



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:28 AM UTC

PDB ID : 7SXX / pdb_00007sxx
EMDB ID : EMD-25500
Title : Kinetically trapped Pseudomonas-phage PaP3 portal protein - Full Length
Authors : Hou, C.F.D.; Swanson, N.A.; Li, F.; Yang, R.; Lokareddy, R.K.; Cingolani, G.
Deposited on : 2021-11-23
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

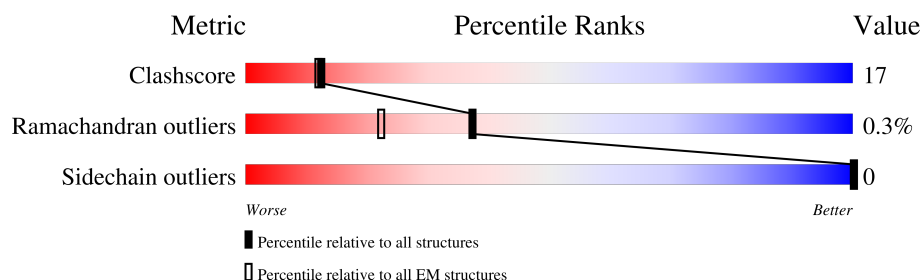
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	705	 54% 25% 21%
1	b	705	 58% 22% 19%
1	c	705	 52% 28% 19%
1	d	705	 52% 28% 19%
1	e	705	 51% 28% 20%
1	f	705	 45% 29% 27%
1	g	705	 46% 51%
1	h	705	 55% 25% 21%
1	i	705	 52% 28% 20%

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Mol	Chain	Length	Quality of chain
1	j	705	 54% 28% 18%
1	k	705	 53% 27% 20%
1	l	705	 52% 27% 21%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 48937 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.

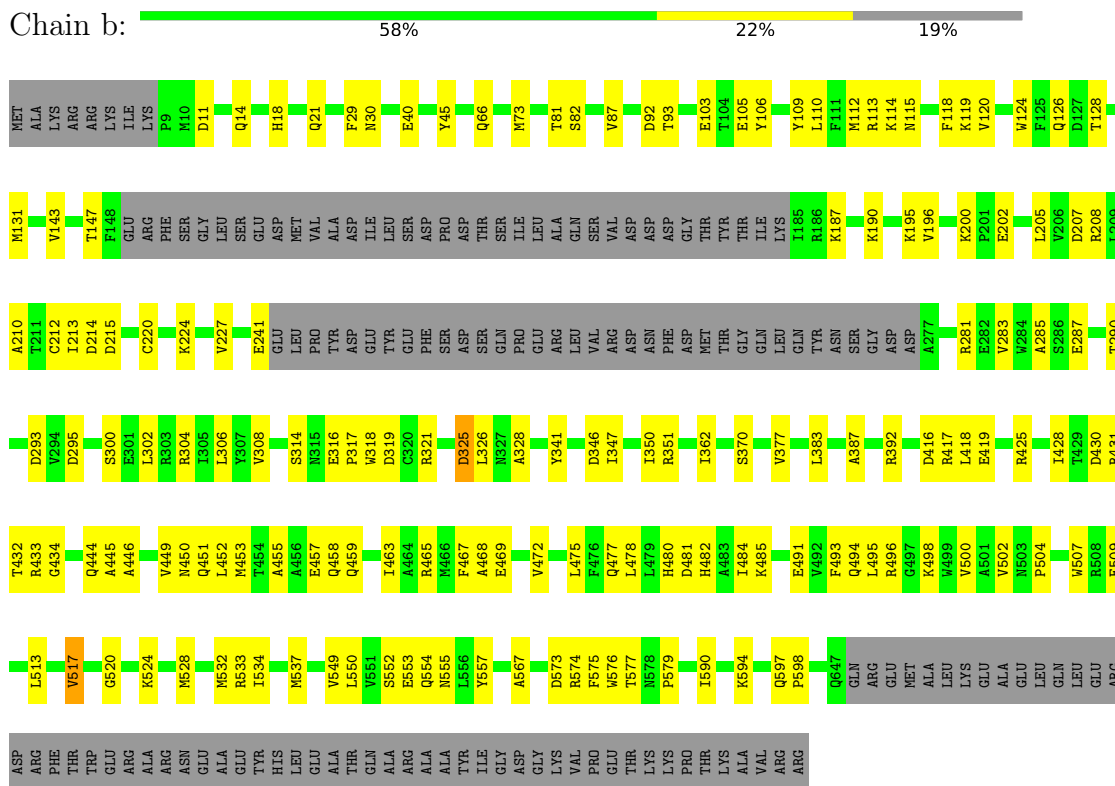
- Molecule 1 is a protein called Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	b	568	Total	C	N	O	S	0	0
			4325	2706	767	829	23		
1	a	558	Total	C	N	O	S	0	0
			4293	2689	758	823	23		
1	l	555	Total	C	N	O	S	0	0
			4281	2682	757	819	23		
1	k	565	Total	C	N	O	S	0	0
			4345	2719	770	833	23		
1	j	578	Total	C	N	O	S	0	0
			4405	2755	782	845	23		
1	i	564	Total	C	N	O	S	0	0
			4322	2705	767	828	22		
1	h	559	Total	C	N	O	S	0	0
			4108	2563	745	778	22		
1	c	569	Total	C	N	O	S	0	0
			4377	2740	776	838	23		
1	d	569	Total	C	N	O	S	0	0
			4358	2727	773	835	23		
1	e	562	Total	C	N	O	S	0	0
			4323	2706	766	828	23		
1	f	518	Total	C	N	O	S	0	0
			4077	2560	717	777	23		
1	g	348	Total	C	N	O		0	0
			1723	1027	348	348			

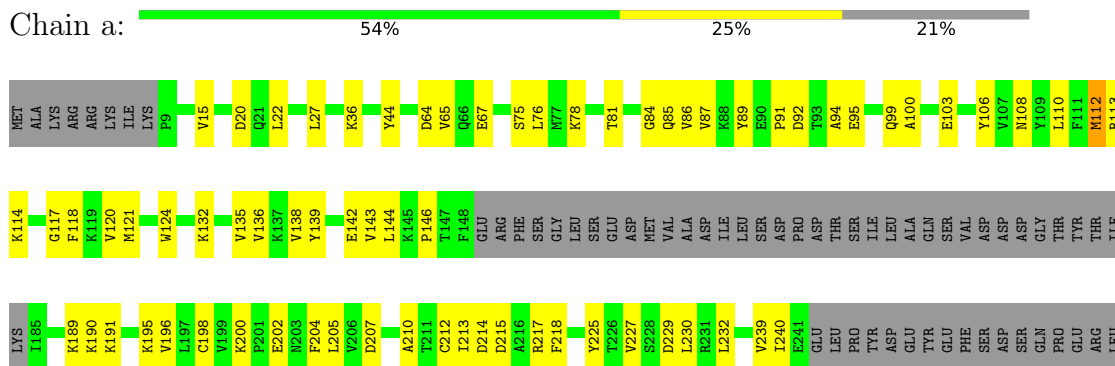
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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: Portal protein

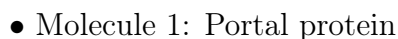
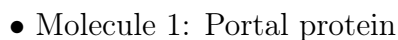


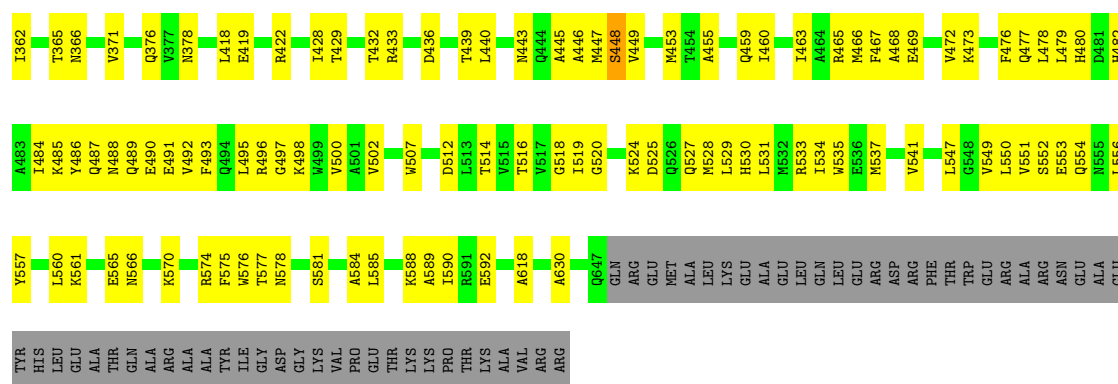
• Molecule 1: Portal protein





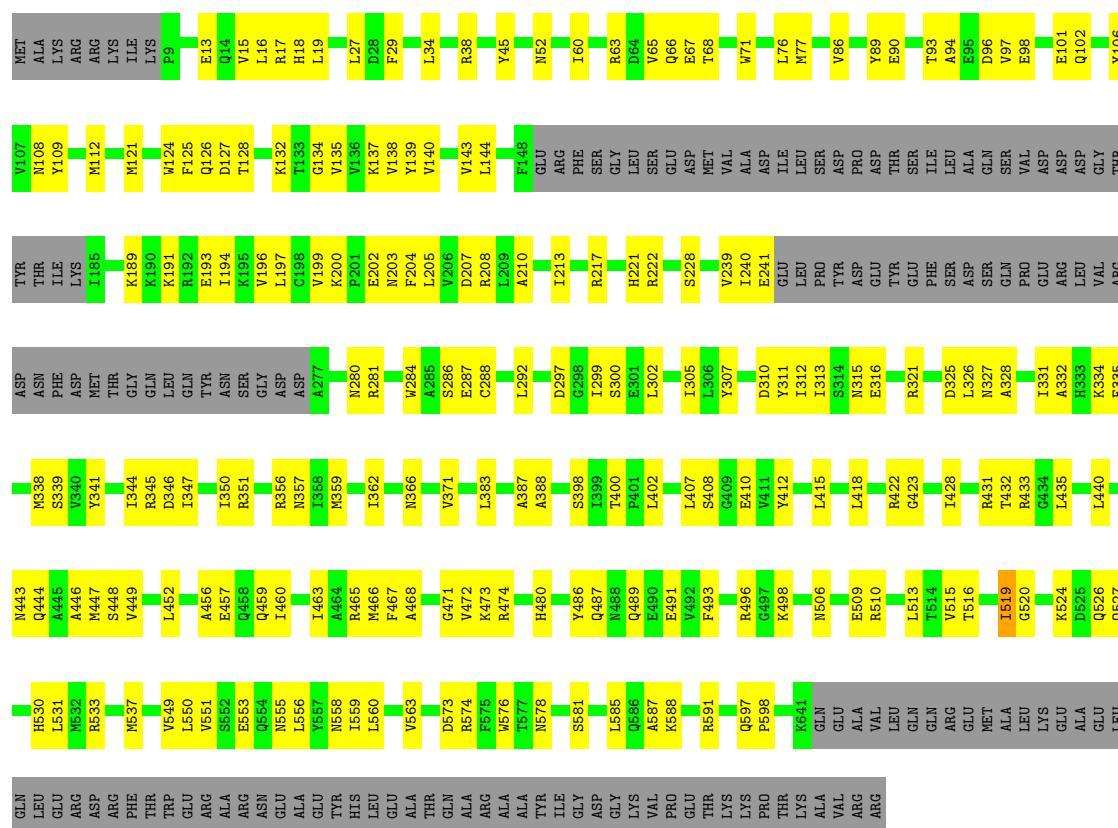






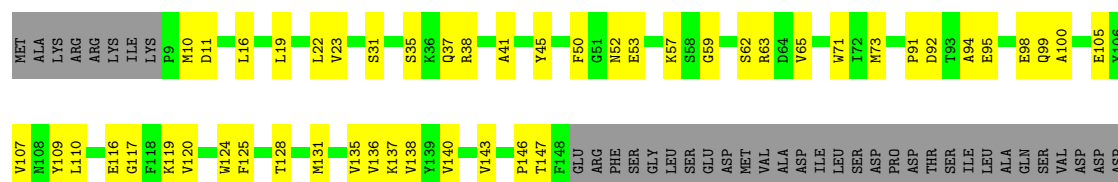
• Molecule 1: Portal protein

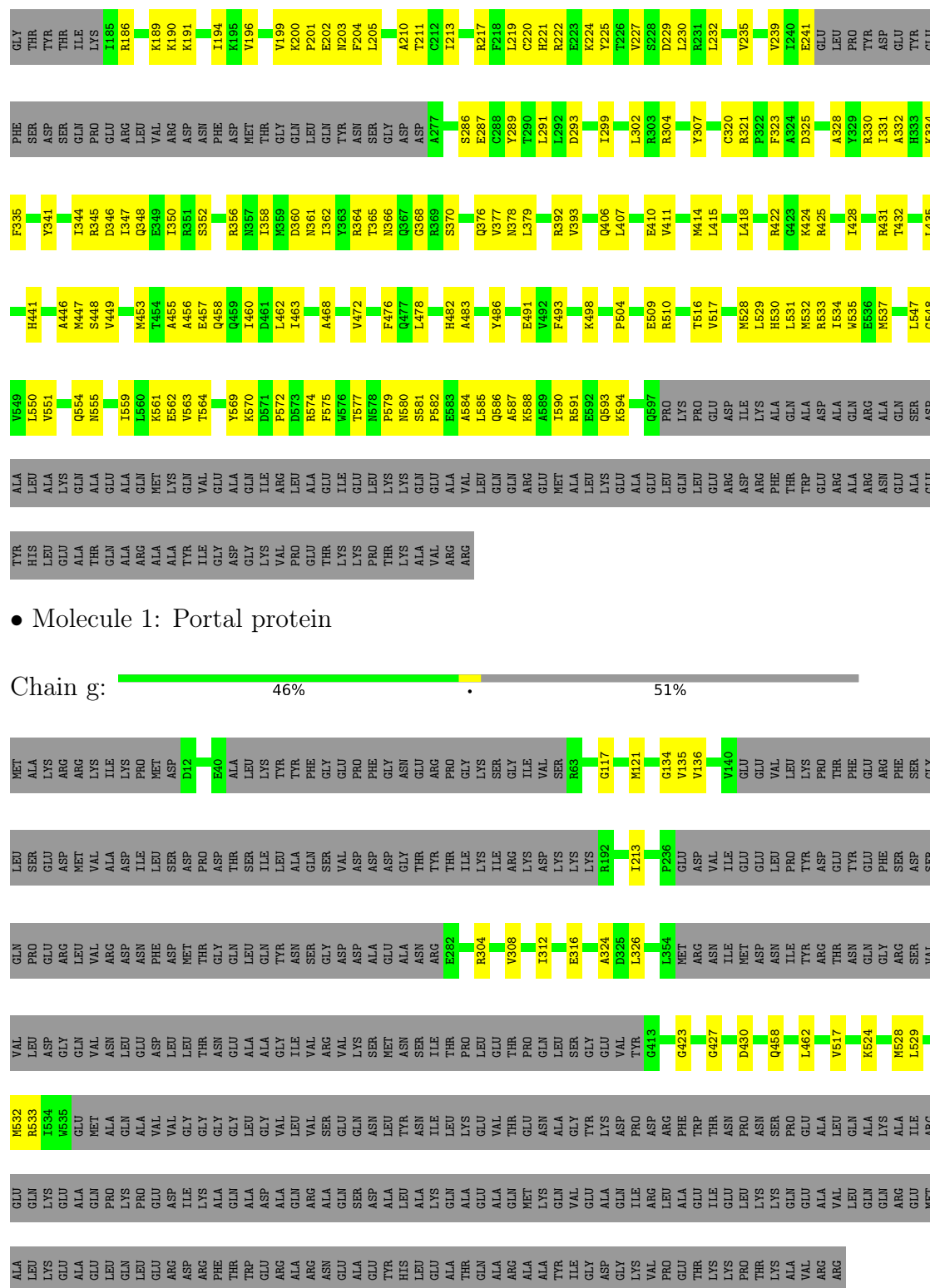
Chain e: 51% 28% 20%



• Molecule 1: Portal protein

Chain f: 45% 29% 27%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28000	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k 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 >5	RMSZ	# Z >5
1	a	0.16	0/4366	0.43	0/5911
1	b	0.15	0/4397	0.41	0/5956
1	c	0.15	0/4450	0.42	0/6025
1	d	0.14	0/4431	0.40	0/6000
1	e	0.13	0/4396	0.40	0/5951
1	f	0.13	0/4148	0.41	0/5607
1	g	0.09	0/1718	0.31	0/2387
1	h	0.14	0/4169	0.41	0/5657
1	i	0.13	0/4394	0.39	1/5950 (0.0%)
1	j	0.27	0/4478	0.51	0/6065
1	k	0.14	0/4418	0.42	0/5981
1	l	0.15	0/4354	0.44	0/5893
All	All	0.16	0/49719	0.42	1/67383 (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	2
1	b	0	1
1	c	0	2
1	d	0	2
1	e	0	2
1	f	0	1
1	i	0	2
1	j	0	2
1	k	0	3
1	l	0	3
All	All	0	20

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	i	294	VAL	N-CA-C	-5.27	107.26	113.42

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a	112	MET	Peptide
1	a	448	SER	Peptide
1	b	577	THR	Peptide
1	c	448	SER	Peptide
1	c	518	GLY	Peptide
1	d	448	SER	Peptide
1	d	518	GLY	Peptide
1	e	448	SER	Peptide
1	e	519	ILE	Peptide
1	f	448	SER	Peptide
1	i	448	SER	Peptide
1	i	518	GLY	Peptide
1	j	518	GLY	Peptide
1	j	571	ASP	Peptide
1	k	448	SER	Peptide
1	k	518	GLY	Peptide
1	k	599	LYS	Peptide
1	l	448	SER	Peptide
1	l	518	GLY	Peptide
1	l	600	PRO	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	4293	0	4062	157	0
1	b	4325	0	4062	138	0
1	c	4377	0	4150	179	0
1	d	4358	0	4102	174	0
1	e	4323	0	4087	172	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	f	4077	0	3930	165	0
1	g	1723	0	758	15	0
1	h	4108	0	3742	151	0
1	i	4322	0	4067	187	0
1	j	4405	0	4127	161	0
1	k	4345	0	4112	165	0
1	l	4281	0	4060	160	0
All	All	48937	0	45259	1589	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 17.

All (1589) 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:c:446:ALA:O	1:c:449:VAL:HA	1.64	0.98
1:c:139:TYR:HB2	1:c:195:LYS:HE3	1.50	0.93
1:e:587:ALA:HA	1:e:591:ARG:HB2	1.57	0.86
1:b:496:ARG:HH22	1:c:92:ASP:HB3	1.40	0.86
1:a:569:TYR:HB2	1:a:574:ARG:HH21	1.39	0.85
1:l:558:ASN:HB2	1:k:574:ARG:HH22	1.43	0.84
1:k:535:TRP:HE1	1:k:563:VAL:HG21	1.43	0.83
1:i:331:ILE:HD11	1:i:338:MET:H	1.44	0.82
1:b:484:ILE:HG23	1:b:485:LYS:HG2	1.62	0.82
1:a:121:MET:HA	1:a:124:TRP:HD1	1.43	0.82
1:h:351:ARG:HE	1:h:418:LEU:HB3	1.43	0.81
1:c:557:TYR:HE2	1:c:578:ASN:HB3	1.47	0.80
1:i:484:ILE:HG22	1:i:485:LYS:HG2	1.64	0.80
1:c:574:ARG:HD3	1:c:576:TRP:CE3	2.17	0.79
1:c:143:VAL:HB	1:c:191:LYS:HB3	1.62	0.79
1:h:479:LEU:HG	1:h:510:ARG:HH21	1.45	0.79
1:h:72:ILE:HG23	1:h:76:LEU:HD12	1.64	0.78
1:f:532:MET:HG3	1:f:533:ARG:HG2	1.64	0.78
1:a:143:VAL:HB	1:a:191:LYS:HB3	1.65	0.78
1:a:565:GLU:HA	1:a:570:LYS:HE3	1.64	0.78
1:a:132:LYS:HG2	1:a:339:SER:HB3	1.66	0.78
1:f:38:ARG:HH22	1:f:202:GLU:HA	1.49	0.78
1:e:433:ARG:HA	1:f:456:ALA:HB3	1.66	0.77
1:i:71:TRP:NE1	1:i:432:THR:O	2.17	0.77
1:l:549:VAL:O	1:k:578:ASN:ND2	2.17	0.77
1:j:500:VAL:HG12	1:j:502:VAL:H	1.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:86:VAL:HG13	1:a:87:VAL:HG23	1.67	0.77
1:c:541:VAL:HG22	1:c:550:LEU:HD13	1.67	0.77
1:a:22:LEU:HD21	1:a:218:PHE:HB3	1.67	0.76
1:k:301:GLU:HG2	1:k:302:LEU:H	1.51	0.76
1:e:143:VAL:HB	1:e:191:LYS:HB2	1.67	0.76
1:l:143:VAL:HB	1:l:191:LYS:HB2	1.68	0.76
1:j:617:LEU:HA	1:j:621:ALA:HB3	1.65	0.76
1:d:561:LYS:HE3	1:d:577:THR:HG22	1.67	0.76
1:a:112:MET:HB3	1:a:113:ARG:HG3	1.68	0.76
1:f:140:VAL:HA	1:f:194:ILE:HG12	1.68	0.76
1:l:588:LYS:O	1:l:593:GLN:NE2	2.18	0.75
1:c:500:VAL:HG12	1:c:502:VAL:H	1.52	0.75
1:h:303:ARG:HE	1:h:315:ASN:HB3	1.48	0.75
1:h:484:ILE:HG13	1:h:485:LYS:H	1.52	0.75
1:k:456:ALA:HB3	1:j:433:ARG:HA	1.69	0.74
1:i:424:LYS:HA	1:i:428:ILE:HG12	1.67	0.74
1:a:355:MET:HE2	1:a:415:LEU:HD11	1.68	0.74
1:b:304:ARG:HB3	1:b:318:TRP:HD1	1.51	0.74
1:d:241:GLU:HG2	1:d:283:VAL:HG22	1.70	0.74
1:k:446:ALA:HB3	1:k:449:VAL:HG22	1.68	0.74
1:b:434:GLY:HA2	1:a:437:GLN:HE21	1.51	0.74
1:h:553:GLU:HA	1:h:556:LEU:HB2	1.69	0.74
1:d:138:VAL:HG22	1:d:196:VAL:HG22	1.70	0.73
1:c:577:THR:HG22	1:c:579:PRO:HD3	1.70	0.73
1:d:478:LEU:O	1:d:482:HIS:ND1	2.22	0.72
1:k:484:ILE:HG22	1:k:485:LYS:HG2	1.70	0.72
1:f:476:PHE:HB2	1:f:510:ARG:HH22	1.53	0.72
1:k:64:ASP:OD1	1:k:422:ARG:NH1	2.23	0.72
1:i:38:ARG:NH2	1:i:133:THR:OG1	2.22	0.72
1:d:218:PHE:HA	1:d:290:THR:HG22	1.71	0.72
1:b:93:THR:OG1	1:a:496:ARG:NE	2.22	0.72
1:k:517:VAL:HG13	1:j:78:LYS:HG2	1.71	0.72
1:j:84:GLY:O	1:j:108:ASN:ND2	2.23	0.72
1:c:586:GLN:HB3	1:c:591:ARG:HH12	1.55	0.72
1:c:443:ASN:HD22	1:d:445:ALA:HB3	1.55	0.72
1:d:326:LEU:HD23	1:d:467:PHE:HD1	1.55	0.72
1:f:199:VAL:HG11	1:f:221:HIS:HB3	1.72	0.72
1:k:131:MET:HG2	1:k:201:PRO:HG2	1.71	0.71
1:j:124:TRP:HZ2	1:j:199:VAL:H	1.36	0.71
1:k:603:ILE:O	1:k:607:ALA:N	2.23	0.71
1:i:338:MET:HE1	1:i:343:LYS:HB3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:121:MET:HA	1:e:124:TRP:HD1	1.55	0.71
1:f:361:ASN:HB2	1:f:407:LEU:HD13	1.71	0.71
1:e:109:TYR:HA	1:e:112:MET:HB2	1.71	0.71
1:i:343:LYS:HD3	1:i:425:ARG:HE	1.56	0.71
1:f:107:VAL:HA	1:f:110:LEU:HG	1.73	0.71
1:l:495:LEU:O	1:l:498:LYS:NZ	2.24	0.71
1:l:241:GLU:HG2	1:l:283:VAL:HG22	1.73	0.70
1:e:519:ILE:HG13	1:e:520:GLY:H	1.56	0.70
1:b:417:ARG:NH1	1:a:416:ASP:OD1	2.25	0.70
1:i:86:VAL:HG13	1:i:87:VAL:HG23	1.73	0.70
1:h:550:LEU:HD21	1:g:423:GLY:HA2	1.72	0.70
1:f:320:CYS:SG	1:f:321:ARG:N	2.64	0.70
1:i:330:ARG:HH21	1:i:470:THR:HG23	1.56	0.70
1:d:578:ASN:O	1:d:588:LYS:NZ	2.24	0.70
1:k:135:VAL:HG23	1:k:199:VAL:HG21	1.74	0.70
1:i:128:THR:HB	1:i:328:ALA:HB2	1.73	0.70
1:e:27:LEU:HG	1:e:205:LEU:HD21	1.72	0.70
1:b:110:LEU:HA	1:b:114:LYS:HB3	1.73	0.70
1:j:353:VAL:HG11	1:i:359:MET:HE1	1.74	0.70
1:h:212:CYS:HB3	1:h:215:ASP:HB2	1.74	0.70
1:i:124:TRP:HZ2	1:i:326:LEU:HD23	1.55	0.70
1:b:241:GLU:HG2	1:b:283:VAL:HG22	1.74	0.69
1:j:321:ARG:O	1:j:477:GLN:NE2	2.25	0.69
1:e:98:GLU:O	1:e:102:GLN:NE2	2.24	0.69
1:f:135:VAL:HG22	1:f:325:ASP:HA	1.74	0.69
1:a:429:THR:OG1	1:l:433:ARG:NH1	2.25	0.69
1:e:440:LEU:HD21	1:f:441:HIS:HD1	1.56	0.69
1:a:330:ARG:HH11	1:a:466:MET:HE1	1.56	0.69
1:k:143:VAL:HB	1:k:191:LYS:HB2	1.74	0.69
1:c:62:SER:OG	1:c:351:ARG:NH1	2.25	0.69
1:e:71:TRP:HE1	1:e:433:ARG:HE	1.41	0.69
1:l:515:VAL:HG22	1:l:516:THR:HG23	1.75	0.69
1:i:457:GLU:HB3	1:h:78:LYS:HD2	1.73	0.69
1:d:500:VAL:HG12	1:d:502:VAL:H	1.58	0.69
1:i:590:ILE:HG23	1:i:594:LYS:HD2	1.75	0.69
1:c:343:LYS:O	1:c:425:ARG:NH1	2.26	0.68
1:f:446:ALA:HA	1:f:532:MET:HE1	1.76	0.68
1:i:105:GLU:OE1	1:i:498:LYS:NZ	2.27	0.68
1:c:602:ASP:O	1:c:606:GLN:N	2.23	0.68
1:a:64:ASP:OD2	1:a:422:ARG:NH1	2.26	0.68
1:j:47:GLY:HA3	1:j:63:ARG:HH11	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:110:LEU:HD21	1:c:194:ILE:HD12	1.76	0.68
1:f:446:ALA:O	1:f:449:VAL:HA	1.93	0.68
1:e:222:ARG:HD2	1:e:284:TRP:HE1	1.59	0.68
1:b:517:VAL:HG23	1:b:520:GLY:H	1.59	0.68
1:l:91:PRO:HD3	1:l:100:ALA:HB2	1.76	0.68
1:k:590:ILE:HG13	1:k:591:ARG:HD2	1.75	0.68
1:j:241:GLU:HA	1:j:283:VAL:HG23	1.76	0.67
1:l:478:LEU:O	1:l:482:HIS:ND1	2.25	0.67
1:b:227:VAL:HG21	1:b:281:ARG:HD3	1.77	0.67
1:b:478:LEU:O	1:b:482:HIS:ND1	2.19	0.67
1:l:500:VAL:HG12	1:l:502:VAL:H	1.59	0.67
1:j:495:LEU:O	1:j:498:LYS:NZ	2.26	0.67
1:d:443:ASN:ND2	1:d:447:MET:SD	2.67	0.67
1:b:575:PHE:HB2	1:c:551:VAL:HA	1.75	0.67
1:b:433:ARG:O	1:a:437:GLN:NE2	2.27	0.67
1:j:350:ILE:HD11	1:i:60:ILE:HG21	1.76	0.67
1:d:205:LEU:HD11	1:d:222:ARG:HE	1.59	0.67
1:b:29:PHE:HB3	1:b:208:ARG:HH21	1.59	0.67
1:k:500:VAL:HG12	1:k:502:VAL:H	1.59	0.67
1:d:496:ARG:HG3	1:e:94:ALA:HB2	1.75	0.67
1:f:35:SER:HA	1:f:38:ARG:HE	1.59	0.66
1:k:446:ALA:O	1:k:449:VAL:HA	1.95	0.66
1:i:549:VAL:HG13	1:i:550:LEU:HG	1.76	0.66
1:c:524:LYS:HE2	1:d:449:VAL:HB	1.76	0.66
1:a:92:ASP:HB3	1:l:496:ARG:HE	1.59	0.66
1:k:590:ILE:HA	1:k:594:LYS:HB2	1.76	0.66
1:j:450:ASN:OD1	1:j:524:LYS:NZ	2.28	0.66
1:d:110:LEU:HA	1:d:114:LYS:HD3	1.78	0.66
1:k:86:VAL:HG12	1:k:87:VAL:HG23	1.78	0.66
1:j:458:GLN:HB3	1:j:460:ILE:HG12	1.78	0.66
1:i:479:LEU:HA	1:i:482:HIS:CD2	2.30	0.66
1:b:524:LYS:HE3	1:c:453:MET:HG3	1.78	0.66
1:e:527:GLN:HG3	1:e:531:LEU:HD12	1.78	0.66
1:l:213:ILE:HD12	1:l:325:ASP:HB2	1.77	0.66
1:i:360:ASP:O	1:i:363:TYR:HB3	1.96	0.66
1:i:456:ALA:HB3	1:h:433:ARG:HG2	1.77	0.66
1:a:84:GLY:O	1:a:108:ASN:ND2	2.29	0.65
1:h:534:ILE:HG12	1:h:559:ILE:HD11	1.77	0.65
1:c:420:ALA:O	1:c:424:LYS:N	2.29	0.65
1:d:588:LYS:HG2	1:e:549:VAL:HA	1.78	0.65
1:i:330:ARG:HH22	1:i:469:GLU:HB2	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:574:ARG:HA	1:c:555:ASN:HB3	1.78	0.65
1:f:574:ARG:NH1	1:g:524:LYS:O	2.28	0.65
1:f:581:SER:O	1:f:585:LEU:N	2.25	0.65
1:l:86:VAL:HG12	1:l:87:VAL:HG23	1.77	0.65
1:j:95:GLU:H	1:i:496:ARG:NH2	1.94	0.65
1:i:241:GLU:HG2	1:i:283:VAL:HG22	1.77	0.65
1:i:569:TYR:HB2	1:i:574:ARG:HH21	1.60	0.65
1:h:425:ARG:NH1	1:f:392:ARG:O	2.30	0.65
1:c:138:VAL:HG22	1:c:196:VAL:HG22	1.78	0.65
1:c:332:ALA:O	1:c:334:LYS:N	2.29	0.65
1:d:574:ARG:HB3	1:d:576:TRP:CD1	2.31	0.65
1:f:41:ALA:HB2	1:f:345:ARG:HH21	1.62	0.65
1:f:584:ALA:O	1:f:588:LYS:N	2.29	0.65
1:l:19:LEU:HD11	1:l:307:TYR:CE2	2.32	0.65
1:i:428:ILE:HB	1:h:433:ARG:HD2	1.79	0.65
1:b:105:GLU:O	1:b:109:TYR:N	2.28	0.64
1:a:472:VAL:O	1:a:510:ARG:NH2	2.29	0.64
1:j:476:PHE:HA	1:j:510:ARG:HH22	1.61	0.64
1:e:86:VAL:HG23	1:e:515:VAL:HG11	1.77	0.64
1:e:412:TYR:HA	1:e:415:LEU:HD23	1.79	0.64
1:l:332:ALA:O	1:l:334:LYS:N	2.30	0.64
1:c:632:ILE:HA	1:d:630:ALA:HB2	1.79	0.64
1:e:433:ARG:HD2	1:f:428:ILE:HG21	1.77	0.64
1:a:488:ASN:HA	1:a:500:VAL:HG23	1.80	0.64
1:k:490:GLU:HG2	1:k:498:LYS:HB2	1.80	0.64
1:k:554:GLN:NE2	1:k:578:ASN:O	2.30	0.64
1:h:221:HIS:O	1:h:286:SER:HA	1.98	0.64
1:h:493:PHE:O	1:h:498:LYS:NZ	2.31	0.64
1:l:138:VAL:HG22	1:l:196:VAL:HG12	1.80	0.64
1:k:189:LYS:HG2	1:k:190:LYS:H	1.62	0.64
1:i:561:LYS:HE2	1:i:577:THR:HG22	1.79	0.64
1:h:143:VAL:HB	1:h:191:LYS:HB2	1.80	0.64
1:c:364:ARG:HH12	1:c:405:PRO:HD2	1.63	0.64
1:e:344:ILE:HG13	1:e:347:ILE:HD12	1.79	0.64
1:f:572:PRO:HA	1:f:575:PHE:HE1	1.61	0.64
1:a:332:ALA:O	1:a:334:LYS:N	2.31	0.64
1:j:113:ARG:HH22	1:j:492:VAL:HB	1.61	0.64
1:h:356:ARG:O	1:h:360:ASP:N	2.28	0.64
1:d:491:GLU:HG2	1:d:498:LYS:HG2	1.79	0.64
1:j:420:ALA:HB1	1:i:431:ARG:HG3	1.79	0.64
1:i:212:CYS:SG	1:i:213:ILE:N	2.70	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:364:ARG:NH2	1:h:404:THR:OG1	2.29	0.64
1:f:143:VAL:HB	1:f:191:LYS:HB2	1.80	0.64
1:b:444:GLN:NE2	1:a:441:HIS:O	2.30	0.63
1:j:71:TRP:NE1	1:j:432:THR:OG1	2.31	0.63
1:j:478:LEU:HG	1:j:482:HIS:CE1	2.33	0.63
1:d:556:LEU:O	1:d:560:LEU:HG	1.97	0.63
1:e:135:VAL:HG22	1:e:325:ASP:HA	1.80	0.63
1:l:441:HIS:NE2	1:k:437:GLN:O	2.26	0.63
1:k:45:TYR:O	1:k:66:GLN:NE2	2.26	0.63
1:e:108:ASN:O	1:e:112:MET:N	2.31	0.63
1:e:213:ILE:O	1:e:321:ARG:NH1	2.30	0.63
1:j:27:LEU:HB2	1:j:205:LEU:HD21	1.80	0.63
1:j:329:TYR:HD2	1:j:338:MET:HG3	1.62	0.63
1:i:124:TRP:CZ3	1:i:136:VAL:HG23	2.33	0.63
1:f:98:GLU:HG2	1:f:99:GLN:HG3	1.78	0.63
1:l:484:ILE:HG22	1:l:485:LYS:HG2	1.79	0.63
1:l:549:VAL:HB	1:k:588:LYS:HB3	1.80	0.63
1:k:332:ALA:O	1:k:334:LYS:N	2.31	0.63
1:l:456:ALA:HB2	1:k:433:ARG:HB3	1.80	0.63
1:k:81:THR:HG21	1:k:118:PHE:HD1	1.62	0.63
1:c:557:TYR:HE1	1:d:550:LEU:HD23	1.63	0.63
1:f:591:ARG:NH2	1:g:517:VAL:O	2.32	0.63
1:a:307:TYR:HA	1:a:313:ILE:HD12	1.80	0.63
1:c:139:TYR:OH	1:c:287:GLU:OE2	2.17	0.63
1:d:332:ALA:O	1:d:334:LYS:N	2.30	0.63
1:i:124:TRP:CZ2	1:i:326:LEU:HD23	2.34	0.63
1:i:472:VAL:O	1:i:510:ARG:NH2	2.32	0.63
1:d:351:ARG:HG2	1:d:418:LEU:HD23	1.81	0.63
1:c:466:MET:HE2	1:c:466:MET:HA	1.81	0.62
1:e:487:GLN:HB3	1:e:489:GLN:HG2	1.80	0.62
1:f:205:LEU:HB3	1:f:220:CYS:HB2	1.81	0.62
1:f:577:THR:HG22	1:f:579:PRO:HD3	1.81	0.62
1:a:124:TRP:CH2	1:a:136:VAL:HA	2.33	0.62
1:j:478:LEU:HG	1:j:482:HIS:HE1	1.64	0.62
1:b:597:GLN:HG2	1:b:598:PRO:HD3	1.81	0.62
1:a:227:VAL:HB	1:a:280:ASN:HA	1.81	0.62
1:h:216:ALA:O	1:h:321:ARG:NH2	2.33	0.62
1:e:189:LYS:HA	1:e:191:LYS:HE2	1.81	0.62
1:j:549:VAL:HA	1:i:587:ALA:HB1	1.80	0.62
1:l:278:GLU:O	1:l:281:ARG:NH1	2.32	0.62
1:e:60:ILE:HD13	1:f:350:ILE:HG22	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:107:VAL:HG13	1:j:478:LEU:HD23	1.82	0.62
1:j:350:ILE:HD11	1:i:60:ILE:HD13	1.81	0.62
1:h:211:THR:HA	1:h:335:PHE:HA	1.80	0.62
1:j:91:PRO:HG3	1:j:507:TRP:HZ3	1.64	0.62
1:i:143:VAL:O	1:i:190:LYS:N	2.33	0.62
1:d:113:ARG:NH2	1:e:90:GLU:OE1	2.32	0.62
1:f:116:GLU:HG3	1:f:119:LYS:HB2	1.82	0.62
1:k:98:GLU:HG2	1:k:99:GLN:HG2	1.80	0.62
1:d:574:ARG:HB3	1:d:576:TRP:HD1	1.64	0.62
1:e:45:TYR:HE2	1:f:331:ILE:HD11	1.64	0.62
1:l:327:ASN:HD21	1:l:330:ARG:HD2	1.65	0.62
1:h:344:ILE:HG22	1:h:348:GLN:HB2	1.82	0.62
1:e:431:ARG:NH1	1:e:433:ARG:O	2.32	0.62
1:b:321:ARG:O	1:b:477:GLN:NE2	2.33	0.61
1:k:41:ALA:HA	1:k:341:TYR:CE1	2.35	0.61
1:a:594:LYS:HD2	1:a:598:PRO:HG2	1.81	0.61
1:c:60:ILE:O	1:c:356:ARG:NH2	2.34	0.61
1:c:565:GLU:HG2	1:c:570:LYS:HG3	1.81	0.61
1:l:212:CYS:SG	1:l:213:ILE:N	2.74	0.61
1:h:63:ARG:HB3	1:h:66:GLN:HB2	1.80	0.61
1:c:621:ALA:HB1	1:d:618:ALA:HB3	1.83	0.61
1:a:435:LEU:O	1:l:437:GLN:NE2	2.25	0.61
1:l:217:ARG:NH2	1:k:282:GLU:OE2	2.32	0.61
1:i:330:ARG:NH2	1:i:466:MET:O	2.33	0.61
1:h:138:VAL:HB	1:h:322:PRO:HB2	1.82	0.61
1:f:62:SER:HB3	1:f:352:SER:HB3	1.83	0.61
1:f:554:GLN:OE1	1:f:580:ASN:ND2	2.33	0.61
1:b:465:ARG:NH1	1:b:469:GLU:OE2	2.33	0.61
1:k:347:ILE:HD11	1:k:425:ARG:HD2	1.83	0.61
1:j:478:LEU:O	1:j:482:HIS:ND1	2.32	0.61
1:c:438:ASN:HD21	1:d:439:THR:HB	1.66	0.61
1:a:225:TYR:HB3	1:a:230:LEU:HD21	1.81	0.61
1:k:459:GLN:H	1:j:433:ARG:NH2	1.98	0.61
1:f:341:TYR:O	1:f:345:ARG:HG3	2.00	0.61
1:h:290:THR:HB	1:h:292:LEU:HD13	1.83	0.61
1:h:557:TYR:HA	1:h:576:TRP:HB3	1.82	0.61
1:b:458:GLN:HG2	1:a:433:ARG:HD3	1.83	0.60
1:a:120:VAL:HG12	1:a:124:TRP:HE1	1.66	0.60
1:d:484:ILE:HG22	1:d:485:LYS:HG2	1.83	0.60
1:j:138:VAL:HG22	1:j:196:VAL:HG22	1.81	0.60
1:j:217:ARG:NH1	1:j:291:LEU:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:462:LEU:HD23	1:i:517:VAL:HG11	1.83	0.60
1:e:591:ARG:NH2	1:f:548:GLY:O	2.33	0.60
1:f:124:TRP:CE2	1:f:136:VAL:HG22	2.36	0.60
1:d:29:PHE:HB3	1:d:208:ARG:HH21	1.66	0.60
1:e:496:ARG:NE	1:f:94:ALA:H	2.00	0.60
1:j:411:VAL:O	1:j:414:MET:HB3	2.01	0.60
1:c:228:SER:HB2	1:d:299:ILE:HG21	1.83	0.60
1:c:554:GLN:NE2	1:c:579:PRO:O	2.35	0.60
1:e:239:VAL:HG22	1:e:240:ILE:H	1.66	0.60
1:l:465:ARG:HH12	1:l:513:LEU:HD12	1.66	0.60
1:i:344:ILE:HD11	1:i:425:ARG:HG2	1.83	0.60
1:d:527:GLN:HB2	1:e:533:ARG:HH22	1.67	0.60
1:b:115:ASN:HD22	1:b:195:LYS:HA	1.66	0.60
1:l:308:VAL:HG23	1:l:309:GLY:H	1.67	0.60
1:k:230:LEU:HD11	1:k:308:VAL:HG11	1.82	0.60
1:d:341:TYR:HB3	1:d:345:ARG:HH21	1.66	0.60
1:k:526:GLN:O	1:k:530:HIS:ND1	2.30	0.60
1:c:205:LEU:HB2	1:c:220:CYS:HB2	1.84	0.60
1:c:364:ARG:NH2	1:c:405:PRO:O	2.35	0.60
1:c:414:MET:O	1:c:418:LEU:N	2.32	0.60
1:d:295:ASP:OD1	1:d:303:ARG:NH2	2.34	0.60
1:k:490:GLU:OE2	1:k:497:GLY:N	2.35	0.60
1:k:132:LYS:HG2	1:k:339:SER:HB3	1.84	0.59
1:i:465:ARG:NH1	1:i:512:ASP:O	2.28	0.59
1:i:551:VAL:HB	1:h:575:PHE:HD1	1.66	0.59
1:d:429:THR:HB	1:d:432:THR:HG22	1.84	0.59
1:i:289:TYR:HB3	1:i:302:LEU:HD11	1.83	0.59
1:f:201:PRO:HA	1:f:204:PHE:CD1	2.37	0.59
1:a:557:TYR:HB2	1:a:576:TRP:HB2	1.85	0.59
1:h:13:GLU:HA	1:h:16:LEU:HD13	1.83	0.59
1:b:143:VAL:O	1:b:190:LYS:HA	2.03	0.59
1:f:476:PHE:HB2	1:f:510:ARG:NH2	2.17	0.59
1:a:522:MET:SD	1:a:522:MET:N	2.75	0.59
1:e:341:TYR:HB3	1:e:345:ARG:HH12	1.66	0.59
1:g:117:GLY:O	1:g:121:MET:N	2.31	0.59
1:h:125:PHE:HA	1:h:128:THR:HG22	1.83	0.59
1:c:592:GLU:HA	1:c:595:GLU:HG2	1.83	0.59
1:e:77:MET:HE3	1:e:77:MET:HA	1.85	0.59
1:l:595:GLU:HA	1:l:599:LYS:HB2	1.84	0.59
1:f:453:MET:O	1:f:456:ALA:N	2.35	0.59
1:d:493:PHE:HB3	1:d:498:LYS:HE2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:64:ASP:OD1	1:h:422:ARG:NH1	2.36	0.59
1:h:89:TYR:HE2	1:h:103:GLU:HB2	1.68	0.59
1:c:515:VAL:HG13	1:c:516:THR:HG23	1.84	0.59
1:d:27:LEU:HD11	1:d:205:LEU:HD13	1.84	0.59
1:l:43:LYS:HG3	1:l:48:GLU:HB2	1.84	0.58
1:k:424:LYS:HA	1:k:428:ILE:HG12	1.85	0.58
1:j:476:PHE:N	1:j:510:ARG:HH12	2.00	0.58
1:i:562:GLU:O	1:i:565:GLU:HG3	2.02	0.58
1:a:476:PHE:HD1	1:a:510:ARG:HH12	1.50	0.58
1:l:93:THR:HG22	1:k:492:VAL:HG13	1.84	0.58
1:i:38:ARG:HD3	1:i:131:MET:HE3	1.86	0.58
1:i:574:ARG:HB3	1:i:576:TRP:CD1	2.38	0.58
1:h:91:PRO:HB3	1:h:100:ALA:HB2	1.83	0.58
1:c:143:VAL:O	1:c:190:LYS:N	2.37	0.58
1:c:221:HIS:ND1	1:c:223:GLU:OE2	2.36	0.58
1:b:119:LYS:HB2	1:c:330:ARG:HH21	1.68	0.58
1:a:555:ASN:O	1:a:558:ASN:HB2	2.03	0.58
1:c:495:LEU:O	1:c:498:LYS:NZ	2.37	0.58
1:d:97:VAL:HA	1:d:101:GLU:HB2	1.84	0.58
1:d:581:SER:H	1:d:584:ALA:HB3	1.69	0.58
1:i:137:LYS:NZ	1:i:223:GLU:OE2	2.32	0.58
1:d:527:GLN:OE1	1:e:533:ARG:NH1	2.36	0.58
1:a:138:VAL:HG22	1:a:196:VAL:HG22	1.85	0.58
1:l:555:ASN:HD21	1:k:575:PHE:HB2	1.69	0.58
1:d:495:LEU:O	1:d:498:LYS:NZ	2.36	0.58
1:c:361:ASN:HD22	1:c:407:LEU:HG	1.68	0.58
1:l:574:ARG:HB3	1:l:576:TRP:CE3	2.39	0.58
1:k:137:LYS:NZ	1:k:287:GLU:OE2	2.37	0.58
1:h:195:LYS:HB3	1:h:197:LEU:HD23	1.86	0.58
1:k:91:PRO:HG3	1:k:100:ALA:HB2	1.85	0.58
1:j:593:GLN:O	1:j:597:GLN:N	2.26	0.58
1:i:212:CYS:HB3	1:i:215:ASP:HB2	1.85	0.58
1:i:535:TRP:CH2	1:i:556:LEU:HD22	2.38	0.58
1:h:221:HIS:HB3	1:h:287:GLU:HG3	1.85	0.57
1:d:514:THR:HA	1:d:520:GLY:HA2	1.86	0.57
1:e:408:SER:OG	1:e:410:GLU:OE1	2.18	0.57
1:e:286:SER:HB2	1:e:307:TYR:HB3	1.86	0.57
1:a:452:LEU:HD13	1:l:434:GLY:HA3	1.87	0.57
1:l:88:LYS:HA	1:l:104:THR:HG21	1.86	0.57
1:h:490:GLU:HB2	1:h:498:LYS:H	1.69	0.57
1:i:515:VAL:HG12	1:i:516:THR:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:447:MET:HG2	1:h:532:MET:HE1	1.84	0.57
1:c:446:ALA:HB3	1:c:449:VAL:HG22	1.87	0.57
1:d:487:GLN:HG3	1:d:488:ASN:H	1.69	0.57
1:l:135:VAL:HB	1:l:199:VAL:HG21	1.85	0.57
1:i:300:SER:OG	1:i:303:ARG:NH1	2.37	0.57
1:f:446:ALA:HB1	1:f:449:VAL:HG13	1.86	0.57
1:b:40:GLU:OE1	1:b:341:TYR:OH	2.19	0.57
1:b:81:THR:HG23	1:b:118:PHE:CE2	2.38	0.57
1:b:428:ILE:HD13	1:a:431:ARG:HG3	1.85	0.57
1:b:446:ALA:N	1:b:532:MET:HE1	2.19	0.57
1:a:568:GLY:HA2	1:a:570:LYS:HZ2	1.70	0.57
1:i:541:VAL:HG21	1:h:576:TRP:HZ2	1.68	0.57
1:h:487:GLN:HE22	1:h:489:GLN:HG3	1.69	0.57
1:c:91:PRO:HB3	1:c:507:TRP:HZ3	1.69	0.57
1:f:530:HIS:HA	1:f:534:ILE:HD13	1.86	0.57
1:h:560:LEU:O	1:h:574:ARG:NH1	2.37	0.57
1:c:45:TYR:CE1	1:c:66:GLN:HG2	2.40	0.57
1:c:110:LEU:O	1:c:114:LYS:HB3	2.05	0.57
1:h:452:LEU:HA	1:f:366:ASN:HB3	1.86	0.57
1:e:553:GLU:HA	1:e:556:LEU:HB2	1.87	0.57
1:f:116:GLU:HB3	1:f:120:VAL:HG13	1.86	0.57
1:a:569:TYR:HB2	1:a:574:ARG:NH2	2.15	0.57
1:l:22:LEU:HD22	1:l:218:PHE:CD2	2.40	0.57
1:c:60:ILE:HD11	1:c:359:MET:SD	2.45	0.57
1:e:460:ILE:HA	1:e:463:ILE:HD12	1.86	0.57
1:j:479:LEU:HA	1:j:482:HIS:HD1	1.68	0.57
1:c:124:TRP:HZ2	1:c:136:VAL:HG12	1.70	0.57
1:c:213:ILE:HG12	1:c:325:ASP:HB2	1.87	0.57
1:d:560:LEU:HD22	1:e:537:MET:HE1	1.87	0.57
1:e:332:ALA:O	1:e:334:LYS:N	2.37	0.57
1:e:45:TYR:HB2	1:e:341:TYR:OH	2.05	0.56
1:a:239:VAL:HG12	1:a:240:ILE:H	1.70	0.56
1:k:192:ARG:H	1:k:487:GLN:HE21	1.52	0.56
1:k:557:TYR:HA	1:k:560:LEU:HD12	1.87	0.56
1:j:33:GLU:OE1	1:j:208:ARG:NH1	2.38	0.56
1:e:327:ASN:HD21	1:e:331:ILE:HG22	1.70	0.56
1:f:446:ALA:HB3	1:f:449:VAL:HG22	1.87	0.56
1:b:555:ASN:H	1:a:575:PHE:HE2	1.51	0.56
1:l:34:LEU:HD12	1:l:132:LYS:HE2	1.87	0.56
1:k:359:MET:HE3	1:k:359:MET:HA	1.87	0.56
1:h:516:THR:O	1:h:520:GLY:HA3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:144:LEU:HD23	1:d:190:LYS:H	1.70	0.56
1:e:200:LYS:O	1:e:203:ASN:N	2.37	0.56
1:e:463:ILE:HA	1:e:466:MET:SD	2.44	0.56
1:f:229:ASP:HA	1:f:232:LEU:HD12	1.87	0.56
1:b:557:TYR:OH	1:c:549:VAL:O	2.22	0.56
1:i:226:THR:OG1	1:i:280:ASN:OD1	2.15	0.56
1:e:121:MET:HA	1:e:124:TRP:CD1	2.39	0.56
1:f:304:ARG:NH2	1:f:320:CYS:O	2.36	0.56
1:j:302:LEU:HD11	1:j:321:ARG:HE	1.70	0.56
1:i:550:LEU:HB3	1:h:575:PHE:HB3	1.88	0.56
1:h:69:VAL:O	1:h:73:MET:HG2	2.04	0.56
1:d:433:ARG:NH1	1:e:456:ALA:O	2.38	0.56
1:b:517:VAL:O	1:a:78:LYS:NZ	2.35	0.56
1:j:561:LYS:HZ2	1:j:577:THR:HG23	1.69	0.56
1:e:431:ARG:HG3	1:e:433:ARG:HB2	1.87	0.56
1:h:338:MET:HE3	1:h:338:MET:HA	1.87	0.56
1:f:10:MET:HE3	1:f:10:MET:HA	1.88	0.56
1:b:82:SER:HB2	1:c:519:ILE:HG13	1.87	0.56
1:a:146:PRO:HG3	1:a:189:LYS:HE2	1.86	0.56
1:k:351:ARG:HG2	1:k:418:LEU:HD23	1.88	0.56
1:l:476:PHE:O	1:l:480:HIS:ND1	2.37	0.56
1:h:39:SER:O	1:h:43:LYS:HG2	2.06	0.56
1:e:578:ASN:O	1:e:588:LYS:NZ	2.30	0.56
1:a:121:MET:HA	1:a:124:TRP:CD1	2.33	0.56
1:a:200:LYS:O	1:a:202:GLU:N	2.38	0.56
1:a:491:GLU:HB2	1:a:498:LYS:HG3	1.88	0.55
1:j:555:ASN:OD1	1:j:558:ASN:ND2	2.39	0.55
1:c:590:ILE:HB	1:c:591:ARG:NH1	2.21	0.55
1:h:227:VAL:HB	1:h:280:ASN:HA	1.87	0.55
1:c:590:ILE:HB	1:c:591:ARG:HH11	1.71	0.55
1:d:67:GLU:OE2	1:d:422:ARG:NH1	2.39	0.55
1:f:50:PHE:HB2	1:f:356:ARG:HH12	1.70	0.55
1:k:26:ALA:O	1:k:30:ASN:ND2	2.30	0.55
1:j:379:LEU:HA	1:i:398:SER:HA	1.88	0.55
1:h:556:LEU:HA	1:h:559:ILE:HG22	1.89	0.55
1:h:577:THR:HG23	1:h:578:ASN:H	1.71	0.55
1:d:446:ALA:O	1:d:449:VAL:HA	2.06	0.55
1:f:224:LYS:HD2	1:f:225:TYR:N	2.21	0.55
1:l:472:VAL:HG11	1:l:510:ARG:HE	1.72	0.55
1:d:366:ASN:ND2	1:e:407:LEU:HD11	2.21	0.55
1:l:474:ARG:HA	1:l:477:GLN:HE21	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:69:VAL:HG21	1:k:130:MET:HE3	1.89	0.55
1:j:13:GLU:HA	1:j:16:LEU:HD12	1.87	0.55
1:d:106:TYR:OH	1:d:489:GLN:OE1	2.24	0.55
1:k:578:ASN:OD1	1:k:581:SER:OG	2.20	0.55
1:j:465:ARG:HH12	1:j:513:LEU:HD23	1.71	0.55
1:h:475:LEU:HB3	1:h:510:ARG:CZ	2.36	0.55
1:e:513:LEU:HG	1:e:519:ILE:HG12	1.88	0.55
1:f:45:TYR:O	1:f:63:ARG:NH1	2.40	0.55
1:b:92:ASP:HA	1:a:492:VAL:HG23	1.88	0.55
1:a:555:ASN:HB2	1:l:575:PHE:CE1	2.42	0.55
1:h:102:GLN:NE2	1:h:491:GLU:OE2	2.39	0.55
1:d:132:LYS:HG2	1:d:339:SER:HB3	1.88	0.55
1:e:576:TRP:HE1	1:f:551:VAL:HB	1.71	0.55
1:h:68:THR:O	1:h:72:ILE:HD12	2.06	0.55
1:d:139:TYR:HB3	1:d:195:LYS:HE3	1.88	0.55
1:b:30:ASN:HD21	1:b:208:ARG:HG2	1.70	0.54
1:b:370:SER:HA	1:b:392:ARG:HA	1.88	0.54
1:i:465:ARG:NE	1:i:469:GLU:OE2	2.41	0.54
1:c:481:ASP:HB3	1:c:486:TYR:OH	2.07	0.54
1:i:357:ASN:OD1	1:i:361:ASN:ND2	2.29	0.54
1:c:588:LYS:HA	1:c:592:GLU:HB3	1.89	0.54
1:d:60:ILE:HG12	1:e:350:ILE:HD11	1.88	0.54
1:a:590:ILE:HG13	1:a:591:ARG:HG3	1.89	0.54
1:i:19:LEU:HB3	1:i:307:TYR:OH	2.08	0.54
1:c:235:VAL:HG12	1:c:312:ILE:HD12	1.90	0.54
1:d:45:TYR:O	1:d:66:GLN:NE2	2.41	0.54
1:d:460:ILE:HA	1:d:463:ILE:HD12	1.88	0.54
1:b:304:ARG:HB3	1:b:318:TRP:CD1	2.38	0.54
1:h:351:ARG:NH2	1:h:418:LEU:O	2.40	0.54
1:d:446:ALA:HB3	1:d:449:VAL:HG22	1.89	0.54
1:e:97:VAL:HA	1:e:101:GLU:HB2	1.88	0.54
1:a:120:VAL:HG12	1:a:124:TRP:NE1	2.21	0.54
1:l:200:LYS:O	1:l:202:GLU:N	2.40	0.54
1:k:194:ILE:HG13	1:k:486:TYR:CZ	2.43	0.54
1:j:140:VAL:HG12	1:j:194:ILE:HG22	1.89	0.54
1:i:192:ARG:HE	1:i:485:LYS:HD3	1.73	0.54
1:i:490:GLU:HB2	1:i:498:LYS:H	1.73	0.54
1:h:456:ALA:HB2	1:f:368:GLY:H	1.73	0.54
1:h:491:GLU:HB2	1:h:498:LYS:HD3	1.88	0.54
1:e:573:ASP:O	1:f:555:ASN:ND2	2.33	0.54
1:k:13:GLU:O	1:k:17:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:547:LEU:N	1:j:591:ARG:HH12	2.06	0.54
1:j:436:ASP:HB2	1:j:440:LEU:HD23	1.89	0.54
1:i:338:MET:HE2	1:i:342:ASP:HB2	1.90	0.54
1:h:351:ARG:HG3	1:h:418:LEU:HD13	1.88	0.54
1:c:96:ASP:O	1:c:100:ALA:N	2.35	0.54
1:e:63:ARG:HH22	1:f:346:ASP:HB2	1.73	0.54
1:b:575:PHE:CZ	1:c:554:GLN:HB2	2.42	0.54
1:k:491:GLU:H	1:k:498:LYS:HD3	1.72	0.54
1:j:332:ALA:O	1:j:334:LYS:N	2.40	0.54
1:b:131:MET:HE3	1:b:131:MET:HA	1.90	0.54
1:i:292:LEU:O	1:i:300:SER:OG	2.25	0.54
1:i:500:VAL:HG12	1:i:502:VAL:H	1.73	0.54
1:i:205:LEU:HB2	1:i:220:CYS:HB3	1.90	0.54
1:e:446:ALA:HB3	1:e:449:VAL:HG22	1.90	0.54
1:b:293:ASP:HA	1:b:300:SER:HB3	1.89	0.54
1:a:568:GLY:HA2	1:a:570:LYS:NZ	2.23	0.54
1:l:31:SER:O	1:l:35:SER:HB3	2.08	0.54
1:b:290:THR:O	1:b:302:LEU:HA	2.07	0.53
1:b:453:MET:HE3	1:b:453:MET:HA	1.90	0.53
1:l:102:GLN:HB3	1:l:499:TRP:HE1	1.73	0.53
1:l:222:ARG:HB3	1:l:284:TRP:HE1	1.73	0.53
1:k:551:VAL:HG11	1:k:555:ASN:HD22	1.73	0.53
1:e:135:VAL:HB	1:e:199:VAL:HG11	1.88	0.53
1:f:19:LEU:O	1:f:23:VAL:HG23	2.08	0.53
1:b:496:ARG:NH2	1:c:94:ALA:H	2.05	0.53
1:l:490:GLU:OE2	1:l:497:GLY:N	2.39	0.53
1:j:590:ILE:HA	1:j:594:LYS:HB3	1.90	0.53
1:i:436:ASP:OD2	1:i:441:HIS:NE2	2.41	0.53
1:c:488:ASN:HA	1:c:500:VAL:HA	1.90	0.53
1:f:105:GLU:HB3	1:f:493:PHE:CD2	2.44	0.53
1:f:128:THR:HB	1:f:328:ALA:HB2	1.90	0.53
1:a:562:GLU:HA	1:a:565:GLU:HG2	1.89	0.53
1:j:557:TYR:CZ	1:j:578:ASN:HB2	2.42	0.53
1:i:328:ALA:HA	1:i:467:PHE:HE1	1.74	0.53
1:k:138:VAL:HG22	1:k:196:VAL:HG22	1.89	0.53
1:i:430:ASP:H	1:h:435:LEU:HD21	1.74	0.53
1:c:496:ARG:HH22	1:d:95:GLU:CD	2.15	0.53
1:d:376:GLN:O	1:d:378:ASN:N	2.40	0.53
1:f:211:THR:H	1:f:335:PHE:HD1	1.55	0.53
1:h:359:MET:O	1:h:362:ILE:HB	2.08	0.53
1:a:110:LEU:HD22	1:a:482:HIS:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:135:VAL:HG11	1:k:204:PHE:CE2	2.44	0.53
1:h:599:LYS:HB2	1:h:600:PRO:HD3	1.90	0.53
1:d:146:PRO:HG3	1:d:189:LYS:HD2	1.90	0.53
1:e:128:THR:HB	1:e:328:ALA:HB2	1.90	0.53
1:e:140:VAL:HG22	1:e:194:ILE:HG12	1.91	0.53
1:e:210:ALA:H	1:e:335:PHE:HZ	1.55	0.53
1:l:519:ILE:H	1:l:519:ILE:HD12	1.73	0.53
1:k:239:VAL:HG12	1:k:241:GLU:H	1.73	0.53
1:k:560:LEU:HB3	1:k:576:TRP:HB3	1.90	0.53
1:i:189:LYS:HE3	1:i:190:LYS:HB2	1.91	0.53
1:h:419:GLU:HA	1:h:422:ARG:HE	1.74	0.53
1:c:575:PHE:CE2	1:d:554:GLN:HB2	2.44	0.53
1:b:147:THR:H	1:b:187:LYS:HZ2	1.55	0.53
1:a:330:ARG:NH2	1:l:123:ASP:OD2	2.39	0.53
1:a:343:LYS:O	1:a:425:ARG:NH1	2.42	0.53
1:a:586:GLN:O	1:a:590:ILE:HG12	2.09	0.53
1:h:73:MET:HE1	1:h:125:PHE:HB3	1.91	0.53
1:d:530:HIS:HA	1:d:534:ILE:HD13	1.90	0.53
1:b:452:LEU:HD23	1:b:453:MET:HG2	1.91	0.53
1:a:430:ASP:O	1:a:431:ARG:HG2	2.09	0.53
1:j:524:LYS:O	1:j:528:MET:HG2	2.09	0.53
1:i:530:HIS:CE1	1:i:562:GLU:HB3	2.44	0.53
1:d:497:GLY:C	1:d:498:LYS:HD2	2.34	0.53
1:e:531:LEU:HD11	1:e:563:VAL:HG13	1.91	0.53
1:c:200:LYS:O	1:c:202:GLU:N	2.42	0.53
1:c:212:CYS:SG	1:c:213:ILE:N	2.80	0.53
1:c:216:ALA:O	1:c:321:ARG:NH1	2.41	0.53
1:f:447:MET:SD	1:f:528:MET:HB2	2.48	0.53
1:b:534:ILE:HG13	1:a:574:ARG:HH12	1.75	0.52
1:b:537:MET:HE1	1:a:563:VAL:HG11	1.91	0.52
1:l:524:LYS:O	1:l:527:GLN:HG3	2.09	0.52
1:k:191:LYS:HD3	1:k:487:GLN:HE22	1.74	0.52
1:d:228:SER:HB2	1:e:299:ILE:HB	1.91	0.52
1:b:73:MET:HE1	1:b:126:GLN:HA	1.91	0.52
1:a:139:TYR:CE1	1:a:195:LYS:HB2	2.44	0.52
1:l:420:ALA:O	1:l:424:LYS:N	2.42	0.52
1:k:495:LEU:O	1:k:498:LYS:NZ	2.42	0.52
1:h:358:ILE:HD12	1:h:415:LEU:HD12	1.91	0.52
1:c:321:ARG:O	1:c:477:GLN:NE2	2.38	0.52
1:f:91:PRO:HG3	1:f:100:ALA:HB2	1.90	0.52
1:f:199:VAL:HB	1:f:204:PHE:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:488:ASN:HA	1:k:500:VAL:HA	1.90	0.52
1:h:351:ARG:NE	1:h:418:LEU:HB3	2.21	0.52
1:f:186:ARG:O	1:f:186:ARG:HD3	2.09	0.52
1:f:219:LEU:HB3	1:f:289:TYR:HB2	1.91	0.52
1:l:465:ARG:N	1:l:516:THR:HG21	2.24	0.52
1:i:328:ALA:HA	1:i:467:PHE:CE1	2.44	0.52
1:h:484:ILE:HG13	1:h:485:LYS:N	2.22	0.52
1:f:361:ASN:O	1:f:365:THR:OG1	2.25	0.52
1:j:308:VAL:HG23	1:j:309:GLY:H	1.74	0.52
1:e:29:PHE:HB3	1:e:208:ARG:CZ	2.39	0.52
1:f:424:LYS:HA	1:f:428:ILE:HG22	1.91	0.52
1:j:287:GLU:HB2	1:j:306:LEU:HD23	1.92	0.52
1:i:143:VAL:HB	1:i:191:LYS:HB2	1.90	0.52
1:h:347:ILE:HD12	1:h:351:ARG:NH2	2.25	0.52
1:d:581:SER:O	1:d:585:LEU:N	2.34	0.52
1:e:292:LEU:O	1:e:300:SER:OG	2.20	0.52
1:e:326:LEU:HD13	1:e:467:PHE:HD1	1.75	0.52
1:e:351:ARG:HH12	1:e:422:ARG:HD3	1.75	0.52
1:k:515:VAL:HG12	1:k:516:THR:HG23	1.91	0.52
1:j:73:MET:SD	1:j:126:GLN:NE2	2.80	0.52
1:j:487:GLN:HG3	1:j:488:ASN:H	1.74	0.52
1:c:292:LEU:HD21	1:c:303:ARG:HB2	1.91	0.52
1:d:285:ALA:HB2	1:d:308:VAL:HG23	1.91	0.52
1:d:575:PHE:H	1:e:555:ASN:ND2	2.08	0.52
1:h:411:VAL:HA	1:h:414:MET:SD	2.50	0.52
1:h:428:ILE:H	1:h:428:ILE:HD12	1.75	0.52
1:h:546:GLY:HA2	1:g:430:ASP:HA	1.92	0.52
1:e:471:GLY:O	1:e:473:LYS:N	2.43	0.52
1:l:302:LEU:O	1:l:318:TRP:N	2.36	0.52
1:j:95:GLU:HB2	1:i:496:ARG:HH22	1.75	0.52
1:i:93:THR:OG1	1:h:496:ARG:HA	2.09	0.52
1:i:146:PRO:HG3	1:i:189:LYS:HB2	1.92	0.52
1:i:343:LYS:HG3	1:i:344:ILE:HG12	1.92	0.52
1:h:423:GLY:O	1:h:427:GLY:N	2.37	0.52
1:d:557:TYR:OH	1:e:549:VAL:O	2.21	0.52
1:e:400:THR:HG22	1:e:402:LEU:H	1.75	0.52
1:b:493:PHE:O	1:b:494:GLN:HG2	2.10	0.52
1:a:330:ARG:HH12	1:l:119:LYS:HB3	1.76	0.52
1:k:26:ALA:HB1	1:k:205:LEU:HB3	1.92	0.52
1:c:118:PHE:HB3	1:d:469:GLU:HG2	1.90	0.52
1:c:523:ASN:O	1:c:527:GLN:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:462:LEU:HD13	1:k:77:MET:HG3	1.91	0.51
1:j:574:ARG:HE	1:j:576:TRP:NE1	2.08	0.51
1:c:433:ARG:HB3	1:d:455:ALA:HB1	1.92	0.51
1:b:444:GLN:HE22	1:a:443:ASN:HB2	1.75	0.51
1:k:110:LEU:O	1:k:114:LYS:HB3	2.10	0.51
1:k:465:ARG:HD3	1:k:516:THR:OG1	2.11	0.51
1:j:423:GLY:C	1:j:428:ILE:HG13	2.35	0.51
1:i:507:TRP:O	1:i:509:GLU:HG3	2.10	0.51
1:j:105:GLU:CD	1:j:493:PHE:HB2	2.35	0.51
1:j:343:LYS:O	1:j:425:ARG:NH1	2.43	0.51
1:c:239:VAL:HA	1:c:311:TYR:HE2	1.75	0.51
1:f:346:ASP:O	1:f:350:ILE:HG23	2.10	0.51
1:b:554:GLN:HA	1:b:579:PRO:HG2	1.93	0.51
1:a:87:VAL:HG12	1:a:510:ARG:HG2	1.91	0.51
1:l:555:ASN:ND2	1:k:575:PHE:HB2	2.25	0.51
1:j:68:THR:O	1:j:72:ILE:HG12	2.11	0.51
1:j:450:ASN:ND2	1:j:525:ASP:OD2	2.43	0.51
1:c:192:ARG:HB3	1:c:486:TYR:HD1	1.76	0.51
1:d:135:VAL:HG12	1:d:199:VAL:HG21	1.93	0.51
1:e:132:LYS:HG2	1:e:339:SER:HB3	1.91	0.51
1:f:194:ILE:HB	1:f:486:TYR:OH	2.11	0.51
1:b:213:ILE:O	1:b:321:ARG:NH1	2.43	0.51
1:k:124:TRP:CH2	1:k:136:VAL:HG22	2.45	0.51
1:j:494:GLN:HA	1:j:571:ASP:OD2	2.11	0.51
1:i:145:LYS:HD2	1:i:145:LYS:O	2.11	0.51
1:i:477:GLN:HA	1:i:480:HIS:ND1	2.25	0.51
1:c:19:LEU:HD22	1:c:307:TYR:CD2	2.45	0.51
1:c:433:ARG:HG3	1:d:428:ILE:HG21	1.92	0.51
1:c:440:LEU:HD13	1:d:448:SER:HB3	1.92	0.51
1:d:473:LYS:O	1:d:477:GLN:HG2	2.11	0.51
1:k:428:ILE:HB	1:j:433:ARG:HD2	1.93	0.51
1:j:91:PRO:HG3	1:j:507:TRP:CZ3	2.44	0.51
1:i:471:GLY:HA2	1:i:474:ARG:HE	1.76	0.51
1:f:73:MET:HE1	1:f:125:PHE:HD2	1.76	0.51
1:f:535:TRP:HE1	1:f:563:VAL:HG21	1.76	0.51
1:a:212:CYS:SG	1:a:213:ILE:N	2.84	0.51
1:l:93:THR:OG1	1:k:496:ARG:HB2	2.10	0.51
1:l:112:MET:HE1	1:l:118:PHE:CZ	2.46	0.51
1:k:44:TYR:HB2	1:k:341:TYR:CE1	2.45	0.51
1:k:121:MET:HE1	1:k:474:ARG:NH1	2.24	0.51
1:j:43:LYS:HG3	1:j:48:GLU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:435:LEU:HD23	1:f:441:HIS:CD2	2.45	0.51
1:a:449:VAL:HG11	1:l:524:LYS:HE3	1.92	0.51
1:l:98:GLU:O	1:l:99:GLN:NE2	2.41	0.51
1:l:522:MET:SD	1:l:524:LYS:HB3	2.51	0.51
1:k:532:MET:SD	1:k:533:ARG:HG2	2.50	0.51
1:f:483:ALA:HA	1:f:504:PRO:HD2	1.93	0.51
1:b:319:ASP:OD2	1:b:480:HIS:NE2	2.43	0.51
1:l:428:ILE:HG23	1:k:433:ARG:HD2	1.93	0.51
1:l:482:HIS:HA	1:l:486:TYR:HD2	1.75	0.51
1:d:565:GLU:HG2	1:d:570:LYS:HB3	1.93	0.51
1:e:398:SER:HA	1:f:379:LEU:HA	1.93	0.51
1:e:597:GLN:HB2	1:e:598:PRO:HD3	1.93	0.51
1:f:509:GLU:C	1:f:510:ARG:HD3	2.35	0.51
1:b:295:ASP:OD1	1:b:295:ASP:N	2.42	0.51
1:a:89:TYR:HA	1:a:510:ARG:HG3	1.92	0.51
1:h:209:LEU:HD23	1:h:217:ARG:HG3	1.92	0.51
1:c:554:GLN:O	1:c:557:TYR:HB2	2.11	0.51
1:g:304:ARG:N	1:g:316:GLU:O	2.35	0.51
1:i:29:PHE:HB3	1:i:208:ARG:HE	1.76	0.50
1:i:110:LEU:HD22	1:i:482:HIS:HE1	1.75	0.50
1:c:227:VAL:HB	1:c:280:ASN:HA	1.94	0.50
1:c:331:ILE:HD11	1:c:338:MET:HG3	1.92	0.50
1:c:496:ARG:HE	1:d:94:ALA:H	1.57	0.50
1:d:478:LEU:C	1:d:482:HIS:HD1	2.19	0.50
1:e:496:ARG:HH22	1:f:95:GLU:HG2	1.76	0.50
1:f:117:GLY:O	1:f:120:VAL:HG22	2.11	0.50
1:b:110:LEU:HD21	1:b:482:HIS:NE2	2.26	0.50
1:b:304:ARG:HD2	1:b:318:TRP:HE1	1.77	0.50
1:a:286:SER:OG	1:a:307:TYR:O	2.24	0.50
1:d:203:ASN:O	1:d:221:HIS:ND1	2.41	0.50
1:e:17:ARG:NH1	1:e:310:ASP:OD2	2.44	0.50
1:f:213:ILE:HD13	1:f:325:ASP:HB2	1.92	0.50
1:b:207:ASP:OD1	1:b:208:ARG:N	2.45	0.50
1:b:459:GLN:O	1:b:463:ILE:HG12	2.10	0.50
1:a:213:ILE:HD11	1:a:325:ASP:HB2	1.93	0.50
1:l:465:ARG:HD3	1:l:516:THR:OG1	2.12	0.50
1:k:41:ALA:HA	1:k:341:TYR:HE1	1.74	0.50
1:j:503:ASN:N	1:j:504:PRO:HD3	2.26	0.50
1:c:303:ARG:HG2	1:c:317:PRO:HA	1.93	0.50
1:c:331:ILE:HG22	1:c:332:ALA:H	1.76	0.50
1:d:360:ASP:OD1	1:d:361:ASN:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:433:ARG:HH22	1:e:459:GLN:H	1.60	0.50
1:f:572:PRO:HA	1:f:575:PHE:CE1	2.45	0.50
1:b:110:LEU:HD11	1:b:482:HIS:CE1	2.46	0.50
1:a:189:LYS:HG2	1:a:190:LYS:H	1.77	0.50
1:l:499:TRP:H	1:l:499:TRP:CD1	2.28	0.50
1:k:468:ALA:O	1:k:472:VAL:HG23	2.10	0.50
1:j:64:ASP:OD2	1:j:422:ARG:NE	2.45	0.50
1:i:332:ALA:HB2	1:h:126:GLN:HG2	1.92	0.50
1:d:531:LEU:O	1:d:535:TRP:HB3	2.11	0.50
1:e:331:ILE:HG13	1:e:332:ALA:H	1.77	0.50
1:f:478:LEU:HB3	1:f:482:HIS:NE2	2.26	0.50
1:b:554:GLN:O	1:b:554:GLN:NE2	2.44	0.50
1:k:531:LEU:HD23	1:k:532:MET:HB3	1.93	0.50
1:i:92:ASP:HA	1:h:492:VAL:HG12	1.92	0.50
1:i:482:HIS:HD1	1:i:486:TYR:HE1	1.56	0.50
1:b:124:TRP:CZ2	1:b:326:LEU:HD13	2.47	0.50
1:l:597:GLN:HB2	1:l:598:PRO:HD3	1.94	0.50
1:h:418:LEU:O	1:h:422:ARG:HG3	2.11	0.50
1:c:121:MET:HA	1:c:124:TRP:HD1	1.76	0.50
1:l:331:ILE:HG22	1:l:332:ALA:N	2.27	0.50
1:j:92:ASP:HB2	1:i:496:ARG:HE	1.77	0.50
1:j:420:ALA:O	1:j:424:LYS:N	2.45	0.50
1:h:463:ILE:HG23	1:h:467:PHE:HE2	1.77	0.50
1:h:556:LEU:HB3	1:h:576:TRP:HZ3	1.77	0.50
1:c:587:ALA:HA	1:c:591:ARG:HG2	1.93	0.50
1:d:557:TYR:HA	1:d:560:LEU:HD12	1.94	0.50
1:f:213:ILE:HD11	1:f:323:PHE:HB2	1.94	0.50
1:b:416:ASP:OD1	1:b:417:ARG:N	2.44	0.50
1:l:419:GLU:HB3	1:l:422:ARG:HH21	1.76	0.50
1:k:466:MET:HE2	1:k:466:MET:HA	1.94	0.50
1:j:19:LEU:HD22	1:j:307:TYR:CE1	2.46	0.50
1:i:220:CYS:SG	1:i:221:HIS:N	2.85	0.50
1:h:359:MET:HA	1:h:362:ILE:HD12	1.93	0.50
1:d:110:LEU:HD13	1:d:482:HIS:NE2	2.27	0.50
1:d:490:GLU:HG2	1:d:498:LYS:HB2	1.94	0.50
1:b:326:LEU:HD23	1:b:467:PHE:CD1	2.47	0.50
1:b:455:ALA:HB1	1:a:433:ARG:HG2	1.94	0.50
1:a:112:MET:O	1:a:114:LYS:N	2.45	0.50
1:i:555:ASN:HB3	1:h:575:PHE:CE1	2.46	0.50
1:i:586:GLN:HG2	1:i:590:ILE:HD12	1.93	0.50
1:d:436:ASP:HB3	1:d:440:LEU:HD23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:126:GLN:NE2	1:f:330:ARG:O	2.45	0.50
1:b:430:ASP:OD1	1:b:430:ASP:N	2.43	0.49
1:b:524:LYS:CE	1:c:453:MET:HG3	2.41	0.49
1:j:139:TYR:CD1	1:j:197:LEU:HD22	2.46	0.49
1:i:306:LEU:O	1:i:313:ILE:HG12	2.12	0.49
1:h:320:CYS:SG	1:h:321:ARG:N	2.81	0.49
1:h:466:MET:HA	1:h:469:GLU:HG2	1.93	0.49
1:d:362:ILE:O	1:d:365:THR:OG1	2.29	0.49
1:d:465:ARG:HD3	1:d:516:THR:OG1	2.12	0.49
1:e:45:TYR:O	1:e:66:GLN:NE2	2.39	0.49
1:f:31:SER:O	1:f:35:SER:OG	2.18	0.49
1:f:569:TYR:HB3	1:f:572:PRO:HD2	1.94	0.49
1:j:227:VAL:HG23	1:j:281:ARG:H	1.77	0.49
1:j:364:ARG:HA	1:j:367:GLN:HB2	1.94	0.49
1:b:494:GLN:O	1:b:495:LEU:HD12	2.11	0.49
1:l:18:HIS:NE2	1:k:278:GLU:HG3	2.27	0.49
1:k:76:LEU:HA	1:k:79:VAL:HG12	1.94	0.49
1:i:60:ILE:HD11	1:i:355:MET:HB3	1.94	0.49
1:i:210:ALA:O	1:i:211:THR:OG1	2.27	0.49
1:d:560:LEU:HD13	1:d:576:TRP:CE3	2.48	0.49
1:e:213:ILE:HD11	1:e:325:ASP:HB2	1.94	0.49
1:g:308:VAL:O	1:g:312:ILE:N	2.40	0.49
1:l:12:ASP:OD1	1:l:12:ASP:N	2.44	0.49
1:l:428:ILE:O	1:k:433:ARG:NH1	2.46	0.49
1:j:488:ASN:HA	1:j:500:VAL:HG22	1.93	0.49
1:e:71:TRP:HH2	1:f:425:ARG:HA	1.77	0.49
1:e:315:ASN:OD1	1:e:316:GLU:N	2.45	0.49
1:f:455:ALA:HB3	1:f:458:GLN:HG3	1.94	0.49
1:l:87:VAL:HG22	1:l:512:ASP:HB3	1.93	0.49
1:k:586:GLN:O	1:k:590:ILE:HG12	2.13	0.49
1:i:425:ARG:O	1:i:425:ARG:NH1	2.44	0.49
1:c:564:THR:O	1:c:568:GLY:N	2.29	0.49
1:f:200:LYS:O	1:f:202:GLU:N	2.45	0.49
1:l:554:GLN:HA	1:l:557:TYR:HD2	1.77	0.49
1:k:110:LEU:HD23	1:k:478:LEU:HD13	1.93	0.49
1:j:503:ASN:N	1:j:503:ASN:OD1	2.46	0.49
1:i:535:TRP:HH2	1:i:556:LEU:HD22	1.76	0.49
1:i:542:VAL:HG21	1:i:556:LEU:HD21	1.95	0.49
1:e:331:ILE:HD13	1:e:338:MET:HE1	1.94	0.49
1:e:383:LEU:O	1:e:388:ALA:N	2.46	0.49
1:f:344:ILE:HG22	1:f:348:GLN:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:574:ARG:HH12	1:g:528:MET:N	2.10	0.49
1:a:528:MET:HE1	1:a:533:ARG:HH12	1.78	0.49
1:k:137:LYS:HB3	1:k:197:LEU:HB3	1.95	0.49
1:k:425:ARG:HG2	1:j:67:GLU:HG2	1.95	0.49
1:d:213:ILE:O	1:d:321:ARG:NH1	2.46	0.49
1:d:592:GLU:N	1:d:592:GLU:OE1	2.46	0.49
1:e:341:TYR:HB3	1:e:345:ARG:NH1	2.28	0.49
1:a:95:GLU:H	1:l:496:ARG:CZ	2.26	0.49
1:l:189:LYS:O	1:l:191:LYS:NZ	2.46	0.49
1:k:136:VAL:HG11	1:k:138:VAL:HG23	1.95	0.49
1:i:19:LEU:HD23	1:i:307:TYR:CE2	2.48	0.49
1:c:433:ARG:HH21	1:d:459:GLN:H	1.59	0.49
1:e:106:TYR:HB2	1:e:493:PHE:HZ	1.78	0.49
1:e:228:SER:HB3	1:f:299:ILE:HD12	1.94	0.49
1:f:35:SER:HA	1:f:38:ARG:NE	2.27	0.49
1:a:110:LEU:HD22	1:a:482:HIS:NE2	2.28	0.49
1:l:91:PRO:HG2	1:l:96:ASP:HA	1.95	0.49
1:k:94:ALA:HB3	1:j:496:ARG:CZ	2.43	0.49
1:d:86:VAL:HG12	1:d:87:VAL:HG23	1.95	0.49
1:e:207:ASP:OD2	1:e:217:ARG:N	2.43	0.49
1:e:496:ARG:HE	1:f:94:ALA:H	1.60	0.49
1:f:493:PHE:HB2	1:f:498:LYS:HZ1	1.78	0.49
1:b:205:LEU:HB2	1:b:220:CYS:HB3	1.95	0.48
1:b:557:TYR:CD2	1:b:579:PRO:HD3	2.48	0.48
1:l:103:GLU:HG3	1:l:499:TRP:HZ2	1.77	0.48
1:l:147:THR:HG22	1:l:186:ARG:HG2	1.95	0.48
1:l:443:ASN:ND2	1:l:532:MET:SD	2.86	0.48
1:i:124:TRP:NE1	1:i:474:ARG:HH22	2.12	0.48
1:c:16:LEU:HD21	1:c:313:ILE:HD11	1.95	0.48
1:d:130:MET:C	1:d:131:MET:HE2	2.38	0.48
1:e:67:GLU:O	1:e:71:TRP:HE3	1.95	0.48
1:b:468:ALA:O	1:b:472:VAL:HG23	2.13	0.48
1:a:218:PHE:CE1	1:a:290:THR:HG23	2.48	0.48
1:l:424:LYS:NZ	1:k:422:ARG:HH22	2.11	0.48
1:j:347:ILE:HD13	1:j:422:ARG:HA	1.94	0.48
1:c:62:SER:HG	1:c:351:ARG:NH1	2.10	0.48
1:c:222:ARG:HD2	1:c:286:SER:HB3	1.95	0.48
1:b:513:LEU:HA	1:b:517:VAL:HG11	1.94	0.48
1:a:331:ILE:HG13	1:a:332:ALA:H	1.79	0.48
1:l:27:LEU:O	1:l:31:SER:OG	2.31	0.48
1:k:304:ARG:HG2	1:k:318:TRP:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:351:ARG:NH1	1:j:419:GLU:OE1	2.46	0.48
1:j:578:ASN:HB3	1:j:584:ALA:HB2	1.95	0.48
1:i:194:ILE:HB	1:i:486:TYR:OH	2.13	0.48
1:h:88:LYS:O	1:h:511:SER:OG	2.32	0.48
1:c:575:PHE:HE2	1:d:554:GLN:HB2	1.78	0.48
1:d:358:ILE:O	1:d:362:ILE:HG12	2.12	0.48
1:d:465:ARG:HB2	1:d:516:THR:HB	1.95	0.48
1:f:41:ALA:HB2	1:f:345:ARG:NH2	2.27	0.48
1:b:493:PHE:C	1:b:495:LEU:H	2.21	0.48
1:b:590:ILE:O	1:b:594:LYS:HE2	2.14	0.48
1:a:594:LYS:O	1:a:598:PRO:HD2	2.13	0.48
1:j:94:ALA:HB3	1:i:496:ARG:NH1	2.29	0.48
1:j:110:LEU:HD23	1:j:482:HIS:NE2	2.27	0.48
1:j:458:GLN:HE21	1:j:460:ILE:HG12	1.78	0.48
1:i:558:ASN:HA	1:i:561:LYS:HD2	1.95	0.48
1:c:62:SER:H	1:c:352:SER:HB3	1.77	0.48
1:d:216:ALA:H	1:d:321:ARG:HH12	1.60	0.48
1:e:52:ASN:O	1:e:356:ARG:NH1	2.46	0.48
1:l:376:GLN:O	1:l:378:ASN:N	2.47	0.48
1:l:482:HIS:HA	1:l:486:TYR:CD2	2.48	0.48
1:l:557:TYR:HB3	1:l:561:LYS:NZ	2.27	0.48
1:j:596:ALA:O	1:j:600:PRO:HA	2.13	0.48
1:b:494:GLN:HG3	1:b:495:LEU:HD12	1.96	0.48
1:a:515:VAL:HG13	1:a:516:THR:HG23	1.96	0.48
1:j:428:ILE:HD13	1:i:431:ARG:HB3	1.95	0.48
1:i:92:ASP:OD1	1:i:92:ASP:N	2.44	0.48
1:d:45:TYR:CD1	1:d:130:MET:HE1	2.47	0.48
1:d:65:VAL:HG21	1:d:341:TYR:OH	2.14	0.48
1:d:77:MET:O	1:d:81:THR:OG1	2.30	0.48
1:d:143:VAL:HB	1:d:191:LYS:HB2	1.94	0.48
1:d:476:PHE:O	1:d:480:HIS:ND1	2.46	0.48
1:a:537:MET:HE3	1:l:560:LEU:HG	1.95	0.48
1:l:81:THR:HG22	1:l:118:PHE:CD2	2.49	0.48
1:l:468:ALA:O	1:l:472:VAL:HG23	2.14	0.48
1:j:19:LEU:HD21	1:j:288:CYS:SG	2.53	0.48
1:d:529:LEU:HB3	1:d:533:ARG:HH21	1.79	0.48
1:e:203:ASN:O	1:e:221:HIS:HA	2.13	0.48
1:a:212:CYS:HB3	1:a:215:ASP:HB2	1.96	0.48
1:c:484:ILE:HG22	1:c:485:LYS:HG2	1.95	0.48
1:c:557:TYR:CE2	1:c:578:ASN:HB3	2.38	0.48
1:e:471:GLY:C	1:e:474:ARG:HH11	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:458:GLN:O	1:g:462:LEU:N	2.41	0.48
1:b:14:GLN:O	1:b:18:HIS:ND1	2.47	0.48
1:a:106:TYR:HB2	1:a:491:GLU:OE2	2.13	0.48
1:l:65:VAL:HG21	1:l:341:TYR:CE1	2.49	0.48
1:k:64:ASP:OD2	1:k:351:ARG:NH1	2.46	0.48
1:j:514:THR:HA	1:j:520:GLY:HA2	1.95	0.48
1:h:347:ILE:HD12	1:h:351:ARG:HH22	1.79	0.48
1:d:200:LYS:O	1:d:202:GLU:N	2.47	0.48
1:d:326:LEU:HD23	1:d:467:PHE:CD1	2.42	0.48
1:e:383:LEU:O	1:e:387:ALA:N	2.45	0.48
1:l:488:ASN:HB3	1:l:500:VAL:HG13	1.95	0.48
1:k:330:ARG:NH2	1:j:123:ASP:OD2	2.47	0.48
1:c:102:GLN:OE1	1:c:499:TRP:NE1	2.47	0.48
1:c:524:LYS:HD2	1:d:453:MET:SD	2.54	0.48
1:d:87:VAL:HG22	1:d:512:ASP:HB3	1.95	0.48
1:f:37:GLN:O	1:f:345:ARG:NH2	2.47	0.48
1:b:93:THR:H	1:a:496:ARG:NH2	2.11	0.47
1:b:481:ASP:HA	1:b:484:ILE:HG22	1.95	0.47
1:b:507:TRP:O	1:b:509:GLU:N	2.47	0.47
1:j:306:LEU:HB2	1:j:314:SER:OG	2.14	0.47
1:i:517:VAL:HG21	1:h:78:LYS:HG2	1.96	0.47
1:h:212:CYS:SG	1:h:213:ILE:N	2.81	0.47
1:c:65:VAL:HB	1:c:341:TYR:CE1	2.49	0.47
1:c:576:TRP:HE1	1:d:541:VAL:HG11	1.79	0.47
1:f:516:THR:OG1	1:f:517:VAL:N	2.45	0.47
1:k:548:GLY:H	1:j:591:ARG:NH1	2.11	0.47
1:k:590:ILE:O	1:k:595:GLU:N	2.47	0.47
1:i:524:LYS:O	1:i:528:MET:HG2	2.14	0.47
1:h:138:VAL:HG12	1:h:194:ILE:HD11	1.96	0.47
1:c:433:ARG:NH2	1:d:428:ILE:HD13	2.30	0.47
1:d:128:THR:HG21	1:d:467:PHE:CE1	2.48	0.47
1:d:147:THR:CG2	1:d:186:ARG:H	2.27	0.47
1:d:214:ASP:OD1	1:d:214:ASP:N	2.47	0.47
1:b:346:ASP:OD1	1:b:347:ILE:N	2.47	0.47
1:l:137:LYS:NZ	1:l:223:GLU:OE2	2.41	0.47
1:l:143:VAL:C	1:l:144:LEU:HD12	2.38	0.47
1:k:121:MET:HA	1:k:121:MET:HE2	1.95	0.47
1:j:200:LYS:O	1:j:202:GLU:N	2.46	0.47
1:j:541:VAL:HG11	1:j:551:VAL:HG23	1.94	0.47
1:j:549:VAL:HG21	1:i:592:GLU:HG3	1.96	0.47
1:d:574:ARG:HA	1:d:574:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:533:ARG:O	1:b:537:MET:HG3	2.15	0.47
1:a:20:ASP:OD1	1:a:307:TYR:OH	2.20	0.47
1:a:76:LEU:HD13	1:a:467:PHE:HE2	1.79	0.47
1:k:568:GLY:O	1:k:570:LYS:NZ	2.38	0.47
1:i:462:LEU:CD1	1:h:74:PRO:HA	2.44	0.47
1:c:359:MET:HA	1:c:362:ILE:HG22	1.95	0.47
1:e:496:ARG:NH2	1:f:95:GLU:H	2.13	0.47
1:b:528:MET:HE2	1:b:528:MET:N	2.29	0.47
1:a:124:TRP:CZ2	1:a:136:VAL:HG22	2.50	0.47
1:l:29:PHE:HB3	1:l:208:ARG:HD2	1.95	0.47
1:l:212:CYS:HB3	1:l:215:ASP:HB2	1.96	0.47
1:l:343:LYS:O	1:l:425:ARG:NH1	2.45	0.47
1:j:461:ASP:O	1:j:516:THR:OG1	2.32	0.47
1:i:579:PRO:O	1:i:588:LYS:NZ	2.48	0.47
1:h:341:TYR:O	1:h:345:ARG:HG2	2.14	0.47
1:e:288:CYS:SG	1:e:305:ILE:HB	2.54	0.47
1:a:27:LEU:HA	1:a:205:LEU:HD11	1.96	0.47
1:a:210:ALA:HB3	1:a:335:PHE:HB2	1.96	0.47
1:l:135:VAL:HG21	1:l:204:PHE:CD2	2.50	0.47
1:j:135:VAL:HG23	1:j:199:VAL:HB	1.97	0.47
1:i:491:GLU:HB2	1:i:498:LYS:HD2	1.96	0.47
1:c:32:SER:OG	1:c:33:GLU:OE1	2.29	0.47
1:c:474:ARG:O	1:c:478:LEU:HG	2.15	0.47
1:f:136:VAL:O	1:f:323:PHE:HA	2.15	0.47
1:f:200:LYS:O	1:f:203:ASN:N	2.45	0.47
1:a:553:GLU:HG2	1:a:556:LEU:HB2	1.95	0.47
1:l:346:ASP:N	1:l:346:ASP:OD1	2.45	0.47
1:k:77:MET:HE2	1:k:77:MET:HA	1.95	0.47
1:k:301:GLU:HG2	1:k:302:LEU:N	2.27	0.47
1:k:449:VAL:HG21	1:j:528:MET:HE1	1.97	0.47
1:k:594:LYS:HD2	1:k:594:LYS:HA	1.78	0.47
1:j:338:MET:HE3	1:j:342:ASP:HB2	1.95	0.47
1:i:338:MET:HE1	1:i:343:LYS:HE3	1.97	0.47
1:h:289:TYR:CE2	1:h:304:ARG:HD3	2.50	0.47
1:c:546:GLY:H	1:c:550:LEU:HD12	1.80	0.47
1:d:366:ASN:HD21	1:e:407:LEU:HD11	1.78	0.47
1:e:200:LYS:O	1:e:202:GLU:N	2.47	0.47
1:f:291:LEU:HA	1:f:302:LEU:HA	1.96	0.47
1:f:407:LEU:HD23	1:f:411:VAL:HG21	1.96	0.47
1:f:460:ILE:HA	1:f:463:ILE:HD12	1.97	0.47
1:f:555:ASN:O	1:f:559:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:500:VAL:HG22	1:b:502:VAL:H	1.79	0.47
1:k:497:GLY:C	1:k:498:LYS:HD2	2.39	0.47
1:i:45:TYR:O	1:i:66:GLN:NE2	2.44	0.47
1:i:353:VAL:HA	1:i:356:ARG:HB2	1.95	0.47
1:h:62:SER:HB2	1:h:422:ARG:HH12	1.80	0.47
1:h:146:PRO:HG3	1:h:189:LYS:HB3	1.97	0.47
1:h:329:TYR:OH	1:h:340:VAL:HG22	2.14	0.47
1:d:124:TRP:CZ2	1:d:324:ALA:HB1	2.49	0.47
1:a:95:GLU:H	1:l:496:ARG:NH2	2.13	0.47
1:a:135:VAL:HG11	1:a:204:PHE:CE2	2.50	0.47
1:l:15:VAL:HA	1:l:18:HIS:HB3	1.96	0.47
1:i:58:SER:OG	1:i:60:ILE:HG12	2.15	0.47
1:i:525:ASP:HA	1:i:528:MET:HG2	1.97	0.47
1:i:558:ASN:OD1	1:i:561:LYS:NZ	2.41	0.47
1:h:139:TYR:O	1:h:194:ILE:HG13	2.15	0.47
1:e:138:VAL:HG22	1:e:196:VAL:HG22	1.95	0.47
1:e:359:MET:O	1:e:362:ILE:HG22	2.15	0.47
1:f:362:ILE:O	1:f:366:ASN:ND2	2.48	0.47
1:j:38:ARG:HD3	1:j:131:MET:HE3	1.97	0.47
1:i:192:ARG:HG2	1:i:485:LYS:HD2	1.97	0.47
1:h:71:TRP:O	1:h:74:PRO:HD2	2.14	0.47
1:h:364:ARG:HH21	1:h:404:THR:HG1	1.59	0.47
1:c:549:VAL:HG23	1:c:550:LEU:HG	1.97	0.47
1:d:482:HIS:HA	1:d:486:TYR:CD2	2.51	0.47
1:e:493:PHE:HB2	1:e:498:LYS:HE2	1.96	0.47
1:f:415:LEU:HD23	1:f:418:LEU:HD21	1.97	0.47
1:b:450:ASN:OD1	1:b:451:GLN:NE2	2.49	0.46
1:l:125:PHE:HA	1:l:128:THR:HG22	1.97	0.46
1:k:560:LEU:HD22	1:k:576:TRP:CD2	2.50	0.46
1:i:417:ARG:HG2	1:h:419:GLU:OE1	2.16	0.46
1:f:559:ILE:O	1:f:562:GLU:HG3	2.15	0.46
1:b:110:LEU:HD11	1:b:482:HIS:NE2	2.30	0.46
1:b:316:GLU:HG3	1:b:317:PRO:HD2	1.97	0.46
1:a:350:ILE:HG22	1:a:418:LEU:HD11	1.97	0.46
1:a:590:ILE:HG13	1:a:591:ARG:N	2.30	0.46
1:j:428:ILE:HG22	1:i:435:LEU:HD12	1.96	0.46
1:c:111:PHE:CD2	1:c:112:MET:HE3	2.51	0.46
1:e:241:GLU:HB3	1:e:281:ARG:HB2	1.96	0.46
1:e:581:SER:O	1:e:585:LEU:N	2.35	0.46
1:f:138:VAL:HG22	1:f:196:VAL:HG12	1.97	0.46
1:f:529:LEU:HA	1:f:532:MET:HE2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:558:ASN:HB2	1:k:574:ARG:NH2	2.20	0.46
1:j:493:PHE:HB3	1:j:498:LYS:HE2	1.97	0.46
1:h:304:ARG:HE	1:h:318:TRP:NE1	2.13	0.46
1:h:383:LEU:O	1:h:387:ALA:N	2.45	0.46
1:c:31:SER:HA	1:c:35:SER:HB3	1.96	0.46
1:e:433:ARG:HB3	1:f:428:ILE:HD13	1.97	0.46
1:e:435:LEU:HD11	1:f:428:ILE:HB	1.97	0.46
1:a:456:ALA:HB3	1:l:433:ARG:HA	1.96	0.46
1:j:468:ALA:O	1:j:472:VAL:HG13	2.15	0.46
1:i:110:LEU:O	1:i:115:ASN:ND2	2.48	0.46
1:d:74:PRO:HB2	1:e:457:GLU:OE1	2.15	0.46
1:b:18:HIS:O	1:b:21:GLN:HG2	2.16	0.46
1:b:433:ARG:NH2	1:c:458:GLN:HG2	2.31	0.46
1:k:575:PHE:O	1:k:577:THR:N	2.47	0.46
1:i:140:VAL:HA	1:i:194:ILE:HD13	1.96	0.46
1:h:89:TYR:HD2	1:h:100:ALA:HA	1.79	0.46
1:h:205:LEU:HD13	1:h:222:ARG:HD3	1.97	0.46
1:d:304:ARG:HD2	1:d:316:GLU:OE2	2.16	0.46
1:b:552:SER:HB3	1:a:575:PHE:CZ	2.50	0.46
1:a:44:TYR:CE2	1:a:345:ARG:HG2	2.51	0.46
1:l:81:THR:HG22	1:l:118:PHE:CE2	2.51	0.46
1:j:211:THR:HA	1:j:335:PHE:N	2.31	0.46
1:j:333:HIS:HB2	1:i:200:LYS:NZ	2.31	0.46
1:i:465:ARG:CZ	1:i:518:GLY:HA3	2.46	0.46
1:h:345:ARG:HG3	1:h:346:ASP:N	2.30	0.46
1:h:577:THR:HG23	1:h:578:ASN:N	2.30	0.46
1:c:557:TYR:CE1	1:d:550:LEU:HD23	2.49	0.46
1:d:308:VAL:HG13	1:d:309:GLY:N	2.31	0.46
1:b:465:ARG:HH21	1:a:81:THR:HG21	1.80	0.46
1:a:124:TRP:CH2	1:a:198:CYS:HA	2.51	0.46
1:a:207:ASP:OD2	1:a:217:ARG:NH1	2.48	0.46
1:i:541:VAL:O	1:i:546:GLY:N	2.40	0.46
1:c:204:PHE:O	1:c:206:VAL:HG23	2.16	0.46
1:d:280:ASN:OD1	1:e:217:ARG:NH2	2.38	0.46
1:e:519:ILE:HG13	1:e:520:GLY:N	2.24	0.46
1:g:528:MET:O	1:g:532:MET:N	2.48	0.46
1:j:303:ARG:HG2	1:j:317:PRO:HA	1.97	0.46
1:h:308:VAL:HG13	1:h:309:GLY:N	2.30	0.46
1:h:514:THR:HA	1:h:520:GLY:H	1.81	0.46
1:d:466:MET:HA	1:d:466:MET:HE2	1.96	0.46
1:f:135:VAL:HB	1:f:204:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:507:TRP:O	1:a:509:GLU:N	2.48	0.46
1:l:461:ASP:HB3	1:l:517:VAL:HG23	1.98	0.46
1:l:549:VAL:HG13	1:l:550:LEU:HG	1.98	0.46
1:i:135:VAL:HG13	1:i:199:VAL:HG12	1.98	0.46
1:i:535:TRP:HE3	1:i:559:ILE:HG21	1.81	0.46
1:h:138:VAL:HG22	1:h:196:VAL:HG13	1.96	0.46
1:c:82:SER:HB2	1:d:519:ILE:HB	1.98	0.46
1:e:297:ASP:OD1	1:e:297:ASP:N	2.47	0.46
1:f:428:ILE:HD11	1:f:455:ALA:HB1	1.98	0.46
1:l:43:LYS:NZ	1:l:48:GLU:OE1	2.45	0.46
1:l:311:TYR:O	1:l:313:ILE:HG13	2.16	0.46
1:i:429:THR:HA	1:h:435:LEU:HD21	1.97	0.46
1:h:138:VAL:HG13	1:h:196:VAL:HG22	1.97	0.46
1:h:210:ALA:HA	1:h:216:ALA:HA	1.98	0.46
1:c:438:ASN:ND2	1:d:439:THR:HB	2.31	0.46
1:b:11:ASP:OD1	1:b:11:ASP:N	2.49	0.45
1:a:135:VAL:HG12	1:a:325:ASP:HA	1.97	0.45
1:a:142:GLU:HG2	1:a:190:LYS:HA	1.97	0.45
1:k:350:ILE:HD11	1:j:60:ILE:HG12	1.98	0.45
1:i:110:LEU:O	1:i:114:LYS:HB3	2.15	0.45
1:i:512:ASP:H	1:h:113:ARG:NH2	2.15	0.45
1:c:45:TYR:CE1	1:c:130:MET:HE1	2.51	0.45
1:d:91:PRO:HB3	1:d:507:TRP:CZ3	2.51	0.45
1:d:468:ALA:O	1:d:472:VAL:HG23	2.15	0.45
1:d:549:VAL:HG23	1:d:550:LEU:HG	1.97	0.45
1:k:19:LEU:HA	1:k:22:LEU:HD12	1.99	0.45
1:k:84:GLY:N	1:k:85:GLN:OE1	2.50	0.45
1:k:347:ILE:HD13	1:k:422:ARG:HA	1.98	0.45
1:k:588:LYS:O	1:k:592:GLU:HB2	2.16	0.45
1:i:42:LEU:HD23	1:i:42:LEU:HA	1.81	0.45
1:i:289:TYR:CD1	1:i:304:ARG:HG2	2.51	0.45
1:h:303:ARG:NE	1:h:315:ASN:HB3	2.25	0.45
1:c:212:CYS:HB3	1:c:215:ASP:HB2	1.99	0.45
1:c:555:ASN:OD1	1:c:558:ASN:ND2	2.47	0.45
1:c:599:LYS:O	1:c:601:GLU:N	2.47	0.45
1:d:135:VAL:HG21	1:d:204:PHE:CE2	2.51	0.45
1:f:410:GLU:O	1:f:414:MET:N	2.48	0.45
1:f:591:ARG:HA	1:f:594:LYS:HD2	1.98	0.45
1:l:16:LEU:HD12	1:l:307:TYR:CE1	2.50	0.45
1:j:92:ASP:HA	1:i:492:VAL:HG12	1.97	0.45
1:i:461:ASP:OD1	1:i:517:VAL:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:118:PHE:HA	1:h:121:MET:HE2	1.98	0.45
1:h:425:ARG:HH12	1:f:393:VAL:HA	1.80	0.45
1:h:436:ASP:OD1	1:h:436:ASP:N	2.49	0.45
1:c:491:GLU:HB2	1:c:498:LYS:HG3	1.97	0.45
1:e:491:GLU:HB2	1:e:498:LYS:HB2	1.98	0.45
1:l:469:GLU:HG3	1:k:118:PHE:CD2	2.51	0.45
1:l:499:TRP:CH2	1:l:504:PRO:HB3	2.51	0.45
1:k:429:THR:HG23	1:j:433:ARG:NH1	2.31	0.45
1:j:135:VAL:HG11	1:j:204:PHE:CE2	2.52	0.45
1:c:121:MET:HE3	1:c:121:MET:HB3	1.84	0.45
1:d:22:LEU:HD21	1:d:218:PHE:HB2	1.98	0.45
1:d:124:TRP:CZ2	1:d:326:LEU:HD22	2.52	0.45
1:e:351:ARG:HE	1:e:418:LEU:HD23	1.80	0.45
1:f:109:TYR:CE2	1:f:491:GLU:HB3	2.52	0.45
1:b:112:MET:O	1:b:113:ARG:HG2	2.16	0.45
1:l:497:GLY:C	1:l:498:LYS:HD2	2.41	0.45
1:j:16:LEU:HD11	1:j:313:ILE:HD11	1.98	0.45
1:d:362:ILE:HG22	1:e:357:ASN:ND2	2.32	0.45
1:e:371:VAL:HA	1:e:400:THR:O	2.16	0.45
1:e:496:ARG:HH21	1:f:92:ASP:C	2.25	0.45
1:e:560:LEU:HB3	1:e:576:TRP:CE3	2.52	0.45
1:b:304:ARG:HD2	1:b:318:TRP:NE1	2.32	0.45
1:a:135:VAL:HG21	1:a:204:PHE:CG	2.51	0.45
1:l:46:PHE:C	1:l:63:ARG:HH12	2.24	0.45
1:l:103:GLU:HG3	1:l:499:TRP:CZ2	2.52	0.45
1:d:143:VAL:O	1:d:190:LYS:N	2.50	0.45
1:d:419:GLU:OE2	1:d:422:ARG:NH2	2.49	0.45
1:d:519:ILE:HG23	1:d:520:GLY:H	1.82	0.45
1:b:190:LYS:HA	1:b:190:LYS:HD2	1.76	0.45
1:b:200:LYS:O	1:b:202:GLU:N	2.50	0.45
1:a:217:ARG:HG3	1:a:218:PHE:CG	2.51	0.45
1:j:41:ALA:O	1:j:341:TYR:HE2	1.99	0.45
1:j:213:ILE:HB	1:j:325:ASP:OD2	2.16	0.45
1:j:551:VAL:HA	1:i:575:PHE:HZ	1.82	0.45
1:i:204:PHE:O	1:i:206:VAL:HG23	2.17	0.45
1:i:535:TRP:CE3	1:i:559:ILE:HG21	2.51	0.45
1:h:530:HIS:O	1:h:534:ILE:HG22	2.16	0.45
1:e:135:VAL:HG21	1:e:204:PHE:CE2	2.51	0.45
1:e:555:ASN:OD1	1:e:558:ASN:HB3	2.16	0.45
1:f:533:ARG:O	1:f:537:MET:HE3	2.16	0.45
1:f:587:ALA:HA	1:f:590:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:287:GLU:CD	1:b:304:ARG:HH21	2.25	0.45
1:a:330:ARG:HH22	1:l:119:LYS:HB3	1.82	0.45
1:l:515:VAL:HG13	1:l:516:THR:OG1	2.17	0.45
1:k:443:ASN:HB3	1:k:447:MET:HA	1.99	0.45
1:i:424:LYS:HE2	1:h:431:ARG:O	2.17	0.45
1:i:471:GLY:O	1:i:474:ARG:HG2	2.17	0.45
1:h:502:VAL:C	1:h:504:PRO:HD3	2.42	0.45
1:d:139:TYR:CB	1:d:195:LYS:HE3	2.46	0.45
1:e:108:ASN:O	1:e:112:MET:HG2	2.17	0.45
1:b:425:ARG:HD3	1:a:67:GLU:HG2	1.98	0.45
1:a:550:LEU:HD23	1:a:550:LEU:HA	1.86	0.45
1:j:124:TRP:NE1	1:j:198:CYS:SG	2.89	0.45
1:j:318:TRP:CG	1:j:319:ASP:H	2.34	0.45
1:i:207:ASP:OD1	1:i:207:ASP:N	2.46	0.45
1:h:124:TRP:NE1	1:h:326:LEU:HD11	2.32	0.45
1:c:135:VAL:HG22	1:c:199:VAL:HG21	1.99	0.45
1:c:488:ASN:HB3	1:c:500:VAL:HG22	1.97	0.45
1:e:202:GLU:N	1:e:202:GLU:OE1	2.48	0.45
1:f:52:ASN:HB2	1:f:356:ARG:NH1	2.31	0.45
1:l:559:ILE:HG13	1:k:574:ARG:NH2	2.32	0.45
1:j:218:PHE:HA	1:j:290:THR:HG22	1.99	0.45
1:i:460:ILE:HA	1:i:463:ILE:HD12	1.99	0.45
1:h:424:LYS:NZ	1:f:370:SER:O	2.46	0.45
1:c:503:ASN:N	1:c:504:PRO:HD3	2.32	0.45
1:e:137:LYS:HZ1	1:e:197:LEU:HD11	1.81	0.45
1:e:307:TYR:HA	1:e:313:ILE:HD13	1.99	0.45
1:f:547:LEU:HA	1:f:550:LEU:HB2	1.98	0.45
1:k:110:LEU:HD22	1:k:482:HIS:NE2	2.32	0.44
1:k:207:ASP:OD1	1:k:208:ARG:N	2.51	0.44
1:h:227:VAL:HG21	1:h:281:ARG:HG2	1.99	0.44
1:d:570:LYS:H	1:d:570:LYS:HG2	1.55	0.44
1:b:428:ILE:H	1:a:433:ARG:CZ	2.29	0.44
1:a:239:VAL:HG12	1:a:240:ILE:N	2.32	0.44
1:l:499:TRP:HH2	1:l:504:PRO:HB3	1.82	0.44
1:k:491:GLU:HB2	1:k:498:LYS:HD3	2.00	0.44
1:h:552:SER:O	1:h:556:LEU:N	2.47	0.44
1:d:124:TRP:HZ2	1:d:324:ALA:HB1	1.81	0.44
1:d:287:GLU:O	1:d:287:GLU:HG2	2.17	0.44
1:d:525:ASP:HA	1:d:528:MET:HG3	1.99	0.44
1:e:302:LEU:HD22	1:e:321:ARG:HG2	1.99	0.44
1:e:452:LEU:HD23	1:e:452:LEU:HA	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:57:LYS:HE2	1:f:364:ARG:HH21	1.82	0.44
1:b:431:ARG:HG3	1:b:433:ARG:HB2	1.98	0.44
1:k:110:LEU:HD21	1:k:194:ILE:HG21	1.99	0.44
1:j:456:ALA:HB3	1:i:433:ARG:HG2	1.98	0.44
1:i:493:PHE:HD2	1:i:498:LYS:HZ1	1.65	0.44
1:c:230:LEU:HD11	1:c:283:VAL:HG11	1.98	0.44
1:c:326:LEU:HD11	1:c:474:ARG:NH2	2.32	0.44
1:d:574:ARG:CZ	1:e:559:ILE:HD11	2.48	0.44
1:e:346:ASP:OD1	1:e:346:ASP:N	2.48	0.44
1:f:468:ALA:O	1:f:472:VAL:HG23	2.18	0.44
1:b:106:TYR:HE1	1:b:491:GLU:HG2	1.83	0.44
1:a:555:ASN:OD1	1:a:558:ASN:ND2	2.51	0.44
1:k:121:MET:HA	1:k:124:TRP:HD1	1.82	0.44
1:i:523:ASN:O	1:i:527:GLN:HG3	2.16	0.44
1:c:472:VAL:HG11	1:c:510:ARG:NE	2.33	0.44
1:c:486:TYR:O	1:c:487:GLN:HG3	2.17	0.44
1:e:89:TYR:CD1	1:e:510:ARG:HD2	2.52	0.44
1:e:331:ILE:HG13	1:e:332:ALA:N	2.32	0.44
1:e:463:ILE:HG23	1:e:467:PHE:HE2	1.81	0.44
1:b:428:ILE:H	1:a:433:ARG:NH1	2.16	0.44
1:a:360:ASP:OD1	1:a:361:ASN:N	2.50	0.44
1:i:462:LEU:HD12	1:h:74:PRO:HA	1.99	0.44
1:h:134:GLY:H	1:h:326:LEU:HB2	1.82	0.44
1:h:545:GLY:HA2	1:f:431:ARG:HH12	1.82	0.44
1:a:229:ASP:O	1:a:232:LEU:HG	2.18	0.44
1:a:500:VAL:HG22	1:a:502:VAL:H	1.82	0.44
1:l:76:LEU:HD13	1:l:467:PHE:HE2	1.82	0.44
1:l:338:MET:HE2	1:l:338:MET:HB3	1.90	0.44
1:l:443:ASN:OD1	1:l:447:MET:N	2.30	0.44
1:k:450:ASN:HB2	1:k:453:MET:HA	1.98	0.44
1:j:73:MET:HE3	1:j:73:MET:HA	1.99	0.44
1:d:213:ILE:HD13	1:d:325:ASP:OD2	2.17	0.44
1:e:465:ARG:HA	1:e:516:THR:HG21	1.99	0.44
1:b:445:ALA:O	1:b:449:VAL:N	2.44	0.44
1:b:557:TYR:OH	1:c:550:LEU:HD23	2.17	0.44
1:a:465:ARG:HB2	1:a:516:THR:HB	2.00	0.44
1:a:473:LYS:HA	1:a:476:PHE:CD2	2.53	0.44
1:a:588:LYS:O	1:a:592:GLU:HB3	2.17	0.44
1:k:29:PHE:HB3	1:k:208:ARG:NE	2.33	0.44
1:k:331:ILE:HD12	1:k:331:ILE:HA	1.92	0.44
1:i:425:ARG:HG3	1:i:426:THR:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:192:ARG:HB2	1:h:486:TYR:O	2.18	0.44
1:c:47:GLY:HA3	1:c:63:ARG:NH2	2.33	0.44
1:c:125:PHE:HA	1:c:128:THR:HG22	1.98	0.44
1:c:586:GLN:HB3	1:c:591:ARG:NH1	2.29	0.44
1:d:351:ARG:NH1	1:d:419:GLU:OE1	2.51	0.44
1:e:63:ARG:HD2	1:e:66:GLN:NE2	2.33	0.44
1:e:555:ASN:O	1:e:559:ILE:HG13	2.17	0.44
1:l:38:ARG:NH2	1:l:133:THR:OG1	2.51	0.44
1:c:575:PHE:HB2	1:d:551:VAL:HG23	1.99	0.44
1:e:127:ASP:HB3	1:e:134:GLY:HA2	1.99	0.44
1:f:210:ALA:H	1:f:335:PHE:HE1	1.66	0.44
1:f:222:ARG:HG2	1:f:286:SER:HA	2.00	0.44
1:f:561:LYS:HB3	1:f:570:LYS:HZ3	1.83	0.44
1:b:446:ALA:H	1:b:532:MET:HE1	1.82	0.44
1:l:444:GLN:CD	1:k:443:ASN:HB2	2.43	0.44
1:l:575:PHE:N	1:l:576:TRP:HE3	2.16	0.44
1:k:144:LEU:HA	1:k:189:LYS:HA	1.99	0.44
1:j:408:SER:O	1:j:411:VAL:HG12	2.17	0.44
1:j:417:ARG:O	1:j:420:ALA:HB3	2.18	0.44
1:i:346:ASP:OD1	1:i:347:ILE:N	2.50	0.44
1:h:502:VAL:HG12	1:h:502:VAL:O	2.18	0.44
1:c:121:MET:HA	1:c:124:TRP:CD1	2.53	0.44
1:e:137:LYS:NZ	1:e:197:LEU:HD21	2.33	0.44
1:e:423:GLY:HA3	1:e:428:ILE:HA	2.00	0.44
1:b:287:GLU:OE2	1:b:304:ARG:NH2	2.50	0.43
1:b:575:PHE:CD2	1:c:555:ASN:HB2	2.52	0.43
1:k:446:ALA:HA	1:k:532:MET:HE3	2.00	0.43
1:k:465:ARG:N	1:k:516:THR:HG21	2.33	0.43
1:j:86:VAL:HG12	1:j:87:VAL:HG23	2.00	0.43
1:j:416:ASP:O	1:j:419:GLU:HB3	2.18	0.43
1:h:463:ILE:HG23	1:h:467:PHE:CE2	2.53	0.43
1:c:144:LEU:HD23	1:c:189:LYS:HB2	2.00	0.43
1:c:228:SER:O	1:c:232:LEU:HG	2.17	0.43
1:d:443:ASN:N	1:e:444:GLN:OE1	2.43	0.43
1:d:480:HIS:O	1:d:484:ILE:HG13	2.18	0.43
1:e:239:VAL:HG13	1:e:241:GLU:H	1.82	0.43
1:f:19:LEU:HA	1:f:22:LEU:HD12	1.99	0.43
1:a:143:VAL:HG12	1:a:144:LEU:H	1.83	0.43
1:l:110:LEU:HD22	1:l:482:HIS:CE1	2.52	0.43
1:l:214:ASP:OD1	1:l:321:ARG:NH1	2.52	0.43
1:l:446:ALA:HB3	1:l:449:VAL:HG13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:595:GLU:N	1:l:595:GLU:OE1	2.51	0.43
1:k:9:PRO:HA	1:k:296:GLY:HA3	1.99	0.43
1:k:239:VAL:HG11	1:k:309:GLY:HA3	2.00	0.43
1:k:493:PHE:O	1:k:495:LEU:HD23	2.18	0.43
1:k:577:THR:HG22	1:k:579:PRO:HG3	2.00	0.43
1:i:30:ASN:OD1	1:i:34:LEU:HB3	2.18	0.43
1:i:581:SER:H	1:i:584:ALA:HB3	1.83	0.43
1:d:95:GLU:HG2	1:d:95:GLU:O	2.18	0.43
1:d:492:VAL:HG12	1:e:93:THR:HG23	1.99	0.43
1:d:527:GLN:HB3	1:d:566:ASN:CG	2.43	0.43
1:a:135:VAL:HG21	1:a:204:PHE:CD2	2.54	0.43
1:a:430:ASP:HB3	1:a:431:ARG:NH1	2.34	0.43
1:i:196:VAL:C	1:i:197:LEU:HD12	2.43	0.43
1:h:226:THR:HG22	1:h:282:GLU:HA	2.00	0.43
1:c:47:GLY:HA3	1:c:63:ARG:HH22	1.83	0.43
1:c:65:VAL:HB	1:c:341:TYR:HE1	1.83	0.43
1:c:140:VAL:HA	1:c:193:GLU:O	2.18	0.43
1:c:415:LEU:O	1:c:418:LEU:HB2	2.18	0.43
1:e:139:TYR:OH	1:e:287:GLU:OE2	2.35	0.43
1:a:65:VAL:HG21	1:a:341:TYR:CD1	2.54	0.43
1:a:583:GLU:O	1:a:586:GLN:HG3	2.19	0.43
1:k:442:SER:H	1:j:440:LEU:HD12	1.83	0.43
1:k:537:MET:HE3	1:j:535:TRP:CD2	2.53	0.43
1:j:303:ARG:HH11	1:j:315:ASN:HD21	1.66	0.43
1:i:137:LYS:NZ	1:i:287:GLU:OE2	2.38	0.43
1:d:128:THR:HG21	1:d:467:PHE:HE1	1.82	0.43
1:d:497:GLY:O	1:d:498:LYS:HD2	2.18	0.43
1:e:550:LEU:HD23	1:e:551:VAL:HG12	1.99	0.43
1:f:38:ARG:HD2	1:f:131:MET:SD	2.58	0.43
1:l:308:VAL:HG23	1:l:311:TYR:HB2	2.01	0.43
1:k:201:PRO:C	1:k:203:ASN:H	2.26	0.43
1:j:428:ILE:HD12	1:i:433:ARG:HD2	2.00	0.43
1:i:19:LEU:HD12	1:i:22:LEU:HB2	1.98	0.43
1:i:220:CYS:O	1:i:221:HIS:ND1	2.51	0.43
1:i:458:GLN:HB3	1:i:460:ILE:HG12	1.99	0.43
1:e:76:LEU:HB3	1:e:125:PHE:CE2	2.54	0.43
1:b:113:ARG:NH1	1:c:90:GLU:OE1	2.51	0.43
1:l:192:ARG:H	1:l:487:GLN:NE2	2.17	0.43
1:k:115:ASN:C	1:k:117:GLY:H	2.27	0.43
1:k:503:ASN:N	1:k:504:PRO:HD3	2.34	0.43
1:j:144:LEU:HG	1:j:145:LYS:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:124:TRP:HE1	1:i:474:ARG:HH22	1.65	0.43
1:i:330:ARG:NE	1:i:466:MET:HB2	2.33	0.43
1:i:563:VAL:HA	1:i:566:ASN:ND2	2.33	0.43
1:h:140:VAL:HG22	1:h:194:ILE:HD12	2.01	0.43
1:c:91:PRO:HB3	1:c:507:TRP:CZ3	2.53	0.43
1:c:211:THR:H	1:c:335:PHE:HB2	1.83	0.43
1:d:366:ASN:ND2	1:e:357:ASN:OD1	2.39	0.43
1:e:71:TRP:CD1	1:e:432:THR:HG1	2.37	0.43
1:e:468:ALA:O	1:e:472:VAL:HG13	2.18	0.43
1:f:16:LEU:HD23	1:f:307:TYR:OH	2.18	0.43
1:l:110:LEU:HD22	1:l:482:HIS:NE2	2.34	0.43
1:l:110:LEU:O	1:l:114:LYS:HB3	2.18	0.43
1:l:486:TYR:HB3	1:l:487:GLN:OE1	2.18	0.43
1:k:449:VAL:HG11	1:j:528:MET:HE1	2.00	0.43
1:d:331:ILE:HG12	1:d:332:ALA:H	1.83	0.43
1:f:57:LYS:HE2	1:f:364:ARG:NH2	2.33	0.43
1:f:358:ILE:O	1:f:362:ILE:HG12	2.19	0.43
1:l:492:VAL:HG12	1:l:492:VAL:O	2.18	0.43
1:l:590:ILE:O	1:l:594:LYS:HG2	2.18	0.43
1:h:359:MET:HG3	1:h:362:ILE:HD12	2.01	0.43
1:d:346:ASP:OD1	1:d:346:ASP:N	2.51	0.43
1:b:444:GLN:NE2	1:a:443:ASN:H	2.17	0.43
1:a:36:LYS:HB3	1:a:36:LYS:HE2	1.79	0.43
1:l:91:PRO:CD	1:l:100:ALA:HB2	2.46	0.43
1:l:376:GLN:O	1:l:379:LEU:N	2.38	0.43
1:k:371:VAL:HA	1:k:402:LEU:HG	2.01	0.43
1:k:455:ALA:HB3	1:k:458:GLN:HE21	1.84	0.43
1:j:217:ARG:NH2	1:i:280:ASN:HB3	2.33	0.43
1:j:507:TRP:O	1:j:509:GLU:N	2.51	0.43
1:i:330:ARG:NH2	1:i:470:THR:HG23	2.30	0.43
1:i:530:HIS:ND1	1:i:562:GLU:OE1	2.51	0.43
1:h:128:THR:OG1	1:h:328:ALA:HB2	2.19	0.43
1:c:32:SER:HG	1:c:33:GLU:CD	2.25	0.43
1:d:459:GLN:O	1:d:463:ILE:HG13	2.19	0.43
1:b:433:ARG:HH21	1:c:458:GLN:HG2	1.83	0.43
1:k:120:VAL:O	1:k:124:TRP:CD1	2.72	0.43
1:k:581:SER:OG	1:k:584:ALA:HB3	2.18	0.43
1:j:429:THR:HA	1:i:435:LEU:HD11	2.01	0.43
1:j:490:GLU:OE2	1:j:497:GLY:N	2.23	0.43
1:i:465:ARG:HD3	1:i:516:THR:OG1	2.18	0.43
1:h:362:ILE:O	1:h:365:THR:OG1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:371:VAL:HG22	1:c:402:LEU:HD12	2.01	0.43
1:d:115:ASN:C	1:d:116:GLU:HG3	2.44	0.43
1:f:140:VAL:HG22	1:f:194:ILE:HD11	2.00	0.43
1:b:293:ASP:OD1	1:b:293:ASP:N	2.51	0.42
1:b:573:ASP:C	1:b:574:ARG:HD2	2.44	0.42
1:b:575:PHE:HE2	1:c:555:ASN:H	1.64	0.42
1:c:96:ASP:OD1	1:c:97:VAL:N	2.49	0.42
1:c:241:GLU:HA	1:c:283:VAL:HG23	2.01	0.42
1:c:557:TYR:OH	1:d:549:VAL:O	2.34	0.42
1:e:366:ASN:ND2	1:f:360:ASP:OD2	2.51	0.42
1:f:137:LYS:NZ	1:f:287:GLU:OE1	2.41	0.42
1:f:291:LEU:HD23	1:f:291:LEU:H	1.84	0.42
1:b:383:LEU:O	1:b:387:ALA:N	2.50	0.42
1:l:239:VAL:HG12	1:l:240:ILE:N	2.34	0.42
1:i:298:GLY:HA2	1:h:231:ARG:NH1	2.34	0.42
1:e:207:ASP:OD1	1:e:207:ASP:N	2.44	0.42
1:f:347:ILE:HG21	1:f:422:ARG:HG3	2.00	0.42
1:k:136:VAL:HG12	1:k:137:LYS:N	2.34	0.42
1:k:218:PHE:CZ	1:k:220:CYS:HB2	2.54	0.42
1:k:326:LEU:HD11	1:k:474:ARG:HH22	1.84	0.42
1:k:530:HIS:O	1:k:535:TRP:HD1	2.02	0.42
1:j:474:ARG:HE	1:j:475:LEU:HD23	1.84	0.42
1:j:552:SER:H	1:i:575:PHE:HZ	1.67	0.42
1:c:110:LEU:HD22	1:c:482:HIS:CE1	2.55	0.42
1:c:416:ASP:OD1	1:c:417:ARG:N	2.51	0.42
1:d:560:LEU:HD13	1:d:576:TRP:CZ3	2.54	0.42
1:b:128:THR:HG22	1:b:328:ALA:HB2	2.01	0.42
1:b:351:ARG:NE	1:b:419:GLU:OE2	2.47	0.42
1:a:78:LYS:HD3	1:a:78:LYS:HA	1.89	0.42
1:a:92:ASP:HB2	1:l:496:ARG:HH21	1.84	0.42
1:a:407:LEU:HD21	1:a:411:VAL:HG21	2.00	0.42
1:a:515:VAL:HG22	1:a:516:THR:HG23	2.02	0.42
1:a:560:LEU:O	1:a:564:THR:HG23	2.19	0.42
1:i:535:TRP:CZ2	1:i:560:LEU:HD21	2.55	0.42
1:h:308:VAL:HG13	1:h:309:GLY:H	1.84	0.42
1:c:280:ASN:HB2	1:d:217:ARG:NH2	2.35	0.42
1:d:547:LEU:HG	1:d:552:SER:HA	2.01	0.42
1:f:376:GLN:O	1:f:378:ASN:N	2.52	0.42
1:b:120:VAL:HG21	1:b:196:VAL:HG23	2.01	0.42
1:a:110:LEU:HD23	1:a:478:LEU:HD22	2.01	0.42
1:l:561:LYS:NZ	1:l:577:THR:O	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:358:ILE:O	1:k:362:ILE:HG12	2.19	0.42
1:j:106:TYR:OH	1:j:489:GLN:OE1	2.27	0.42
1:i:188:ASP:OD1	1:i:188:ASP:N	2.44	0.42
1:i:357:ASN:ND2	1:h:362:ILE:HG12	2.35	0.42
1:h:89:TYR:CE2	1:h:103:GLU:HB2	2.53	0.42
1:c:303:ARG:NH1	1:c:315:ASN:HB3	2.35	0.42
1:e:60:ILE:HD12	1:e:359:MET:HG3	2.02	0.42
1:f:230:LEU:HD23	1:f:235:VAL:HG21	2.02	0.42
1:b:554:GLN:HB3	1:a:575:PHE:CZ	2.55	0.42
1:a:214:ASP:OD1	1:a:214:ASP:N	2.51	0.42
1:a:465:ARG:HD3	1:a:516:THR:OG1	2.19	0.42
1:j:428:ILE:HB	1:i:433:ARG:HH11	1.83	0.42
1:j:454:THR:O	1:j:458:GLN:HG2	2.20	0.42
1:j:487:GLN:O	1:j:500:VAL:HG13	2.20	0.42
1:i:58:SER:N	1:i:360:ASP:OD1	2.52	0.42
1:i:223:GLU:HB2	1:i:225:TYR:CE2	2.54	0.42
1:i:421:ASP:O	1:i:424:LYS:HB3	2.18	0.42
1:e:443:ASN:HB3	1:e:447:MET:HA	2.01	0.42
1:f:564:THR:HG22	1:f:574:ARG:HB3	2.01	0.42
1:g:135:VAL:HA	1:g:324:ALA:HB3	2.02	0.42
1:b:325:ASP:C	1:b:326:LEU:HD12	2.45	0.42
1:l:22:LEU:HD22	1:l:218:PHE:CE2	2.54	0.42
1:k:62:SER:O	1:k:348:GLN:HG3	2.20	0.42
1:k:331:ILE:HG13	1:k:332:ALA:H	1.85	0.42
1:c:19:LEU:HB3	1:c:307:TYR:HE2	1.85	0.42
1:c:527:GLN:OE1	1:c:566:ASN:ND2	2.52	0.42
1:c:569:TYR:HE2	1:d:530:HIS:HE2	1.68	0.42
1:e:143:VAL:HG12	1:e:144:LEU:N	2.35	0.42
1:f:53:GLU:HG2	1:f:59:GLY:HA2	2.02	0.42
1:f:361:ASN:OD1	1:f:406:GLN:HB3	2.20	0.42
1:b:224:LYS:HA	1:b:224:LYS:HD3	1.76	0.42
1:b:554:GLN:HB3	1:a:575:PHE:HZ	1.84	0.42
1:l:530:HIS:O	1:l:534:ILE:HB	2.19	0.42
1:k:548:GLY:H	1:j:591:ARG:HH11	1.67	0.42
1:j:132:LYS:HG2	1:j:339:SER:HB3	2.02	0.42
1:d:89:TYR:CZ	1:d:479:LEU:HD22	2.55	0.42
1:d:433:ARG:NH2	1:e:459:GLN:H	2.16	0.42
1:a:85:GLN:OE1	1:a:85:GLN:N	2.53	0.42
1:a:514:THR:C	1:a:520:GLY:HA2	2.45	0.42
1:l:302:LEU:HD11	1:l:321:ARG:HE	1.85	0.42
1:l:507:TRP:O	1:l:509:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:62:SER:HB3	1:h:355:MET:HG3	2.01	0.42
1:c:359:MET:O	1:c:362:ILE:HG22	2.19	0.42
1:c:468:ALA:O	1:c:472:VAL:HG23	2.20	0.42
1:d:306:LEU:C	1:d:313:ILE:HG23	2.45	0.42
1:f:219:LEU:HG	1:f:221:HIS:CE1	2.55	0.42
1:f:453:MET:O	1:f:456:ALA:CA	2.68	0.42
1:b:210:ALA:C	1:b:212:CYS:H	2.28	0.42
1:b:432:THR:O	1:c:456:ALA:HB3	2.20	0.42
1:a:407:LEU:HD23	1:a:408:SER:O	2.19	0.42
1:l:36:LYS:O	1:l:40:GLU:HG2	2.20	0.42
1:l:321:ARG:HA	1:l:322:PRO:HD3	1.89	0.42
1:l:518:GLY:O	1:l:520:GLY:N	2.53	0.42
1:l:534:ILE:HG23	1:k:576:TRP:CH2	2.54	0.42
1:k:136:VAL:CG1	1:k:138:VAL:HG23	2.50	0.42
1:k:227:VAL:HG23	1:k:281:ARG:H	1.83	0.42
1:i:124:TRP:O	1:i:128:THR:HG23	2.19	0.42
1:i:560:LEU:O	1:i:564:THR:HG23	2.20	0.42
1:h:545:GLY:HA2	1:f:431:ARG:NH1	2.34	0.42
1:c:76:LEU:HB3	1:c:125:PHE:CE2	2.55	0.42
1:c:77:MET:HE3	1:c:118:PHE:CE1	2.55	0.42
1:d:443:ASN:H	1:e:444:GLN:CD	2.26	0.42
1:e:18:HIS:ND1	1:e:19:LEU:HD12	2.35	0.42
1:e:65:VAL:O	1:e:68:THR:OG1	2.34	0.42
1:e:496:ARG:HH22	1:f:95:GLU:CG	2.33	0.42
1:f:227:VAL:HA	1:f:230:LEU:HD13	2.01	0.42
1:b:87:VAL:HG11	1:b:475:LEU:HG	2.02	0.41
1:a:218:PHE:CD1	1:a:290:THR:HG23	2.55	0.41
1:a:487:GLN:HG3	1:a:488:ASN:H	1.84	0.41
1:k:301:GLU:OE2	1:k:319:ASP:HA	2.20	0.41
1:j:237:GLU:HG2	1:j:238:ASP:N	2.34	0.41
1:i:448:SER:OG	1:h:441:HIS:NE2	2.50	0.41
1:e:506:ASN:O	1:e:510:ARG:NH2	2.53	0.41
1:f:332:ALA:O	1:f:334:LYS:N	2.54	0.41
1:f:491:GLU:HB2	1:f:498:LYS:HD2	2.02	0.41
1:b:555:ASN:HB2	1:a:575:PHE:CD2	2.55	0.41
1:b:597:GLN:HG2	1:b:598:PRO:CD	2.50	0.41
1:a:369:ARG:HA	1:a:402:LEU:HD22	2.02	0.41
1:a:590:ILE:O	1:a:594:LYS:HB3	2.20	0.41
1:l:503:ASN:N	1:l:504:PRO:HD3	2.35	0.41
1:k:575:PHE:HE2	1:k:578:ASN:CG	2.29	0.41
1:c:496:ARG:NE	1:d:94:ALA:H	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:567:ALA:HB2	1:d:533:ARG:HH22	1.86	0.41
1:e:15:VAL:HG23	1:e:16:LEU:HD12	2.02	0.41
1:f:330:ARG:HD2	1:f:330:ARG:HA	1.75	0.41
1:b:498:LYS:HA	1:b:498:LYS:HD3	1.76	0.41
1:a:558:ASN:O	1:a:562:GLU:N	2.47	0.41
1:l:549:VAL:HA	1:k:584:ALA:HB1	2.03	0.41
1:j:416:ASP:OD1	1:j:416:ASP:N	2.52	0.41
1:j:432:THR:HG22	1:j:432:THR:O	2.20	0.41
1:j:440:LEU:HD23	1:j:440:LEU:HA	1.88	0.41
1:i:204:PHE:CD1	1:i:221:HIS:HE1	2.39	0.41
1:i:226:THR:OG1	1:i:227:VAL:N	2.53	0.41
1:h:426:THR:O	1:h:460:ILE:HG23	2.20	0.41
1:h:475:LEU:HB3	1:h:510:ARG:NH1	2.35	0.41
1:c:482:HIS:HA	1:c:486:TYR:CD2	2.56	0.41
1:d:295:ASP:OD2	1:d:300:SER:OG	2.27	0.41
1:d:533:ARG:O	1:d:537:MET:HG2	2.20	0.41
1:e:524:LYS:HG3	1:f:449:VAL:HG11	2.01	0.41
1:f:147:THR:HG23	1:f:186:ARG:C	2.45	0.41
1:b:214:ASP:OD1	1:b:215:ASP:N	2.54	0.41
1:b:457:GLU:OE2	1:a:75:SER:HA	2.20	0.41
1:a:15:VAL:HG12	1:a:292:LEU:HD13	2.02	0.41
1:k:128:THR:HG21	1:k:467:PHE:HE1	1.86	0.41
1:j:78:LYS:HB3	1:j:78:LYS:HE2	1.72	0.41
1:j:484:ILE:O	1:j:485:LYS:HG3	2.21	0.41
1:i:575:PHE:HE2	1:i:578:ASN:HD21	1.68	0.41
1:h:67:GLU:OE2	1:h:422:ARG:HD3	2.20	0.41
1:c:144:LEU:HD21	1:c:190:LYS:HE3	2.02	0.41
1:c:235:VAL:HA	1:c:236:PRO:HD3	1.92	0.41
1:e:280:ASN:HD22	1:f:217:ARG:NH1	2.18	0.41
1:e:460:ILE:HD12	1:e:460:ILE:H	1.85	0.41
1:e:574:ARG:CZ	1:f:559:ILE:HD11	2.49	0.41
1:f:19:LEU:HD11	1:f:307:TYR:CZ	2.56	0.41
1:f:65:VAL:HG23	1:f:348:GLN:HE22	1.84	0.41
1:f:189:LYS:C	1:f:190:LYS:HG2	2.45	0.41
1:f:590:ILE:O	1:f:593:GLN:HG2	2.21	0.41
1:b:103:GLU:CD	1:b:504:PRO:HG3	2.45	0.41
1:b:306:LEU:HB3	1:b:314:SER:OG	2.19	0.41
1:a:117:GLY:C	1:a:118:PHE:HD1	2.28	0.41
1:a:414:MET:HA	1:a:417:ARG:HD2	2.02	0.41
1:a:530:HIS:CE1	1:a:562:GLU:HB3	2.55	0.41
1:l:99:GLN:O	1:l:103:GLU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:291:LEU:H	1:l:291:LEU:HD23	1.84	0.41
1:j:94:ALA:HB3	1:i:496:ARG:CZ	2.50	0.41
1:j:131:MET:SD	1:j:131:MET:N	2.94	0.41
1:j:444:GLN:OE1	1:i:443:ASN:ND2	2.38	0.41
1:h:531:LEU:HA	1:h:535:TRP:HD1	1.86	0.41
1:h:549:VAL:HG11	1:g:427:GLY:O	2.21	0.41
1:h:557:TYR:CD2	1:h:578:ASN:HB2	2.55	0.41
1:c:76:LEU:HA	1:c:79:VAL:HG12	2.02	0.41
1:c:498:LYS:HA	1:c:498:LYS:HD3	1.80	0.41
1:d:496:ARG:HE	1:e:94:ALA:HB3	1.86	0.41
1:e:493:PHE:CD2	1:e:498:LYS:HD3	2.55	0.41
1:e:526:GLN:O	1:e:530:HIS:HB2	2.19	0.41
1:e:559:ILE:O	1:e:563:VAL:HG23	2.21	0.41
1:f:146:PRO:HG3	1:f:189:LYS:HG3	2.02	0.41
1:g:529:LEU:HA	1:g:533:ARG:H	1.86	0.41
1:a:99:GLN:O	1:a:103:GLU:HB2	2.21	0.41
1:k:15:VAL:HG12	1:k:292:LEU:HD13	2.01	0.41
1:k:378:ASN:HA	1:j:396:MET:HA	2.02	0.41
1:j:144:LEU:HA	1:j:189:LYS:HZ3	1.86	0.41
1:j:240:ILE:H	1:j:311:TYR:HE2	1.68	0.41
1:j:422:ARG:O	1:j:422:ARG:NH1	2.54	0.41
1:j:518:GLY:O	1:j:520:GLY:N	2.53	0.41
1:i:507:TRP:O	1:i:508:ARG:HG2	2.20	0.41
1:i:519:ILE:O	1:i:521:ASN:N	2.54	0.41
1:h:135:VAL:HG22	1:h:325:ASP:H	1.86	0.41
1:c:45:TYR:CD1	1:c:130:MET:HE1	2.55	0.41
1:c:135:VAL:HG11	1:c:204:PHE:CE2	2.55	0.41
1:c:423:GLY:O	1:c:428:ILE:HG13	2.21	0.41
1:f:582:PRO:O	1:f:586:GLN:HB3	2.20	0.41
1:b:552:SER:OG	1:b:553:GLU:N	2.51	0.41
1:l:361:ASN:C	1:l:361:ASN:HD22	2.28	0.41
1:k:106:TYR:HA	1:k:491:GLU:OE2	2.20	0.41
1:k:110:LEU:HD11	1:k:194:ILE:HB	2.03	0.41
1:k:193:GLU:OE2	1:k:195:LYS:HE3	2.20	0.41
1:k:197:LEU:HG	1:k:198:CYS:O	2.20	0.41
1:k:302:LEU:HD21	1:k:321:ARG:HE	1.85	0.41
1:k:450:ASN:ND2	1:k:453:MET:SD	2.88	0.41
1:k:471:GLY:O	1:k:474:ARG:HG2	2.19	0.41
1:i:351:ARG:HE	1:i:415:LEU:HD11	1.86	0.41
1:c:361:ASN:ND2	1:c:407:LEU:HG	2.34	0.41
1:c:578:ASN:HD21	1:c:588:LYS:NZ	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:326:LEU:HD13	1:e:467:PHE:CD1	2.55	0.41
1:e:509:GLU:O	1:e:510:ARG:HD3	2.20	0.41
1:a:94:ALA:HB3	1:l:496:ARG:NH1	2.36	0.41
1:l:502:VAL:C	1:l:504:PRO:HD3	2.46	0.41
1:i:40:GLU:HG2	1:i:345:ARG:HH22	1.86	0.41
1:i:304:ARG:O	1:i:305:ILE:HD13	2.21	0.41
1:i:574:ARG:HB3	1:i:576:TRP:NE1	2.35	0.41
1:d:589:ALA:C	1:d:590:ILE:HD13	2.46	0.41
1:e:96:ASP:OD1	1:e:97:VAL:N	2.53	0.41
1:e:471:GLY:C	1:e:473:LYS:N	2.78	0.41
1:f:11:ASP:HB3	1:f:293:ASP:O	2.21	0.41
1:a:65:VAL:HG21	1:a:341:TYR:HD1	1.86	0.41
1:a:293:ASP:OD1	1:a:299:ILE:HA	2.21	0.41
1:l:16:LEU:HA	1:l:307:TYR:OH	2.21	0.41
1:j:344:ILE:HA	1:j:347:ILE:HD12	2.03	0.41
1:i:561:LYS:O	1:i:564:THR:OG1	2.28	0.41
1:h:13:GLU:O	1:h:16:LEU:HB2	2.21	0.41
1:h:89:TYR:HB3	1:h:507:TRP:HZ3	1.86	0.41
1:h:144:LEU:HG	1:h:146:PRO:HD3	2.02	0.41
1:h:302:LEU:HD13	1:h:321:ARG:HG3	2.02	0.41
1:h:477:GLN:NE2	1:h:481:ASP:OD1	2.54	0.41
1:h:550:LEU:HD23	1:h:550:LEU:HA	1.94	0.41
1:c:101:GLU:O	1:c:105:GLU:N	2.38	0.41
1:c:522:MET:O	1:c:526:GLN:N	2.43	0.41
1:e:480:HIS:HE1	1:e:506:ASN:HB3	1.86	0.41
1:f:71:TRP:CD1	1:f:432:THR:HG22	2.56	0.41
1:f:531:LEU:HA	1:f:535:TRP:HB2	2.03	0.41
1:g:136:VAL:H	1:g:324:ALA:HB3	1.86	0.41
1:b:45:TYR:CE1	1:b:66:GLN:HG2	2.56	0.41
1:b:350:ILE:HD13	1:b:418:LEU:HD21	2.02	0.41
1:b:567:ALA:HA	1:c:529:LEU:HD21	2.03	0.41
1:b:575:PHE:O	1:b:576:TRP:C	2.63	0.41
1:a:424:LYS:HA	1:a:428:ILE:HG13	2.03	0.41
1:l:94:ALA:HB3	1:k:496:ARG:CZ	2.51	0.41
1:l:431:ARG:HG3	1:l:433:ARG:HB2	2.02	0.41
1:l:450:ASN:HB2	1:l:453:MET:HA	2.03	0.41
1:i:135:VAL:HG11	1:i:204:PHE:CG	2.56	0.41
1:i:341:TYR:HA	1:i:345:ARG:HG3	2.02	0.41
1:f:456:ALA:C	1:f:457:GLU:HG2	2.46	0.41
1:a:91:PRO:HG3	1:a:100:ALA:HB2	2.03	0.40
1:a:513:LEU:O	1:a:520:GLY:N	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:555:ASN:N	1:l:575:PHE:CE1	2.89	0.40
1:l:575:PHE:H	1:l:576:TRP:HE3	1.68	0.40
1:h:73:MET:HB2	1:h:74:PRO:HD3	2.03	0.40
1:h:431:ARG:C	1:h:433:ARG:H	2.29	0.40
1:c:192:ARG:HB3	1:c:486:TYR:CD1	2.55	0.40
1:d:123:ASP:HB2	1:d:198:CYS:SG	2.61	0.40
1:d:237:GLU:HB2	1:d:311:TYR:OH	2.20	0.40
1:e:34:LEU:HD13	1:e:38:ARG:NH2	2.36	0.40
1:g:134:GLY:O	1:g:326:LEU:N	2.45	0.40
1:b:285:ALA:HB2	1:b:308:VAL:HG23	2.03	0.40
1:b:362:ILE:HD13	1:b:362:ILE:HA	1.94	0.40
1:b:549:VAL:HG23	1:b:550:LEU:H	1.87	0.40
1:k:299:ILE:N	1:j:228:SER:OG	2.47	0.40
1:j:69:VAL:HG11	1:j:130:MET:HE1	2.02	0.40
1:i:200:LYS:HE3	1:i:202:GLU:OE2	2.21	0.40
1:d:14:GLN:HG3	1:d:17:ARG:HD2	2.03	0.40
1:d:65:VAL:HG21	1:d:341:TYR:CZ	2.56	0.40
1:a:547:LEU:HB3	1:a:552:SER:HA	2.03	0.40
1:k:204:PHE:O	1:k:206:VAL:HG23	2.22	0.40
1:j:546:GLY:N	1:j:550:LEU:HD13	2.36	0.40
1:i:200:LYS:O	1:i:202:GLU:N	2.54	0.40
1:c:16:LEU:HB3	1:c:310:ASP:OD1	2.21	0.40
1:c:575:PHE:O	1:c:577:THR:N	2.55	0.40
1:d:290:THR:O	1:d:302:LEU:HA	2.20	0.40
1:d:524:LYS:O	1:d:527:GLN:HG3	2.21	0.40
1:d:553:GLU:HB3	1:d:557:TYR:CZ	2.56	0.40
1:f:320:CYS:HG	1:f:321:ARG:H	1.67	0.40
1:b:575:PHE:HZ	1:c:554:GLN:HB2	1.85	0.40
1:l:562:GLU:O	1:l:565:GLU:HG3	2.21	0.40
1:k:124:TRP:HH2	1:k:136:VAL:HG22	1.85	0.40
1:j:19:LEU:HD11	1:j:288:CYS:HB2	2.03	0.40
1:j:92:ASP:OD1	1:j:92:ASP:N	2.54	0.40
1:j:292:LEU:O	1:j:300:SER:OG	2.26	0.40
1:c:575:PHE:O	1:c:576:TRP:C	2.64	0.40
1:e:13:GLU:HA	1:e:16:LEU:HD13	2.03	0.40
1:f:239:VAL:HG23	1:f:241:GLU:H	1.87	0.40
1:f:462:LEU:HD13	1:f:517:VAL:HG21	2.04	0.40
1:a:283:VAL:HG12	1:a:284:TRP:N	2.37	0.40
1:j:29:PHE:HB3	1:j:208:ARG:NH2	2.37	0.40
1:j:68:THR:HB	1:j:422:ARG:HH22	1.86	0.40
1:i:132:LYS:HE2	1:i:132:LYS:HB3	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:290:THR:O	1:i:302:LEU:HD12	2.21	0.40
1:i:468:ALA:O	1:i:472:VAL:HG23	2.21	0.40
1:h:460:ILE:HG13	1:h:461:ASP:N	2.36	0.40
1:e:193:GLU:HG2	1:e:486:TYR:HE1	1.87	0.40
1:e:311:TYR:CG	1:e:312:ILE:N	2.89	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	552/705 (78%)	442 (80%)	107 (19%)	3 (0%)	24	54
1	b	562/705 (80%)	480 (85%)	79 (14%)	3 (0%)	24	54
1	c	563/705 (80%)	454 (81%)	106 (19%)	3 (0%)	24	54
1	d	563/705 (80%)	453 (80%)	109 (19%)	1 (0%)	43	71
1	e	556/705 (79%)	464 (84%)	92 (16%)	0	100	100
1	f	512/705 (73%)	398 (78%)	113 (22%)	1 (0%)	43	71
1	g	338/705 (48%)	275 (81%)	62 (18%)	1 (0%)	36	65
1	h	553/705 (78%)	434 (78%)	118 (21%)	1 (0%)	43	71
1	i	558/705 (79%)	451 (81%)	107 (19%)	0	100	100
1	j	572/705 (81%)	475 (83%)	94 (16%)	3 (0%)	24	54
1	k	559/705 (79%)	450 (80%)	109 (20%)	0	100	100
1	l	549/705 (78%)	439 (80%)	106 (19%)	4 (1%)	18	47
All	All	6437/8460 (76%)	5215 (81%)	1202 (19%)	20 (0%)	37	65

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	j	371	VAL
1	b	325	ASP
1	b	517	VAL
1	a	377	VAL
1	a	508	ARG
1	c	576	TRP
1	d	371	VAL
1	l	371	VAL
1	l	377	VAL
1	l	575	PHE
1	j	449	VAL
1	c	371	VAL
1	g	213	ILE
1	a	371	VAL
1	h	371	VAL
1	c	507	TRP
1	j	377	VAL
1	f	377	VAL
1	b	377	VAL
1	l	449	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	430/614 (70%)	430 (100%)	0	100	100
1	b	426/614 (69%)	426 (100%)	0	100	100
1	c	439/614 (72%)	439 (100%)	0	100	100
1	d	432/614 (70%)	432 (100%)	0	100	100
1	e	432/614 (70%)	432 (100%)	0	100	100
1	f	425/614 (69%)	425 (100%)	0	100	100
1	h	375/614 (61%)	375 (100%)	0	100	100
1	i	428/614 (70%)	428 (100%)	0	100	100
1	j	432/614 (70%)	432 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	k	435/614 (71%)	435 (100%)	0	100	100
1	l	430/614 (70%)	430 (100%)	0	100	100
All	All	4684/6754 (69%)	4684 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	b	21	GLN
1	b	66	GLN
1	b	444	GLN
1	b	451	GLN
1	b	458	GLN
1	b	566	ASN
1	b	578	ASN
1	a	37	GLN
1	a	361	ASN
1	a	437	GLN
1	a	482	HIS
1	a	539	GLN
1	a	558	ASN
1	a	580	ASN
1	a	593	GLN
1	l	539	GLN
1	k	102	GLN
1	k	108	ASN
1	k	203	ASN
1	k	221	HIS
1	k	361	ASN
1	k	438	ASN
1	k	443	ASN
1	k	458	GLN
1	k	487	GLN
1	k	506	ASN
1	j	477	GLN
1	j	597	GLN
1	i	115	ASN
1	i	489	GLN
1	i	526	GLN
1	h	66	GLN

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Mol	Chain	Res	Type
1	h	203	ASN
1	h	458	GLN
1	h	494	GLN
1	h	526	GLN
1	c	438	ASN
1	c	443	ASN
1	c	527	GLN
1	c	566	ASN
1	d	24	ASN
1	d	450	ASN
1	d	494	GLN
1	e	102	GLN
1	e	203	ASN
1	f	85	GLN
1	f	108	ASN
1	f	221	HIS
1	f	357	ASN
1	f	450	ASN
1	f	487	GLN
1	f	526	GLN
1	f	558	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-25500. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.