



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jul 24, 2017 – 04:21 PM EDT

PDB ID : 5FJ5
EMDB ID: : EMD-3185
Title : Structure of the in vitro assembled bacteriophage phi6 polymerase complex
Authors : Ilca, S.; Kotecha, A.; Sun, X.; Poranen, M.P.; Stuart, D.I.; Huiskonen, J.T.
Deposited on : unknown
Resolution : 4.80 Å(reported)
Based on PDB ID : 4K7H

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

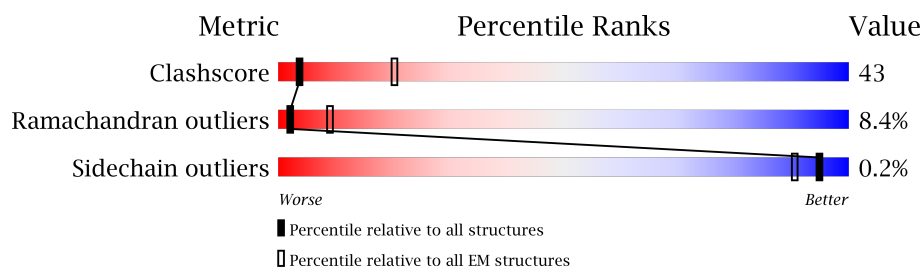
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY



The reported resolution of this entry is 4.80 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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

Mol	Chain	Length	Quality of chain
1	A	761	 <div>33% 59% 7% .</div>
1	B	761	 <div>36% 59% 5%</div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11840 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called MAJOR INNER PROTEIN P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	761	Total	C	N	O	S	0	0
			5920	3741	1048	1109	22		
1	B	761	Total	C	N	O	S	0	0
			5920	3741	1048	1109	22		

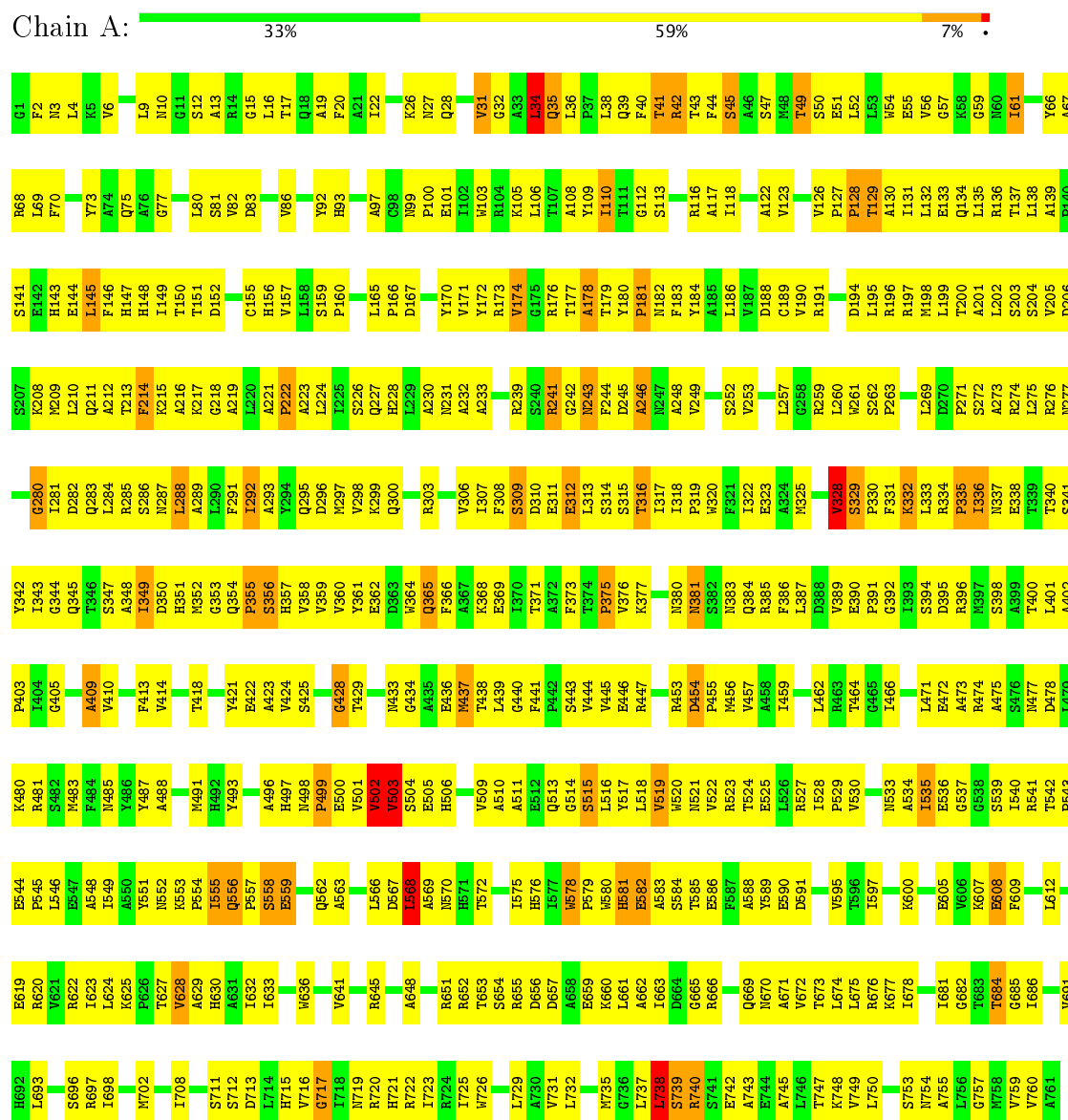
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P11126
B	1	GLY	-	expression tag	UNP P11126

3 Residue-property plots

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

• Molecule 1: MAJOR INNER PROTEIN P1



• Molecule 1: MAJOR INNER PROTEIN P1






4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	4379	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	16	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	37037	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	A	0.43	0/6040	0.70	7/8206 (0.1%)
1	B	0.40	0/6040	0.68	1/8206 (0.0%)
All	All	0.41	0/12080	0.69	8/16412 (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	A	0	5
1	B	0	3
All	All	0	8

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	PRO	CA-C-N	6.74	132.03	117.20
1	A	128	PRO	C-N-CA	6.09	136.93	121.70
1	A	568	LEU	CA-CB-CG	5.92	128.90	115.30
1	A	502	VAL	C-N-CA	5.79	136.19	121.70
1	B	313	LEU	CA-CB-CG	5.67	128.35	115.30
1	A	128	PRO	N-CA-C	5.33	125.97	112.10
1	A	738	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	128	PRO	CA-C-O	-5.16	107.83	120.20

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	328	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	A	34	LEU	Peptide
1	A	35	GLN	Peptide
1	A	365	GLN	Peptide
1	A	437	MET	Peptide
1	B	165	LEU	Peptide
1	B	171	VAL	Peptide
1	B	508	GLY	Peptide

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	5920	0	5913	515	0
1	B	5920	0	5913	504	0
All	All	11840	0	11826	1011	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 43.

All (1011) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ARG:HD2	1:B:339:THR:H	1.30	0.96
1:A:117:ALA:H	1:A:221:ALA:H	1.10	0.93
1:B:117:ALA:HB1	1:B:221:ALA:HB1	1.50	0.91
1:B:80:LEU:HD12	1:B:81:SER:H	1.36	0.88
1:A:342:TYR:HA	1:A:559:GLU:HG3	1.57	0.86
1:B:259:ARG:HG2	1:B:269:LEU:HG	1.56	0.85
1:A:108:ALA:HA	1:A:112:GLY:HA3	1.59	0.85
1:B:103:TRP:HE1	1:B:230:ALA:H	1.23	0.85
1:B:400:THR:HG21	1:B:686:ILE:HG12	1.59	0.84
1:B:63:PRO:HB3	1:B:199:LEU:HB2	1.60	0.83
1:B:128:PRO:O	1:B:132:LEU:N	2.12	0.83
1:B:172:TYR:HD1	1:B:578:TRP:HB2	1.42	0.83
1:B:254:LEU:HD11	1:B:294:TYR:HA	1.60	0.82
1:B:733:GLN:HG3	1:B:734:MET:HG2	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:THR:HG21	1:B:547:GLU:HB2	1.62	0.82
1:A:502:VAL:HA	1:A:503:VAL:HG12	1.62	0.81
1:A:4:LEU:HG	1:A:436:GLU:HB2	1.60	0.81
1:A:527:ARG:HG3	1:A:529:PRO:HD3	1.61	0.81
1:B:281:ILE:HA	1:B:284:LEU:HB3	1.63	0.80
1:A:44:PHE:HA	1:A:333:LEU:HA	1.64	0.80
1:B:42:ARG:HD3	1:B:337:ASN:H	1.45	0.80
1:A:582:GLU:O	1:A:625:LYS:NZ	2.15	0.80
1:A:715:HIS:HD2	1:A:716:VAL:HG22	1.43	0.80
1:A:16:LEU:HA	1:A:487:TYR:HE1	1.46	0.80
1:B:135:LEU:O	1:B:139:ALA:N	2.15	0.80
1:A:651:ARG:HB2	1:A:663:ILE:HD11	1.63	0.80
1:B:93:HIS:O	1:B:96:THR:OG1	1.99	0.80
1:A:436:GLU:OE2	1:A:439:LEU:N	2.12	0.80
1:A:528:ILE:HG12	1:A:536:GLU:HB3	1.65	0.79
1:A:173:ARG:HB2	1:A:579:PRO:HG2	1.64	0.79
1:B:53:LEU:HD21	1:B:171:VAL:HG23	1.64	0.79
1:B:756:LEU:HG	1:B:757:GLY:H	1.48	0.79
1:A:117:ALA:N	1:A:221:ALA:H	1.81	0.78
1:A:197:ARG:HA	1:A:200:THR:HG22	1.66	0.78
1:B:407:THR:OG1	1:B:680:MET:SD	2.42	0.77
1:A:581:HIS:O	1:A:583:ALA:N	2.17	0.77
1:A:195:LEU:HA	1:A:198:MET:HB3	1.67	0.77
1:B:408:PHE:HD1	1:B:413:PHE:HZ	1.33	0.77
1:B:609:PHE:HB3	1:B:611:LEU:H	1.49	0.77
1:B:106:LEU:HD13	1:B:154:VAL:HG21	1.67	0.76
1:A:189:CYS:HB3	1:A:323:GLU:HG3	1.67	0.76
1:B:7:LYS:HD3	1:B:531:GLY:H	1.51	0.76
1:A:176:ARG:HH12	1:A:447:ARG:HA	1.49	0.75
1:B:451:LEU:O	1:B:453:ARG:NH1	2.19	0.75
1:A:387:LEU:HG	1:A:572:THR:HG21	1.66	0.75
1:B:647:LEU:HD23	1:B:667:ARG:HG3	1.67	0.75
1:A:588:ALA:HB1	1:A:589:TYR:HB2	1.67	0.75
1:A:200:THR:HA	1:A:203:SER:HB3	1.67	0.75
1:A:480:LYS:HA	1:A:483:MET:HG2	1.68	0.75
1:B:608:GLU:N	1:B:609:PHE:HB2	2.01	0.75
1:B:575:ILE:HA	1:B:576:HIS:HB2	1.68	0.75
1:A:410:VAL:HA	1:A:413:PHE:HB3	1.66	0.74
1:A:148:HIS:O	1:A:151:THR:OG1	2.04	0.74
1:A:208:LYS:O	1:A:211:GLN:NE2	2.19	0.74
1:B:75:GLN:OE1	1:B:447:ARG:NH2	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:ILE:HD13	1:A:738:LEU:HB3	1.69	0.74
1:B:182:ASN:ND2	1:B:296:ASP:OD2	2.21	0.74
1:A:134:GLN:O	1:A:137:THR:OG1	2.06	0.74
1:A:347:SER:HA	1:A:358:VAL:HG13	1.70	0.73
1:A:717:GLY:O	1:A:721:HIS:N	2.16	0.73
1:B:95:SER:OG	1:B:99:ASN:ND2	2.21	0.73
1:B:134:GLN:O	1:B:137:THR:OG1	2.06	0.73
1:A:530:VAL:O	1:A:551:TYR:OH	2.07	0.73
1:A:619:GLU:OE2	1:A:620:ARG:NH1	2.21	0.72
1:B:323:GLU:O	1:B:326:SER:OG	2.05	0.72
1:A:359:VAL:HA	1:A:438:THR:HA	1.71	0.72
1:B:14:ARG:HB2	1:B:465:GLY:HA3	1.70	0.72
1:B:46:ALA:HA	1:B:331:PHE:HA	1.71	0.72
1:B:342:TYR:HB3	1:B:559:GLU:HG2	1.72	0.72
1:A:55:GLU:HG3	1:A:171:VAL:HG22	1.70	0.72
1:A:365:GLN:HA	1:A:562:GLN:HB2	1.70	0.72
1:B:348:ALA:HB3	1:B:356:SER:H	1.55	0.72
1:A:352:MET:N	1:A:353:GLY:HA2	2.05	0.72
1:A:533:ASN:HD22	1:A:543:PRO:HD2	1.55	0.72
1:B:152:ASP:O	1:B:156:HIS:N	2.23	0.72
1:B:714:LEU:HB3	1:B:719:ASN:HD22	1.54	0.72
1:A:132:LEU:HD21	1:A:136:ARG:HH21	1.53	0.72
1:B:644:ASP:OD2	1:B:748:LYS:NZ	2.23	0.71
1:A:272:SER:HB2	1:A:275:LEU:HB3	1.72	0.71
1:B:42:ARG:HD2	1:B:339:THR:N	2.05	0.71
1:A:40:PHE:HB2	1:A:288:LEU:HB3	1.73	0.71
1:B:224:LEU:O	1:B:228:HIS:N	2.24	0.71
1:A:630:HIS:HB2	1:A:737:LEU:HD22	1.73	0.71
1:A:334:ARG:HD3	1:A:338:GLU:HB2	1.72	0.71
1:B:35:GLN:NE2	1:B:504:SER:OG	2.24	0.71
1:A:392:GLY:O	1:A:396:ARG:NH1	2.24	0.70
1:B:231:ASN:O	1:B:234:THR:OG1	2.08	0.70
1:A:172:TYR:CD1	1:A:578:TRP:HB2	2.26	0.70
1:A:73:TYR:O	1:A:77:GLY:N	2.25	0.70
1:B:4:LEU:HD21	1:B:13:ALA:HB3	1.73	0.70
1:B:584:SER:H	1:B:622:ARG:NH1	1.90	0.70
1:A:385:ARG:HD2	1:A:580:TRP:HE1	1.57	0.70
1:A:242:GLY:O	1:A:244:PHE:N	2.24	0.70
1:B:182:ASN:OD1	1:B:183:PHE:N	2.25	0.70
1:A:655:ARG:N	1:A:656:ASP:HB2	2.07	0.69
1:B:163:PHE:HA	1:B:164:ILE:HB	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:ALA:H	1:B:536:GLU:HG3	1.57	0.69
1:B:213:THR:O	1:B:215:LYS:N	2.25	0.69
1:A:31:VAL:HG22	1:A:32:GLY:H	1.58	0.69
1:A:453:ARG:NH2	1:A:474:ARG:O	2.26	0.69
1:A:534:ALA:O	1:A:536:GLU:N	2.26	0.69
1:A:97:ALA:HA	1:A:103:TRP:HZ2	1.58	0.69
1:A:40:PHE:HD2	1:A:289:ALA:HA	1.57	0.69
1:A:45:SER:OG	1:A:332:LYS:HB2	1.93	0.68
1:B:46:ALA:O	1:B:334:ARG:NH2	2.27	0.68
1:A:368:LYS:HG2	1:A:402:ALA:HA	1.76	0.68
1:A:126:VAL:HG13	1:A:166:PRO:HD3	1.75	0.67
1:B:678:ILE:HA	1:B:681:ILE:HD12	1.76	0.67
1:A:51:GLU:HA	1:A:174:VAL:HG21	1.75	0.67
1:A:194:ASP:O	1:A:198:MET:N	2.25	0.67
1:A:315:SER:O	1:A:317:ILE:N	2.28	0.67
1:A:580:TRP:HA	1:A:581:HIS:O	1.95	0.67
1:A:712:SER:O	1:A:715:HIS:ND1	2.22	0.67
1:A:739:SER:OG	1:A:740:ARG:N	2.28	0.67
1:A:283:GLN:O	1:A:286:SER:OG	2.09	0.67
1:B:15:GLY:HA3	1:B:462:LEU:HG	1.76	0.67
1:B:10:ASN:HD22	1:B:29:LEU:HD21	1.59	0.66
1:B:337:ASN:OD1	1:B:338:GLU:N	2.28	0.66
1:B:237:PHE:O	1:B:240:SER:OG	2.14	0.66
1:B:334:ARG:HD3	1:B:335:PRO:HD2	1.77	0.66
1:A:179:THR:N	1:A:180:TYR:HA	2.11	0.66
1:A:456:MET:HA	1:A:459:ILE:HD12	1.78	0.66
1:A:627:THR:O	1:A:629:ALA:N	2.29	0.66
1:A:112:GLY:HA2	1:A:116:ARG:HD3	1.76	0.66
1:B:667:ARG:NH2	1:B:752:ASP:OD2	2.29	0.66
1:B:30:SER:HB2	1:B:517:TYR:CZ	2.31	0.65
1:A:296:ASP:O	1:A:300:GLN:N	2.19	0.65
1:B:349:ILE:HG13	1:B:351:HIS:H	1.61	0.65
1:B:275:LEU:HB2	1:B:312:GLU:HG2	1.78	0.65
1:A:283:GLN:NE2	1:A:286:SER:OG	2.30	0.65
1:A:395:ASP:OD1	1:A:396:ARG:N	2.30	0.65
1:A:92:TYR:HE2	1:A:150:THR:HG21	1.62	0.65
1:B:45:SER:OG	1:B:46:ALA:N	2.29	0.65
1:A:505:GLU:HG2	1:A:515:SER:H	1.61	0.65
1:B:274:ARG:HB3	1:B:312:GLU:HG3	1.79	0.65
1:A:306:VAL:O	1:A:308:PHE:N	2.30	0.65
1:A:655:ARG:H	1:A:656:ASP:HB2	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:TYR:HA	1:B:576:HIS:CD2	2.31	0.65
1:A:358:VAL:H	1:A:437:MET:HB3	1.60	0.65
1:A:691:VAL:HG12	1:A:723:ILE:HG12	1.77	0.65
1:B:18:GLN:HE22	1:B:518:LEU:HB2	1.62	0.64
1:A:535:ILE:HD12	1:A:541:ARG:H	1.61	0.64
1:A:729:LEU:HD21	1:A:743:ALA:HB1	1.79	0.64
1:A:501:VAL:HG23	1:A:502:VAL:HG12	1.78	0.64
1:B:125:LYS:HE2	1:B:163:PHE:HB2	1.80	0.64
1:A:45:SER:HB3	1:A:334:ARG:HB2	1.80	0.64
1:B:506:HIS:HB2	1:B:517:TYR:HE2	1.62	0.64
1:B:66:TYR:HD1	1:B:69:LEU:HD12	1.63	0.64
1:A:57:GLY:H	1:A:170:TYR:HB2	1.62	0.64
1:A:315:SER:OG	1:A:316:THR:N	2.30	0.64
1:B:156:HIS:NE2	1:B:206:ASP:OD2	2.16	0.64
1:B:233:ALA:O	1:B:237:PHE:N	2.30	0.64
1:B:606:VAL:HB	1:B:697:ARG:NH2	2.12	0.64
1:A:520:TRP:H	1:A:542:THR:H	1.46	0.64
1:B:44:PHE:HE2	1:B:181:PRO:HG3	1.63	0.64
1:A:580:TRP:CD2	1:A:581:HIS:HA	2.33	0.64
1:B:420:VAL:HG13	1:B:669:GLN:HE22	1.62	0.64
1:B:132:LEU:HD13	1:B:151:THR:HG22	1.80	0.64
1:A:358:VAL:N	1:A:437:MET:SD	2.71	0.64
1:A:77:GLY:O	1:A:474:ARG:NH1	2.28	0.64
1:A:178:ALA:O	1:A:332:LYS:NZ	2.31	0.63
1:B:205:VAL:O	1:B:209:MET:HG2	1.98	0.63
1:B:83:ASP:HA	1:B:191:ARG:HG2	1.79	0.63
1:A:144:GLU:HG2	1:A:145:LEU:H	1.63	0.63
1:A:554:PRO:O	1:A:556:GLN:N	2.22	0.63
1:B:616:GLN:HG3	1:B:617:ARG:HG2	1.78	0.63
1:A:42:ARG:NH2	1:A:283:GLN:HE21	1.96	0.63
1:B:225:ILE:HA	1:B:228:HIS:HB3	1.79	0.63
1:B:449:TYR:HH	1:B:630:HIS:HD1	0.65	0.63
1:B:485:ASN:OD1	1:B:486:TYR:N	2.32	0.63
1:B:593:TYR:HB3	1:B:604:ALA:HB3	1.80	0.63
1:A:597:ILE:HD11	1:A:600:LYS:HE3	1.81	0.63
1:A:498:ASN:HD22	1:A:500:GLU:HG2	1.64	0.63
1:B:312:GLU:O	1:B:315:SER:N	2.24	0.63
1:B:317:ILE:HG12	1:B:320:TRP:CZ2	2.34	0.63
1:B:370:ILE:HG12	1:B:626:PRO:HG3	1.80	0.63
1:A:4:LEU:H	1:A:436:GLU:HB2	1.64	0.63
1:B:35:GLN:HE21	1:B:502:VAL:HG23	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ARG:HB2	1:B:147:HIS:NE2	2.14	0.63
1:A:375:PRO:HG3	1:A:622:ARG:HE	1.63	0.62
1:B:77:GLY:HA3	1:B:474:ARG:HH22	1.63	0.62
1:B:608:GLU:HA	1:B:609:PHE:O	1.99	0.62
1:A:10:ASN:HA	1:A:17:THR:HG21	1.81	0.62
1:A:666:ARG:HD3	1:A:669:GLN:NE2	2.14	0.62
1:B:153:PHE:HB3	1:B:229:LEU:HD21	1.80	0.62
1:B:2:PHE:O	1:B:439:LEU:N	2.30	0.62
1:B:635:MET:O	1:B:638:SER:OG	2.10	0.62
1:B:408:PHE:HD1	1:B:413:PHE:CZ	2.16	0.62
1:B:472:GLU:O	1:B:476:SER:N	2.30	0.62
1:A:607:LYS:O	1:A:609:PHE:N	2.32	0.62
1:A:715:HIS:CD2	1:A:716:VAL:HG22	2.31	0.62
1:B:123:VAL:HG23	1:B:164:ILE:HG12	1.80	0.62
1:A:360:VAL:HG22	1:A:438:THR:HG22	1.80	0.62
1:B:132:LEU:HA	1:B:135:LEU:HB2	1.82	0.62
1:B:16:LEU:HD23	1:B:546:LEU:HD21	1.81	0.62
1:A:173:ARG:HD3	1:A:579:PRO:HG2	1.82	0.62
1:A:61:ILE:HD11	1:A:199:LEU:HD21	1.80	0.62
1:A:172:TYR:HD1	1:A:578:TRP:HB2	1.65	0.62
1:B:128:PRO:HA	1:B:131:ILE:HG22	1.81	0.62
1:B:136:ARG:HB2	1:B:147:HIS:CD2	2.35	0.62
1:B:209:MET:O	1:B:213:THR:OG1	2.09	0.62
1:B:41:THR:N	1:B:286:SER:OG	2.32	0.62
1:B:421:TYR:HE2	1:B:427:ARG:HH22	1.47	0.62
1:B:637:TYR:HA	1:B:640:PHE:CD2	2.34	0.62
1:A:40:PHE:CD2	1:A:289:ALA:HA	2.35	0.62
1:B:61:ILE:HG12	1:B:152:ASP:HB2	1.82	0.62
1:A:100:PRO:HA	1:A:103:TRP:HD1	1.63	0.61
1:A:190:VAL:HG12	1:A:323:GLU:HB2	1.81	0.61
1:A:502:VAL:HA	1:A:503:VAL:CG1	2.28	0.61
1:B:481:ARG:HA	1:B:484:PHE:CE2	2.34	0.61
1:A:287:ASN:O	1:A:289:ALA:N	2.33	0.61
1:A:349:ILE:HG13	1:A:350:ASP:H	1.65	0.61
1:A:666:ARG:HG3	1:A:670:ASN:HD21	1.65	0.61
1:B:630:HIS:NE2	1:B:738:LEU:HA	2.15	0.61
1:A:173:ARG:HE	1:A:566:LEU:HD21	1.65	0.61
1:A:183:PHE:HA	1:A:186:LEU:HD13	1.82	0.61
1:B:153:PHE:CZ	1:B:202:LEU:HB3	2.36	0.61
1:B:745:ALA:O	1:B:748:LYS:HG2	2.01	0.61
1:A:128:PRO:N	1:A:129:THR:HB	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:GLU:HA	1:A:516:LEU:HB3	1.83	0.61
1:A:713:ASP:HA	1:A:715:HIS:CE1	2.36	0.61
1:B:231:ASN:OD1	1:B:232:ALA:N	2.34	0.61
1:A:296:ASP:HA	1:A:299:LYS:HB3	1.82	0.60
1:B:388:ASP:HA	1:B:572:THR:HG21	1.82	0.60
1:A:127:PRO:HG2	1:A:130:ALA:HB2	1.83	0.60
1:A:176:ARG:NH2	1:A:447:ARG:HD2	2.17	0.60
1:A:9:LEU:HA	1:A:12:SER:HB3	1.84	0.60
1:B:75:GLN:HB3	1:B:447:ARG:HH22	1.66	0.60
1:A:135:LEU:HD12	1:A:151:THR:HG22	1.84	0.60
1:A:214:PHE:HA	1:A:215:LYS:O	2.02	0.60
1:A:666:ARG:HA	1:A:669:GLN:HE22	1.65	0.60
1:A:754:ASN:N	1:A:755:ALA:HA	2.16	0.60
1:B:163:PHE:HB3	1:B:164:ILE:HG22	1.84	0.60
1:A:493:TYR:CE2	1:A:549:ILE:HG12	2.36	0.60
1:B:543:PRO:HG2	1:B:544:GLU:HG3	1.83	0.60
1:B:636:TRP:HB3	1:B:640:PHE:CZ	2.37	0.60
1:A:13:ALA:HB1	1:A:16:LEU:HD12	1.83	0.60
1:A:4:LEU:N	1:A:436:GLU:HB2	2.17	0.60
1:B:37:PRO:HA	1:B:502:VAL:HG12	1.84	0.60
1:B:131:ILE:O	1:B:134:GLN:HB3	2.02	0.60
1:B:715:HIS:HB3	1:B:720:ARG:NH2	2.17	0.60
1:B:744:GLU:O	1:B:747:THR:OG1	2.17	0.60
1:A:472:GLU:HB3	1:A:475:ALA:HB3	1.83	0.60
1:B:598:ARG:NH1	1:B:710:ASP:OD1	2.35	0.60
1:A:116:ARG:HB2	1:A:222:PRO:HA	1.83	0.59
1:A:181:PRO:HD3	1:A:485:ASN:HD21	1.67	0.59
1:A:360:VAL:HG13	1:A:438:THR:HG23	1.84	0.59
1:A:671:ALA:O	1:A:674:LEU:HG	2.01	0.59
1:B:583:ALA:N	1:B:584:SER:HA	2.16	0.59
1:A:715:HIS:CD2	1:A:716:VAL:H	2.21	0.59
1:B:521:ASN:HA	1:B:540:ILE:HB	1.84	0.59
1:B:732:LEU:HG	1:B:738:LEU:HD22	1.83	0.59
1:A:660:LYS:O	1:A:663:ILE:HG13	2.02	0.59
1:A:678:ILE:HG21	1:A:725:ILE:HG23	1.85	0.59
1:B:8:ASP:OD1	1:B:9:LEU:N	2.35	0.59
1:B:288:LEU:O	1:B:291:PHE:HB3	2.03	0.59
1:B:159:SER:OG	1:B:162:GLY:O	2.21	0.59
1:B:656:ASP:HB3	1:B:659:GLU:HG2	1.84	0.59
1:B:264:SER:HB3	1:B:269:LEU:HD22	1.85	0.59
1:B:279:ASN:O	1:B:281:ILE:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:LEU:HB3	1:B:475:ALA:HB3	1.85	0.59
1:B:363:ASP:OD1	1:B:561:LEU:HD22	2.03	0.59
1:A:173:ARG:HB2	1:A:579:PRO:CG	2.33	0.59
1:A:306:VAL:HG12	1:A:309:SER:HA	1.85	0.59
1:B:145:LEU:HD12	1:B:146:PHE:N	2.18	0.59
1:B:332:LYS:HE2	1:B:334:ARG:HH12	1.67	0.59
1:B:478:ASP:OD1	1:B:479:LEU:N	2.36	0.59
1:A:505:GLU:OE2	1:A:515:SER:OG	2.15	0.58
1:A:661:LEU:O	1:A:665:GLY:N	2.35	0.58
1:A:144:GLU:O	1:A:146:PHE:N	2.36	0.58
1:A:445:VAL:HG13	1:A:455:PRO:HG3	1.85	0.58
1:A:347:SER:H	1:A:554:PRO:HB3	1.68	0.58
1:A:589:TYR:OH	1:A:740:ARG:NE	2.26	0.58
1:A:61:ILE:HG13	1:A:66:TYR:HE2	1.68	0.58
1:B:479:LEU:O	1:B:482:SER:OG	2.18	0.58
1:A:395:ASP:O	1:A:398:SER:OG	2.14	0.58
1:A:669:GLN:HA	1:A:672:VAL:HB	1.86	0.58
1:B:562:GLN:HG2	1:B:564:LYS:H	1.68	0.58
1:B:746:LEU:HA	1:B:749:VAL:HG22	1.85	0.58
1:A:180:TYR:CE1	1:A:331:PHE:HA	2.38	0.58
1:A:740:ARG:N	1:A:742:GLU:OE1	2.36	0.58
1:B:476:SER:O	1:B:480:LYS:HG2	2.04	0.58
1:A:530:VAL:HG13	1:A:551:TYR:CZ	2.38	0.58
1:A:568:LEU:HD12	1:A:569:ALA:N	2.19	0.58
1:B:407:THR:HG23	1:B:408:PHE:CD2	2.39	0.58
1:B:424:VAL:HG23	1:B:430:VAL:HA	1.85	0.58
1:B:617:ARG:N	1:B:618:ARG:HA	2.18	0.58
1:A:284:LEU:HG	1:A:287:ASN:ND2	2.19	0.58
1:B:170:TYR:HA	1:B:576:HIS:CG	2.39	0.58
1:B:506:HIS:HA	1:B:507:GLN:HB3	1.86	0.58
1:B:506:HIS:HB2	1:B:517:TYR:CE2	2.39	0.58
1:A:47:SER:HB3	1:A:332:LYS:HD3	1.84	0.58
1:A:358:VAL:H	1:A:437:MET:CB	2.17	0.58
1:B:443:SER:HA	1:B:446:GLU:HG2	1.85	0.58
1:B:587:PHE:HB3	1:B:621:VAL:HG23	1.85	0.58
1:A:210:LEU:HD22	1:A:228:HIS:ND1	2.18	0.57
1:A:343:ILE:N	1:A:559:GLU:OE2	2.34	0.57
1:B:182:ASN:H	1:B:185:ALA:HB3	1.69	0.57
1:B:467:VAL:HG13	1:B:469:GLU:HB2	1.86	0.57
1:A:4:LEU:O	1:A:436:GLU:N	2.37	0.57
1:B:194:ASP:OD1	1:B:195:LEU:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:669:GLN:HA	1:B:672:VAL:HG12	1.85	0.57
1:A:661:LEU:HD22	1:B:105:LYS:HD2	1.84	0.57
1:B:75:GLN:OE1	1:B:481:ARG:NH1	2.37	0.57
1:B:560:VAL:O	1:B:561:LEU:HG	2.04	0.57
1:B:324:ALA:HB1	1:B:333:LEU:HB2	1.86	0.57
1:A:97:ALA:HA	1:A:103:TRP:CZ2	2.37	0.57
1:A:375:PRO:HB2	1:A:385:ARG:HD3	1.86	0.57
1:A:702:MET:HG3	1:A:711:SER:HB3	1.86	0.57
1:A:732:LEU:HG	1:A:738:LEU:HD11	1.86	0.57
1:B:216:ALA:HA	1:B:217:LYS:C	2.25	0.57
1:A:433:ASN:HB3	1:A:434:GLY:CA	2.35	0.57
1:A:200:THR:O	1:A:204:SER:N	2.37	0.57
1:B:607:LYS:HB2	1:B:608:GLU:O	2.05	0.57
1:B:693:LEU:HD23	1:B:697:ARG:HH11	1.70	0.57
1:B:707:LEU:HD12	1:B:708:ILE:HG23	1.86	0.57
1:B:56:VAL:HG23	1:B:170:TYR:HB3	1.86	0.57
1:B:609:PHE:HB3	1:B:611:LEU:N	2.19	0.57
1:B:87:ASN:OD1	1:B:88:GLN:N	2.37	0.57
1:A:179:THR:HG21	1:A:488:ALA:HB1	1.87	0.56
1:A:544:GLU:CD	1:A:546:LEU:H	2.08	0.56
1:A:67:ALA:HA	1:A:70:PHE:HD2	1.68	0.56
1:B:489:ALA:HA	1:B:492:HIS:CE1	2.40	0.56
1:A:354:GLN:NE2	1:A:525:GLU:OE1	2.38	0.56
1:A:400:THR:HG21	1:A:731:VAL:HG21	1.87	0.56
1:B:70:PHE:CE1	1:B:145:LEU:HD13	2.40	0.56
1:A:342:TYR:O	1:A:362:GLU:HG2	2.05	0.56
1:B:345:GLN:HB2	1:B:554:PRO:HA	1.87	0.56
1:B:586:GLU:O	1:B:622:ARG:NH2	2.38	0.56
1:A:52:LEU:O	1:A:174:VAL:HG13	2.05	0.56
1:B:153:PHE:HZ	1:B:202:LEU:HD23	1.70	0.56
1:B:377:LYS:HB2	1:B:385:ARG:HG2	1.86	0.56
1:B:647:LEU:HD21	1:B:663:ILE:HA	1.88	0.56
1:B:199:LEU:HD23	1:B:202:LEU:HD22	1.88	0.56
1:A:557:PRO:HB2	1:A:559:GLU:HB2	1.87	0.56
1:A:591:ASP:OD2	1:A:726:TRP:NE1	2.38	0.56
1:B:738:LEU:HD23	1:B:742:GLU:HG2	1.86	0.56
1:B:651:ARG:HG2	1:B:663:ILE:HD13	1.88	0.56
1:B:125:LYS:NZ	1:B:158:LEU:O	2.38	0.56
1:B:291:PHE:O	1:B:294:TYR:HB3	2.05	0.56
1:A:422:GLU:OE2	1:B:116:ARG:HB3	2.06	0.56
1:A:473:ALA:O	1:A:477:ASN:ND2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:ASP:OD1	1:B:568:LEU:N	2.34	0.56
1:A:337:ASN:ND2	1:A:496:ALA:HB2	2.21	0.56
1:A:93:HIS:NE2	1:A:202:LEU:HD13	2.21	0.56
1:B:43:THR:HG21	1:B:289:ALA:H	1.70	0.56
1:A:558:SER:N	1:A:559:GLU:OE1	2.39	0.55
1:B:43:THR:OG1	1:B:288:LEU:N	2.35	0.55
1:A:274:ARG:HH12	1:A:312:GLU:HG3	1.71	0.55
1:A:344:GLY:N	1:A:361:TYR:O	2.27	0.55
1:A:196:ARG:HD3	1:A:328:VAL:HG12	1.89	0.55
1:B:456:MET:HA	1:B:459:ILE:HD12	1.87	0.55
1:B:344:GLY:HA2	1:B:555:ILE:HG13	1.88	0.55
1:B:640:PHE:CZ	1:B:674:LEU:HD21	2.41	0.55
1:A:291:PHE:HZ	1:A:517:TYR:HA	1.71	0.55
1:A:568:LEU:HD12	1:A:569:ALA:H	1.71	0.55
1:B:597:ILE:O	1:B:602:TYR:OH	2.17	0.55
1:B:93:HIS:CE1	1:B:96:THR:HA	2.41	0.55
1:B:4:LEU:O	1:B:437:MET:N	2.40	0.55
1:A:196:ARG:HH11	1:A:328:VAL:HG12	1.72	0.55
1:A:210:LEU:HG	1:A:213:THR:HA	1.88	0.55
1:A:585:THR:N	1:A:586:GLU:HB2	2.22	0.55
1:B:272:SER:O	1:B:276:ARG:HG3	2.06	0.55
1:B:68:ARG:NH1	1:B:327:GLU:O	2.38	0.55
1:A:533:ASN:ND2	1:A:543:PRO:HD2	2.21	0.55
1:A:605:GLU:N	1:A:605:GLU:OE1	2.40	0.55
1:B:3:ASN:HB3	1:B:438:THR:HA	1.88	0.55
1:A:42:ARG:NH2	1:A:283:GLN:O	2.40	0.54
1:A:42:ARG:CZ	1:A:283:GLN:HE21	2.20	0.54
1:A:45:SER:HB2	1:A:334:ARG:CZ	2.38	0.54
1:A:586:GLU:HB3	1:A:623:ILE:HG22	1.89	0.54
1:A:693:LEU:O	1:A:697:ARG:HG2	2.08	0.54
1:B:193:SER:HA	1:B:328:VAL:HG11	1.89	0.54
1:B:249:VAL:HG23	1:B:318:ILE:HG23	1.90	0.54
1:B:347:SER:HB3	1:B:355:PRO:HB3	1.88	0.54
1:A:214:PHE:HA	1:A:215:LYS:C	2.28	0.54
1:A:42:ARG:NH2	1:A:286:SER:OG	2.40	0.54
1:B:312:GLU:C	1:B:315:SER:H	2.10	0.54
1:B:358:VAL:HG11	1:B:437:MET:SD	2.47	0.54
1:B:666:ARG:O	1:B:669:GLN:HG2	2.07	0.54
1:A:446:GLU:HG3	1:A:627:THR:HB	1.90	0.54
1:B:467:VAL:HG22	1:B:469:GLU:H	1.71	0.54
1:A:22:ILE:HG21	1:A:515:SER:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:PHE:HE1	1:A:629:ALA:HB2	1.73	0.54
1:B:132:LEU:O	1:B:136:ARG:N	2.40	0.54
1:A:15:GLY:HA2	1:A:20:PHE:CG	2.42	0.54
1:A:350:ASP:O	1:A:352:MET:N	2.36	0.54
1:A:558:SER:OG	1:A:559:GLU:N	2.40	0.54
1:B:42:ARG:NH1	1:B:339:THR:O	2.40	0.54
1:B:35:GLN:HB3	1:B:502:VAL:HB	1.88	0.54
1:A:272:SER:HB2	1:A:275:LEU:CB	2.38	0.54
1:B:501:VAL:HG11	1:B:518:LEU:HD13	1.89	0.54
1:B:702:MET:HA	1:B:708:ILE:HD12	1.90	0.54
1:A:349:ILE:HD13	1:A:357:HIS:H	1.71	0.54
1:A:572:THR:HA	1:A:575:ILE:O	2.08	0.54
1:B:100:PRO:HA	1:B:103:TRP:CE3	2.43	0.54
1:B:354:GLN:HE21	1:B:431:ASN:HB3	1.73	0.53
1:A:144:GLU:HB2	1:A:147:HIS:HB3	1.90	0.53
1:A:165:LEU:N	1:A:166:PRO:HD2	2.23	0.53
1:B:143:HIS:HB2	1:B:146:PHE:CE2	2.43	0.53
1:A:99:ASN:ND2	1:A:101:GLU:OE2	2.41	0.53
1:B:443:SER:O	1:B:446:GLU:HG2	2.08	0.53
1:B:124:GLY:H	1:B:164:ILE:HG21	1.73	0.53
1:B:50:SER:H	1:B:176:ARG:HB3	1.74	0.53
1:A:42:ARG:HH21	1:A:286:SER:HG	1.55	0.53
1:B:272:SER:O	1:B:276:ARG:N	2.42	0.53
1:B:354:GLN:HE22	1:B:431:ASN:HD22	1.57	0.53
1:A:42:ARG:H	1:A:336:ILE:HD13	1.73	0.53
1:A:383:ASN:O	1:A:385:ARG:N	2.38	0.53
1:B:394:SER:OG	1:B:395:ASP:N	2.41	0.53
1:B:404:ILE:HG23	1:B:408:PHE:CD2	2.44	0.53
1:A:26:LYS:HE3	1:A:509:VAL:HG22	1.91	0.53
1:A:527:ARG:HH11	1:A:528:ILE:H	1.56	0.53
1:B:275:LEU:HD13	1:B:315:SER:HB2	1.91	0.53
1:A:285:ARG:O	1:A:288:LEU:HD13	2.09	0.53
1:A:310:ASP:OD2	1:A:313:LEU:N	2.42	0.53
1:A:170:TYR:HD1	1:A:576:HIS:CE1	2.27	0.53
1:B:42:ARG:HB2	1:B:339:THR:HA	1.91	0.53
1:B:345:GLN:CB	1:B:554:PRO:HA	2.39	0.53
1:B:86:VAL:HG21	1:B:191:ARG:HG3	1.90	0.53
1:A:182:ASN:ND2	1:A:184:TYR:HB2	2.23	0.53
1:B:128:PRO:O	1:B:131:ILE:N	2.42	0.53
1:B:709:ASP:O	1:B:711:SER:N	2.41	0.53
1:B:733:GLN:OE1	1:B:740:ARG:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:PHE:HE1	1:A:180:TYR:H	1.57	0.53
1:A:2:PHE:H	1:A:439:LEU:HD11	1.74	0.53
1:A:365:GLN:OE1	1:A:563:ALA:HB3	2.09	0.53
1:A:368:LYS:HE2	1:A:402:ALA:HA	1.91	0.53
1:A:702:MET:HB3	1:A:708:ILE:HA	1.91	0.53
1:B:467:VAL:HG22	1:B:469:GLU:N	2.24	0.53
1:B:570:ASN:O	1:B:573:THR:HG22	2.08	0.53
1:B:616:GLN:O	1:B:617:ARG:HB2	2.08	0.53
1:A:143:HIS:CD2	1:A:146:PHE:HE2	2.26	0.52
1:A:585:THR:HB	1:A:586:GLU:HA	1.91	0.52
1:A:641:VAL:O	1:A:645:ARG:HG2	2.08	0.52
1:B:16:LEU:HD13	1:B:462:LEU:HD21	1.91	0.52
1:B:459:ILE:O	1:B:463:ARG:HG3	2.09	0.52
1:B:571:HIS:O	1:B:575:ILE:HG23	2.09	0.52
1:B:610:GLU:C	1:B:612:LEU:H	2.12	0.52
1:A:231:ASN:OD1	1:A:232:ALA:N	2.42	0.52
1:A:287:ASN:C	1:A:289:ALA:H	2.13	0.52
1:A:34:LEU:HG	1:A:35:GLN:HG3	1.89	0.52
1:A:630:HIS:N	1:A:737:LEU:HD13	2.24	0.52
1:B:377:LYS:HG3	1:B:384:GLN:O	2.10	0.52
1:B:487:TYR:O	1:B:491:MET:HG2	2.10	0.52
1:A:519:VAL:HG22	1:A:542:THR:N	2.25	0.52
1:A:223:ALA:O	1:A:227:GLN:N	2.34	0.52
1:A:472:GLU:HB3	1:A:475:ALA:CB	2.40	0.52
1:B:133:GLU:OE2	1:B:136:ARG:HD2	2.09	0.52
1:B:80:LEU:CD1	1:B:81:SER:H	2.14	0.52
1:B:114:SER:HB2	1:B:223:ALA:HB2	1.90	0.52
1:B:610:GLU:OE2	1:B:614:LEU:N	2.40	0.52
1:A:345:GLN:HG2	1:A:555:ILE:HG12	1.91	0.52
1:A:732:LEU:HD21	1:A:738:LEU:HD21	1.91	0.52
1:A:38:LEU:H	1:A:501:VAL:HG21	1.73	0.52
1:B:42:ARG:HH11	1:B:339:THR:N	2.07	0.52
1:B:378:LEU:HD12	1:B:379:ALA:N	2.24	0.52
1:B:400:THR:O	1:B:403:PRO:HD2	2.10	0.52
1:B:575:ILE:HB	1:B:576:HIS:O	2.09	0.52
1:A:524:THR:HG21	1:A:540:ILE:HG12	1.92	0.52
1:B:346:THR:OG1	1:B:359:VAL:HG11	2.10	0.52
1:B:445:VAL:O	1:B:449:TYR:HB3	2.09	0.52
1:B:35:GLN:NE2	1:B:503:VAL:O	2.42	0.52
1:A:713:ASP:HA	1:A:715:HIS:ND1	2.24	0.52
1:B:587:PHE:HA	1:B:622:ARG:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:PRO:O	1:A:130:ALA:N	2.36	0.51
1:A:159:SER:OG	1:A:160:PRO:HD3	2.09	0.51
1:B:107:THR:HA	1:B:110:ILE:HD12	1.92	0.51
1:B:110:ILE:O	1:B:111:THR:OG1	2.28	0.51
1:B:152:ASP:OD1	1:B:153:PHE:N	2.43	0.51
1:B:408:PHE:CD1	1:B:413:PHE:HZ	2.22	0.51
1:B:42:ARG:CZ	1:B:334:ARG:HG3	2.39	0.51
1:A:100:PRO:HA	1:A:103:TRP:CD1	2.45	0.51
1:B:338:GLU:OE2	1:B:341:SER:N	2.43	0.51
1:B:387:LEU:HD23	1:B:578:TRP:HH2	1.75	0.51
1:A:105:LYS:HE2	1:A:138:LEU:HD11	1.91	0.51
1:A:296:ASP:HB2	1:A:300:GLN:HG2	1.92	0.51
1:B:482:SER:HA	1:B:485:ASN:HD21	1.76	0.51
1:A:245:ASP:HB2	1:A:248:ALA:HB3	1.93	0.51
1:A:32:GLY:H	1:A:541:ARG:HH21	1.59	0.51
1:A:580:TRP:CH2	1:A:622:ARG:HD3	2.45	0.51
1:B:326:SER:HB2	1:B:328:VAL:HG22	1.92	0.51
1:A:144:GLU:HG2	1:A:145:LEU:N	2.26	0.51
1:A:157:VAL:O	1:A:160:PRO:HD2	2.10	0.51
1:A:39:GLN:HA	1:A:501:VAL:HG11	1.92	0.51
1:B:132:LEU:HG	1:B:135:LEU:HB2	1.91	0.51
1:B:198:MET:O	1:B:202:LEU:HD13	2.11	0.51
1:A:252:SER:HB3	1:A:306:VAL:HG13	1.93	0.51
1:B:154:VAL:HA	1:B:229:LEU:HD11	1.92	0.51
1:B:25:LEU:O	1:B:27:ASN:ND2	2.44	0.51
1:B:343:ILE:HB	1:B:493:TYR:OH	2.10	0.51
1:B:568:LEU:O	1:B:572:THR:N	2.38	0.51
1:A:103:TRP:O	1:A:226:SER:OG	2.26	0.51
1:A:106:LEU:O	1:A:110:ILE:HG12	2.10	0.51
1:A:720:ARG:HD2	1:A:760:VAL:HG21	1.91	0.51
1:B:100:PRO:HA	1:B:103:TRP:HE3	1.74	0.51
1:A:284:LEU:C	1:A:287:ASN:H	2.14	0.51
1:B:145:LEU:HD12	1:B:146:PHE:H	1.76	0.51
1:B:7:LYS:HA	1:B:531:GLY:HA2	1.93	0.51
1:B:363:ASP:OD2	1:B:557:PRO:HB2	2.11	0.51
1:A:196:ARG:O	1:A:197:ARG:NH1	2.40	0.51
1:A:698:ILE:O	1:A:702:MET:HE2	2.11	0.51
1:B:387:LEU:H	1:B:575:ILE:HD11	1.76	0.51
1:B:45:SER:HG	1:B:180:TYR:HE1	1.57	0.51
1:A:54:TRP:CZ3	1:A:174:VAL:HG12	2.46	0.50
1:A:261:TRP:CE2	1:A:288:LEU:HG	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:GLN:O	1:A:673:THR:N	2.39	0.50
1:B:183:PHE:HB2	1:B:297:MET:HB3	1.92	0.50
1:B:42:ARG:HE	1:B:335:PRO:C	2.15	0.50
1:A:276:ARG:HB2	1:A:281:ILE:HD11	1.93	0.50
1:B:114:SER:HB3	1:B:222:PRO:HG2	1.92	0.50
1:B:321:PHE:HA	1:B:325:MET:SD	2.51	0.50
1:A:340:THR:O	1:A:343:ILE:HG22	2.12	0.50
1:A:369:GLU:HA	1:A:398:SER:HB2	1.94	0.50
1:A:387:LEU:H	1:A:572:THR:HG22	1.76	0.50
1:B:4:LEU:H	1:B:437:MET:HB3	1.76	0.50
1:B:16:LEU:HB3	1:B:546:LEU:HD11	1.94	0.50
1:A:409:ALA:O	1:A:413:PHE:N	2.38	0.50
1:B:18:GLN:O	1:B:22:ILE:HG12	2.11	0.50
1:B:413:PHE:HB3	1:B:636:TRP:HZ2	1.76	0.50
1:A:715:HIS:CG	1:A:716:VAL:H	2.29	0.50
1:B:597:ILE:HG22	1:B:602:TYR:CE2	2.47	0.50
1:A:347:SER:O	1:A:358:VAL:HG22	2.11	0.50
1:A:352:MET:SD	1:A:355:PRO:HD2	2.51	0.50
1:B:352:MET:H	1:B:353:GLY:HA2	1.75	0.50
1:A:366:PHE:HD2	1:A:405:GLY:HA2	1.77	0.50
1:B:24:GLU:OE2	1:B:28:GLN:N	2.45	0.50
1:B:342:TYR:HB3	1:B:559:GLU:CG	2.42	0.50
1:B:586:GLU:C	1:B:622:ARG:HE	2.15	0.50
1:B:71:PHE:O	1:B:75:GLN:HG2	2.12	0.50
1:A:502:VAL:HA	1:A:503:VAL:CB	2.42	0.50
1:A:745:ALA:O	1:A:749:VAL:HG23	2.12	0.50
1:B:560:VAL:O	1:B:562:GLN:N	2.45	0.50
1:A:16:LEU:HD11	1:A:462:LEU:HB3	1.94	0.49
1:B:352:MET:H	1:B:353:GLY:CA	2.26	0.49
1:B:58:LYS:HE2	1:B:60:ASN:HD22	1.77	0.49
1:B:666:ARG:HA	1:B:669:GLN:HG2	1.93	0.49
1:A:128:PRO:HG2	1:A:129:THR:OG1	2.13	0.49
1:A:196:ARG:HB3	1:A:197:ARG:NH1	2.27	0.49
1:A:81:SER:HB2	1:A:188:ASP:OD2	2.12	0.49
1:A:127:PRO:C	1:A:129:THR:HB	2.33	0.49
1:A:42:ARG:H	1:A:336:ILE:CD1	2.25	0.49
1:A:477:ASN:OD1	1:A:478:ASP:N	2.45	0.49
1:B:199:LEU:HA	1:B:202:LEU:HB2	1.93	0.49
1:B:209:MET:SD	1:B:228:HIS:HE1	2.35	0.49
1:B:45:SER:O	1:B:332:LYS:N	2.45	0.49
1:A:567:ASP:O	1:A:569:ALA:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:PHE:CZ	1:B:405:GLY:HA2	2.47	0.49
1:B:676:ARG:O	1:B:679:GLU:HB3	2.12	0.49
1:A:253:VAL:HG11	1:A:322:ILE:HD13	1.95	0.49
1:B:232:ALA:O	1:B:236:ALA:N	2.43	0.49
1:A:156:HIS:O	1:A:159:SER:OG	2.30	0.49
1:A:585:THR:O	1:A:622:ARG:HG2	2.12	0.49
1:B:379:ALA:O	1:B:381:ASN:N	2.45	0.49
1:B:403:PRO:O	1:B:407:THR:HG22	2.13	0.49
1:A:433:ASN:HB3	1:A:434:GLY:C	2.33	0.49
1:A:433:ASN:HB3	1:A:434:GLY:HA3	1.95	0.49
1:A:443:SER:O	1:A:447:ARG:HG2	2.11	0.49
1:A:365:GLN:CA	1:A:562:GLN:HB2	2.41	0.49
1:B:296:ASP:O	1:B:299:LYS:HB3	2.13	0.49
1:A:716:VAL:HG21	1:B:386:PHE:CE2	2.48	0.49
1:B:415:LYS:O	1:B:418:THR:OG1	2.28	0.49
1:A:155:CYS:O	1:A:159:SER:N	2.45	0.49
1:B:42:ARG:HD3	1:B:337:ASN:N	2.21	0.49
1:A:15:GLY:O	1:A:487:TYR:OH	2.21	0.48
1:A:396:ARG:HE	1:A:612:LEU:HB3	1.78	0.48
1:B:136:ARG:HE	1:B:147:HIS:CD2	2.31	0.48
1:B:125:LYS:HZ2	1:B:155:CYS:HA	1.78	0.48
1:B:726:TRP:HA	1:B:729:LEU:HD12	1.95	0.48
1:B:737:LEU:HB3	1:B:738:LEU:HD12	1.95	0.48
1:A:391:PRO:HA	1:A:394:SER:HB2	1.93	0.48
1:B:396:ARG:HD2	1:B:612:LEU:HD13	1.95	0.48
1:B:30:SER:HB2	1:B:517:TYR:CE2	2.47	0.48
1:A:16:LEU:HA	1:A:487:TYR:CE1	2.36	0.48
1:B:610:GLU:CD	1:B:614:LEU:H	2.15	0.48
1:A:556:GLN:OE1	1:A:557:PRO:HD2	2.13	0.48
1:A:747:THR:HA	1:A:750:LEU:HG	1.96	0.48
1:B:743:ALA:O	1:B:747:THR:N	2.36	0.48
1:A:418:THR:O	1:A:421:TYR:CD1	2.66	0.48
1:A:61:ILE:HG13	1:A:66:TYR:CE2	2.47	0.48
1:A:719:ASN:OD1	1:A:720:ARG:N	2.46	0.48
1:B:41:THR:O	1:B:42:ARG:HG2	2.14	0.48
1:B:30:SER:O	1:B:543:PRO:HG3	2.13	0.48
1:A:729:LEU:O	1:A:732:LEU:HB3	2.14	0.48
1:A:355:PRO:O	1:A:356:SER:OG	2.28	0.48
1:A:477:ASN:O	1:A:481:ARG:N	2.47	0.48
1:A:516:LEU:O	1:A:516:LEU:HD12	2.13	0.48
1:A:66:TYR:HA	1:A:69:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:GLY:HA2	1:B:261:TRP:HD1	1.78	0.48
1:B:314:SER:OG	1:B:317:ILE:N	2.31	0.48
1:A:696:SER:OG	1:A:697:ARG:NH1	2.47	0.48
1:B:660:LYS:O	1:B:663:ILE:HG13	2.13	0.48
1:A:335:PRO:HB2	1:A:338:GLU:OE2	2.14	0.48
1:A:648:ALA:O	1:A:652:ARG:HG3	2.14	0.48
1:A:109:TYR:OH	1:A:130:ALA:HB1	2.14	0.48
1:A:16:LEU:HD21	1:A:462:LEU:HD13	1.96	0.48
1:A:257:LEU:HB3	1:A:261:TRP:CZ2	2.48	0.48
1:B:164:ILE:HG13	1:B:165:LEU:H	1.79	0.48
1:B:254:LEU:HD22	1:B:297:MET:SD	2.54	0.48
1:B:747:THR:O	1:B:750:LEU:HG	2.13	0.48
1:A:533:ASN:ND2	1:A:542:THR:OG1	2.47	0.47
1:A:672:VAL:HA	1:A:675:LEU:HD12	1.96	0.47
1:B:132:LEU:HA	1:B:135:LEU:HD13	1.95	0.47
1:B:357:HIS:O	1:B:359:VAL:HG23	2.14	0.47
1:B:510:ALA:HB1	1:B:513:GLN:H	1.79	0.47
1:A:362:GLU:HB2	1:A:364:TRP:HE1	1.79	0.47
1:A:4:LEU:HG	1:A:436:GLU:CB	2.37	0.47
1:B:197:ARG:NH2	1:B:240:SER:HA	2.29	0.47
1:B:288:LEU:O	1:B:292:ILE:HD12	2.14	0.47
1:B:356:SER:HA	1:B:435:ALA:HB1	1.96	0.47
1:B:719:ASN:OD1	1:B:720:ARG:N	2.47	0.47
1:A:334:ARG:HD3	1:A:338:GLU:CB	2.41	0.47
1:B:525:GLU:OE2	1:B:535:ILE:HG12	2.14	0.47
1:A:83:ASP:OD1	1:A:191:ARG:NE	2.47	0.47
1:B:345:GLN:OE1	1:B:360:VAL:HG12	2.14	0.47
1:B:449:TYR:OH	1:B:630:HIS:ND1	2.13	0.47
1:A:375:PRO:CG	1:A:622:ARG:HE	2.26	0.47
1:A:441:PHE:HB2	1:A:444:VAL:HG22	1.96	0.47
1:B:379:ALA:C	1:B:381:ASN:H	2.17	0.47
1:A:282:ASP:O	1:A:285:ARG:HB3	2.14	0.47
1:A:308:PHE:HE2	1:A:318:ILE:HG13	1.80	0.47
1:A:745:ALA:O	1:A:748:LYS:HB3	2.15	0.47
1:B:111:THR:HA	1:B:112:GLY:HA3	1.65	0.47
1:B:725:ILE:O	1:B:729:LEU:HG	2.15	0.47
1:A:344:GLY:HA2	1:A:557:PRO:HB3	1.96	0.47
1:A:376:VAL:O	1:A:386:PHE:N	2.47	0.47
1:A:80:LEU:HD21	1:A:477:ASN:HD21	1.79	0.47
1:A:580:TRP:CE3	1:A:581:HIS:HA	2.49	0.47
1:A:757:GLY:HA3	1:A:759:VAL:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:LEU:O	1:B:149:ILE:HG12	2.14	0.47
1:B:195:LEU:O	1:B:198:MET:HB3	2.14	0.47
1:A:739:SER:OG	1:A:742:GLU:OE1	2.32	0.47
1:B:585:THR:C	1:B:622:ARG:HB2	2.35	0.47
1:A:6:VAL:HG11	1:A:530:VAL:HG23	1.96	0.47
1:B:437:MET:HE2	1:B:546:LEU:HD22	1.96	0.47
1:B:474:ARG:O	1:B:477:ASN:HB3	2.15	0.47
1:A:493:TYR:CZ	1:A:549:ILE:HG12	2.49	0.47
1:A:56:VAL:HG13	1:A:66:TYR:CE1	2.50	0.47
1:A:712:SER:C	1:A:715:HIS:HD1	2.16	0.47
1:B:125:LYS:NZ	1:B:155:CYS:HA	2.29	0.47
1:B:144:GLU:N	1:B:144:GLU:OE1	2.45	0.47
1:B:54:TRP:CZ3	1:B:65:MET:HG2	2.50	0.47
1:B:619:GLU:N	1:B:619:GLU:OE1	2.48	0.47
1:B:630:HIS:HE1	1:B:739:SER:HB3	1.80	0.47
1:B:7:LYS:HD3	1:B:531:GLY:N	2.22	0.47
1:A:280:GLY:N	1:A:282:ASP:OD1	2.48	0.47
1:B:136:ARG:HH21	1:B:147:HIS:CG	2.33	0.47
1:B:9:LEU:HD22	1:B:546:LEU:HD12	1.97	0.47
1:B:686:ILE:O	1:B:689:SER:OG	2.21	0.47
1:A:149:ILE:HA	1:A:152:ASP:OD2	2.15	0.46
1:A:535:ILE:HG13	1:A:540:ILE:HG23	1.96	0.46
1:B:129:THR:HG22	1:B:151:THR:HG21	1.96	0.46
1:B:297:MET:HA	1:B:300:GLN:OE1	2.15	0.46
1:B:414:VAL:O	1:B:418:THR:HG23	2.15	0.46
1:B:41:THR:C	1:B:43:THR:H	2.17	0.46
1:B:449:TYR:HH	1:B:630:HIS:CE1	2.19	0.46
1:B:154:VAL:HG22	1:B:229:LEU:HD13	1.97	0.46
1:B:317:ILE:HA	1:B:320:TRP:CE2	2.50	0.46
1:B:354:GLN:NE2	1:B:431:ASN:HD22	2.12	0.46
1:B:176:ARG:NH2	1:B:446:GLU:O	2.44	0.46
1:B:677:LYS:O	1:B:680:MET:HG2	2.15	0.46
1:A:212:ALA:HB3	1:A:219:ALA:HB3	1.97	0.46
1:B:386:PHE:CE1	1:B:576:HIS:N	2.83	0.46
1:B:427:ARG:HB3	1:B:428:GLY:HA3	1.97	0.46
1:B:481:ARG:O	1:B:485:ASN:ND2	2.48	0.46
1:B:577:ILE:HG13	1:B:578:TRP:H	1.80	0.46
1:B:673:THR:O	1:B:677:LYS:HD3	2.14	0.46
1:A:337:ASN:HD21	1:A:496:ALA:HB2	1.80	0.46
1:B:529:PRO:O	1:B:530:VAL:HG13	2.16	0.46
1:B:606:VAL:HB	1:B:697:ARG:CZ	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:610:GLU:OE1	1:B:610:GLU:N	2.42	0.46
1:B:648:ALA:HA	1:B:651:ARG:HD3	1.98	0.46
1:B:657:ASP:O	1:B:660:LYS:HB3	2.15	0.46
1:A:176:ARG:C	1:A:447:ARG:HH12	2.19	0.46
1:A:282:ASP:N	1:A:282:ASP:OD1	2.48	0.46
1:A:418:THR:O	1:A:421:TYR:HD1	1.99	0.46
1:B:53:LEU:HD22	1:B:571:HIS:ND1	2.30	0.46
1:A:36:LEU:C	1:A:502:VAL:HG11	2.36	0.46
1:B:318:ILE:H	1:B:318:ILE:HD12	1.80	0.46
1:B:368:LYS:O	1:B:398:SER:OG	2.32	0.46
1:A:210:LEU:HB3	1:A:212:ALA:O	2.16	0.46
1:A:281:ILE:HG22	1:A:319:PRO:HB2	1.98	0.46
1:A:329:SER:HB3	1:A:331:PHE:HB3	1.98	0.46
1:A:349:ILE:HD11	1:A:356:SER:HB2	1.96	0.46
1:A:678:ILE:HA	1:A:681:ILE:HG12	1.97	0.46
1:B:164:ILE:HG23	1:B:165:LEU:N	2.31	0.46
1:B:374:THR:N	1:B:387:LEU:O	2.43	0.46
1:B:18:GLN:OE1	1:B:517:TYR:HB2	2.16	0.46
1:A:261:TRP:HE1	1:A:288:LEU:HD11	1.81	0.46
1:A:303:ARG:HB2	1:A:513:GLN:OE1	2.15	0.46
1:A:45:SER:C	1:A:332:LYS:HD2	2.37	0.46
1:B:10:ASN:HB2	1:B:14:ARG:HH11	1.81	0.46
1:B:376:VAL:HG12	1:B:378:LEU:HD23	1.98	0.46
1:B:641:VAL:HG23	1:B:645:ARG:HH12	1.80	0.46
1:B:62:ASP:CG	1:B:64:VAL:HG22	2.37	0.46
1:B:677:LYS:O	1:B:681:ILE:HG13	2.15	0.46
1:A:328:VAL:HG23	1:A:329:SER:CB	2.46	0.46
1:A:350:ASP:N	1:A:350:ASP:OD1	2.49	0.46
1:A:559:GLU:OE1	1:A:559:GLU:N	2.49	0.46
1:A:371:THR:O	1:A:623:ILE:HD12	2.16	0.46
1:A:666:ARG:O	1:A:670:ASN:ND2	2.49	0.46
1:B:317:ILE:HA	1:B:320:TRP:CD2	2.51	0.46
1:B:590:GLU:HB2	1:B:606:VAL:O	2.16	0.46
1:B:596:THR:HG22	1:B:601:ARG:HD2	1.97	0.46
1:B:584:SER:C	1:B:622:ARG:HG2	2.35	0.46
1:A:328:VAL:HG23	1:A:329:SER:HB2	1.97	0.45
1:A:3:ASN:HA	1:A:436:GLU:HB3	1.98	0.45
1:A:685:GLY:HA2	1:A:686:ILE:HA	1.53	0.45
1:B:63:PRO:HG3	1:B:200:THR:HB	1.98	0.45
1:B:754:ASN:OD1	1:B:755:ALA:N	2.49	0.45
1:A:17:THR:O	1:A:19:ALA:N	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:VAL:CA	1:A:413:PHE:HB3	2.41	0.45
1:B:334:ARG:HA	1:B:335:PRO:HD3	1.80	0.45
1:A:263:PRO:HG3	1:A:504:SER:HA	1.97	0.45
1:A:317:ILE:O	1:A:320:TRP:HB3	2.16	0.45
1:A:662:ALA:HA	1:B:108:ALA:O	2.17	0.45
1:B:10:ASN:ND2	1:B:29:LEU:HD21	2.30	0.45
1:B:413:PHE:HB3	1:B:636:TRP:CZ2	2.51	0.45
1:A:146:PHE:HA	1:A:149:ILE:HB	1.97	0.45
1:A:498:ASN:OD1	1:A:499:PRO:HD2	2.15	0.45
1:A:69:LEU:HD22	1:A:172:TYR:HD2	1.80	0.45
1:A:298:VAL:HG21	1:A:514:GLY:O	2.17	0.45
1:A:315:SER:O	1:A:319:PRO:HD2	2.16	0.45
1:A:371:THR:HB	1:A:389:VAL:HG23	1.96	0.45
1:A:497:HIS:HE2	1:A:548:ALA:C	2.20	0.45
1:A:502:VAL:HG23	1:A:503:VAL:HG12	1.97	0.45
1:A:566:LEU:HD12	1:A:568:LEU:HD23	1.98	0.45
1:B:89:PHE:O	1:B:92:TYR:HB3	2.16	0.45
1:A:16:LEU:HD21	1:A:462:LEU:HB3	1.99	0.45
1:A:410:VAL:O	1:A:414:VAL:HG23	2.16	0.45
1:A:428:GLY:HA3	1:A:429:THR:HA	1.59	0.45
1:A:652:ARG:O	1:A:653:THR:OG1	2.30	0.45
1:A:75:GLN:HE22	1:A:447:ARG:NH2	2.14	0.45
1:B:254:LEU:O	1:B:257:LEU:HB3	2.17	0.45
1:B:55:GLU:O	1:B:58:LYS:NZ	2.49	0.45
1:A:209:MET:O	1:A:210:LEU:HB2	2.16	0.45
1:A:201:ALA:HB1	1:A:239:ARG:HD3	1.98	0.45
1:A:320:TRP:HA	1:A:325:MET:HE1	1.99	0.45
1:A:503:VAL:HG11	1:A:517:TYR:O	2.16	0.45
1:A:595:VAL:HG12	1:A:597:ILE:HG23	1.99	0.45
1:B:25:LEU:O	1:B:27:ASN:N	2.49	0.45
1:B:326:SER:CB	1:B:328:VAL:HG22	2.47	0.45
1:B:42:ARG:HG2	1:B:335:PRO:O	2.17	0.45
1:B:560:VAL:C	1:B:561:LEU:HG	2.36	0.45
1:A:138:LEU:HB3	1:A:139:ALA:H	1.69	0.45
1:A:674:LEU:HA	1:A:677:LYS:NZ	2.32	0.45
1:B:607:LYS:C	1:B:609:PHE:HB2	2.36	0.45
1:B:628:VAL:O	1:B:632:ILE:HG22	2.17	0.45
1:A:224:LEU:HA	1:A:227:GLN:HB3	1.99	0.45
1:A:503:VAL:HG22	1:A:504:SER:H	1.81	0.45
1:B:42:ARG:HH11	1:B:339:THR:CA	2.30	0.45
1:B:426:GLN:HA	1:B:427:ARG:HA	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:HIS:HE1	1:B:555:ILE:HD13	1.82	0.45
1:A:211:GLN:O	1:A:218:GLY:HA3	2.18	0.44
1:B:143:HIS:HB3	1:B:145:LEU:HG	1.98	0.44
1:B:321:PHE:CE1	1:B:325:MET:HG3	2.52	0.44
1:B:346:THR:OG1	1:B:359:VAL:HG21	2.17	0.44
1:A:503:VAL:HG21	1:A:517:TYR:C	2.36	0.44
1:B:125:LYS:HB2	1:B:163:PHE:HB3	1.98	0.44
1:B:454:ASP:O	1:B:457:VAL:HG22	2.17	0.44
1:A:313:LEU:HB3	1:A:314:SER:HB3	1.99	0.44
1:A:366:PHE:O	1:A:368:LYS:HD2	2.17	0.44
1:A:500:GLU:HB3	1:A:521:ASN:H	1.83	0.44
1:B:125:LYS:HB3	1:B:165:LEU:O	2.18	0.44
1:B:609:PHE:HA	1:B:616:GLN:OE1	2.18	0.44
1:A:57:GLY:N	1:A:170:TYR:HB2	2.30	0.44
1:A:51:GLU:CA	1:A:174:VAL:HG21	2.44	0.44
1:A:271:PRO:HA	1:A:276:ARG:HD3	2.00	0.44
1:B:122:ALA:H	1:B:163:PHE:HE1	1.64	0.44
1:B:125:LYS:HE2	1:B:163:PHE:CB	2.47	0.44
1:A:55:GLU:N	1:A:55:GLU:OE1	2.51	0.44
1:A:580:TRP:HA	1:A:581:HIS:C	2.36	0.44
1:A:719:ASN:O	1:A:722:ARG:HB3	2.18	0.44
1:B:61:ILE:HD13	1:B:156:HIS:HB3	1.99	0.44
1:B:274:ARG:CB	1:B:312:GLU:HG3	2.46	0.44
1:B:332:LYS:HE2	1:B:334:ARG:NH1	2.30	0.44
1:A:423:ALA:HA	1:A:424:VAL:HA	1.48	0.44
1:A:66:TYR:HD1	1:A:69:LEU:HD12	1.83	0.44
1:B:233:ALA:HA	1:B:236:ALA:HB3	1.98	0.44
1:B:280:GLY:HA2	1:B:283:GLN:HE22	1.83	0.44
1:B:292:ILE:HG21	1:B:488:ALA:HB2	1.98	0.44
1:B:577:ILE:HG13	1:B:578:TRP:N	2.33	0.44
1:A:366:PHE:CD2	1:A:405:GLY:HA2	2.52	0.44
1:A:549:ILE:HA	1:A:552:ASN:HB2	2.00	0.44
1:A:590:GLU:OE1	1:A:607:LYS:HD3	2.18	0.44
1:B:106:LEU:O	1:B:109:TYR:HB3	2.17	0.44
1:B:56:VAL:O	1:B:170:TYR:N	2.50	0.44
1:A:260:LEU:HD11	1:A:285:ARG:HH12	1.82	0.44
1:A:337:ASN:O	1:A:341:SER:N	2.50	0.44
1:B:225:ILE:O	1:B:228:HIS:HB3	2.18	0.44
1:B:387:LEU:HD23	1:B:578:TRP:CH2	2.53	0.44
1:B:172:TYR:CE1	1:B:579:PRO:HG2	2.51	0.44
1:A:199:LEU:HD23	1:A:203:SER:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ARG:HD2	1:A:580:TRP:NE1	2.29	0.44
1:A:56:VAL:HB	1:A:170:TYR:HB2	2.00	0.44
1:A:737:LEU:O	1:A:738:LEU:HG	2.18	0.44
1:B:14:ARG:CZ	1:B:26:LYS:HA	2.48	0.44
1:B:321:PHE:CD1	1:B:325:MET:HG3	2.53	0.44
1:B:656:ASP:HB3	1:B:659:GLU:CG	2.48	0.44
1:A:116:ARG:HA	1:A:118:ILE:H	1.82	0.43
1:A:348:ALA:O	1:A:349:ILE:HG22	2.18	0.43
1:B:251:SER:O	1:B:254:LEU:HB3	2.18	0.43
1:B:610:GLU:HG2	1:B:612:LEU:N	2.33	0.43
1:B:675:LEU:HD21	1:B:757:GLY:O	2.18	0.43
1:B:9:LEU:HD12	1:B:10:ASN:N	2.33	0.43
1:A:293:ALA:O	1:A:297:MET:HB2	2.19	0.43
1:A:402:ALA:HB3	1:A:403:PRO:HD3	2.00	0.43
1:A:454:ASP:O	1:A:457:VAL:HG12	2.18	0.43
1:B:66:TYR:CD1	1:B:69:LEU:HD12	2.49	0.43
1:A:389:VAL:HG13	1:A:391:PRO:HD3	1.99	0.43
1:A:655:ARG:H	1:A:656:ASP:CB	2.30	0.43
1:A:68:ARG:CZ	1:A:330:PRO:HG3	2.49	0.43
1:B:228:HIS:O	1:B:230:ALA:N	2.51	0.43
1:B:349:ILE:HD12	1:B:353:GLY:HA3	2.00	0.43
1:A:259:ARG:O	1:A:262:SER:OG	2.23	0.43
1:A:359:VAL:HG22	1:A:437:MET:O	2.19	0.43
1:A:590:GLU:OE2	1:A:607:LYS:HA	2.18	0.43
1:A:682:GLY:O	1:A:684:THR:N	2.51	0.43
1:B:133:GLU:O	1:B:136:ARG:HB3	2.18	0.43
1:B:209:MET:HG3	1:B:228:HIS:CE1	2.54	0.43
1:B:230:ALA:HB1	1:B:233:ALA:HB3	2.00	0.43
1:B:225:ILE:O	1:B:229:LEU:N	2.23	0.43
1:B:234:THR:O	1:B:237:PHE:HB3	2.17	0.43
1:B:313:LEU:HD12	1:B:313:LEU:O	2.18	0.43
1:B:681:ILE:HG21	1:B:728:GLY:HA2	1.99	0.43
1:A:204:SER:O	1:A:206:ASP:N	2.52	0.43
1:A:221:ALA:HB1	1:A:224:LEU:HB3	1.99	0.43
1:A:362:GLU:OE1	1:A:443:SER:OG	2.35	0.43
1:A:424:VAL:HG12	1:A:425:SER:O	2.18	0.43
1:A:59:GLY:HA3	1:A:155:CYS:HB3	2.00	0.43
1:A:754:ASN:HB3	1:A:755:ALA:C	2.39	0.43
1:B:604:ALA:HB1	1:B:697:ARG:NH2	2.32	0.43
1:A:349:ILE:HA	1:A:349:ILE:HD12	1.79	0.43
1:A:49:THR:OG1	1:A:50:SER:N	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:LEU:HA	1:A:677:LYS:HG2	2.00	0.43
1:B:675:LEU:O	1:B:678:ILE:HG13	2.19	0.43
1:A:241:ARG:HG3	1:A:243:ASN:H	1.84	0.43
1:A:369:GLU:HA	1:A:398:SER:CB	2.49	0.43
1:A:368:LYS:HE2	1:A:402:ALA:O	2.18	0.43
1:A:544:GLU:HG2	1:A:545:PRO:HD2	2.01	0.43
1:A:345:GLN:HE22	1:A:549:ILE:HG23	1.83	0.43
1:A:715:HIS:HB2	1:A:716:VAL:HG13	2.01	0.43
1:A:754:ASN:H	1:A:755:ALA:HA	1.82	0.43
1:B:521:ASN:OD1	1:B:539:SER:HB3	2.18	0.43
1:B:721:HIS:CD2	1:B:757:GLY:HA2	2.54	0.43
1:B:732:LEU:HD13	1:B:743:ALA:HB2	2.00	0.43
1:A:177:THR:HA	1:A:447:ARG:HH22	1.83	0.43
1:A:368:LYS:HA	1:A:401:LEU:HD23	2.01	0.43
1:B:160:PRO:HG3	1:B:210:LEU:HD22	2.00	0.43
1:B:2:PHE:N	1:B:439:LEU:O	2.50	0.43
1:B:604:ALA:HB1	1:B:697:ARG:HH21	1.83	0.43
1:A:176:ARG:NH1	1:A:447:ARG:HA	2.26	0.43
1:A:54:TRP:CH2	1:A:174:VAL:HG12	2.54	0.43
1:A:566:LEU:CD1	1:A:568:LEU:HB3	2.49	0.43
1:B:153:PHE:CZ	1:B:202:LEU:HD23	2.51	0.43
1:B:359:VAL:HG22	1:B:418:THR:HG22	2.00	0.43
1:B:360:VAL:HG23	1:B:439:LEU:HB3	2.00	0.43
1:B:376:VAL:N	1:B:386:PHE:O	2.50	0.43
1:B:3:ASN:HA	1:B:437:MET:O	2.19	0.43
1:A:182:ASN:HD21	1:A:184:TYR:HD2	1.67	0.42
1:A:41:THR:OG1	1:A:42:ARG:N	2.51	0.42
1:A:536:GLU:N	1:A:536:GLU:OE1	2.40	0.42
1:A:628:VAL:O	1:A:632:ILE:HD12	2.19	0.42
1:A:666:ARG:HA	1:A:669:GLN:NE2	2.31	0.42
1:A:732:LEU:O	1:A:735:MET:HB3	2.18	0.42
1:B:13:ALA:HA	1:B:463:ARG:O	2.19	0.42
1:B:423:ALA:O	1:B:430:VAL:HG22	2.19	0.42
1:A:289:ALA:C	1:A:291:PHE:H	2.22	0.42
1:A:520:TRP:CH2	1:A:545:PRO:HG3	2.54	0.42
1:A:80:LEU:HA	1:A:81:SER:HA	1.78	0.42
1:B:257:LEU:HG	1:B:261:TRP:HE1	1.84	0.42
1:B:316:THR:HG22	1:B:320:TRP:CD1	2.53	0.42
1:A:716:VAL:HG21	1:B:386:PHE:CD2	2.54	0.42
1:B:675:LEU:HD21	1:B:758:MET:N	2.34	0.42
1:A:521:ASN:O	1:A:539:SER:OG	2.10	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:HIS:HD2	1:A:633:ILE:HD11	1.83	0.42
1:A:246:ALA:O	1:A:249:VAL:HG22	2.19	0.42
1:A:292:ILE:HD11	1:A:491:MET:HG3	2.02	0.42
1:A:523:ARG:HA	1:A:539:SER:HB2	2.01	0.42
1:B:130:ALA:O	1:B:133:GLU:HB3	2.20	0.42
1:B:345:GLN:O	1:B:554:PRO:HB3	2.20	0.42
1:B:606:VAL:HG22	1:B:607:LYS:O	2.20	0.42
1:A:212:ALA:H	1:A:218:GLY:C	2.23	0.42
1:A:43:THR:HA	1:A:289:ALA:CB	2.50	0.42
1:A:2:PHE:HE2	1:A:4:LEU:HD23	1.85	0.42
1:A:259:ARG:HG3	1:A:269:LEU:HD13	2.01	0.42
1:A:291:PHE:O	1:A:292:ILE:HB	2.19	0.42
1:B:40:PHE:CZ	1:B:495:VAL:HG13	2.54	0.42
1:A:474:ARG:HA	1:A:474:ARG:HD3	1.82	0.42
1:A:498:ASN:ND2	1:A:500:GLU:HG2	2.33	0.42
1:A:510:ALA:HA	1:A:511:ALA:HA	1.72	0.42
1:B:43:THR:HG21	1:B:289:ALA:N	2.34	0.42
1:B:518:LEU:O	1:B:543:PRO:HA	2.19	0.42
1:A:608:GLU:HG3	1:A:609:PHE:N	2.35	0.42
1:A:676:ARG:NH1	1:B:165:LEU:HD23	2.34	0.42
1:B:684:THR:O	1:B:688:ALA:N	2.51	0.42
1:A:331:PHE:O	1:A:332:LYS:HG2	2.19	0.42
1:A:373:PHE:CE1	1:A:387:LEU:HD22	2.54	0.42
1:B:19:ALA:HB1	1:B:24:GLU:HB3	2.02	0.42
1:B:2:PHE:CZ	1:B:463:ARG:HG2	2.55	0.42
1:B:494:ALA:HB2	1:B:549:ILE:HD11	2.02	0.42
1:A:101:GLU:OE1	1:A:101:GLU:N	2.49	0.42
1:A:133:GLU:O	1:A:137:THR:HG23	2.20	0.42
1:A:41:THR:HG23	1:A:286:SER:O	2.20	0.42
1:A:292:ILE:HA	1:A:295:GLN:CG	2.50	0.42
1:A:331:PHE:C	1:A:332:LYS:HG2	2.40	0.42
1:A:377:LYS:HD2	1:A:380:ASN:HA	2.01	0.42
1:A:436:GLU:CD	1:A:438:THR:H	2.23	0.42
1:A:629:ALA:HA	1:A:632:ILE:HD13	2.02	0.42
1:A:82:VAL:O	1:A:86:VAL:HG23	2.19	0.42
1:B:257:LEU:HG	1:B:261:TRP:NE1	2.34	0.42
1:B:387:LEU:HD11	1:B:568:LEU:HD13	2.02	0.42
1:B:522:VAL:HB	1:B:540:ILE:HD11	2.02	0.42
1:B:546:LEU:O	1:B:549:ILE:HB	2.19	0.42
1:B:610:GLU:CG	1:B:614:LEU:H	2.33	0.42
1:A:117:ALA:H	1:A:221:ALA:N	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:PRO:HB2	1:A:182:ASN:H	1.43	0.41
1:A:386:PHE:HE1	1:A:576:HIS:H	1.68	0.41
1:A:413:PHE:CZ	1:A:636:TRP:HA	2.54	0.41
1:B:19:ALA:HB1	1:B:24:GLU:CB	2.50	0.41
1:B:43:THR:HG21	1:B:289:ALA:HB3	2.02	0.41
1:B:610:GLU:HG3	1:B:614:LEU:H	1.85	0.41
1:B:640:PHE:HA	1:B:670:ASN:HD21	1.85	0.41
1:B:757:GLY:N	1:B:758:MET:HA	2.35	0.41
1:A:358:VAL:N	1:A:437:MET:HB3	2.31	0.41
1:A:753:SER:HA	1:A:754:ASN:HA	1.85	0.41
1:B:313:LEU:HA	1:B:314:SER:HA	1.32	0.41
1:B:384:GLN:HA	1:B:577:ILE:HG21	2.01	0.41
1:A:230:ALA:HA	1:A:233:ALA:HB3	2.03	0.41
1:A:349:ILE:HG21	1:A:354:GLN:O	2.20	0.41
1:A:38:LEU:HD23	1:A:39:GLN:O	2.19	0.41
1:A:708:ILE:O	1:A:711:SER:OG	2.22	0.41
1:B:401:LEU:O	1:B:405:GLY:N	2.53	0.41
1:A:314:SER:HA	1:A:315:SER:C	2.41	0.41
1:A:349:ILE:HG13	1:A:353:GLY:O	2.21	0.41
1:A:383:ASN:C	1:A:385:ARG:H	2.22	0.41
1:A:553:LYS:O	1:A:555:ILE:HG23	2.20	0.41
1:B:118:ILE:H	1:B:222:PRO:HD2	1.85	0.41
1:B:284:LEU:HA	1:B:287:ASN:HD22	1.86	0.41
1:B:410:VAL:HA	1:B:413:PHE:HD2	1.85	0.41
1:B:522:VAL:O	1:B:540:ILE:HG13	2.20	0.41
1:A:281:ILE:O	1:A:284:LEU:HB2	2.21	0.41
1:A:366:PHE:CE1	1:A:629:ALA:HB2	2.54	0.41
1:B:198:MET:HG3	1:B:202:LEU:HD22	2.02	0.41
1:B:289:ALA:HA	1:B:292:ILE:HD13	2.02	0.41
1:B:637:TYR:O	1:B:641:VAL:HG22	2.20	0.41
1:A:128:PRO:O	1:A:131:ILE:HB	2.21	0.41
1:A:128:PRO:HD3	1:A:166:PRO:HB2	2.03	0.41
1:A:357:HIS:HA	1:A:437:MET:HG2	2.02	0.41
1:A:44:PHE:HE1	1:A:180:TYR:N	2.18	0.41
1:A:657:ASP:O	1:A:660:LYS:HG2	2.20	0.41
1:B:13:ALA:HB1	1:B:462:LEU:HD23	2.03	0.41
1:B:62:ASP:HB3	1:B:65:MET:HG3	2.03	0.41
1:B:669:GLN:O	1:B:672:VAL:HG12	2.21	0.41
1:B:132:LEU:HD23	1:B:147:HIS:NE2	2.35	0.41
1:B:92:TYR:OH	1:B:150:THR:HG21	2.21	0.41
1:B:427:ARG:H	1:B:428:GLY:HA3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:THR:HG22	1:B:44:PHE:O	2.21	0.41
1:B:383:ASN:O	1:B:577:ILE:HG12	2.20	0.41
1:A:186:LEU:O	1:A:190:VAL:HG13	2.21	0.41
1:A:257:LEU:O	1:A:260:LEU:HB3	2.21	0.41
1:A:334:ARG:HG3	1:A:335:PRO:HD2	2.03	0.41
1:A:349:ILE:CD1	1:A:356:SER:HB2	2.51	0.41
1:A:521:ASN:HA	1:A:540:ILE:O	2.21	0.41
1:A:173:ARG:HH11	1:A:579:PRO:HG2	1.86	0.41
1:A:659:GLU:O	1:A:662:ALA:HB3	2.20	0.41
1:B:171:VAL:HG12	1:B:576:HIS:HB3	2.03	0.41
1:B:342:TYR:HA	1:B:558:SER:H	1.86	0.41
1:B:35:GLN:HE21	1:B:502:VAL:CG2	2.32	0.41
1:B:505:GLU:HB2	1:B:506:HIS:O	2.20	0.41
1:B:674:LEU:HA	1:B:674:LEU:HD23	1.82	0.41
1:B:676:ARG:HA	1:B:679:GLU:OE1	2.21	0.41
1:A:216:ALA:HA	1:A:217:LYS:HA	1.72	0.41
1:A:27:ASN:OD1	1:A:28:GLN:N	2.54	0.41
1:A:657:ASP:HA	1:A:660:LYS:HE3	2.03	0.41
1:B:210:LEU:HD12	1:B:211:GLN:N	2.36	0.41
1:A:436:GLU:O	1:A:438:THR:N	2.54	0.41
1:B:135:LEU:HG	1:B:138:LEU:HD12	2.02	0.41
1:A:141:SER:HB3	1:A:144:GLU:HA	2.03	0.41
1:A:310:ASP:CG	1:A:311:GLU:H	2.25	0.41
1:A:506:HIS:CD2	1:A:517:TYR:CE2	3.09	0.41
1:B:132:LEU:CA	1:B:135:LEU:HB2	2.49	0.41
1:B:141:SER:CB	1:B:147:HIS:HB2	2.50	0.41
1:B:451:LEU:HG	1:B:453:ARG:CZ	2.51	0.41
1:B:510:ALA:N	1:B:511:ALA:HA	2.35	0.41
1:B:173:ARG:CZ	1:B:578:TRP:HE1	2.34	0.41
1:B:607:LYS:HB2	1:B:608:GLU:C	2.40	0.41
1:B:68:ARG:NH1	1:B:328:VAL:O	2.54	0.41
1:A:674:LEU:O	1:A:678:ILE:HG13	2.22	0.40
1:B:303:ARG:HB2	1:B:305:GLU:OE2	2.20	0.40
1:B:519:VAL:HG12	1:B:543:PRO:HA	2.03	0.40
1:A:517:TYR:HD1	1:A:518:LEU:H	1.69	0.40
1:B:103:TRP:HH2	1:B:234:THR:HG21	1.86	0.40
1:B:493:TYR:O	1:B:496:ALA:HB3	2.22	0.40
1:B:747:THR:HA	1:B:750:LEU:HG	2.02	0.40
1:A:381:ASN:OD1	1:A:381:ASN:N	2.54	0.40
1:A:3:ASN:HA	1:A:436:GLU:CB	2.50	0.40
1:A:464:THR:HG23	1:A:466:ILE:HG13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:ASP:OD2	1:A:570:ASN:ND2	2.31	0.40
1:B:118:ILE:O	1:B:120:ALA:N	2.54	0.40
1:B:321:PHE:CZ	1:B:326:SER:HB3	2.57	0.40
1:B:501:VAL:HG22	1:B:520:TRP:CD1	2.56	0.40
1:B:6:VAL:HG12	1:B:435:ALA:N	2.36	0.40
1:A:361:TYR:CD1	1:A:414:VAL:HG21	2.57	0.40
1:A:666:ARG:HD3	1:A:669:GLN:HE22	1.87	0.40
1:B:497:HIS:HE1	1:B:555:ILE:CD1	2.35	0.40
1:A:389:VAL:HG22	1:A:390:GLU:N	2.37	0.40
1:A:361:TYR:CG	1:A:414:VAL:HG21	2.56	0.40
1:A:716:VAL:HG11	1:B:386:PHE:CD2	2.56	0.40
1:A:425:SER:CB	1:B:116:ARG:HE	2.35	0.40
1:B:230:ALA:O	1:B:234:THR:HG23	2.22	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	759/761 (100%)	593 (78%)	92 (12%)	74 (10%)	1	13
1	B	759/761 (100%)	597 (79%)	108 (14%)	54 (7%)	1	20
All	All	1518/1522 (100%)	1190 (78%)	200 (13%)	128 (8%)	2	16

All (128) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	VAL
1	A	41	THR
1	A	129	THR
1	A	145	LEU
1	A	174	VAL

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Mol	Chain	Res	Type
1	A	222	PRO
1	A	243	ASN
1	A	288	LEU
1	A	292	ILE
1	A	307	ILE
1	A	349	ILE
1	A	503	VAL
1	A	535	ILE
1	A	568	LEU
1	A	581	HIS
1	A	582	GLU
1	A	608	GLU
1	A	684	THR
1	A	738	LEU
1	B	27	ASN
1	B	31	VAL
1	B	126	VAL
1	B	127	PRO
1	B	164	ILE
1	B	280	GLY
1	B	335	PRO
1	B	337	ASN
1	B	359	VAL
1	B	424	VAL
1	B	582	GLU
1	A	45	SER
1	A	61	ILE
1	A	110	ILE
1	A	122	ALA
1	A	181	PRO
1	A	241	ARG
1	A	277	ASN
1	A	309	SER
1	A	316	THR
1	A	332	LYS
1	A	355	PRO
1	A	356	SER
1	A	381	ASN
1	A	502	VAL
1	A	522	VAL
1	A	537	GLY
1	A	555	ILE

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Mol	Chain	Res	Type
1	A	558	SER
1	A	559	GLU
1	A	717	GLY
1	A	740	ARG
1	B	43	THR
1	B	44	PHE
1	B	48	MET
1	B	61	ILE
1	B	80	LEU
1	B	129	THR
1	B	229	LEU
1	B	342	TYR
1	B	388	ASP
1	B	394	SER
1	B	421	TYR
1	B	565	VAL
1	B	583	ALA
1	B	605	GLU
1	B	609	PHE
1	B	717	GLY
1	B	732	LEU
1	A	34	LEU
1	A	167	ASP
1	A	205	VAL
1	A	214	PHE
1	A	335	PRO
1	A	351	HIS
1	A	384	GLN
1	A	409	ALA
1	A	584	SER
1	A	654	SER
1	A	739	SER
1	B	216	ALA
1	B	710	ASP
1	B	755	ALA
1	B	760	VAL
1	A	49	THR
1	A	113	SER
1	A	178	ALA
1	A	273	ALA
1	A	312	GLU
1	A	375	PRO

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Mol	Chain	Res	Type
1	A	556	GLN
1	B	157	VAL
1	B	254	LEU
1	B	363	ASP
1	B	378	LEU
1	B	506	HIS
1	B	527	ARG
1	B	530	VAL
1	B	603	THR
1	B	617	ARG
1	B	644	ASP
1	A	42	ARG
1	A	123	VAL
1	A	328	VAL
1	A	454	ASP
1	A	499	PRO
1	A	515	SER
1	A	624	LEU
1	A	628	VAL
1	B	34	LEU
1	B	214	PHE
1	B	277	ASN
1	B	454	ASP
1	B	704	GLY
1	A	246	ALA
1	A	329	SER
1	A	471	LEU
1	A	578	TRP
1	B	305	GLU
1	B	568	LEU
1	A	336	ILE
1	A	440	GLY
1	A	428	GLY
1	B	162	GLY
1	B	222	PRO
1	A	280	GLY
1	B	322	ILE
1	B	716	VAL
1	B	118	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	629/629 (100%)	627 (100%)	2 (0%)	94	96
1	B	629/629 (100%)	628 (100%)	1 (0%)	94	96
All	All	1258/1258 (100%)	1255 (100%)	3 (0%)	95	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	503	VAL
1	A	519	VAL
1	B	530	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	HIS
1	A	283	GLN
1	A	337	ASN
1	A	345	GLN
1	A	485	ASN
1	A	492	HIS
1	A	506	HIS
1	A	670	ASN
1	A	695	GLN
1	B	27	ASN
1	B	35	GLN
1	B	39	GLN
1	B	72	GLN
1	B	93	HIS
1	B	228	HIS
1	B	384	GLN
1	B	431	ASN
1	B	492	HIS
1	B	497	HIS

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Mol	Chain	Res	Type
1	B	507	GLN
1	B	634	GLN
1	B	669	GLN
1	B	670	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.