL:C	2.50	0.50
1:E:40:THR:O	1:E:41:LEU:HD23	2.11	0.50
1:A:58:LYS:HB3	1:A:221:LEU:HB3	1.94	0.50
1:A:113:ILE:HG23	1:A:113:ILE:O	2.11	0.50
1:A:201:MET:HG2	1:A:261:HIS:NE2	2.27	0.50
1:C:208:VAL:HG12	1:C:267:ALA:CB	2.41	0.50
1:E:53:PRO:HB3	1:E:130:VAL:HG13	1.93	0.50
1:E:260:MET:C	1:E:263:ALA:H	2.15	0.50
1:E:407:ARG:O	1:E:408:GLY:C	2.49	0.50
2:F:46:ALA:O	2:F:47:ALA:C	2.49	0.50
1:C:24:VAL:HG12	1:C:25:LEU:N	2.25	0.50
1:C:49:GLU:O	1:C:136:GLU:HG2	2.11	0.50
1:C:59:TYR:N	1:C:59:TYR:CD1	2.79	0.50
1:C:212:TRP:CE3	1:C:216:LEU:HD21	2.46	0.50
1:C:231:TRP:O	1:C:234:LYS:HE3	2.10	0.50
1:C:241:LYS:HZ2	2:F:19:TRP:HZ3	1.57	0.50
1:C:488:TYR:O	1:C:489:LEU:C	2.47	0.50
1:E:19:SER:HA	1:E:289:MET:HB2	1.93	0.50
1:E:187:PRO:O	1:E:188:ARG:C	2.49	0.50
1:A:2:ARG:HG3	1:A:153:ASN:H	1.76	0.50
1:A:233:GLN:O	1:A:234:LYS:HB2	2.12	0.50
1:A:233:GLN:O	1:A:235:GLU:HG2	2.12	0.50
2:B:70:VAL:O	2:B:72:PRO:HD3	2.12	0.50
1:C:36:LYS:HZ3	1:C:36:LYS:HB2	1.76	0.50
1:C:38:LYS:N	1:C:294:LEU:HD21	2.26	0.50
1:C:58:LYS:HE3	1:C:126:LYS:HZ3	1.74	0.50
1:C:100:GLY:HA2	1:C:108:PHE:CD2	2.47	0.50
1:C:227:GLN:OE1	1:C:227:GLN:HA	2.12	0.50
1:C:262:THR:O	1:C:265:THR:OG1	2.29	0.50
1:C:295:LYS:O	1:C:295:LYS:HG2	2.11	0.50
1:C:452:SER:CA	1:C:494:GLN:NE2	2.72	0.50
1:C:466:ILE:HG23	1:C:467:GLY:N	2.26	0.50
1:E:322:ILE:HD12	1:E:322:ILE:N	2.25	0.50
1:E:343:GLU:O	1:E:345:ARG:HD3	2.11	0.50
1:E:389:LEU:N	1:E:389:LEU:CD2	2.72	0.50
1:E:487:LEU:C	1:E:491:VAL:HG22	2.32	0.50
2:F:35:TRP:CE3	2:F:36:ILE:HA	2.47	0.50
2:F:62:LEU:O	2:F:63:ILE:C	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:PRO:C	1:A:168:SER:N	2.65	0.50
1:A:205:ALA:C	1:A:206:TRP:CD2	2.85	0.50
1:A:297:MET:O	1:A:298:SER:HB2	2.12	0.50
1:A:342:LEU:HA	1:A:377:TYR:CE1	2.46	0.50
1:A:438:GLN:OE1	1:A:438:GLN:HA	2.12	0.50
1:C:414:ILE:HD12	2:D:14:THR:O	2.11	0.50
1:E:415:LEU:O	1:E:416:GLY:O	2.29	0.50
2:F:67:LEU:HA	2:F:70:VAL:CG2	2.41	0.50
1:A:39:PRO:O	1:A:41:LEU:HG	2.10	0.50
1:A:99:ARG:HB2	1:A:99:ARG:CZ	2.42	0.50
1:A:99:ARG:NH2	1:A:99:ARG:CB	2.75	0.50
1:A:139:ILE:HG22	1:A:162:ILE:HG23	1.93	0.50
1:A:146:GLY:O	1:A:147:GLU:CB	2.56	0.50
1:A:205:ALA:O	1:A:270:ILE:HG22	2.11	0.50
1:A:245:ALA:HB3	1:A:246:LYS:HE3	1.92	0.50
1:A:323:ARG:HB2	1:A:323:ARG:HH21	1.77	0.50
1:A:436:LEU:HD13	1:A:437:HIS:N	2.26	0.50
2:B:1:SER:OG	2:B:2:VAL:N	2.44	0.50
2:B:29:ALA:O	2:B:32:ILE:HG13	2.12	0.50
1:C:460:GLY:HA2	1:C:463:ILE:HG22	1.93	0.50
1:E:35:ALA:C	1:E:37:ASN:N	2.65	0.50
1:E:221:LEU:HD13	1:E:222:PRO:HD2	1.91	0.50
1:E:304:GLY:HA2	1:E:306:PHE:HE1	1.75	0.50
1:E:401:MET:O	1:E:404:THR:HB	2.12	0.50
1:E:453:TRP:CE3	1:E:454:ILE:HA	2.47	0.50
1:A:39:PRO:O	1:A:40:THR:C	2.50	0.50
1:C:149:HIS:CG	1:C:150:ALA:N	2.79	0.50
1:E:67:ASN:HB2	1:E:118:MET:SD	2.51	0.50
1:A:24:VAL:CG2	1:A:421:ASP:HB3	2.38	0.50
1:C:27:HIS:CD2	1:C:45:LEU:HD12	2.47	0.50
1:C:144:HIS:ND1	1:C:144:HIS:N	2.60	0.50
1:C:205:ALA:HB2	1:C:272:MET:HB3	1.94	0.50
1:C:450:GLY:HA2	2:D:9:GLY:HA3	1.93	0.50
1:E:91:VAL:O	1:E:116:CYS:HA	2.12	0.50
1:E:302:CYS:H	1:E:333:CYS:HB3	1.77	0.50
2:F:59:GLN:HE21	2:F:63:ILE:HD13	1.75	0.50
1:C:404:THR:O	1:C:405:THR:C	2.50	0.50
2:D:34:THR:CG2	2:D:38:ARG:HH11	2.25	0.50
2:D:48:ILE:O	2:D:49:LEU:C	2.49	0.50
1:E:57:ARG:HH22	1:E:214:LEU:CA	2.14	0.50
1:A:89:ARG:HH21	1:A:89:ARG:HG2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:THR:O	1:A:156:GLY:O	2.30	0.49
1:A:407:ARG:HH21	1:A:407:ARG:CG	2.23	0.49
2:B:3:ALA:HB3	2:B:4:LEU:HD22	1.92	0.49
1:C:350:ARG:HG2	1:C:351:LEU:O	2.12	0.49
1:E:35:ALA:C	1:E:37:ASN:H	2.12	0.49
1:E:157:LYS:C	1:E:158:HIS:ND1	2.65	0.49
1:E:242:ASN:CB	1:E:248:GLN:HB3	2.41	0.49
1:E:243:PRO:O	1:E:245:ALA:N	2.45	0.49
1:E:397:SER:O	1:E:400:GLN:N	2.45	0.49
1:A:193:PHE:C	1:A:195:GLU:N	2.62	0.49
1:A:315:THR:O	1:A:316:GLN:C	2.49	0.49
1:C:296:GLY:O	1:C:299:TYR:CB	2.60	0.49
1:C:434:LYS:C	1:C:436:LEU:N	2.66	0.49
1:C:463:ILE:CG1	1:C:482:VAL:HG22	2.42	0.49
1:E:57:ARG:NH1	1:E:220:TRP:CZ2	2.80	0.49
1:E:90:PHE:CZ	1:E:118:MET:SD	3.05	0.49
1:E:191:LEU:CD1	1:E:191:LEU:H	2.25	0.49
1:E:212:TRP:O	1:E:215:ASP:N	2.45	0.49
1:E:417:ASP:N	1:E:437:HIS:CE1	2.80	0.49
1:E:493:VAL:O	1:E:494:GLN:HB2	2.11	0.49
2:F:1:SER:H3	2:F:4:LEU:HD12	1.76	0.49
1:A:58:LYS:CD	1:A:221:LEU:HD23	2.35	0.49
1:A:64:LYS:NZ	1:A:64:LYS:HB3	2.27	0.49
1:A:216:LEU:O	1:A:217:PRO:O	2.30	0.49
1:A:233:GLN:O	1:A:234:LYS:CB	2.61	0.49
1:C:92:CYS:HA	1:C:115:THR:O	2.12	0.49
1:C:218:LEU:N	1:C:218:LEU:CD1	2.75	0.49
1:C:222:PRO:CG	1:C:223:GLY:H	2.20	0.49
1:E:191:LEU:HB3	1:E:193:PHE:CE2	2.47	0.49
1:E:194:ASN:HD22	1:E:194:ASN:N	2.08	0.49
1:A:140:VAL:HG12	1:A:161:GLU:CA	2.29	0.49
1:A:240:PHE:CD2	1:A:250:VAL:HG12	2.46	0.49
1:A:278:LEU:HD23	1:A:278:LEU:N	2.27	0.49
1:C:119:PHE:CE2	1:C:234:LYS:HB3	2.47	0.49
1:C:183:MET:HG2	1:C:287:LEU:HD21	1.94	0.49
1:E:65:LEU:HD11	1:E:238:VAL:CB	2.42	0.49
1:E:296:GLY:C	1:E:298:SER:N	2.65	0.49
1:E:447:ALA:O	1:E:448:PHE:CB	2.50	0.49
2:F:35:TRP:HH2	2:F:42:PHE:CD2	2.30	0.49
1:A:37:ASN:O	1:A:38:LYS:CB	2.61	0.49
1:A:57:ARG:NH2	1:A:214:LEU:HD23	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ARG:O	1:A:74:CYS:HB2	2.13	0.49
1:A:216:LEU:O	1:A:216:LEU:HG	2.12	0.49
1:A:271:GLN:O	1:A:272:MET:HB2	2.12	0.49
1:A:489:LEU:C	1:A:493:VAL:HG13	2.32	0.49
2:B:41:GLY:O	2:B:44:ILE:N	2.46	0.49
1:C:85:GLU:O	1:C:85:GLU:HG2	2.11	0.49
1:C:484:VAL:O	1:C:488:TYR:HB3	2.11	0.49
2:D:48:ILE:C	2:D:50:ALA:N	2.64	0.49
1:E:46:ILE:CG2	1:E:140:VAL:HG13	2.43	0.49
1:A:166:PRO:CB	1:A:187:PRO:HG2	2.25	0.49
1:A:482:VAL:HG12	1:A:487:LEU:CD2	2.42	0.49
2:B:60:ARG:O	2:B:61:ALA:C	2.51	0.49
1:C:39:PRO:N	1:C:294:LEU:HG	2.28	0.49
1:C:309:VAL:O	1:C:323:ARG:HB2	2.12	0.49
2:D:13:GLU:O	2:D:14:THR:HB	2.12	0.49
2:D:32:ILE:HD12	2:D:33:GLU:N	2.27	0.49
1:E:9:ARG:HH12	1:E:319:THR:HG21	1.77	0.49
1:E:38:LYS:CG	1:E:292:LEU:HD23	2.42	0.49
1:E:58:LYS:HB3	1:E:58:LYS:HZ2	1.76	0.49
1:E:141:ILE:O	1:E:159:GLY:O	2.29	0.49
1:E:407:ARG:HD2	1:E:407:ARG:H	1.77	0.49
1:E:452:SER:O	1:E:453:TRP:C	2.50	0.49
1:A:8:ASN:HB3	1:A:29:SER:CB	2.43	0.49
1:A:201:MET:HE3	1:A:201:MET:HA	1.95	0.49
1:A:246:LYS:HZ2	1:A:246:LYS:HB2	1.78	0.49
1:C:89:ARG:HH21	1:C:89:ARG:HB2	1.75	0.49
1:C:202:GLU:HG2	1:C:203:ASN:ND2	2.27	0.49
1:C:388:LYS:C	1:C:389:LEU:HG	2.33	0.49
1:C:410:LYS:HE3	1:C:414:ILE:HG12	1.95	0.49
2:D:27:LYS:O	2:D:28:HIS:C	2.49	0.49
2:F:51:TYR:HA	2:F:60:ARG:CD	2.43	0.49
1:A:19:SER:HB3	1:A:289:MET:HB2	1.93	0.49
1:A:101:TRP:HE3	1:A:108:PHE:CD2	2.29	0.49
1:A:309:VAL:O	1:A:310:LYS:HE2	2.12	0.49
2:B:62:LEU:HD13	2:B:63:ILE:CA	2.43	0.49
1:C:144:HIS:O	1:C:145:SER:C	2.51	0.49
1:C:210:ARG:CG	1:C:210:ARG:NH2	2.74	0.49
1:C:383:GLU:HG3	1:C:384:PRO:HD3	1.94	0.49
1:E:68:THR:HA	1:E:116:CYS:O	2.13	0.49
1:E:123:LYS:N	1:E:123:LYS:NZ	2.61	0.49
1:E:240:PHE:HA	1:E:249:ASP:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:ALA:O	1:E:265:THR:N	2.46	0.49
1:E:280:THR:HG22	2:F:16:THR:HG21	1.95	0.49
1:A:221:LEU:HG	1:A:222:PRO:HD2	1.93	0.49
1:A:278:LEU:H	1:A:278:LEU:CD2	2.25	0.49
1:C:57:ARG:NH2	1:C:214:LEU:CD2	2.76	0.49
1:E:40:THR:HG22	1:E:41:LEU:N	2.27	0.49
1:E:52:GLN:H	1:E:134:ASN:CG	2.14	0.49
1:A:27:HIS:CE1	1:A:279:PHE:CD1	3.00	0.49
1:A:27:HIS:NE2	1:A:279:PHE:HB3	2.27	0.49
1:A:193:PHE:HA	1:A:196:MET:CG	2.43	0.49
1:C:60:CYS:SG	1:C:219:PRO:HD2	2.53	0.49
1:C:270:ILE:CD1	1:C:272:MET:HB2	2.43	0.49
1:C:279:PHE:O	1:C:280:THR:O	2.30	0.49
1:E:170:ILE:HA	1:E:183:MET:O	2.13	0.49
1:A:218:LEU:N	1:A:236:THR:HG21	2.27	0.48
1:A:473:THR:HG22	1:A:474:SER:N	2.28	0.48
1:C:197:VAL:HG11	1:C:213:PHE:CG	2.48	0.48
1:C:201:MET:HB3	1:C:206:TRP:HZ3	1.77	0.48
1:C:226:THR:O	1:C:227:GLN:CB	2.61	0.48
1:C:326:TYR:CZ	1:C:327:GLU:O	2.66	0.48
2:D:60:ARG:O	2:D:61:ALA:C	2.51	0.48
1:E:131:GLN:O	1:E:133:GLU:N	2.45	0.48
1:E:464:THR:HB	1:E:482:VAL:HG21	1.95	0.48
1:A:3:CYS:O	1:A:9:ARG:NH2	2.46	0.48
1:A:25:LEU:HD22	1:A:31:VAL:HG21	1.94	0.48
1:A:408:GLY:O	1:A:411:ARG:N	2.46	0.48
1:C:61:ILE:HD11	1:C:123:LYS:HB3	1.95	0.48
1:C:146:GLY:HA3	1:C:365:VAL:HB	1.95	0.48
1:C:418:THR:O	1:C:421:ASP:HB2	2.13	0.48
1:C:453:TRP:N	1:C:494:GLN:NE2	2.57	0.48
1:E:100:GLY:H	1:E:103:ASN:ND2	2.08	0.48
1:E:175:LEU:HD23	1:E:175:LEU:C	2.32	0.48
1:E:188:ARG:NH2	1:E:188:ARG:CA	2.76	0.48
1:E:322:ILE:O	1:E:366:ASN:HB2	2.12	0.48
1:E:453:TRP:CE3	1:E:454:ILE:N	2.77	0.48
2:F:59:GLN:HE22	2:F:63:ILE:CD1	2.26	0.48
1:A:21:VAL:HG12	1:A:22:ASP:N	2.27	0.48
1:A:101:TRP:HB2	1:A:108:PHE:CD2	2.46	0.48
1:A:133:GLU:O	1:A:134:ASN:CB	2.62	0.48
1:A:350:ARG:NH1	1:A:372:PRO:CB	2.74	0.48
1:A:420:TRP:CD1	1:A:420:TRP:N	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:PHE:O	1:C:194:ASN:C	2.52	0.48
1:C:473:THR:O	1:C:474:SER:C	2.52	0.48
1:E:1:MET:CA	1:E:151:VAL:HA	2.43	0.48
1:E:21:VAL:HA	1:E:424:SER:HB3	1.95	0.48
1:E:85:GLU:HG2	1:E:85:GLU:O	2.12	0.48
1:E:150:ALA:C	1:E:152:GLY:H	2.15	0.48
1:E:306:PHE:CE2	1:E:326:TYR:HB2	2.49	0.48
1:E:367:ILE:HD12	1:E:367:ILE:C	2.32	0.48
1:A:339:ILE:HB	1:A:349:GLY:CA	2.44	0.48
1:A:369:ALA:C	1:A:371:PRO:HD3	2.33	0.48
1:C:440:PHE:C	1:C:440:PHE:CD2	2.86	0.48
1:E:384:PRO:HD2	1:E:386:GLN:NE2	2.28	0.48
1:E:450:GLY:HA2	2:F:9:GLY:CA	2.43	0.48
1:E:450:GLY:C	2:F:9:GLY:HA3	2.34	0.48
1:A:69:THR:O	1:A:70:THR:HB	2.14	0.48
2:B:41:GLY:O	2:B:44:ILE:HB	2.12	0.48
1:E:3:CYS:SG	1:E:9:ARG:HG3	2.53	0.48
1:E:11:PHE:CD2	1:E:32:THR:HB	2.38	0.48
1:E:193:PHE:O	1:E:195:GLU:N	2.46	0.48
1:E:382:VAL:O	1:E:383:GLU:O	2.31	0.48
1:A:144:HIS:CD2	1:A:368:GLU:HG3	2.43	0.48
1:A:201:MET:O	1:A:202:GLU:HG2	2.13	0.48
1:A:284:LYS:O	1:A:285:CYS:CB	2.62	0.48
1:A:335:ILE:HD13	1:A:335:ILE:HA	1.77	0.48
1:A:348:LEU:O	1:A:350:ARG:NE	2.42	0.48
1:C:58:LYS:NZ	1:C:126:LYS:NZ	2.61	0.48
1:C:97:VAL:HG13	1:C:113:ILE:CG2	2.43	0.48
1:C:191:LEU:HD21	1:C:281:GLY:HA2	1.96	0.48
1:C:229:SER:HA	1:C:231:TRP:NE1	2.26	0.48
1:C:475:LEU:HD23	1:C:476:SER:CA	2.43	0.48
1:E:24:VAL:HG11	1:E:415:LEU:CD1	2.44	0.48
1:E:310:LYS:CG	1:E:323:ARG:HD2	2.42	0.48
1:E:337:PHE:HE1	1:E:339:ILE:HG12	1.79	0.48
1:E:413:ALA:HB3	1:E:414:ILE:CD1	2.41	0.48
1:A:91:VAL:HG12	1:A:117:ALA:O	2.14	0.48
1:A:246:LYS:N	1:A:246:LYS:NZ	2.56	0.48
1:A:284:LYS:HZ3	1:A:418:THR:HG22	1.77	0.48
1:A:417:ASP:O	1:A:420:TRP:HD1	1.96	0.48
1:C:40:THR:HG23	1:C:144:HIS:CE1	2.48	0.48
1:C:343:GLU:O	1:C:344:LYS:C	2.52	0.48
1:C:383:GLU:C	1:C:385:GLY:N	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:462:ILE:C	1:C:464:THR:N	2.64	0.48
1:E:206:TRP:CE3	1:E:206:TRP:N	2.82	0.48
1:A:33:THR:O	1:A:40:THR:CB	2.60	0.48
1:A:56:LEU:C	1:A:56:LEU:HD12	2.34	0.48
1:A:170:ILE:HD13	1:A:170:ILE:C	2.34	0.48
1:A:454:ILE:HG23	1:A:455:MET:N	2.21	0.48
1:C:16:SER:C	1:C:18:GLY:H	2.16	0.48
1:C:86:GLN:NE2	1:C:87:ASP:N	2.61	0.48
1:C:197:VAL:HB	1:C:208:VAL:O	2.14	0.48
1:C:434:LYS:HZ3	1:C:435:ALA:N	2.11	0.48
1:E:38:LYS:CG	1:E:292:LEU:HB3	2.37	0.48
1:E:74:CYS:HB3	1:E:77:GLN:OE1	2.14	0.48
1:E:165:THR:OG1	1:E:167:GLN:HG2	2.14	0.48
1:E:348:LEU:H	1:E:348:LEU:HD12	1.78	0.48
1:A:19:SER:O	1:A:288:ARG:HA	2.13	0.48
1:A:39:PRO:HA	1:A:354:VAL:HG21	1.94	0.48
1:A:248:GLN:NE2	1:A:248:GLN:O	2.46	0.48
1:C:318:GLY:H	1:C:393:LYS:HE3	1.79	0.48
1:C:337:PHE:CD1	1:C:338:GLU:N	2.82	0.48
1:C:487:LEU:HD23	1:C:487:LEU:C	2.34	0.48
2:D:29:ALA:O	2:D:32:ILE:CG1	2.53	0.48
2:D:55:THR:OG1	2:D:60:ARG:NE	2.46	0.48
1:E:1:MET:C	1:E:3:CYS:H	2.16	0.48
1:E:79:GLU:O	1:E:80:PRO:O	2.32	0.48
1:E:370:GLU:HG2	1:E:370:GLU:O	2.14	0.48
1:A:437:HIS:O	1:A:438:GLN:C	2.52	0.48
1:C:94:HIS:ND1	1:C:114:VAL:CG1	2.76	0.48
1:C:315:THR:CG2	1:E:108:PHE:HB3	2.42	0.48
1:E:6:ILE:HG13	1:E:6:ILE:O	2.13	0.48
1:E:17:GLY:O	1:E:20:TRP:CB	2.62	0.48
1:E:74:CYS:HB3	1:E:77:GLN:CD	2.33	0.48
1:E:388:LYS:NZ	1:E:388:LYS:CB	2.76	0.48
1:E:411:ARG:O	1:E:413:ALA:O	2.31	0.48
2:F:12:LEU:HD22	2:F:12:LEU:N	2.29	0.48
2:F:24:GLY:O	2:F:26:TRP:N	2.46	0.48
2:F:64:PHE:O	2:F:66:LEU:N	2.47	0.48
1:A:338:GLU:O	1:A:339:ILE:HD13	2.14	0.47
1:A:403:GLU:HA	1:A:406:MET:HE2	1.95	0.47
1:C:237:LEU:O	1:C:238:VAL:C	2.53	0.47
1:C:260:MET:O	1:C:261:HIS:C	2.52	0.47
1:C:357:ILE:HD12	1:C:357:ILE:C	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:217:PRO:C	1:E:218:LEU:HG	2.35	0.47
1:E:330:GLY:HA3	1:E:333:CYS:SG	2.54	0.47
1:E:453:TRP:HB2	1:E:494:GLN:CG	2.30	0.47
1:A:61:ILE:O	1:A:255:SER:HA	2.14	0.47
1:A:82:LEU:HD23	1:A:82:LEU:N	2.30	0.47
1:A:130:VAL:O	1:A:194:ASN:OD1	2.32	0.47
1:A:373:PHE:O	1:A:394:LYS:N	2.48	0.47
1:A:383:GLU:CB	1:A:384:PRO:CD	2.81	0.47
1:A:454:ILE:O	1:A:455:MET:C	2.53	0.47
1:C:205:ALA:C	1:C:206:TRP:CE3	2.88	0.47
1:C:485:VAL:O	1:C:486:THR:C	2.52	0.47
1:E:96:MET:HA	1:E:113:ILE:HG22	1.96	0.47
1:E:101:TRP:CZ3	1:E:107:LEU:HA	2.49	0.47
1:A:162:ILE:O	1:A:162:ILE:HG12	2.13	0.47
1:A:199:LEU:HD23	1:A:208:VAL:HG21	1.95	0.47
1:A:239:THR:CG2	1:A:240:PHE:N	2.78	0.47
1:A:461:VAL:O	1:A:463:ILE:N	2.48	0.47
1:C:264:LEU:HD21	1:C:267:ALA:HB3	1.96	0.47
2:D:53:ILE:CG2	2:D:54:GLY:H	2.16	0.47
1:E:45:LEU:C	1:E:45:LEU:CD2	2.82	0.47
1:E:87:ASP:O	1:E:89:ARG:CG	2.62	0.47
1:E:122:LYS:CB	1:E:123:LYS:HZ3	2.28	0.47
1:E:355:ASN:N	1:E:356:PRO:CD	2.77	0.47
1:A:55:THR:HA	1:A:128:LYS:HG3	1.96	0.47
1:A:380:ILE:CG2	1:A:382:VAL:HG23	2.30	0.47
2:B:50:ALA:CB	2:B:63:ILE:HD11	2.44	0.47
1:C:132:PRO:HD3	1:C:194:ASN:OD1	2.14	0.47
1:C:332:PRO:HG2	1:C:360:GLU:N	2.30	0.47
1:C:470:SER:O	1:C:471:ARG:O	2.31	0.47
1:E:66:THR:C	1:E:118:MET:HG2	2.34	0.47
1:E:203:ASN:C	1:E:204:LYS:HE3	2.35	0.47
1:E:207:LEU:H	1:E:207:LEU:HD12	1.78	0.47
1:E:267:ALA:HB2	2:F:7:HIS:CD2	2.50	0.47
1:E:482:VAL:HA	1:E:486:THR:OG1	2.14	0.47
1:A:73:ARG:HG2	1:A:80:PRO:HG3	1.94	0.47
1:A:367:ILE:CG2	1:A:368:GLU:N	2.78	0.47
1:A:463:ILE:CG2	1:A:464:THR:N	2.78	0.47
1:A:488:TYR:O	1:A:492:MET:HB2	2.15	0.47
1:C:59:TYR:N	1:C:59:TYR:HD1	2.12	0.47
1:C:89:ARG:HB3	1:C:89:ARG:CZ	2.43	0.47
1:C:446:ALA:O	1:C:447:ALA:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:HIS:C	2:D:41:GLY:N	2.67	0.47
1:E:15:VAL:O	1:E:16:SER:HB2	2.14	0.47
1:E:233:GLN:C	1:E:234:LYS:HG3	2.33	0.47
2:F:38:ARG:HB2	2:F:38:ARG:HH21	1.78	0.47
1:A:210:ARG:O	1:A:212:TRP:N	2.47	0.47
1:C:37:ASN:N	1:C:37:ASN:HD22	2.12	0.47
1:C:38:LYS:C	1:C:294:LEU:HD21	2.35	0.47
1:C:115:THR:CG2	1:C:248:GLN:HE22	2.16	0.47
1:C:147:GLU:C	1:C:149:HIS:H	2.18	0.47
1:C:270:ILE:HG12	1:C:271:GLN:N	2.28	0.47
1:C:420:TRP:C	1:C:422:PHE:H	2.17	0.47
1:C:436:LEU:C	1:C:438:GLN:N	2.65	0.47
1:E:75:PRO:O	1:E:77:GLN:NE2	2.48	0.47
1:E:148:GLU:HG3	1:E:323:ARG:NH2	2.29	0.47
1:E:162:ILE:HD13	1:E:172:GLU:O	2.15	0.47
1:E:172:GLU:HG2	1:E:173:ALA:N	2.30	0.47
1:E:186:SER:O	1:E:187:PRO:C	2.51	0.47
1:E:242:ASN:ND2	1:E:247:LYS:O	2.48	0.47
1:A:88:LYS:O	1:A:88:LYS:HD2	2.15	0.47
1:A:221:LEU:CD1	1:A:222:PRO:HD3	2.45	0.47
1:A:317:HIS:C	1:A:319:THR:N	2.68	0.47
1:A:337:PHE:CE1	1:A:351:LEU:HD23	2.49	0.47
1:A:403:GLU:O	1:A:407:ARG:HB2	2.15	0.47
1:A:410:LYS:HA	1:A:488:TYR:OH	2.15	0.47
1:A:458:LEU:C	1:A:458:LEU:HD13	2.35	0.47
1:C:11:PHE:CE2	1:C:352:ILE:HG12	2.50	0.47
1:C:197:VAL:HB	1:C:208:VAL:HG23	1.97	0.47
1:C:297:MET:O	1:C:298:SER:HB3	2.13	0.47
1:C:417:ASP:N	1:C:437:HIS:HE1	2.12	0.47
1:C:451:VAL:HG13	1:C:455:MET:CB	2.38	0.47
2:D:50:ALA:CB	2:D:63:ILE:HD11	2.44	0.47
1:E:42:ASP:HB2	1:E:142:THR:HG22	1.96	0.47
1:E:74:CYS:C	1:E:77:GLN:NE2	2.67	0.47
1:E:94:HIS:HA	1:E:114:VAL:HG23	1.96	0.47
1:E:132:PRO:CA	1:E:135:LEU:HD21	2.45	0.47
1:E:166:PRO:CA	1:E:187:PRO:HG3	2.44	0.47
1:E:227:GLN:O	1:E:227:GLN:HG2	2.15	0.47
2:F:38:ARG:HG3	2:F:39:HIS:CE1	2.50	0.47
2:F:51:TYR:HA	2:F:60:ARG:HD3	1.96	0.47
1:A:149:HIS:CA	1:A:153:ASN:OD1	2.62	0.47
1:A:197:VAL:HG11	1:A:213:PHE:CG	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ILE:HG23	1:A:399:GLY:N	2.30	0.47
1:A:435:ALA:O	1:A:438:GLN:N	2.48	0.47
2:B:1:SER:O	2:B:4:LEU:O	2.33	0.47
2:B:32:ILE:HD12	2:B:32:ILE:C	2.34	0.47
1:C:63:ALA:CB	1:C:237:LEU:HD12	2.45	0.47
1:C:169:SER:OG	1:C:170:ILE:N	2.48	0.47
1:C:362:ASP:O	1:C:363:SER:HB3	2.15	0.47
2:D:50:ALA:C	2:D:52:THR:N	2.66	0.47
1:E:148:GLU:CB	1:E:364:PRO:HG2	2.45	0.47
1:E:463:ILE:CA	1:E:466:ILE:HG22	2.44	0.47
2:F:12:LEU:O	2:F:14:THR:N	2.48	0.47
2:F:33:GLU:O	2:F:34:THR:C	2.53	0.47
1:A:20:TRP:CE3	1:A:20:TRP:CA	2.93	0.47
1:A:391:TRP:CZ3	1:A:393:LYS:CA	2.95	0.47
1:C:46:ILE:CG2	1:C:140:VAL:HG22	2.44	0.47
1:C:394:LYS:O	1:C:395:GLY:C	2.53	0.47
1:E:62:GLU:O	1:E:122:LYS:HB2	2.15	0.47
1:E:101:TRP:CD2	1:E:108:PHE:HE2	2.32	0.47
2:F:45:MET:O	2:F:46:ALA:C	2.53	0.47
1:A:74:CYS:N	1:A:99:ARG:HE	2.12	0.47
1:A:122:LYS:CB	1:A:122:LYS:NZ	2.78	0.47
1:A:373:PHE:CG	1:A:374:GLY:N	2.83	0.47
1:A:388:LYS:HB3	1:A:388:LYS:HZ3	1.80	0.47
1:C:294:LEU:HD23	1:C:354:VAL:HG23	1.95	0.47
1:C:460:GLY:HA2	1:C:463:ILE:CG2	2.45	0.47
2:D:41:GLY:O	2:D:44:ILE:HG22	2.15	0.47
1:E:100:GLY:C	1:E:102:GLY:N	2.65	0.47
1:E:187:PRO:O	1:E:189:THR:N	2.47	0.47
1:E:372:PRO:O	1:E:393:LYS:HD2	2.15	0.47
1:A:50:ALA:HB2	1:A:135:LEU:HD22	1.97	0.46
1:A:139:ILE:O	1:A:162:ILE:HG23	2.15	0.46
1:A:211:GLN:OE1	1:A:211:GLN:HA	2.15	0.46
1:A:414:ILE:HG22	1:A:415:LEU:HD23	1.96	0.46
1:C:60:CYS:SG	1:C:219:PRO:CG	3.03	0.46
1:C:119:PHE:CE2	1:C:234:LYS:HG2	2.49	0.46
1:C:258:GLY:O	1:C:259:ALA:C	2.53	0.46
1:E:46:ILE:HG23	1:E:47:GLU:N	2.30	0.46
1:E:60:CYS:SG	1:E:61:ILE:N	2.87	0.46
1:E:460:GLY:O	1:E:461:VAL:C	2.53	0.46
2:F:32:ILE:O	2:F:35:TRP:HB3	2.15	0.46
1:A:353:THR:O	1:A:354:VAL:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ALA:C	1:A:446:ALA:HB3	2.36	0.46
1:C:46:ILE:O	1:C:47:GLU:CB	2.62	0.46
1:E:37:ASN:CA	1:E:294:LEU:HD21	2.40	0.46
1:E:143:PRO:HB2	1:E:178:TYR:CE1	2.50	0.46
1:E:344:LYS:O	1:E:345:ARG:C	2.53	0.46
1:E:470:SER:OG	1:E:475:LEU:HB3	2.15	0.46
1:A:71:ASP:O	1:A:113:ILE:HG13	2.15	0.46
1:A:88:LYS:HB2	1:C:88:LYS:HG2	1.97	0.46
1:A:148:GLU:C	1:A:150:ALA:H	2.17	0.46
1:A:193:PHE:O	1:A:195:GLU:N	2.48	0.46
1:A:209:HIS:H	2:B:7:HIS:CE1	2.32	0.46
1:A:340:MET:HE1	1:A:345:ARG:HE	1.81	0.46
1:C:89:ARG:NH2	1:C:89:ARG:CB	2.54	0.46
1:C:220:TRP:CD1	1:C:221:LEU:N	2.83	0.46
1:C:410:LYS:C	1:C:410:LYS:CD	2.79	0.46
1:E:59:TYR:O	1:E:124:ASN:HA	2.15	0.46
1:E:75:PRO:O	1:E:76:THR:HB	2.15	0.46
1:E:413:ALA:C	1:E:414:ILE:HG12	2.36	0.46
2:F:18:THR:HB	2:F:21:SER:OG	2.15	0.46
1:A:2:ARG:HH12	1:A:44:GLU:CG	2.20	0.46
1:A:122:LYS:HB2	1:A:122:LYS:NZ	2.31	0.46
1:A:240:PHE:N	1:A:240:PHE:HD2	2.13	0.46
1:C:63:ALA:HB1	1:C:119:PHE:HE1	1.79	0.46
1:C:259:ALA:O	1:C:260:MET:C	2.53	0.46
1:C:451:VAL:HG11	1:C:456:LYS:CA	2.45	0.46
1:C:455:MET:HE3	2:F:67:LEU:HD11	1.97	0.46
1:E:207:LEU:H	1:E:207:LEU:HD13	1.79	0.46
2:F:52:THR:HG1	2:F:53:ILE:H	1.64	0.46
1:A:43:PHE:CD2	1:A:141:ILE:HG22	2.50	0.46
1:A:126:LYS:HZ2	1:A:128:LYS:HE3	1.80	0.46
1:A:171:THR:HG22	1:A:172:GLU:N	2.30	0.46
1:A:229:SER:HA	1:A:231:TRP:NE1	2.30	0.46
1:A:257:GLU:O	1:A:260:MET:HB3	2.16	0.46
1:A:260:MET:HA	1:A:260:MET:HE3	1.98	0.46
1:A:356:PRO:C	1:A:357:ILE:HG22	2.36	0.46
2:B:27:LYS:HA	2:B:30:GLN:HB3	1.97	0.46
1:C:1:MET:SD	1:C:2:ARG:CG	2.95	0.46
1:C:27:HIS:C	1:C:29:SER:H	2.18	0.46
1:C:28:GLY:HA3	1:E:244:HIS:HB2	1.98	0.46
1:C:46:ILE:HG22	1:C:140:VAL:HG22	1.96	0.46
1:C:252:VAL:O	1:C:253:LEU:CB	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:MET:HA	1:C:334:LYS:HB2	1.96	0.46
1:C:325:GLN:HE22	1:C:362:ASP:HA	1.81	0.46
2:D:71:ALA:O	2:D:72:PRO:O	2.33	0.46
1:E:1:MET:HA	1:E:151:VAL:HA	1.95	0.46
1:E:83:ASN:CG	1:E:84:GLU:N	2.69	0.46
1:E:131:GLN:C	1:E:133:GLU:N	2.69	0.46
1:E:233:GLN:C	1:E:235:GLU:N	2.69	0.46
1:E:315:THR:O	1:E:316:GLN:C	2.53	0.46
1:E:337:PHE:CE2	1:E:367:ILE:HG12	2.51	0.46
1:E:394:LYS:O	1:E:395:GLY:O	2.34	0.46
1:A:323:ARG:HA	1:A:366:ASN:CA	2.39	0.46
1:C:39:PRO:HG3	1:C:178:TYR:CD1	2.50	0.46
1:C:101:TRP:N	1:C:108:PHE:CE2	2.84	0.46
1:C:305:LYS:H	1:C:386:GLN:CG	2.17	0.46
1:C:473:THR:O	1:C:475:LEU:N	2.48	0.46
2:D:34:THR:O	2:D:38:ARG:HG2	2.15	0.46
2:D:55:THR:OG1	2:D:60:ARG:HG3	2.16	0.46
1:E:70:THR:OG1	1:E:115:THR:HB	2.15	0.46
1:E:230:ASN:O	1:E:232:ILE:HD13	2.15	0.46
1:E:231:TRP:HB2	1:E:234:LYS:HZ1	1.74	0.46
1:E:307:LYS:HB2	1:E:307:LYS:NZ	2.31	0.46
1:E:413:ALA:O	1:E:414:ILE:HG12	2.15	0.46
1:E:471:ARG:O	1:E:472:SER:CB	2.63	0.46
2:F:62:LEU:C	2:F:62:LEU:HD13	2.36	0.46
1:A:50:ALA:HA	1:A:134:ASN:O	2.16	0.46
1:A:139:ILE:HG23	1:A:162:ILE:HG23	1.98	0.46
1:A:448:PHE:CZ	1:A:451:VAL:HG21	2.51	0.46
1:A:457:ILE:O	1:A:461:VAL:HG22	2.16	0.46
1:C:352:ILE:HG22	1:C:369:ALA:HA	1.98	0.46
1:C:451:VAL:HG12	1:C:455:MET:HB3	1.97	0.46
2:D:50:ALA:HA	2:D:63:ILE:HD11	1.96	0.46
2:D:66:LEU:CD1	2:F:66:LEU:HD23	2.45	0.46
1:E:61:ILE:CG2	1:E:256:GLN:HB2	2.46	0.46
1:E:102:GLY:O	1:E:103:ASN:C	2.53	0.46
1:E:409:ALA:C	1:E:411:ARG:N	2.66	0.46
1:E:420:TRP:C	1:E:422:PHE:N	2.69	0.46
2:F:3:ALA:O	2:F:4:LEU:HD23	2.16	0.46
1:A:21:VAL:CG1	1:A:22:ASP:N	2.78	0.46
1:A:270:ILE:HD12	1:A:270:ILE:HA	1.68	0.46
1:A:377:TYR:CE2	1:A:390:ASN:OD1	2.69	0.46
1:A:484:VAL:HA	1:A:488:TYR:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:ALA:HA	2:B:53:ILE:HG22	1.97	0.46
1:C:75:PRO:HA	1:C:111:GLY:HA2	1.98	0.46
1:C:410:LYS:HE3	1:C:414:ILE:CG1	2.46	0.46
1:C:476:SER:O	1:C:479:LEU:N	2.48	0.46
2:D:3:ALA:HB2	2:F:3:ALA:HB1	1.97	0.46
2:D:34:THR:HG23	2:D:38:ARG:HH11	1.79	0.46
1:E:332:PRO:HA	1:E:358:VAL:O	2.16	0.46
1:E:378:ILE:HG21	1:E:389:LEU:HG	1.95	0.46
1:A:78:GLY:O	1:A:80:PRO:HD3	2.16	0.46
1:A:173:ALA:HB3	1:A:181:VAL:H	1.79	0.46
1:A:220:TRP:C	1:A:220:TRP:HD1	2.14	0.46
1:A:241:LYS:C	1:A:243:PRO:HD3	2.36	0.46
1:A:246:LYS:HZ2	1:A:246:LYS:CB	2.29	0.46
1:A:305:LYS:HG3	1:A:327:GLU:HB3	1.98	0.46
1:A:413:ALA:O	1:A:414:ILE:CG1	2.60	0.46
1:A:463:ILE:HG23	1:A:482:VAL:CG2	2.37	0.46
1:E:101:TRP:HZ3	1:E:107:LEU:HA	1.81	0.46
2:F:67:LEU:O	2:F:68:THR:C	2.54	0.46
1:A:24:VAL:HG13	1:A:284:LYS:HB3	1.98	0.46
1:A:206:TRP:CE2	1:A:264:LEU:HD21	2.50	0.46
1:C:119:PHE:HD1	1:C:120:THR:H	1.62	0.46
1:C:204:LYS:HB2	1:C:206:TRP:CH2	2.51	0.46
1:C:212:TRP:O	1:C:216:LEU:HG	2.15	0.46
1:C:392:PHE:CD2	1:C:392:PHE:O	2.69	0.46
1:C:477:VAL:O	1:C:481:LEU:HB2	2.16	0.46
1:E:4:ILE:HB	1:E:151:VAL:HB	1.97	0.46
1:E:488:TYR:HA	1:E:491:VAL:CG2	2.45	0.46
1:A:73:ARG:CG	1:A:80:PRO:HG3	2.47	0.45
1:A:135:LEU:HD22	1:A:135:LEU:HA	1.70	0.45
1:A:343:GLU:O	1:A:345:ARG:HD2	2.16	0.45
1:A:407:ARG:CG	1:A:407:ARG:NH2	2.78	0.45
1:C:3:CYS:HA	1:C:6:ILE:HG21	1.97	0.45
1:C:99:ARG:CB	1:C:103:ASN:HD21	2.03	0.45
1:C:121:CYS:C	1:C:122:LYS:HD2	2.35	0.45
1:C:148:GLU:CG	1:C:323:ARG:NH1	2.79	0.45
1:C:386:GLN:O	1:C:387:LEU:CB	2.61	0.45
1:C:430:THR:O	1:C:431:SER:C	2.54	0.45
2:D:51:TYR:HD2	2:D:60:ARG:NH1	2.14	0.45
1:E:60:CYS:SG	1:E:219:PRO:HG3	2.56	0.45
1:E:147:GLU:HG2	1:E:149:HIS:H	1.81	0.45
1:E:418:THR:O	1:E:419:ALA:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:471:ARG:HH21	1:E:471:ARG:HG3	1.81	0.45
2:F:1:SER:O	2:F:3:ALA:N	2.48	0.45
2:F:22:SER:O	2:F:23:GLU:C	2.54	0.45
1:A:57:ARG:NH2	1:A:214:LEU:CD2	2.79	0.45
1:A:90:PHE:CE2	1:A:118:MET:HG3	2.51	0.45
1:A:277:LEU:O	1:A:279:PHE:HD2	1.99	0.45
1:A:375:ASP:O	1:A:376:SER:HB2	2.16	0.45
1:A:379:ILE:HG12	1:A:381:GLY:N	2.30	0.45
1:C:39:PRO:HD3	1:C:293:GLN:O	2.17	0.45
1:C:278:LEU:O	1:C:278:LEU:HG	2.15	0.45
1:C:308:VAL:CG2	1:C:387:LEU:HD11	2.46	0.45
2:D:32:ILE:HG13	2:D:33:GLU:N	2.32	0.45
1:E:36:LYS:NZ	1:E:36:LYS:CA	2.73	0.45
1:E:351:LEU:CD1	1:E:353:THR:H	2.29	0.45
1:E:463:ILE:CG2	1:E:464:THR:H	2.29	0.45
1:A:49:GLU:HG2	1:A:50:ALA:N	2.31	0.45
1:A:91:VAL:HG13	1:A:117:ALA:HB3	1.97	0.45
1:A:450:GLY:O	1:A:451:VAL:O	2.33	0.45
1:A:479:LEU:O	1:A:482:VAL:HB	2.16	0.45
2:B:63:ILE:HD13	2:B:64:PHE:N	2.30	0.45
1:C:239:THR:HG22	1:C:240:PHE:N	2.30	0.45
2:D:35:TRP:HH2	2:D:42:PHE:CD2	2.34	0.45
1:E:65:LEU:HD21	1:E:238:VAL:HG21	1.97	0.45
1:E:84:GLU:C	1:E:86:GLN:N	2.69	0.45
1:E:97:VAL:HG23	1:E:98:ASP:O	2.16	0.45
1:E:102:GLY:C	1:E:104:GLY:H	2.20	0.45
1:E:351:LEU:HD12	1:E:351:LEU:C	2.36	0.45
1:E:396:SER:O	1:E:397:SER:C	2.53	0.45
2:F:59:GLN:NE2	2:F:63:ILE:CD1	2.75	0.45
1:A:1:MET:O	1:A:2:ARG:C	2.55	0.45
1:A:27:HIS:NE2	1:A:279:PHE:CB	2.79	0.45
1:A:43:PHE:CE2	1:A:141:ILE:HG21	2.51	0.45
1:A:47:GLU:HG3	1:A:138:THR:CB	2.44	0.45
1:A:61:ILE:CD1	1:A:255:SER:HB2	2.46	0.45
1:A:125:MET:HB3	1:A:201:MET:CE	2.46	0.45
1:A:260:MET:HA	1:A:260:MET:CE	2.46	0.45
1:A:309:VAL:O	1:A:309:VAL:HG12	2.16	0.45
1:A:444:TYR:O	1:A:446:ALA:N	2.50	0.45
1:C:2:ARG:C	1:C:4:ILE:N	2.70	0.45
1:C:84:GLU:C	1:C:86:GLN:H	2.20	0.45
1:C:119:PHE:CD2	1:C:234:LYS:CD	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:216:LEU:HD23	1:E:217:PRO:CD	2.46	0.45
1:E:303:THR:CG2	1:E:304:GLY:N	2.80	0.45
1:A:148:GLU:C	1:A:150:ALA:N	2.70	0.45
1:A:420:TRP:CB	1:A:434:LYS:HG3	2.36	0.45
1:A:487:LEU:N	1:A:487:LEU:CD2	2.79	0.45
2:B:48:ILE:C	2:B:50:ALA:N	2.66	0.45
2:B:51:TYR:HA	2:B:60:ARG:HD3	1.98	0.45
1:C:64:LYS:HG2	1:C:122:LYS:HE2	1.99	0.45
1:C:131:GLN:C	1:C:133:GLU:H	2.20	0.45
1:C:132:PRO:HB2	1:C:188:ARG:NH1	2.31	0.45
1:C:420:TRP:CG	1:C:434:LYS:HB2	2.52	0.45
1:C:462:ILE:HG13	1:C:463:ILE:N	2.32	0.45
2:D:32:ILE:CG1	2:D:33:GLU:N	2.80	0.45
2:D:65:ILE:HG22	2:D:66:LEU:N	2.31	0.45
1:A:51:LYS:O	1:A:52:GLN:CB	2.65	0.45
1:A:213:PHE:CD2	1:A:213:PHE:O	2.69	0.45
2:D:22:SER:O	2:D:23:GLU:C	2.55	0.45
2:D:26:TRP:O	2:D:27:LYS:C	2.55	0.45
1:E:32:THR:HA	1:E:41:LEU:O	2.17	0.45
1:E:34:MET:H	1:E:34:MET:CE	2.30	0.45
1:E:190:GLY:HA2	1:E:284:LYS:NZ	2.31	0.45
1:E:333:CYS:C	1:E:357:ILE:HD12	2.36	0.45
1:E:406:MET:O	1:E:407:ARG:C	2.54	0.45
2:F:69:ALA:O	2:F:70:VAL:C	2.54	0.45
1:A:142:THR:OG1	1:A:143:PRO:HD2	2.17	0.45
1:A:264:LEU:O	1:A:267:ALA:HB3	2.16	0.45
2:B:47:ALA:HB2	2:B:64:PHE:CE1	2.51	0.45
1:C:57:ARG:HB3	1:C:58:LYS:H	1.65	0.45
1:E:9:ARG:HH22	1:E:319:THR:CG2	2.27	0.45
1:E:280:THR:HG21	2:F:16:THR:OG1	2.17	0.45
1:E:403:GLU:O	1:E:407:ARG:HG2	2.17	0.45
1:E:492:MET:HA	1:E:492:MET:HE1	1.99	0.45
2:F:44:ILE:O	2:F:47:ALA:HB3	2.16	0.45
1:A:6:ILE:HG22	1:A:6:ILE:O	2.17	0.45
1:A:185:CYS:CB	1:A:187:PRO:HD3	2.45	0.45
1:A:318:GLY:C	1:A:320:ILE:N	2.70	0.45
1:A:352:ILE:HG23	1:A:352:ILE:O	2.16	0.45
1:A:386:GLN:NE2	1:A:386:GLN:CA	2.77	0.45
2:B:50:ALA:HB1	2:B:63:ILE:HD11	1.98	0.45
1:C:37:ASN:HB2	1:C:38:LYS:NZ	2.32	0.45
1:C:270:ILE:C	1:C:270:ILE:HD13	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:51:TYR:HA	2:D:60:ARG:CD	2.47	0.45
1:E:211:GLN:O	1:E:211:GLN:HG2	2.17	0.45
1:E:343:GLU:O	1:E:345:ARG:NH2	2.50	0.45
1:E:411:ARG:HA	1:E:415:LEU:HD21	1.98	0.45
1:E:420:TRP:CB	1:E:434:LYS:HG3	2.46	0.45
1:E:470:SER:OG	1:E:473:THR:HA	2.16	0.45
2:F:24:GLY:O	2:F:25:ALA:C	2.55	0.45
2:F:47:ALA:O	2:F:50:ALA:HB3	2.16	0.45
1:A:39:PRO:HA	1:A:354:VAL:CG2	2.47	0.45
1:A:98:ASP:HA	1:A:110:LYS:HA	1.98	0.45
1:A:125:MET:CB	1:A:201:MET:HE3	2.47	0.45
1:A:373:PHE:HB3	1:A:395:GLY:O	2.16	0.45
2:B:71:ALA:O	2:B:72:PRO:C	2.55	0.45
1:C:73:ARG:HB3	1:C:80:PRO:HB3	1.98	0.45
1:C:209:HIS:H	2:D:7:HIS:CE1	2.35	0.45
1:C:220:TRP:HD1	1:C:221:LEU:N	2.14	0.45
1:C:451:VAL:HG12	1:C:456:LYS:H	1.82	0.45
1:C:487:LEU:O	1:C:488:TYR:C	2.54	0.45
2:D:56:THR:C	2:D:58:PHE:H	2.20	0.45
1:E:201:MET:HA	1:E:201:MET:CE	2.46	0.45
1:E:208:VAL:HG12	2:F:7:HIS:ND1	2.32	0.45
1:E:305:LYS:HD3	1:E:305:LYS:C	2.37	0.45
2:F:35:TRP:O	2:F:38:ARG:N	2.50	0.45
1:A:27:HIS:HA	1:A:45:LEU:HD12	1.99	0.45
1:A:62:GLU:CG	1:A:122:LYS:HB3	2.46	0.45
1:A:210:ARG:C	1:A:212:TRP:H	2.20	0.45
1:A:387:LEU:HD13	1:A:388:LYS:N	2.32	0.45
1:A:406:MET:O	1:A:408:GLY:N	2.50	0.45
1:C:80:PRO:HD3	1:C:112:GLY:HA3	1.98	0.45
1:C:119:PHE:CD1	1:C:120:THR:N	2.84	0.45
1:C:176:THR:C	1:C:178:TYR:H	2.20	0.45
1:C:217:PRO:C	1:C:218:LEU:HD12	2.37	0.45
2:D:2:VAL:O	2:D:5:VAL:CG2	2.65	0.45
2:D:13:GLU:HB3	2:D:14:THR:H	1.59	0.45
1:E:65:LEU:HD11	1:E:238:VAL:CG1	2.47	0.45
1:E:145:SER:HB3	1:E:353:THR:HG22	1.93	0.45
3:I:1:NAG:C7	3:I:1:NAG:O3	2.65	0.45
1:A:205:ALA:O	1:A:206:TRP:CD2	2.70	0.44
1:A:340:MET:HA	1:A:347:VAL:HG12	1.99	0.44
1:A:370:GLU:O	1:A:370:GLU:HG2	2.17	0.44
1:A:371:PRO:HB3	1:A:372:PRO:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:TRP:CD1	2:B:20:MET:SD	3.10	0.44
2:B:50:ALA:HA	2:B:63:ILE:HD11	1.98	0.44
2:B:67:LEU:C	2:B:67:LEU:HD23	2.37	0.44
1:C:345:ARG:O	1:C:346:HIS:CG	2.70	0.44
1:C:452:SER:C	1:C:494:GLN:HE22	2.20	0.44
1:E:56:LEU:HD11	1:E:210:ARG:HH22	1.81	0.44
1:E:65:LEU:HG	1:E:252:VAL:HG22	1.99	0.44
1:E:453:TRP:CD1	1:E:494:GLN:HG3	2.52	0.44
1:A:192:ASP:O	1:A:196:MET:HG2	2.17	0.44
1:A:277:LEU:O	1:A:279:PHE:CD2	2.70	0.44
1:A:314:GLU:HG2	1:A:320:ILE:HD13	1.97	0.44
1:A:329:ASP:O	1:A:333:CYS:SG	2.75	0.44
1:A:388:LYS:HB3	1:A:388:LYS:HZ2	1.82	0.44
1:A:399:GLY:HA2	1:A:402:ILE:CG2	2.47	0.44
1:C:25:LEU:HD12	1:C:25:LEU:N	2.31	0.44
1:C:62:GLU:HB3	1:C:122:LYS:HB2	1.98	0.44
1:C:198:LEU:HD23	1:C:198:LEU:C	2.37	0.44
1:C:439:VAL:O	1:C:440:PHE:C	2.53	0.44
1:C:452:SER:O	1:C:456:LYS:HB3	2.17	0.44
1:C:461:VAL:O	1:C:464:THR:HB	2.18	0.44
1:E:90:PHE:CA	1:E:117:ALA:O	2.64	0.44
1:E:260:MET:HB2	2:F:2:VAL:HG21	2.00	0.44
1:E:396:SER:O	1:E:398:ILE:HG22	2.17	0.44
1:A:70:THR:HA	1:A:82:LEU:HD11	1.99	0.44
1:A:197:VAL:HG23	1:A:210:ARG:CA	2.42	0.44
1:A:311:GLU:O	1:A:322:ILE:HD13	2.17	0.44
1:A:390:ASN:ND2	1:A:390:ASN:C	2.71	0.44
1:C:336:PRO:HG2	1:C:382:VAL:HG13	1.98	0.44
1:C:386:GLN:O	1:C:387:LEU:CG	2.66	0.44
1:E:74:CYS:HA	1:E:99:ARG:HG2	1.98	0.44
1:E:233:GLN:O	1:E:234:LYS:CB	2.64	0.44
1:E:240:PHE:CA	1:E:249:ASP:O	2.65	0.44
1:E:265:THR:CG2	2:F:20:MET:HB2	2.47	0.44
1:E:457:ILE:O	1:E:460:GLY:N	2.50	0.44
1:E:488:TYR:O	1:E:489:LEU:C	2.55	0.44
1:A:297:MET:O	1:A:298:SER:CB	2.66	0.44
1:A:383:GLU:C	1:A:385:GLY:H	2.21	0.44
1:A:411:ARG:NH2	1:A:411:ARG:HB2	2.31	0.44
2:B:19:TRP:CD1	2:B:20:MET:HG2	2.53	0.44
1:C:13:GLU:HA	1:C:34:MET:HE1	2.00	0.44
1:C:274:SER:C	1:C:276:ASN:N	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:VAL:CG2	1:C:322:ILE:N	2.80	0.44
1:C:377:TYR:OH	1:C:388:LYS:HD2	2.17	0.44
1:C:451:VAL:O	1:C:452:SER:HB3	2.17	0.44
1:C:475:LEU:CD2	1:C:476:SER:N	2.69	0.44
1:E:44:GLU:HB3	1:E:140:VAL:CG2	2.47	0.44
1:E:159:GLY:O	1:E:160:LYS:CB	2.64	0.44
1:E:177:GLY:O	1:E:178:TYR:C	2.54	0.44
1:E:297:MET:C	1:E:334:LYS:HZ1	2.20	0.44
1:E:316:GLN:O	1:E:317:HIS:CG	2.71	0.44
1:A:66:THR:CG2	1:A:118:MET:HB3	2.44	0.44
1:A:149:HIS:ND1	1:A:158:HIS:HE1	2.15	0.44
1:A:210:ARG:HG3	1:A:210:ARG:HH21	1.83	0.44
1:A:320:ILE:C	1:A:321:VAL:HG13	2.37	0.44
1:A:434:LYS:HZ2	1:A:434:LYS:HB3	1.83	0.44
1:C:304:GLY:O	1:C:305:LYS:HB2	2.18	0.44
1:C:352:ILE:CG2	1:C:368:GLU:O	2.66	0.44
1:E:83:ASN:O	1:E:85:GLU:N	2.50	0.44
1:E:191:LEU:HB3	1:E:193:PHE:CD2	2.52	0.44
1:E:196:MET:HE2	1:E:209:HIS:HB3	1.99	0.44
1:E:464:THR:CB	1:E:482:VAL:HG21	2.48	0.44
1:A:229:SER:O	1:A:231:TRP:HD1	2.00	0.44
1:A:231:TRP:O	1:A:234:LYS:HG3	2.17	0.44
1:A:270:ILE:CG2	1:A:271:GLN:N	2.71	0.44
1:C:182:THR:O	1:C:287:LEU:HD13	2.17	0.44
1:C:245:ALA:O	1:C:246:LYS:C	2.55	0.44
1:C:299:TYR:CE1	1:C:332:PRO:O	2.71	0.44
1:E:15:VAL:HG23	1:E:21:VAL:CG1	2.47	0.44
1:E:49:GLU:O	1:E:136:GLU:HG2	2.17	0.44
1:E:99:ARG:CZ	1:E:105:CYS:SG	3.06	0.44
1:E:220:TRP:O	1:E:231:TRP:CE3	2.71	0.44
1:A:93:LYS:HZ3	1:A:240:PHE:HB2	1.81	0.44
1:A:99:ARG:CB	1:A:99:ARG:HH21	2.31	0.44
1:A:154:ASP:O	1:A:155:THR:HG23	2.18	0.44
1:A:193:PHE:CE2	1:A:278:LEU:HD11	2.53	0.44
1:A:199:LEU:O	1:A:205:ALA:HB1	2.18	0.44
1:A:411:ARG:NH2	1:A:422:PHE:CE1	2.86	0.44
1:A:463:ILE:O	1:A:464:THR:C	2.55	0.44
2:B:37:LEU:CD2	2:B:38:ARG:N	2.69	0.44
1:E:38:LYS:N	1:E:294:LEU:HG	2.30	0.44
1:E:167:GLN:NE2	1:E:167:GLN:HA	2.32	0.44
1:E:172:GLU:CG	1:E:180:THR:HB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:217:PRO:C	1:E:218:LEU:CG	2.85	0.44
1:E:232:ILE:O	1:E:232:ILE:HG22	2.18	0.44
1:E:263:ALA:C	1:E:265:THR:H	2.21	0.44
1:E:310:LYS:O	1:E:311:GLU:C	2.55	0.44
1:E:490:GLY:C	1:E:492:MET:H	2.20	0.44
2:F:32:ILE:HD12	2:F:33:GLU:N	2.33	0.44
1:A:97:VAL:HB	1:A:245:ALA:O	2.18	0.44
1:A:166:PRO:CB	1:A:187:PRO:CG	2.93	0.44
1:A:259:ALA:HA	1:A:262:THR:HB	2.00	0.44
1:A:307:LYS:CG	1:A:308:VAL:N	2.73	0.44
1:A:450:GLY:HA2	2:B:9:GLY:O	2.18	0.44
1:C:34:MET:HB3	1:C:40:THR:CA	2.45	0.44
1:C:119:PHE:HD1	1:C:120:THR:N	2.15	0.44
1:C:169:SER:O	1:C:170:ILE:C	2.55	0.44
1:C:318:GLY:O	1:C:370:GLU:HA	2.18	0.44
1:E:164:ILE:HD11	1:E:283:LEU:HD21	1.99	0.44
1:E:268:THR:N	2:F:18:THR:HG23	2.32	0.44
1:E:460:GLY:O	1:E:463:ILE:N	2.49	0.44
1:E:479:LEU:O	1:E:480:VAL:C	2.55	0.44
1:A:3:CYS:SG	1:A:30:CYS:HB3	2.58	0.44
1:A:206:TRP:CG	1:A:264:LEU:HD11	2.53	0.44
1:A:252:VAL:O	1:A:253:LEU:CB	2.53	0.44
1:A:350:ARG:CZ	1:A:372:PRO:HA	2.47	0.44
1:C:148:GLU:HG2	1:C:323:ARG:NH1	2.32	0.44
1:C:205:ALA:O	1:C:206:TRP:CD2	2.71	0.44
1:C:261:HIS:O	1:C:264:LEU:N	2.43	0.44
1:E:73:ARG:CG	1:E:80:PRO:HG3	2.48	0.44
1:E:131:GLN:HA	1:E:194:ASN:HD21	1.82	0.44
1:E:270:ILE:HG23	1:E:270:ILE:O	2.17	0.44
1:E:279:PHE:HD2	1:E:279:PHE:N	2.16	0.44
1:A:46:ILE:HG13	1:A:47:GLU:HG2	2.00	0.43
1:A:61:ILE:HG21	1:A:201:MET:HE2	2.00	0.43
1:A:99:ARG:CD	1:A:111:GLY:HA3	2.45	0.43
1:A:201:MET:HB2	1:A:206:TRP:HZ3	1.83	0.43
1:A:219:PRO:HD3	1:A:236:THR:OG1	2.18	0.43
1:A:232:ILE:O	1:A:233:GLN:CG	2.66	0.43
1:A:450:GLY:C	1:A:451:VAL:O	2.56	0.43
2:B:59:GLN:O	2:B:60:ARG:C	2.55	0.43
1:C:37:ASN:H	1:C:37:ASN:HD22	1.66	0.43
1:C:72:SER:HB3	1:C:113:ILE:CD1	2.39	0.43
1:C:80:PRO:HG3	1:C:112:GLY:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:MET:HB3	1:C:110:LYS:HG3	1.99	0.43
1:C:118:MET:HG2	1:C:119:PHE:N	2.33	0.43
1:C:165:THR:O	1:C:167:GLN:N	2.51	0.43
1:C:379:ILE:O	1:C:380:ILE:HG23	2.18	0.43
2:D:51:TYR:C	2:D:51:TYR:CD2	2.92	0.43
1:E:9:ARG:HH12	1:E:319:THR:CG2	2.30	0.43
1:E:42:ASP:HB2	1:E:142:THR:HG23	2.00	0.43
1:E:65:LEU:HA	1:E:118:MET:O	2.18	0.43
1:E:148:GLU:C	1:E:150:ALA:H	2.21	0.43
1:E:167:GLN:HA	1:E:167:GLN:HE21	1.83	0.43
1:E:305:LYS:O	1:E:326:TYR:HA	2.18	0.43
1:E:335:ILE:HA	1:E:335:ILE:HD13	1.77	0.43
1:E:429:PHE:O	1:E:431:SER:N	2.51	0.43
2:F:8:VAL:HG13	2:F:9:GLY:N	2.27	0.43
2:F:9:GLY:O	2:F:11:GLY:N	2.51	0.43
1:A:9:ARG:HG2	1:A:316:GLN:HG2	2.00	0.43
1:A:41:LEU:HD23	1:A:143:PRO:HA	2.00	0.43
1:A:212:TRP:C	1:A:214:LEU:N	2.69	0.43
1:A:240:PHE:CG	1:A:250:VAL:HG12	2.52	0.43
1:A:333:CYS:HB2	1:A:358:VAL:CG2	2.48	0.43
1:A:403:GLU:HA	1:A:406:MET:CE	2.48	0.43
1:A:415:LEU:HB2	1:A:419:ALA:HB2	1.99	0.43
1:A:463:ILE:CG2	1:A:482:VAL:HG22	2.40	0.43
1:C:86:GLN:HE21	1:C:87:ASP:N	2.14	0.43
1:C:199:LEU:CD1	1:C:200:GLN:N	2.76	0.43
1:E:150:ALA:HB2	3:I:1:NAG:O7	2.18	0.43
1:E:240:PHE:HB3	1:E:250:VAL:CG1	2.48	0.43
1:E:463:ILE:HA	1:E:466:ILE:CG2	2.46	0.43
1:A:140:VAL:HG23	1:A:140:VAL:O	2.18	0.43
1:A:146:GLY:HA2	1:A:366:ASN:OD1	2.18	0.43
1:A:255:SER:O	1:A:257:GLU:N	2.51	0.43
1:A:306:PHE:HD2	1:A:306:PHE:HA	1.64	0.43
1:A:323:ARG:HB2	1:A:323:ARG:CZ	2.47	0.43
1:C:65:LEU:CD2	1:C:252:VAL:HG12	2.48	0.43
1:C:355:ASN:O	1:C:357:ILE:HG23	2.18	0.43
1:C:464:THR:CG2	1:C:465:TRP:N	2.81	0.43
1:E:41:LEU:HD23	1:E:41:LEU:HA	1.76	0.43
1:E:125:MET:HB3	1:E:199:LEU:CD1	2.48	0.43
1:E:351:LEU:HD12	1:E:353:THR:H	1.83	0.43
1:C:312:ILE:O	1:C:312:ILE:CD1	2.64	0.43
1:C:439:VAL:O	1:C:443:ILE:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ARG:NH1	1:A:425:LEU:CD2	2.80	0.43
1:A:324:VAL:HG23	1:A:325:GLN:N	2.31	0.43
1:A:457:ILE:HG22	1:A:490:GLY:CA	2.42	0.43
2:B:31:ARG:HH21	2:B:31:ARG:CG	2.27	0.43
2:B:60:ARG:O	2:B:63:ILE:CD1	2.61	0.43
1:C:38:LYS:C	1:C:40:THR:H	2.22	0.43
1:C:122:LYS:HD2	1:C:122:LYS:N	2.33	0.43
1:C:143:PRO:CB	1:C:178:TYR:HE1	2.32	0.43
1:C:246:LYS:HD2	1:C:246:LYS:O	2.19	0.43
1:C:246:LYS:O	1:C:247:LYS:HB3	2.18	0.43
1:C:282:HIS:CD2	1:C:415:LEU:HD12	2.53	0.43
1:C:369:ALA:O	1:C:371:PRO:HD3	2.18	0.43
1:C:425:LEU:N	1:C:425:LEU:HD23	2.34	0.43
1:E:325:GLN:OE1	1:E:325:GLN:HA	2.18	0.43
1:E:408:GLY:O	1:E:412:MET:HB2	2.19	0.43
1:E:417:ASP:C	1:E:419:ALA:N	2.69	0.43
1:A:166:PRO:CD	1:A:187:PRO:HB2	2.48	0.43
1:A:420:TRP:CD2	1:A:434:LYS:HA	2.53	0.43
1:A:487:LEU:O	1:A:489:LEU:N	2.51	0.43
2:B:4:LEU:N	2:B:4:LEU:CD2	2.81	0.43
2:B:32:ILE:O	2:B:36:ILE:HG22	2.18	0.43
1:C:209:HIS:CB	2:D:10:MET:HG2	2.49	0.43
1:C:460:GLY:O	1:C:461:VAL:C	2.57	0.43
2:D:6:PRO:O	2:D:8:VAL:N	2.51	0.43
1:E:11:PHE:CA	1:E:32:THR:O	2.61	0.43
1:E:147:GLU:HG2	1:E:149:HIS:N	2.33	0.43
1:E:148:GLU:O	1:E:148:GLU:CG	2.66	0.43
1:E:207:LEU:CD1	1:E:207:LEU:N	2.77	0.43
1:E:217:PRO:HB2	1:E:218:LEU:HD23	2.01	0.43
1:E:242:ASN:HD22	1:E:243:PRO:N	2.15	0.43
1:E:351:LEU:CD1	1:E:353:THR:N	2.81	0.43
1:A:27:HIS:O	1:A:45:LEU:O	2.37	0.43
1:A:325:GLN:HG3	1:A:326:TYR:N	2.34	0.43
1:A:406:MET:O	1:A:407:ARG:C	2.57	0.43
1:A:495:ALA:O	2:B:17:GLU:HA	2.19	0.43
2:B:9:GLY:O	2:B:10:MET:C	2.57	0.43
1:C:27:HIS:CD2	1:C:45:LEU:CD1	3.02	0.43
1:C:130:VAL:C	1:C:131:GLN:HG3	2.39	0.43
1:C:299:TYR:CE1	1:C:333:CYS:HA	2.53	0.43
1:C:315:THR:HB	1:C:316:GLN:H	1.52	0.43
1:C:343:GLU:O	1:C:345:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:GLU:HG3	1:C:384:PRO:CD	2.49	0.43
1:C:402:ILE:O	1:C:403:GLU:C	2.57	0.43
1:C:411:ARG:CZ	1:C:411:ARG:HB2	2.48	0.43
1:E:93:LYS:HE2	1:E:240:PHE:CZ	2.53	0.43
1:E:188:ARG:HH21	1:E:188:ARG:HB3	1.83	0.43
1:A:191:LEU:HD23	1:A:191:LEU:C	2.38	0.43
1:A:246:LYS:NZ	1:A:246:LYS:CB	2.82	0.43
2:B:8:VAL:HG23	2:B:9:GLY:H	1.83	0.43
1:C:197:VAL:O	1:C:208:VAL:HG22	2.19	0.43
1:C:200:GLN:O	1:C:201:MET:HB2	2.18	0.43
1:C:247:LYS:HG3	1:C:248:GLN:N	2.34	0.43
2:D:44:ILE:HG22	2:D:45:MET:N	2.33	0.43
1:E:6:ILE:HG12	1:E:30:CYS:SG	2.59	0.43
1:E:345:ARG:HH21	1:E:345:ARG:HG2	1.84	0.43
1:E:439:VAL:O	1:E:440:PHE:C	2.55	0.43
2:F:53:ILE:HD12	2:F:54:GLY:N	2.33	0.43
1:A:9:ARG:HG2	1:A:316:GLN:CG	2.48	0.43
1:A:197:VAL:HG21	1:A:210:ARG:HA	1.99	0.43
1:A:234:LYS:O	1:A:238:VAL:HG22	2.18	0.43
1:A:364:PRO:O	1:A:365:VAL:HG13	2.19	0.43
1:A:461:VAL:CA	1:A:464:THR:HG22	2.42	0.43
1:A:480:VAL:O	1:A:481:LEU:C	2.57	0.43
1:C:36:LYS:HD3	1:C:37:ASN:HD22	1.83	0.43
1:C:178:TYR:N	1:C:178:TYR:CD2	2.86	0.43
1:C:408:GLY:O	1:C:409:ALA:C	2.57	0.43
1:E:80:PRO:HG2	1:E:112:GLY:C	2.38	0.43
1:E:145:SER:CB	1:E:353:THR:HG22	2.48	0.43
1:E:170:ILE:HG12	1:E:184:GLU:CG	2.45	0.43
1:E:279:PHE:CD2	1:E:279:PHE:N	2.86	0.43
2:F:40:PRO:O	2:F:41:GLY:C	2.56	0.43
1:A:2:ARG:NH2	1:A:2:ARG:HB3	2.34	0.43
1:A:58:LYS:O	1:A:231:TRP:HZ3	2.02	0.43
1:A:122:LYS:HA	1:A:122:LYS:NZ	2.31	0.43
1:A:256:GLN:O	1:A:258:GLY:N	2.51	0.43
1:C:93:LYS:O	1:C:114:VAL:HA	2.19	0.43
1:C:241:LYS:O	1:C:248:GLN:HA	2.19	0.43
1:C:270:ILE:O	1:C:270:ILE:HD13	2.18	0.43
1:C:332:PRO:HB3	1:C:358:VAL:C	2.39	0.43
1:C:425:LEU:HD23	1:C:425:LEU:H	1.82	0.43
1:C:439:VAL:HG23	1:C:440:PHE:N	2.34	0.43
1:E:20:TRP:HZ3	1:E:425:LEU:HB2	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:335:ILE:HA	1:E:336:PRO:HD3	1.74	0.43
1:E:350:ARG:NH1	1:E:372:PRO:HB3	2.34	0.43
1:A:9:ARG:HG2	1:A:316:GLN:CD	2.38	0.42
1:A:55:THR:HB	1:A:128:LYS:HG3	2.01	0.42
1:A:224:ALA:CB	1:C:73:ARG:HH12	2.31	0.42
1:A:225:ASP:O	1:A:226:THR:C	2.58	0.42
1:A:453:TRP:HE3	1:A:454:ILE:HA	1.84	0.42
1:C:45:LEU:HD13	1:C:46:ILE:CA	2.48	0.42
1:C:89:ARG:HG3	1:C:229:SER:O	2.18	0.42
1:E:30:CYS:HA	1:E:43:PHE:O	2.19	0.42
1:E:198:LEU:HA	1:E:198:LEU:HD23	1.80	0.42
1:E:240:PHE:CB	1:E:250:VAL:HG12	2.49	0.42
1:E:280:THR:CG2	2:F:16:THR:OG1	2.67	0.42
1:E:333:CYS:O	1:E:357:ILE:HD12	2.19	0.42
2:F:28:HIS:O	2:F:31:ARG:HB3	2.19	0.42
2:F:33:GLU:O	2:F:36:ILE:HB	2.19	0.42
1:A:102:GLY:C	1:A:104:GLY:N	2.71	0.42
1:A:165:THR:HG22	1:A:167:GLN:H	1.83	0.42
1:A:202:GLU:O	1:A:204:LYS:HG2	2.19	0.42
1:A:338:GLU:HB2	1:A:379:ILE:CG2	2.49	0.42
1:A:461:VAL:O	1:A:464:THR:N	2.52	0.42
1:C:239:THR:CG2	1:C:240:PHE:N	2.81	0.42
1:C:253:LEU:HD12	1:C:253:LEU:HA	1.82	0.42
1:C:261:HIS:O	1:C:264:LEU:CB	2.67	0.42
1:C:385:GLY:C	1:C:387:LEU:H	2.21	0.42
1:C:433:GLY:O	1:C:436:LEU:HB3	2.19	0.42
1:E:66:THR:O	1:E:67:ASN:HB2	2.20	0.42
1:E:123:LYS:CD	1:E:123:LYS:N	2.82	0.42
1:E:210:ARG:C	1:E:212:TRP:N	2.71	0.42
1:E:457:ILE:HD13	1:E:457:ILE:HA	1.64	0.42
1:E:474:SER:O	1:E:477:VAL:HB	2.19	0.42
1:A:100:GLY:HA3	1:A:108:PHE:HB2	2.01	0.42
1:A:221:LEU:CG	1:A:222:PRO:CD	2.96	0.42
1:A:263:ALA:O	2:B:6:PRO:HA	2.19	0.42
1:C:57:ARG:HD3	1:C:57:ARG:HA	1.79	0.42
1:C:75:PRO:C	1:C:76:THR:HG1	2.20	0.42
1:C:201:MET:CB	1:C:206:TRP:HZ3	2.31	0.42
1:C:226:THR:HG22	1:C:227:GLN:HG2	2.01	0.42
1:C:292:LEU:O	1:C:293:GLN:HG2	2.19	0.42
1:C:403:GLU:HG2	1:C:407:ARG:HH21	1.84	0.42
1:C:417:ASP:C	1:C:419:ALA:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:451:VAL:CG1	1:C:456:LYS:H	2.33	0.42
1:C:462:ILE:O	1:C:463:ILE:C	2.57	0.42
1:C:476:SER:O	1:C:479:LEU:HG	2.19	0.42
1:E:40:THR:CG2	1:E:41:LEU:N	2.82	0.42
4:E:501:NAG:H5	4:E:501:NAG:N2	2.29	0.42
1:A:284:LYS:HG3	1:A:285:CYS:N	2.33	0.42
1:A:450:GLY:O	2:B:9:GLY:HA3	2.19	0.42
1:C:142:THR:HB	1:C:159:GLY:CA	2.42	0.42
1:C:411:ARG:NH2	1:C:411:ARG:HB2	2.34	0.42
1:E:279:PHE:O	1:E:280:THR:O	2.37	0.42
1:E:309:VAL:O	1:E:310:LYS:HG2	2.20	0.42
1:E:406:MET:HA	1:E:406:MET:CE	2.49	0.42
1:E:479:LEU:O	1:E:482:VAL:N	2.52	0.42
2:F:35:TRP:NE1	2:F:39:HIS:CD2	2.88	0.42
1:A:59:TYR:N	1:A:59:TYR:CD1	2.87	0.42
1:A:198:LEU:HD12	1:A:272:MET:HE1	2.02	0.42
1:A:256:GLN:HA	1:A:256:GLN:NE2	2.34	0.42
1:A:308:VAL:HA	1:A:324:VAL:HA	2.01	0.42
1:C:53:PRO:HG3	1:C:130:VAL:HG13	2.01	0.42
1:C:248:GLN:NE2	1:C:248:GLN:C	2.73	0.42
2:D:48:ILE:HA	2:D:48:ILE:HD13	1.79	0.42
1:E:70:THR:HB	1:E:115:THR:OG1	2.20	0.42
1:E:150:ALA:HB2	3:I:1:NAG:C7	2.49	0.42
1:E:203:ASN:CB	1:E:204:LYS:NZ	2.71	0.42
1:E:242:ASN:HB2	1:E:248:GLN:CB	2.49	0.42
1:E:310:LYS:HD3	1:E:310:LYS:HA	1.72	0.42
1:E:373:PHE:CB	1:E:397:SER:H	2.32	0.42
1:E:443:ILE:O	1:E:446:ALA:N	2.53	0.42
1:E:470:SER:HB2	1:E:475:LEU:HB3	2.01	0.42
1:A:61:ILE:HD13	1:A:255:SER:HB2	2.01	0.42
1:A:99:ARG:CZ	1:A:105:CYS:SG	3.07	0.42
1:A:218:LEU:HB3	1:A:219:PRO:HD2	2.01	0.42
1:A:318:GLY:O	1:A:320:ILE:N	2.46	0.42
1:A:330:GLY:HA2	1:A:361:LYS:HD2	2.02	0.42
1:A:367:ILE:HG22	1:A:368:GLU:N	2.34	0.42
1:A:487:LEU:O	1:A:488:TYR:C	2.57	0.42
1:C:173:ALA:HB3	1:C:181:VAL:CG1	2.47	0.42
1:C:195:GLU:O	1:C:209:HIS:CD2	2.72	0.42
1:C:196:MET:HE3	2:D:12:LEU:HD23	2.02	0.42
1:C:331:SER:O	1:C:332:PRO:O	2.37	0.42
1:E:37:ASN:HB2	1:E:38:LYS:HZ2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:LYS:HB3	1:E:58:LYS:HZ3	1.83	0.42
1:E:282:HIS:O	1:E:282:HIS:ND1	2.49	0.42
1:E:463:ILE:HG12	1:E:481:LEU:HD23	2.02	0.42
1:A:3:CYS:O	1:A:3:CYS:SG	2.78	0.42
1:A:98:ASP:O	1:A:100:GLY:N	2.53	0.42
1:A:169:SER:HB2	1:E:389:LEU:HA	2.02	0.42
1:A:185:CYS:C	1:A:187:PRO:HD3	2.40	0.42
1:A:283:LEU:HD11	1:A:284:LYS:O	2.19	0.42
1:C:239:THR:O	1:C:250:VAL:HA	2.20	0.42
1:C:302:CYS:SG	1:C:333:CYS:N	2.93	0.42
2:D:67:LEU:O	2:D:68:THR:C	2.58	0.42
2:D:69:ALA:O	2:D:70:VAL:C	2.58	0.42
1:E:19:SER:CA	1:E:289:MET:HB2	2.49	0.42
1:E:183:MET:SD	1:E:183:MET:N	2.90	0.42
1:E:204:LYS:HE3	1:E:204:LYS:CA	2.49	0.42
1:E:456:LYS:O	1:E:457:ILE:C	2.57	0.42
2:F:38:ARG:CZ	2:F:38:ARG:CA	2.94	0.42
2:F:45:MET:O	2:F:48:ILE:HB	2.20	0.42
1:A:337:PHE:HD2	1:A:367:ILE:HD13	1.79	0.42
1:A:414:ILE:HA	1:A:414:ILE:HD13	1.63	0.42
1:C:141:ILE:O	1:C:142:THR:CB	2.68	0.42
1:C:398:ILE:HA	1:C:401:MET:HB2	2.02	0.42
1:C:455:MET:HE2	1:C:455:MET:O	2.20	0.42
2:D:29:ALA:O	2:D:30:GLN:C	2.56	0.42
2:D:52:THR:HG23	2:D:53:ILE:N	2.34	0.42
1:E:135:LEU:N	1:E:135:LEU:CD2	2.71	0.42
1:E:348:LEU:HD22	1:E:350:ARG:NH1	2.35	0.42
1:A:404:THR:O	1:A:405:THR:C	2.58	0.42
1:A:475:LEU:O	1:A:478:SER:N	2.53	0.42
1:C:108:PHE:HD1	1:E:315:THR:HG21	1.83	0.42
1:C:312:ILE:CD1	1:C:391:TRP:HE1	2.04	0.42
2:D:19:TRP:HD1	2:D:20:MET:SD	2.43	0.42
1:E:46:ILE:HG22	1:E:140:VAL:HG13	2.02	0.42
1:E:86:GLN:C	1:E:88:LYS:H	2.23	0.42
1:E:305:LYS:HD2	1:E:327:GLU:CA	2.50	0.42
1:E:351:LEU:HD13	1:E:367:ILE:HD13	2.02	0.42
1:E:351:LEU:HD21	1:E:356:PRO:CD	2.50	0.42
1:E:414:ILE:N	1:E:414:ILE:CD1	2.73	0.42
1:A:74:CYS:O	1:A:75:PRO:O	2.37	0.42
1:A:339:ILE:CB	1:A:349:GLY:HA2	2.50	0.42
1:A:459:ILE:O	1:A:463:ILE:CG2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:SER:O	1:C:276:ASN:N	2.53	0.42
1:C:384:PRO:HB2	1:C:386:GLN:OE1	2.20	0.42
1:C:464:THR:O	1:C:468:MET:N	2.53	0.42
1:C:489:LEU:HD22	1:C:493:VAL:CG2	2.50	0.42
1:E:37:ASN:O	1:E:38:LYS:HB2	2.20	0.42
1:E:122:LYS:HB3	1:E:123:LYS:HZ3	1.85	0.42
1:E:126:LYS:O	1:E:128:LYS:N	2.52	0.42
1:E:220:TRP:CB	1:E:232:ILE:O	2.68	0.42
1:E:267:ALA:N	2:F:18:THR:HG21	2.35	0.42
1:E:315:THR:CG2	1:E:316:GLN:N	2.82	0.42
1:E:367:ILE:HD12	1:E:368:GLU:H	1.75	0.42
1:E:476:SER:HA	1:E:479:LEU:CG	2.46	0.42
1:E:478:SER:O	1:E:481:LEU:N	2.51	0.42
2:F:56:THR:CA	2:F:59:GLN:HB3	2.50	0.42
1:A:56:LEU:CD1	1:A:214:LEU:HD21	2.47	0.41
1:A:356:PRO:O	1:A:357:ILE:HG22	2.19	0.41
1:A:376:SER:C	1:A:377:TYR:HD2	2.22	0.41
2:B:32:ILE:CG1	2:B:33:GLU:N	2.83	0.41
2:B:56:THR:CB	2:B:59:GLN:HB2	2.49	0.41
1:C:19:SER:HB2	1:C:20:TRP:CE3	2.55	0.41
1:C:93:LYS:HG2	1:C:240:PHE:CD2	2.55	0.41
1:C:97:VAL:CG1	1:C:113:ILE:CG2	2.98	0.41
1:C:295:LYS:HB3	1:C:295:LYS:HZ2	1.85	0.41
1:C:440:PHE:O	1:C:443:ILE:HG22	2.20	0.41
1:A:27:HIS:NE2	1:A:279:PHE:CG	2.88	0.41
1:A:59:TYR:O	1:A:124:ASN:HB2	2.20	0.41
1:A:78:GLY:C	1:A:80:PRO:HD3	2.40	0.41
1:A:277:LEU:HD23	1:A:277:LEU:N	2.34	0.41
1:A:317:HIS:C	1:A:319:THR:H	2.23	0.41
1:A:338:GLU:HB2	1:A:379:ILE:HG23	2.01	0.41
2:B:33:GLU:CA	2:B:36:ILE:HG22	2.50	0.41
2:B:37:LEU:HD23	2:B:38:ARG:CA	2.50	0.41
1:C:30:CYS:O	1:C:30:CYS:SG	2.78	0.41
1:C:290:ASP:O	1:C:291:LYS:C	2.59	0.41
1:C:324:VAL:O	1:C:324:VAL:CG2	2.65	0.41
1:C:378:ILE:CG2	1:C:389:LEU:HB2	2.50	0.41
1:C:464:THR:OG1	1:C:482:VAL:HG11	2.20	0.41
2:D:19:TRP:CD1	2:D:19:TRP:C	2.92	0.41
1:E:138:THR:HG22	1:E:163:LYS:CD	2.38	0.41
1:E:200:GLN:N	1:E:200:GLN:OE1	2.53	0.41
1:E:305:LYS:HE3	1:E:327:GLU:HB3	1.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:310:LYS:HG2	1:E:323:ARG:HD2	2.01	0.41
1:A:339:ILE:HB	1:A:349:GLY:HA2	2.01	0.41
1:A:360:GLU:C	1:A:362:ASP:N	2.71	0.41
1:A:452:SER:O	1:A:453:TRP:C	2.59	0.41
1:A:482:VAL:O	1:A:483:GLY:O	2.38	0.41
2:B:37:LEU:HD21	2:B:38:ARG:CZ	2.49	0.41
1:C:2:ARG:O	1:C:6:ILE:HG21	2.19	0.41
1:C:318:GLY:CA	1:C:393:LYS:NZ	2.83	0.41
1:E:152:GLY:O	1:E:153:ASN:C	2.59	0.41
1:E:473:THR:HA	1:E:475:LEU:HD22	2.01	0.41
2:F:7:HIS:CD2	2:F:7:HIS:O	2.73	0.41
1:A:37:ASN:O	1:A:38:LYS:HD2	2.20	0.41
1:A:441:GLY:O	1:A:443:ILE:O	2.39	0.41
2:B:31:ARG:O	2:B:34:THR:HB	2.19	0.41
1:C:85:GLU:HG3	1:C:92:CYS:SG	2.60	0.41
1:C:205:ALA:O	1:C:206:TRP:CG	2.73	0.41
1:C:231:TRP:H	1:C:231:TRP:HD1	1.68	0.41
1:C:332:PRO:HG2	1:C:360:GLU:HA	2.02	0.41
1:E:34:MET:HE3	1:E:34:MET:H	1.86	0.41
1:E:106:GLY:C	1:E:107:LEU:CD1	2.78	0.41
1:A:39:PRO:O	1:A:39:PRO:HG2	2.21	0.41
1:A:206:TRP:CG	1:A:264:LEU:HD21	2.55	0.41
1:A:212:TRP:O	1:A:214:LEU:N	2.54	0.41
1:A:337:PHE:CD1	1:A:338:GLU:N	2.88	0.41
1:A:436:LEU:HD22	1:A:436:LEU:O	2.19	0.41
1:A:444:TYR:HB3	1:A:445:GLY:H	1.62	0.41
1:C:403:GLU:HG2	1:C:407:ARG:NH2	2.35	0.41
1:C:434:LYS:C	1:C:434:LYS:CD	2.84	0.41
2:D:70:VAL:HG23	2:D:71:ALA:N	2.36	0.41
1:E:148:GLU:HG3	1:E:323:ARG:NH1	2.32	0.41
1:E:303:THR:CG2	1:E:304:GLY:H	2.33	0.41
1:E:397:SER:O	1:E:398:ILE:C	2.57	0.41
1:A:22:ASP:HB2	1:A:424:SER:CA	2.48	0.41
1:A:43:PHE:CD2	1:A:141:ILE:CG2	3.04	0.41
1:A:90:PHE:HA	1:A:118:MET:HA	2.03	0.41
1:A:97:VAL:O	1:A:99:ARG:N	2.43	0.41
1:A:208:VAL:O	1:A:209:HIS:C	2.59	0.41
1:A:256:GLN:OE1	2:B:2:VAL:HG21	2.21	0.41
1:A:259:ALA:O	1:A:260:MET:C	2.58	0.41
1:A:312:ILE:C	1:A:320:ILE:HD11	2.41	0.41
1:A:318:GLY:H	1:A:393:LYS:HE3	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:GLY:O	1:A:428:VAL:CB	2.68	0.41
1:C:145:SER:O	1:C:146:GLY:C	2.58	0.41
1:E:232:ILE:HD13	1:E:232:ILE:N	2.35	0.41
1:E:237:LEU:HD12	1:E:237:LEU:HA	1.73	0.41
1:E:316:GLN:O	1:E:317:HIS:CD2	2.74	0.41
1:E:321:VAL:HG23	1:E:367:ILE:O	2.20	0.41
1:E:403:GLU:HA	1:E:406:MET:HB2	2.03	0.41
1:E:411:ARG:HD2	1:E:422:PHE:CE1	2.55	0.41
2:F:5:VAL:HG23	2:F:5:VAL:O	2.21	0.41
2:F:48:ILE:O	2:F:50:ALA:N	2.53	0.41
1:A:191:LEU:HD13	1:A:193:PHE:CZ	2.55	0.41
1:A:194:ASN:C	1:A:195:GLU:HG2	2.40	0.41
1:A:231:TRP:O	1:A:232:ILE:C	2.59	0.41
1:A:358:VAL:C	1:A:359:THR:HG1	2.24	0.41
1:C:24:VAL:HG12	1:C:25:LEU:H	1.84	0.41
1:C:97:VAL:O	1:C:97:VAL:CG2	2.68	0.41
1:C:323:ARG:HG2	1:C:366:ASN:HB3	2.03	0.41
1:C:341:ASP:HB2	1:C:348:LEU:CD1	2.50	0.41
2:D:65:ILE:HG22	2:D:66:LEU:H	1.86	0.41
1:E:99:ARG:CB	1:E:109:GLY:O	2.66	0.41
1:E:191:LEU:CD1	1:E:191:LEU:N	2.84	0.41
1:E:195:GLU:O	1:E:209:HIS:CB	2.64	0.41
1:E:207:LEU:HD13	1:E:207:LEU:N	2.36	0.41
1:E:233:GLN:O	1:E:234:LYS:HB2	2.21	0.41
1:E:247:LYS:O	1:E:248:GLN:HB3	2.20	0.41
1:E:304:GLY:HA2	1:E:306:PHE:CE1	2.56	0.41
1:E:405:THR:O	1:E:406:MET:C	2.58	0.41
2:F:56:THR:C	2:F:59:GLN:HB3	2.41	0.41
1:A:57:ARG:NH1	1:A:220:TRP:CZ3	2.89	0.41
1:A:144:HIS:ND1	1:A:144:HIS:N	2.69	0.41
1:A:166:PRO:HG3	1:A:187:PRO:HB2	2.03	0.41
1:A:277:LEU:HG	1:A:277:LEU:O	2.20	0.41
1:A:339:ILE:HD13	1:A:339:ILE:HA	1.80	0.41
1:A:342:LEU:O	1:A:344:LYS:N	2.54	0.41
1:A:346:HIS:O	1:A:346:HIS:CG	2.73	0.41
1:A:398:ILE:C	1:A:400:GLN:N	2.73	0.41
1:A:465:TRP:C	1:A:467:GLY:H	2.22	0.41
2:B:41:GLY:O	2:B:44:ILE:CB	2.69	0.41
1:E:35:ALA:HB3	1:E:38:LYS:CE	2.45	0.41
1:E:39:PRO:CD	1:E:294:LEU:HA	2.47	0.41
1:E:61:ILE:CD1	1:E:124:ASN:HA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:443:ILE:C	1:E:445:GLY:N	2.73	0.41
1:A:2:ARG:NH2	1:A:44:GLU:HG2	2.35	0.41
1:A:144:HIS:O	1:A:145:SER:OG	2.36	0.41
1:A:160:LYS:HE3	1:A:160:LYS:HA	2.02	0.41
1:A:186:SER:O	1:A:188:ARG:N	2.54	0.41
1:A:191:LEU:CD2	1:A:196:MET:HG3	2.51	0.41
1:A:239:THR:C	1:A:240:PHE:HD2	2.24	0.41
1:A:243:PRO:O	1:A:244:HIS:CB	2.68	0.41
1:A:246:LYS:HB3	1:A:247:LYS:H	1.75	0.41
1:A:316:GLN:O	1:A:317:HIS:CB	2.68	0.41
1:A:335:ILE:HG12	1:A:358:VAL:HG13	2.02	0.41
1:A:342:LEU:HD11	1:A:375:ASP:HB2	2.03	0.41
1:A:355:ASN:O	1:A:356:PRO:O	2.39	0.41
1:A:411:ARG:CZ	1:A:422:PHE:CE1	3.04	0.41
2:B:14:THR:OG1	2:B:15:ALA:N	2.50	0.41
1:C:108:PHE:O	1:C:109:GLY:C	2.59	0.41
1:C:142:THR:OG1	1:C:143:PRO:CD	2.69	0.41
1:C:247:LYS:HA	1:C:247:LYS:CE	2.49	0.41
1:C:338:GLU:HB2	1:C:379:ILE:HG13	2.03	0.41
1:C:354:VAL:C	1:C:356:PRO:HD3	2.41	0.41
2:D:51:TYR:CD2	2:D:60:ARG:NH1	2.89	0.41
1:E:25:LEU:HD11	1:E:283:LEU:CD2	2.41	0.41
1:E:34:MET:SD	1:E:34:MET:C	2.99	0.41
1:E:57:ARG:HH12	1:E:214:LEU:HD22	1.85	0.41
1:E:72:SER:HB3	1:E:113:ILE:HG13	2.02	0.41
1:E:74:CYS:O	1:E:77:GLN:NE2	2.54	0.41
1:E:80:PRO:HG2	1:E:113:ILE:N	2.36	0.41
1:E:93:LYS:N	1:E:240:PHE:HE2	2.19	0.41
1:E:206:TRP:CD1	1:E:264:LEU:HD13	2.55	0.41
1:E:216:LEU:HD21	2:F:2:VAL:HG12	2.03	0.41
1:E:252:VAL:HG12	1:E:254:GLY:N	2.23	0.41
1:E:307:LYS:NZ	1:E:307:LYS:CB	2.83	0.41
1:E:350:ARG:HH22	1:E:372:PRO:HD3	1.86	0.41
1:A:123:LYS:C	1:A:124:ASN:O	2.59	0.41
1:A:141:ILE:HD13	1:A:141:ILE:H	1.86	0.41
1:A:360:GLU:O	1:A:362:ASP:N	2.53	0.41
1:A:373:PHE:HB2	1:A:395:GLY:C	2.41	0.41
1:A:493:VAL:O	1:A:494:GLN:C	2.59	0.41
1:C:100:GLY:C	1:C:102:GLY:N	2.73	0.41
1:C:147:GLU:HB3	1:C:149:HIS:ND1	2.36	0.41
1:C:191:LEU:HD21	1:C:281:GLY:CA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:ALA:C	1:C:206:TRP:CD2	2.95	0.41
1:C:296:GLY:O	1:C:297:MET:C	2.60	0.41
1:C:320:ILE:H	1:C:320:ILE:HG23	1.63	0.41
1:E:67:ASN:HB2	1:E:118:MET:CG	2.51	0.41
1:E:134:ASN:C	1:E:135:LEU:HD23	2.41	0.41
1:E:257:GLU:O	1:E:258:GLY:C	2.58	0.41
1:E:402:ILE:HD13	1:E:402:ILE:HA	1.95	0.41
1:E:437:HIS:ND1	1:E:437:HIS:C	2.74	0.41
1:E:471:ARG:HB3	1:E:471:ARG:CZ	2.51	0.41
1:A:62:GLU:HB3	1:A:122:LYS:HB3	2.02	0.40
1:A:73:ARG:O	1:A:74:CYS:CB	2.69	0.40
1:A:90:PHE:HE2	1:A:118:MET:HE2	1.85	0.40
1:A:256:GLN:NE2	1:A:256:GLN:CA	2.85	0.40
1:A:276:ASN:C	1:A:276:ASN:OD1	2.59	0.40
1:A:441:GLY:O	1:A:446:ALA:CB	2.63	0.40
1:C:40:THR:O	1:C:40:THR:HG23	2.21	0.40
1:C:130:VAL:O	1:C:131:GLN:CB	2.68	0.40
1:C:372:PRO:HG2	1:C:376:SER:OG	2.20	0.40
1:C:409:ALA:O	1:C:412:MET:N	2.54	0.40
1:C:431:SER:O	1:C:434:LYS:HB3	2.21	0.40
1:E:15:VAL:HG23	1:E:21:VAL:HG12	2.03	0.40
1:E:60:CYS:C	1:E:61:ILE:HD12	2.41	0.40
1:E:114:VAL:HG22	1:E:115:THR:N	2.35	0.40
1:E:169:SER:O	1:E:170:ILE:O	2.39	0.40
1:E:265:THR:HG22	2:F:19:TRP:CD1	2.56	0.40
1:E:457:ILE:HG22	1:E:458:LEU:N	2.36	0.40
2:F:34:THR:O	2:F:35:TRP:C	2.60	0.40
2:F:56:THR:HB	2:F:59:GLN:HB2	2.01	0.40
1:A:16:SER:HB2	1:A:425:LEU:HD12	2.03	0.40
1:A:25:LEU:HD12	1:A:45:LEU:CB	2.44	0.40
1:A:48:THR:O	1:A:48:THR:HG23	2.21	0.40
1:A:135:LEU:HD11	1:A:193:PHE:CZ	2.56	0.40
2:B:39:HIS:O	2:B:40:PRO:C	2.60	0.40
1:C:191:LEU:O	1:C:193:PHE:CD2	2.73	0.40
1:C:202:GLU:O	1:C:203:ASN:HB3	2.20	0.40
1:C:214:LEU:HD22	1:C:214:LEU:HA	1.78	0.40
1:C:237:LEU:CA	1:C:253:LEU:HD23	2.40	0.40
1:C:383:GLU:O	1:C:385:GLY:N	2.54	0.40
1:E:99:ARG:N	1:E:103:ASN:HD21	2.20	0.40
1:E:212:TRP:C	1:E:214:LEU:N	2.73	0.40
1:E:339:ILE:HD13	1:E:339:ILE:HA	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:373:PHE:HA	1:E:393:LYS:HD3	1.97	0.40
2:F:68:THR:O	2:F:69:ALA:C	2.60	0.40
1:A:23:ILE:HD12	1:A:23:ILE:H	1.87	0.40
1:A:121:CYS:SG	1:A:231:TRP:CZ2	3.13	0.40
1:A:199:LEU:C	1:A:199:LEU:CD1	2.85	0.40
1:A:229:SER:O	1:A:231:TRP:CD1	2.74	0.40
1:A:295:LYS:C	1:A:297:MET:N	2.73	0.40
1:C:9:ARG:HA	1:C:30:CYS:O	2.21	0.40
1:C:65:LEU:HG	1:C:252:VAL:HG12	2.03	0.40
1:C:152:GLY:O	1:C:154:ASP:N	2.55	0.40
1:C:237:LEU:HD23	1:C:237:LEU:N	2.33	0.40
1:C:301:MET:O	1:C:301:MET:HG3	2.21	0.40
1:C:304:GLY:N	1:C:382:VAL:HG21	2.21	0.40
1:C:402:ILE:HG23	1:C:403:GLU:N	2.36	0.40
1:C:485:VAL:HG12	1:C:486:THR:N	2.36	0.40
2:D:56:THR:C	2:D:58:PHE:N	2.74	0.40
1:E:25:LEU:O	1:E:45:LEU:HD12	2.21	0.40
1:E:94:HIS:N	1:E:114:VAL:HG23	2.37	0.40
1:E:170:ILE:HG23	1:E:184:GLU:HA	2.04	0.40
1:E:339:ILE:O	1:E:348:LEU:C	2.60	0.40
1:E:451:VAL:CG1	1:E:455:MET:HB3	2.52	0.40
1:E:463:ILE:O	1:E:464:THR:C	2.57	0.40
1:A:330:GLY:HA2	1:A:361:LYS:CG	2.51	0.40
1:C:149:HIS:HD2	1:C:158:HIS:CE1	2.39	0.40
1:C:355:ASN:ND2	1:C:357:ILE:HG12	2.37	0.40
1:C:430:THR:O	1:C:433:GLY:N	2.54	0.40
1:E:46:ILE:O	1:E:47:GLU:C	2.60	0.40
1:E:265:THR:CB	2:F:20:MET:HB2	2.51	0.40
1:E:393:LYS:HB3	1:E:394:LYS:H	1.60	0.40
1:E:465:TRP:O	1:E:468:MET:HB3	2.22	0.40
1:A:45:LEU:HD22	1:A:45:LEU:HA	1.84	0.40
1:A:46:ILE:O	1:A:47:GLU:C	2.60	0.40
1:A:49:GLU:CG	1:A:50:ALA:N	2.85	0.40
1:A:86:GLN:HA	1:C:230:ASN:ND2	2.35	0.40
1:A:131:GLN:HE21	1:A:131:GLN:N	2.14	0.40
1:A:181:VAL:CG1	1:A:182:THR:N	2.84	0.40
1:A:420:TRP:HD1	1:A:420:TRP:H	1.68	0.40
1:A:438:GLN:OE1	1:A:438:GLN:CA	2.68	0.40
1:A:454:ILE:HG12	1:A:455:MET:N	2.36	0.40
1:A:457:ILE:C	1:A:457:ILE:HD12	2.42	0.40
1:C:73:ARG:CD	1:C:77:GLN:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:ALA:HB2	1:E:259:ALA:HB2	2.04	0.40
1:C:310:LYS:HD2	1:E:101:TRP:CH2	2.57	0.40
1:E:209:HIS:CD2	2:F:10:MET:HB3	2.56	0.40
1:E:262:THR:C	1:E:265:THR:HG23	2.41	0.40
1:E:413:ALA:O	1:E:414:ILE:C	2.59	0.40
1:E:488:TYR:O	1:E:492:MET:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	493/495 (100%)	238 (48%)	130 (26%)	125 (25%)	0	0
1	C	493/495 (100%)	260 (53%)	113 (23%)	120 (24%)	0	0
1	E	493/495 (100%)	253 (51%)	123 (25%)	117 (24%)	0	0
2	B	70/75 (93%)	32 (46%)	22 (31%)	16 (23%)	0	1
2	D	70/75 (93%)	32 (46%)	20 (29%)	18 (26%)	0	0
2	F	70/75 (93%)	26 (37%)	27 (39%)	17 (24%)	0	0
All	All	1689/1710 (99%)	841 (50%)	435 (26%)	413 (24%)	0	0

All (413) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	27	HIS
1	A	36	LYS
1	A	74	CYS
1	A	75	PRO
1	A	77	GLN

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Mol	Chain	Res	Type
1	A	80	PRO
1	A	134	ASN
1	A	150	ALA
1	A	192	ASP
1	A	202	GLU
1	A	217	PRO
1	A	222	PRO
1	A	224	ALA
1	A	233	GLN
1	A	238	VAL
1	A	247	LYS
1	A	253	LEU
1	A	256	GLN
1	A	270	ILE
1	A	279	PHE
1	A	295	LYS
1	A	298	SER
1	A	300	SER
1	A	310	LYS
1	A	316	GLN
1	A	317	HIS
1	A	342	LEU
1	A	346	HIS
1	A	347	VAL
1	A	355	ASN
1	A	356	PRO
1	A	357	ILE
1	A	365	VAL
1	A	383	GLU
1	A	386	GLN
1	A	392	PHE
1	A	394	LYS
1	A	414	ILE
1	A	429	PHE
1	A	453	TRP
1	A	468	MET
1	A	472	SER
1	A	483	GLY
1	A	485	VAL
2	B	8	VAL
2	B	9	GLY
2	B	23	GLU

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Mol	Chain	Res	Type
2	B	41	GLY
1	C	16	SER
1	C	37	ASN
1	C	40	THR
1	C	46	ILE
1	C	58	LYS
1	C	68	THR
1	C	77	GLN
1	C	84	GLU
1	C	88	LYS
1	C	108	PHE
1	C	109	GLY
1	C	150	ALA
1	C	160	LYS
1	C	170	ILE
1	C	192	ASP
1	C	203	ASN
1	C	217	PRO
1	C	222	PRO
1	C	229	SER
1	C	238	VAL
1	C	257	GLU
1	C	264	LEU
1	C	274	SER
1	C	276	ASN
1	C	280	THR
1	C	300	SER
1	C	302	CYS
1	C	304	GLY
1	C	317	HIS
1	C	318	GLY
1	C	332	PRO
1	C	346	HIS
1	C	347	VAL
1	C	353	THR
1	C	354	VAL
1	C	363	SER
1	C	382	VAL
1	C	386	GLN
1	C	394	LYS
1	C	414	ILE
1	C	416	GLY

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Mol	Chain	Res	Type
1	C	427	GLY
1	C	428	VAL
1	C	438	GLN
1	C	447	ALA
1	C	454	ILE
1	C	471	ARG
1	C	484	VAL
1	C	494	GLN
2	D	8	VAL
2	D	9	GLY
2	D	19	TRP
2	D	51	TYR
2	D	53	ILE
2	D	70	VAL
2	D	71	ALA
1	E	8	ASN
1	E	57	ARG
1	E	59	TYR
1	E	80	PRO
1	E	88	LYS
1	E	106	GLY
1	E	108	PHE
1	E	113	ILE
1	E	127	GLY
1	E	134	ASN
1	E	144	HIS
1	E	145	SER
1	E	150	ALA
1	E	169	SER
1	E	188	ARG
1	E	193	PHE
1	E	203	ASN
1	E	211	GLN
1	E	222	PRO
1	E	233	GLN
1	E	237	LEU
1	E	238	VAL
1	E	244	HIS
1	E	247	LYS
1	E	270	ILE
1	E	278	LEU
1	E	280	THR

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Mol	Chain	Res	Type
1	E	290	ASP
1	E	291	LYS
1	E	305	LYS
1	E	311	GLU
1	E	312	ILE
1	E	316	GLN
1	E	319	THR
1	E	332	PRO
1	E	344	LYS
1	E	345	ARG
1	E	347	VAL
1	E	354	VAL
1	E	362	ASP
1	E	382	VAL
1	E	383	GLU
1	E	393	LYS
1	E	397	SER
1	E	410	LYS
1	E	414	ILE
1	E	417	ASP
1	E	421	ASP
1	E	425	LEU
1	E	428	VAL
1	E	429	PHE
1	E	443	ILE
1	E	448	PHE
1	E	468	MET
1	E	470	SER
1	E	473	THR
1	E	491	VAL
2	F	7	HIS
2	F	10	MET
2	F	13	GLU
2	F	55	THR
2	F	56	THR
2	F	70	VAL
1	A	2	ARG
1	A	18	GLY
1	A	37	ASN
1	A	58	LYS
1	A	99	ARG
1	A	101	TRP

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Mol	Chain	Res	Type
1	A	126	LYS
1	A	144	HIS
1	A	146	GLY
1	A	156	GLY
1	A	176	THR
1	A	188	ARG
1	A	195	GLU
1	A	211	GLN
1	A	215	ASP
1	A	228	GLY
1	A	245	ALA
1	A	258	GLY
1	A	262	THR
1	A	272	MET
1	A	278	LEU
1	A	285	CYS
1	A	301	MET
1	A	344	LYS
1	A	381	GLY
1	A	395	GLY
1	A	406	MET
1	A	407	ARG
1	A	417	ASP
1	A	418	THR
1	A	428	VAL
1	A	438	GLN
1	A	451	VAL
1	A	454	ILE
1	A	474	SER
1	A	484	VAL
1	A	487	LEU
1	A	493	VAL
1	A	494	GLN
2	B	6	PRO
2	B	10	MET
2	B	57	HIS
1	C	9	ARG
1	C	27	HIS
1	C	30	CYS
1	C	123	LYS
1	C	145	SER
1	C	146	GLY

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Mol	Chain	Res	Type
1	C	147	GLU
1	C	153	ASN
1	C	176	THR
1	C	177	GLY
1	C	210	ARG
1	C	226	THR
1	C	228	GLY
1	C	253	LEU
1	C	254	GLY
1	C	270	ILE
1	C	278	LEU
1	C	289	MET
1	C	365	VAL
1	C	376	SER
1	C	395	GLY
1	C	435	ALA
1	C	474	SER
1	C	482	VAL
2	D	7	HIS
2	D	14	THR
2	D	28	HIS
2	D	50	ALA
2	D	59	GLN
2	D	69	ALA
1	E	7	SER
1	E	40	THR
1	E	77	GLN
1	E	84	GLU
1	E	105	CYS
1	E	112	GLY
1	E	147	GLU
1	E	153	ASN
1	E	170	ILE
1	E	218	LEU
1	E	225	ASP
1	E	258	GLY
1	E	264	LEU
1	E	313	ALA
1	E	330	GLY
1	E	359	THR
1	E	394	LYS
1	E	408	GLY

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Mol	Chain	Res	Type
1	E	416	GLY
1	E	450	GLY
1	E	453	TRP
1	E	461	VAL
1	E	472	SER
1	E	483	GLY
2	F	2	VAL
2	F	15	ALA
2	F	17	GLU
1	A	88	LYS
1	A	98	ASP
1	A	106	GLY
1	A	110	LYS
1	A	124	ASN
1	A	231	TRP
1	A	290	ASP
1	A	332	PRO
1	A	382	VAL
1	A	444	TYR
2	B	18	THR
2	B	40	PRO
2	B	46	ALA
2	B	66	LEU
1	C	7	SER
1	C	19	SER
1	C	35	ALA
1	C	57	ARG
1	C	106	GLY
1	C	164	ILE
1	C	201	MET
1	C	234	LYS
1	C	245	ALA
1	C	255	SER
1	C	261	HIS
1	C	273	SER
1	C	279	PHE
1	C	364	PRO
1	C	444	TYR
1	C	453	TRP
2	D	49	LEU
1	E	68	THR
1	E	76	THR

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Mol	Chain	Res	Type
1	E	78	GLY
1	E	151	VAL
1	E	160	LYS
1	E	176	THR
1	E	257	GLU
1	E	271	GLN
1	E	276	ASN
1	E	295	LYS
1	E	302	CYS
1	E	317	HIS
1	E	395	GLY
1	E	487	LEU
2	F	22	SER
2	F	25	ALA
2	F	54	GLY
2	F	64	PHE
1	A	38	LYS
1	A	84	GLU
1	A	155	THR
1	A	178	TYR
1	A	193	PHE
1	A	221	LEU
1	A	289	MET
1	A	343	GLU
1	A	354	VAL
1	A	361	LYS
1	A	371	PRO
1	A	393	LYS
1	A	430	THR
1	A	435	ALA
1	A	473	THR
1	A	488	TYR
2	B	34	THR
2	B	55	THR
2	B	71	ALA
1	C	47	GLU
1	C	110	LYS
1	C	131	GLN
1	C	269	GLU
1	C	344	LYS
1	C	424	SER
1	C	451	VAL

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Mol	Chain	Res	Type
2	D	48	ILE
2	D	60	ARG
1	E	2	ARG
1	E	46	ILE
1	E	126	LYS
1	E	268	THR
1	E	361	LYS
1	A	40	THR
1	A	128	LYS
1	A	147	GLU
1	A	166	PRO
1	A	225	ASP
1	A	255	SER
1	A	292	LEU
1	A	312	ILE
2	B	56	THR
1	C	169	SER
1	C	186	SER
1	C	221	LEU
1	C	305	LYS
1	C	310	LYS
1	C	387	LEU
1	C	396	SER
1	C	430	THR
2	D	16	THR
2	D	55	THR
1	E	16	SER
1	E	18	GLY
1	E	38	LYS
1	E	53	PRO
1	E	194	ASN
1	E	205	ALA
1	E	279	PHE
1	E	430	THR
2	F	6	PRO
2	F	44	ILE
2	F	48	ILE
1	A	76	THR
1	A	445	GLY
2	B	44	ILE
1	C	6	ILE
1	C	125	MET

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Mol	Chain	Res	Type
1	C	190	GLY
1	C	195	GLU
1	C	314	GLU
1	C	329	ASP
1	C	423	GLY
1	C	426	GLY
1	E	75	PRO
1	E	331	SER
1	E	364	PRO
1	E	482	VAL
1	A	46	ILE
1	C	28	GLY
1	C	218	LEU
1	C	243	PRO
1	C	356	PRO
1	C	461	VAL
1	E	493	VAL
1	A	15	VAL
1	A	328	GLY
1	A	490	GLY
1	E	454	ILE
2	F	65	ILE
1	C	132	PRO
1	C	151	VAL
1	A	462	ILE
1	C	5	GLY
1	E	217	PRO
1	E	372	PRO
1	E	485	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	420/420 (100%)	344 (82%)	76 (18%)	1 11
1	C	420/420 (100%)	344 (82%)	76 (18%)	1 11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	420/420 (100%)	328 (78%)	92 (22%)	1 6
2	B	57/60 (95%)	48 (84%)	9 (16%)	2 17
2	D	57/60 (95%)	43 (75%)	14 (25%)	0 4
2	F	57/60 (95%)	52 (91%)	5 (9%)	10 40
All	All	1431/1440 (99%)	1159 (81%)	272 (19%)	4 9

All (272) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	9	ARG
1	A	15	VAL
1	A	20	TRP
1	A	23	ILE
1	A	24	VAL
1	A	25	LEU
1	A	26	GLU
1	A	36	LYS
1	A	51	LYS
1	A	55	THR
1	A	64	LYS
1	A	75	PRO
1	A	77	GLN
1	A	80	PRO
1	A	83	ASN
1	A	97	VAL
1	A	103	ASN
1	A	122	LYS
1	A	125	MET
1	A	131	GLN
1	A	133	GLU
1	A	135	LEU
1	A	139	ILE
1	A	141	ILE
1	A	153	ASN
1	A	160	LYS
1	A	162	ILE
1	A	164	ILE
1	A	170	ILE
1	A	198	LEU
1	A	204	LYS

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Mol	Chain	Res	Type
1	A	207	LEU
1	A	208	VAL
1	A	217	PRO
1	A	220	TRP
1	A	221	LEU
1	A	222	PRO
1	A	246	LYS
1	A	248	GLN
1	A	265	THR
1	A	269	GLU
1	A	278	LEU
1	A	291	LYS
1	A	294	LEU
1	A	305	LYS
1	A	306	PHE
1	A	310	LYS
1	A	312	ILE
1	A	314	GLU
1	A	316	GLN
1	A	317	HIS
1	A	319	THR
1	A	332	PRO
1	A	335	ILE
1	A	337	PHE
1	A	350	ARG
1	A	386	GLN
1	A	390	ASN
1	A	400	GLN
1	A	407	ARG
1	A	414	ILE
1	A	429	PHE
1	A	430	THR
1	A	432	ILE
1	A	436	LEU
1	A	440	PHE
1	A	444	TYR
1	A	448	PHE
1	A	451	VAL
1	A	457	ILE
1	A	461	VAL
1	A	466	ILE
1	A	468	MET

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Mol	Chain	Res	Type
1	A	474	SER
1	A	492	MET
2	B	14	THR
2	B	26	TRP
2	B	31	ARG
2	B	37	LEU
2	B	38	ARG
2	B	42	PHE
2	B	63	ILE
2	B	65	ILE
2	B	72	PRO
1	C	1	MET
1	C	2	ARG
1	C	6	ILE
1	C	11	PHE
1	C	22	ASP
1	C	34	MET
1	C	36	LYS
1	C	38	LYS
1	C	46	ILE
1	C	48	THR
1	C	52	GLN
1	C	59	TYR
1	C	65	LEU
1	C	69	THR
1	C	74	CYS
1	C	86	GLN
1	C	91	VAL
1	C	97	VAL
1	C	110	LYS
1	C	119	PHE
1	C	139	ILE
1	C	141	ILE
1	C	144	HIS
1	C	153	ASN
1	C	157	LYS
1	C	164	ILE
1	C	175	LEU
1	C	176	THR
1	C	187	PRO
1	C	204	LYS
1	C	210	ARG

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Mol	Chain	Res	Type
1	C	214	LEU
1	C	220	TRP
1	C	231	TRP
1	C	242	ASN
1	C	244	HIS
1	C	246	LYS
1	C	270	ILE
1	C	271	GLN
1	C	272	MET
1	C	280	THR
1	C	287	LEU
1	C	299	TYR
1	C	301	MET
1	C	303	THR
1	C	316	GLN
1	C	320	ILE
1	C	321	VAL
1	C	322	ILE
1	C	332	PRO
1	C	339	ILE
1	C	340	MET
1	C	346	HIS
1	C	347	VAL
1	C	377	TYR
1	C	378	ILE
1	C	379	ILE
1	C	380	ILE
1	C	382	VAL
1	C	394	LYS
1	C	404	THR
1	C	405	THR
1	C	407	ARG
1	C	410	LYS
1	C	415	LEU
1	C	434	LYS
1	C	437	HIS
1	C	438	GLN
1	C	440	PHE
1	C	455	MET
1	C	464	THR
1	C	471	ARG
1	C	475	LEU

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Mol	Chain	Res	Type
1	C	478	SER
1	C	479	LEU
1	C	489	LEU
2	D	2	VAL
2	D	5	VAL
2	D	10	MET
2	D	20	MET
2	D	28	HIS
2	D	32	ILE
2	D	44	ILE
2	D	48	ILE
2	D	49	LEU
2	D	51	TYR
2	D	57	HIS
2	D	62	LEU
2	D	68	THR
2	D	72	PRO
1	E	9	ARG
1	E	11	PHE
1	E	21	VAL
1	E	30	CYS
1	E	34	MET
1	E	36	LYS
1	E	45	LEU
1	E	52	GLN
1	E	53	PRO
1	E	55	THR
1	E	56	LEU
1	E	58	LYS
1	E	60	CYS
1	E	61	ILE
1	E	73	ARG
1	E	74	CYS
1	E	77	GLN
1	E	88	LYS
1	E	94	HIS
1	E	96	MET
1	E	101	TRP
1	E	118	MET
1	E	122	LYS
1	E	123	LYS
1	E	134	ASN

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Mol	Chain	Res	Type
1	E	135	LEU
1	E	137	TYR
1	E	141	ILE
1	E	144	HIS
1	E	149	HIS
1	E	157	LYS
1	E	165	THR
1	E	171	THR
1	E	178	TYR
1	E	183	MET
1	E	188	ARG
1	E	194	ASN
1	E	196	MET
1	E	200	GLN
1	E	204	LYS
1	E	207	LEU
1	E	218	LEU
1	E	233	GLN
1	E	240	PHE
1	E	241	LYS
1	E	242	ASN
1	E	261	HIS
1	E	268	THR
1	E	269	GLU
1	E	270	ILE
1	E	276	ASN
1	E	284	LYS
1	E	286	ARG
1	E	294	LEU
1	E	299	TYR
1	E	300	SER
1	E	301	MET
1	E	309	VAL
1	E	312	ILE
1	E	332	PRO
1	E	335	ILE
1	E	348	LEU
1	E	350	ARG
1	E	351	LEU
1	E	353	THR
1	E	354	VAL
1	E	355	ASN

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Mol	Chain	Res	Type
1	E	363	SER
1	E	367	ILE
1	E	371	PRO
1	E	373	PHE
1	E	379	ILE
1	E	380	ILE
1	E	382	VAL
1	E	389	LEU
1	E	391	TRP
1	E	398	ILE
1	E	406	MET
1	E	414	ILE
1	E	418	THR
1	E	420	TRP
1	E	422	PHE
1	E	425	LEU
1	E	448	PHE
1	E	457	ILE
1	E	458	LEU
1	E	464	THR
1	E	470	SER
1	E	476	SER
1	E	487	LEU
1	E	488	TYR
1	E	492	MET
2	F	12	LEU
2	F	32	ILE
2	F	37	LEU
2	F	38	ARG
2	F	68	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) 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	144	HIS
1	A	158	HIS
1	A	167	GLN
1	A	233	GLN

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Mol	Chain	Res	Type
1	A	242	ASN
1	A	248	GLN
1	A	386	GLN
1	A	390	ASN
1	A	400	GLN
2	B	7	HIS
1	C	8	ASN
1	C	27	HIS
1	C	37	ASN
1	C	52	GLN
1	C	86	GLN
1	C	124	ASN
1	C	134	ASN
1	C	144	HIS
1	C	200	GLN
1	C	242	ASN
1	C	248	GLN
1	C	293	GLN
1	C	316	GLN
1	C	355	ASN
1	C	494	GLN
2	D	30	GLN
2	D	59	GLN
1	E	52	GLN
1	E	103	ASN
1	E	167	GLN
1	E	194	ASN
1	E	233	GLN
1	E	242	ASN
1	E	248	GLN
1	E	271	GLN
1	E	293	GLN
1	E	355	ASN
1	E	386	GLN
1	E	437	HIS
2	F	57	HIS
2	F	59	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

6 monosaccharides 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	G	1	1,3	14,14,15	0.56	0	17,19,21	0.99	1 (5%)
3	NAG	G	2	3	14,14,15	0.57	0	17,19,21	0.76	1 (5%)
3	NAG	H	1	1,3	14,14,15	0.60	0	17,19,21	0.67	0
3	NAG	H	2	3	14,14,15	0.57	0	17,19,21	0.59	0
3	NAG	I	1	1,3	14,14,15	0.80	0	17,19,21	0.91	2 (11%)
3	NAG	I	2	3	14,14,15	0.83	0	17,19,21	0.89	0

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	G	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	5/6/23/26	0/1/1/1
3	NAG	H	2	3	-	4/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	4/6/23/26	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(^{o})	Ideal(^{o})
3	I	1	NAG	O5-C1-C2	-2.28	107.69	111.29
3	G	2	NAG	C2-N2-C7	-2.23	119.72	122.90
3	I	1	NAG	C2-N2-C7	-2.16	119.83	122.90
3	G	1	NAG	C4-C3-C2	2.09	114.09	111.02

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
3	H	1	NAG	C8-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	I	1	NAG	C1-C2-N2-C7
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
3	G	1	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	I	1	NAG	C8-C7-N2-C2
3	H	2	NAG	O5-C5-C6-O6
3	H	1	NAG	C1-C2-N2-C7
3	I	1	NAG	O7-C7-N2-C2
3	H	1	NAG	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	I	1	NAG	C3-C2-N2-C7

There are no ring outliers.

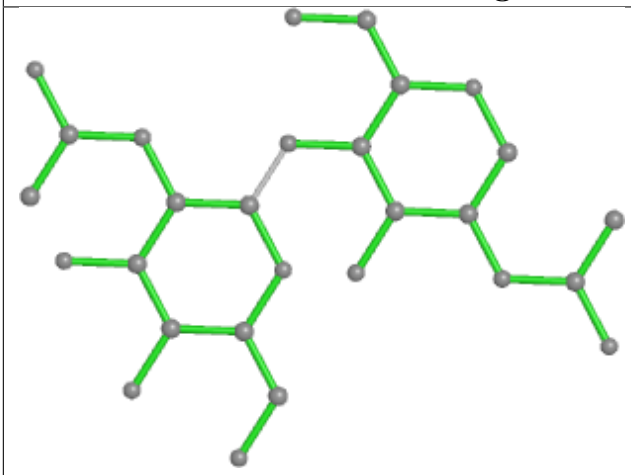
3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NAG	3	0
3	I	1	NAG	7	0
3	H	2	NAG	2	0

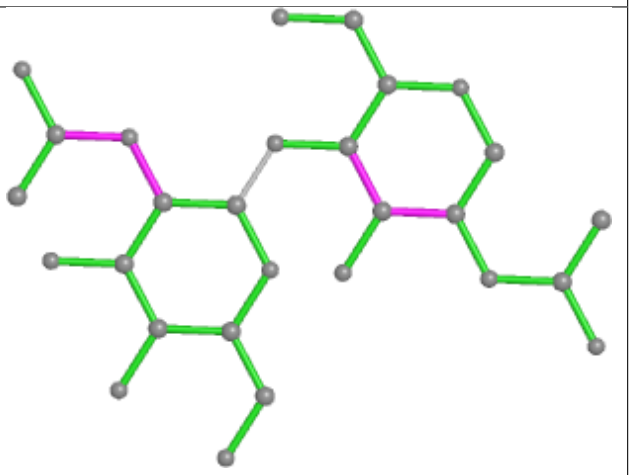
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.

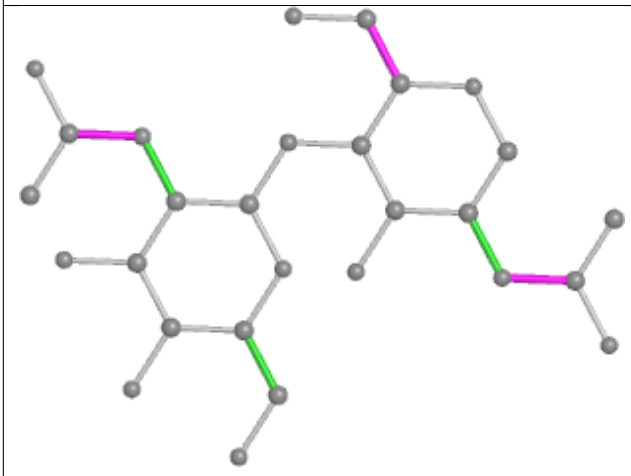
Oligosaccharide Chain G



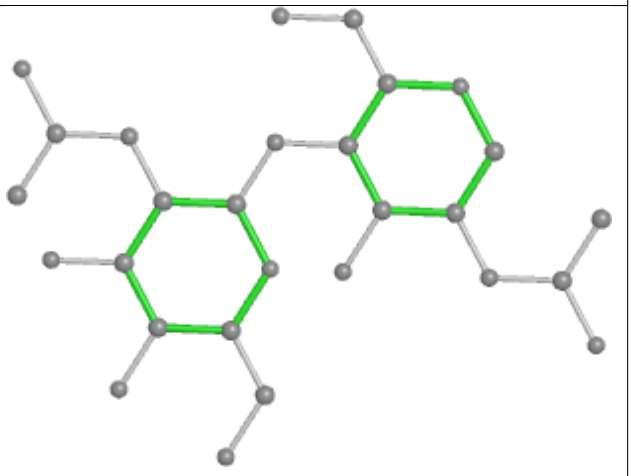
Bond lengths



Bond angles

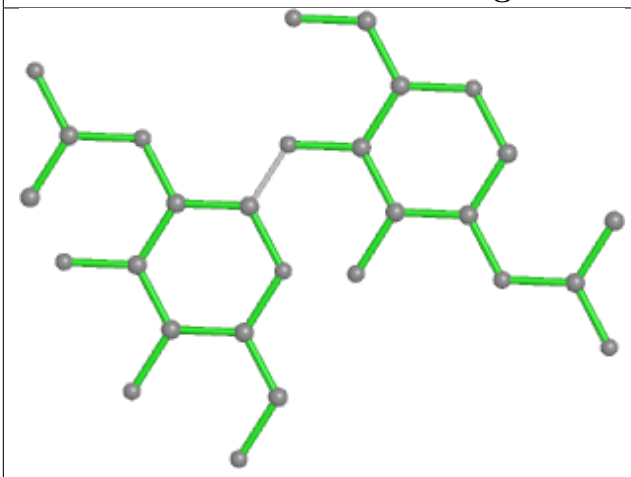


Torsions

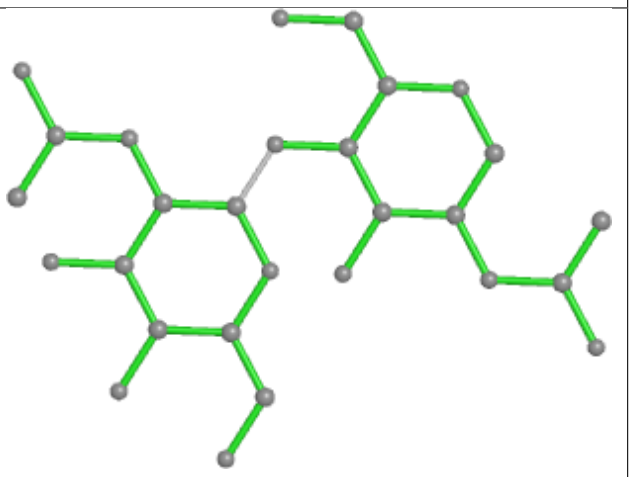


Rings

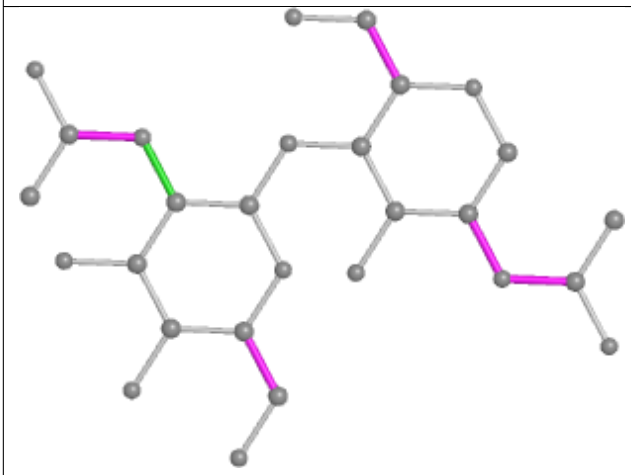
Oligosaccharide Chain H



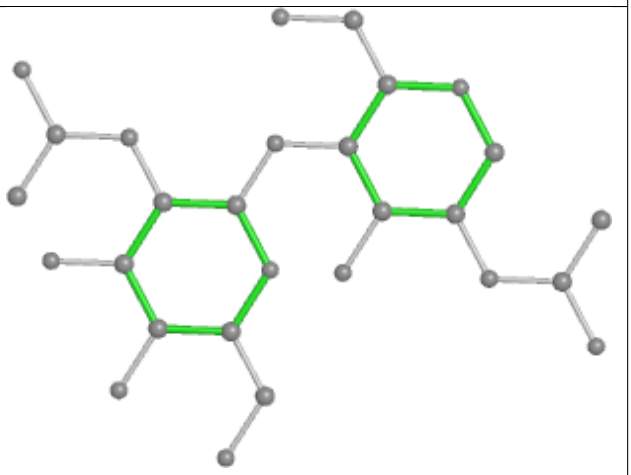
Bond lengths



Bond angles

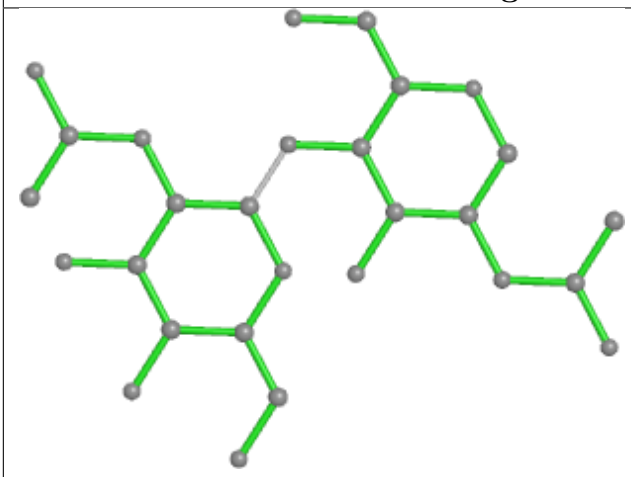


Torsions

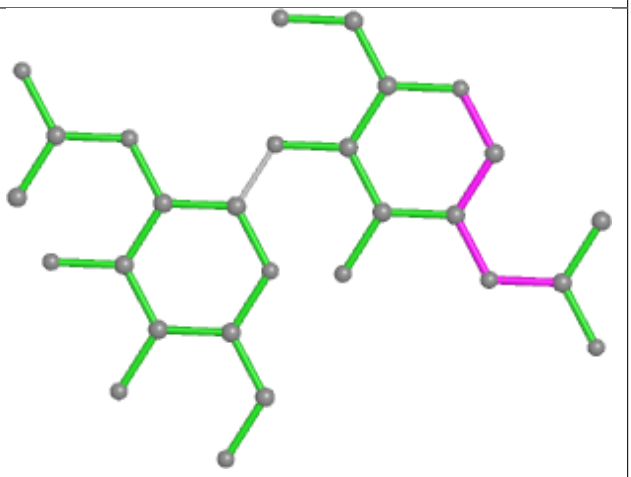


Rings

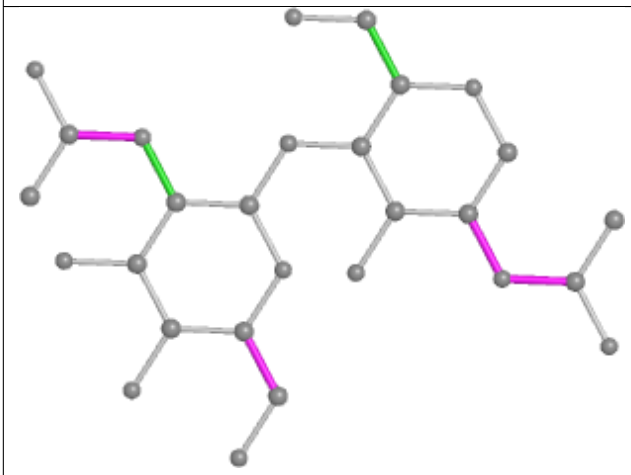
Oligosaccharide Chain I



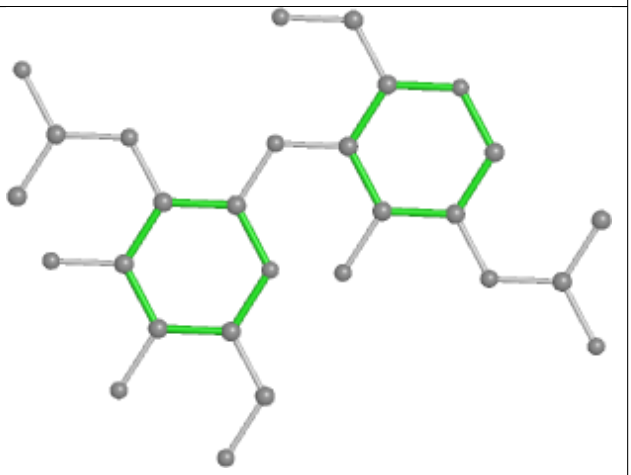
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
4	NAG	A	501	1	14,14,15	0.52	0	17,19,21	0.63	0
4	NAG	E	501	1	14,14,15	0.66	0	17,19,21	0.68	0
4	NAG	C	501	1	14,14,15	0.54	0	17,19,21	0.62	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	501	1	-	4/6/23/26	0/1/1/1
4	NAG	E	501	1	-	4/6/23/26	0/1/1/1
4	NAG	C	501	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	NAG	C8-C7-N2-C2
4	A	501	NAG	O7-C7-N2-C2
4	C	501	NAG	C1-C2-N2-C7
4	C	501	NAG	C8-C7-N2-C2
4	C	501	NAG	O7-C7-N2-C2
4	E	501	NAG	C8-C7-N2-C2
4	E	501	NAG	O7-C7-N2-C2
4	A	501	NAG	O5-C5-C6-O6
4	E	501	NAG	O5-C5-C6-O6
4	A	501	NAG	C4-C5-C6-O6
4	E	501	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	501	NAG	2	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.

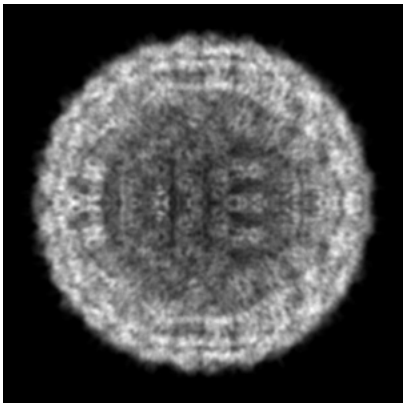
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-5520. These allow visual inspection of the internal detail of the map and identification of artifacts.

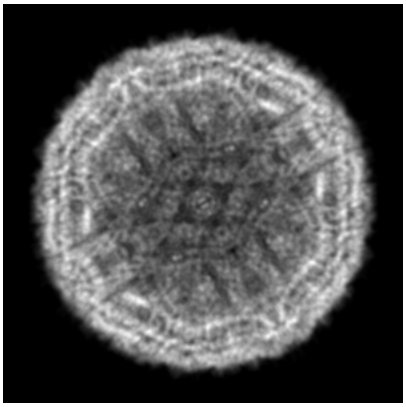
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

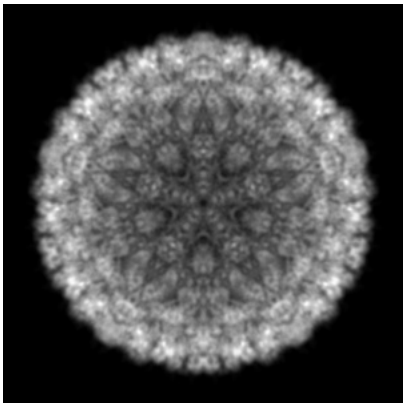
6.1.1 Primary map



X



Y



Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 240

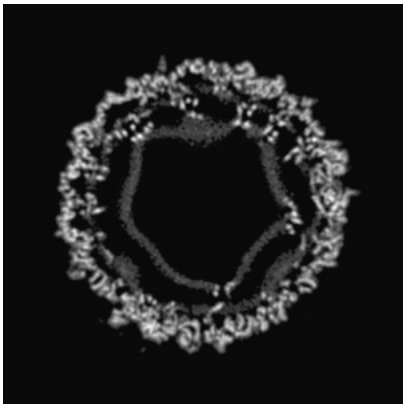
Y Index: 240

Z Index: 240

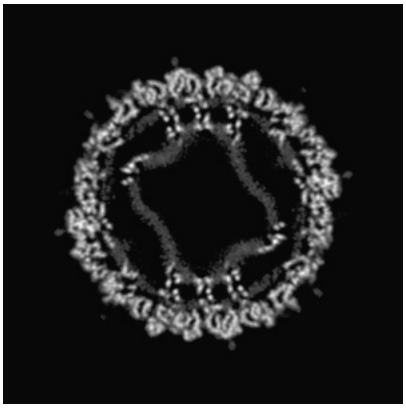
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 353



Y Index: 114

Z Index: 147

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

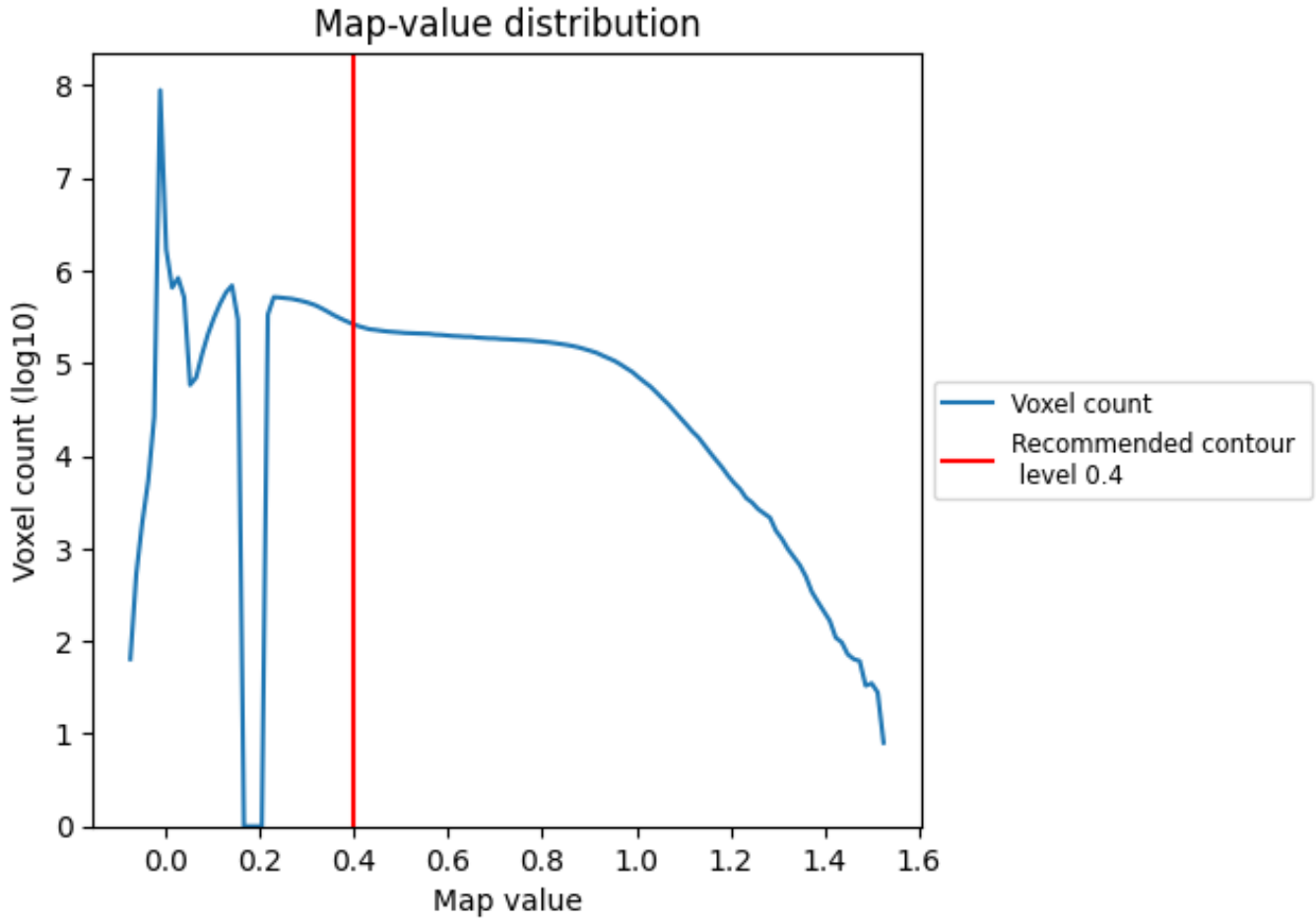
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

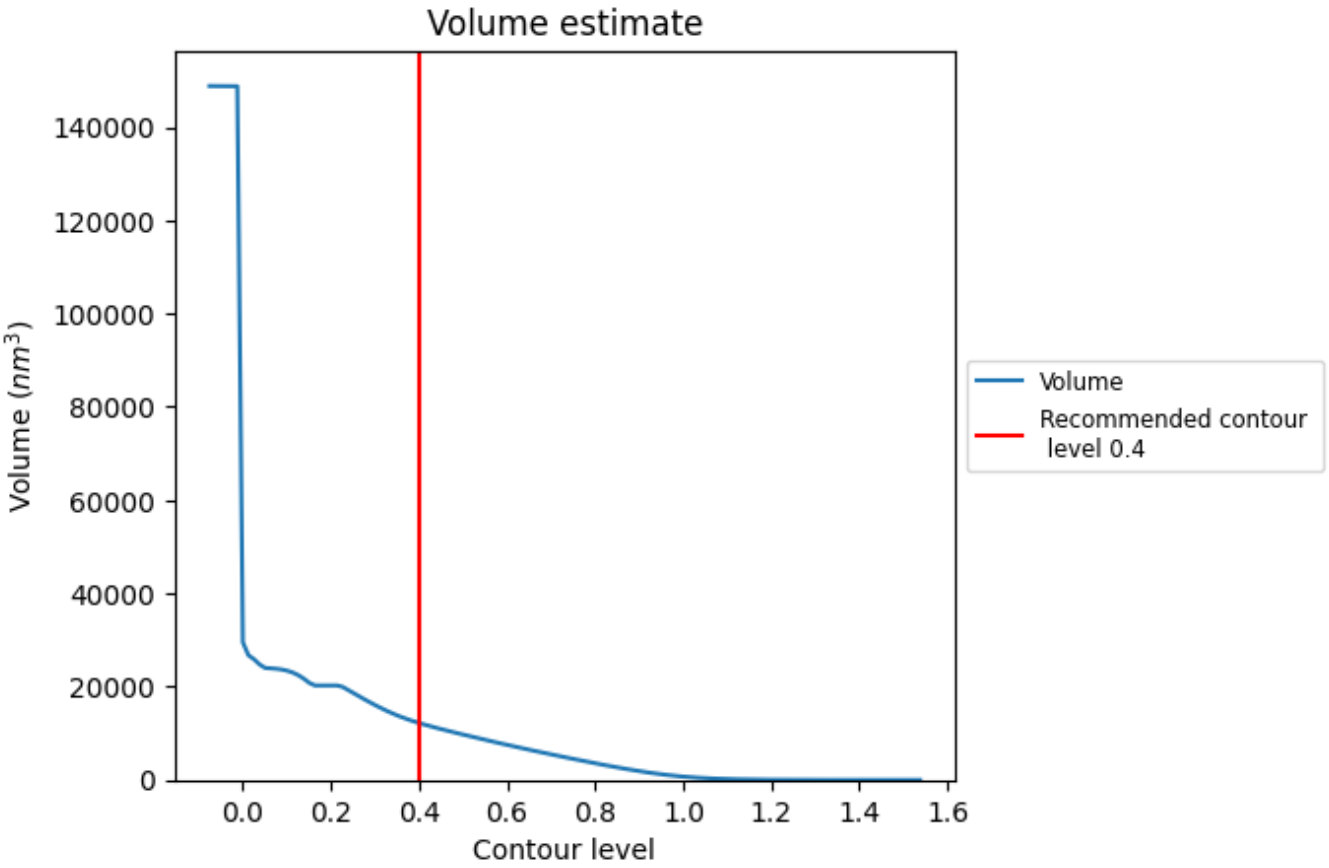
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

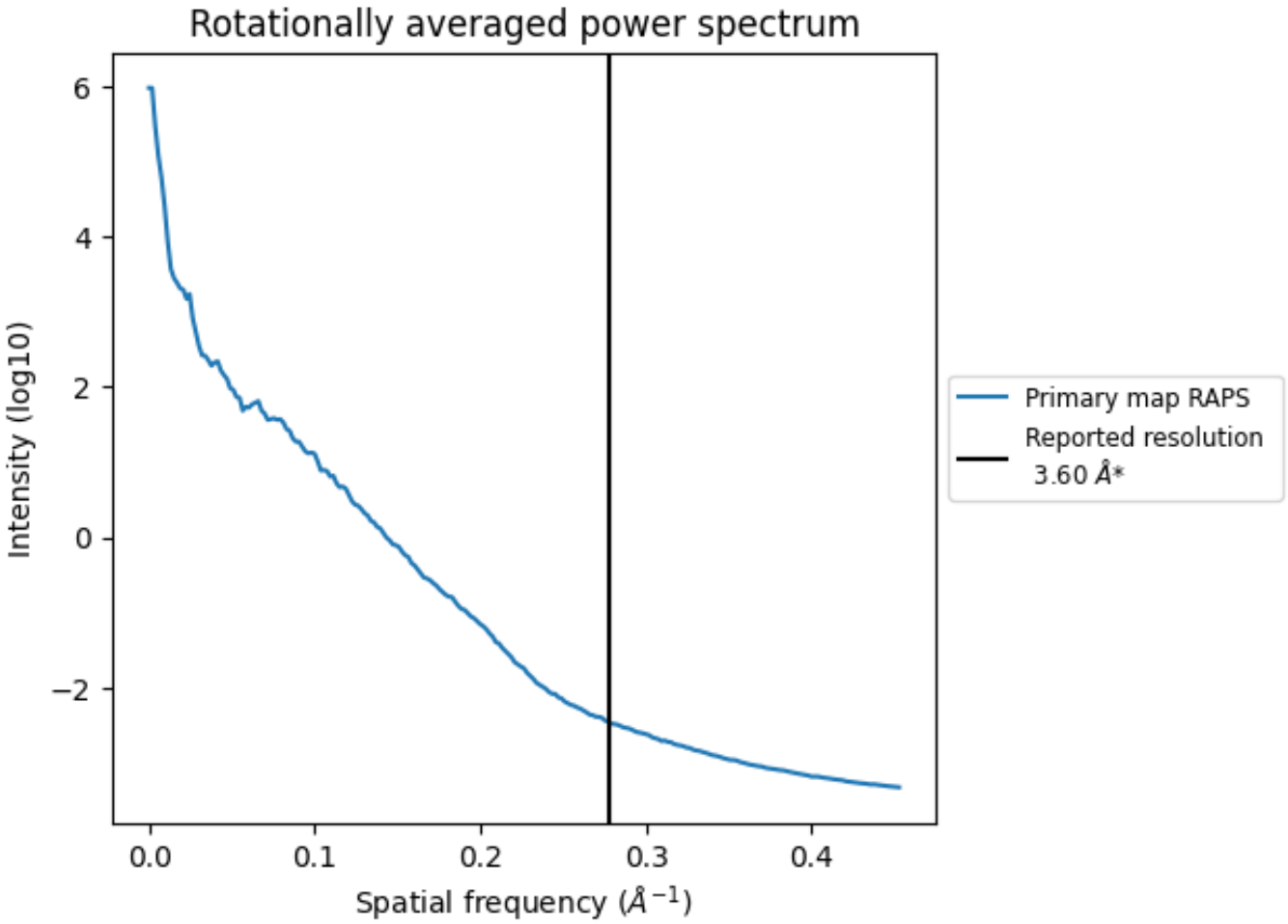
7.2 Volume estimate



The volume at the recommended contour level is 12223 nm^3; this corresponds to an approximate mass of 11041 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation (i)

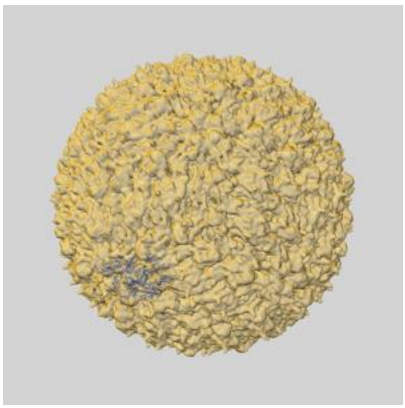
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

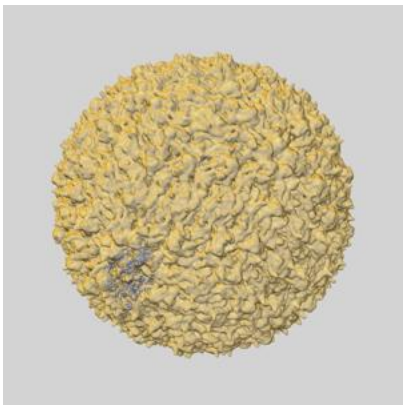
This section contains information regarding the fit between EMDB map EMD-5520 and PDB model 3J27. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

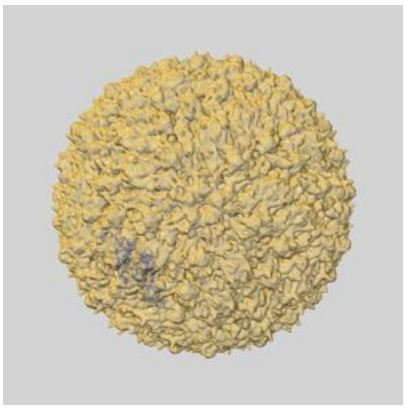
9.1.1 Map-model overlay



X

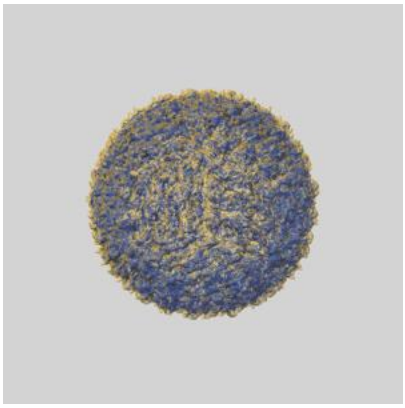


Y

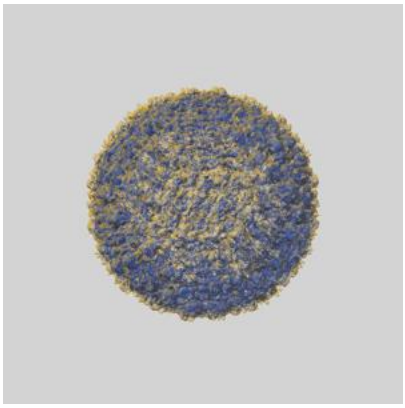


Z

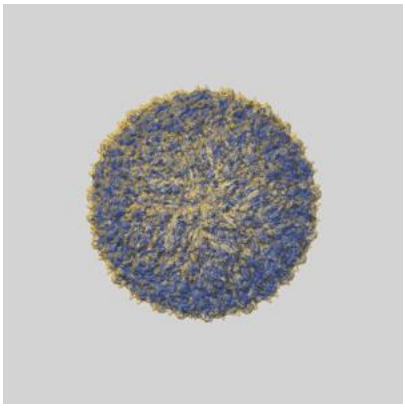
9.1.2 Map-model assembly overlay



X



Y



Z

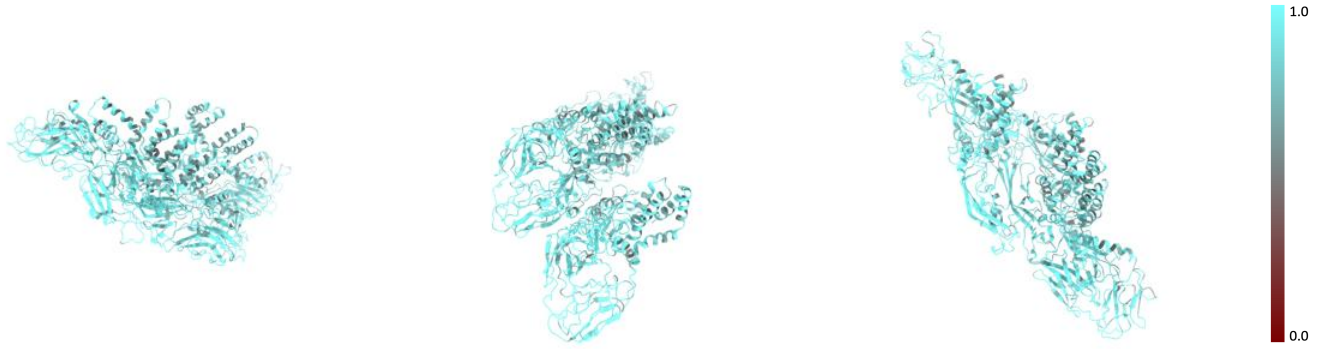
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model

X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

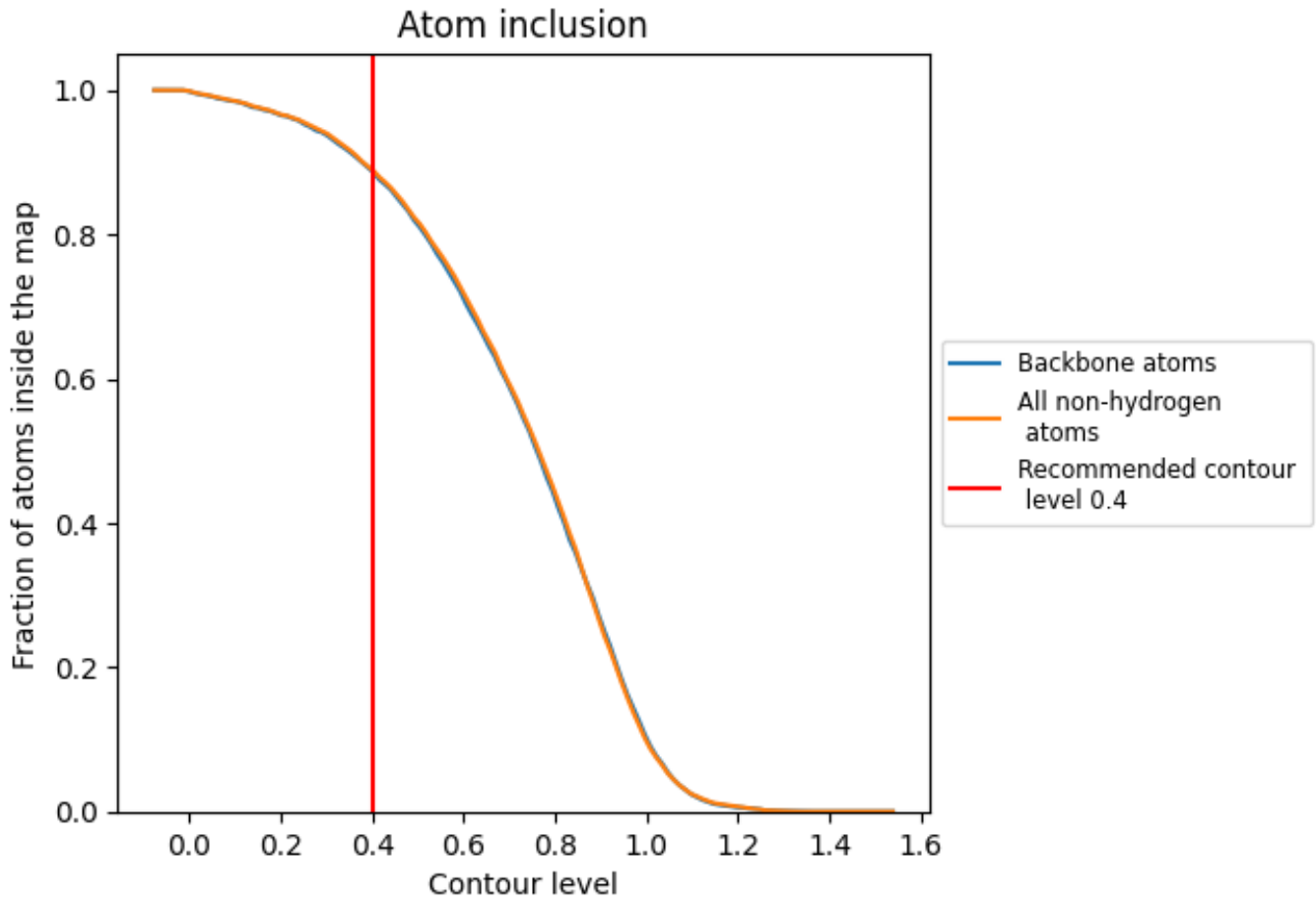
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8896	0.2730
A	0.9089	0.2760
B	0.8452	0.2690
C	0.8954	0.2710
D	0.8634	0.2810
E	0.8967	0.2740
F	0.8288	0.2700
G	0.8929	0.3160
H	0.9643	0.3100
I	0.9643	0.3000