



Full wwPDB EM Validation Report ⓘ

Jun 26, 2025 – 12:40 AM JST

PDB ID : 9IM3 / pdb_00009im3
EMDB ID : EMD-60684
Title : The Cryo-EM structure of MPXV E5 head-to-head double hexamer conformation
Authors : Cheng, Y.X.; Han, P.; Wang, H.
Deposited on : 2024-07-01
Resolution : 3.31 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 : **FAILED**
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

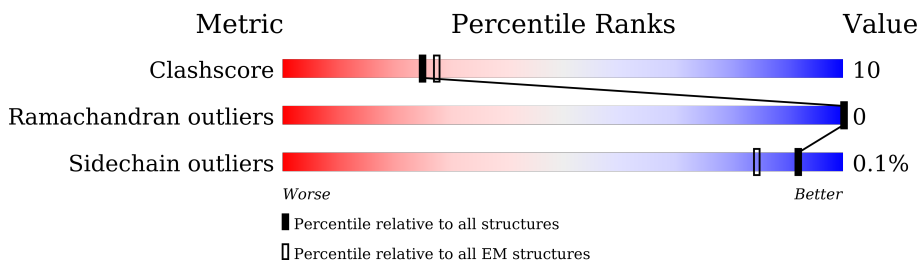
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.31 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	785	48% 17% 35%
1	B	785	49% 16% 35%
1	C	785	49% 16% 35%
1	E	785	52% 13% 35%
1	F	785	46% 18% 35%
1	J	785	45% 20% 35%
1	M	785	46% 18% 35%
1	N	785	52% 13% 35%
1	O	785	48% 17% 35%

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Mol	Chain	Length	Quality of chain
1	Q	785	 49% 16% 35%
1	R	785	 50% 15% 35%
1	S	785	 48% 17% 35%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 49692 atoms, of which 0 are hydrogens and 0 are deuteriums.

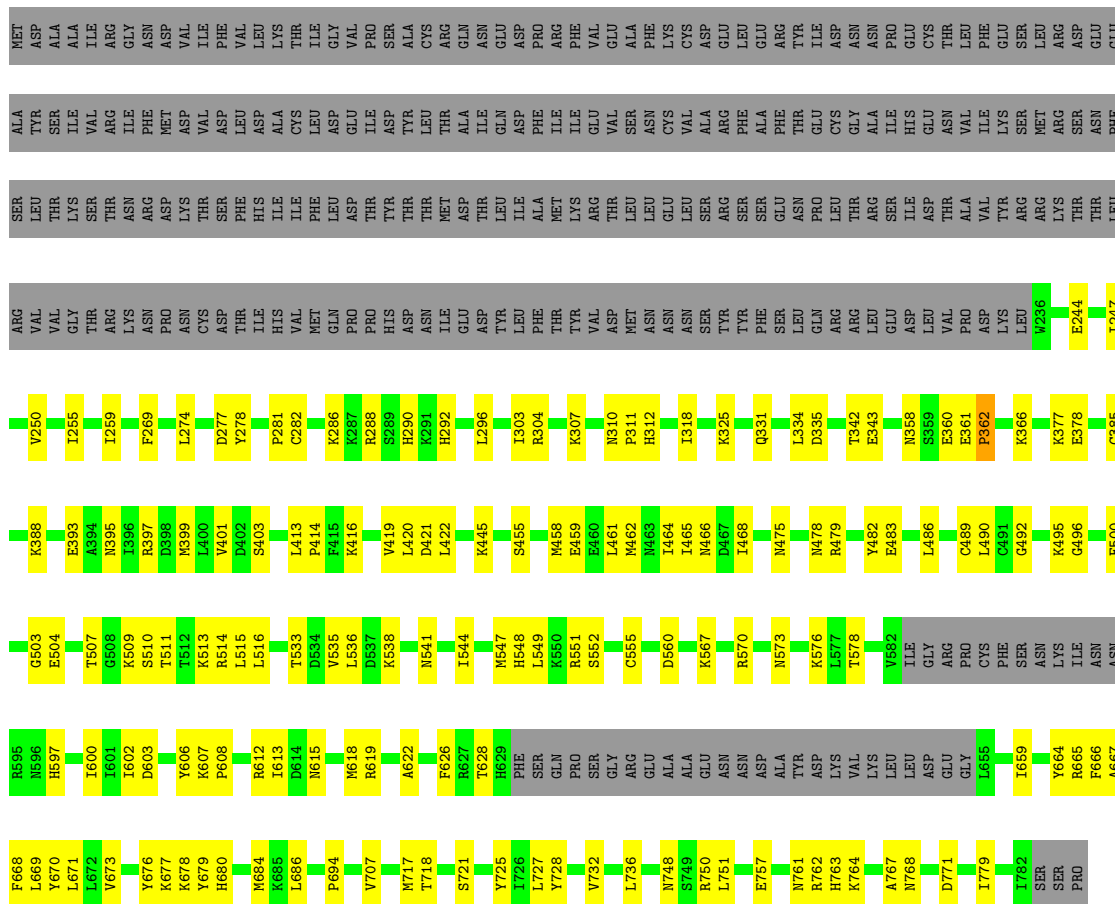
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Primase D5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	510	Total 4141	C 2665	N 696	O 761	S 19	0	0
1	B	510	Total 4141	C 2665	N 696	O 761	S 19	0	0
1	C	510	Total 4141	C 2665	N 696	O 761	S 19	0	0
1	E	510	Total 4141	C 2665	N 696	O 761	S 19	0	0
1	F	510	Total 4141	C 2665	N 696	O 761	S 19	0	0
1	J	510	Total 4141	C 2665	N 696	O 761	S 19	0	0
1	M	510	Total 4141	C 2665	N 696	O 761	S 19	0	0
1	N	510	Total 4141	C 2665	N 696	O 761	S 19	0	0
1	O	510	Total 4141	C 2665	N 696	O 761	S 19	0	0
1	Q	510	Total 4141	C 2665	N 696	O 761	S 19	0	0
1	R	510	Total 4141	C 2665	N 696	O 761	S 19	0	0
1	S	510	Total 4141	C 2665	N 696	O 761	S 19	0	0

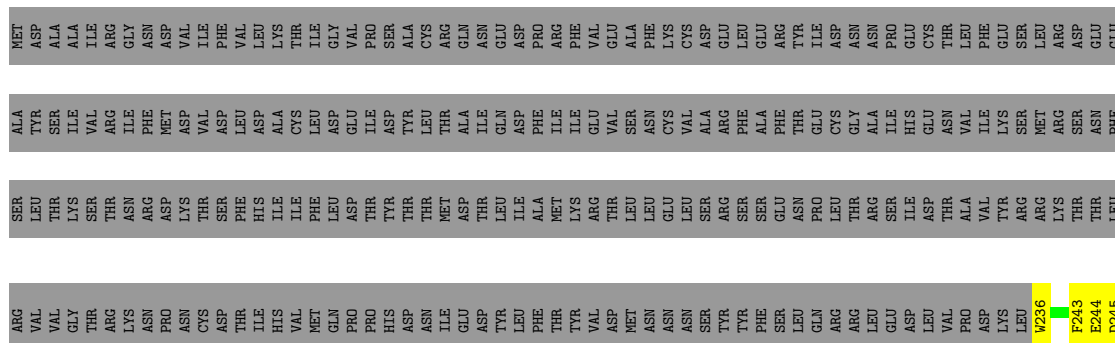
- Molecule 1: Primase D5

Chain J: 45% 20% 35%



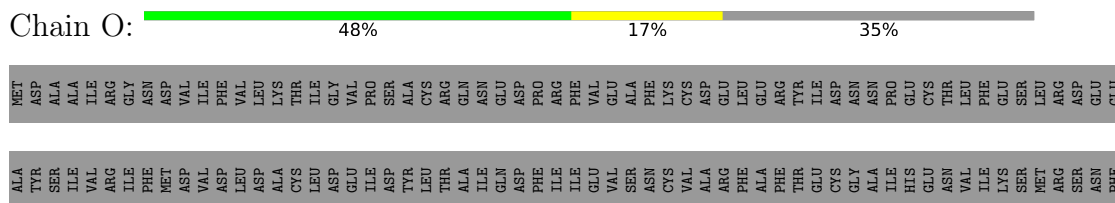
- Molecule 1: Primase D5

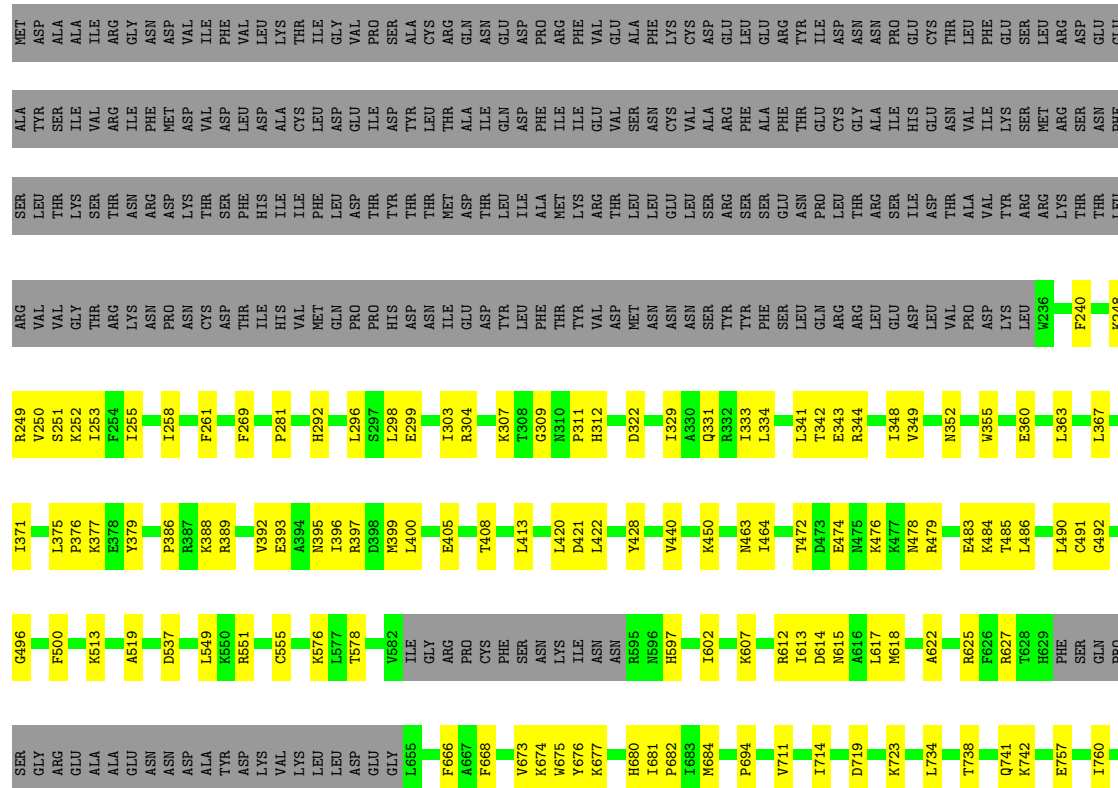
Chain M: 46% 18% 35%



- Molecule 1: Primase D5

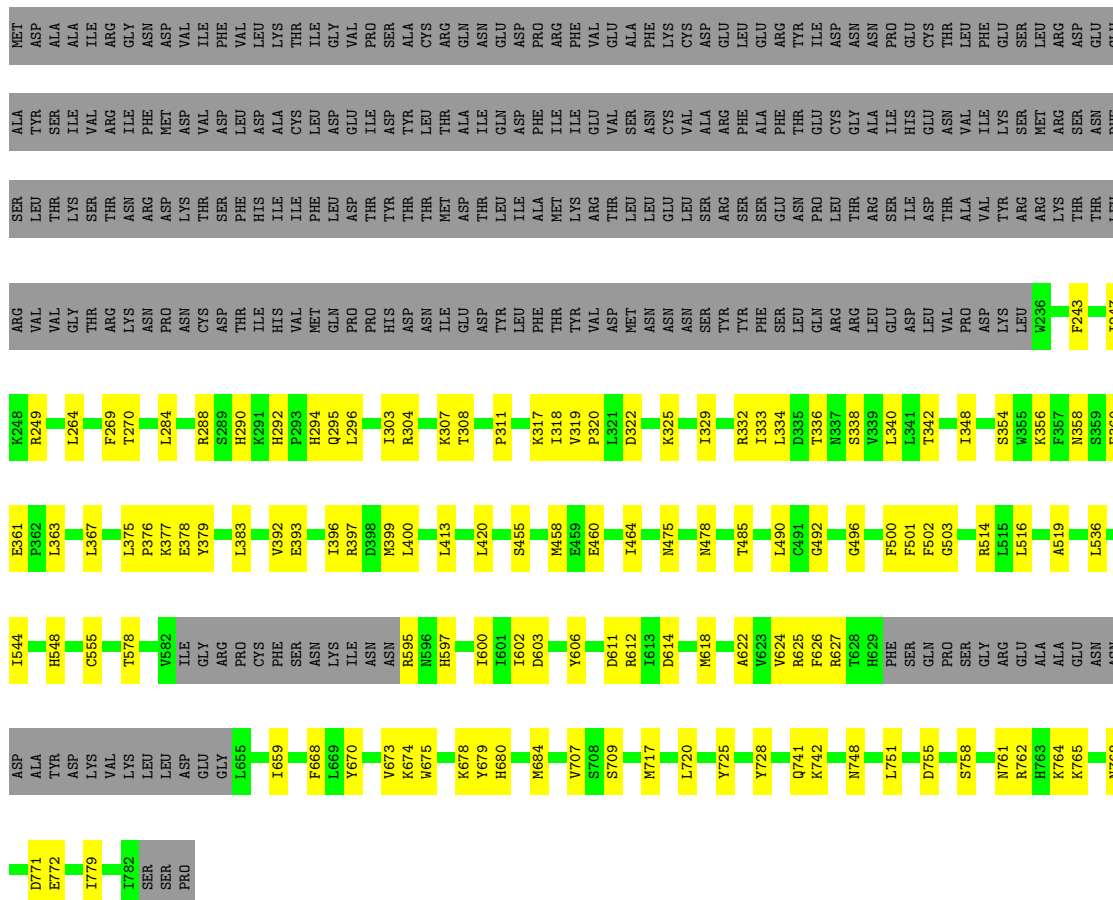
- Molecule 1: Primase D5





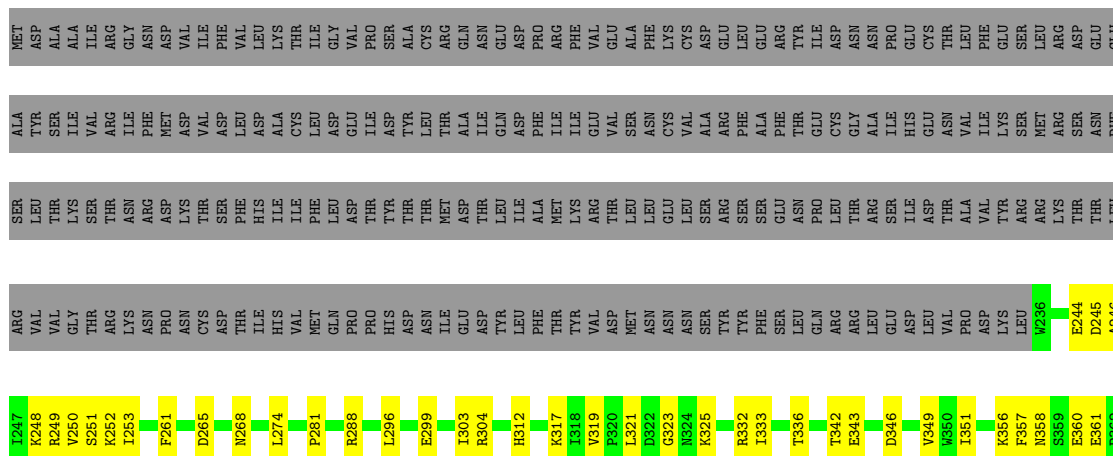
- Molecule 1: Primase D5

Chain R: 50% 15% 35%



- Molecule 1: Primase D5

Chain S: 48% 17% 35%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	311720	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	0.11	0/4233	0.32	0/5721
1	B	0.11	0/4233	0.32	0/5721
1	C	0.11	0/4233	0.32	0/5721
1	E	0.10	0/4233	0.30	0/5721
1	F	0.11	0/4233	0.32	0/5721
1	J	0.14	0/4233	0.38	2/5721 (0.0%)
1	M	0.11	0/4233	0.30	0/5721
1	N	0.09	0/4233	0.27	0/5721
1	O	0.12	0/4233	0.33	1/5721 (0.0%)
1	Q	0.10	0/4233	0.28	0/5721
1	R	0.10	0/4233	0.30	0/5721
1	S	0.10	0/4233	0.30	0/5721
All	All	0.11	0/50796	0.31	3/68652 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	362	PRO	CA-N-CD	-11.03	96.55	112.00
1	O	320	PRO	CA-N-CD	-8.11	100.64	112.00
1	J	362	PRO	N-CD-CG	-5.74	94.59	103.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4141	0	4187	101	0
1	B	4141	0	4187	92	0
1	C	4141	0	4187	89	0
1	E	4141	0	4187	74	0
1	F	4141	0	4187	109	0
1	J	4141	0	4187	116	0
1	M	4141	0	4187	95	0
1	N	4141	0	4187	70	0
1	O	4141	0	4187	98	0
1	Q	4141	0	4187	83	0
1	R	4141	0	4187	85	0
1	S	4141	0	4187	95	0
All	All	49692	0	50244	1031	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 10.

All (1031) 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:M:341:LEU:HD11	1:M:400:LEU:HB3	1.65	0.79
1:F:471:LEU:HD23	1:F:479:ARG:HH12	1.47	0.78
1:F:358:ASN:ND2	1:F:361:GLU:O	2.17	0.77
1:J:483:GLU:HA	1:J:486:LEU:HD12	1.65	0.77
1:C:255:ILE:HG12	1:C:283:ALA:HB2	1.65	0.76
1:F:255:ILE:HG12	1:F:283:ALA:HB2	1.67	0.76
1:E:607:LYS:HB2	1:E:694:PRO:HG3	1.68	0.75
1:F:281:PRO:HD3	1:J:311:PRO:HB2	1.66	0.75
1:Q:281:PRO:HD3	1:R:311:PRO:HG2	1.66	0.75
1:J:462:MET:HA	1:J:465:ILE:HG12	1.70	0.73
1:B:245:ASP:HB3	1:B:249:ARG:HH12	1.54	0.73
1:M:711:VAL:HG11	1:Q:627:ARG:HH22	1.53	0.73
1:Q:478:ASN:ND2	1:Q:625:ARG:O	2.22	0.73
1:M:332:ARG:HH22	1:M:375:LEU:HA	1.53	0.72
1:A:676:TYR:HA	1:A:680:HIS:HB2	1.71	0.72
1:Q:491:CYS:HB3	1:Q:684:MET:HE2	1.71	0.72
1:O:358:ASN:ND2	1:O:361:GLU:OE1	2.23	0.72
1:C:680:HIS:HB3	1:C:684:MET:HE1	1.72	0.71
1:J:536:LEU:HB3	1:J:544:ILE:HG13	1.71	0.71
1:R:519:ALA:HB2	1:R:668:PHE:HB3	1.71	0.71
1:N:717:MET:HE1	1:N:732:VAL:HG22	1.72	0.71
1:A:299:GLU:OE2	1:A:304:ARG:NH2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:281:PRO:HD3	1:O:311:PRO:HG2	1.72	0.71
1:F:349:VAL:HG13	1:F:367:LEU:HD22	1.72	0.70
1:O:478:ASN:ND2	1:O:625:ARG:O	2.25	0.70
1:E:496:GLY:HA3	1:E:578:THR:HA	1.74	0.70
1:B:417:ASN:HB3	1:B:445:LYS:HZ1	1.57	0.70
1:F:296:LEU:HD11	1:F:303:ILE:HD12	1.74	0.70
1:E:244:GLU:OE1	1:F:377:LYS:NZ	2.24	0.70
1:F:348:ILE:HD12	1:F:355:TRP:HE1	1.56	0.70
1:O:459:GLU:O	1:O:463:ASN:ND2	2.25	0.70
1:S:607:LYS:HB3	1:S:694:PRO:HB3	1.74	0.69
1:A:490:LEU:O	1:A:551:ARG:NH1	2.25	0.69
1:R:761:ASN:HA	1:R:764:LYS:HG3	1.74	0.69
1:S:459:GLU:HA	1:S:462:MET:SD	2.32	0.69
1:C:478:ASN:ND2	1:C:625:ARG:O	2.26	0.68
1:O:560:ASP:HB2	1:O:606:TYR:HB2	1.75	0.68
1:Q:386:PRO:HA	1:Q:389:ARG:HD3	1.75	0.68
1:Q:375:LEU:HD12	1:Q:376:PRO:HD2	1.74	0.68
1:S:455:SER:HB3	1:S:458:MET:HG2	1.75	0.68
1:B:625:ARG:NH1	1:B:626:PHE:O	2.27	0.68
1:Q:341:LEU:HB2	1:Q:400:LEU:HD21	1.75	0.67
1:J:492:GLY:O	1:J:597:HIS:ND1	2.27	0.67
1:J:757:GLU:O	1:J:761:ASN:ND2	2.25	0.67
1:R:334:LEU:HD13	1:R:399:MET:HG2	1.77	0.67
1:B:382:GLU:OE1	1:B:382:GLU:N	2.20	0.67
1:R:358:ASN:ND2	1:R:361:GLU:OE1	2.28	0.67
1:F:385:CYS:SG	1:F:387:ARG:NH1	2.67	0.67
1:F:492:GLY:O	1:F:597:HIS:ND1	2.28	0.67
1:J:286:LYS:O	1:J:288:ARG:NH2	2.27	0.67
1:A:269:PHE:HB2	1:A:296:LEU:HD11	1.75	0.67
1:C:459:GLU:HA	1:C:462:MET:HE3	1.77	0.66
1:B:398:ASP:OD2	1:C:389:ARG:NH1	2.28	0.66
1:A:288:ARG:HH22	1:E:310:ASN:HA	1.61	0.66
1:E:536:LEU:HD12	1:E:576:LYS:HD2	1.77	0.66
1:J:680:HIS:ND1	1:J:684:MET:SD	2.63	0.66
1:N:398:ASP:OD2	1:O:389:ARG:NH1	2.28	0.66
1:J:362:PRO:HD2	1:J:362:PRO:O	1.96	0.66
1:M:281:PRO:HD3	1:Q:311:PRO:HB2	1.76	0.66
1:Q:349:VAL:HG21	1:Q:363:LEU:HB2	1.78	0.66
1:E:674:LYS:HA	1:E:677:LYS:HE2	1.78	0.66
1:O:296:LEU:HB3	1:O:303:ILE:HD11	1.78	0.66
1:E:358:ASN:HB2	1:E:363:LEU:HD11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:548:HIS:HB3	1:J:549:LEU:HD12	1.77	0.65
1:M:255:ILE:O	1:Q:304:ARG:NH1	2.28	0.65
1:O:502:PHE:HE1	1:O:606:TYR:HA	1.61	0.65
1:F:477:LYS:HZ3	1:F:481:LEU:HD11	1.60	0.65
1:E:518:SER:HB2	1:E:659:ILE:HG23	1.79	0.65
1:Q:413:LEU:HD23	1:Q:420:LEU:HD23	1.79	0.65
1:B:750:ARG:HD3	1:J:768:ASN:HD22	1.62	0.65
1:F:416:LYS:HD2	1:F:445:LYS:HG3	1.79	0.64
1:J:618:MET:HE3	1:J:618:MET:H	1.62	0.64
1:J:750:ARG:HD3	1:J:751:LEU:HG	1.79	0.64
1:O:729:ASP:O	1:O:730:ASN:ND2	2.30	0.64
1:S:424:ASP:HB2	1:S:426:MET:HE1	1.78	0.64
1:S:533:THR:HA	1:S:567:LYS:HZ3	1.61	0.64
1:A:416:LYS:HE3	1:A:445:LYS:HG3	1.79	0.64
1:E:717:MET:HE3	1:E:717:MET:HA	1.78	0.64
1:J:668:PHE:HD1	1:J:671:LEU:HD12	1.61	0.64
1:B:486:LEU:HD12	1:B:675:TRP:HZ3	1.62	0.64
1:E:612:ARG:NH1	1:E:613:ILE:O	2.31	0.64
1:F:478:ASN:ND2	1:F:625:ARG:O	2.27	0.64
1:O:264:LEU:HD12	1:O:269:PHE:HA	1.80	0.64
1:A:244:GLU:OE1	1:E:377:LYS:NZ	2.29	0.64
1:B:490:LEU:O	1:B:551:ARG:NH1	2.31	0.64
1:C:519:ALA:HB2	1:C:668:PHE:HB3	1.79	0.64
1:E:349:VAL:HG21	1:E:363:LEU:HB2	1.80	0.64
1:F:297:SER:OG	1:F:304:ARG:NE	2.30	0.64
1:Q:440:VAL:HG21	1:Q:549:LEU:HD21	1.78	0.64
1:A:256:ASN:ND2	1:A:280:THR:OG1	2.30	0.63
1:R:680:HIS:HB3	1:R:684:MET:HE1	1.79	0.63
1:M:389:ARG:NH2	1:O:395:ASN:OD1	2.31	0.63
1:B:484:LYS:NZ	1:B:685:LYS:O	2.26	0.63
1:B:349:VAL:HG13	1:B:367:LEU:HD22	1.80	0.63
1:B:472:THR:OG1	1:B:474:GLU:OE2	2.17	0.63
1:N:255:ILE:HG12	1:N:283:ALA:HB2	1.80	0.63
1:J:255:ILE:H	1:J:255:ILE:HD12	1.64	0.63
1:S:519:ALA:HB2	1:S:668:PHE:HB3	1.81	0.62
1:A:384:LEU:HB3	1:C:324:ASN:HD22	1.65	0.62
1:C:618:MET:HG3	1:C:696:PHE:HE2	1.65	0.62
1:E:490:LEU:O	1:E:551:ARG:NH1	2.31	0.62
1:E:417:ASN:HD21	1:E:446:PHE:H	1.46	0.62
1:B:253:ILE:HG23	1:B:317:LYS:HZ3	1.65	0.62
1:F:701:LYS:HD2	1:F:747:PHE:HZ	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:736:LEU:HD22	1:J:764:LYS:HZ1	1.65	0.62
1:R:478:ASN:ND2	1:R:625:ARG:O	2.25	0.62
1:S:303:ILE:HG13	1:S:321:LEU:HD11	1.81	0.62
1:B:417:ASN:HD22	1:B:445:LYS:HE3	1.66	0.61
1:C:625:ARG:HH12	1:C:627:ARG:HD2	1.64	0.61
1:E:250:VAL:HA	1:E:253:ILE:HD12	1.83	0.61
1:J:490:LEU:O	1:J:551:ARG:NH1	2.34	0.61
1:Q:250:VAL:HA	1:Q:253:ILE:HD12	1.81	0.61
1:C:284:LEU:HD13	1:C:317:LYS:HG2	1.81	0.61
1:R:400:LEU:O	1:S:366:LYS:NZ	2.31	0.61
1:S:536:LEU:HB3	1:S:544:ILE:HG13	1.82	0.61
1:F:719:ASP:O	1:F:722:LYS:NZ	2.34	0.61
1:C:358:ASN:ND2	1:C:361:GLU:O	2.34	0.61
1:F:393:GLU:O	1:F:397:ARG:HG3	2.01	0.61
1:J:768:ASN:OD1	1:J:771:ASP:N	2.31	0.61
1:S:358:ASN:ND2	1:S:361:GLU:OE1	2.31	0.61
1:E:459:GLU:HA	1:E:462:MET:HE3	1.82	0.61
1:R:303:ILE:HB	1:R:319:VAL:HB	1.83	0.61
1:R:768:ASN:HD21	1:R:771:ASP:HB3	1.66	0.61
1:S:299:GLU:OE1	1:S:304:ARG:NH1	2.34	0.61
1:Q:496:GLY:HA3	1:Q:578:THR:HA	1.82	0.60
1:A:681:ILE:H	1:A:681:ILE:HD12	1.66	0.60
1:E:519:ALA:HB2	1:E:668:PHE:HB3	1.83	0.60
1:N:532:LEU:O	1:N:570:ARG:NH2	2.34	0.60
1:Q:537:ASP:OD1	1:Q:576:LYS:NZ	2.34	0.60
1:N:244:GLU:HB3	1:O:377:LYS:HE3	1.81	0.60
1:M:304:ARG:NH1	1:O:255:ILE:O	2.34	0.60
1:N:299:GLU:O	1:N:300:ASN:ND2	2.35	0.60
1:N:514:ARG:HB3	1:N:659:ILE:HG21	1.84	0.60
1:O:502:PHE:HD2	1:O:625:ARG:HG3	1.66	0.60
1:Q:673:VAL:HG22	1:Q:677:LYS:HE2	1.82	0.60
1:S:490:LEU:O	1:S:551:ARG:NH1	2.34	0.60
1:A:548:HIS:HE1	1:A:595:ARG:HB2	1.66	0.60
1:J:509:LYS:HD2	1:J:603:ASP:HB2	1.83	0.60
1:N:325:LYS:H	1:N:325:LYS:HD2	1.66	0.60
1:B:513:LYS:HG2	1:B:514:ARG:HH11	1.67	0.60
1:C:560:ASP:HB2	1:C:606:TYR:HB2	1.83	0.60
1:C:616:ALA:HA	1:C:619:ARG:HH21	1.67	0.60
1:R:492:GLY:O	1:R:597:HIS:ND1	2.34	0.60
1:B:292:HIS:HB2	1:B:307:LYS:HE2	1.82	0.60
1:F:248:LYS:O	1:F:252:LYS:HG3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:468:ILE:O	1:S:628:THR:OG1	2.20	0.60
1:A:242:SER:HB2	1:E:377:LYS:HZ2	1.67	0.59
1:B:532:LEU:O	1:B:570:ARG:NH2	2.34	0.59
1:A:358:ASN:ND2	1:A:361:GLU:O	2.35	0.59
1:A:496:GLY:HA3	1:A:578:THR:HA	1.84	0.59
1:J:468:ILE:O	1:J:628:THR:OG1	2.21	0.59
1:J:490:LEU:HD21	1:J:676:TYR:HB2	1.84	0.59
1:B:385:CYS:HB3	1:B:388:LYS:HD2	1.85	0.59
1:B:311:PRO:HB2	1:J:281:PRO:HD3	1.84	0.59
1:M:483:GLU:OE1	1:M:678:LYS:NZ	2.34	0.59
1:F:618:MET:SD	1:F:618:MET:N	2.75	0.59
1:O:750:ARG:HD3	1:O:751:LEU:HG	1.85	0.59
1:Q:472:THR:OG1	1:Q:474:GLU:OE2	2.19	0.59
1:S:496:GLY:HA3	1:S:578:THR:HA	1.84	0.59
1:O:315:LYS:HB2	1:O:317:LYS:HZ2	1.67	0.58
1:R:269:PHE:HB2	1:R:296:LEU:HD22	1.84	0.58
1:R:413:LEU:HD23	1:R:420:LEU:HD23	1.84	0.58
1:R:728:TYR:OH	1:S:748:ASN:ND2	2.36	0.58
1:C:768:ASN:ND2	1:C:771:ASP:OD2	2.34	0.58
1:F:455:SER:HB3	1:F:458:MET:HG3	1.84	0.58
1:J:459:GLU:HA	1:J:462:MET:HE3	1.84	0.58
1:A:514:ARG:HB3	1:A:659:ILE:HG21	1.84	0.58
1:C:738:THR:O	1:C:741:GLN:NE2	2.25	0.58
1:Q:612:ARG:NH1	1:Q:613:ILE:O	2.36	0.58
1:R:292:HIS:HB2	1:R:307:LYS:HE2	1.86	0.58
1:S:665:ARG:HG3	1:S:666:PHE:HD1	1.68	0.58
1:J:482:TYR:CE1	1:J:486:LEU:HD11	2.38	0.58
1:C:655:LEU:HB2	1:C:658:LYS:HE2	1.85	0.58
1:E:500:PHE:HE1	1:E:602:ILE:HD12	1.68	0.58
1:O:384:LEU:O	1:O:389:ARG:NH2	2.37	0.58
1:A:288:ARG:NH1	1:E:310:ASN:OD1	2.36	0.58
1:E:492:GLY:O	1:E:597:HIS:ND1	2.36	0.58
1:B:303:ILE:HG22	1:B:319:VAL:HB	1.86	0.58
1:J:360:GLU:OE1	1:J:360:GLU:N	2.37	0.58
1:M:490:LEU:O	1:M:551:ARG:NH1	2.37	0.58
1:A:389:ARG:NH2	1:C:395:ASN:OD1	2.37	0.57
1:C:555:CYS:HB2	1:C:600:ILE:HG23	1.85	0.57
1:F:668:PHE:O	1:F:672:LEU:HD22	2.04	0.57
1:M:424:ASP:HB3	1:M:426:MET:HE1	1.85	0.57
1:N:496:GLY:HA3	1:N:578:THR:HA	1.85	0.57
1:Q:490:LEU:O	1:Q:551:ARG:NH1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:GLU:O	1:E:248:LYS:HG2	2.04	0.57
1:M:570:ARG:NH2	1:M:572:ASP:OD2	2.37	0.57
1:C:607:LYS:HD2	1:C:694:PRO:HD3	1.87	0.57
1:A:746:TYR:OH	1:A:780:GLU:OE1	2.15	0.57
1:E:759:PHE:HB3	1:E:763:HIS:HE1	1.68	0.57
1:A:312:HIS:CD2	1:C:288:ARG:HA	2.40	0.57
1:R:375:LEU:HD12	1:R:376:PRO:HD2	1.86	0.57
1:M:249:ARG:HB2	1:M:249:ARG:NH1	2.19	0.57
1:M:310:ASN:HD21	1:M:313:SER:HB3	1.69	0.57
1:E:305:ILE:HD11	1:E:317:LYS:HD2	1.85	0.57
1:N:720:LEU:HB3	1:N:725:TYR:HD2	1.69	0.57
1:O:351:ILE:HB	1:O:356:LYS:HE3	1.85	0.57
1:J:343:GLU:HB2	1:J:403:SER:HB3	1.87	0.57
1:B:360:GLU:OE1	1:B:360:GLU:N	2.38	0.57
1:C:757:GLU:O	1:C:761:ASN:ND2	2.38	0.57
1:F:498:LEU:HD11	1:F:577:LEU:HD11	1.86	0.57
1:N:349:VAL:HG13	1:N:367:LEU:HD22	1.87	0.57
1:O:250:VAL:HA	1:O:253:ILE:HD12	1.87	0.57
1:C:612:ARG:NH1	1:C:613:ILE:O	2.38	0.56
1:J:560:ASP:HB2	1:J:606:TYR:HD2	1.70	0.56
1:A:292:HIS:HB2	1:A:307:LYS:HE2	1.87	0.56
1:C:675:TRP:HA	1:C:678:LYS:HZ2	1.69	0.56
1:N:297:SER:OG	1:N:304:ARG:NH1	2.38	0.56
1:O:349:VAL:HG13	1:O:367:LEU:HD22	1.86	0.56
1:O:458:MET:O	1:O:462:MET:HG3	2.05	0.56
1:O:516:LEU:HD12	1:O:520:ILE:HD11	1.87	0.56
1:R:329:ILE:O	1:R:333:ILE:HG12	2.06	0.56
1:A:734:LEU:HD12	1:A:735:PRO:HD2	1.87	0.56
1:N:490:LEU:O	1:N:551:ARG:NH1	2.39	0.56
1:N:768:ASN:OD1	1:N:771:ASP:N	2.37	0.56
1:O:757:GLU:O	1:O:761:ASN:ND2	2.38	0.56
1:Q:292:HIS:HB2	1:Q:307:LYS:HE2	1.86	0.56
1:S:431:ASP:OD1	1:S:431:ASP:N	2.39	0.56
1:A:536:LEU:HD12	1:A:576:LYS:HD2	1.86	0.56
1:E:351:ILE:O	1:E:356:LYS:NZ	2.36	0.56
1:J:489:CYS:HB3	1:J:552:SER:HB2	1.87	0.56
1:B:701:LYS:HD2	1:B:747:PHE:HE1	1.70	0.56
1:R:765:LYS:HE2	1:S:563:CYS:HA	1.87	0.56
1:B:249:ARG:HA	1:B:252:LYS:HZ2	1.70	0.56
1:B:670:TYR:O	1:B:674:LYS:HG2	2.06	0.56
1:M:299:GLU:OE1	1:M:304:ARG:NH1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:478:ASN:ND2	1:M:625:ARG:O	2.30	0.56
1:E:711:VAL:HG13	1:E:714:ILE:HD12	1.86	0.56
1:F:728:TYR:OH	1:J:748:ASN:ND2	2.39	0.56
1:J:259:ILE:HD11	1:J:277:ASP:HB2	1.87	0.56
1:J:395:ASN:O	1:J:399:MET:HG3	2.05	0.56
1:S:729:ASP:O	1:S:730:ASN:ND2	2.39	0.56
1:C:244:GLU:O	1:C:248:LYS:HG2	2.06	0.56
1:B:244:GLU:O	1:B:247:ILE:HG12	2.06	0.55
1:C:303:ILE:HG12	1:C:321:LEU:HD11	1.87	0.55
1:C:490:LEU:O	1:C:551:ARG:NH1	2.39	0.55
1:C:509:LYS:HD3	1:C:626:PHE:HE2	1.71	0.55
1:J:247:ILE:HA	1:J:250:VAL:HG22	1.88	0.55
1:F:422:LEU:H	1:F:422:LEU:HD23	1.72	0.55
1:Q:329:ILE:O	1:Q:333:ILE:HG12	2.05	0.55
1:R:516:LEU:HD22	1:R:668:PHE:HE2	1.70	0.55
1:F:577:LEU:HD13	1:F:600:ILE:HD12	1.87	0.55
1:J:292:HIS:HB2	1:J:307:LYS:HE2	1.88	0.55
1:E:401:VAL:HG12	1:F:366:LYS:HD3	1.89	0.55
1:J:500:PHE:HE1	1:J:602:ILE:HD12	1.70	0.55
1:M:322:ASP:N	1:M:322:ASP:OD1	2.39	0.55
1:A:753:GLY:O	1:A:757:GLU:HG2	2.07	0.55
1:E:734:LEU:H	1:E:773:TYR:HB2	1.72	0.55
1:M:676:TYR:HA	1:M:680:HIS:HB2	1.88	0.55
1:N:377:LYS:HZ3	1:S:244:GLU:HB3	1.69	0.55
1:F:244:GLU:OE1	1:F:244:GLU:N	2.38	0.55
1:J:607:LYS:HE3	1:J:608:PRO:HD2	1.88	0.55
1:O:671:LEU:O	1:O:674:LYS:NZ	2.40	0.55
1:Q:734:LEU:H	1:Q:773:TYR:HB2	1.72	0.55
1:R:536:LEU:HD22	1:R:544:ILE:HD11	1.88	0.55
1:N:573:ASN:HA	1:N:576:LYS:HE2	1.88	0.55
1:B:534:ASP:O	1:B:570:ARG:NH2	2.35	0.55
1:N:385:CYS:HB3	1:N:388:LYS:HD2	1.87	0.55
1:S:274:LEU:HD11	1:S:296:LEU:HD21	1.87	0.55
1:F:707:VAL:HB	1:F:779:ILE:HD11	1.88	0.55
1:O:768:ASN:ND2	1:O:771:ASP:OD2	2.39	0.55
1:Q:395:ASN:O	1:Q:399:MET:HG2	2.07	0.55
1:F:413:LEU:HB3	1:F:420:LEU:HB3	1.89	0.54
1:M:349:VAL:HG23	1:M:367:LEU:HD22	1.89	0.54
1:M:607:LYS:HB3	1:M:694:PRO:HB3	1.89	0.54
1:R:458:MET:SD	1:R:458:MET:N	2.81	0.54
1:A:270:THR:HG22	1:A:297:SER:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:768:ASN:HD21	1:F:771:ASP:HB3	1.72	0.54
1:J:464:ILE:O	1:J:468:ILE:HG12	2.07	0.54
1:M:284:LEU:HD22	1:M:317:LYS:HD3	1.89	0.54
1:S:472:THR:OG1	1:S:474:GLU:OE2	2.24	0.54
1:J:358:ASN:ND2	1:J:361:GLU:OE1	2.40	0.54
1:B:673:VAL:HG13	1:B:674:LYS:HD2	1.90	0.54
1:F:340:LEU:HB2	1:F:348:ILE:HD11	1.90	0.54
1:Q:676:TYR:HA	1:Q:680:HIS:HB2	1.90	0.54
1:A:282:CYS:SG	1:A:290:HIS:NE2	2.77	0.54
1:A:500:PHE:HE1	1:A:602:ILE:HD12	1.73	0.54
1:A:618:MET:SD	1:A:618:MET:N	2.81	0.54
1:J:475:ASN:O	1:J:479:ARG:HG2	2.07	0.54
1:R:318:ILE:HG22	1:R:320:PRO:HD3	1.89	0.54
1:A:691:GLU:OE2	1:A:692:GLU:HB2	2.08	0.54
1:M:312:HIS:CE1	1:O:288:ARG:HA	2.43	0.54
1:N:392:VAL:O	1:N:396:ILE:HG12	2.08	0.54
1:S:483:GLU:HA	1:S:486:LEU:HD12	1.89	0.54
1:S:511:THR:HG22	1:S:515:LEU:HD13	1.90	0.54
1:A:487:SER:HB3	1:A:680:HIS:NE2	2.22	0.54
1:E:469:GLN:O	1:E:479:ARG:NH2	2.40	0.54
1:A:717:MET:HE3	1:A:717:MET:HA	1.90	0.54
1:O:342:THR:O	1:O:343:GLU:HG2	2.08	0.54
1:N:378:GLU:HB3	1:S:248:LYS:HZ3	1.73	0.54
1:B:768:ASN:OD1	1:B:771:ASP:N	2.37	0.53
1:Q:388:LYS:O	1:Q:392:VAL:HG23	2.08	0.53
1:R:555:CYS:HB2	1:R:600:ILE:HG23	1.91	0.53
1:S:250:VAL:HA	1:S:253:ILE:HD12	1.89	0.53
1:B:767:ALA:O	1:C:754:HIS:NE2	2.37	0.53
1:J:413:LEU:HB2	1:J:422:LEU:HD21	1.90	0.53
1:C:358:ASN:HD22	1:C:363:LEU:HG	1.73	0.53
1:F:450:LYS:HB2	1:F:666:PHE:HD2	1.74	0.53
1:O:458:MET:HE2	1:O:667:ALA:HA	1.89	0.53
1:Q:299:GLU:OE1	1:Q:304:ARG:NH1	2.41	0.53
1:Q:479:ARG:HD3	1:Q:483:GLU:HB2	1.89	0.53
1:B:720:LEU:HB3	1:B:725:TYR:HD2	1.73	0.53
1:C:536:LEU:HD12	1:C:576:LYS:HD2	1.90	0.53
1:S:702:ILE:HA	1:S:705:LEU:HB2	1.91	0.53
1:B:374:GLN:N	1:B:374:GLN:OE1	2.37	0.53
1:Q:341:LEU:HG	1:Q:343:GLU:H	1.73	0.53
1:R:755:ASP:O	1:R:758:SER:OG	2.26	0.53
1:F:494:THR:HG21	1:F:580:PRO:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:500:PHE:HE1	1:M:602:ILE:HD12	1.73	0.53
1:O:520:ILE:HG22	1:O:523:LEU:HB2	1.90	0.53
1:S:246:ALA:HA	1:S:249:ARG:HD3	1.89	0.53
1:J:514:ARG:HB3	1:J:659:ILE:HG21	1.90	0.53
1:J:555:CYS:HB3	1:J:602:ILE:HG12	1.91	0.53
1:O:294:HIS:HB3	1:O:305:ILE:HD11	1.91	0.53
1:Q:492:GLY:O	1:Q:597:HIS:ND1	2.41	0.53
1:S:342:THR:OG1	1:S:346:ASP:OD1	2.23	0.53
1:M:387:ARG:O	1:M:390:LYS:HG3	2.09	0.52
1:N:768:ASN:HD21	1:N:771:ASP:HB2	1.74	0.52
1:O:255:ILE:HG13	1:O:283:ALA:HB2	1.91	0.52
1:O:607:LYS:HD2	1:O:694:PRO:HB3	1.91	0.52
1:R:707:VAL:HB	1:R:779:ILE:HD11	1.90	0.52
1:R:748:ASN:HD21	1:R:751:LEU:HD12	1.74	0.52
1:E:759:PHE:O	1:E:763:HIS:ND1	2.42	0.52
1:F:674:LYS:O	1:F:678:LYS:HG2	2.09	0.52
1:J:665:ARG:HG2	1:J:666:PHE:HD1	1.74	0.52
1:R:611:ASP:OD1	1:R:612:ARG:N	2.42	0.52
1:C:302:ALA:HA	1:C:321:LEU:HG	1.90	0.52
1:A:750:ARG:NH1	1:A:750:ARG:O	2.42	0.52
1:B:573:ASN:HA	1:B:576:LYS:HE2	1.91	0.52
1:J:665:ARG:HG2	1:J:666:PHE:CD1	2.45	0.52
1:Q:450:LYS:HB2	1:Q:666:PHE:HD2	1.73	0.52
1:S:555:CYS:HB3	1:S:602:ILE:HG12	1.92	0.52
1:F:611:ASP:OD1	1:F:612:ARG:N	2.43	0.52
1:J:717:MET:HE3	1:J:732:VAL:HG21	1.90	0.52
1:M:398:ASP:HB3	1:Q:389:ARG:HH22	1.73	0.52
1:O:612:ARG:NH1	1:O:613:ILE:O	2.43	0.52
1:A:516:LEU:HD22	1:A:668:PHE:HE2	1.74	0.52
1:C:484:LYS:NZ	1:C:685:LYS:O	2.40	0.52
1:J:511:THR:HG22	1:J:515:LEU:HD13	1.91	0.52
1:R:455:SER:HB3	1:R:458:MET:HG2	1.91	0.52
1:R:674:LYS:O	1:R:678:LYS:HG3	2.09	0.52
1:S:509:LYS:HD2	1:S:603:ASP:HB2	1.92	0.52
1:B:343:GLU:HB2	1:B:403:SER:HB3	1.91	0.52
1:B:504:GLU:O	1:B:507:THR:OG1	2.23	0.52
1:M:519:ALA:HB2	1:M:668:PHE:HB3	1.90	0.52
1:A:311:PRO:HB2	1:C:281:PRO:HD3	1.92	0.52
1:A:458:MET:SD	1:A:459:GLU:N	2.83	0.52
1:A:504:GLU:O	1:A:507:THR:OG1	2.23	0.52
1:B:560:ASP:HB3	1:B:606:TYR:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:768:ASN:OD1	1:E:771:ASP:N	2.37	0.52
1:S:248:LYS:O	1:S:252:LYS:HG3	2.10	0.52
1:S:413:LEU:HD23	1:S:420:LEU:HD23	1.92	0.52
1:S:500:PHE:HE1	1:S:602:ILE:HD12	1.74	0.52
1:B:517:LYS:HG2	1:B:524:PHE:CE2	2.45	0.51
1:C:533:THR:HA	1:C:567:LYS:HE2	1.90	0.51
1:S:462:MET:C	1:S:462:MET:HE2	2.35	0.51
1:A:248:LYS:O	1:A:252:LYS:HG3	2.10	0.51
1:B:555:CYS:HB3	1:B:602:ILE:HG12	1.92	0.51
1:M:413:LEU:HD23	1:M:420:LEU:HD23	1.91	0.51
1:S:332:ARG:HH12	1:S:376:PRO:HD3	1.75	0.51
1:B:247:ILE:HA	1:B:250:VAL:HG12	1.92	0.51
1:B:288:ARG:HA	1:C:312:HIS:CD2	2.45	0.51
1:B:693:ILE:HB	1:B:696:PHE:HB2	1.93	0.51
1:F:460:GLU:O	1:F:464:ILE:HG13	2.10	0.51
1:J:334:LEU:HD12	1:J:399:MET:HE2	1.92	0.51
1:O:255:ILE:H	1:O:283:ALA:HB2	1.74	0.51
1:E:340:LEU:HD13	1:E:404:VAL:HG21	1.92	0.51
1:J:718:THR:O	1:J:721:SER:OG	2.26	0.51
1:S:351:ILE:HG23	1:S:356:LYS:HD2	1.92	0.51
1:E:288:ARG:HD2	1:F:312:HIS:HB3	1.92	0.51
1:F:401:VAL:HG12	1:J:366:LYS:HD3	1.93	0.51
1:O:519:ALA:HB2	1:O:668:PHE:HB3	1.91	0.51
1:J:455:SER:HB3	1:J:458:MET:HG3	1.93	0.51
1:N:395:ASN:O	1:N:399:MET:HG3	2.11	0.51
1:N:717:MET:HA	1:N:720:LEU:HB2	1.93	0.51
1:R:460:GLU:O	1:R:464:ILE:HG13	2.10	0.51
1:A:388:LYS:O	1:A:392:VAL:HG23	2.11	0.51
1:Q:500:PHE:HE1	1:Q:602:ILE:HD12	1.75	0.51
1:S:386:PRO:HA	1:S:389:ARG:HE	1.76	0.51
1:A:495:LYS:HZ1	1:A:686:LEU:N	2.08	0.51
1:M:393:GLU:OE2	1:M:397:ARG:NH2	2.44	0.51
1:Q:392:VAL:O	1:Q:396:ILE:HG22	2.10	0.51
1:S:392:VAL:O	1:S:396:ILE:HG12	2.11	0.51
1:S:464:ILE:O	1:S:468:ILE:HG12	2.11	0.51
1:S:555:CYS:HB2	1:S:600:ILE:HG23	1.93	0.51
1:A:607:LYS:HB3	1:A:694:PRO:HB3	1.92	0.51
1:F:358:ASN:HD22	1:F:363:LEU:HG	1.76	0.51
1:M:340:LEU:HD12	1:M:404:VAL:HG21	1.92	0.51
1:O:292:HIS:HB2	1:O:307:LYS:HE2	1.93	0.51
1:R:490:LEU:HD12	1:R:490:LEU:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:504:GLU:O	1:S:507:THR:OG1	2.27	0.51
1:B:478:ASN:ND2	1:B:625:ARG:O	2.44	0.50
1:F:536:LEU:HD22	1:F:544:ILE:HD11	1.93	0.50
1:O:484:LYS:HE2	1:O:686:LEU:HA	1.93	0.50
1:B:505:THR:HB	1:B:605:ASN:HD21	1.76	0.50
1:O:363:LEU:HD23	1:O:363:LEU:H	1.77	0.50
1:O:618:MET:SD	1:O:618:MET:N	2.82	0.50
1:Q:485:THR:HG23	1:Q:486:LEU:HD12	1.93	0.50
1:M:613:ILE:HG21	1:M:699:TYR:HE2	1.76	0.50
1:N:364:ILE:HD12	1:N:364:ILE:H	1.77	0.50
1:N:386:PRO:O	1:N:390:LYS:HG2	2.11	0.50
1:R:325:LYS:NZ	1:R:378:GLU:O	2.42	0.50
1:B:701:LYS:HD2	1:B:747:PHE:CE1	2.45	0.50
1:C:244:GLU:O	1:C:247:ILE:HG12	2.12	0.50
1:C:426:MET:SD	1:C:426:MET:N	2.84	0.50
1:E:360:GLU:OE1	1:E:360:GLU:N	2.44	0.50
1:J:612:ARG:NH1	1:J:613:ILE:O	2.44	0.50
1:N:413:LEU:HD23	1:N:420:LEU:HD23	1.94	0.50
1:O:574:ILE:HG22	1:O:620:ARG:HD3	1.94	0.50
1:O:618:MET:HG3	1:O:696:PHE:HE2	1.76	0.50
1:S:535:VAL:HG12	1:S:538:LYS:H	1.76	0.50
1:A:249:ARG:HA	1:A:252:LYS:HD2	1.93	0.50
1:M:392:VAL:O	1:M:396:ILE:HG12	2.12	0.50
1:S:349:VAL:HG11	1:S:363:LEU:HB3	1.93	0.50
1:N:670:TYR:HA	1:N:673:VAL:HG12	1.93	0.50
1:Q:248:LYS:NZ	1:Q:252:LYS:HB3	2.26	0.50
1:B:750:ARG:HD3	1:J:768:ASN:ND2	2.27	0.50
1:C:460:GLU:O	1:C:464:ILE:HG13	2.12	0.50
1:C:574:ILE:HG22	1:C:620:ARG:HD3	1.92	0.50
1:J:495:LYS:HZ3	1:J:686:LEU:HG	1.76	0.50
1:M:426:MET:SD	1:M:426:MET:N	2.83	0.50
1:R:270:THR:O	1:R:295:GLN:NE2	2.42	0.50
1:B:280:THR:OG1	1:C:304:ARG:NH1	2.44	0.50
1:C:402:ASP:OD1	1:C:403:SER:N	2.44	0.50
1:F:256:ASN:OD1	1:F:280:THR:OG1	2.24	0.50
1:R:284:LEU:HD22	1:R:317:LYS:HG2	1.94	0.50
1:R:342:THR:HG22	1:R:348:ILE:HG23	1.93	0.50
1:J:475:ASN:ND2	1:J:478:ASN:HB3	2.27	0.50
1:N:375:LEU:HD21	1:N:379:TYR:HB2	1.93	0.50
1:O:717:MET:SD	1:O:720:LEU:HD12	2.51	0.50
1:C:707:VAL:HB	1:C:779:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:THR:HG23	1:C:344:ARG:H	1.77	0.49
1:F:741:GLN:NE2	1:F:742:LYS:HG3	2.28	0.49
1:M:520:ILE:HB	1:M:524:PHE:HB2	1.94	0.49
1:N:278:TYR:HE1	1:N:282:CYS:HB2	1.76	0.49
1:J:515:LEU:HB3	1:J:668:PHE:CE2	2.47	0.49
1:R:678:LYS:HE2	1:R:679:TYR:CE2	2.47	0.49
1:J:274:LEU:HD21	1:J:296:LEU:HD13	1.94	0.49
1:J:475:ASN:HD22	1:J:479:ARG:HD2	1.78	0.49
1:J:536:LEU:HD12	1:J:576:LYS:HE2	1.93	0.49
1:R:269:PHE:HD1	1:R:270:THR:HG23	1.77	0.49
1:A:484:LYS:HD3	1:A:680:HIS:CE1	2.48	0.49
1:C:348:ILE:HG22	1:C:355:TRP:HE3	1.78	0.49
1:C:674:LYS:O	1:C:678:LYS:HG2	2.13	0.49
1:E:244:GLU:O	1:E:247:ILE:HG12	2.13	0.49
1:F:625:ARG:CZ	1:F:627:ARG:HB2	2.42	0.49
1:O:253:ILE:HD11	1:O:319:VAL:HG21	1.95	0.49
1:R:500:PHE:HE1	1:R:602:ILE:HD12	1.78	0.49
1:A:490:LEU:HD11	1:A:672:LEU:HB3	1.94	0.49
1:B:571:SER:O	1:B:575:LYS:HG2	2.12	0.49
1:E:618:MET:HA	1:E:618:MET:HE3	1.95	0.49
1:J:504:GLU:O	1:J:507:THR:OG1	2.26	0.49
1:N:290:HIS:HB3	1:N:307:LYS:HE3	1.93	0.49
1:M:355:TRP:HZ2	1:M:434:LYS:HG2	1.78	0.49
1:Q:296:LEU:HB3	1:Q:303:ILE:HD11	1.94	0.49
1:N:363:LEU:HA	1:N:366:LYS:NZ	2.28	0.49
1:O:348:ILE:HG22	1:O:355:TRP:CE3	2.48	0.49
1:R:500:PHE:N	1:R:622:ALA:O	2.44	0.49
1:S:618:MET:SD	1:S:690:PRO:HB3	2.53	0.49
1:A:249:ARG:O	1:A:253:ILE:HG13	2.13	0.49
1:A:490:LEU:HD12	1:A:490:LEU:H	1.77	0.49
1:J:503:GLY:HA3	1:J:626:PHE:HB2	1.94	0.49
1:R:288:ARG:HA	1:S:312:HIS:CD2	2.48	0.49
1:A:487:SER:HB3	1:A:680:HIS:CD2	2.48	0.49
1:F:697:ALA:O	1:F:701:LYS:HG2	2.13	0.49
1:N:251:SER:HB3	1:N:261:PHE:CE1	2.48	0.49
1:E:681:ILE:HD12	1:E:681:ILE:H	1.77	0.48
1:F:475:ASN:O	1:F:479:ARG:HG2	2.13	0.48
1:M:236:TRP:CD1	1:M:243:PHE:HB2	2.48	0.48
1:M:725:TYR:CE1	1:M:734:LEU:HB2	2.48	0.48
1:Q:615:ASN:HA	1:Q:618:MET:HE1	1.95	0.48
1:Q:768:ASN:OD1	1:Q:771:ASP:N	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:ASN:O	1:B:399:MET:HG3	2.13	0.48
1:C:305:ILE:HB	1:C:317:LYS:HB2	1.93	0.48
1:M:245:ASP:O	1:M:249:ARG:HG3	2.14	0.48
1:R:761:ASN:OD1	1:R:762:ARG:N	2.46	0.48
1:Q:607:LYS:HB2	1:Q:694:PRO:HB3	1.94	0.48
1:B:683:ILE:C	1:B:684:MET:HE2	2.39	0.48
1:B:720:LEU:HD11	1:B:782:ILE:HD11	1.95	0.48
1:C:558:LEU:HD12	1:C:559:PRO:O	2.14	0.48
1:C:665:ARG:HG2	1:C:666:PHE:HD1	1.78	0.48
1:F:755:ASP:O	1:F:758:SER:OG	2.30	0.48
1:O:520:ILE:HB	1:O:524:PHE:HB2	1.95	0.48
1:E:736:LEU:HD23	1:E:736:LEU:H	1.78	0.48
1:J:278:TYR:CG	1:J:278:TYR:O	2.66	0.48
1:S:249:ARG:HH21	1:S:319:VAL:HG13	1.78	0.48
1:B:670:TYR:HA	1:B:673:VAL:HG12	1.95	0.48
1:E:548:HIS:CD2	1:E:549:LEU:HD23	2.48	0.48
1:F:612:ARG:HH22	1:F:614:ASP:CG	2.21	0.48
1:J:677:LYS:O	1:J:677:LYS:NZ	2.40	0.48
1:Q:393:GLU:OE2	1:Q:397:ARG:NH2	2.46	0.48
1:A:245:ASP:O	1:A:249:ARG:HG2	2.14	0.48
1:F:572:ASP:O	1:F:576:LYS:NZ	2.41	0.48
1:A:285:CYS:SG	1:A:287:LYS:HG2	2.54	0.48
1:A:725:TYR:HE1	1:A:734:LEU:HD13	1.79	0.48
1:E:253:ILE:HG12	1:E:317:LYS:HZ2	1.79	0.48
1:J:331:GLN:NE2	1:J:335:ASP:OD1	2.46	0.48
1:A:367:LEU:O	1:A:371:ILE:HG12	2.14	0.48
1:F:555:CYS:HB2	1:F:600:ILE:HG23	1.95	0.48
1:S:332:ARG:O	1:S:336:THR:HG23	2.13	0.48
1:A:360:GLU:N	1:A:360:GLU:OE1	2.46	0.48
1:A:563:CYS:SG	1:A:564:SER:N	2.87	0.48
1:F:348:ILE:HD12	1:F:355:TRP:NE1	2.25	0.48
1:M:342:THR:HG23	1:M:344:ARG:H	1.79	0.48
1:S:388:LYS:O	1:S:392:VAL:HG23	2.14	0.48
1:B:561:PHE:HD1	1:B:566:SER:HB2	1.79	0.47
1:M:464:ILE:O	1:M:468:ILE:HG12	2.14	0.47
1:M:747:PHE:CZ	1:M:756:ILE:HG21	2.49	0.47
1:N:768:ASN:ND2	1:O:750:ARG:HG2	2.29	0.47
1:Q:375:LEU:HG	1:Q:379:TYR:HB2	1.96	0.47
1:A:754:HIS:HE2	1:C:767:ALA:HA	1.78	0.47
1:C:476:LYS:O	1:C:480:GLU:HG2	2.14	0.47
1:E:707:VAL:HB	1:E:779:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:500:PHE:N	1:O:622:ALA:O	2.39	0.47
1:A:720:LEU:HB3	1:A:725:TYR:HD2	1.78	0.47
1:B:474:GLU:OE1	1:B:628:THR:OG1	2.32	0.47
1:F:317:LYS:HA	1:F:317:LYS:HD3	1.73	0.47
1:F:455:SER:O	1:F:458:MET:N	2.46	0.47
1:F:762:ARG:O	1:F:762:ARG:NH1	2.34	0.47
1:S:244:GLU:CD	1:S:244:GLU:H	2.22	0.47
1:F:701:LYS:HD2	1:F:747:PHE:CZ	2.48	0.47
1:M:465:ILE:HD12	1:M:465:ILE:H	1.79	0.47
1:S:245:ASP:O	1:S:248:LYS:HG2	2.15	0.47
1:S:413:LEU:HB2	1:S:422:LEU:HD21	1.97	0.47
1:A:348:ILE:HG22	1:A:355:TRP:HE3	1.80	0.47
1:J:533:THR:HA	1:J:567:LYS:HZ3	1.79	0.47
1:M:514:ARG:HB3	1:M:659:ILE:HG21	1.96	0.47
1:O:358:ASN:HB3	1:O:363:LEU:HD22	1.95	0.47
1:R:340:LEU:HD12	1:R:348:ILE:HD11	1.96	0.47
1:B:243:PHE:O	1:B:247:ILE:HG23	2.15	0.47
1:B:253:ILE:HD12	1:B:317:LYS:NZ	2.30	0.47
1:B:290:HIS:HB3	1:B:307:LYS:HE3	1.97	0.47
1:B:426:MET:HE1	1:B:428:TYR:CE2	2.50	0.47
1:B:462:MET:SD	1:B:466:ASN:ND2	2.88	0.47
1:B:524:PHE:HE1	1:B:554:PHE:H	1.63	0.47
1:B:564:SER:OG	1:J:761:ASN:O	2.28	0.47
1:C:237:GLU:HB3	1:C:240:PHE:CE2	2.50	0.47
1:C:455:SER:HB3	1:C:458:MET:HG3	1.97	0.47
1:C:458:MET:O	1:C:462:MET:HE2	2.15	0.47
1:F:459:GLU:O	1:F:462:MET:HG3	2.15	0.47
1:J:500:PHE:N	1:J:622:ALA:O	2.38	0.47
1:M:367:LEU:O	1:M:371:ILE:HG12	2.14	0.47
1:M:458:MET:HE1	1:M:667:ALA:HA	1.96	0.47
1:M:491:CYS:HB3	1:M:684:MET:HE2	1.96	0.47
1:O:342:THR:HG23	1:O:344:ARG:H	1.80	0.47
1:J:618:MET:SD	1:J:619:ARG:HG3	2.55	0.47
1:Q:674:LYS:HG3	1:Q:675:TRP:CD1	2.50	0.47
1:B:494:THR:HG21	1:B:580:PRO:HG3	1.96	0.47
1:B:665:ARG:HG3	1:B:666:PHE:HD1	1.79	0.47
1:M:360:GLU:N	1:M:360:GLU:OE1	2.48	0.47
1:M:417:ASN:HD21	1:M:446:PHE:H	1.62	0.47
1:Q:331:GLN:HA	1:Q:334:LEU:HG	1.97	0.47
1:Q:422:LEU:O	1:Q:677:LYS:NZ	2.26	0.47
1:R:360:GLU:N	1:R:360:GLU:OE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:GLU:CD	1:A:244:GLU:H	2.23	0.47
1:A:417:ASN:HD21	1:A:446:PHE:H	1.61	0.47
1:B:526:GLU:HB2	1:B:554:PHE:HD2	1.80	0.47
1:E:471:LEU:HD23	1:E:479:ARG:HH21	1.80	0.47
1:E:513:LYS:HE2	1:E:513:LYS:HB3	1.75	0.47
1:E:719:ASP:O	1:E:723:LYS:HG2	2.15	0.47
1:M:608:PRO:HD2	1:M:694:PRO:HG3	1.96	0.47
1:M:768:ASN:OD1	1:M:771:ASP:N	2.46	0.47
1:Q:607:LYS:HD3	1:Q:694:PRO:HB3	1.96	0.47
1:R:392:VAL:O	1:R:396:ILE:HG12	2.14	0.47
1:S:251:SER:HB3	1:S:261:PHE:CE1	2.50	0.47
1:A:699:TYR:HE1	1:A:755:ASP:HB3	1.80	0.46
1:C:250:VAL:O	1:C:253:ILE:HG22	2.14	0.46
1:E:334:LEU:HD21	1:E:396:ILE:HG23	1.97	0.46
1:E:677:LYS:O	1:E:681:ILE:HD11	2.15	0.46
1:J:269:PHE:HE2	1:J:303:ILE:HD11	1.79	0.46
1:N:669:LEU:HD12	1:N:670:TYR:N	2.30	0.46
1:R:290:HIS:HB3	1:R:307:LYS:HE3	1.97	0.46
1:R:741:GLN:NE2	1:R:742:LYS:HG3	2.30	0.46
1:A:613:ILE:HG21	1:A:699:TYR:HE2	1.81	0.46
1:C:568:LYS:HB2	1:C:611:ASP:HB3	1.97	0.46
1:E:342:THR:O	1:E:343:GLU:HG2	2.16	0.46
1:F:767:ALA:HB1	1:J:750:ARG:HH12	1.80	0.46
1:F:767:ALA:HB1	1:J:750:ARG:HH22	1.81	0.46
1:M:673:VAL:O	1:M:677:LYS:HG2	2.15	0.46
1:O:240:PHE:HZ	1:O:301:GLY:HA2	1.79	0.46
1:O:329:ILE:HD11	1:O:379:TYR:HB3	1.96	0.46
1:O:460:GLU:O	1:O:464:ILE:HG13	2.15	0.46
1:O:707:VAL:HB	1:O:779:ILE:HD11	1.97	0.46
1:Q:296:LEU:HD12	1:Q:303:ILE:HD11	1.96	0.46
1:R:717:MET:HE2	1:R:725:TYR:HB3	1.96	0.46
1:F:273:PRO:HB2	1:F:293:PRO:HB2	1.98	0.46
1:Q:463:ASN:OD1	1:Q:464:ILE:N	2.48	0.46
1:A:259:ILE:HD12	1:A:275:VAL:HG12	1.98	0.46
1:A:482:TYR:O	1:A:486:LEU:HG	2.14	0.46
1:B:411:ASP:O	1:B:412:LYS:HD2	2.16	0.46
1:J:465:ILE:HG13	1:J:466:ASN:N	2.29	0.46
1:M:713:HIS:HA	1:M:716:LEU:HD23	1.98	0.46
1:S:369:LEU:HD13	1:S:389:ARG:HH11	1.79	0.46
1:B:281:PRO:HB3	1:C:312:HIS:CD2	2.50	0.46
1:E:495:LYS:HZ2	1:E:686:LEU:HB2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:250:VAL:HA	1:N:253:ILE:HD12	1.98	0.46
1:N:572:ASP:OD1	1:N:573:ASN:N	2.48	0.46
1:O:455:SER:O	1:O:459:GLU:HG2	2.15	0.46
1:O:496:GLY:HA3	1:O:578:THR:HA	1.98	0.46
1:Q:618:MET:SD	1:Q:618:MET:N	2.82	0.46
1:C:484:LYS:HE2	1:C:686:LEU:HD23	1.98	0.46
1:E:476:LYS:HD2	1:E:477:LYS:N	2.31	0.46
1:M:482:TYR:CZ	1:M:486:LEU:HD11	2.51	0.46
1:N:363:LEU:HA	1:N:366:LYS:HZ3	1.80	0.46
1:O:343:GLU:HB3	1:O:403:SER:HB3	1.98	0.46
1:A:502:PHE:HD2	1:A:625:ARG:HG3	1.80	0.46
1:F:288:ARG:HA	1:J:312:HIS:CE1	2.50	0.46
1:F:670:TYR:HA	1:F:673:VAL:HG12	1.98	0.46
1:M:413:LEU:HB2	1:M:422:LEU:HD21	1.98	0.46
1:N:720:LEU:HD11	1:N:782:ILE:HD11	1.98	0.46
1:Q:549:LEU:O	1:Q:549:LEU:HD23	2.16	0.46
1:R:332:ARG:O	1:R:336:THR:HG23	2.16	0.46
1:B:270:THR:HG22	1:B:297:SER:HA	1.96	0.46
1:C:324:ASN:ND2	1:C:327:PHE:HB2	2.31	0.46
1:F:258:ILE:HB	1:F:261:PHE:HB2	1.98	0.46
1:J:678:LYS:HE3	1:J:679:TYR:CE2	2.50	0.46
1:M:248:LYS:O	1:M:252:LYS:HG2	2.16	0.46
1:M:341:LEU:HD13	1:M:402:ASP:O	2.16	0.46
1:F:503:GLY:HA3	1:F:626:PHE:HB2	1.98	0.46
1:F:760:ILE:O	1:F:764:LYS:N	2.48	0.46
1:R:709:SER:O	1:S:606:TYR:OH	2.33	0.46
1:S:343:GLU:HB2	1:S:403:SER:HB3	1.98	0.46
1:A:245:ASP:H	1:E:377:LYS:HZ1	1.63	0.46
1:B:516:LEU:HG	1:B:524:PHE:CE2	2.51	0.46
1:B:760:ILE:O	1:B:764:LYS:HG2	2.16	0.46
1:C:471:LEU:HD23	1:C:479:ARG:NH1	2.31	0.46
1:E:662:ASN:OD1	1:E:665:ARG:NH2	2.44	0.46
1:J:282:CYS:SG	1:J:290:HIS:HE1	2.39	0.46
1:N:626:PHE:HB3	1:N:629:HIS:HE2	1.81	0.46
1:O:244:GLU:H	1:O:244:GLU:CD	2.24	0.46
1:O:558:LEU:HD22	1:O:561:PHE:HE2	1.80	0.46
1:O:711:VAL:HG13	1:O:714:ILE:HD12	1.97	0.46
1:R:358:ASN:HD22	1:R:363:LEU:HG	1.80	0.46
1:M:490:LEU:HD21	1:M:672:LEU:HD13	1.98	0.45
1:O:458:MET:C	1:O:462:MET:HE3	2.41	0.45
1:Q:614:ASP:OD1	1:Q:617:LEU:HD13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:338:SER:HB3	1:R:367:LEU:HD21	1.99	0.45
1:A:464:ILE:O	1:A:468:ILE:HG12	2.16	0.45
1:C:244:GLU:H	1:C:244:GLU:CD	2.24	0.45
1:E:421:ASP:HB2	1:E:428:TYR:HE1	1.81	0.45
1:J:378:GLU:H	1:J:378:GLU:CD	2.23	0.45
1:J:573:ASN:HA	1:J:576:LYS:NZ	2.32	0.45
1:M:496:GLY:HA3	1:M:578:THR:HA	1.97	0.45
1:N:768:ASN:HD22	1:O:750:ARG:HG2	1.82	0.45
1:R:496:GLY:HA3	1:R:578:THR:HA	1.98	0.45
1:R:720:LEU:HB3	1:R:725:TYR:HD2	1.81	0.45
1:A:325:LYS:HE3	1:A:382:GLU:OE2	2.16	0.45
1:E:759:PHE:HB3	1:E:763:HIS:CE1	2.48	0.45
1:B:760:ILE:HG23	1:B:764:LYS:HD3	1.98	0.45
1:E:244:GLU:HB2	1:F:377:LYS:NZ	2.31	0.45
1:F:357:PHE:HE1	1:F:439:THR:HG21	1.81	0.45
1:M:329:ILE:HD13	1:M:383:LEU:HD21	1.98	0.45
1:N:607:LYS:HB3	1:N:694:PRO:HB3	1.98	0.45
1:F:350:TRP:CE3	1:F:355:TRP:HE3	2.35	0.45
1:F:665:ARG:O	1:F:669:LEU:HD23	2.15	0.45
1:F:768:ASN:OD1	1:F:771:ASP:N	2.48	0.45
1:Q:342:THR:C	1:Q:344:ARG:H	2.25	0.45
1:R:618:MET:SD	1:R:618:MET:N	2.89	0.45
1:S:775:GLN:O	1:S:775:GLN:HG2	2.16	0.45
1:F:305:ILE:HD11	1:F:317:LYS:HB2	1.97	0.45
1:M:402:ASP:OD1	1:Q:352:ASN:ND2	2.49	0.45
1:Q:292:HIS:ND1	1:Q:309:GLY:HA3	2.31	0.45
1:S:323:GLY:O	1:S:325:LYS:NZ	2.45	0.45
1:A:377:LYS:HD2	1:C:244:GLU:HB2	1.99	0.45
1:A:608:PRO:HD2	1:A:694:PRO:HG3	1.99	0.45
1:F:502:PHE:HE1	1:F:606:TYR:HA	1.82	0.45
1:J:707:VAL:HG12	1:J:779:ILE:HD11	1.99	0.45
1:R:378:GLU:HG3	1:R:379:TYR:CD1	2.52	0.45
1:S:245:ASP:HA	1:S:248:LYS:HD3	1.99	0.45
1:A:570:ARG:NH1	1:A:573:ASN:OD1	2.50	0.45
1:A:754:HIS:NE2	1:C:767:ALA:HA	2.32	0.45
1:B:278:TYR:O	1:B:278:TYR:CG	2.69	0.45
1:B:563:CYS:O	1:B:566:SER:OG	2.31	0.45
1:F:299:GLU:OE1	1:F:299:GLU:N	2.50	0.45
1:J:607:LYS:HE2	1:J:694:PRO:HD3	1.98	0.45
1:M:294:HIS:HA	1:M:307:LYS:HA	1.98	0.45
1:O:509:LYS:HD3	1:O:626:PHE:HE2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:684:MET:HE2	1:C:684:MET:HA	1.98	0.45
1:F:244:GLU:O	1:F:247:ILE:HG12	2.17	0.45
1:F:360:GLU:HG2	1:F:361:GLU:H	1.81	0.45
1:J:458:MET:HB3	1:J:667:ALA:HB1	1.99	0.45
1:J:495:LYS:HZ1	1:J:684:MET:C	2.25	0.45
1:M:563:CYS:SG	1:M:564:SER:N	2.89	0.45
1:R:501:PHE:HB2	1:R:603:ASP:HA	1.98	0.45
1:A:259:ILE:HD11	1:A:277:ASP:HB2	1.97	0.45
1:A:324:ASN:OD1	1:A:327:PHE:HB2	2.16	0.45
1:C:536:LEU:HD22	1:C:544:ILE:HD11	1.98	0.45
1:E:500:PHE:N	1:E:622:ALA:O	2.47	0.45
1:F:500:PHE:N	1:F:622:ALA:O	2.47	0.45
1:F:675:TRP:CD1	1:F:678:LYS:HZ3	2.35	0.45
1:J:544:ILE:HA	1:J:547:MET:HG3	1.99	0.45
1:M:502:PHE:HD2	1:M:625:ARG:HG3	1.82	0.45
1:M:738:THR:HA	1:M:741:GLN:NE2	2.32	0.45
1:Q:360:GLU:OE1	1:Q:360:GLU:N	2.50	0.45
1:Q:405:GLU:HG3	1:Q:408:THR:HG22	1.99	0.45
1:C:560:ASP:HB2	1:C:606:TYR:HD2	1.82	0.44
1:C:761:ASN:HA	1:C:764:LYS:HD3	1.99	0.44
1:F:255:ILE:HG22	1:J:318:ILE:HD11	1.99	0.44
1:F:269:PHE:CD1	1:F:270:THR:HG23	2.52	0.44
1:J:244:GLU:O	1:J:247:ILE:HG12	2.16	0.44
1:J:414:PRO:HA	1:J:419:VAL:HG12	1.98	0.44
1:N:502:PHE:HE2	1:N:606:TYR:HA	1.82	0.44
1:N:707:VAL:HG23	1:N:779:ILE:HD11	1.98	0.44
1:O:477:LYS:NZ	1:O:627:ARG:HH22	2.15	0.44
1:F:296:LEU:HD12	1:F:297:SER:N	2.31	0.44
1:M:288:ARG:HD2	1:Q:312:HIS:NE2	2.32	0.44
1:M:476:LYS:NZ	1:M:480:GLU:OE1	2.50	0.44
1:O:240:PHE:CZ	1:O:301:GLY:HA2	2.51	0.44
1:Q:500:PHE:N	1:Q:622:ALA:O	2.44	0.44
1:R:269:PHE:CD1	1:R:270:THR:HG23	2.52	0.44
1:R:329:ILE:HD13	1:R:383:LEU:HD21	1.99	0.44
1:A:779:ILE:HD12	1:A:779:ILE:H	1.82	0.44
1:B:625:ARG:HH22	1:B:627:ARG:HA	1.82	0.44
1:F:255:ILE:HD11	1:F:281:PRO:O	2.18	0.44
1:J:342:THR:O	1:J:343:GLU:HB3	2.17	0.44
1:A:736:LEU:O	1:A:740:GLN:HG2	2.17	0.44
1:C:611:ASP:OD1	1:C:612:ARG:N	2.50	0.44
1:F:351:ILE:HD12	1:F:351:ILE:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:548:HIS:HE1	1:R:595:ARG:HB2	1.82	0.44
1:R:768:ASN:OD1	1:R:771:ASP:N	2.50	0.44
1:A:243:PHE:CZ	1:A:247:ILE:HD11	2.52	0.44
1:O:460:GLU:HA	1:O:463:ASN:HD22	1.83	0.44
1:S:462:MET:HA	1:S:465:ILE:HB	1.98	0.44
1:S:475:ASN:OD1	1:S:475:ASN:O	2.36	0.44
1:A:490:LEU:HD21	1:A:672:LEU:HB3	1.99	0.44
1:B:249:ARG:HG2	1:B:252:LYS:NZ	2.32	0.44
1:C:303:ILE:HD13	1:C:303:ILE:HA	1.91	0.44
1:F:288:ARG:HA	1:J:312:HIS:NE2	2.33	0.44
1:J:281:PRO:HB2	1:J:286:LYS:HD3	1.99	0.44
1:J:762:ARG:HG3	1:J:763:HIS:N	2.31	0.44
1:M:504:GLU:O	1:M:507:THR:OG1	2.26	0.44
1:M:570:ARG:NH1	1:M:573:ASN:OD1	2.50	0.44
1:N:270:THR:HG22	1:N:297:SER:HA	2.00	0.44
1:N:329:ILE:HD13	1:N:383:LEU:HD21	1.98	0.44
1:O:274:LEU:HD11	1:O:296:LEU:HD21	2.00	0.44
1:S:342:THR:HG21	1:S:357:PHE:CE1	2.53	0.44
1:B:764:LYS:O	1:C:564:SER:OG	2.24	0.44
1:C:350:TRP:CZ2	1:C:353:ASN:HA	2.52	0.44
1:C:516:LEU:HD23	1:C:668:PHE:HE2	1.83	0.44
1:J:535:VAL:HG12	1:J:538:LYS:H	1.83	0.44
1:M:501:PHE:HB2	1:M:603:ASP:HA	2.00	0.44
1:N:312:HIS:HE2	1:S:288:ARG:HA	1.83	0.44
1:O:761:ASN:HA	1:O:764:LYS:HD3	1.99	0.44
1:R:288:ARG:HG2	1:S:312:HIS:CD2	2.53	0.44
1:R:475:ASN:OD1	1:R:478:ASN:HB3	2.18	0.44
1:F:470:PRO:HD2	1:F:627:ARG:HH21	1.83	0.44
1:R:243:PHE:O	1:R:247:ILE:HG12	2.18	0.44
1:R:377:LYS:HG3	1:R:378:GLU:N	2.33	0.44
1:E:475:ASN:O	1:E:475:ASN:ND2	2.51	0.44
1:N:500:PHE:N	1:N:622:ALA:O	2.48	0.44
1:N:560:ASP:HB3	1:N:606:TYR:HB2	1.99	0.44
1:O:536:LEU:HD22	1:O:544:ILE:HD11	1.99	0.44
1:B:269:PHE:CD1	1:B:270:THR:HG23	2.53	0.43
1:C:520:ILE:HB	1:C:524:PHE:HB2	1.99	0.43
1:E:547:MET:HE2	1:E:547:MET:O	2.18	0.43
1:J:510:SER:O	1:J:513:LYS:HG2	2.18	0.43
1:J:727:LEU:HA	1:J:732:VAL:HG22	1.99	0.43
1:N:618:MET:SD	1:N:618:MET:N	2.91	0.43
1:O:325:LYS:HA	1:O:325:LYS:HD3	1.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:354:SER:OG	1:R:356:LYS:NZ	2.50	0.43
1:R:548:HIS:CE1	1:R:595:ARG:HB2	2.52	0.43
1:S:490:LEU:HD11	1:S:672:LEU:HB3	2.00	0.43
1:M:332:ARG:O	1:M:336:THR:HG23	2.18	0.43
1:M:369:LEU:HD12	1:M:372:ARG:HD3	1.99	0.43
1:M:603:ASP:OD1	1:M:603:ASP:N	2.49	0.43
1:N:311:PRO:HB2	1:S:281:PRO:HD3	2.00	0.43
1:N:555:CYS:HB3	1:N:602:ILE:HG12	1.99	0.43
1:O:354:SER:OG	1:O:356:LYS:NZ	2.49	0.43
1:A:315:LYS:HD2	1:A:315:LYS:N	2.33	0.43
1:M:292:HIS:HB2	1:M:307:LYS:HE2	2.01	0.43
1:N:374:GLN:CD	1:N:374:GLN:H	2.26	0.43
1:Q:249:ARG:O	1:Q:252:LYS:HG3	2.18	0.43
1:Q:484:LYS:HD3	1:Q:484:LYS:HA	1.90	0.43
1:S:492:GLY:O	1:S:597:HIS:ND1	2.34	0.43
1:A:312:HIS:CD2	1:C:281:PRO:HG3	2.53	0.43
1:A:395:ASN:O	1:A:399:MET:HG3	2.19	0.43
1:A:734:LEU:HD11	1:A:738:THR:HB	2.00	0.43
1:A:768:ASN:OD1	1:A:771:ASP:N	2.47	0.43
1:C:475:ASN:O	1:C:479:ARG:HG2	2.19	0.43
1:F:568:LYS:HB2	1:F:611:ASP:HB3	1.99	0.43
1:J:461:LEU:O	1:J:465:ILE:HG23	2.18	0.43
1:M:495:LYS:HZ1	1:M:686:LEU:N	2.16	0.43
1:S:386:PRO:HG3	1:S:389:ARG:HH21	1.84	0.43
1:B:366:LYS:HD3	1:J:401:VAL:HG12	2.01	0.43
1:B:496:GLY:HA3	1:B:578:THR:HA	2.00	0.43
1:B:516:LEU:HG	1:B:524:PHE:CD2	2.52	0.43
1:C:393:GLU:HA	1:C:396:ILE:HG22	2.01	0.43
1:C:406:THR:HG22	1:C:437:THR:HB	2.00	0.43
1:F:245:ASP:HB3	1:F:249:ARG:HH22	1.83	0.43
1:F:295:GLN:HB3	1:F:306:TYR:CZ	2.54	0.43
1:F:491:CYS:SG	1:F:684:MET:HG3	2.59	0.43
1:F:757:GLU:HA	1:F:760:ILE:HB	1.99	0.43
1:J:393:GLU:O	1:J:397:ARG:HG3	2.19	0.43
1:O:375:LEU:HD12	1:O:376:PRO:O	2.19	0.43
1:Q:348:ILE:HG22	1:Q:355:TRP:HE3	1.83	0.43
1:Q:555:CYS:HB3	1:Q:602:ILE:HG12	2.00	0.43
1:R:322:ASP:OD1	1:R:322:ASP:N	2.50	0.43
1:R:500:PHE:O	1:R:624:VAL:N	2.48	0.43
1:R:612:ARG:HH22	1:R:614:ASP:CG	2.26	0.43
1:R:625:ARG:HH21	1:R:627:ARG:CZ	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:681:ILE:HB	1:E:682:PRO:HD3	1.98	0.43
1:M:475:ASN:OD1	1:M:478:ASN:HB3	2.18	0.43
1:N:671:LEU:HA	1:N:674:LYS:HZ2	1.83	0.43
1:N:727:LEU:HD11	1:N:730:ASN:HA	2.00	0.43
1:O:358:ASN:HD21	1:O:361:GLU:HB3	1.82	0.43
1:O:364:ILE:O	1:O:368:ILE:HG13	2.19	0.43
1:O:458:MET:HE1	1:O:670:TYR:HB3	1.99	0.43
1:Q:269:PHE:HZ	1:Q:298:LEU:HD22	1.83	0.43
1:Q:719:ASP:O	1:Q:723:LYS:HG2	2.18	0.43
1:R:514:ARG:HB3	1:R:659:ILE:HG21	1.99	0.43
1:B:457:GLU:OE2	1:B:663:ARG:NH2	2.52	0.43
1:S:747:PHE:HB3	1:S:752:PHE:HD2	1.83	0.43
1:O:360:GLU:N	1:O:360:GLU:OE1	2.51	0.43
1:A:555:CYS:HB3	1:A:602:ILE:HG12	1.99	0.43
1:B:258:ILE:HB	1:B:261:PHE:HB2	2.00	0.43
1:C:343:GLU:HB2	1:C:403:SER:HB3	2.00	0.43
1:E:299:GLU:N	1:E:299:GLU:OE1	2.52	0.43
1:F:482:TYR:CE1	1:F:486:LEU:HD11	2.53	0.43
1:M:750:ARG:HG3	1:M:751:LEU:HG	2.01	0.43
1:O:350:TRP:CZ2	1:O:353:ASN:HA	2.53	0.43
1:O:500:PHE:HE1	1:O:602:ILE:HD12	1.82	0.43
1:F:244:GLU:HB2	1:J:377:LYS:HE2	2.01	0.43
1:F:457:GLU:O	1:F:460:GLU:HG2	2.19	0.43
1:N:712:LYS:HG2	1:O:629:HIS:NE2	2.34	0.43
1:O:386:PRO:O	1:O:390:LYS:HG2	2.19	0.43
1:A:242:SER:HB2	1:E:377:LYS:NZ	2.32	0.42
1:B:509:LYS:HB2	1:B:626:PHE:HZ	1.84	0.42
1:B:529:GLN:HB3	1:B:558:LEU:HD23	2.00	0.42
1:B:697:ALA:O	1:B:701:LYS:HG2	2.19	0.42
1:B:707:VAL:HB	1:B:779:ILE:HD11	2.01	0.42
1:Q:513:LYS:HB3	1:Q:513:LYS:HE2	1.75	0.42
1:Q:519:ALA:HB2	1:Q:668:PHE:HD2	1.84	0.42
1:R:670:TYR:HA	1:R:673:VAL:HG12	2.00	0.42
1:A:241:ILE:HG23	1:A:321:LEU:O	2.19	0.42
1:A:256:ASN:OD1	1:A:279:VAL:N	2.51	0.42
1:E:625:ARG:NH1	1:E:627:ARG:HB3	2.34	0.42
1:N:458:MET:O	1:N:462:MET:HE3	2.19	0.42
1:N:560:ASP:N	1:N:560:ASP:OD1	2.52	0.42
1:Q:757:GLU:HA	1:Q:760:ILE:HB	2.01	0.42
1:R:675:TRP:HA	1:R:678:LYS:HZ2	1.83	0.42
1:S:265:ASP:N	1:S:268:ASN:OD1	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:333:ILE:O	1:S:336:THR:OG1	2.29	0.42
1:F:292:HIS:ND1	1:F:309:GLY:HA3	2.34	0.42
1:N:366:LYS:HG2	1:S:398:ASP:O	2.19	0.42
1:Q:251:SER:HB3	1:Q:261:PHE:CE1	2.53	0.42
1:S:491:CYS:HB2	1:S:676:TYR:HE2	1.84	0.42
1:S:536:LEU:HD12	1:S:576:LYS:HE2	2.00	0.42
1:C:496:GLY:HA3	1:C:578:THR:HA	2.01	0.42
1:E:757:GLU:HA	1:E:760:ILE:HB	2.01	0.42
1:F:725:TYR:HE1	1:F:734:LEU:HB2	1.85	0.42
1:J:416:LYS:NZ	1:J:445:LYS:HG3	2.34	0.42
1:J:615:ASN:O	1:J:619:ARG:NH2	2.52	0.42
1:N:350:TRP:HB2	1:N:355:TRP:CZ3	2.54	0.42
1:R:393:GLU:OE2	1:R:397:ARG:NH2	2.53	0.42
1:R:728:TYR:HE2	1:S:751:LEU:HD12	1.85	0.42
1:S:393:GLU:O	1:S:397:ARG:HG3	2.19	0.42
1:A:548:HIS:CE1	1:A:595:ARG:HB2	2.49	0.42
1:C:752:PHE:O	1:C:756:ILE:HG13	2.19	0.42
1:E:243:PHE:O	1:E:247:ILE:HG23	2.20	0.42
1:J:541:ASN:HB3	1:J:544:ILE:HB	2.00	0.42
1:M:742:LYS:HZ3	1:M:778:PHE:HB3	1.83	0.42
1:N:326:LEU:HD12	1:N:326:LEU:H	1.83	0.42
1:O:244:GLU:HA	1:O:247:ILE:HG12	2.00	0.42
1:O:292:HIS:HB3	1:O:308:THR:OG1	2.19	0.42
1:S:533:THR:O	1:S:570:ARG:NH2	2.52	0.42
1:F:471:LEU:HD23	1:F:479:ARG:NH1	2.25	0.42
1:O:284:LEU:O	1:O:317:LYS:NZ	2.50	0.42
1:Q:421:ASP:HB2	1:Q:428:TYR:CE2	2.55	0.42
1:R:294:HIS:HA	1:R:307:LYS:HA	2.00	0.42
1:S:610:PHE:HE2	1:S:694:PRO:HG2	1.84	0.42
1:B:534:ASP:C	1:B:570:ARG:HH22	2.24	0.42
1:J:461:LEU:HD11	1:J:664:TYR:HB3	2.02	0.42
1:M:248:LYS:O	1:M:251:SER:OG	2.30	0.42
1:M:414:PRO:HB2	1:M:441:SER:HA	2.02	0.42
1:O:237:GLU:H	1:O:240:PHE:HD2	1.67	0.42
1:R:502:PHE:HE1	1:R:606:TYR:HA	1.84	0.42
1:S:503:GLY:HA3	1:S:626:PHE:HB2	2.02	0.42
1:S:544:ILE:O	1:S:547:MET:HG3	2.19	0.42
1:B:517:LYS:HE3	1:B:517:LYS:HB3	1.86	0.42
1:E:348:ILE:HG22	1:E:355:TRP:HE3	1.85	0.42
1:E:485:THR:HG23	1:E:486:LEU:HD12	2.02	0.42
1:E:658:LYS:HD3	1:E:664:TYR:HE2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:547:MET:HE2	1:M:547:MET:O	2.20	0.42
1:O:385:CYS:HB3	1:O:388:LYS:HG3	2.02	0.42
1:S:547:MET:HE2	1:S:547:MET:O	2.20	0.42
1:A:243:PHE:O	1:A:247:ILE:HG12	2.20	0.42
1:A:284:LEU:HD23	1:A:317:LYS:HE2	2.02	0.42
1:C:470:PRO:HB2	1:C:472:THR:HG23	2.00	0.42
1:M:250:VAL:HA	1:M:253:ILE:HD12	2.01	0.42
1:N:312:HIS:CE1	1:S:288:ARG:HG2	2.55	0.42
1:O:733:THR:HG21	1:O:773:TYR:CD2	2.54	0.42
1:Q:240:PHE:HA	1:Q:322:ASP:HA	2.00	0.42
1:R:249:ARG:HH22	1:S:378:GLU:HA	1.85	0.42
1:S:475:ASN:OD1	1:S:478:ASN:HB3	2.19	0.42
1:S:573:ASN:HA	1:S:576:LYS:NZ	2.35	0.42
1:A:371:ILE:HG22	1:A:371:ILE:O	2.20	0.42
1:B:750:ARG:NE	1:J:767:ALA:HB1	2.34	0.42
1:C:600:ILE:HD13	1:C:600:ILE:HA	1.89	0.42
1:E:537:ASP:OD1	1:E:576:LYS:NZ	2.53	0.42
1:F:280:THR:OG1	1:J:304:ARG:NH1	2.53	0.42
1:N:464:ILE:O	1:N:468:ILE:HG12	2.20	0.42
1:N:563:CYS:O	1:N:566:SER:OG	2.38	0.42
1:O:315:LYS:HB2	1:O:317:LYS:NZ	2.32	0.42
1:O:333:ILE:HD13	1:O:333:ILE:HA	1.90	0.42
1:O:516:LEU:HD22	1:O:668:PHE:CE2	2.54	0.42
1:B:750:ARG:O	1:B:750:ARG:NH1	2.42	0.41
1:C:555:CYS:HB3	1:C:602:ILE:HG12	2.02	0.41
1:F:541:ASN:HB3	1:F:544:ILE:HG12	2.02	0.41
1:R:503:GLY:HA3	1:R:626:PHE:HB2	2.00	0.41
1:A:325:LYS:H	1:A:325:LYS:HG3	1.56	0.41
1:B:621:ILE:HD13	1:B:621:ILE:HA	1.90	0.41
1:E:544:ILE:O	1:E:547:MET:HG3	2.20	0.41
1:J:533:THR:O	1:J:570:ARG:NH2	2.53	0.41
1:M:512:THR:HG22	1:M:516:LEU:HD23	2.00	0.41
1:M:611:ASP:OD1	1:M:612:ARG:N	2.53	0.41
1:Q:476:LYS:HD3	1:Q:476:LYS:HA	1.76	0.41
1:A:288:ARG:NH2	1:E:311:PRO:HD2	2.35	0.41
1:E:412:LYS:NZ	1:E:421:ASP:OD1	2.39	0.41
1:F:342:THR:HG22	1:F:348:ILE:HG23	2.03	0.41
1:F:364:ILE:HB	1:F:393:GLU:HG3	2.03	0.41
1:F:761:ASN:OD1	1:F:762:ARG:N	2.54	0.41
1:M:779:ILE:HD12	1:M:779:ILE:H	1.84	0.41
1:Q:255:ILE:O	1:R:304:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:612:ARG:NH1	1:S:613:ILE:O	2.53	0.41
1:A:256:ASN:HD21	1:A:280:THR:C	2.28	0.41
1:A:516:LEU:HD22	1:A:668:PHE:CE2	2.55	0.41
1:B:249:ARG:O	1:B:253:ILE:HG12	2.20	0.41
1:C:278:TYR:O	1:C:278:TYR:CG	2.73	0.41
1:E:515:LEU:HG	1:E:668:PHE:CD2	2.55	0.41
1:N:684:MET:HA	1:N:684:MET:HE2	2.02	0.41
1:R:485:THR:HG21	1:R:624:VAL:HG21	2.02	0.41
1:S:385:CYS:HB3	1:S:388:LYS:HG3	2.02	0.41
1:A:477:LYS:HG3	1:A:478:ASN:N	2.34	0.41
1:E:519:ALA:HB1	1:E:669:LEU:HD23	2.03	0.41
1:E:668:PHE:HD1	1:E:671:LEU:HD12	1.86	0.41
1:F:447:ASP:HB3	1:F:666:PHE:HE2	1.85	0.41
1:F:484:LYS:HD3	1:F:680:HIS:NE2	2.35	0.41
1:J:385:CYS:HB3	1:J:388:LYS:HG3	2.03	0.41
1:J:496:GLY:HA3	1:J:578:THR:HA	2.03	0.41
1:M:288:ARG:HD2	1:M:288:ARG:HA	1.89	0.41
1:S:509:LYS:O	1:S:512:THR:HG22	2.21	0.41
1:F:361:GLU:OE1	1:F:361:GLU:N	2.50	0.41
1:F:658:LYS:HG2	1:F:663:ARG:NH1	2.35	0.41
1:J:533:THR:HA	1:J:567:LYS:NZ	2.36	0.41
1:J:667:ALA:O	1:J:671:LEU:HG	2.20	0.41
1:N:413:LEU:HB3	1:N:420:LEU:HB3	2.02	0.41
1:N:413:LEU:HB2	1:N:422:LEU:HD21	2.03	0.41
1:O:665:ARG:HG3	1:O:666:PHE:HD1	1.85	0.41
1:A:417:ASN:ND2	1:A:446:PHE:H	2.19	0.41
1:B:742:LYS:HG2	1:B:778:PHE:CE2	2.55	0.41
1:C:413:LEU:HD12	1:C:422:LEU:HD11	2.02	0.41
1:F:248:LYS:HB3	1:F:252:LYS:NZ	2.35	0.41
1:F:728:TYR:HE2	1:J:751:LEU:HD12	1.86	0.41
1:M:519:ALA:O	1:M:669:LEU:HD21	2.21	0.41
1:Q:367:LEU:O	1:Q:371:ILE:HG13	2.21	0.41
1:Q:738:THR:HA	1:Q:741:GLN:HE21	1.85	0.41
1:R:764:LYS:NZ	1:R:772:GLU:OE1	2.43	0.41
1:S:461:LEU:HD13	1:S:664:TYR:CD1	2.56	0.41
1:A:725:TYR:CE1	1:A:734:LEU:HD13	2.54	0.41
1:A:747:PHE:CZ	1:A:756:ILE:HG21	2.56	0.41
1:C:502:PHE:HD2	1:C:625:ARG:HG3	1.86	0.41
1:M:328:ASN:O	1:M:332:ARG:HG3	2.20	0.41
1:M:419:VAL:HG11	1:M:436:TYR:HD2	1.86	0.41
1:N:625:ARG:HB3	1:N:627:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:681:ILE:HB	1:Q:682:PRO:HD3	2.02	0.41
1:S:360:GLU:HG2	1:S:361:GLU:OE1	2.21	0.41
1:A:611:ASP:OD1	1:A:612:ARG:N	2.54	0.41
1:B:367:LEU:O	1:B:371:ILE:HG12	2.21	0.41
1:C:244:GLU:HA	1:C:247:ILE:HG12	2.03	0.41
1:F:278:TYR:O	1:F:278:TYR:CG	2.74	0.41
1:J:307:LYS:NZ	1:J:310:ASN:OD1	2.45	0.41
1:J:536:LEU:HD22	1:J:544:ILE:HD11	2.03	0.41
1:M:292:HIS:HB3	1:M:308:THR:OG1	2.20	0.41
1:M:519:ALA:HB1	1:M:669:LEU:HD23	2.03	0.41
1:N:327:PHE:O	1:N:331:GLN:HG2	2.21	0.41
1:O:555:CYS:HB2	1:O:600:ILE:HG23	2.03	0.41
1:O:726:ILE:O	1:O:732:VAL:HG13	2.20	0.41
1:Q:258:ILE:HB	1:Q:261:PHE:HB2	2.03	0.41
1:Q:322:ASP:OD1	1:Q:322:ASP:N	2.52	0.41
1:Q:371:ILE:HG22	1:Q:371:ILE:O	2.21	0.41
1:Q:711:VAL:HG13	1:Q:714:ILE:HD12	2.02	0.41
1:R:264:LEU:HD12	1:R:269:PHE:HA	2.03	0.41
1:S:665:ARG:HG3	1:S:666:PHE:CD1	2.52	0.41
1:A:303:ILE:HD13	1:A:303:ILE:HA	1.89	0.41
1:E:284:LEU:H	1:E:284:LEU:HD12	1.84	0.41
1:F:250:VAL:O	1:F:253:ILE:HG22	2.21	0.41
1:J:325:LYS:HE3	1:J:325:LYS:HB3	1.98	0.41
1:M:288:ARG:HA	1:Q:312:HIS:CE1	2.55	0.41
1:N:555:CYS:HB2	1:N:600:ILE:HG23	2.03	0.41
1:O:367:LEU:O	1:O:371:ILE:HG12	2.21	0.41
1:O:611:ASP:OD1	1:O:612:ARG:N	2.53	0.41
1:Q:421:ASP:HB2	1:Q:428:TYR:HE2	1.86	0.41
1:B:455:SER:HB3	1:B:458:MET:HG3	2.04	0.40
1:C:567:LYS:HD2	1:C:568:LYS:O	2.20	0.40
1:J:721:SER:HA	1:J:725:TYR:HB2	2.03	0.40
1:O:701:LYS:HE2	1:O:746:TYR:CE2	2.56	0.40
1:A:461:LEU:HD13	1:A:664:TYR:CE1	2.57	0.40
1:F:259:ILE:HD11	1:F:277:ASP:HB2	2.02	0.40
1:M:572:ASP:OD1	1:M:573:ASN:N	2.54	0.40
1:O:743:ILE:HD12	1:O:743:ILE:HA	1.91	0.40
1:S:382:GLU:OE1	1:S:382:GLU:N	2.49	0.40
1:S:519:ALA:HB1	1:S:669:LEU:HD23	2.02	0.40
1:A:674:LYS:HA	1:A:677:LYS:HG2	2.04	0.40
1:B:750:ARG:HH21	1:J:728:TYR:HE1	1.70	0.40
1:C:469:GLN:O	1:C:479:ARG:NH1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:675:TRP:HA	1:F:678:LYS:HZ2	1.85	0.40
1:J:555:CYS:HB2	1:J:600:ILE:HG23	2.04	0.40
1:M:251:SER:HB3	1:M:261:PHE:CE1	2.56	0.40
1:N:367:LEU:O	1:N:371:ILE:HG12	2.21	0.40
1:Q:741:GLN:NE2	1:Q:742:LYS:HG3	2.37	0.40
1:R:379:TYR:O	1:R:383:LEU:HD23	2.21	0.40
1:S:533:THR:HA	1:S:567:LYS:NZ	2.34	0.40
1:A:671:LEU:O	1:A:674:LYS:HG2	2.20	0.40
1:A:764:LYS:HD2	1:A:764:LYS:HA	1.93	0.40
1:C:351:ILE:O	1:C:356:LYS:NZ	2.51	0.40
1:J:420:LEU:HD12	1:J:421:ASP:N	2.35	0.40
1:J:516:LEU:HD22	1:J:668:PHE:HE2	1.85	0.40
1:J:669:LEU:HD23	1:J:669:LEU:HA	1.93	0.40
1:M:282:CYS:O	1:M:286:LYS:HD3	2.22	0.40
1:M:296:LEU:HG	1:M:303:ILE:HD11	2.03	0.40
1:M:671:LEU:O	1:M:674:LYS:HG2	2.21	0.40
1:O:322:ASP:OD1	1:O:322:ASP:N	2.54	0.40
1:O:538:LYS:HD2	1:O:538:LYS:O	2.21	0.40
1:Q:249:ARG:HA	1:Q:252:LYS:HG3	2.02	0.40
1:R:292:HIS:HB3	1:R:308:THR:OG1	2.21	0.40
1:F:303:ILE:O	1:F:318:ILE:HD12	2.21	0.40
1:J:670:TYR:HA	1:J:673:VAL:HG12	2.04	0.40
1:M:244:GLU:CD	1:Q:377:LYS:HD2	2.47	0.40
1:O:431:ASP:OD1	1:O:432:ASP:N	2.55	0.40
1:S:253:ILE:HG23	1:S:317:LYS:NZ	2.37	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	504/785 (64%)	481 (95%)	23 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	504/785 (64%)	491 (97%)	13 (3%)	0	100	100
1	C	504/785 (64%)	485 (96%)	19 (4%)	0	100	100
1	E	504/785 (64%)	492 (98%)	12 (2%)	0	100	100
1	F	504/785 (64%)	486 (96%)	18 (4%)	0	100	100
1	J	504/785 (64%)	486 (96%)	18 (4%)	0	100	100
1	M	504/785 (64%)	486 (96%)	18 (4%)	0	100	100
1	N	504/785 (64%)	489 (97%)	15 (3%)	0	100	100
1	O	504/785 (64%)	490 (97%)	14 (3%)	0	100	100
1	Q	504/785 (64%)	485 (96%)	19 (4%)	0	100	100
1	R	504/785 (64%)	491 (97%)	13 (3%)	0	100	100
1	S	504/785 (64%)	486 (96%)	18 (4%)	0	100	100
All	All	6048/9420 (64%)	5848 (97%)	200 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	472/725 (65%)	472 (100%)	0	100	100
1	B	472/725 (65%)	472 (100%)	0	100	100
1	C	472/725 (65%)	471 (100%)	1 (0%)	92	95
1	E	472/725 (65%)	470 (100%)	2 (0%)	89	93
1	F	472/725 (65%)	472 (100%)	0	100	100
1	J	472/725 (65%)	472 (100%)	0	100	100
1	M	472/725 (65%)	471 (100%)	1 (0%)	92	95
1	N	472/725 (65%)	472 (100%)	0	100	100
1	O	472/725 (65%)	472 (100%)	0	100	100
1	Q	472/725 (65%)	472 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	472/725 (65%)	472 (100%)	0	100	100
1	S	472/725 (65%)	472 (100%)	0	100	100
All	All	5664/8700 (65%)	5660 (100%)	4 (0%)	92	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	426	MET
1	E	349	VAL
1	E	426	MET
1	M	439	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	337	ASN
1	A	347	HIS
1	A	358	ASN
1	A	605	ASN
1	B	267	ASN
1	B	417	ASN
1	B	463	ASN
1	B	763	HIS
1	C	312	HIS
1	C	324	ASN
1	C	347	HIS
1	C	358	ASN
1	C	373	HIS
1	C	529	GLN
1	C	597	HIS
1	C	713	HIS
1	C	761	ASN
1	E	417	ASN
1	E	475	ASN
1	E	541	ASN
1	E	660	GLN
1	F	267	ASN
1	F	347	HIS
1	F	475	ASN
1	F	529	GLN

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Mol	Chain	Res	Type
1	J	374	GLN
1	J	475	ASN
1	J	740	GLN
1	J	748	ASN
1	M	331	GLN
1	M	417	ASN
1	M	463	ASN
1	M	660	GLN
1	N	292	HIS
1	N	300	ASN
1	O	292	HIS
1	O	353	ASN
1	O	358	ASN
1	O	463	ASN
1	O	730	ASN
1	Q	478	ASN
1	Q	741	GLN
1	Q	763	HIS
1	R	292	HIS
1	R	331	GLN
1	R	358	ASN
1	R	529	GLN
1	R	741	GLN
1	R	775	GLN
1	S	312	HIS
1	S	331	GLN
1	S	337	ASN
1	S	475	ASN
1	S	730	ASN
1	S	748	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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.