Full wwPDB EM Validation Report ⓘ

Jan 22, 2025 – 07:04 PM JST

PDB ID	:	8ZB7
EMDB ID	:	EMD-39896
Title	:	Human left ventricle ATM complex
Authors	:	Li, D.N.; Zhao, Q.Y.; Liu, C.
Deposited on	:	2024-04-26
Resolution	:	3.19 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:

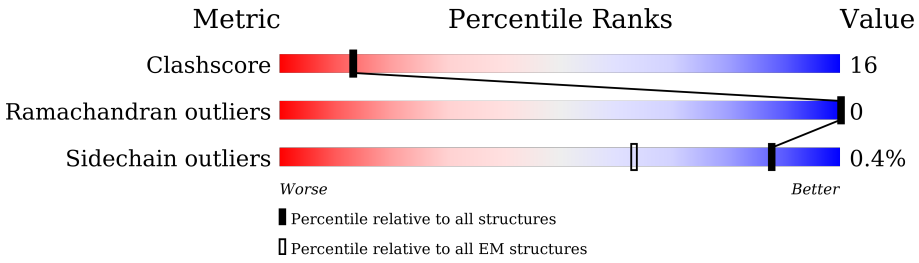
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.19 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 <=5%

Mol	Chain	Length	Quality of chain
1	G	776	58% 37% .
1	H	776	59% 36% .
1	I	776	58% 38% .
1	J	776	57% 38% .
1	K	776	58% 37% .
1	M	776	59% 37% .
2	A	371	78% 22%
2	B	371	81% 19%
2	C	371	79% 21%

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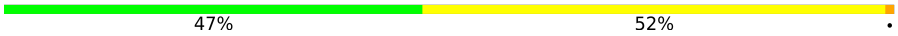
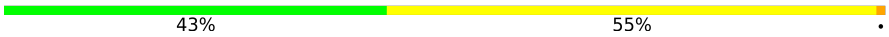
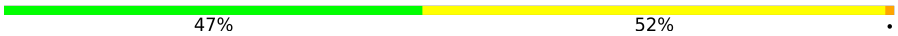
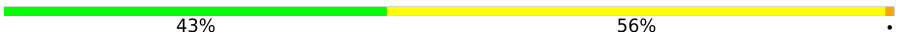
Mol	Chain	Length	Quality of chain
2	D	371	
2	E	371	
2	F	371	
3	L	166	
3	N	166	
3	O	166	
3	P	166	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 58698 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 Myosin-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	742	Total	C	N	O	S	0	0
			5974	3824	1016	1102	32		
1	G	742	Total	C	N	O	S	0	0
			5974	3824	1016	1102	32		
1	H	742	Total	C	N	O	S	0	0
			5974	3824	1016	1102	32		
1	I	742	Total	C	N	O	S	0	0
			5974	3824	1016	1102	32		
1	J	742	Total	C	N	O	S	0	0
			5974	3824	1016	1102	32		
1	K	742	Total	C	N	O	S	0	0
			5974	3824	1016	1102	32		

- Molecule 2 is a protein called Actin, alpha cardiac muscle 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		
2	C	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		
2	D	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		
2	E	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		
2	F	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		
2	A	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		

- Molecule 3 is a protein called Tropomyosin alpha-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	166	Total	C	N	O	S	0	0
			1326	806	230	287	3		

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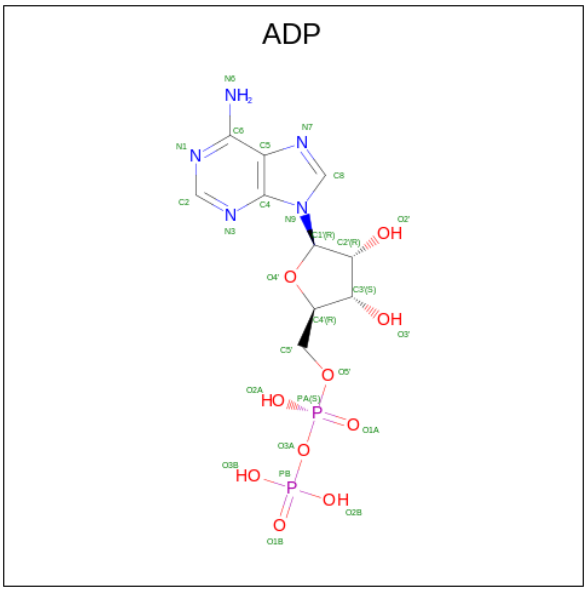
Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	166	Total	C	N	O	S	0	0
			1326	806	230	287	3		
3	L	166	Total	C	N	O	S	0	0
			1326	806	230	287	3		
3	N	166	Total	C	N	O	S	0	0
			1326	806	230	287	3		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



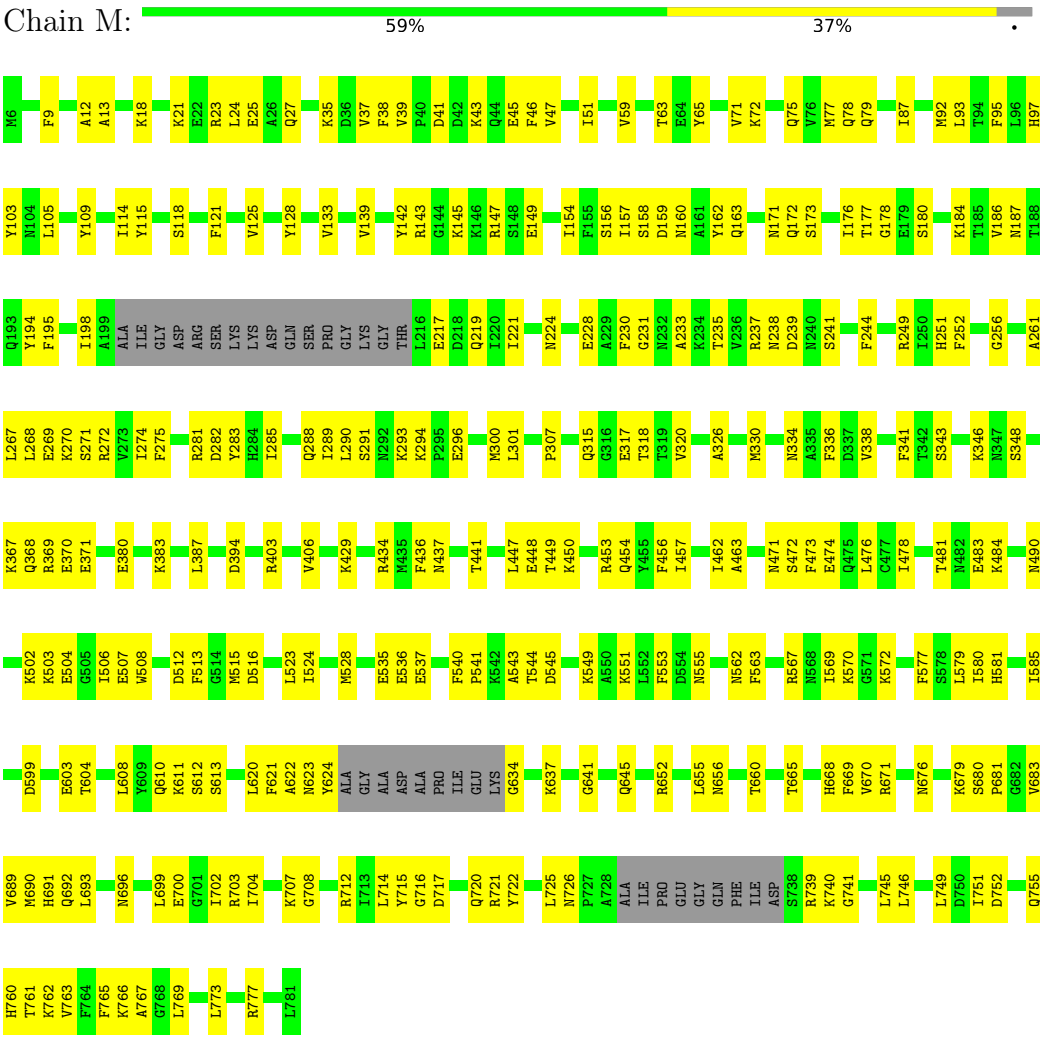
Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

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.

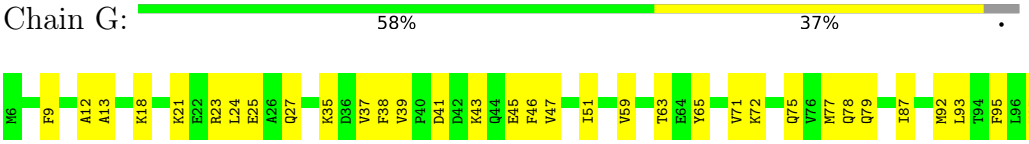
- Molecule 1: Myosin-7

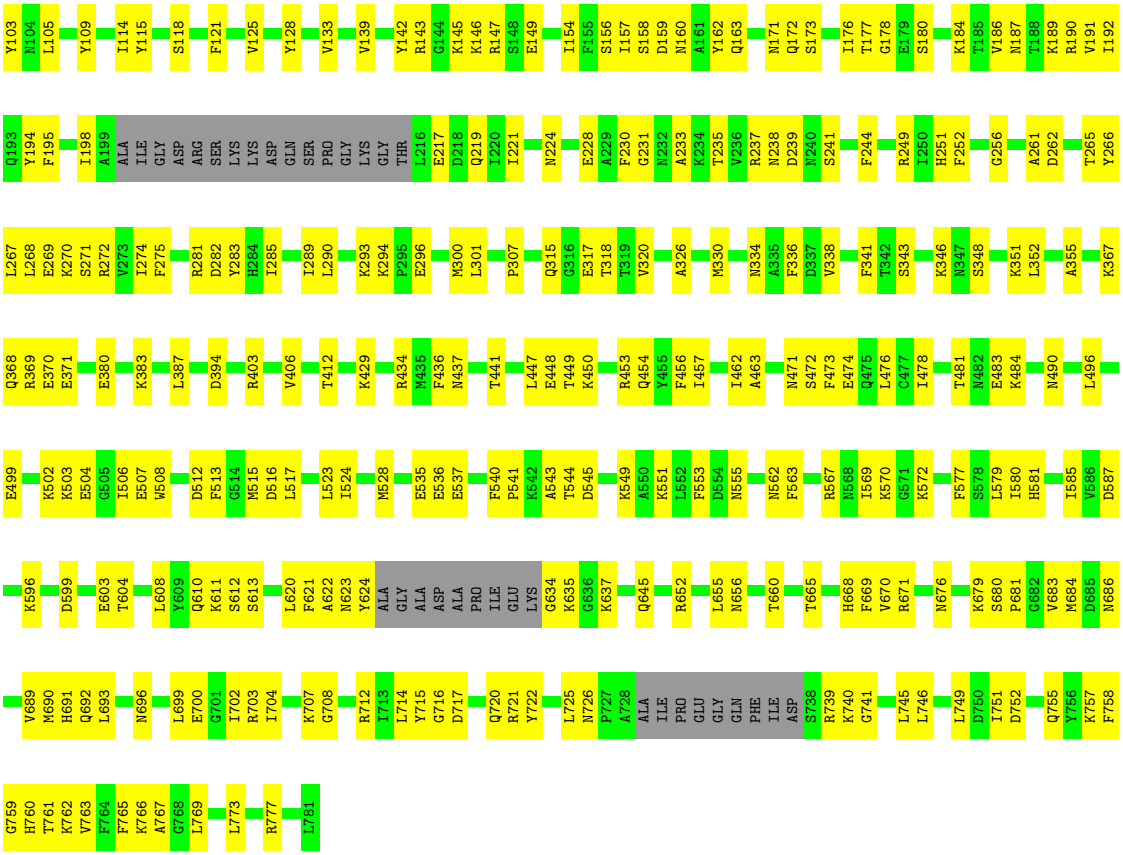
Chain M:



- Molecule 1: Myosin-7

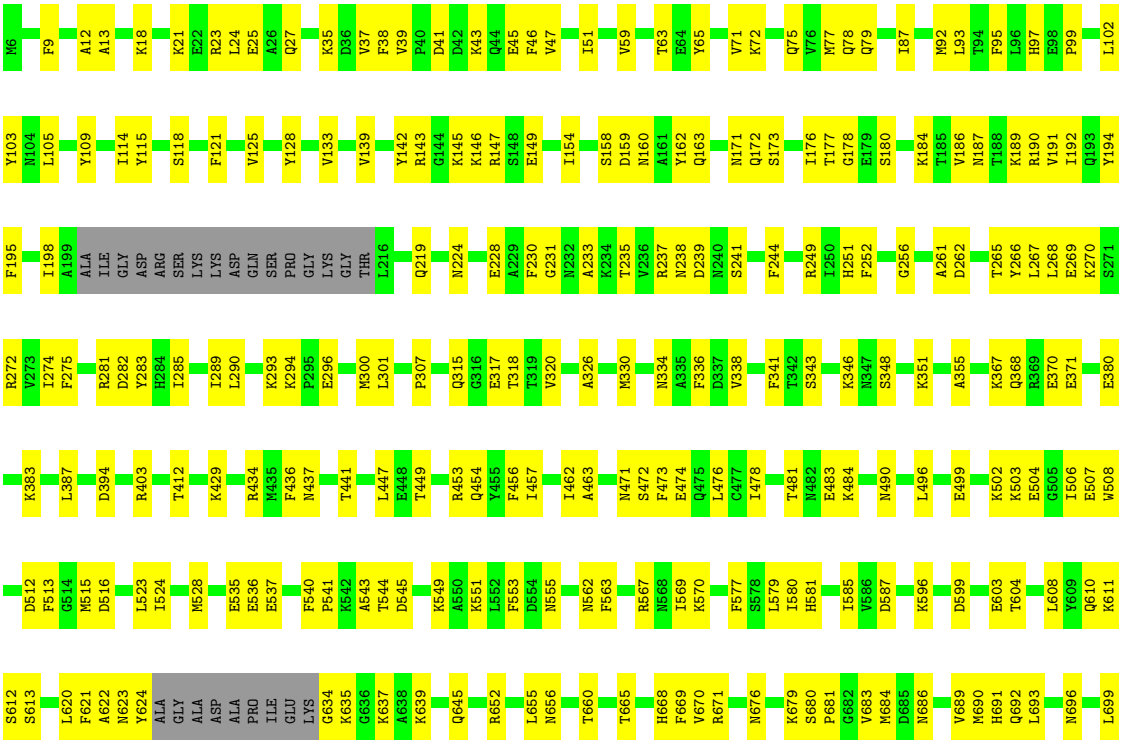
Chain G:

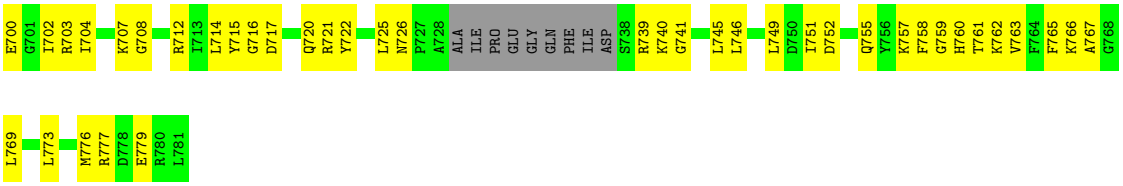




• Molecule 1: Myosin-7

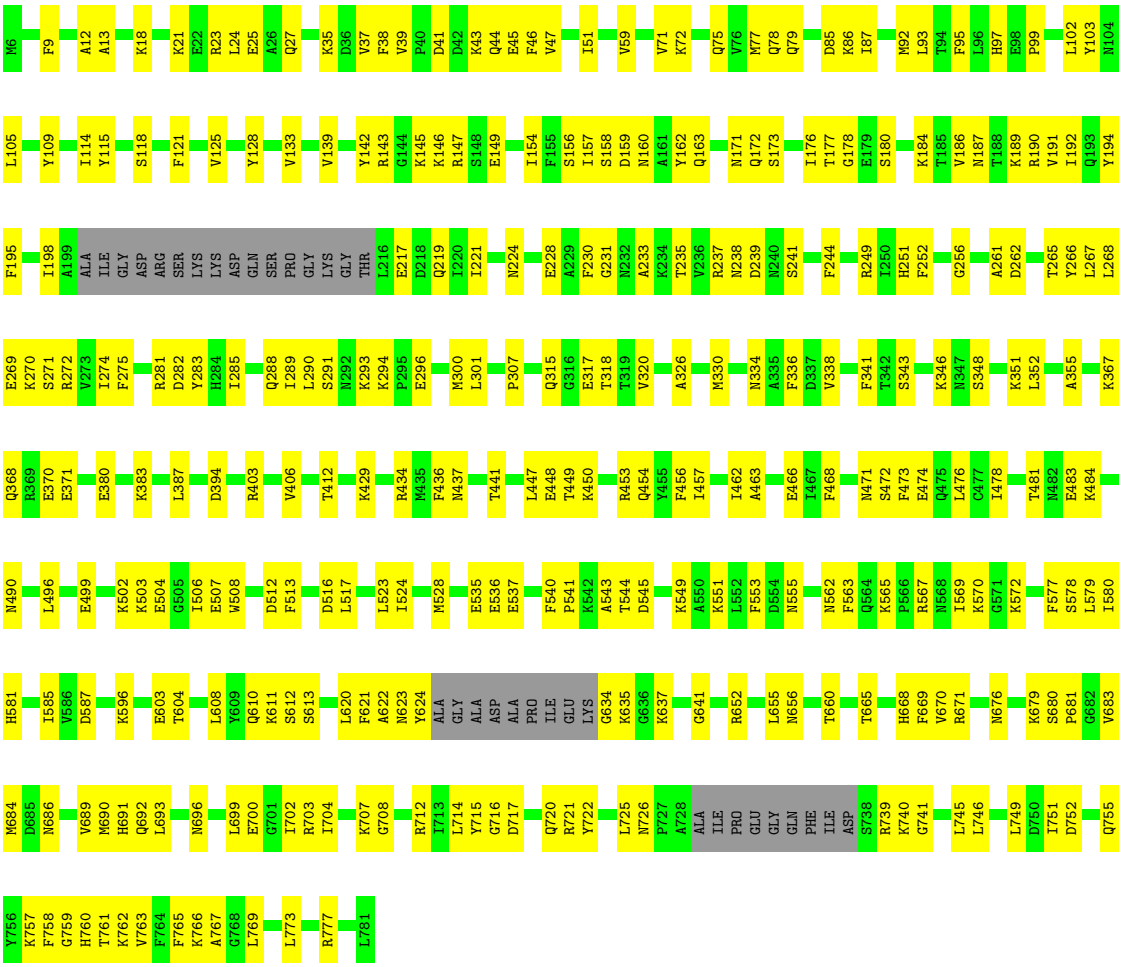
Chain H:





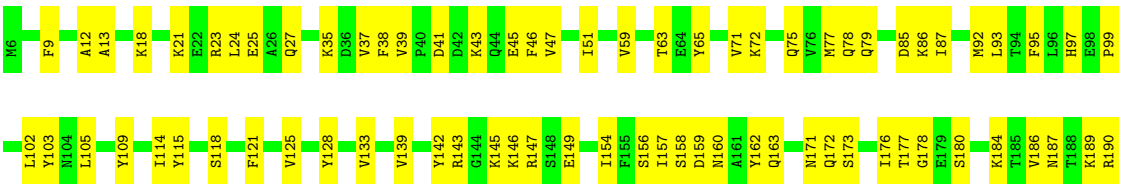
• Molecule 1: Myosin-7

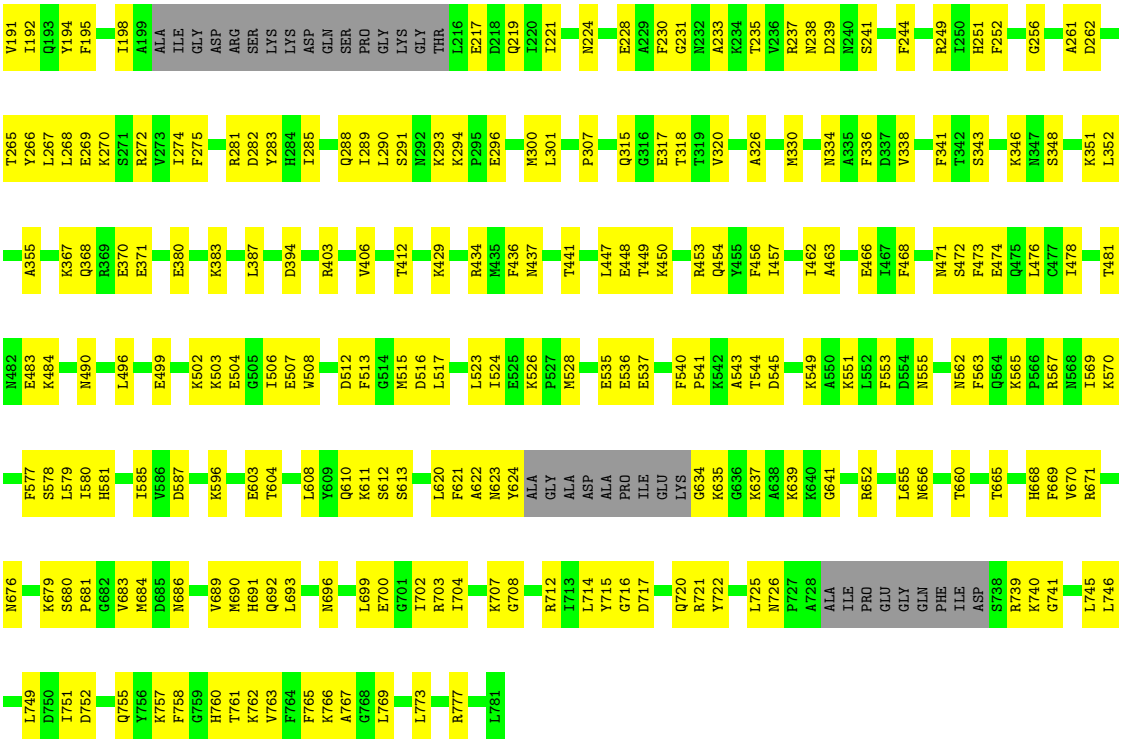
Chain I:



• Molecule 1: Myosin-7

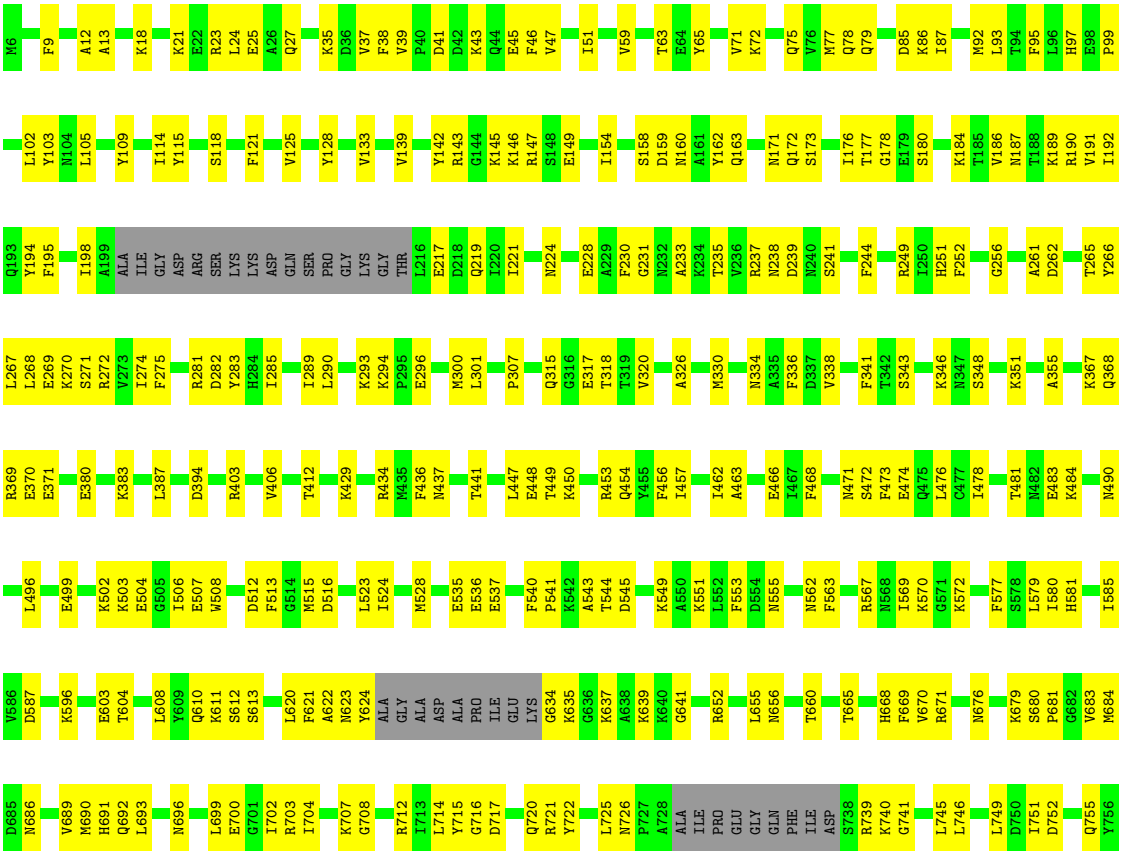
Chain J:

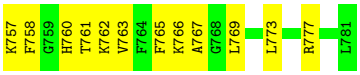




• Molecule 1: Myosin-7

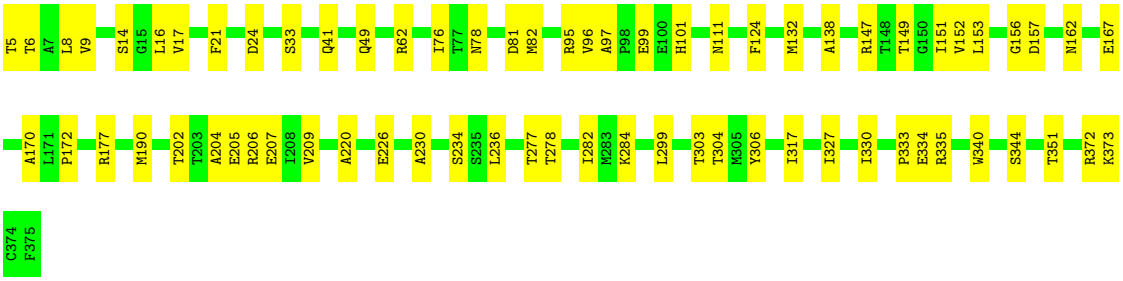
Chain K:





• Molecule 2: Actin, alpha cardiac muscle 1

Chain B:

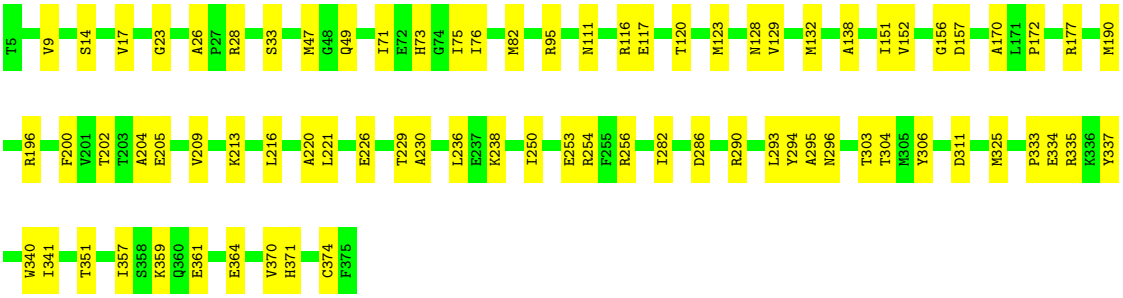


• Molecule 2: Actin, alpha cardiac muscle 1

Chain C:

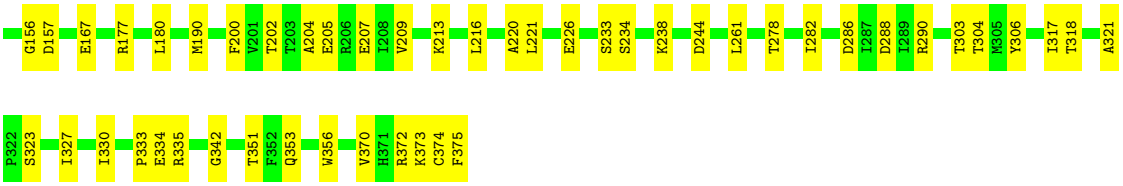
• Molecule 2: Actin, alpha cardiac muscle 1

Chain D:



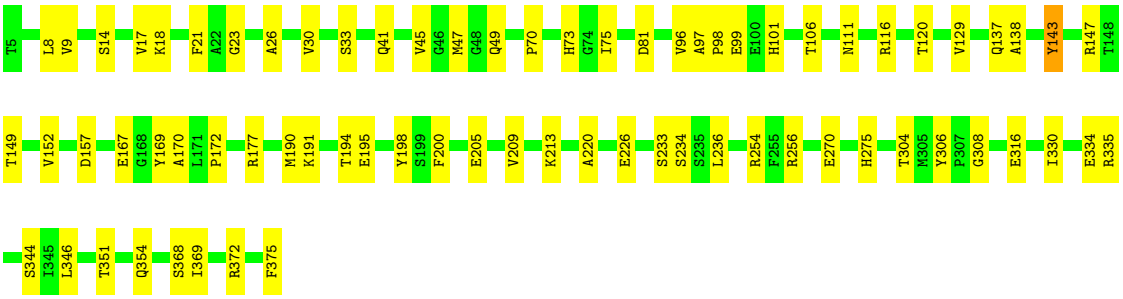
• Molecule 2: Actin, alpha cardiac muscle 1

Chain E:



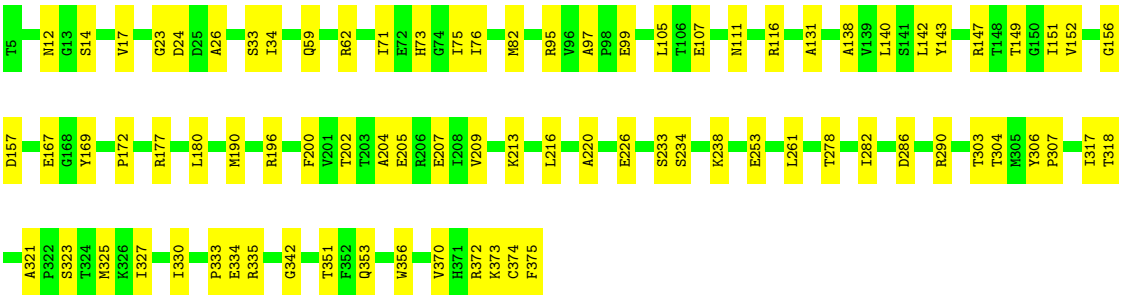
• Molecule 2: Actin, alpha cardiac muscle 1

Chain F:



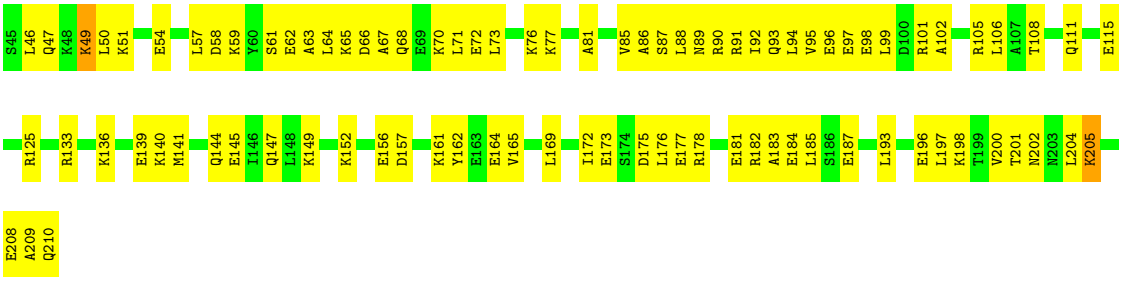
• Molecule 2: Actin, alpha cardiac muscle 1

Chain A:



• Molecule 3: Tropomyosin alpha-1 chain

Chain O:

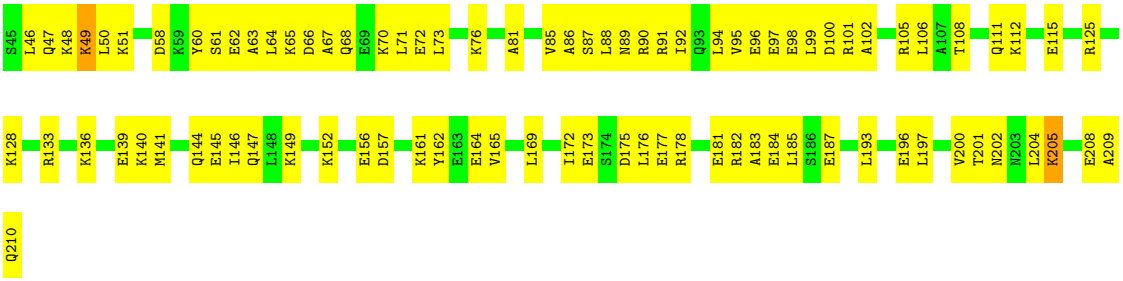


• Molecule 3: Tropomyosin alpha-1 chain

Chain P:

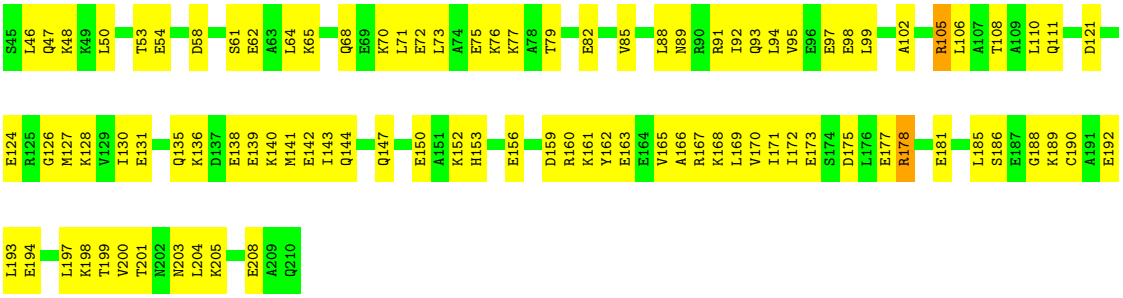
• Molecule 3: Tropomyosin alpha-1 chain

Chain L:



• Molecule 3: Tropomyosin alpha-1 chain

Chain N:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-166.66°, rise=27.3 Å, axial sym=C1	Depositor
Number of segments used	69013	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	55	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

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	G	0.32	0/6101	0.45	0/8217
1	H	0.32	0/6101	0.45	0/8217
1	I	0.32	0/6101	0.45	0/8217
1	J	0.32	0/6101	0.45	0/8217
1	K	0.32	0/6101	0.45	0/8217
1	M	0.32	0/6101	0.45	0/8217
2	A	0.58	0/2961	0.51	0/4011
2	B	0.53	0/2961	0.50	0/4011
2	C	0.55	0/2961	0.50	0/4011
2	D	0.57	0/2961	0.51	0/4011
2	E	0.58	0/2961	0.51	0/4011
2	F	0.57	0/2961	0.50	0/4011
3	L	0.28	0/1328	0.48	0/1770
3	N	0.28	0/1328	0.46	0/1770
3	O	0.28	0/1328	0.48	0/1770
3	P	0.28	0/1328	0.46	0/1770
All	All	0.40	0/59684	0.47	0/80448

There are no bond length outliers.

There are no bond angle outliers.

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	G	5974	0	5961	217	0
1	H	5974	0	5961	212	0
1	I	5974	0	5961	221	0
1	J	5974	0	5961	233	0
1	K	5974	0	5961	224	0
1	M	5974	0	5961	204	0
2	A	2898	0	2870	63	0
2	B	2898	0	2871	53	0
2	C	2898	0	2871	56	0
2	D	2898	0	2868	73	0
2	E	2898	0	2871	61	0
2	F	2898	0	2871	54	0
3	L	1326	0	1330	120	0
3	N	1326	0	1332	106	0
3	O	1326	0	1332	90	0
3	P	1326	0	1332	90	0
4	A	27	0	12	3	0
4	B	27	0	12	1	0
4	C	27	0	12	2	0
4	D	27	0	12	2	0
4	E	27	0	12	3	0
4	F	27	0	12	2	0
All	All	58698	0	58386	1879	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 16.

All (1879) 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:I:368:GLN:HE22	3:N:142:GLU:CB	1.15	1.57
1:J:368:GLN:HE22	3:L:100:ASP:CA	1.21	1.49
1:I:368:GLN:HE22	3:N:142:GLU:CA	1.21	1.48
1:I:368:GLN:NE2	3:N:142:GLU:HB3	1.30	1.45
1:J:368:GLN:NE2	3:L:100:ASP:CA	1.78	1.45
1:K:368:GLN:NE2	3:N:61:SER:HB3	1.28	1.43
2:D:254:ARG:HH12	3:L:128:LYS:NZ	1.13	1.42
1:K:368:GLN:NE2	3:N:61:SER:CB	1.80	1.41
3:O:173:GLU:CG	1:H:368:GLN:HE21	1.36	1.39
1:J:368:GLN:HG2	3:L:99:LEU:CD1	1.52	1.38
1:I:368:GLN:NE2	3:N:142:GLU:CA	1.92	1.33
1:J:368:GLN:NE2	3:L:100:ASP:HA	1.32	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:368:GLN:HE22	3:N:61:SER:CB	1.42	1.20
1:J:368:GLN:HE22	3:L:100:ASP:CB	1.52	1.19
1:J:368:GLN:HG2	3:L:99:LEU:HD12	1.27	1.17
1:K:368:GLN:HE22	3:N:61:SER:CA	1.56	1.16
1:J:368:GLN:NE2	3:L:100:ASP:CB	2.10	1.15
2:D:254:ARG:NH1	3:L:128:LYS:NZ	1.99	1.11
3:O:173:GLU:HG2	1:H:368:GLN:NE2	1.63	1.11
2:D:221:LEU:HD21	3:L:136:LYS:HZ3	1.16	1.11
2:D:311:ASP:HB3	3:L:136:LYS:HE2	1.23	1.11
2:D:221:LEU:CD2	3:L:136:LYS:HZ3	1.66	1.07
1:I:368:GLN:NE2	3:N:142:GLU:CB	1.88	1.06
3:O:173:GLU:CG	1:H:368:GLN:NE2	2.19	1.04
2:D:238:LYS:NZ	3:L:125:ARG:CD	2.18	1.03
2:D:221:LEU:HD21	3:L:136:LYS:NZ	1.73	1.02
3:O:173:GLU:HG2	1:H:368:GLN:HE21	0.86	1.01
2:D:238:LYS:HZ1	3:L:125:ARG:HG2	1.24	0.98
1:I:368:GLN:NE2	3:N:142:GLU:HA	1.81	0.95
1:I:368:GLN:HE22	3:N:142:GLU:HA	1.31	0.95
1:K:368:GLN:HE22	3:N:61:SER:HA	1.29	0.95
2:D:238:LYS:NZ	3:L:125:ARG:HD2	1.82	0.94
1:J:368:GLN:HG2	3:L:99:LEU:HD11	1.48	0.94
2:D:221:LEU:HD11	3:L:136:LYS:NZ	1.81	0.94
1:J:368:GLN:NE2	3:L:100:ASP:HB2	1.80	0.94
1:J:368:GLN:CG	3:L:99:LEU:CD1	2.45	0.94
1:I:368:GLN:NE2	3:N:142:GLU:N	2.13	0.94
2:D:254:ARG:HH12	3:L:128:LYS:HZ1	1.05	0.92
1:K:368:GLN:NE2	3:N:61:SER:CA	2.25	0.91
2:A:149:THR:HG22	2:A:167:GLU:H	1.35	0.91
3:O:96:GLU:HG3	1:G:368:GLN:OE1	1.69	0.91
2:D:254:ARG:HH12	3:L:128:LYS:HZ2	1.20	0.90
1:J:368:GLN:HE22	3:L:100:ASP:HA	0.86	0.90
2:E:41:GLN:HE21	2:A:172:PRO:HG3	1.37	0.89
2:E:149:THR:HG22	2:E:167:GLU:H	1.35	0.89
1:J:142:TYR:HA	1:J:145:LYS:HE2	1.55	0.88
2:E:147:ARG:HH21	2:E:330:ILE:HG12	1.38	0.88
1:K:142:TYR:HA	1:K:145:LYS:HE2	1.55	0.88
1:I:142:TYR:HA	1:I:145:LYS:HE2	1.55	0.87
1:K:368:GLN:HE21	3:N:61:SER:HB3	1.12	0.87
2:A:147:ARG:HH21	2:A:330:ILE:HG12	1.38	0.87
1:M:142:TYR:HA	1:M:145:LYS:HE2	1.55	0.87
2:B:149:THR:HG22	2:B:167:GLU:H	1.39	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:149:THR:HG22	2:F:167:GLU:H	1.39	0.86
1:K:369:ARG:CB	3:L:60:TYR:OH	2.24	0.86
1:G:142:TYR:HA	1:G:145:LYS:HE2	1.55	0.85
1:H:142:TYR:HA	1:H:145:LYS:HE2	1.55	0.85
1:J:368:GLN:NE2	3:L:100:ASP:N	2.25	0.84
1:K:369:ARG:HB2	3:L:60:TYR:OH	1.78	0.83
1:J:368:GLN:CG	3:L:99:LEU:HD12	2.07	0.83
2:D:254:ARG:NH1	3:L:128:LYS:HZ1	1.68	0.83
2:D:238:LYS:HZ1	3:L:125:ARG:CG	1.91	0.82
2:E:351:THR:OG1	1:J:536:GLU:OE2	1.96	0.82
1:H:230:PHE:HA	1:H:285:ILE:HD11	1.61	0.82
1:G:230:PHE:HA	1:G:285:ILE:HD11	1.61	0.82
2:F:47:MET:HB3	1:G:540:PHE:CZ	2.14	0.82
1:I:293:LYS:HE2	1:I:326:ALA:HB1	1.62	0.81
1:G:293:LYS:HE2	1:G:326:ALA:HB1	1.62	0.81
1:J:230:PHE:HA	1:J:285:ILE:HD11	1.61	0.81
1:K:368:GLN:NE2	3:N:61:SER:HA	1.89	0.81
3:L:73:LEU:HA	3:L:76:LYS:HD3	1.62	0.81
1:M:293:LYS:HE2	1:M:326:ALA:HB1	1.62	0.81
1:J:293:LYS:HE2	1:J:326:ALA:HB1	1.62	0.81
1:K:230:PHE:HA	1:K:285:ILE:HD11	1.61	0.81
2:D:221:LEU:HD11	3:L:136:LYS:HZ1	1.44	0.81
1:K:293:LYS:HE2	1:K:326:ALA:HB1	1.62	0.81
1:M:230:PHE:HA	1:M:285:ILE:HD11	1.61	0.81
1:I:230:PHE:HA	1:I:285:ILE:HD11	1.61	0.80
1:H:293:LYS:HE2	1:H:326:ALA:HB1	1.62	0.80
2:C:149:THR:HG22	2:C:167:GLU:H	1.46	0.80
2:D:238:LYS:NZ	3:L:125:ARG:CG	2.45	0.80
2:C:351:THR:OG1	1:G:536:GLU:OE2	1.99	0.80
1:K:536:GLU:OE2	2:A:351:THR:OG1	1.98	0.80
1:H:528:MET:SD	1:H:555:ASN:ND2	2.55	0.80
2:B:351:THR:HG23	1:H:536:GLU:OE1	1.81	0.79
2:D:238:LYS:NZ	3:L:125:ARG:HG2	1.98	0.79
3:O:73:LEU:HA	3:O:76:LYS:HD3	1.62	0.79
1:K:528:MET:SD	1:K:555:ASN:ND2	2.55	0.79
2:D:351:THR:OG1	1:I:536:GLU:OE2	1.99	0.79
3:P:91:ARG:HE	1:G:369:ARG:HH21	1.28	0.79
1:G:528:MET:SD	1:G:555:ASN:ND2	2.55	0.79
1:M:528:MET:SD	1:M:555:ASN:ND2	2.55	0.79
2:C:147:ARG:HH21	2:C:330:ILE:HG12	1.46	0.79
2:D:202:THR:HG22	2:D:204:ALA:H	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:105:ARG:HG3	3:P:106:LEU:HD11	1.65	0.79
3:L:105:ARG:HG3	3:N:106:LEU:HD11	1.64	0.79
1:I:528:MET:SD	1:I:555:ASN:ND2	2.55	0.79
2:D:254:ARG:HH12	3:L:128:LYS:HZ3	1.31	0.78
1:J:528:MET:SD	1:J:555:ASN:ND2	2.55	0.78
3:P:165:VAL:HA	3:P:168:LYS:HD2	1.67	0.77
1:K:368:GLN:NE2	3:N:61:SER:HB2	1.96	0.77
3:N:165:VAL:HA	3:N:168:LYS:HD2	1.67	0.77
3:L:71:LEU:HD22	3:N:70:LYS:HD2	1.68	0.75
2:C:35:VAL:HG21	2:C:81:ASP:HB2	1.69	0.75
3:P:91:ARG:HE	1:G:369:ARG:NH2	1.85	0.75
2:C:351:THR:HG1	1:G:536:GLU:CD	1.91	0.73
2:D:221:LEU:CD1	3:L:136:LYS:HZ3	2.00	0.73
2:B:24:ASP:OD1	1:H:639:LYS:O	2.06	0.73
1:I:128:TYR:HB2	1:I:681:PRO:HG3	1.70	0.73
3:O:173:GLU:CB	1:H:368:GLN:NE2	2.51	0.73
3:O:71:LEU:HD22	3:P:70:LYS:HD2	1.68	0.73
1:K:281:ARG:NH2	1:K:318:THR:O	2.22	0.73
1:K:128:TYR:HB2	1:K:681:PRO:HG3	1.69	0.73
1:M:281:ARG:NH2	1:M:318:THR:O	2.22	0.73
3:L:71:LEU:HD21	3:N:71:LEU:HA	1.70	0.73
1:G:281:ARG:NH2	1:G:318:THR:O	2.22	0.72
1:M:128:TYR:HB2	1:M:681:PRO:HG3	1.69	0.72
1:G:536:GLU:OE2	1:G:551:LYS:NZ	2.22	0.72
2:F:106:THR:HG22	2:F:137:GLN:HG2	1.69	0.72
1:G:45:GLU:HG2	1:G:46:PHE:HD2	1.54	0.72
1:J:281:ARG:NH2	1:J:318:THR:O	2.22	0.72
1:J:128:TYR:HB2	1:J:681:PRO:HG3	1.70	0.72
1:M:536:GLU:OE2	1:M:551:LYS:NZ	2.22	0.72
1:G:490:ASN:ND2	1:G:513:PHE:O	2.23	0.72
1:I:281:ARG:NH2	1:I:318:THR:O	2.22	0.72
1:H:281:ARG:NH2	1:H:318:THR:O	2.22	0.72
1:H:490:ASN:ND2	1:H:513:PHE:O	2.23	0.72
1:H:128:TYR:HB2	1:H:681:PRO:HG3	1.70	0.72
1:G:128:TYR:HB2	1:G:681:PRO:HG3	1.69	0.72
1:J:490:ASN:ND2	1:J:513:PHE:O	2.23	0.72
1:H:536:GLU:OE2	1:H:551:LYS:NZ	2.22	0.72
1:I:490:ASN:ND2	1:I:513:PHE:O	2.23	0.72
1:I:536:GLU:OE2	1:I:551:LYS:NZ	2.22	0.72
1:H:45:GLU:HG2	1:H:46:PHE:HD2	1.54	0.71
3:O:71:LEU:HD21	3:P:71:LEU:HA	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:96:GLU:HG3	1:G:368:GLN:CD	2.09	0.71
1:K:536:GLU:OE2	1:K:551:LYS:NZ	2.22	0.71
1:I:45:GLU:HG2	1:I:46:PHE:HD2	1.54	0.71
1:J:536:GLU:OE2	1:J:551:LYS:NZ	2.22	0.71
2:C:202:THR:HG22	2:C:204:ALA:H	1.56	0.71
1:K:45:GLU:HG2	1:K:46:PHE:HD2	1.54	0.71
1:M:45:GLU:HG2	1:M:46:PHE:HD2	1.54	0.71
2:D:221:LEU:CD1	3:L:136:LYS:NZ	2.54	0.71
1:H:739:ARG:NH2	1:H:760:HIS:O	2.24	0.71
1:J:739:ARG:NH2	1:J:760:HIS:O	2.24	0.71
1:K:490:ASN:ND2	1:K:513:PHE:O	2.23	0.71
1:K:739:ARG:NH2	1:K:760:HIS:O	2.24	0.71
2:A:307:PRO:CB	3:L:48:LYS:HE2	2.21	0.71
1:H:512:ASP:OD1	1:H:513:PHE:N	2.24	0.71
1:H:755:GLN:HB3	1:H:769:LEU:HD11	1.73	0.71
1:M:739:ARG:NH2	1:M:760:HIS:O	2.24	0.70
1:K:512:ASP:OD1	1:K:513:PHE:N	2.24	0.70
1:M:490:ASN:ND2	1:M:513:PHE:O	2.23	0.70
1:M:755:GLN:HB3	1:M:769:LEU:HD11	1.73	0.70
3:P:138:GLU:HA	3:P:141:MET:HG2	1.74	0.70
1:J:45:GLU:HG2	1:J:46:PHE:HD2	1.54	0.70
1:G:512:ASP:OD1	1:G:513:PHE:N	2.24	0.70
1:G:755:GLN:HB3	1:G:769:LEU:HD11	1.73	0.70
1:I:512:ASP:OD1	1:I:513:PHE:N	2.24	0.70
1:I:739:ARG:NH2	1:I:760:HIS:O	2.24	0.70
2:E:244:ASP:O	2:A:325:MET:CE	2.39	0.70
3:O:133:ARG:NH2	3:P:138:GLU:OE2	2.25	0.70
1:J:368:GLN:CD	3:L:100:ASP:HA	2.11	0.70
1:J:512:ASP:OD1	1:J:513:PHE:N	2.24	0.70
3:N:102:ALA:O	3:N:105:ARG:NH1	2.25	0.70
1:M:512:ASP:OD1	1:M:513:PHE:N	2.24	0.70
2:B:351:THR:HG23	1:H:536:GLU:CD	2.12	0.70
2:A:317:ILE:HG22	2:A:327:ILE:HD13	1.74	0.69
1:G:739:ARG:NH2	1:G:760:HIS:O	2.24	0.69
3:L:133:ARG:NH2	3:N:138:GLU:OE2	2.25	0.69
1:K:639:LYS:O	2:A:24:ASP:OD1	2.11	0.69
1:K:755:GLN:HB3	1:K:769:LEU:HD11	1.73	0.69
3:N:138:GLU:HA	3:N:141:MET:HG2	1.74	0.69
1:J:18:LYS:O	1:J:23:ARG:NH1	2.26	0.69
3:P:102:ALA:O	3:P:105:ARG:NH1	2.25	0.69
1:G:523:LEU:HD21	1:G:563:PHE:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:17:VAL:HG23	2:D:33:SER:HB3	1.74	0.69
1:G:18:LYS:O	1:G:23:ARG:NH1	2.26	0.69
1:I:18:LYS:O	1:I:23:ARG:NH1	2.26	0.69
1:I:523:LEU:HD21	1:I:563:PHE:HB2	1.74	0.69
1:K:18:LYS:O	1:K:23:ARG:NH1	2.26	0.69
1:H:18:LYS:O	1:H:23:ARG:NH1	2.26	0.68
1:J:755:GLN:HB3	1:J:769:LEU:HD11	1.73	0.68
3:O:97:GLU:HB3	3:O:101:ARG:HH12	1.59	0.68
1:J:523:LEU:HD21	1:J:563:PHE:HB2	1.74	0.68
1:G:355:ALA:HB2	1:G:387:LEU:HD22	1.76	0.68
1:M:523:LEU:HD21	1:M:563:PHE:HB2	1.74	0.68
3:O:157:ASP:O	3:O:161:LYS:HG2	1.93	0.68
1:H:523:LEU:HD21	1:H:563:PHE:HB2	1.74	0.68
3:L:157:ASP:O	3:L:161:LYS:HG2	1.93	0.68
1:J:355:ALA:HB2	1:J:387:LEU:HD22	1.76	0.68
1:K:355:ALA:HB2	1:K:387:LEU:HD22	1.76	0.68
1:M:355:ALA:HB2	1:M:387:LEU:HD22	1.76	0.68
1:H:355:ALA:HB2	1:H:387:LEU:HD22	1.76	0.68
1:I:755:GLN:HB3	1:I:769:LEU:HD11	1.73	0.68
1:M:18:LYS:O	1:M:23:ARG:NH1	2.26	0.68
1:I:355:ALA:HB2	1:I:387:LEU:HD22	1.76	0.68
1:K:523:LEU:HD21	1:K:563:PHE:HB2	1.74	0.68
3:O:173:GLU:CD	1:H:368:GLN:HE21	1.98	0.67
3:L:67:ALA:HA	3:L:70:LYS:HD2	1.76	0.67
2:B:41:GLN:HE22	2:F:172:PRO:HG3	1.57	0.67
2:E:317:ILE:HG22	2:E:327:ILE:HD13	1.74	0.67
3:N:140:LYS:O	3:N:144:GLN:NE2	2.27	0.67
2:B:17:VAL:HG23	2:B:33:SER:HB3	1.76	0.67
3:P:140:LYS:O	3:P:144:GLN:NE2	2.27	0.67
2:C:213:LYS:NZ	4:C:401:ADP:O2'	2.26	0.67
2:D:200:PHE:HB3	2:D:205:GLU:HB3	1.76	0.67
3:O:67:ALA:HA	3:O:70:LYS:HD2	1.76	0.67
2:A:156:GLY:O	2:A:303:THR:OG1	2.11	0.67
1:K:368:GLN:HE22	3:N:61:SER:HB2	1.50	0.67
3:L:97:GLU:HB3	3:L:101:ARG:HH12	1.59	0.66
1:M:348:SER:HA	1:M:351:LYS:HG2	1.78	0.66
2:F:200:PHE:HB3	2:F:205:GLU:HB3	1.77	0.66
3:O:193:LEU:HD21	3:P:197:LEU:HD22	1.76	0.66
1:H:348:SER:HA	1:H:351:LYS:HG2	1.78	0.66
3:O:62:GLU:HA	3:O:65:LYS:HD2	1.78	0.66
2:E:156:GLY:O	2:E:303:THR:OG1	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:102:ALA:O	3:P:106:LEU:HB2	1.95	0.65
3:O:182:ARG:NH2	3:P:186:SER:OG	2.29	0.65
1:G:274:ILE:O	1:G:315:GLN:NE2	2.30	0.65
1:I:348:SER:HA	1:I:351:LYS:HG2	1.78	0.65
1:J:348:SER:HA	1:J:351:LYS:HG2	1.78	0.65
2:E:24:ASP:OD1	1:J:639:LYS:O	2.13	0.65
1:G:37:VAL:HG12	1:G:78:GLN:HA	1.77	0.65
1:I:37:VAL:HG12	1:I:78:GLN:HA	1.77	0.65
3:N:102:ALA:O	3:N:106:LEU:HB2	1.95	0.65
3:L:62:GLU:HA	3:L:65:LYS:HD2	1.78	0.65
3:L:182:ARG:NH2	3:N:186:SER:OG	2.29	0.65
3:L:193:LEU:HD21	3:N:197:LEU:HD22	1.76	0.65
2:B:351:THR:HG21	1:H:551:LYS:NZ	2.12	0.65
2:F:213:LYS:NZ	4:F:401:ADP:O2'	2.27	0.65
1:I:274:ILE:O	1:I:315:GLN:NE2	2.30	0.65
1:K:274:ILE:O	1:K:315:GLN:NE2	2.30	0.65
1:H:37:VAL:HG12	1:H:78:GLN:HA	1.77	0.65
1:M:37:VAL:HG12	1:M:78:GLN:HA	1.77	0.65
1:M:274:ILE:O	1:M:315:GLN:NE2	2.30	0.65
1:H:274:ILE:O	1:H:315:GLN:NE2	2.30	0.65
1:G:348:SER:HA	1:G:351:LYS:HG2	1.78	0.64
1:K:610:GLN:NE2	1:K:621:PHE:O	2.30	0.64
3:O:93:GLN:HA	1:G:368:GLN:HE22	1.62	0.64
1:K:37:VAL:HG12	1:K:78:GLN:HA	1.77	0.64
1:K:252:PHE:O	1:K:454:GLN:N	2.28	0.64
1:K:348:SER:HA	1:K:351:LYS:HG2	1.78	0.64
1:H:610:GLN:NE2	1:H:621:PHE:O	2.30	0.64
1:H:252:PHE:O	1:H:454:GLN:N	2.28	0.64
2:C:156:GLY:O	2:C:303:THR:OG1	2.15	0.64
1:J:37:VAL:HG12	1:J:78:GLN:HA	1.77	0.64
1:M:265:THR:HG21	1:M:436:PHE:HE2	1.63	0.64
1:J:274:ILE:O	1:J:315:GLN:NE2	2.30	0.64
2:E:41:GLN:NE2	2:A:172:PRO:HG3	2.12	0.64
1:I:610:GLN:NE2	1:I:621:PHE:O	2.30	0.64
1:J:610:GLN:NE2	1:J:621:PHE:O	2.30	0.64
1:H:516:ASP:N	1:H:516:ASP:OD1	2.30	0.64
2:A:307:PRO:HB3	3:L:48:LYS:HE2	1.80	0.64
1:G:265:THR:HG21	1:G:436:PHE:HE2	1.63	0.63
2:C:220:ALA:HB1	2:C:226:GLU:HG3	1.79	0.63
1:G:610:GLN:NE2	1:G:621:PHE:O	2.30	0.63
1:H:265:THR:HG21	1:H:436:PHE:HE2	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:351:THR:HG23	1:H:536:GLU:OE2	1.98	0.63
1:M:162:TYR:OH	1:M:256:GLY:O	2.16	0.63
2:B:202:THR:HG22	2:B:204:ALA:H	1.63	0.63
1:J:265:THR:HG21	1:J:436:PHE:HE2	1.63	0.63
1:K:516:ASP:N	1:K:516:ASP:OD1	2.30	0.63
1:K:265:THR:HG21	1:K:436:PHE:HE2	1.63	0.63
2:A:220:ALA:HB1	2:A:226:GLU:HG3	1.81	0.63
1:I:700:GLU:O	1:I:704:ILE:HG12	1.99	0.63
1:J:252:PHE:O	1:J:454:GLN:N	2.28	0.63
2:D:190:MET:HG2	2:D:209:VAL:HG21	1.81	0.63
1:I:265:THR:HG21	1:I:436:PHE:HE2	1.63	0.63
1:J:516:ASP:N	1:J:516:ASP:OD1	2.30	0.63
2:E:220:ALA:HB1	2:E:226:GLU:HG3	1.81	0.62
1:M:610:GLN:NE2	1:M:621:PHE:O	2.30	0.62
2:C:14:SER:O	2:C:157:ASP:HB3	2.00	0.62
2:D:304:THR:O	2:D:335:ARG:NH1	2.32	0.62
1:G:700:GLU:O	1:G:704:ILE:HG12	1.99	0.62
1:I:506:ILE:HD11	1:I:757:LYS:HG2	1.82	0.62
1:K:700:GLU:O	1:K:704:ILE:HG12	1.99	0.62
3:O:144:GLN:NE2	3:P:144:GLN:HB3	2.15	0.62
1:K:506:ILE:HD11	1:K:757:LYS:HG2	1.82	0.62
3:L:144:GLN:NE2	3:N:144:GLN:HB3	2.15	0.62
2:A:286:ASP:O	2:A:290:ARG:NE	2.33	0.62
1:M:252:PHE:O	1:M:454:GLN:N	2.28	0.62
1:M:549:LYS:HE3	1:M:553:PHE:HE2	1.65	0.62
3:O:102:ALA:HA	3:O:105:ARG:HE	1.65	0.62
1:H:700:GLU:O	1:H:704:ILE:HG12	1.99	0.62
1:M:700:GLU:O	1:M:704:ILE:HG12	1.99	0.62
2:E:286:ASP:O	2:E:290:ARG:NE	2.33	0.62
1:I:162:TYR:OH	1:I:256:GLY:O	2.16	0.62
2:A:334:GLU:OE1	2:A:334:GLU:N	2.29	0.62
1:H:549:LYS:HE3	1:H:553:PHE:HE2	1.65	0.62
1:G:549:LYS:HE3	1:G:553:PHE:HE2	1.65	0.61
1:J:700:GLU:O	1:J:704:ILE:HG12	1.99	0.61
3:L:102:ALA:HA	3:L:105:ARG:HE	1.65	0.61
2:E:213:LYS:NZ	4:E:401:ADP:O2'	2.28	0.61
1:H:506:ILE:HD11	1:H:757:LYS:HG2	1.82	0.61
1:J:506:ILE:HD11	1:J:757:LYS:HG2	1.82	0.61
2:C:351:THR:O	2:C:354:GLN:NE2	2.33	0.61
1:G:285:ILE:O	1:G:289:ILE:HG12	2.01	0.61
2:B:8:LEU:HD13	2:B:101:HIS:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:116:ARG:NH2	2:F:375:PHE:O	2.33	0.61
3:P:89:ASN:HA	3:P:92:ILE:HD12	1.82	0.61
1:J:187:ASN:O	1:J:191:VAL:HG23	2.00	0.61
1:K:549:LYS:HE3	1:K:553:PHE:HE2	1.65	0.61
1:M:285:ILE:O	1:M:289:ILE:HG12	2.01	0.61
2:D:334:GLU:OE1	2:D:334:GLU:N	2.30	0.61
1:H:380:GLU:HA	1:H:383:LYS:HG2	1.83	0.61
1:J:368:GLN:HE21	3:L:100:ASP:N	1.94	0.61
1:I:187:ASN:O	1:I:191:VAL:HG23	2.00	0.61
1:I:285:ILE:O	1:I:289:ILE:HG12	2.01	0.61
2:E:351:THR:OG1	1:J:536:GLU:CD	2.38	0.61
1:K:162:TYR:OH	1:K:256:GLY:O	2.16	0.61
1:K:187:ASN:O	1:K:191:VAL:HG23	2.00	0.61
1:M:506:ILE:HD11	1:M:757:LYS:HG2	1.82	0.61
2:B:351:THR:CG2	1:H:536:GLU:OE2	2.49	0.61
2:F:8:LEU:HD13	2:F:101:HIS:HB3	1.83	0.61
1:J:549:LYS:HE3	1:J:553:PHE:HE2	1.65	0.61
1:K:285:ILE:O	1:K:289:ILE:HG12	2.01	0.61
2:E:111:ASN:OD1	2:E:177:ARG:NH1	2.33	0.60
1:I:294:LYS:NZ	1:I:296:GLU:OE2	2.30	0.60
1:J:162:TYR:OH	1:J:256:GLY:O	2.16	0.60
3:N:89:ASN:HA	3:N:92:ILE:HD12	1.82	0.60
3:P:91:ARG:NE	1:G:369:ARG:NH2	2.49	0.60
1:G:187:ASN:O	1:G:191:VAL:HG23	2.00	0.60
1:H:285:ILE:O	1:H:289:ILE:HG12	2.01	0.60
1:J:285:ILE:O	1:J:289:ILE:HG12	2.01	0.60
1:K:380:GLU:HA	1:K:383:LYS:HG2	1.83	0.60
1:K:536:GLU:CD	2:A:351:THR:OG1	2.39	0.60
3:P:175:ASP:O	3:P:178:ARG:NH1	2.35	0.60
1:G:516:ASP:OD1	1:G:516:ASP:N	2.30	0.60
1:I:549:LYS:HE3	1:I:553:PHE:HE2	1.65	0.60
1:J:380:GLU:HA	1:J:383:LYS:HG2	1.82	0.60
1:K:294:LYS:NZ	1:K:296:GLU:OE2	2.30	0.60
3:N:175:ASP:O	3:N:178:ARG:NH1	2.35	0.60
1:H:187:ASN:O	1:H:191:VAL:HG23	2.00	0.60
1:I:380:GLU:HA	1:I:383:LYS:HG2	1.83	0.60
1:M:516:ASP:N	1:M:516:ASP:OD1	2.30	0.60
1:H:162:TYR:OH	1:H:256:GLY:O	2.16	0.60
1:I:472:SER:OG	1:I:473:PHE:N	2.35	0.60
1:J:233:ALA:O	1:J:241:SER:OG	2.20	0.60
2:A:202:THR:HG22	2:A:204:ALA:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:252:PHE:HE1	1:M:457:ILE:HD12	1.67	0.60
2:C:111:ASN:OD1	2:C:177:ARG:NH1	2.35	0.60
1:K:252:PHE:HE1	1:K:457:ILE:HD12	1.67	0.60
1:M:187:ASN:O	1:M:191:VAL:HG23	2.00	0.60
2:F:143:TYR:HE2	2:F:346:LEU:HD13	1.66	0.60
1:G:380:GLU:HA	1:G:383:LYS:HG2	1.82	0.60
1:I:39:VAL:HG23	1:I:71:VAL:HG21	1.84	0.60
1:I:233:ALA:O	1:I:241:SER:OG	2.20	0.60
1:G:506:ILE:HD11	1:G:757:LYS:HG2	1.82	0.60
1:J:294:LYS:NZ	1:J:296:GLU:OE2	2.30	0.60
3:O:173:GLU:HB3	1:H:368:GLN:NE2	2.17	0.60
1:G:252:PHE:HE1	1:G:457:ILE:HD12	1.67	0.60
1:J:39:VAL:HG23	1:J:71:VAL:HG21	1.84	0.60
1:K:472:SER:OG	1:K:473:PHE:N	2.35	0.60
1:M:656:ASN:O	1:M:660:THR:HG23	2.02	0.59
1:M:676:ASN:ND2	1:M:683:VAL:O	2.36	0.59
2:B:334:GLU:OE1	2:B:334:GLU:N	2.31	0.59
2:F:334:GLU:OE1	2:F:334:GLU:N	2.29	0.59
1:I:656:ASN:O	1:I:660:THR:HG23	2.02	0.59
1:J:656:ASN:O	1:J:660:THR:HG23	2.02	0.59
1:M:380:GLU:HA	1:M:383:LYS:HG2	1.83	0.59
2:E:334:GLU:OE1	2:E:334:GLU:N	2.29	0.59
1:J:252:PHE:HE1	1:J:457:ILE:HD12	1.67	0.59
1:K:656:ASN:O	1:K:660:THR:HG23	2.02	0.59
2:E:318:THR:HA	2:E:327:ILE:HD12	1.84	0.59
1:H:233:ALA:O	1:H:241:SER:OG	2.20	0.59
1:H:252:PHE:HE1	1:H:457:ILE:HD12	1.67	0.59
1:I:516:ASP:OD1	1:I:516:ASP:N	2.30	0.59
1:I:676:ASN:ND2	1:I:683:VAL:O	2.36	0.59
1:J:437:ASN:O	1:J:441:THR:HG23	2.02	0.59
1:J:676:ASN:ND2	1:J:683:VAL:O	2.35	0.59
1:H:143:ARG:NH1	1:H:159:ASP:OD2	2.36	0.59
1:H:656:ASN:O	1:H:660:THR:HG23	2.02	0.59
1:H:676:ASN:ND2	1:H:683:VAL:O	2.36	0.59
1:I:143:ARG:NH1	1:I:159:ASP:OD2	2.36	0.59
1:J:472:SER:OG	1:J:473:PHE:N	2.35	0.59
1:K:437:ASN:O	1:K:441:THR:HG23	2.02	0.59
1:K:676:ASN:ND2	1:K:683:VAL:O	2.36	0.59
2:A:318:THR:HA	2:A:327:ILE:HD12	1.84	0.59
3:O:88:LEU:O	3:O:92:ILE:HG23	2.03	0.59
1:G:676:ASN:ND2	1:G:683:VAL:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:437:ASN:O	1:I:441:THR:HG23	2.02	0.59
3:N:189:LYS:O	3:N:193:LEU:HG	2.02	0.59
2:E:202:THR:HG22	2:E:204:ALA:H	1.66	0.59
1:G:39:VAL:HG23	1:G:71:VAL:HG21	1.84	0.59
1:G:143:ARG:NH1	1:G:159:ASP:OD2	2.36	0.59
1:K:233:ALA:O	1:K:241:SER:OG	2.20	0.59
1:M:437:ASN:O	1:M:441:THR:HG23	2.02	0.59
2:B:21:PHE:HZ	2:B:96:VAL:HG11	1.67	0.59
1:G:233:ALA:O	1:G:241:SER:OG	2.20	0.59
1:K:39:VAL:HG23	1:K:71:VAL:HG21	1.84	0.59
2:D:213:LYS:NZ	4:D:401:ADP:O2'	2.28	0.59
1:G:437:ASN:O	1:G:441:THR:HG23	2.02	0.59
1:M:472:SER:OG	1:M:473:PHE:N	2.35	0.59
1:H:437:ASN:O	1:H:441:THR:HG23	2.02	0.59
1:K:143:ARG:NH1	1:K:159:ASP:OD2	2.36	0.59
2:A:111:ASN:OD1	2:A:177:ARG:NH1	2.33	0.59
1:M:143:ARG:NH1	1:M:159:ASP:OD2	2.36	0.58
1:M:39:VAL:HG23	1:M:71:VAL:HG21	1.84	0.58
1:J:143:ARG:NH1	1:J:159:ASP:OD2	2.36	0.58
2:D:351:THR:OG1	1:I:536:GLU:CD	2.41	0.58
1:G:656:ASN:O	1:G:660:THR:HG23	2.02	0.58
3:L:144:GLN:O	3:L:147:GLN:NE2	2.35	0.58
1:M:233:ALA:O	1:M:241:SER:OG	2.20	0.58
1:M:746:LEU:HG	1:M:751:ILE:HD12	1.86	0.58
2:B:111:ASN:OD1	2:B:177:ARG:NH1	2.32	0.58
2:D:221:LEU:CG	3:L:136:LYS:HZ3	2.15	0.58
1:H:746:LEU:HG	1:H:751:ILE:HD12	1.86	0.58
1:K:708:GLY:O	1:K:766:LYS:NZ	2.28	0.58
2:A:200:PHE:HB3	2:A:205:GLU:HB3	1.86	0.58
3:L:105:ARG:HE	3:N:106:LEU:HD21	1.68	0.58
3:P:189:LYS:O	3:P:193:LEU:HG	2.02	0.58
1:G:162:TYR:OH	1:G:256:GLY:O	2.16	0.58
1:G:746:LEU:HG	1:G:751:ILE:HD12	1.86	0.58
1:H:39:VAL:HG23	1:H:71:VAL:HG21	1.84	0.58
2:E:200:PHE:HB3	2:E:205:GLU:HB3	1.86	0.58
1:I:252:PHE:HE1	1:I:457:ILE:HD12	1.67	0.58
1:I:676:ASN:ND2	1:I:680:SER:O	2.28	0.58
1:K:72:LYS:H	1:K:75:GLN:HE21	1.52	0.58
3:L:88:LEU:O	3:L:92:ILE:HG23	2.03	0.58
2:F:111:ASN:OD1	2:F:177:ARG:NH1	2.35	0.58
1:I:72:LYS:H	1:I:75:GLN:HE21	1.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:708:GLY:O	1:I:766:LYS:NZ	2.28	0.58
1:J:72:LYS:H	1:J:75:GLN:HE21	1.52	0.58
1:M:708:GLY:O	1:M:766:LYS:NZ	2.28	0.58
3:L:144:GLN:HA	3:L:147:GLN:HG3	1.84	0.58
1:H:270:LYS:HB3	1:H:429:LYS:HD2	1.86	0.58
2:F:47:MET:HB3	1:G:540:PHE:HZ	1.65	0.58
3:L:141:MET:O	3:L:145:GLU:HG2	2.04	0.58
3:O:144:GLN:HA	3:O:147:GLN:HG3	1.84	0.57
1:I:746:LEU:HG	1:I:751:ILE:HD12	1.86	0.57
1:M:270:LYS:HB3	1:M:429:LYS:HD2	1.86	0.57
1:G:472:SER:OG	1:G:473:PHE:N	2.35	0.57
1:J:725:LEU:O	1:J:726:ASN:ND2	2.37	0.57
1:K:269:GLU:HG3	1:K:272:ARG:HG2	1.86	0.57
1:K:293:LYS:HE3	1:K:330:MET:HE2	1.85	0.57
1:K:478:ILE:O	1:K:481:THR:OG1	2.22	0.57
1:G:72:LYS:H	1:G:75:GLN:HE21	1.52	0.57
1:G:269:GLU:HG3	1:G:272:ARG:HG2	1.86	0.57
1:I:252:PHE:O	1:I:454:GLN:N	2.28	0.57
1:J:269:GLU:HG3	1:J:272:ARG:HG2	1.86	0.57
1:J:761:THR:HG23	1:J:762:LYS:HG3	1.86	0.57
2:C:189:LEU:HA	2:C:192:ILE:HG22	1.86	0.57
2:D:156:GLY:O	2:D:303:THR:OG1	2.19	0.57
3:O:141:MET:O	3:O:145:GLU:HG2	2.04	0.57
1:I:269:GLU:HG3	1:I:272:ARG:HG2	1.86	0.57
1:I:368:GLN:HG2	3:N:141:MET:HG3	1.87	0.57
2:D:111:ASN:OD1	2:D:177:ARG:NH1	2.31	0.57
1:I:270:LYS:HB3	1:I:429:LYS:HD2	1.86	0.57
1:M:269:GLU:HG3	1:M:272:ARG:HG2	1.86	0.57
1:I:725:LEU:O	1:I:726:ASN:ND2	2.37	0.57
1:K:368:GLN:HG3	3:L:60:TYR:HE2	1.68	0.57
1:G:270:LYS:HB3	1:G:429:LYS:HD2	1.86	0.57
1:G:294:LYS:NZ	1:G:296:GLU:OE2	2.30	0.57
1:G:474:GLU:OE2	1:G:596:LYS:NZ	2.38	0.57
1:H:269:GLU:HG3	1:H:272:ARG:HG2	1.86	0.57
1:J:270:LYS:HB3	1:J:429:LYS:HD2	1.86	0.57
1:K:109:TYR:HB3	1:K:684:MET:HE1	1.86	0.57
1:K:536:GLU:OE1	2:A:351:THR:OG1	2.23	0.57
1:M:92:MET:HE1	1:M:712:ARG:H	1.70	0.57
2:B:351:THR:HG21	1:H:551:LYS:HZ1	1.69	0.57
1:I:761:THR:HG23	1:I:762:LYS:HG3	1.86	0.57
1:M:725:LEU:O	1:M:726:ASN:ND2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:MET:HG3	2:B:209:VAL:HG11	1.87	0.56
2:E:351:THR:OG1	1:J:536:GLU:OE1	2.23	0.56
2:F:116:ARG:O	2:F:120:THR:HG23	2.05	0.56
1:G:252:PHE:O	1:G:454:GLN:N	2.28	0.56
1:H:761:THR:HG23	1:H:762:LYS:HG3	1.86	0.56
1:M:478:ILE:O	1:M:481:THR:OG1	2.22	0.56
2:C:351:THR:OG1	1:G:536:GLU:CD	2.40	0.56
1:H:676:ASN:ND2	1:H:680:SER:O	2.28	0.56
2:C:192:ILE:HD11	2:C:256:ARG:CZ	2.36	0.56
2:D:357:ILE:HG12	2:D:374:CYS:HB3	1.86	0.56
3:P:108:THR:HA	3:P:111:GLN:HG2	1.86	0.56
3:P:159:ASP:O	3:P:163:GLU:HG2	2.06	0.56
1:G:761:THR:HG23	1:G:762:LYS:HG3	1.86	0.56
1:H:725:LEU:O	1:H:726:ASN:ND2	2.37	0.56
1:I:474:GLU:OE2	1:I:596:LYS:NZ	2.38	0.56
1:J:293:LYS:HE3	1:J:330:MET:HE2	1.86	0.56
1:J:746:LEU:HG	1:J:751:ILE:HD12	1.86	0.56
1:K:270:LYS:HB3	1:K:429:LYS:HD2	1.86	0.56
1:K:725:LEU:O	1:K:726:ASN:ND2	2.37	0.56
1:M:610:GLN:HG2	1:M:620:LEU:O	2.05	0.56
1:H:471:ASN:ND2	1:H:587:ASP:O	2.36	0.56
1:H:610:GLN:HG2	1:H:620:LEU:O	2.05	0.56
1:K:610:GLN:HG2	1:K:620:LEU:O	2.05	0.56
1:M:761:THR:HG23	1:M:762:LYS:HG3	1.86	0.56
1:H:72:LYS:H	1:H:75:GLN:HE21	1.52	0.56
1:H:294:LYS:NZ	1:H:296:GLU:OE2	2.30	0.56
1:K:746:LEU:HG	1:K:751:ILE:HD12	1.86	0.56
1:M:72:LYS:H	1:M:75:GLN:HE21	1.52	0.56
2:C:351:THR:OG1	1:G:536:GLU:OE1	2.23	0.56
2:F:14:SER:O	2:F:157:ASP:HB3	2.06	0.56
1:G:610:GLN:HG2	1:G:620:LEU:O	2.05	0.56
1:I:504:GLU:OE2	1:I:761:THR:HG22	2.06	0.56
3:N:108:THR:HA	3:N:111:GLN:HG2	1.86	0.56
1:K:761:THR:HG23	1:K:762:LYS:HG3	1.86	0.56
2:A:14:SER:O	2:A:157:ASP:HB3	2.06	0.56
2:E:14:SER:O	2:E:157:ASP:HB3	2.06	0.56
2:E:41:GLN:HE21	2:A:172:PRO:CG	2.14	0.56
1:G:293:LYS:HE3	1:G:330:MET:HE2	1.86	0.56
1:G:504:GLU:OE2	1:G:761:THR:HG22	2.06	0.56
1:I:478:ILE:O	1:I:481:THR:OG1	2.22	0.56
3:O:105:ARG:HE	3:P:106:LEU:HD21	1.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:92:MET:HE1	1:H:712:ARG:H	1.71	0.56
1:H:109:TYR:HB3	1:H:684:MET:HE1	1.86	0.56
1:J:471:ASN:ND2	1:J:587:ASP:O	2.36	0.56
1:M:504:GLU:OE2	1:M:761:THR:HG22	2.06	0.56
2:D:220:ALA:HB1	2:D:226:GLU:HG3	1.88	0.56
1:G:725:LEU:O	1:G:726:ASN:ND2	2.37	0.56
1:M:474:GLU:OE2	1:M:596:LYS:NZ	2.38	0.55
2:B:317:ILE:HG23	2:B:327:ILE:HG21	1.88	0.55
1:G:109:TYR:HB3	1:G:684:MET:HE1	1.88	0.55
1:I:721:ARG:O	1:I:777:ARG:HD3	2.06	0.55
1:K:504:GLU:OE2	1:K:761:THR:HG22	2.06	0.55
1:H:472:SER:OG	1:H:473:PHE:N	2.35	0.55
1:H:474:GLU:OE2	1:H:596:LYS:NZ	2.38	0.55
1:H:504:GLU:OE2	1:H:761:THR:HG22	2.06	0.55
1:H:535:GLU:OE2	1:H:652:ARG:NH2	2.39	0.55
1:I:535:GLU:OE2	1:I:652:ARG:NH2	2.39	0.55
1:J:504:GLU:OE2	1:J:761:THR:HG22	2.06	0.55
1:J:535:GLU:OE2	1:J:652:ARG:NH2	2.39	0.55
1:K:535:GLU:OE2	1:K:652:ARG:NH2	2.39	0.55
1:M:109:TYR:HB3	1:M:684:MET:HE1	1.87	0.55
1:H:721:ARG:O	1:H:777:ARG:HD3	2.06	0.55
1:I:610:GLN:HG2	1:I:620:LEU:O	2.05	0.55
1:M:721:ARG:O	1:M:777:ARG:HD3	2.06	0.55
1:J:610:GLN:HG2	1:J:620:LEU:O	2.05	0.55
3:N:159:ASP:O	3:N:163:GLU:HG2	2.06	0.55
2:B:95:ARG:O	1:H:635:LYS:HA	2.05	0.55
1:H:478:ILE:O	1:H:481:THR:OG1	2.22	0.55
1:H:506:ILE:HG13	1:H:508:TRP:CZ3	2.42	0.55
1:J:24:LEU:HA	1:J:27:GLN:HG2	1.89	0.55
1:K:24:LEU:HA	1:K:27:GLN:HG2	1.89	0.55
1:K:281:ARG:HG2	1:K:317:GLU:HB2	1.88	0.55
1:K:721:ARG:O	1:K:777:ARG:HD3	2.06	0.55
2:C:369:ILE:HG12	2:C:374:CYS:SG	2.46	0.55
2:D:351:THR:OG1	1:I:536:GLU:OE1	2.25	0.55
1:J:721:ARG:O	1:J:777:ARG:HD3	2.07	0.55
2:A:213:LYS:NZ	4:A:401:ADP:O2'	2.28	0.55
1:M:24:LEU:HA	1:M:27:GLN:HG2	1.89	0.55
2:B:202:THR:HB	2:B:205:GLU:HG3	1.88	0.55
1:K:474:GLU:OE2	1:K:596:LYS:NZ	2.38	0.55
3:N:82:GLU:HA	3:N:85:VAL:HG12	1.88	0.55
1:M:506:ILE:HG13	1:M:508:TRP:CZ3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:47:GLN:OE1	3:P:47:GLN:N	2.39	0.55
1:G:24:LEU:HA	1:G:27:GLN:HG2	1.89	0.55
1:G:535:GLU:OE2	1:G:652:ARG:NH2	2.39	0.55
1:H:24:LEU:HA	1:H:27:GLN:HG2	1.89	0.55
1:I:293:LYS:HE3	1:I:330:MET:HE2	1.88	0.55
3:P:82:GLU:HA	3:P:85:VAL:HG12	1.88	0.55
1:G:173:SER:O	1:G:668:HIS:N	2.39	0.55
1:H:281:ARG:HG2	1:H:317:GLU:HB2	1.88	0.55
1:I:24:LEU:HA	1:I:27:GLN:HG2	1.89	0.55
1:I:471:ASN:ND2	1:I:587:ASP:O	2.36	0.55
1:J:281:ARG:HG2	1:J:317:GLU:HB2	1.88	0.55
1:J:474:GLU:OE2	1:J:596:LYS:NZ	2.38	0.55
1:M:281:ARG:HG2	1:M:317:GLU:HB2	1.88	0.54
1:M:535:GLU:OE2	1:M:652:ARG:NH2	2.39	0.54
2:F:369:ILE:HD12	2:F:372:ARG:HG3	1.88	0.54
3:O:144:GLN:O	3:O:147:GLN:NE2	2.35	0.54
1:G:471:ASN:ND2	1:G:587:ASP:O	2.36	0.54
1:G:478:ILE:O	1:G:481:THR:OG1	2.22	0.54
1:M:173:SER:O	1:M:668:HIS:N	2.39	0.54
2:D:116:ARG:O	2:D:120:THR:HG23	2.07	0.54
2:D:221:LEU:HD21	3:L:136:LYS:HZ2	1.70	0.54
2:F:147:ARG:HH22	2:F:330:ILE:HG12	1.73	0.54
3:P:98:GLU:OE2	3:P:99:LEU:HD12	2.08	0.54
1:G:721:ARG:O	1:G:777:ARG:HD3	2.07	0.54
2:A:321:ALA:HB3	2:A:327:ILE:HD11	1.89	0.54
3:N:173:GLU:O	3:N:177:GLU:HG2	2.07	0.54
3:O:61:SER:O	3:O:65:LYS:HG3	2.07	0.54
3:O:105:ARG:NE	3:P:106:LEU:HD21	2.22	0.54
1:J:478:ILE:O	1:J:481:THR:OG1	2.22	0.54
3:P:173:GLU:O	3:P:177:GLU:HG2	2.07	0.54
1:G:281:ARG:HG2	1:G:317:GLU:HB2	1.88	0.54
1:G:506:ILE:HG13	1:G:508:TRP:CZ3	2.42	0.54
1:G:676:ASN:ND2	1:G:680:SER:O	2.28	0.54
3:L:201:THR:HA	3:L:204:LEU:HG	1.89	0.54
1:J:368:GLN:HE21	3:L:100:ASP:HB2	1.70	0.54
1:M:294:LYS:NZ	1:M:296:GLU:OE2	2.30	0.54
2:E:321:ALA:HB3	2:E:327:ILE:HD11	1.89	0.54
1:I:281:ARG:HG2	1:I:317:GLU:HB2	1.88	0.54
1:M:676:ASN:ND2	1:M:680:SER:O	2.28	0.54
1:K:471:ASN:ND2	1:K:587:ASP:O	2.36	0.54
1:H:173:SER:O	1:H:668:HIS:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:506:ILE:HG13	1:K:508:TRP:CZ3	2.42	0.54
2:B:220:ALA:HB1	2:B:226:GLU:HG3	1.90	0.54
1:K:368:GLN:HG3	3:L:60:TYR:CE2	2.43	0.54
1:M:562:ASN:HD22	1:M:580:ILE:HD11	1.73	0.54
3:O:161:LYS:O	3:O:165:VAL:HG23	2.08	0.54
3:P:75:GLU:O	3:P:79:THR:HG23	2.08	0.54
1:G:562:ASN:HD22	1:G:580:ILE:HD11	1.73	0.54
1:I:562:ASN:HD22	1:I:580:ILE:HD11	1.73	0.54
3:L:105:ARG:NE	3:N:106:LEU:HD21	2.22	0.54
3:N:98:GLU:OE2	3:N:99:LEU:HD12	2.08	0.54
2:E:244:ASP:O	2:A:325:MET:HE1	2.07	0.53
1:J:562:ASN:HD22	1:J:580:ILE:HD11	1.73	0.53
1:K:173:SER:O	1:K:668:HIS:N	2.39	0.53
3:L:61:SER:O	3:L:65:LYS:HG3	2.07	0.53
3:N:75:GLU:O	3:N:79:THR:HG23	2.08	0.53
2:D:286:ASP:O	2:D:290:ARG:NE	2.40	0.53
2:F:304:THR:O	2:F:335:ARG:NH1	2.42	0.53
3:P:124:GLU:O	3:P:128:LYS:HG2	2.08	0.53
1:I:244:PHE:HB3	1:I:268:LEU:HD13	1.91	0.53
2:B:151:ILE:HG21	2:B:282:ILE:HD11	1.89	0.53
3:O:68:GLN:O	3:O:72:GLU:HG2	2.09	0.53
3:O:201:THR:HA	3:O:204:LEU:HG	1.89	0.53
1:H:244:PHE:HB3	1:H:268:LEU:HD13	1.91	0.53
1:I:506:ILE:HG13	1:I:508:TRP:CZ3	2.42	0.53
3:L:161:LYS:O	3:L:165:VAL:HG23	2.08	0.53
1:I:109:TYR:HB3	1:I:684:MET:HE1	1.90	0.53
1:J:244:PHE:HB3	1:J:268:LEU:HD13	1.91	0.53
3:N:197:LEU:HD23	3:N:198:LYS:NZ	2.24	0.53
1:M:244:PHE:HB3	1:M:268:LEU:HD13	1.91	0.53
1:M:334:ASN:O	1:M:338:VAL:HG22	2.09	0.53
1:G:334:ASN:O	1:G:338:VAL:HG22	2.09	0.53
1:J:173:SER:O	1:J:668:HIS:N	2.39	0.53
3:N:124:GLU:O	3:N:128:LYS:HG2	2.08	0.53
1:H:334:ASN:O	1:H:338:VAL:HG22	2.09	0.53
1:I:173:SER:O	1:I:668:HIS:N	2.39	0.53
1:I:580:ILE:HG22	1:I:585:ILE:HG12	1.90	0.53
1:K:244:PHE:HB3	1:K:268:LEU:HD13	1.91	0.53
2:C:116:ARG:O	2:C:120:THR:HG23	2.07	0.53
2:C:172:PRO:HG3	2:F:41:GLN:HE21	1.73	0.53
2:C:233:SER:OG	2:C:234:SER:N	2.41	0.53
1:H:293:LYS:HE3	1:H:330:MET:HE2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:235:THR:HG23	1:J:241:SER:OG	2.09	0.53
1:J:506:ILE:HG13	1:J:508:TRP:CZ3	2.42	0.53
3:N:73:LEU:O	3:N:77:LYS:NZ	2.42	0.53
2:D:120:THR:HG21	2:D:370:VAL:HG21	1.90	0.53
1:H:580:ILE:HG22	1:H:585:ILE:HG12	1.90	0.53
1:M:249:ARG:HB2	1:M:262:ASP:HB2	1.91	0.53
1:M:692:GLN:O	1:M:696:ASN:HB2	2.09	0.53
2:B:306:TYR:CE1	4:B:401:ADP:H2	2.27	0.53
1:I:692:GLN:O	1:I:696:ASN:HB2	2.09	0.53
1:K:235:THR:HG23	1:K:241:SER:OG	2.09	0.53
1:K:562:ASN:HD22	1:K:580:ILE:HD11	1.73	0.53
2:E:26:ALA:HB1	1:J:406:VAL:HG12	1.91	0.52
2:F:220:ALA:HB1	2:F:226:GLU:HG3	1.91	0.52
3:P:197:LEU:HD23	3:P:198:LYS:NZ	2.24	0.52
1:G:244:PHE:HB3	1:G:268:LEU:HD13	1.91	0.52
1:H:249:ARG:HB2	1:H:262:ASP:HB2	1.91	0.52
1:I:235:THR:HG23	1:I:241:SER:OG	2.09	0.52
1:J:334:ASN:O	1:J:338:VAL:HG22	2.09	0.52
1:J:580:ILE:HG22	1:J:585:ILE:HG12	1.90	0.52
3:O:91:ARG:O	3:O:95:VAL:HG23	2.10	0.52
1:H:562:ASN:HD22	1:H:580:ILE:HD11	1.73	0.52
3:O:81:ALA:O	3:O:85:VAL:HG13	2.09	0.52
1:G:580:ILE:HG22	1:G:585:ILE:HG12	1.90	0.52
1:H:722:TYR:CE2	1:H:773:LEU:HB3	2.44	0.52
1:I:334:ASN:O	1:I:338:VAL:HG22	2.09	0.52
1:M:471:ASN:ND2	1:M:587:ASP:O	2.36	0.52
1:G:235:THR:HG23	1:G:241:SER:OG	2.09	0.52
1:G:249:ARG:HB2	1:G:262:ASP:HB2	1.91	0.52
1:K:692:GLN:O	1:K:696:ASN:HB2	2.09	0.52
1:K:722:TYR:CE2	1:K:773:LEU:HB3	2.44	0.52
1:I:92:MET:HE1	1:I:712:ARG:H	1.73	0.52
1:J:109:TYR:HB3	1:J:684:MET:HE1	1.91	0.52
1:K:92:MET:HE1	1:K:712:ARG:H	1.73	0.52
1:K:249:ARG:HB2	1:K:262:ASP:HB2	1.91	0.52
3:L:81:ALA:O	3:L:85:VAL:HG13	2.10	0.52
1:I:249:ARG:N	1:I:262:ASP:O	2.41	0.52
1:M:235:THR:HG23	1:M:241:SER:OG	2.09	0.52
1:J:154:ILE:HD11	1:J:190:ARG:HG3	1.92	0.52
1:K:334:ASN:O	1:K:338:VAL:HG22	2.09	0.52
3:L:68:GLN:O	3:L:72:GLU:HG2	2.09	0.52
3:L:91:ARG:O	3:L:95:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:722:TYR:CE2	1:M:773:LEU:HB3	2.44	0.52
3:P:181:GLU:O	3:P:185:LEU:HG	2.10	0.52
1:I:368:GLN:CD	3:N:142:GLU:HA	2.30	0.52
1:J:92:MET:HE1	1:J:712:ARG:H	1.73	0.52
1:J:249:ARG:HB2	1:J:262:ASP:HB2	1.91	0.52
2:D:306:TYR:CE2	4:D:401:ADP:H2	2.28	0.52
2:E:62:ARG:HH11	2:E:207:GLU:HB2	1.75	0.52
1:J:692:GLN:O	1:J:696:ASN:HB2	2.09	0.52
1:J:722:TYR:CE2	1:J:773:LEU:HB3	2.44	0.52
3:N:181:GLU:O	3:N:185:LEU:HG	2.10	0.52
2:F:21:PHE:HZ	2:F:96:VAL:HG11	1.75	0.52
1:I:154:ILE:HD11	1:I:190:ARG:HG3	1.92	0.52
1:I:249:ARG:HB2	1:I:262:ASP:HB2	1.91	0.52
1:K:154:ILE:HD11	1:K:190:ARG:HG3	1.92	0.52
1:K:580:ILE:HG22	1:K:585:ILE:HG12	1.90	0.52
2:E:233:SER:OG	2:E:234:SER:N	2.43	0.51
1:G:537:GLU:HG3	1:G:543:ALA:HB1	1.92	0.51
1:H:235:THR:HG23	1:H:241:SER:OG	2.09	0.51
1:M:537:GLU:HG3	1:M:543:ALA:HB1	1.92	0.51
2:F:233:SER:OG	2:F:234:SER:N	2.43	0.51
1:I:265:THR:HG21	1:I:436:PHE:CE2	2.44	0.51
1:I:269:GLU:OE1	1:I:270:LYS:N	2.44	0.51
2:A:233:SER:OG	2:A:234:SER:N	2.43	0.51
3:L:145:GLU:O	3:L:149:LYS:HG2	2.11	0.51
1:M:265:THR:HG21	1:M:436:PHE:CE2	2.44	0.51
1:G:265:THR:HG21	1:G:436:PHE:CE2	2.44	0.51
1:G:722:TYR:CE2	1:G:773:LEU:HB3	2.44	0.51
1:H:269:GLU:OE1	1:H:270:LYS:N	2.44	0.51
1:H:692:GLN:O	1:H:696:ASN:HB2	2.09	0.51
1:J:676:ASN:ND2	1:J:680:SER:O	2.28	0.51
2:B:147:ARG:HH12	2:B:330:ILE:HG13	1.75	0.51
1:J:269:GLU:OE1	1:J:270:LYS:N	2.44	0.51
1:M:580:ILE:HG22	1:M:585:ILE:HG12	1.90	0.51
2:C:365:ALA:HB3	2:C:369:ILE:HD12	1.92	0.51
1:G:249:ARG:N	1:G:262:ASP:O	2.41	0.51
1:H:51:ILE:HD12	1:H:59:VAL:HB	1.92	0.51
1:H:265:THR:HG21	1:H:436:PHE:CE2	2.44	0.51
1:J:265:THR:HG21	1:J:436:PHE:CE2	2.44	0.51
1:H:537:GLU:HG3	1:H:543:ALA:HB1	1.92	0.51
1:I:722:TYR:CE2	1:I:773:LEU:HB3	2.44	0.51
2:A:62:ARG:HH11	2:A:207:GLU:HB2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:51:ILE:HD12	1:M:59:VAL:HB	1.92	0.51
1:M:293:LYS:HE3	1:M:330:MET:HE2	1.91	0.51
1:M:603:GLU:OE2	1:M:624:TYR:HA	2.11	0.51
1:G:449:THR:O	1:G:453:ARG:NH2	2.44	0.51
1:H:449:THR:O	1:H:453:ARG:NH2	2.44	0.51
1:M:269:GLU:OE1	1:M:270:LYS:N	2.44	0.51
1:M:686:ASN:O	1:M:690:MET:HG3	2.11	0.51
3:O:182:ARG:NH2	3:O:183:ALA:HA	2.26	0.51
1:G:603:GLU:OE2	1:G:624:TYR:HA	2.11	0.51
1:G:686:ASN:O	1:G:690:MET:HG3	2.11	0.51
1:G:692:GLN:O	1:G:696:ASN:HB2	2.09	0.51
1:G:708:GLY:O	1:G:766:LYS:NZ	2.28	0.51
1:H:230:PHE:CD1	1:H:285:ILE:HG12	2.46	0.51
1:I:449:THR:O	1:I:453:ARG:NH2	2.44	0.51
2:C:200:PHE:HB3	2:C:205:GLU:HB3	1.93	0.51
3:P:73:LEU:O	3:P:77:LYS:NZ	2.42	0.51
3:P:136:LYS:HG2	3:P:140:LYS:HE2	1.93	0.51
1:H:603:GLU:OE2	1:H:624:TYR:HA	2.11	0.51
1:H:686:ASN:O	1:H:690:MET:HG3	2.11	0.51
1:I:603:GLU:OE2	1:I:624:TYR:HA	2.11	0.51
1:J:537:GLU:HG3	1:J:543:ALA:HB1	1.92	0.51
1:K:449:THR:O	1:K:453:ARG:NH2	2.44	0.51
1:K:537:GLU:HG3	1:K:543:ALA:HB1	1.92	0.51
2:A:17:VAL:HG23	2:A:33:SER:HB2	1.92	0.51
2:C:190:MET:HG3	2:C:209:VAL:HG11	1.92	0.51
1:G:51:ILE:HD12	1:G:59:VAL:HB	1.92	0.51
1:K:265:THR:HG21	1:K:436:PHE:CE2	2.44	0.51
1:K:269:GLU:OE1	1:K:270:LYS:N	2.44	0.51
1:K:603:GLU:OE2	1:K:624:TYR:HA	2.11	0.51
1:K:676:ASN:HB3	1:K:684:MET:HA	1.93	0.51
2:B:21:PHE:CZ	2:B:96:VAL:HG11	2.46	0.50
3:P:72:GLU:O	3:P:76:LYS:HG3	2.12	0.50
1:G:154:ILE:HD11	1:G:190:ARG:HG3	1.92	0.50
1:G:230:PHE:CD1	1:G:285:ILE:HG12	2.46	0.50
1:J:449:THR:O	1:J:453:ARG:NH2	2.44	0.50
1:K:51:ILE:HD12	1:K:59:VAL:HB	1.92	0.50
1:K:230:PHE:CD1	1:K:285:ILE:HG12	2.46	0.50
3:O:145:GLU:O	3:O:149:LYS:HG2	2.11	0.50
1:I:537:GLU:HG3	1:I:543:ALA:HB1	1.92	0.50
1:J:230:PHE:CD1	1:J:285:ILE:HG12	2.46	0.50
1:K:676:ASN:ND2	1:K:680:SER:O	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:686:ASN:O	1:K:690:MET:HG3	2.11	0.50
3:L:182:ARG:NH2	3:L:183:ALA:HA	2.26	0.50
1:M:154:ILE:HD11	1:M:190:ARG:HG3	1.92	0.50
1:M:249:ARG:N	1:M:262:ASP:O	2.41	0.50
2:E:17:VAL:HG23	2:E:33:SER:HB2	1.92	0.50
1:I:230:PHE:CD1	1:I:285:ILE:HG12	2.46	0.50
1:I:752:ASP:HB2	1:I:755:GLN:HG3	1.94	0.50
1:J:676:ASN:HB3	1:J:684:MET:HA	1.93	0.50
1:J:686:ASN:O	1:J:690:MET:HG3	2.11	0.50
1:M:230:PHE:CD1	1:M:285:ILE:HG12	2.46	0.50
1:M:449:THR:O	1:M:453:ARG:NH2	2.44	0.50
2:E:304:THR:O	2:E:335:ARG:NH1	2.45	0.50
1:H:154:ILE:HD11	1:H:190:ARG:HG3	1.92	0.50
2:C:17:VAL:HG23	2:C:33:SER:HB3	1.94	0.50
3:P:204:LEU:O	3:P:208:GLU:HB2	2.12	0.50
1:G:269:GLU:OE1	1:G:270:LYS:N	2.44	0.50
1:I:676:ASN:HB3	1:I:684:MET:HA	1.93	0.50
1:J:51:ILE:HD12	1:J:59:VAL:HB	1.92	0.50
2:A:180:LEU:HD22	2:A:261:LEU:HD23	1.94	0.50
2:B:304:THR:O	2:B:335:ARG:NH1	2.45	0.50
2:D:23:GLY:O	1:I:641:GLY:N	2.40	0.50
1:I:51:ILE:HD12	1:I:59:VAL:HB	1.92	0.50
1:J:603:GLU:OE2	1:J:624:TYR:HA	2.11	0.50
1:J:745:LEU:HG	1:J:749:LEU:HD13	1.94	0.50
1:K:369:ARG:HB3	3:L:60:TYR:OH	2.11	0.50
2:A:304:THR:O	2:A:335:ARG:NH1	2.45	0.50
2:E:180:LEU:HD22	2:E:261:LEU:HD23	1.94	0.50
1:I:189:LYS:O	1:I:192:ILE:HG12	2.12	0.50
3:N:47:GLN:OE1	3:N:47:GLN:N	2.39	0.50
3:N:204:LEU:O	3:N:208:GLU:HB2	2.12	0.50
1:H:189:LYS:O	1:H:192:ILE:HG12	2.12	0.50
1:J:752:ASP:HB2	1:J:755:GLN:HG3	1.94	0.50
3:L:47:GLN:O	3:L:51:LYS:HG2	2.11	0.50
2:B:124:PHE:CZ	2:B:132:MET:HG2	2.47	0.49
1:G:171:ASN:OD1	1:G:456:PHE:N	2.40	0.49
1:G:290:LEU:HD13	1:G:307:PRO:HB3	1.94	0.49
1:H:708:GLY:O	1:H:766:LYS:NZ	2.28	0.49
1:J:115:TYR:HE2	1:J:154:ILE:HG23	1.77	0.49
1:K:219:GLN:OE1	1:K:219:GLN:N	2.42	0.49
2:A:306:TYR:CE2	4:A:401:ADP:H2	2.30	0.49
1:M:189:LYS:O	1:M:192:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:147:ARG:NH2	2:C:330:ILE:HG12	2.21	0.49
2:E:190:MET:HG2	2:E:209:VAL:HG21	1.93	0.49
1:J:45:GLU:HB3	1:J:690:MET:HE1	1.94	0.49
1:J:189:LYS:O	1:J:192:ILE:HG12	2.12	0.49
3:N:136:LYS:HG2	3:N:140:LYS:HE2	1.93	0.49
1:M:745:LEU:HG	1:M:749:LEU:HD13	1.94	0.49
2:D:337:TYR:O	2:D:341:ILE:HG12	2.12	0.49
1:H:281:ARG:HD2	1:H:320:VAL:HG22	1.94	0.49
1:J:219:GLN:OE1	1:J:219:GLN:N	2.42	0.49
1:K:406:VAL:HG12	2:A:26:ALA:HB1	1.94	0.49
1:M:371:GLU:OE1	2:F:147:ARG:NH2	2.44	0.49
1:H:249:ARG:N	1:H:262:ASP:O	2.41	0.49
1:I:171:ASN:OD1	1:I:456:PHE:N	2.40	0.49
1:J:370:GLU:HG2	1:J:371:GLU:H	1.78	0.49
1:M:281:ARG:HD2	1:M:320:VAL:HG22	1.94	0.49
1:M:290:LEU:HD13	1:M:307:PRO:HB3	1.94	0.49
1:M:714:LEU:HA	1:M:762:LYS:HA	1.95	0.49
1:M:752:ASP:HB2	1:M:755:GLN:HG3	1.94	0.49
2:C:143:TYR:OH	2:F:45:VAL:O	2.27	0.49
2:E:306:TYR:CE2	4:E:401:ADP:H2	2.30	0.49
3:O:47:GLN:O	3:O:51:LYS:HG2	2.11	0.49
1:G:281:ARG:HD2	1:G:320:VAL:HG22	1.95	0.49
1:G:714:LEU:HA	1:G:762:LYS:HA	1.95	0.49
1:H:370:GLU:HG2	1:H:371:GLU:H	1.78	0.49
1:I:115:TYR:CE2	1:I:154:ILE:HG23	2.48	0.49
1:J:281:ARG:HD2	1:J:320:VAL:HG22	1.94	0.49
1:J:714:LEU:HA	1:J:762:LYS:HA	1.95	0.49
3:L:71:LEU:HD21	3:N:71:LEU:CA	2.42	0.49
3:N:58:ASP:O	3:N:62:GLU:HG2	2.12	0.49
1:M:506:ILE:HG13	1:M:508:TRP:HZ3	1.78	0.49
2:B:14:SER:O	2:B:157:ASP:HB3	2.12	0.49
1:G:370:GLU:HG2	1:G:371:GLU:H	1.78	0.49
1:G:752:ASP:HB2	1:G:755:GLN:HG3	1.94	0.49
1:H:506:ILE:HG13	1:H:508:TRP:HZ3	1.78	0.49
1:H:752:ASP:HB2	1:H:755:GLN:HG3	1.93	0.49
1:I:290:LEU:HD13	1:I:307:PRO:HB3	1.94	0.49
1:J:716:GLY:O	1:J:720:GLN:HG2	2.13	0.49
1:K:281:ARG:HD2	1:K:320:VAL:HG22	1.94	0.49
1:K:506:ILE:HG13	1:K:508:TRP:HZ3	1.78	0.49
1:K:714:LEU:HA	1:K:762:LYS:HA	1.95	0.49
1:K:745:LEU:HG	1:K:749:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:752:ASP:HB2	1:K:755:GLN:HG3	1.94	0.49
3:N:72:GLU:O	3:N:76:LYS:HG3	2.12	0.49
1:M:115:TYR:HE2	1:M:154:ILE:HG23	1.77	0.49
1:M:434:ARG:HH22	1:M:623:ASN:CG	2.16	0.49
2:F:18:LYS:HG2	2:F:30:VAL:HG22	1.94	0.49
2:F:306:TYR:CE2	4:F:401:ADP:H2	2.30	0.49
3:O:202:ASN:O	3:O:205:LYS:HG3	2.13	0.49
3:P:58:ASP:O	3:P:62:GLU:HG2	2.12	0.49
1:H:115:TYR:HE2	1:H:154:ILE:HG23	1.77	0.49
1:H:745:LEU:HG	1:H:749:LEU:HD13	1.94	0.49
1:I:686:ASN:O	1:I:690:MET:HG3	2.11	0.49
1:J:434:ARG:HH22	1:J:623:ASN:CG	2.16	0.49
1:J:506:ILE:HG13	1:J:508:TRP:HZ3	1.78	0.49
1:J:763:VAL:HG13	1:J:765:PHE:CE2	2.48	0.49
1:K:716:GLY:O	1:K:720:GLN:HG2	2.13	0.49
1:M:716:GLY:O	1:M:720:GLN:HG2	2.13	0.49
2:F:368:SER:HB2	2:F:372:ARG:HH12	1.77	0.49
1:G:434:ARG:HH22	1:G:623:ASN:CG	2.16	0.49
1:H:714:LEU:HA	1:H:762:LYS:HA	1.95	0.49
1:I:434:ARG:HH22	1:I:623:ASN:CG	2.16	0.49
1:I:714:LEU:HA	1:I:762:LYS:HA	1.95	0.49
1:I:716:GLY:O	1:I:720:GLN:HG2	2.13	0.49
2:A:190:MET:HG2	2:A:209:VAL:HG21	1.93	0.49
1:M:676:ASN:HB3	1:M:684:MET:HA	1.93	0.49
3:O:106:LEU:HD22	3:P:105:ARG:CZ	2.43	0.49
1:G:35:LYS:HD2	1:G:51:ILE:HB	1.94	0.49
1:G:115:TYR:CE2	1:G:154:ILE:HG23	2.48	0.49
1:G:139:VAL:HG13	1:G:194:TYR:HD1	1.78	0.49
1:G:676:ASN:HB3	1:G:684:MET:HA	1.93	0.49
1:G:716:GLY:O	1:G:720:GLN:HG2	2.13	0.49
1:H:434:ARG:HH22	1:H:623:ASN:CG	2.16	0.49
1:H:716:GLY:O	1:H:720:GLN:HG2	2.13	0.49
1:I:281:ARG:HD2	1:I:320:VAL:HG22	1.94	0.49
1:K:473:PHE:HB3	1:K:596:LYS:HD2	1.94	0.49
1:K:763:VAL:HG13	1:K:765:PHE:CE2	2.48	0.49
1:M:35:LYS:HD2	1:M:51:ILE:HB	1.94	0.49
1:M:115:TYR:CE2	1:M:154:ILE:HG23	2.48	0.49
1:M:370:GLU:HG2	1:M:371:GLU:H	1.78	0.49
2:E:107:GLU:HG2	2:E:111:ASN:HD22	1.78	0.49
1:I:21:LYS:O	1:I:25:GLU:HG2	2.13	0.49
1:I:219:GLN:OE1	1:I:219:GLN:N	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:699:LEU:HA	1:J:702:ILE:HG12	1.95	0.49
3:L:111:GLN:O	3:L:115:GLU:HG2	2.13	0.49
1:G:189:LYS:O	1:G:192:ILE:HG12	2.12	0.48
1:G:506:ILE:HG13	1:G:508:TRP:HZ3	1.78	0.48
1:H:35:LYS:HD2	1:H:51:ILE:HB	1.94	0.48
1:H:676:ASN:HB3	1:H:684:MET:HA	1.93	0.48
1:I:370:GLU:HG2	1:I:371:GLU:H	1.78	0.48
1:I:473:PHE:HB3	1:I:596:LYS:HD2	1.94	0.48
1:I:506:ILE:HG13	1:I:508:TRP:HZ3	1.78	0.48
1:I:763:VAL:HG13	1:I:765:PHE:CE2	2.48	0.48
1:J:115:TYR:CE2	1:J:154:ILE:HG23	2.48	0.48
1:J:473:PHE:HB3	1:J:596:LYS:HD2	1.94	0.48
1:K:115:TYR:CE2	1:K:154:ILE:HG23	2.48	0.48
1:K:699:LEU:HA	1:K:702:ILE:HG12	1.95	0.48
3:L:108:THR:O	3:L:111:GLN:HG3	2.13	0.48
3:L:202:ASN:O	3:L:205:LYS:HG3	2.13	0.48
1:M:473:PHE:HB3	1:M:596:LYS:HD2	1.94	0.48
1:G:95:PHE:HB3	1:G:97:HIS:NE2	2.29	0.48
1:I:699:LEU:HA	1:I:702:ILE:HG12	1.95	0.48
1:J:290:LEU:HD13	1:J:307:PRO:HB3	1.94	0.48
1:J:499:GLU:HA	1:J:502:LYS:HG2	1.95	0.48
1:K:370:GLU:HG2	1:K:371:GLU:H	1.78	0.48
1:K:434:ARG:HH22	1:K:623:ASN:CG	2.16	0.48
2:D:230:ALA:HB2	2:D:236:LEU:HD12	1.96	0.48
3:O:96:GLU:OE2	3:P:95:VAL:HG11	2.13	0.48
3:P:201:THR:O	3:P:205:LYS:HG2	2.13	0.48
1:G:473:PHE:HB3	1:G:596:LYS:HD2	1.94	0.48
1:I:139:VAL:HG13	1:I:194:TYR:HD1	1.78	0.48
1:I:499:GLU:HA	1:I:502:LYS:HG2	1.95	0.48
1:K:189:LYS:O	1:K:192:ILE:HG12	2.12	0.48
2:A:107:GLU:HG2	2:A:111:ASN:HD22	1.78	0.48
1:M:21:LYS:O	1:M:25:GLU:HG2	2.13	0.48
1:G:699:LEU:HA	1:G:702:ILE:HG12	1.95	0.48
1:H:21:LYS:O	1:H:25:GLU:HG2	2.13	0.48
1:H:95:PHE:HB3	1:H:97:HIS:NE2	2.29	0.48
1:H:115:TYR:CE2	1:H:154:ILE:HG23	2.48	0.48
1:H:290:LEU:HD13	1:H:307:PRO:HB3	1.94	0.48
1:H:473:PHE:HB3	1:H:596:LYS:HD2	1.94	0.48
1:I:9:PHE:HB2	1:I:13:ALA:HB2	1.96	0.48
1:I:115:TYR:HE2	1:I:154:ILE:HG23	1.77	0.48
1:I:715:TYR:OH	1:I:759:GLY:O	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:745:LEU:HG	1:I:749:LEU:HD13	1.94	0.48
1:J:21:LYS:O	1:J:25:GLU:HG2	2.13	0.48
1:K:499:GLU:HA	1:K:502:LYS:HG2	1.95	0.48
1:K:611:LYS:HE2	1:K:611:LYS:HB3	1.61	0.48
1:M:139:VAL:HG13	1:M:194:TYR:HD1	1.78	0.48
2:D:71:ILE:HG12	2:D:76:ILE:HG12	1.95	0.48
1:J:95:PHE:HB3	1:J:97:HIS:NE2	2.29	0.48
1:J:496:LEU:HA	1:J:499:GLU:OE1	2.14	0.48
1:K:95:PHE:HB3	1:K:97:HIS:NE2	2.29	0.48
1:K:115:TYR:HE2	1:K:154:ILE:HG23	1.78	0.48
1:M:699:LEU:HA	1:M:702:ILE:HG12	1.95	0.48
3:O:111:GLN:O	3:O:115:GLU:HG2	2.13	0.48
3:O:202:ASN:OD1	3:O:205:LYS:HE3	2.14	0.48
1:G:92:MET:HE1	1:G:712:ARG:H	1.78	0.48
1:G:172:GLN:HB2	1:G:457:ILE:HG23	1.96	0.48
1:G:187:ASN:O	1:G:190:ARG:HG2	2.14	0.48
1:G:611:LYS:HB3	1:G:611:LYS:HE2	1.61	0.48
1:G:634:GLY:O	1:G:637:LYS:HG2	2.14	0.48
1:I:634:GLY:O	1:I:637:LYS:HG2	2.14	0.48
1:J:139:VAL:HG13	1:J:194:TYR:HD1	1.78	0.48
1:K:9:PHE:HB2	1:K:13:ALA:HB2	1.96	0.48
1:M:45:GLU:HB3	1:M:690:MET:HE1	1.94	0.48
2:E:76:ILE:HD13	2:E:82:MET:HG2	1.95	0.48
1:H:699:LEU:HA	1:H:702:ILE:HG12	1.95	0.48
1:I:95:PHE:HB3	1:I:97:HIS:NE2	2.29	0.48
1:I:496:LEU:HA	1:I:499:GLU:OE1	2.14	0.48
1:J:368:GLN:HG2	3:L:99:LEU:HD13	1.76	0.48
1:J:368:GLN:HE21	3:L:100:ASP:CA	2.01	0.48
1:K:35:LYS:HD2	1:K:51:ILE:HB	1.94	0.48
1:K:290:LEU:HD13	1:K:307:PRO:HB3	1.94	0.48
2:A:76:ILE:HD13	2:A:82:MET:HG2	1.95	0.48
1:M:187:ASN:O	1:M:190:ARG:HG2	2.14	0.48
3:O:70:LYS:HA	3:O:73:LEU:HG	1.96	0.48
3:O:108:THR:O	3:O:111:GLN:HG3	2.13	0.48
1:G:745:LEU:HG	1:G:749:LEU:HD13	1.94	0.48
1:G:763:VAL:HG13	1:G:765:PHE:CE2	2.48	0.48
1:H:562:ASN:HB3	1:H:580:ILE:HG12	1.95	0.48
1:J:634:GLY:O	1:J:637:LYS:HG2	2.14	0.48
1:K:21:LYS:O	1:K:25:GLU:HG2	2.13	0.48
3:L:106:LEU:HD22	3:N:105:ARG:CZ	2.43	0.48
1:M:763:VAL:HG13	1:M:765:PHE:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:226:GLU:HA	2:D:229:THR:HG22	1.96	0.48
1:M:9:PHE:HB2	1:M:13:ALA:HB2	1.96	0.48
1:M:172:GLN:HB2	1:M:457:ILE:HG23	1.96	0.48
2:D:123:MET:O	2:D:129:VAL:HG22	2.14	0.48
1:G:21:LYS:O	1:G:25:GLU:HG2	2.13	0.48
1:G:143:ARG:NH1	1:G:143:ARG:HA	2.29	0.48
1:G:177:THR:OG1	1:G:671:ARG:NH1	2.47	0.48
1:G:275:PHE:HA	1:G:315:GLN:NE2	2.29	0.48
1:G:621:PHE:CG	1:G:622:ALA:N	2.82	0.48
1:H:172:GLN:HB2	1:H:457:ILE:HG23	1.96	0.48
1:H:634:GLY:O	1:H:637:LYS:HG2	2.14	0.48
1:H:763:VAL:HG13	1:H:765:PHE:CE2	2.48	0.48
1:I:160:ASN:HA	1:I:163:GLN:HE21	1.79	0.48
1:K:160:ASN:HA	1:K:163:GLN:HE21	1.79	0.48
1:K:171:ASN:OD1	1:K:456:PHE:N	2.40	0.48
1:M:275:PHE:HA	1:M:315:GLN:NE2	2.29	0.47
1:M:462:ILE:HG23	1:M:463:ALA:O	2.14	0.47
1:G:115:TYR:HE2	1:G:154:ILE:HG23	1.77	0.47
1:H:187:ASN:O	1:H:190:ARG:HG2	2.14	0.47
1:H:462:ILE:HG23	1:H:463:ALA:O	2.14	0.47
1:I:403:ARG:H	1:I:604:THR:HG21	1.79	0.47
1:J:562:ASN:HB3	1:J:580:ILE:HG12	1.95	0.47
1:K:139:VAL:HG13	1:K:194:TYR:HD1	1.78	0.47
1:K:187:ASN:O	1:K:190:ARG:HG2	2.14	0.47
1:K:496:LEU:HA	1:K:499:GLU:OE1	2.14	0.47
1:M:237:ARG:HH12	1:M:691:HIS:CD2	2.33	0.47
1:M:496:LEU:HA	1:M:499:GLU:OE1	2.14	0.47
2:B:162:ASN:ND2	2:B:277:THR:HG22	2.29	0.47
3:O:58:ASP:O	3:O:62:GLU:HG2	2.14	0.47
1:G:237:ARG:HH12	1:G:691:HIS:CD2	2.33	0.47
1:G:499:GLU:HA	1:G:502:LYS:HG2	1.95	0.47
1:G:567:ARG:HH21	1:G:585:ILE:HG22	1.79	0.47
1:I:368:GLN:HE21	3:N:142:GLU:N	2.05	0.47
1:J:35:LYS:HD2	1:J:51:ILE:HB	1.94	0.47
1:J:160:ASN:HA	1:J:163:GLN:HE21	1.79	0.47
1:J:187:ASN:O	1:J:190:ARG:HG2	2.14	0.47
1:J:462:ILE:HG23	1:J:463:ALA:O	2.14	0.47
1:K:634:GLY:O	1:K:637:LYS:HG2	2.14	0.47
3:L:202:ASN:OD1	3:L:205:LYS:HE3	2.14	0.47
3:N:194:GLU:O	3:N:198:LYS:HG2	2.14	0.47
1:M:177:THR:OG1	1:M:671:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:73:LEU:O	3:P:77:LYS:HG2	2.14	0.47
3:P:200:VAL:HA	3:P:203:ASN:HD22	1.79	0.47
1:H:296:GLU:O	1:H:300:MET:HG2	2.15	0.47
1:I:187:ASN:O	1:I:190:ARG:HG2	2.14	0.47
1:I:611:LYS:HB3	1:I:611:LYS:HE2	1.61	0.47
1:J:343:SER:HA	1:J:346:LYS:HE2	1.97	0.47
1:K:249:ARG:N	1:K:262:ASP:O	2.41	0.47
2:A:372:ARG:O	2:A:375:PHE:HB2	2.14	0.47
1:M:143:ARG:NH1	1:M:143:ARG:HA	2.29	0.47
1:M:296:GLU:O	1:M:300:MET:HG2	2.15	0.47
1:M:499:GLU:HA	1:M:502:LYS:HG2	1.95	0.47
2:B:62:ARG:HH11	2:B:207:GLU:HB2	1.78	0.47
2:E:23:GLY:O	1:J:641:GLY:N	2.43	0.47
3:P:194:GLU:O	3:P:198:LYS:HG2	2.14	0.47
1:H:139:VAL:HG13	1:H:194:TYR:HD1	1.78	0.47
1:H:715:TYR:OH	1:H:759:GLY:O	2.26	0.47
1:I:35:LYS:HD2	1:I:51:ILE:HB	1.94	0.47
1:K:343:SER:HA	1:K:346:LYS:HE2	1.97	0.47
3:N:201:THR:O	3:N:205:LYS:HG2	2.13	0.47
1:M:95:PHE:HB3	1:M:97:HIS:NE2	2.29	0.47
1:M:567:ARG:HH21	1:M:585:ILE:HG22	1.79	0.47
2:D:196:ARG:HD2	2:D:253:GLU:OE2	2.14	0.47
3:P:88:LEU:O	3:P:92:ILE:HG13	2.15	0.47
1:G:45:GLU:HB3	1:G:690:MET:HE1	1.95	0.47
1:G:367:LYS:HE2	1:G:367:LYS:HB3	1.63	0.47
1:H:177:THR:OG1	1:H:671:ARG:NH1	2.47	0.47
1:J:143:ARG:NH1	1:J:143:ARG:HA	2.29	0.47
1:K:143:ARG:NH1	1:K:143:ARG:HA	2.29	0.47
3:L:58:ASP:O	3:L:62:GLU:HG2	2.14	0.47
3:N:106:LEU:O	3:N:110:LEU:HG	2.15	0.47
1:M:766:LYS:H	1:M:769:LEU:HD13	1.80	0.47
1:G:562:ASN:HB3	1:G:580:ILE:HG12	1.95	0.47
1:H:143:ARG:NH1	1:H:143:ARG:HA	2.29	0.47
1:H:237:ARG:HH12	1:H:691:HIS:CD2	2.33	0.47
1:I:577:PHE:HE2	1:I:579:LEU:HD13	1.80	0.47
1:I:766:LYS:H	1:I:769:LEU:HD13	1.80	0.47
1:J:403:ARG:H	1:J:604:THR:HG21	1.79	0.47
1:J:621:PHE:CG	1:J:622:ALA:N	2.82	0.47
1:K:296:GLU:O	1:K:300:MET:HG2	2.15	0.47
1:M:368:GLN:NE2	3:P:138:GLU:OE1	2.48	0.47
1:M:634:GLY:O	1:M:637:LYS:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:ALA:HB2	2:B:236:LEU:HD12	1.96	0.47
2:C:221:LEU:HD22	3:P:90:ARG:HB3	1.96	0.47
2:E:147:ARG:NH2	1:J:371:GLU:OE1	2.47	0.47
2:E:372:ARG:O	2:E:375:PHE:HB2	2.14	0.47
2:F:21:PHE:CZ	2:F:96:VAL:HG11	2.49	0.47
3:O:173:GLU:CD	1:H:368:GLN:NE2	2.64	0.47
3:O:177:GLU:O	3:O:181:GLU:HG2	2.15	0.47
3:P:65:LYS:HA	3:P:68:GLN:OE1	2.15	0.47
1:H:9:PHE:HB2	1:H:13:ALA:HB2	1.96	0.47
1:H:275:PHE:HA	1:H:315:GLN:NE2	2.29	0.47
1:H:499:GLU:HA	1:H:502:LYS:HG2	1.95	0.47
1:I:143:ARG:NH1	1:I:143:ARG:HA	2.29	0.47
1:I:343:SER:HA	1:I:346:LYS:HE2	1.97	0.47
1:I:476:LEU:HD11	1:I:524:ILE:HD12	1.97	0.47
1:I:621:PHE:CG	1:I:622:ALA:N	2.82	0.47
1:J:9:PHE:HB2	1:J:13:ALA:HB2	1.96	0.47
1:J:237:ARG:HH12	1:J:691:HIS:CD2	2.33	0.47
1:J:368:GLN:NE2	3:L:99:LEU:HD12	2.29	0.47
1:J:476:LEU:HD11	1:J:524:ILE:HD12	1.97	0.47
1:J:577:PHE:HE2	1:J:579:LEU:HD13	1.80	0.47
1:K:172:GLN:HB2	1:K:457:ILE:HG23	1.96	0.47
1:K:177:THR:OG1	1:K:671:ARG:NH1	2.47	0.47
1:K:476:LEU:HD11	1:K:524:ILE:HD12	1.97	0.47
1:K:567:ARG:HH21	1:K:585:ILE:HG22	1.79	0.47
1:K:641:GLY:N	2:A:23:GLY:O	2.43	0.47
1:M:621:PHE:CG	1:M:622:ALA:N	2.82	0.47
2:E:45:VAL:O	2:A:143:TYR:OH	2.29	0.47
2:F:47:MET:HB3	1:G:540:PHE:CE2	2.50	0.47
1:G:766:LYS:H	1:G:769:LEU:HD13	1.80	0.47
1:H:496:LEU:HA	1:H:499:GLU:OE1	2.14	0.47
1:H:621:PHE:CG	1:H:622:ALA:N	2.82	0.47
1:I:237:ARG:HH12	1:I:691:HIS:CD2	2.33	0.47
1:I:462:ILE:HG23	1:I:463:ALA:O	2.14	0.47
1:I:562:ASN:HB3	1:I:580:ILE:HG12	1.95	0.47
1:K:562:ASN:HB3	1:K:580:ILE:HG12	1.95	0.47
3:L:70:LYS:HA	3:L:73:LEU:HG	1.96	0.47
2:B:5:THR:OG1	2:B:6:THR:N	2.46	0.47
2:E:151:ILE:HG21	2:E:282:ILE:HD11	1.97	0.47
2:F:17:VAL:HG23	2:F:33:SER:HB3	1.97	0.47
1:G:9:PHE:HB2	1:G:13:ALA:HB2	1.96	0.47
1:G:261:ALA:HB3	1:G:447:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:160:ASN:HA	1:H:163:GLN:HE21	1.79	0.47
1:H:766:LYS:H	1:H:769:LEU:HD13	1.80	0.47
1:J:275:PHE:HA	1:J:315:GLN:NE2	2.29	0.47
1:J:708:GLY:O	1:J:766:LYS:NZ	2.28	0.47
1:K:577:PHE:HE2	1:K:579:LEU:HD13	1.80	0.47
1:K:635:LYS:HA	2:A:95:ARG:O	2.14	0.47
3:N:65:LYS:HA	3:N:68:GLN:OE1	2.15	0.47
3:N:73:LEU:O	3:N:77:LYS:HG2	2.14	0.47
1:M:160:ASN:HA	1:M:163:GLN:HE21	1.79	0.47
1:M:562:ASN:HB3	1:M:580:ILE:HG12	1.95	0.47
2:B:76:ILE:HD13	2:B:82:MET:HG2	1.96	0.47
1:H:343:SER:HA	1:H:346:LYS:HE2	1.97	0.47
1:I:177:THR:OG1	1:I:671:ARG:NH1	2.47	0.47
1:J:172:GLN:HB2	1:J:457:ILE:HG23	1.96	0.47
1:K:38:PHE:N	1:K:77:MET:O	2.47	0.47
1:K:261:ALA:HB3	1:K:447:LEU:HD21	1.97	0.47
1:K:462:ILE:HG23	1:K:463:ALA:O	2.14	0.47
1:K:621:PHE:CG	1:K:622:ALA:N	2.82	0.47
3:N:124:GLU:O	3:N:127:MET:HG2	2.15	0.47
3:N:200:VAL:HA	3:N:203:ASN:HD22	1.79	0.47
2:B:162:ASN:HD22	2:B:277:THR:HG22	1.81	0.46
2:E:95:ARG:O	1:J:635:LYS:HA	2.15	0.46
2:F:190:MET:HG3	2:F:209:VAL:HG11	1.96	0.46
1:G:476:LEU:HD11	1:G:524:ILE:HD12	1.97	0.46
1:I:567:ARG:HH21	1:I:585:ILE:HG22	1.79	0.46
1:K:371:GLU:OE1	2:A:147:ARG:NH2	2.49	0.46
3:L:50:LEU:HD11	3:N:53:THR:HG21	1.98	0.46
2:F:195:GLU:OE2	2:F:256:ARG:NH2	2.49	0.46
3:O:94:LEU:O	3:O:98:GLU:HG3	2.15	0.46
1:G:403:ARG:H	1:G:604:THR:HG21	1.79	0.46
1:G:462:ILE:HG23	1:G:463:ALA:O	2.14	0.46
1:G:496:LEU:HA	1:G:499:GLU:OE1	2.14	0.46
1:G:715:TYR:OH	1:G:759:GLY:O	2.26	0.46
1:I:45:GLU:HB3	1:I:690:MET:HE1	1.97	0.46
1:J:766:LYS:H	1:J:769:LEU:HD13	1.80	0.46
1:K:237:ARG:HH12	1:K:691:HIS:CD2	2.33	0.46
1:K:679:LYS:HD3	1:K:679:LYS:HA	1.74	0.46
3:N:188:GLY:O	3:N:192:GLU:HG2	2.15	0.46
1:M:261:ALA:HB3	1:M:447:LEU:HD21	1.97	0.46
3:P:106:LEU:O	3:P:110:LEU:HG	2.15	0.46
3:P:124:GLU:O	3:P:127:MET:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:484:LYS:HG3	1:H:655:LEU:HD21	1.98	0.46
1:I:275:PHE:HA	1:I:315:GLN:NE2	2.29	0.46
1:J:283:TYR:HB3	1:J:285:ILE:HD12	1.98	0.46
1:J:368:GLN:HE21	3:L:99:LEU:HD12	1.80	0.46
1:K:572:LYS:HB3	1:K:572:LYS:HE2	1.69	0.46
3:L:136:LYS:HA	3:L:139:GLU:HG2	1.97	0.46
3:L:177:GLU:O	3:L:181:GLU:HG2	2.15	0.46
3:N:144:GLN:O	3:N:147:GLN:HG3	2.15	0.46
2:C:334:GLU:OE1	2:C:334:GLU:N	2.37	0.46
2:D:216:LEU:HD22	2:D:238:LYS:HD3	1.96	0.46
2:F:97:ALA:HB1	2:F:99:GLU:OE1	2.15	0.46
3:P:153:HIS:O	3:P:156:GLU:HG3	2.15	0.46
1:G:484:LYS:HG3	1:G:655:LEU:HD21	1.98	0.46
1:H:47:VAL:HA	1:H:103:TYR:OH	2.16	0.46
1:H:219:GLN:OE1	1:H:219:GLN:N	2.42	0.46
1:H:567:ARG:HH21	1:H:585:ILE:HG22	1.79	0.46
1:H:637:LYS:HD3	1:H:637:LYS:HA	1.75	0.46
1:I:172:GLN:HB2	1:I:457:ILE:HG23	1.96	0.46
1:J:171:ASN:OD1	1:J:456:PHE:N	2.40	0.46
1:J:177:THR:OG1	1:J:671:ARG:NH1	2.47	0.46
1:J:261:ALA:HB3	1:J:447:LEU:HD21	1.97	0.46
1:J:703:ARG:O	1:J:707:LYS:HE2	2.16	0.46
3:N:88:LEU:O	3:N:92:ILE:HG13	2.15	0.46
1:M:38:PHE:N	1:M:77:MET:O	2.47	0.46
1:M:47:VAL:HA	1:M:103:TYR:OH	2.16	0.46
1:M:343:SER:HA	1:M:346:LYS:HE2	1.97	0.46
1:M:476:LEU:HD11	1:M:524:ILE:HD12	1.97	0.46
1:G:160:ASN:HA	1:G:163:GLN:HE21	1.79	0.46
1:G:296:GLU:O	1:G:300:MET:HG2	2.14	0.46
1:H:261:ALA:HB3	1:H:447:LEU:HD21	1.97	0.46
3:L:161:LYS:O	3:L:164:GLU:HG2	2.16	0.46
3:L:196:GLU:O	3:L:200:VAL:HG22	2.14	0.46
1:M:186:VAL:HG13	1:M:190:ARG:HH21	1.81	0.46
1:M:219:GLN:OE1	1:M:219:GLN:N	2.42	0.46
1:M:483:GLU:OE2	1:M:581:HIS:HB3	2.16	0.46
1:M:484:LYS:HG3	1:M:655:LEU:HD21	1.98	0.46
2:C:301:GLY:O	2:C:304:THR:OG1	2.32	0.46
3:O:165:VAL:O	3:O:169:LEU:HB2	2.16	0.46
3:O:173:GLU:HB3	1:H:368:GLN:HE22	1.80	0.46
1:G:186:VAL:HG13	1:G:190:ARG:HH21	1.81	0.46
1:I:283:TYR:HB3	1:I:285:ILE:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:296:GLU:O	1:J:300:MET:HG2	2.15	0.46
1:K:403:ARG:H	1:K:604:THR:HG21	1.79	0.46
1:K:766:LYS:H	1:K:769:LEU:HD13	1.80	0.46
3:L:94:LEU:O	3:L:98:GLU:HG3	2.15	0.46
2:C:252:ASN:HB3	2:C:256:ARG:HD3	1.97	0.46
1:H:403:ARG:H	1:H:604:THR:HG21	1.79	0.46
1:H:569:ILE:O	1:H:570:LYS:HG2	2.16	0.46
1:K:275:PHE:HA	1:K:315:GLN:NE2	2.29	0.46
1:K:474:GLU:H	1:K:474:GLU:CD	2.18	0.46
1:K:569:ILE:O	1:K:570:LYS:HG2	2.16	0.46
2:A:151:ILE:HG21	2:A:282:ILE:HD11	1.97	0.46
1:M:171:ASN:OD1	1:M:456:PHE:N	2.40	0.46
3:O:87:SER:O	3:O:91:ARG:HG2	2.16	0.46
3:O:196:GLU:O	3:O:200:VAL:HG22	2.15	0.46
1:G:343:SER:HA	1:G:346:LYS:HE2	1.97	0.46
1:I:483:GLU:OE2	1:I:581:HIS:HB3	2.16	0.46
1:K:282:ASP:OD1	1:K:283:TYR:N	2.45	0.46
3:L:87:SER:O	3:L:91:ARG:HG2	2.16	0.46
1:M:703:ARG:O	1:M:707:LYS:HE2	2.16	0.46
2:C:361:GLU:O	2:C:364:GLU:HG3	2.16	0.46
2:E:116:ARG:HG2	2:E:370:VAL:HG11	1.98	0.46
2:F:70:PRO:HB3	2:F:81:ASP:HB3	1.98	0.46
3:P:144:GLN:O	3:P:147:GLN:HG3	2.15	0.46
1:H:186:VAL:HG13	1:H:190:ARG:HH21	1.81	0.46
1:H:282:ASP:OD1	1:H:283:TYR:N	2.45	0.46
1:I:296:GLU:O	1:I:300:MET:HG2	2.15	0.46
1:I:565:LYS:O	1:I:578:SER:OG	2.25	0.46
1:I:703:ARG:O	1:I:707:LYS:HE2	2.16	0.46
1:K:231:GLY:HA3	1:K:244:PHE:CD1	2.51	0.46
1:K:283:TYR:HB3	1:K:285:ILE:HD12	1.98	0.46
1:K:703:ARG:O	1:K:707:LYS:HE2	2.16	0.46
2:A:116:ARG:HG2	2:A:370:VAL:HG11	1.98	0.46
3:N:162:TYR:HA	3:N:165:VAL:HG12	1.97	0.46
3:N:199:THR:HG22	3:N:203:ASN:HD21	1.81	0.46
1:M:577:PHE:HE2	1:M:579:LEU:HD13	1.80	0.46
3:O:71:LEU:HD21	3:P:71:LEU:CA	2.42	0.46
3:O:161:LYS:O	3:O:164:GLU:HG2	2.16	0.46
3:P:188:GLY:O	3:P:192:GLU:HG2	2.15	0.46
1:G:38:PHE:N	1:G:77:MET:O	2.47	0.46
1:G:569:ILE:O	1:G:570:LYS:HG2	2.16	0.46
1:H:476:LEU:HD11	1:H:524:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:766:LYS:HG3	1:H:767:ALA:H	1.81	0.46
1:I:114:ILE:HG23	1:I:125:VAL:O	2.16	0.46
1:I:231:GLY:HA3	1:I:244:PHE:CD1	2.51	0.46
1:I:766:LYS:HG3	1:I:767:ALA:H	1.81	0.46
1:J:567:ARG:HH21	1:J:585:ILE:HG22	1.79	0.46
1:J:739:ARG:HD2	1:J:758:PHE:CZ	2.51	0.46
1:J:766:LYS:HG3	1:J:767:ALA:H	1.81	0.46
3:P:162:TYR:HA	3:P:165:VAL:HG12	1.97	0.45
1:G:158:SER:HB3	1:G:195:PHE:CE1	2.51	0.45
1:H:577:PHE:HE2	1:H:579:LEU:HD13	1.80	0.45
1:J:47:VAL:HA	1:J:103:TYR:OH	2.16	0.45
1:J:114:ILE:HG23	1:J:125:VAL:O	2.16	0.45
1:K:47:VAL:HA	1:K:103:TYR:OH	2.16	0.45
1:M:403:ARG:H	1:M:604:THR:HG21	1.79	0.45
2:C:71:ILE:HG12	2:C:76:ILE:HG12	1.98	0.45
2:C:306:TYR:CE1	4:C:401:ADP:H2	2.34	0.45
2:C:333:PRO:HB2	1:G:412:THR:O	2.16	0.45
3:O:50:LEU:HD11	3:P:53:THR:HG21	1.98	0.45
3:O:63:ALA:HA	3:O:66:ASP:OD2	2.16	0.45
3:P:167:ARG:O	3:P:171:ILE:HG12	2.17	0.45
3:P:199:THR:HG22	3:P:203:ASN:HD21	1.81	0.45
1:G:47:VAL:HA	1:G:103:TYR:OH	2.16	0.45
1:G:739:ARG:HD2	1:G:758:PHE:CZ	2.52	0.45
1:G:766:LYS:HG3	1:G:767:ALA:H	1.81	0.45
1:J:231:GLY:HA3	1:J:244:PHE:CD1	2.51	0.45
1:J:569:ILE:O	1:J:570:LYS:HG2	2.16	0.45
1:K:114:ILE:HG23	1:K:125:VAL:O	2.16	0.45
3:L:184:GLU:O	3:L:187:GLU:HG3	2.16	0.45
3:N:105:ARG:HA	3:N:108:THR:OG1	2.17	0.45
3:N:153:HIS:O	3:N:156:GLU:HG3	2.15	0.45
1:M:38:PHE:CE2	1:M:79:GLN:HA	2.52	0.45
1:M:739:ARG:HD2	1:M:758:PHE:CZ	2.52	0.45
3:O:175:ASP:O	3:O:178:ARG:HG3	2.16	0.45
1:G:577:PHE:HE2	1:G:579:LEU:HD13	1.80	0.45
1:H:38:PHE:N	1:H:77:MET:O	2.47	0.45
1:H:483:GLU:OE2	1:H:581:HIS:HB3	2.16	0.45
1:I:38:PHE:N	1:I:77:MET:O	2.47	0.45
1:I:186:VAL:HG13	1:I:190:ARG:HH21	1.81	0.45
1:I:569:ILE:O	1:I:570:LYS:HG2	2.16	0.45
1:J:671:ARG:HB3	1:J:696:ASN:HD21	1.81	0.45
1:K:45:GLU:HB3	1:K:690:MET:HE1	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:186:VAL:HG13	1:K:190:ARG:HH21	1.81	0.45
1:K:671:ARG:HB3	1:K:696:ASN:HD21	1.82	0.45
1:M:766:LYS:HG3	1:M:767:ALA:H	1.81	0.45
2:B:9:VAL:O	2:B:340:TRP:NE1	2.45	0.45
2:F:170:ALA:O	2:F:172:PRO:HD3	2.15	0.45
1:G:283:TYR:HB3	1:G:285:ILE:HD12	1.98	0.45
1:H:38:PHE:CE2	1:H:79:GLN:HA	2.52	0.45
1:H:611:LYS:HE2	1:H:611:LYS:HB3	1.61	0.45
1:I:47:VAL:HA	1:I:103:TYR:OH	2.16	0.45
1:I:474:GLU:OE1	1:I:474:GLU:N	2.32	0.45
1:M:158:SER:HB3	1:M:195:PHE:CE1	2.51	0.45
2:F:98:PRO:O	2:F:129:VAL:HA	2.16	0.45
3:O:136:LYS:HA	3:O:139:GLU:HG2	1.97	0.45
1:G:483:GLU:OE2	1:G:581:HIS:HB3	2.16	0.45
1:H:671:ARG:HB3	1:H:696:ASN:HD21	1.81	0.45
1:I:671:ARG:HB3	1:I:696:ASN:HD21	1.82	0.45
1:K:38:PHE:CE2	1:K:79:GLN:HA	2.52	0.45
3:L:165:VAL:O	3:L:169:LEU:HB2	2.16	0.45
3:L:175:ASP:O	3:L:178:ARG:HG3	2.16	0.45
1:M:569:ILE:O	1:M:570:LYS:HG2	2.16	0.45
1:H:114:ILE:HG23	1:H:125:VAL:O	2.17	0.45
1:K:484:LYS:HG3	1:K:655:LEU:HD21	1.98	0.45
1:K:766:LYS:HG3	1:K:767:ALA:H	1.81	0.45
3:L:63:ALA:HA	3:L:66:ASP:OD2	2.16	0.45
2:C:50:LYS:HE2	2:C:52:SER:O	2.17	0.45
2:C:305:MET:HA	2:C:335:ARG:NH1	2.32	0.45
3:O:184:GLU:O	3:O:187:GLU:HG3	2.16	0.45
1:G:38:PHE:CE2	1:G:79:GLN:HA	2.52	0.45
1:H:739:ARG:HD2	1:H:758:PHE:CZ	2.51	0.45
1:J:483:GLU:OE2	1:J:581:HIS:HB3	2.16	0.45
1:K:483:GLU:OE2	1:K:581:HIS:HB3	2.16	0.45
2:A:307:PRO:HB2	3:L:48:LYS:HE2	1.98	0.45
1:M:114:ILE:HG23	1:M:125:VAL:O	2.16	0.45
1:M:369:ARG:HE	3:O:133:ARG:NH1	2.14	0.45
1:M:671:ARG:HB3	1:M:696:ASN:HD21	1.81	0.45
1:G:703:ARG:O	1:G:707:LYS:HE2	2.16	0.45
1:H:283:TYR:HB3	1:H:285:ILE:HD12	1.98	0.45
1:H:703:ARG:O	1:H:707:LYS:HE2	2.16	0.45
1:I:261:ALA:HB3	1:I:447:LEU:HD21	1.97	0.45
1:J:186:VAL:HG13	1:J:190:ARG:HH21	1.81	0.45
1:K:158:SER:HB3	1:K:195:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:206:ARG:HE	2:B:206:ARG:HB2	1.54	0.45
2:E:34:ILE:HD11	2:E:59:GLN:HG2	1.98	0.45
2:F:194:THR:HA	2:F:198:TYR:O	2.17	0.45
3:O:173:GLU:O	3:O:176:LEU:HG	2.17	0.45
1:J:282:ASP:OD1	1:J:283:TYR:N	2.45	0.45
1:K:367:LYS:HE2	1:K:367:LYS:HB3	1.63	0.45
2:A:73:HIS:C	2:A:75:ILE:H	2.21	0.45
3:L:102:ALA:HA	3:L:105:ARG:NE	2.31	0.45
3:N:139:GLU:O	3:N:142:GLU:HG3	2.17	0.45
1:M:283:TYR:HB3	1:M:285:ILE:HD12	1.98	0.45
1:M:641:GLY:N	2:F:23:GLY:O	2.42	0.45
2:D:117:GLU:OE2	2:D:371:HIS:NE2	2.46	0.45
2:D:151:ILE:HG21	2:D:282:ILE:HD11	1.98	0.45
2:E:213:LYS:HZ1	4:E:401:ADP:HO2'	1.59	0.45
2:F:47:MET:SD	2:F:49:GLN:NE2	2.90	0.45
3:P:135:GLN:O	3:P:139:GLU:HG2	2.16	0.45
1:H:231:GLY:HA3	1:H:244:PHE:CD1	2.51	0.45
1:H:752:ASP:OD1	1:H:755:GLN:NE2	2.50	0.45
1:J:38:PHE:CE2	1:J:79:GLN:HA	2.52	0.45
1:J:158:SER:HB3	1:J:195:PHE:CE1	2.51	0.45
1:K:739:ARG:HD2	1:K:758:PHE:CZ	2.52	0.45
3:N:167:ARG:O	3:N:171:ILE:HG12	2.17	0.45
1:M:231:GLY:HA3	1:M:244:PHE:CD1	2.51	0.44
1:M:572:LYS:HB3	1:M:572:LYS:HE2	1.69	0.44
2:C:54:VAL:HG13	2:C:85:ILE:HD13	1.98	0.44
2:E:216:LEU:HD22	2:E:238:LYS:HD3	2.00	0.44
3:P:139:GLU:O	3:P:142:GLU:HG3	2.17	0.44
1:H:251:HIS:NE2	1:H:262:ASP:OD2	2.51	0.44
1:I:38:PHE:CE2	1:I:79:GLN:HA	2.52	0.44
1:I:484:LYS:HG3	1:I:655:LEU:HD21	1.98	0.44
1:I:544:THR:HG22	1:I:545:ASP:H	1.82	0.44
1:I:739:ARG:HD2	1:I:758:PHE:CZ	2.51	0.44
1:J:484:LYS:HG3	1:J:655:LEU:HD21	1.98	0.44
3:N:135:GLN:O	3:N:139:GLU:HG2	2.16	0.44
1:M:43:LYS:HB3	1:M:43:LYS:HE3	1.85	0.44
1:M:752:ASP:OD1	1:M:755:GLN:NE2	2.50	0.44
2:C:53:TYR:HB3	2:C:57:GLU:OE1	2.16	0.44
2:F:190:MET:HG2	2:F:209:VAL:HG21	1.98	0.44
3:O:102:ALA:HA	3:O:105:ARG:NE	2.31	0.44
1:G:114:ILE:HG23	1:G:125:VAL:O	2.17	0.44
1:G:251:HIS:NE2	1:G:262:ASP:OD2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:158:SER:HB3	1:H:195:PHE:CE1	2.51	0.44
1:K:637:LYS:HD3	1:K:637:LYS:HA	1.75	0.44
1:M:282:ASP:OD1	1:M:283:TYR:N	2.45	0.44
2:B:147:ARG:NH2	1:H:371:GLU:OE1	2.49	0.44
2:B:284:LYS:HE3	2:B:284:LYS:HB2	1.84	0.44
2:D:253:GLU:HA	2:D:256:ARG:HB2	1.99	0.44
2:E:73:HIS:C	2:E:75:ILE:H	2.21	0.44
2:F:143:TYR:CE2	2:F:346:LEU:HD13	2.49	0.44
3:O:71:LEU:HD23	3:O:71:LEU:HA	1.67	0.44
1:G:544:THR:HG22	1:G:545:ASP:H	1.82	0.44
1:J:249:ARG:N	1:J:262:ASP:O	2.41	0.44
2:B:138:ALA:HB1	2:B:152:VAL:HG11	2.00	0.44
2:E:42:GLY:HA2	2:A:169:TYR:HA	2.00	0.44
1:H:544:THR:HG22	1:H:545:ASP:H	1.82	0.44
1:J:679:LYS:HD3	1:J:679:LYS:HA	1.74	0.44
2:A:216:LEU:HD22	2:A:238:LYS:HD3	2.00	0.44
3:N:89:ASN:O	3:N:93:GLN:NE2	2.51	0.44
1:M:45:GLU:HG2	1:M:46:PHE:CD2	2.44	0.44
2:B:9:VAL:HG21	2:B:344:SER:HA	2.00	0.44
2:E:140:LEU:O	2:E:342:GLY:HA3	2.18	0.44
2:F:149:THR:HG22	2:F:167:GLU:N	2.19	0.44
1:G:102:LEU:HD21	1:G:686:ASN:HD22	1.83	0.44
1:G:231:GLY:HA3	1:G:244:PHE:CD1	2.51	0.44
1:G:671:ARG:HB3	1:G:696:ASN:HD21	1.81	0.44
1:H:149:GLU:OE1	1:H:149:GLU:N	2.51	0.44
1:I:158:SER:HB3	1:I:195:PHE:CE1	2.51	0.44
1:I:752:ASP:OD1	1:I:755:GLN:NE2	2.50	0.44
3:L:197:LEU:HD12	3:N:200:VAL:HG11	2.00	0.44
2:E:323:SER:O	2:E:323:SER:OG	2.36	0.44
2:F:191:LYS:O	2:F:194:THR:HG22	2.17	0.44
1:G:219:GLN:OE1	1:G:219:GLN:N	2.42	0.44
1:H:341:PHE:CE2	1:H:346:LYS:HG2	2.53	0.44
1:J:194:TYR:CE2	1:J:198:ILE:HD13	2.53	0.44
1:K:46:PHE:O	1:K:103:TYR:OH	2.27	0.44
1:K:544:THR:HG22	1:K:545:ASP:H	1.82	0.44
3:N:121:ASP:O	3:N:124:GLU:HG3	2.18	0.44
1:M:149:GLU:OE1	1:M:149:GLU:N	2.51	0.44
1:M:251:HIS:NE2	1:M:262:ASP:OD2	2.51	0.44
2:B:333:PRO:HB2	1:H:412:THR:O	2.18	0.44
1:H:336:PHE:CG	1:H:341:PHE:HZ	2.36	0.44
1:I:149:GLU:N	1:I:149:GLU:OE1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:540:PHE:CG	1:J:541:PRO:HD2	2.53	0.44
1:J:637:LYS:HD3	1:J:637:LYS:HA	1.75	0.44
1:K:149:GLU:OE1	1:K:149:GLU:N	2.51	0.44
1:K:194:TYR:CE2	1:K:198:ILE:HD13	2.53	0.44
1:K:341:PHE:CE2	1:K:346:LYS:HG2	2.53	0.44
1:M:194:TYR:CE2	1:M:198:ILE:HD13	2.53	0.44
1:M:224:ASN:O	1:M:228:GLU:HG2	2.18	0.44
1:M:341:PHE:CE2	1:M:346:LYS:HG2	2.53	0.44
1:G:149:GLU:OE1	1:G:149:GLU:N	2.51	0.44
1:G:474:GLU:H	1:G:474:GLU:CD	2.18	0.44
1:H:224:ASN:O	1:H:228:GLU:HG2	2.18	0.44
1:H:540:PHE:CG	1:H:541:PRO:HD2	2.53	0.44
1:J:43:LYS:HB3	1:J:43:LYS:HE3	1.85	0.44
1:J:544:THR:HG22	1:J:545:ASP:H	1.82	0.44
1:K:224:ASN:O	1:K:228:GLU:HG2	2.18	0.44
1:K:336:PHE:CG	1:K:341:PHE:HZ	2.36	0.44
1:K:752:ASP:OD1	1:K:755:GLN:NE2	2.51	0.44
2:D:95:ARG:O	1:I:635:LYS:HA	2.17	0.44
3:P:89:ASN:O	3:P:93:GLN:NE2	2.51	0.44
3:P:105:ARG:HA	3:P:108:THR:OG1	2.17	0.44
3:P:128:LYS:O	3:P:131:GLU:HG3	2.18	0.44
3:P:190:CYS:HA	3:P:193:LEU:HD12	2.00	0.44
1:G:224:ASN:O	1:G:228:GLU:HG2	2.18	0.44
1:G:544:THR:HG22	1:G:545:ASP:N	2.33	0.44
1:G:637:LYS:HD3	1:G:637:LYS:HA	1.75	0.44
1:I:102:LEU:HD21	1:I:686:ASN:HD22	1.83	0.44
1:I:336:PHE:CG	1:I:341:PHE:HZ	2.36	0.44
1:J:336:PHE:CG	1:J:341:PHE:HZ	2.36	0.44
1:J:752:ASP:OD1	1:J:755:GLN:NE2	2.50	0.44
1:K:102:LEU:HD21	1:K:686:ASN:HD22	1.83	0.44
2:A:34:ILE:HD11	2:A:59:GLN:HG2	1.98	0.44
1:M:102:LEU:HD21	1:M:686:ASN:HD22	1.83	0.43
2:E:288:ASP:OD1	2:E:288:ASP:N	2.43	0.43
3:O:193:LEU:HA	3:O:193:LEU:HD23	1.73	0.43
3:P:175:ASP:O	3:P:178:ARG:HD3	2.18	0.43
3:P:189:LYS:HB3	3:P:189:LYS:HE2	1.87	0.43
1:G:171:ASN:HB2	1:G:665:THR:HG22	2.00	0.43
1:H:176:ILE:HA	1:H:670:VAL:HB	2.01	0.43
1:I:224:ASN:O	1:I:228:GLU:HG2	2.18	0.43
1:J:149:GLU:OE1	1:J:149:GLU:N	2.51	0.43
1:J:224:ASN:O	1:J:228:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:341:PHE:CE2	1:J:346:LYS:HG2	2.53	0.43
1:K:251:HIS:NE2	1:K:262:ASP:OD2	2.51	0.43
3:L:173:GLU:O	3:L:176:LEU:HG	2.17	0.43
1:M:176:ILE:HA	1:M:670:VAL:HB	2.00	0.43
1:M:336:PHE:CG	1:M:341:PHE:HZ	2.36	0.43
1:M:544:THR:HG22	1:M:545:ASP:H	1.82	0.43
1:H:194:TYR:CE2	1:H:198:ILE:HD13	2.53	0.43
1:I:176:ILE:HA	1:I:670:VAL:HB	2.01	0.43
1:I:341:PHE:CE2	1:I:346:LYS:HG2	2.53	0.43
1:I:367:LYS:HE2	1:I:367:LYS:HB3	1.63	0.43
1:J:102:LEU:HD21	1:J:686:ASN:HD22	1.83	0.43
1:J:251:HIS:NE2	1:J:262:ASP:OD2	2.51	0.43
1:K:146:LYS:HA	1:K:146:LYS:HD2	1.76	0.43
1:K:412:THR:O	2:A:333:PRO:HB2	2.18	0.43
3:L:46:LEU:HD12	3:N:46:LEU:HD11	2.00	0.43
1:M:506:ILE:CD1	1:M:757:LYS:HG2	2.48	0.43
1:M:544:THR:HG22	1:M:545:ASP:N	2.33	0.43
2:C:140:LEU:O	2:C:342:GLY:HA3	2.18	0.43
2:D:14:SER:O	2:D:157:ASP:HB3	2.19	0.43
1:G:341:PHE:CE2	1:G:346:LYS:HG2	2.53	0.43
1:H:544:THR:HG22	1:H:545:ASP:N	2.33	0.43
1:I:171:ASN:HB2	1:I:665:THR:HG22	2.00	0.43
1:M:612:SER:OG	1:M:613:SER:N	2.52	0.43
2:D:26:ALA:HB1	1:I:406:VAL:HG12	2.00	0.43
2:D:138:ALA:HB1	2:D:152:VAL:CG1	2.49	0.43
2:D:282:ILE:HD12	2:D:293:LEU:HB3	1.99	0.43
1:G:752:ASP:OD1	1:G:755:GLN:NE2	2.51	0.43
1:I:118:SER:OG	1:I:121:PHE:HB2	2.18	0.43
1:I:251:HIS:NE2	1:I:262:ASP:OD2	2.51	0.43
1:I:506:ILE:CD1	1:I:757:LYS:HG2	2.48	0.43
1:J:176:ILE:HA	1:J:670:VAL:HB	2.00	0.43
1:K:45:GLU:HG2	1:K:46:PHE:CD2	2.44	0.43
1:K:85:ASP:OD1	1:K:86:LYS:N	2.48	0.43
1:M:118:SER:OG	1:M:121:PHE:HB2	2.18	0.43
1:M:180:SER:HB3	1:M:238:ASN:ND2	2.34	0.43
2:B:97:ALA:HB1	2:B:99:GLU:OE2	2.19	0.43
2:B:153:LEU:HD23	2:B:299:LEU:HD22	2.01	0.43
2:F:9:VAL:HG21	2:F:344:SER:HA	2.00	0.43
3:O:92:ILE:HG13	1:G:368:GLN:HE21	1.84	0.43
3:O:209:ALA:O	3:O:210:GLN:HG3	2.19	0.43
1:G:118:SER:OG	1:G:121:PHE:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:612:SER:OG	1:G:613:SER:N	2.52	0.43
1:H:171:ASN:HB2	1:H:665:THR:HG22	2.00	0.43
1:H:394:ASP:OD2	1:H:608:LEU:HD21	2.19	0.43
1:K:540:PHE:CG	1:K:541:PRO:HD2	2.53	0.43
1:K:544:THR:HG22	1:K:545:ASP:N	2.33	0.43
2:A:140:LEU:O	2:A:342:GLY:HA3	2.18	0.43
3:N:175:ASP:O	3:N:178:ARG:HD3	2.18	0.43
1:M:611:LYS:HB3	1:M:611:LYS:HE2	1.61	0.43
2:D:254:ARG:CZ	3:L:128:LYS:HZ1	2.29	0.43
2:F:73:HIS:C	2:F:75:ILE:H	2.22	0.43
3:O:96:GLU:O	3:O:99:LEU:HG	2.18	0.43
3:O:197:LEU:HD12	3:P:200:VAL:HG11	2.00	0.43
3:P:121:ASP:O	3:P:124:GLU:HG3	2.18	0.43
3:P:140:LYS:O	3:P:143:ILE:HG22	2.19	0.43
1:G:43:LYS:HB3	1:G:43:LYS:HE3	1.85	0.43
1:G:194:TYR:CE2	1:G:198:ILE:HD13	2.53	0.43
1:G:336:PHE:CG	1:G:341:PHE:HZ	2.36	0.43
1:G:572:LYS:HE2	1:G:572:LYS:HB3	1.69	0.43
1:H:367:LYS:HE2	1:H:367:LYS:HB3	1.63	0.43
1:I:540:PHE:CG	1:I:541:PRO:HD2	2.53	0.43
1:I:572:LYS:HB3	1:I:572:LYS:HE2	1.69	0.43
1:I:637:LYS:HD3	1:I:637:LYS:HA	1.75	0.43
1:J:118:SER:OG	1:J:121:PHE:HB2	2.18	0.43
1:J:544:THR:HG22	1:J:545:ASP:N	2.33	0.43
1:J:611:LYS:HE2	1:J:611:LYS:HB3	1.61	0.43
1:K:118:SER:OG	1:K:121:PHE:HB2	2.18	0.43
3:N:172:ILE:HG13	3:N:173:GLU:N	2.34	0.43
1:M:171:ASN:HB2	1:M:665:THR:HG22	2.00	0.43
1:M:394:ASP:OD2	1:M:608:LEU:HD21	2.19	0.43
1:M:679:LYS:HD3	1:M:679:LYS:HA	1.74	0.43
2:B:49:GLN:HG2	2:F:169:TYR:CZ	2.53	0.43
2:C:26:ALA:HB1	1:G:406:VAL:HG12	2.00	0.43
1:G:176:ILE:HA	1:G:670:VAL:HB	2.00	0.43
1:G:269:GLU:OE1	1:G:271:SER:N	2.31	0.43
1:G:540:PHE:CG	1:G:541:PRO:HD2	2.53	0.43
1:H:612:SER:OG	1:H:613:SER:N	2.52	0.43
1:I:41:ASP:OD2	1:I:43:LYS:N	2.52	0.43
1:I:394:ASP:OD2	1:I:608:LEU:HD21	2.19	0.43
1:J:41:ASP:OD2	1:J:43:LYS:N	2.52	0.43
1:J:85:ASP:OD1	1:J:86:LYS:N	2.48	0.43
1:K:41:ASP:OD2	1:K:43:LYS:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:95:ARG:O	1:G:635:LYS:HA	2.19	0.43
2:C:300:SER:HA	2:C:335:ARG:HG2	2.00	0.43
2:F:275:HIS:CD2	2:F:316:GLU:HB3	2.53	0.43
3:O:66:ASP:HB2	3:O:70:LYS:NZ	2.34	0.43
1:H:118:SER:OG	1:H:121:PHE:HB2	2.19	0.43
1:H:180:SER:HB3	1:H:238:ASN:ND2	2.34	0.43
1:I:544:THR:HG22	1:I:545:ASP:N	2.33	0.43
1:I:679:LYS:HD3	1:I:679:LYS:HA	1.74	0.43
1:J:171:ASN:HB2	1:J:665:THR:HG22	2.00	0.43
1:J:367:LYS:HB3	1:J:367:LYS:HE2	1.63	0.43
1:J:434:ARG:HH22	1:J:623:ASN:ND2	2.17	0.43
1:K:394:ASP:OD2	1:K:608:LEU:HD21	2.19	0.43
1:K:434:ARG:HH22	1:K:623:ASN:ND2	2.17	0.43
2:A:97:ALA:HB1	2:A:99:GLU:OE2	2.18	0.43
2:A:353:GLN:NE2	2:A:356:TRP:HE1	2.16	0.43
2:C:357:ILE:HG12	2:C:374:CYS:HB2	2.00	0.43
3:O:205:LYS:O	3:O:208:GLU:HG2	2.19	0.43
1:G:394:ASP:OD2	1:G:608:LEU:HD21	2.19	0.43
1:I:269:GLU:OE1	1:I:271:SER:N	2.31	0.43
1:I:282:ASP:OD1	1:I:283:TYR:N	2.45	0.43
1:J:180:SER:HB3	1:J:238:ASN:ND2	2.34	0.43
1:J:352:LEU:HD12	1:J:352:LEU:HA	1.88	0.43
1:K:176:ILE:HA	1:K:670:VAL:HB	2.01	0.43
2:A:213:LYS:HZ1	4:A:401:ADP:HO2'	1.60	0.43
3:L:172:ILE:HB	3:N:172:ILE:HD12	2.01	0.43
3:N:48:LYS:HE2	3:N:48:LYS:HB2	1.87	0.43
3:N:128:LYS:O	3:N:131:GLU:HG3	2.18	0.43
3:N:190:CYS:HA	3:N:193:LEU:HD12	2.00	0.43
1:M:540:PHE:CG	1:M:541:PRO:HD2	2.53	0.43
2:E:97:ALA:HB1	2:E:99:GLU:OE2	2.18	0.43
2:E:147:ARG:NH2	2:E:330:ILE:HG12	2.19	0.43
1:H:102:LEU:HD21	1:H:686:ASN:HD22	1.83	0.43
1:H:434:ARG:HH22	1:H:623:ASN:ND2	2.17	0.43
1:I:194:TYR:CE2	1:I:198:ILE:HD13	2.53	0.43
1:I:715:TYR:CZ	1:I:763:VAL:HB	2.54	0.43
1:J:394:ASP:OD2	1:J:608:LEU:HD21	2.19	0.43
1:K:180:SER:HB3	1:K:238:ASN:ND2	2.34	0.43
1:K:715:TYR:CZ	1:K:763:VAL:HB	2.54	0.43
2:A:12:ASN:HD21	2:A:105:LEU:HD12	1.84	0.43
2:A:323:SER:O	2:A:323:SER:OG	2.36	0.43
1:M:102:LEU:O	1:M:105:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:369:ARG:HE	3:O:133:ARG:CZ	2.31	0.42
1:M:434:ARG:HH22	1:M:623:ASN:ND2	2.17	0.42
2:C:98:PRO:O	2:C:129:VAL:HA	2.18	0.42
2:D:250:ILE:HG23	2:D:253:GLU:HG2	2.01	0.42
1:G:180:SER:HB3	1:G:238:ASN:ND2	2.34	0.42
1:G:502:LYS:HA	1:G:507:GLU:OE1	2.19	0.42
1:H:102:LEU:O	1:H:105:LEU:HG	2.19	0.42
1:H:679:LYS:HD3	1:H:679:LYS:HA	1.74	0.42
1:I:45:GLU:HG2	1:I:46:PHE:CD2	2.44	0.42
1:J:715:TYR:CZ	1:J:763:VAL:HB	2.54	0.42
2:A:147:ARG:NH2	2:A:330:ILE:HG12	2.19	0.42
3:L:152:LYS:O	3:L:156:GLU:HG2	2.19	0.42
3:L:209:ALA:O	3:L:210:GLN:HG3	2.19	0.42
3:N:169:LEU:HA	3:N:172:ILE:HG12	2.01	0.42
1:M:77:MET:HB2	1:M:97:HIS:CE1	2.54	0.42
1:G:77:MET:HB2	1:G:97:HIS:CE1	2.54	0.42
1:G:102:LEU:O	1:G:105:LEU:HG	2.19	0.42
1:H:77:MET:HB2	1:H:97:HIS:CE1	2.54	0.42
1:I:717:ASP:CG	1:I:721:ARG:HE	2.22	0.42
1:J:38:PHE:N	1:J:77:MET:O	2.47	0.42
1:K:171:ASN:HB2	1:K:665:THR:HG22	2.00	0.42
3:L:66:ASP:HB2	3:L:70:LYS:NZ	2.34	0.42
2:C:144:ALA:HB2	2:C:342:GLY:N	2.34	0.42
2:D:47:MET:HB3	2:D:49:GLN:OE1	2.19	0.42
2:D:295:ALA:O	2:D:296:ASN:ND2	2.53	0.42
2:E:71:ILE:HG12	2:E:76:ILE:HG12	2.01	0.42
2:F:138:ALA:HB1	2:F:152:VAL:HG11	2.01	0.42
3:O:46:LEU:HD12	3:P:46:LEU:HD11	2.00	0.42
3:O:152:LYS:O	3:O:156:GLU:HG2	2.19	0.42
3:P:172:ILE:HG13	3:P:173:GLU:N	2.34	0.42
1:G:282:ASP:OD1	1:G:283:TYR:N	2.45	0.42
1:G:717:ASP:CG	1:G:721:ARG:HE	2.22	0.42
1:K:612:SER:OG	1:K:613:SER:N	2.52	0.42
1:M:474:GLU:H	1:M:474:GLU:CD	2.18	0.42
2:B:170:ALA:O	2:B:172:PRO:HD3	2.20	0.42
2:C:353:GLN:NE2	2:C:356:TRP:HE1	2.17	0.42
2:C:369:ILE:HA	2:C:372:ARG:HD3	2.02	0.42
2:E:353:GLN:NE2	2:E:356:TRP:HE1	2.16	0.42
3:O:49:LYS:HZ1	3:P:50:LEU:HD22	1.85	0.42
3:O:71:LEU:CD2	3:P:70:LYS:HD2	2.46	0.42
3:P:169:LEU:HA	3:P:172:ILE:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:45:GLU:HB3	1:H:690:MET:HE1	1.99	0.42
1:I:434:ARG:HH22	1:I:623:ASN:ND2	2.17	0.42
1:I:502:LYS:HA	1:I:507:GLU:OE1	2.19	0.42
1:J:502:LYS:HA	1:J:507:GLU:OE1	2.19	0.42
1:J:506:ILE:CD1	1:J:757:LYS:HG2	2.48	0.42
1:K:717:ASP:CG	1:K:721:ARG:HE	2.23	0.42
3:L:71:LEU:CD2	3:N:70:LYS:HD2	2.46	0.42
3:L:96:GLU:O	3:L:99:LEU:HG	2.18	0.42
3:O:86:ALA:HA	3:O:89:ASN:ND2	2.35	0.42
1:G:434:ARG:HH22	1:G:623:ASN:ND2	2.17	0.42
1:G:506:ILE:CD1	1:G:757:LYS:HG2	2.48	0.42
1:G:679:LYS:HD3	1:G:679:LYS:HA	1.74	0.42
1:H:41:ASP:OD2	1:H:43:LYS:N	2.52	0.42
1:H:301:LEU:HD22	1:H:387:LEU:HD11	2.02	0.42
1:H:715:TYR:CZ	1:H:763:VAL:HB	2.54	0.42
2:A:71:ILE:HG12	2:A:76:ILE:HG12	2.01	0.42
3:N:102:ALA:HA	3:N:105:ARG:NE	2.34	0.42
3:N:140:LYS:O	3:N:143:ILE:HG22	2.19	0.42
1:M:301:LEU:HD22	1:M:387:LEU:HD11	2.02	0.42
1:M:474:GLU:OE1	1:M:474:GLU:N	2.32	0.42
2:D:170:ALA:O	2:D:172:PRO:HD3	2.20	0.42
2:F:351:THR:O	2:F:354:GLN:NE2	2.53	0.42
1:I:612:SER:OG	1:I:613:SER:N	2.52	0.42
1:J:266:TYR:HB3	1:J:267:LEU:HG	2.02	0.42
1:J:612:SER:OG	1:J:613:SER:N	2.52	0.42
3:L:182:ARG:O	3:L:185:LEU:HG	2.19	0.42
3:L:193:LEU:HD23	3:L:193:LEU:HA	1.73	0.42
3:N:166:ALA:O	3:N:170:VAL:HG23	2.20	0.42
1:M:266:TYR:HB3	1:M:267:LEU:HG	2.02	0.42
1:M:717:ASP:CG	1:M:721:ARG:HE	2.23	0.42
2:D:202:THR:HG23	2:F:270:GLU:OE1	2.18	0.42
1:G:352:LEU:HD12	1:G:352:LEU:HA	1.88	0.42
1:I:85:ASP:OD1	1:I:86:LYS:N	2.48	0.42
1:I:178:GLY:C	1:I:184:LYS:HD3	2.40	0.42
1:I:758:PHE:HA	1:I:763:VAL:HG23	2.01	0.42
1:K:102:LEU:O	1:K:105:LEU:HG	2.19	0.42
3:L:205:LYS:O	3:L:208:GLU:HG2	2.19	0.42
1:M:41:ASP:OD2	1:M:43:LYS:N	2.52	0.42
1:M:367:LYS:HB3	1:M:367:LYS:HE2	1.63	0.42
1:M:502:LYS:HA	1:M:507:GLU:OE1	2.19	0.42
1:M:669:PHE:HB3	1:M:671:ARG:CZ	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:73:HIS:C	2:C:75:ILE:H	2.23	0.42
2:C:138:ALA:HB1	2:C:152:VAL:CG1	2.49	0.42
2:C:192:ILE:HD13	2:C:192:ILE:HG21	1.79	0.42
2:E:12:ASN:HD21	2:E:105:LEU:HD12	1.84	0.42
3:O:64:LEU:HG	3:P:64:LEU:HD12	2.01	0.42
3:P:102:ALA:HA	3:P:105:ARG:NE	2.34	0.42
1:G:41:ASP:OD2	1:G:43:LYS:N	2.52	0.42
1:G:301:LEU:HD22	1:G:387:LEU:HD11	2.02	0.42
1:H:266:TYR:HB3	1:H:267:LEU:HG	2.02	0.42
1:I:77:MET:HB2	1:I:97:HIS:CE1	2.54	0.42
1:I:180:SER:HB3	1:I:238:ASN:ND2	2.34	0.42
1:K:474:GLU:OE1	1:K:474:GLU:N	2.32	0.42
1:K:502:LYS:HA	1:K:507:GLU:OE1	2.19	0.42
3:L:64:LEU:HG	3:N:64:LEU:HD12	2.01	0.42
1:M:406:VAL:HG12	2:F:26:ALA:HB1	2.02	0.42
2:B:278:THR:O	2:B:282:ILE:HG12	2.19	0.42
2:E:190:MET:HG3	2:E:209:VAL:HG11	2.02	0.42
2:E:221:LEU:CD2	3:N:97:GLU:OE1	2.68	0.42
3:O:182:ARG:O	3:O:185:LEU:HG	2.19	0.42
1:H:502:LYS:HA	1:H:507:GLU:OE1	2.19	0.42
1:H:758:PHE:HA	1:H:763:VAL:HG23	2.02	0.42
1:I:102:LEU:O	1:I:105:LEU:HG	2.19	0.42
1:I:266:TYR:HB3	1:I:267:LEU:HG	2.02	0.42
1:J:109:TYR:HD2	1:J:684:MET:HE2	1.85	0.42
1:K:266:TYR:HB3	1:K:267:LEU:HG	2.02	0.42
1:K:301:LEU:HD22	1:K:387:LEU:HD11	2.02	0.42
1:K:669:PHE:HB3	1:K:671:ARG:CZ	2.50	0.42
1:M:715:TYR:CZ	1:M:763:VAL:HB	2.54	0.42
1:M:758:PHE:HA	1:M:763:VAL:HG23	2.02	0.42
2:B:149:THR:HG22	2:B:167:GLU:N	2.21	0.42
2:D:76:ILE:HD13	2:D:82:MET:HG2	2.02	0.42
3:P:126:GLY:O	3:P:130:ILE:HG12	2.20	0.42
1:G:266:TYR:HB3	1:G:267:LEU:HG	2.02	0.42
1:J:740:LYS:HG3	1:J:741:GLY:N	2.35	0.42
2:B:138:ALA:HB1	2:B:152:VAL:CG1	2.49	0.41
2:D:73:HIS:C	2:D:75:ILE:H	2.23	0.41
2:E:142:LEU:HD12	2:E:142:LEU:HA	1.88	0.41
1:H:717:ASP:CG	1:H:721:ARG:HE	2.22	0.41
3:N:175:ASP:HA	3:N:178:ARG:NE	2.35	0.41
2:C:305:MET:SD	2:C:335:ARG:NH1	2.93	0.41
1:G:178:GLY:C	1:G:184:LYS:HD3	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:669:PHE:HB3	1:H:671:ARG:CZ	2.50	0.41
1:I:740:LYS:HG3	1:I:741:GLY:N	2.35	0.41
1:K:740:LYS:HG3	1:K:741:GLY:N	2.35	0.41
3:L:86:ALA:HA	3:L:89:ASN:ND2	2.34	0.41
1:M:447:LEU:O	1:M:447:LEU:HD23	2.21	0.41
3:O:172:ILE:HB	3:P:172:ILE:HD12	2.01	0.41
3:P:147:GLN:HA	3:P:150:GLU:OE1	2.21	0.41
1:J:758:PHE:HA	1:J:763:VAL:HG23	2.02	0.41
3:N:136:LYS:HE3	3:N:136:LYS:HB3	1.68	0.41
1:M:740:LYS:HG3	1:M:741:GLY:N	2.35	0.41
2:D:116:ARG:HG2	2:D:370:VAL:HG11	2.02	0.41
2:D:128:ASN:OD1	2:D:359:LYS:NZ	2.42	0.41
1:H:178:GLY:C	1:H:184:LYS:HD3	2.40	0.41
1:I:41:ASP:OD2	1:I:44:GLN:N	2.35	0.41
1:J:102:LEU:O	1:J:105:LEU:HG	2.19	0.41
1:J:301:LEU:HD22	1:J:387:LEU:HD11	2.02	0.41
1:J:526:LYS:HA	1:J:526:LYS:HD3	1.90	0.41
1:J:717:ASP:CG	1:J:721:ARG:HE	2.23	0.41
2:A:190:MET:HG3	2:A:209:VAL:HG11	2.02	0.41
3:N:199:THR:O	3:N:203:ASN:ND2	2.53	0.41
2:B:234:SER:O	2:B:234:SER:OG	2.38	0.41
3:O:66:ASP:HB2	3:O:70:LYS:HZ1	1.85	0.41
1:G:447:LEU:HD23	1:G:447:LEU:O	2.21	0.41
1:G:474:GLU:OE1	1:G:474:GLU:N	2.32	0.41
1:G:669:PHE:HB3	1:G:671:ARG:CZ	2.50	0.41
1:I:669:PHE:HB3	1:I:671:ARG:CZ	2.50	0.41
1:J:146:LYS:HA	1:J:146:LYS:HD2	1.76	0.41
1:J:671:ARG:HB3	1:J:696:ASN:ND2	2.36	0.41
1:K:87:ILE:HG21	1:K:93:LEU:HG	2.03	0.41
3:N:126:GLY:O	3:N:130:ILE:HG12	2.20	0.41
3:N:170:VAL:O	3:N:173:GLU:HG3	2.21	0.41
2:B:16:LEU:HD23	2:B:16:LEU:HA	1.88	0.41
2:D:120:THR:HG22	2:D:132:MET:HE1	2.02	0.41
3:P:152:LYS:HG3	3:P:153:HIS:N	2.36	0.41
1:I:217:GLU:O	1:I:221:ILE:HG12	2.21	0.41
1:J:301:LEU:HA	1:J:301:LEU:HD23	1.75	0.41
1:K:77:MET:HB2	1:K:97:HIS:CE1	2.54	0.41
1:K:506:ILE:CD1	1:K:757:LYS:HG2	2.48	0.41
2:A:196:ARG:HD2	2:A:253:GLU:OE2	2.21	0.41
2:A:278:THR:O	2:A:282:ILE:HG12	2.20	0.41
1:M:178:GLY:C	1:M:184:LYS:HD3	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:269:GLU:OE1	1:M:271:SER:N	2.31	0.41
1:M:599:ASP:O	1:M:645:GLN:HB2	2.21	0.41
1:M:769:LEU:H	1:M:769:LEU:HD12	1.86	0.41
2:C:169:TYR:CZ	2:F:49:GLN:HG2	2.55	0.41
2:D:28:ARG:HH12	1:I:637:LYS:CG	2.33	0.41
2:D:361:GLU:O	2:D:364:GLU:HG3	2.21	0.41
2:F:138:ALA:HB1	2:F:152:VAL:CG1	2.50	0.41
3:P:166:ALA:O	3:P:170:VAL:HG23	2.20	0.41
3:P:199:THR:O	3:P:203:ASN:ND2	2.54	0.41
1:G:517:LEU:HA	1:G:517:LEU:HD12	1.84	0.41
1:H:146:LYS:HA	1:H:146:LYS:HD2	1.76	0.41
1:H:447:LEU:O	1:H:447:LEU:HD23	2.20	0.41
1:H:512:ASP:HB3	1:H:515:MET:CE	2.51	0.41
1:H:599:ASP:O	1:H:645:GLN:HB2	2.21	0.41
1:H:671:ARG:HB3	1:H:696:ASN:ND2	2.36	0.41
1:I:301:LEU:HD22	1:I:387:LEU:HD11	2.02	0.41
1:J:217:GLU:O	1:J:221:ILE:HG12	2.21	0.41
1:J:669:PHE:HB3	1:J:671:ARG:CZ	2.50	0.41
1:K:178:GLY:C	1:K:184:LYS:HD3	2.40	0.41
1:K:447:LEU:O	1:K:447:LEU:HD23	2.21	0.41
1:K:758:PHE:HA	1:K:763:VAL:HG23	2.02	0.41
3:N:197:LEU:O	3:N:201:THR:HG23	2.21	0.41
1:M:671:ARG:HB3	1:M:696:ASN:ND2	2.36	0.41
2:B:78:ASN:HB3	2:B:81:ASP:HB2	2.02	0.41
2:C:78:ASN:HB3	2:C:81:ASP:OD1	2.21	0.41
2:C:138:ALA:HB1	2:C:152:VAL:HG11	2.03	0.41
3:O:57:LEU:HD21	3:P:57:LEU:HG	2.03	0.41
3:P:175:ASP:HA	3:P:178:ARG:NE	2.35	0.41
1:G:599:ASP:O	1:G:645:GLN:HB2	2.21	0.41
1:G:671:ARG:HB3	1:G:696:ASN:ND2	2.36	0.41
1:G:715:TYR:CZ	1:G:763:VAL:HB	2.54	0.41
1:H:238:ASN:OD1	1:H:239:ASP:N	2.54	0.41
1:J:87:ILE:HG21	1:J:93:LEU:HG	2.03	0.41
1:J:156:SER:OG	1:J:157:ILE:N	2.54	0.41
1:M:23:ARG:O	1:M:27:GLN:HG2	2.21	0.41
1:M:156:SER:OG	1:M:157:ILE:N	2.54	0.41
1:M:512:ASP:HB3	1:M:515:MET:CE	2.51	0.41
2:D:294:TYR:CD2	2:D:325:MET:HG2	2.56	0.41
2:D:333:PRO:HB2	1:I:412:THR:O	2.21	0.41
2:E:333:PRO:HB2	1:J:412:THR:O	2.21	0.41
3:P:94:LEU:O	3:P:97:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:46:PHE:CG	1:G:99:PRO:HG3	2.56	0.41
1:G:156:SER:OG	1:G:157:ILE:N	2.54	0.41
1:G:238:ASN:OD1	1:G:239:ASP:N	2.54	0.41
1:H:45:GLU:HG2	1:H:46:PHE:CD2	2.44	0.41
1:H:63:THR:HG23	1:H:65:TYR:H	1.86	0.41
1:H:740:LYS:HG3	1:H:741:GLY:N	2.35	0.41
1:I:23:ARG:O	1:I:27:GLN:HG2	2.21	0.41
1:I:146:LYS:HA	1:I:146:LYS:HD2	1.76	0.41
1:I:238:ASN:OD1	1:I:239:ASP:N	2.54	0.41
1:I:481:THR:HG22	1:I:655:LEU:HD22	2.03	0.41
1:I:671:ARG:HB3	1:I:696:ASN:ND2	2.36	0.41
1:I:689:VAL:O	1:I:693:LEU:HD23	2.21	0.41
1:J:63:THR:HG23	1:J:65:TYR:H	1.86	0.41
1:J:77:MET:HB2	1:J:97:HIS:CE1	2.54	0.41
1:J:178:GLY:C	1:J:184:LYS:HD3	2.40	0.41
1:J:301:LEU:HD21	1:J:351:LYS:HA	2.03	0.41
1:J:517:LEU:HD12	1:J:517:LEU:HA	1.84	0.41
1:J:689:VAL:O	1:J:693:LEU:HD23	2.21	0.41
1:K:43:LYS:HB3	1:K:43:LYS:HE3	1.85	0.41
1:K:238:ASN:OD1	1:K:239:ASP:N	2.54	0.41
1:K:512:ASP:HB3	1:K:515:MET:CE	2.51	0.41
1:K:689:VAL:O	1:K:693:LEU:HD23	2.21	0.41
2:A:131:ALA:HB1	2:A:356:TRP:HB3	2.03	0.41
3:L:86:ALA:HB1	3:L:90:ARG:HH12	1.86	0.41
3:L:139:GLU:HG3	3:L:140:LYS:N	2.36	0.41
3:L:146:ILE:HD13	3:L:146:ILE:HA	1.94	0.41
3:N:94:LEU:O	3:N:97:GLU:HG3	2.21	0.41
3:N:152:LYS:HG3	3:N:153:HIS:N	2.36	0.41
3:N:197:LEU:HD23	3:N:198:LYS:HZ3	1.85	0.41
1:M:87:ILE:HG21	1:M:93:LEU:HG	2.03	0.41
2:B:156:GLY:O	2:B:303:THR:OG1	2.28	0.41
2:F:236:LEU:O	2:F:254:ARG:NH1	2.49	0.41
1:G:63:THR:HG23	1:G:65:TYR:H	1.86	0.41
1:G:146:LYS:HB3	1:G:149:GLU:OE1	2.21	0.41
1:G:740:LYS:HG3	1:G:741:GLY:N	2.35	0.41
1:H:87:ILE:HG21	1:H:93:LEU:HG	2.03	0.41
1:H:171:ASN:OD1	1:H:456:PHE:N	2.40	0.41
1:I:46:PHE:CG	1:I:99:PRO:HG3	2.56	0.41
1:I:146:LYS:HB3	1:I:149:GLU:OE1	2.21	0.41
1:J:23:ARG:O	1:J:27:GLN:HG2	2.21	0.41
1:J:146:LYS:HB3	1:J:149:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:512:ASP:HB3	1:J:515:MET:CE	2.51	0.41
3:L:49:LYS:HZ1	3:N:50:LEU:HD22	1.85	0.41
3:N:50:LEU:O	3:N:54:GLU:HG3	2.21	0.41
1:M:506:ILE:O	1:M:506:ILE:HG23	2.22	0.40
2:C:97:ALA:HB1	2:C:99:GLU:OE2	2.21	0.40
2:E:131:ALA:HB1	2:E:356:TRP:HB3	2.03	0.40
2:E:278:THR:O	2:E:282:ILE:HG12	2.20	0.40
3:O:77:LYS:HB3	3:O:77:LYS:HE2	1.91	0.40
1:G:12:ALA:HB1	1:G:133:VAL:HG12	2.04	0.40
1:G:290:LEU:HD23	1:G:290:LEU:HA	1.92	0.40
1:G:448:GLU:OE1	1:G:450:LYS:HD2	2.22	0.40
1:H:689:VAL:O	1:H:693:LEU:HD23	2.21	0.40
1:H:769:LEU:H	1:H:769:LEU:HD12	1.86	0.40
1:I:156:SER:OG	1:I:157:ILE:N	2.54	0.40
1:I:447:LEU:HD23	1:I:447:LEU:O	2.21	0.40
1:J:447:LEU:HD23	1:J:447:LEU:O	2.21	0.40
1:K:23:ARG:O	1:K:27:GLN:HG2	2.21	0.40
1:K:146:LYS:HB3	1:K:149:GLU:OE1	2.21	0.40
1:K:217:GLU:O	1:K:221:ILE:HG12	2.21	0.40
1:K:301:LEU:HD21	1:K:351:LYS:HA	2.03	0.40
1:K:481:THR:HG22	1:K:655:LEU:HD22	2.03	0.40
1:M:12:ALA:HB1	1:M:133:VAL:HG12	2.04	0.40
2:C:123:MET:O	2:C:129:VAL:HG22	2.21	0.40
2:E:372:ARG:O	2:E:374:CYS:N	2.55	0.40
3:O:162:TYR:CD1	3:P:161:LYS:HD3	2.56	0.40
3:P:48:LYS:HB2	3:P:48:LYS:HE2	1.87	0.40
3:P:50:LEU:O	3:P:54:GLU:HG3	2.21	0.40
1:G:23:ARG:O	1:G:27:GLN:HG2	2.21	0.40
1:G:87:ILE:HG21	1:G:93:LEU:HG	2.03	0.40
1:G:512:ASP:HB3	1:G:515:MET:CE	2.51	0.40
1:H:285:ILE:HD12	1:H:285:ILE:H	1.87	0.40
1:I:12:ALA:HB1	1:I:133:VAL:HG12	2.04	0.40
1:I:301:LEU:HD21	1:I:351:LYS:HA	2.03	0.40
1:J:12:ALA:HB1	1:J:133:VAL:HG12	2.04	0.40
1:J:46:PHE:CG	1:J:99:PRO:HG3	2.56	0.40
1:J:238:ASN:OD1	1:J:239:ASP:N	2.54	0.40
1:J:481:THR:HG22	1:J:655:LEU:HD22	2.03	0.40
1:K:46:PHE:CG	1:K:99:PRO:HG3	2.56	0.40
1:K:269:GLU:OE1	1:K:271:SER:N	2.31	0.40
2:A:138:ALA:HB1	2:A:152:VAL:CG1	2.52	0.40
2:A:372:ARG:O	2:A:374:CYS:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:112:LYS:HA	3:L:112:LYS:HD2	1.83	0.40
1:M:46:PHE:CG	1:M:99:PRO:HG3	2.56	0.40
1:M:63:THR:HG23	1:M:65:TYR:H	1.86	0.40
1:M:238:ASN:OD1	1:M:239:ASP:N	2.54	0.40
1:M:689:VAL:O	1:M:693:LEU:HD23	2.21	0.40
3:O:86:ALA:HB1	3:O:90:ARG:HH12	1.86	0.40
3:O:198:LYS:O	3:O:201:THR:HG22	2.21	0.40
3:P:105:ARG:HH12	3:P:106:LEU:HD13	1.86	0.40
3:P:124:GLU:HA	3:P:127:MET:HG2	2.04	0.40
1:G:285:ILE:HD12	1:G:285:ILE:H	1.87	0.40
1:G:549:LYS:HE3	1:G:553:PHE:CE2	2.52	0.40
1:G:769:LEU:H	1:G:769:LEU:HD12	1.86	0.40
1:H:474:GLU:H	1:H:474:GLU:CD	2.18	0.40
1:I:87:ILE:HG21	1:I:93:LEU:HG	2.03	0.40
1:I:109:TYR:HD2	1:I:684:MET:HE2	1.86	0.40
1:I:288:GLN:O	1:I:291:SER:HB3	2.22	0.40
1:I:352:LEU:HD12	1:I:352:LEU:HA	1.88	0.40
1:I:517:LEU:HD12	1:I:517:LEU:HA	1.84	0.40
1:J:506:ILE:O	1:J:506:ILE:HG23	2.22	0.40
1:K:63:THR:HG23	1:K:65:TYR:H	1.86	0.40
3:L:67:ALA:O	3:L:71:LEU:HG	2.22	0.40
3:N:64:LEU:O	3:N:68:GLN:HG3	2.21	0.40
3:N:147:GLN:HA	3:N:150:GLU:OE1	2.21	0.40
1:M:448:GLU:OE1	1:M:450:LYS:HD2	2.22	0.40
1:M:637:LYS:HA	1:M:637:LYS:HD3	1.75	0.40
2:B:351:THR:HG21	1:H:551:LYS:HZ3	1.84	0.40
2:B:372:ARG:HG2	2:B:373:LYS:H	1.86	0.40
2:D:138:ALA:HB1	2:D:152:VAL:HG11	2.04	0.40
3:O:50:LEU:O	3:O:54:GLU:HG3	2.22	0.40
3:P:91:ARG:O	3:P:95:VAL:HG22	2.22	0.40
3:P:197:LEU:O	3:P:201:THR:HG23	2.21	0.40
1:G:217:GLU:O	1:G:221:ILE:HG12	2.21	0.40
1:G:689:VAL:O	1:G:693:LEU:HD23	2.21	0.40
1:H:23:ARG:O	1:H:27:GLN:HG2	2.21	0.40
1:I:448:GLU:OE1	1:I:450:LYS:HD2	2.21	0.40
1:I:466:GLU:HB2	1:I:468:PHE:CE2	2.57	0.40
1:J:288:GLN:O	1:J:291:SER:HB3	2.22	0.40
1:J:448:GLU:OE1	1:J:450:LYS:HD2	2.22	0.40
1:J:466:GLU:HB2	1:J:468:PHE:CE2	2.57	0.40
1:K:466:GLU:HB2	1:K:468:PHE:CE2	2.57	0.40
1:K:506:ILE:O	1:K:506:ILE:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:91:ARG:O	3:N:95:VAL:HG22	2.22	0.40
1:M:217:GLU:O	1:M:221:ILE:HG12	2.21	0.40
1:M:288:GLN:O	1:M:291:SER:HB3	2.22	0.40
1:M:301:LEU:HD21	1:M:351:LYS:HA	2.03	0.40
2:D:9:VAL:O	2:D:340:TRP:NE1	2.48	0.40
2:E:44:MET:CE	2:A:142:LEU:HD23	2.52	0.40
2:F:308:GLY:HA3	3:O:125:ARG:HH21	1.87	0.40
3:O:59:LYS:HA	3:O:62:GLU:HG2	2.04	0.40
3:O:139:GLU:HG3	3:O:140:LYS:N	2.36	0.40
3:P:50:LEU:O	3:P:53:THR:OG1	2.34	0.40
1:H:12:ALA:HB1	1:H:133:VAL:HG12	2.04	0.40
1:H:46:PHE:CG	1:H:99:PRO:HG3	2.56	0.40
1:H:506:ILE:CD1	1:H:757:LYS:HG2	2.48	0.40
1:H:776:MET:O	1:H:779:GLU:HG3	2.22	0.40
1:J:46:PHE:O	1:J:103:TYR:OH	2.27	0.40
1:J:565:LYS:O	1:J:578:SER:OG	2.25	0.40
1:J:769:LEU:H	1:J:769:LEU:HD12	1.86	0.40
1:K:12:ALA:HB1	1:K:133:VAL:HG12	2.04	0.40
1:K:290:LEU:HD23	1:K:290:LEU:HA	1.92	0.40
1:K:448:GLU:OE1	1:K:450:LYS:HD2	2.22	0.40
3:L:162:TYR:CD1	3:N:161:LYS:HD3	2.56	0.40
3:N:124:GLU:HA	3:N:127:MET:HG2	2.04	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	G	734/776 (95%)	696 (95%)	38 (5%)	0	100	100
1	H	734/776 (95%)	696 (95%)	38 (5%)	0	100	100
1	I	734/776 (95%)	696 (95%)	38 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	734/776 (95%)	696 (95%)	38 (5%)	0	100	100
1	K	734/776 (95%)	696 (95%)	38 (5%)	0	100	100
1	M	734/776 (95%)	696 (95%)	38 (5%)	0	100	100
2	A	369/371 (100%)	347 (94%)	22 (6%)	0	100	100
2	B	369/371 (100%)	349 (95%)	20 (5%)	0	100	100
2	C	369/371 (100%)	352 (95%)	17 (5%)	0	100	100
2	D	369/371 (100%)	344 (93%)	25 (7%)	0	100	100
2	E	369/371 (100%)	347 (94%)	22 (6%)	0	100	100
2	F	369/371 (100%)	348 (94%)	21 (6%)	0	100	100
3	L	164/166 (99%)	164 (100%)	0	0	100	100
3	N	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
3	O	164/166 (99%)	164 (100%)	0	0	100	100
3	P	164/166 (99%)	163 (99%)	1 (1%)	0	100	100
All	All	7274/7546 (96%)	6917 (95%)	357 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	644/668 (96%)	642 (100%)	2 (0%)	91	96
1	H	644/668 (96%)	642 (100%)	2 (0%)	91	96
1	I	644/668 (96%)	642 (100%)	2 (0%)	91	96
1	J	644/668 (96%)	642 (100%)	2 (0%)	91	96
1	K	644/668 (96%)	642 (100%)	2 (0%)	91	96
1	M	644/668 (96%)	642 (100%)	2 (0%)	91	96
2	A	314/314 (100%)	313 (100%)	1 (0%)	91	96
2	B	314/314 (100%)	314 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	C	314/314 (100%)	313 (100%)	1 (0%)	91 96
2	D	314/314 (100%)	314 (100%)	0	100 100
2	E	314/314 (100%)	313 (100%)	1 (0%)	91 96
2	F	314/314 (100%)	313 (100%)	1 (0%)	91 96
3	L	141/141 (100%)	139 (99%)	2 (1%)	62 82
3	N	141/141 (100%)	138 (98%)	3 (2%)	48 74
3	O	141/141 (100%)	139 (99%)	2 (1%)	62 82
3	P	141/141 (100%)	138 (98%)	3 (2%)	48 74
All	All	6312/6456 (98%)	6286 (100%)	26 (0%)	88 94

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	147	ARG
1	M	503	LYS
2	C	373	LYS
2	E	373	LYS
2	F	143	TYR
3	O	49	LYS
3	O	205	LYS
3	P	105	ARG
3	P	160	ARG
3	P	178	ARG
1	G	147	ARG
1	G	503	LYS
1	H	147	ARG
1	H	503	LYS
1	I	147	ARG
1	I	503	LYS
1	J	147	ARG
1	J	503	LYS
1	K	147	ARG
1	K	503	LYS
2	A	373	LYS
3	L	49	LYS
3	L	205	LYS
3	N	105	ARG
3	N	160	ARG
3	N	178	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	75	GLN
1	M	79	GLN
1	M	222	GLN
1	M	224	ASN
1	M	315	GLN
1	M	358	HIS
1	M	418	GLN
1	M	486	GLN
1	M	562	ASN
1	M	623	ASN
1	M	691	HIS
2	B	73	HIS
2	B	88	HIS
2	B	92	ASN
2	B	162	ASN
2	C	275	HIS
2	C	280	ASN
2	C	353	GLN
2	D	88	HIS
2	D	92	ASN
2	D	121	GLN
2	D	275	HIS
2	D	296	ASN
2	D	353	GLN
2	E	41	GLN
2	E	49	GLN
2	E	92	ASN
2	E	162	ASN
2	E	353	GLN
2	E	360	GLN
2	F	41	GLN
2	F	162	ASN
2	F	353	GLN
2	F	371	HIS
3	O	93	GLN
3	O	203	ASN
3	P	144	GLN
3	P	202	ASN
3	P	203	ASN
1	G	75	GLN
1	G	79	GLN

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Mol	Chain	Res	Type
1	G	222	GLN
1	G	224	ASN
1	G	315	GLN
1	G	358	HIS
1	G	368	GLN
1	G	418	GLN
1	G	486	GLN
1	G	562	ASN
1	G	623	ASN
1	G	691	HIS
1	H	75	GLN
1	H	79	GLN
1	H	222	GLN
1	H	224	ASN
1	H	315	GLN
1	H	358	HIS
1	H	368	GLN
1	H	418	GLN
1	H	486	GLN
1	H	562	ASN
1	H	623	ASN
1	H	691	HIS
1	I	75	GLN
1	I	79	GLN
1	I	222	GLN
1	I	224	ASN
1	I	315	GLN
1	I	358	HIS
1	I	368	GLN
1	I	418	GLN
1	I	486	GLN
1	I	562	ASN
1	I	691	HIS
1	J	75	GLN
1	J	79	GLN
1	J	222	GLN
1	J	224	ASN
1	J	315	GLN
1	J	358	HIS
1	J	368	GLN
1	J	418	GLN
1	J	486	GLN

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Mol	Chain	Res	Type
1	J	562	ASN
1	J	691	HIS
1	K	75	GLN
1	K	79	GLN
1	K	222	GLN
1	K	224	ASN
1	K	315	GLN
1	K	358	HIS
1	K	368	GLN
1	K	418	GLN
1	K	486	GLN
1	K	562	ASN
1	K	623	ASN
1	K	691	HIS
2	A	92	ASN
2	A	162	ASN
2	A	353	GLN
2	A	360	GLN
3	L	93	GLN
3	L	203	ASN
3	N	144	GLN
3	N	202	ASN
3	N	203	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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ADP	B	401	-	24,29,29	0.93	1 (4%)	29,45,45	1.45	4 (13%)
4	ADP	E	401	-	24,29,29	0.93	1 (4%)	29,45,45	1.45	4 (13%)
4	ADP	A	401	-	24,29,29	0.94	1 (4%)	29,45,45	1.45	4 (13%)
4	ADP	C	401	-	24,29,29	0.93	1 (4%)	29,45,45	1.50	4 (13%)
4	ADP	F	401	-	24,29,29	0.92	1 (4%)	29,45,45	1.48	4 (13%)
4	ADP	D	401	-	24,29,29	0.93	1 (4%)	29,45,45	1.44	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	B	401	-	-	4/12/32/32	0/3/3/3
4	ADP	E	401	-	-	4/12/32/32	0/3/3/3
4	ADP	A	401	-	-	4/12/32/32	0/3/3/3
4	ADP	C	401	-	-	3/12/32/32	0/3/3/3
4	ADP	F	401	-	-	5/12/32/32	0/3/3/3
4	ADP	D	401	-	-	4/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	ADP	C5-C4	2.28	1.47	1.40
4	B	401	ADP	C5-C4	2.25	1.46	1.40
4	F	401	ADP	C5-C4	2.24	1.46	1.40
4	D	401	ADP	C5-C4	2.23	1.46	1.40
4	A	401	ADP	C5-C4	2.22	1.46	1.40
4	E	401	ADP	C5-C4	2.21	1.46	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	401	ADP	PA-O3A-PB	-3.87	119.54	132.83
4	C	401	ADP	PA-O3A-PB	-3.86	119.59	132.83
4	B	401	ADP	PA-O3A-PB	-3.66	120.26	132.83
4	D	401	ADP	PA-O3A-PB	-3.49	120.86	132.83
4	A	401	ADP	PA-O3A-PB	-3.37	121.26	132.83
4	E	401	ADP	PA-O3A-PB	-3.37	121.26	132.83
4	C	401	ADP	N3-C2-N1	-3.12	123.80	128.68
4	F	401	ADP	N3-C2-N1	-3.08	123.86	128.68
4	A	401	ADP	N3-C2-N1	-3.08	123.86	128.68
4	E	401	ADP	N3-C2-N1	-3.07	123.87	128.68
4	C	401	ADP	C3'-C2'-C1'	3.03	105.54	100.98
4	D	401	ADP	C3'-C2'-C1'	3.03	105.53	100.98
4	B	401	ADP	C3'-C2'-C1'	2.99	105.47	100.98
4	D	401	ADP	N3-C2-N1	-2.92	124.12	128.68
4	A	401	ADP	C3'-C2'-C1'	2.88	105.31	100.98
4	E	401	ADP	C3'-C2'-C1'	2.87	105.30	100.98
4	F	401	ADP	C3'-C2'-C1'	2.85	105.26	100.98
4	B	401	ADP	N3-C2-N1	-2.82	124.28	128.68
4	B	401	ADP	C4-C5-N7	-2.58	106.72	109.40
4	E	401	ADP	C4-C5-N7	-2.56	106.74	109.40
4	A	401	ADP	C4-C5-N7	-2.53	106.77	109.40
4	F	401	ADP	C4-C5-N7	-2.51	106.78	109.40
4	D	401	ADP	C4-C5-N7	-2.50	106.79	109.40
4	C	401	ADP	C4-C5-N7	-2.48	106.82	109.40

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	401	ADP	C5'-O5'-PA-O2A
4	C	401	ADP	C5'-O5'-PA-O2A
4	D	401	ADP	C5'-O5'-PA-O2A
4	E	401	ADP	C5'-O5'-PA-O2A
4	F	401	ADP	C5'-O5'-PA-O2A
4	A	401	ADP	C5'-O5'-PA-O2A
4	B	401	ADP	C5'-O5'-PA-O3A
4	D	401	ADP	C5'-O5'-PA-O3A
4	E	401	ADP	C5'-O5'-PA-O3A
4	F	401	ADP	C5'-O5'-PA-O3A
4	A	401	ADP	C5'-O5'-PA-O3A
4	B	401	ADP	C5'-O5'-PA-O1A
4	D	401	ADP	C5'-O5'-PA-O1A
4	E	401	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
4	F	401	ADP	C5'-O5'-PA-O1A
4	A	401	ADP	C5'-O5'-PA-O1A
4	E	401	ADP	PB-O3A-PA-O2A
4	A	401	ADP	PB-O3A-PA-O2A
4	C	401	ADP	C5'-O5'-PA-O3A
4	B	401	ADP	PB-O3A-PA-O2A
4	D	401	ADP	PB-O3A-PA-O1A
4	F	401	ADP	PB-O3A-PA-O1A
4	F	401	ADP	PB-O3A-PA-O2A
4	C	401	ADP	C5'-O5'-PA-O1A

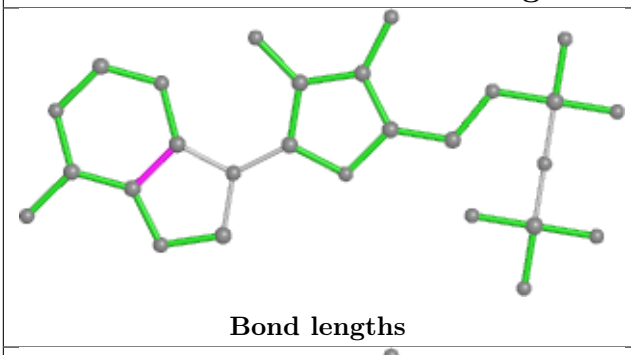
There are no ring outliers.

6 monomers are involved in 13 short contacts:

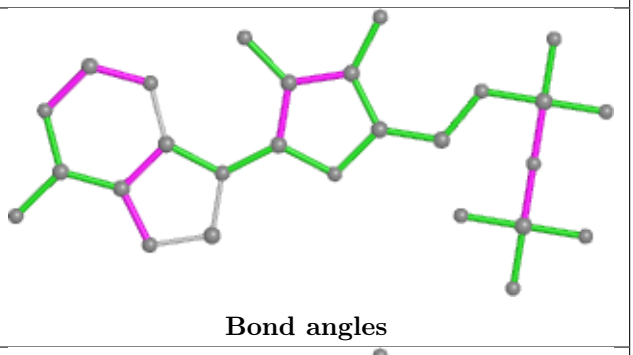
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401	ADP	1	0
4	E	401	ADP	3	0
4	A	401	ADP	3	0
4	C	401	ADP	2	0
4	F	401	ADP	2	0
4	D	401	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

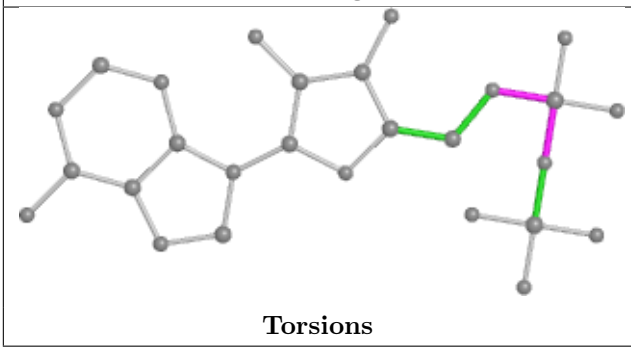
Ligand ADP B 401



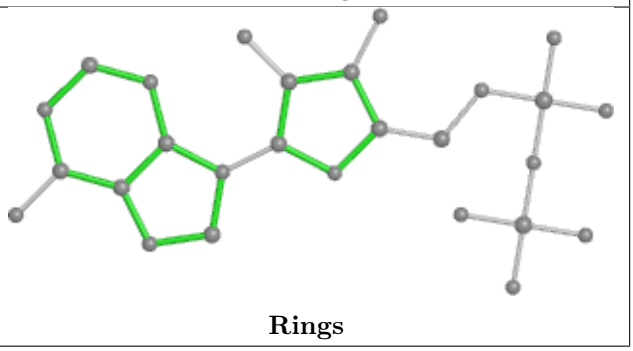
Bond lengths



Bond angles

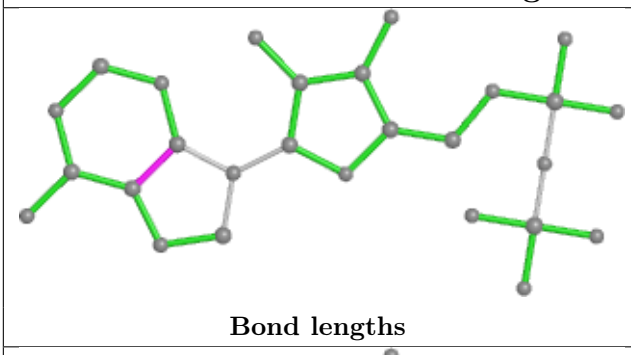


Torsions

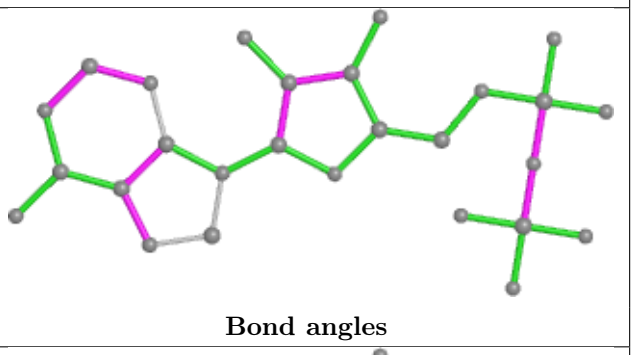


Rings

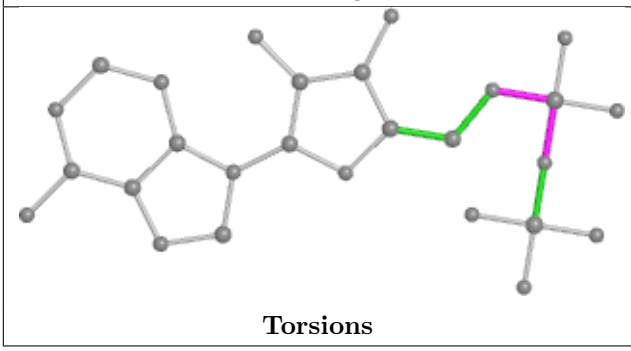
Ligand ADP E 401



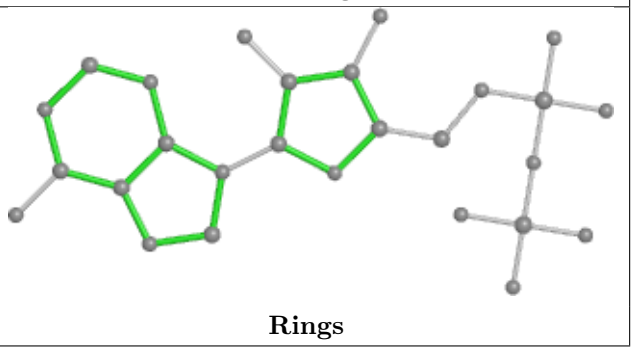
Bond lengths



Bond angles

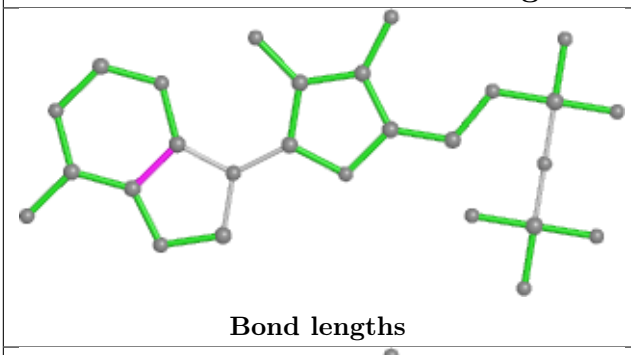


Torsions

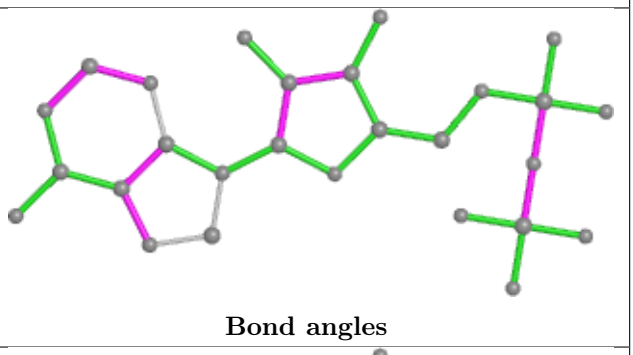


Rings

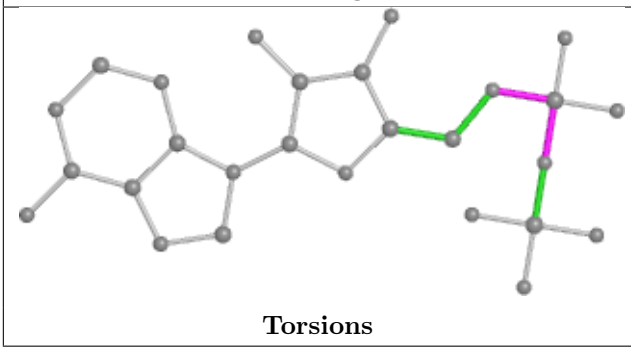
Ligand ADP A 401



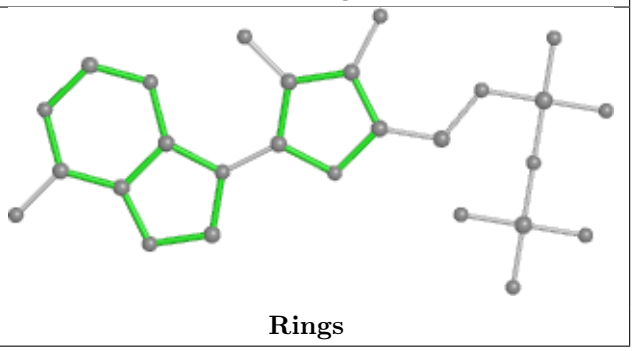
Bond lengths



Bond angles

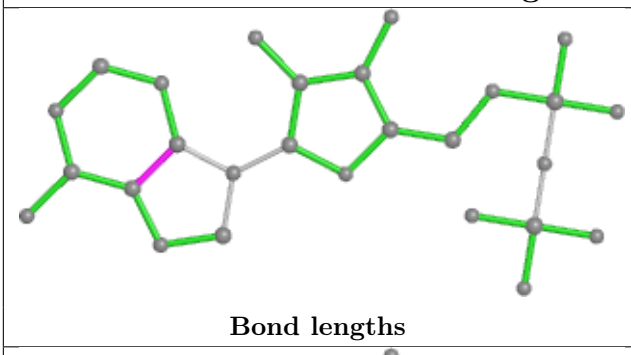


Torsions

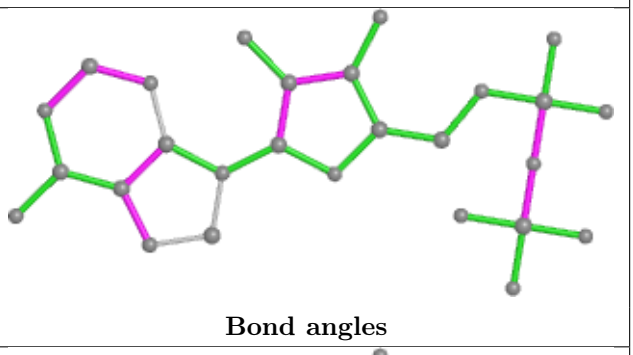


Rings

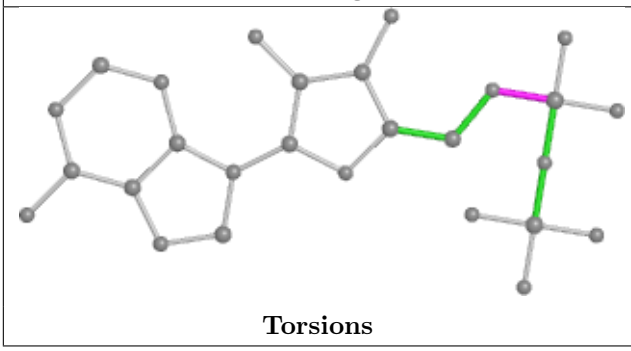
Ligand ADP C 401



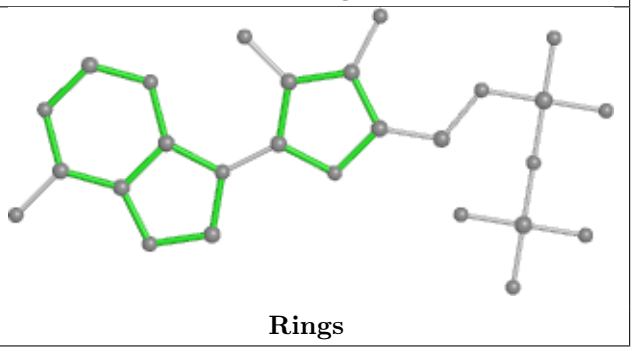
Bond lengths



Bond angles

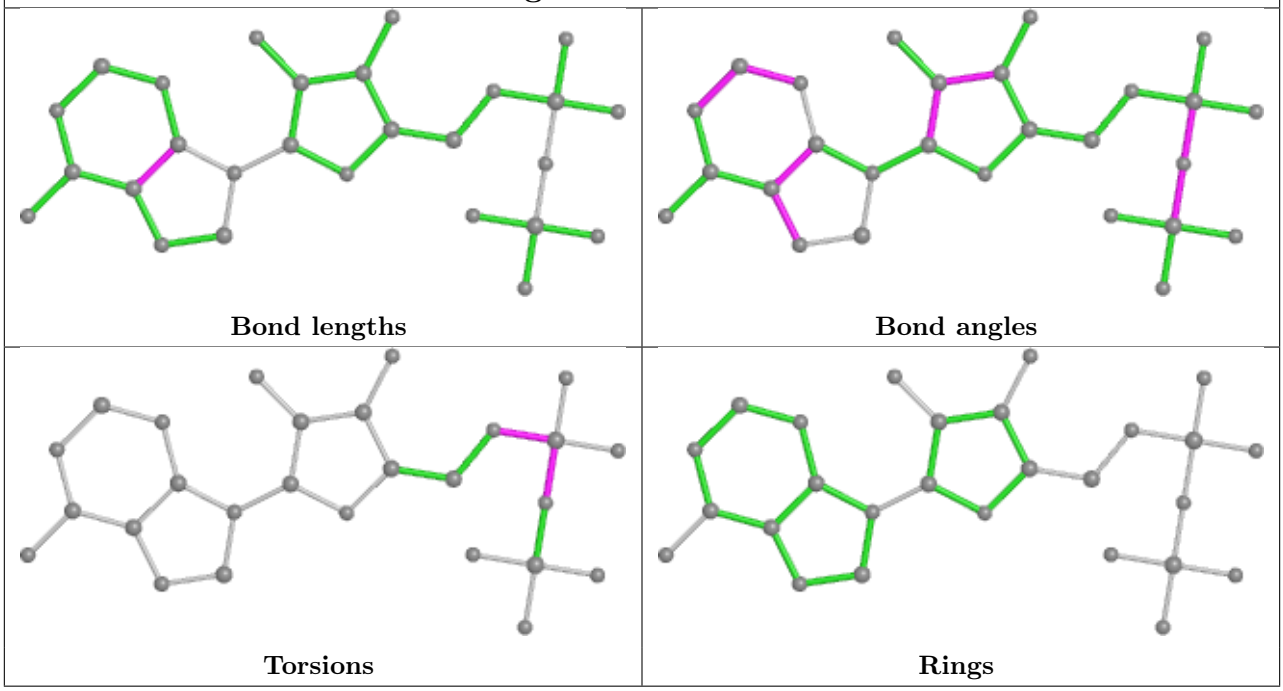


Torsions

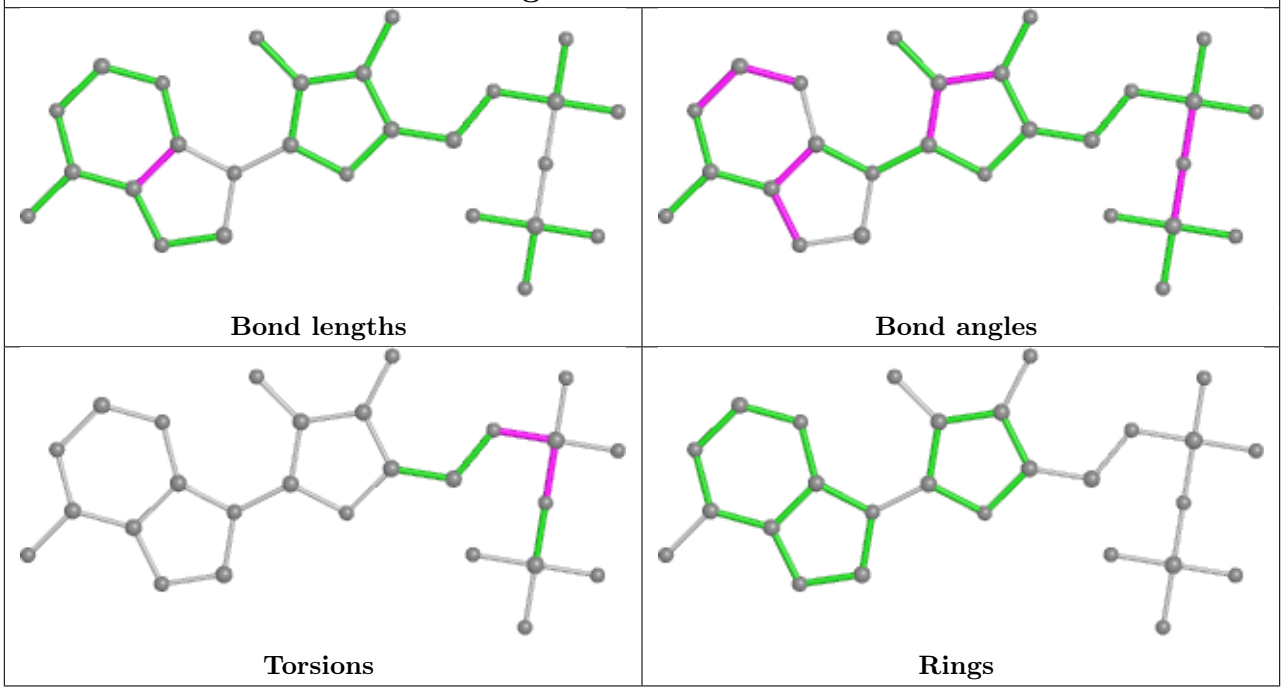


Rings

Ligand ADP F 401



Ligand ADP D 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-39896. 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 (i)

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

9 Map-model fit

This section was not generated.