



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 08:23 AM GMT

PDB ID : 1G4B
Title : CRYSTAL STRUCTURES OF THE HSLVU PEPTIDASE-ATPASE COMPLEX REVEAL AN ATP-DEPENDENT PROTEOLYSIS MECHANISM
Authors : Wang, J.; Song, J.J.; Franklin, M.C.; Kamtekar, S.; Im, Y.J.; Rho, S.H.; Seong, I.S.; Lee, C.S.; Chung, C.H.; Eom, S.H.
Deposited on : 2000-10-26
Resolution : 7.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

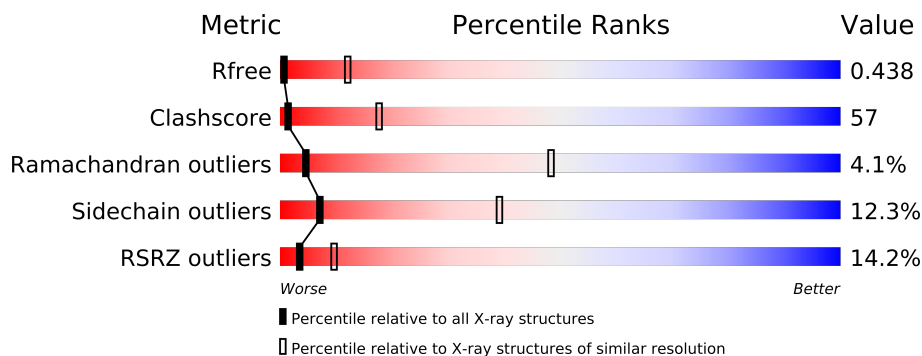
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 7.00 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1098 (10.00-3.50)
Clashscore	79885	1039 (10.00-3.52)
Ramachandran outliers	78287	1291 (9.50-3.50)
Sidechain outliers	78261	1265 (9.50-3.50)
RSRZ outliers	66119	1097 (10.00-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	E	443	
1	F	443	
1	K	443	
1	L	443	
2	M	175	
2	N	175	
2	O	175	
2	P	175	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17660 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUB-UNIT HSLU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	393	Total	C	N	O	S	0	0	0
			3096	1935	551	600	10			
1	F	393	Total	C	N	O	S	0	0	0
			3096	1935	551	600	10			
1	K	393	Total	C	N	O	S	0	0	0
			3096	1935	551	600	10			
1	L	393	Total	C	N	O	S	0	0	0
			3096	1935	551	600	10			

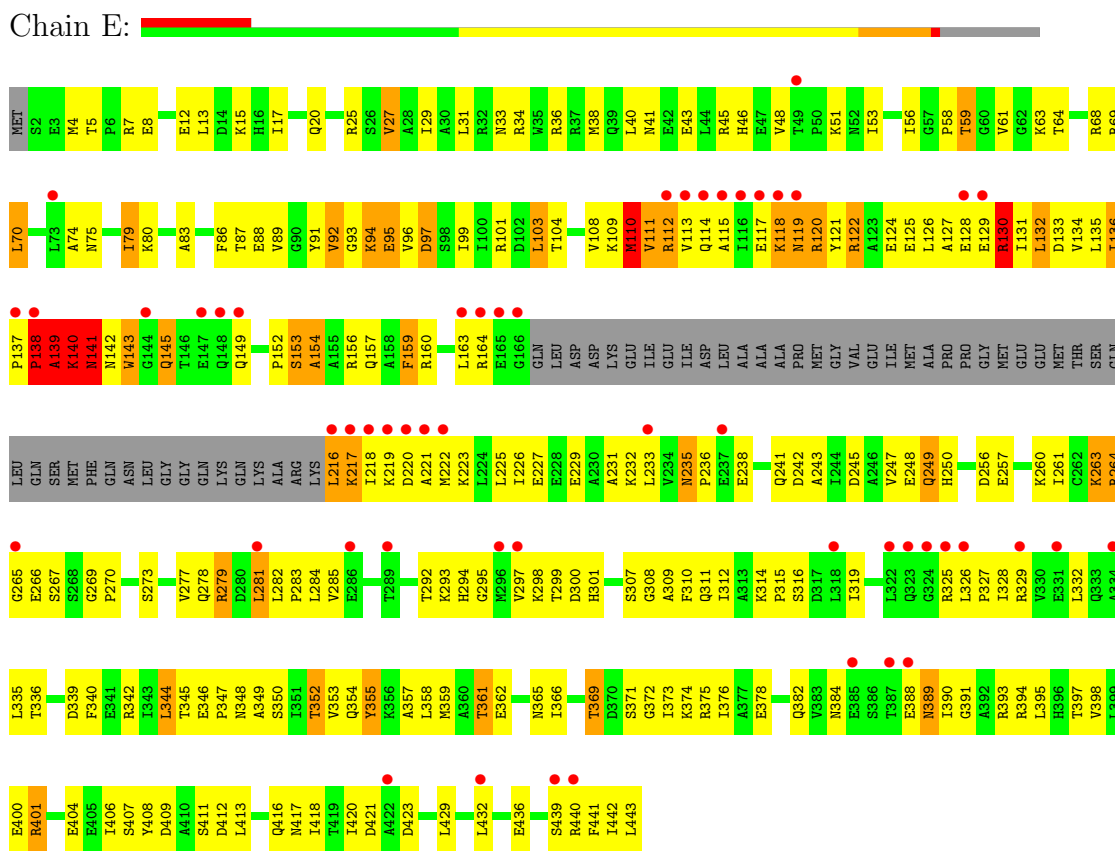
- Molecule 2 is a protein called ATP-DEPENDENT PROTEASE HSLV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	173	Total	C	N	O	S	0	0	0
			1319	828	235	252	4			
2	N	173	Total	C	N	O	S	0	0	0
			1319	828	235	252	4			
2	O	173	Total	C	N	O	S	0	0	0
			1319	828	235	252	4			
2	P	173	Total	C	N	O	S	0	0	0
			1319	828	235	252	4			

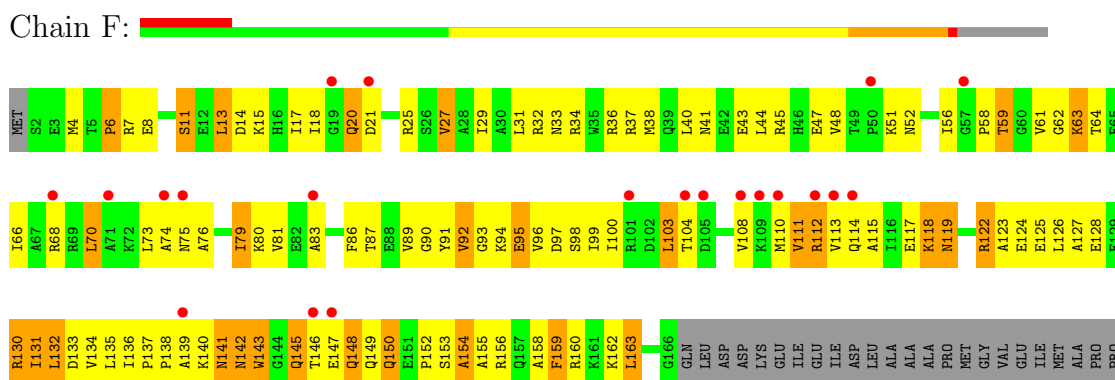
3 Residue-property plots

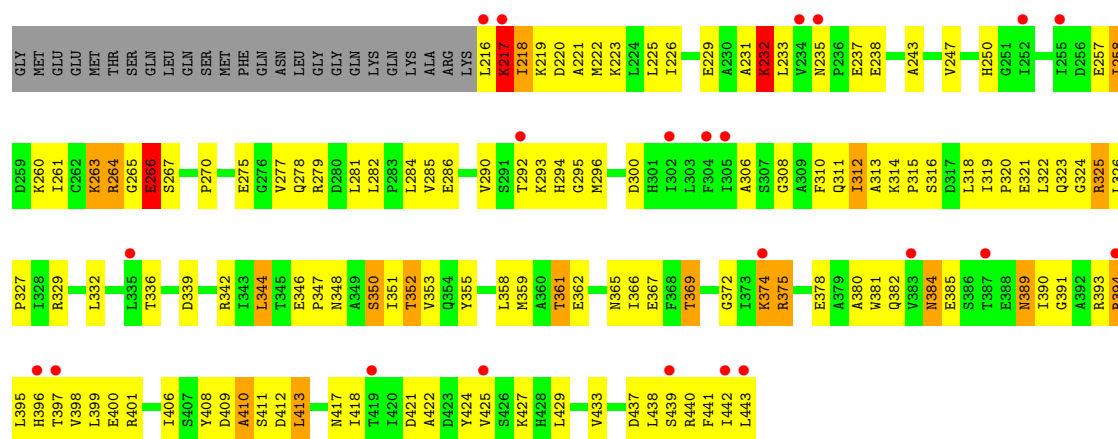
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU



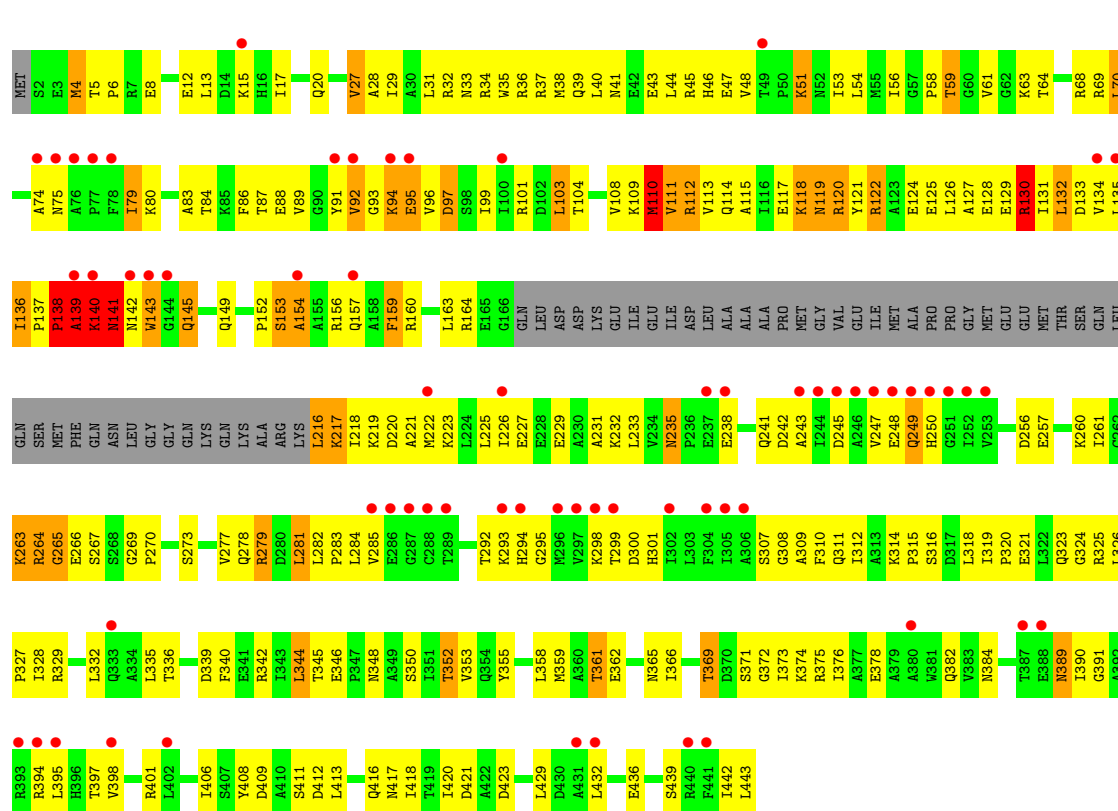
• Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU





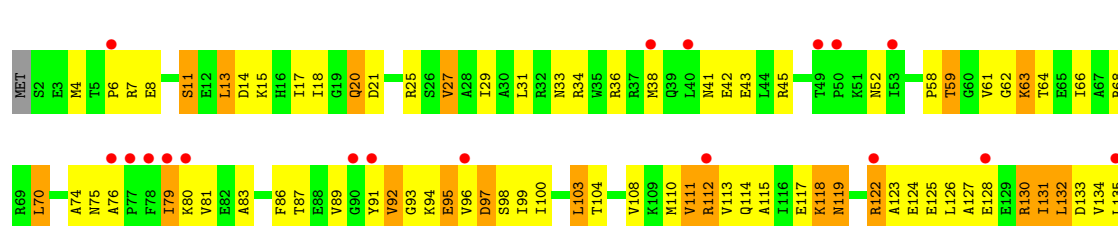
• Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU

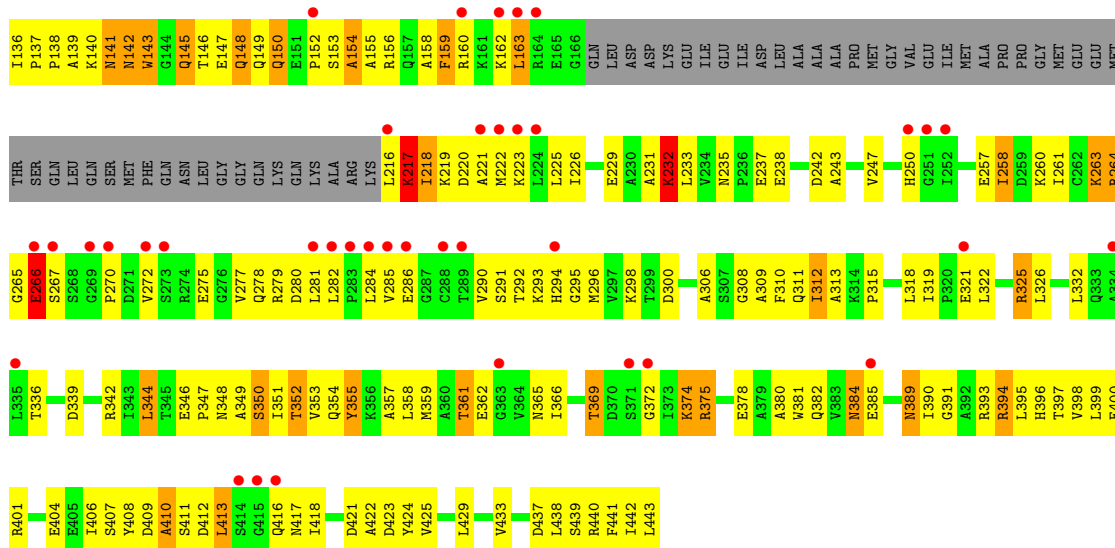
Chain K:



• Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU

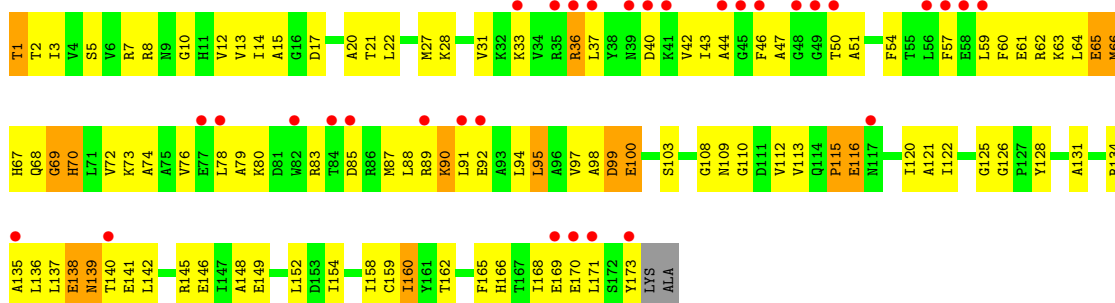
Chain L:





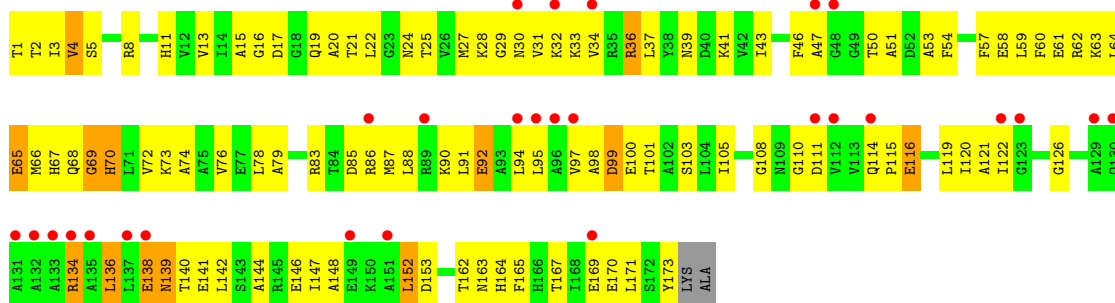
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain M:



• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

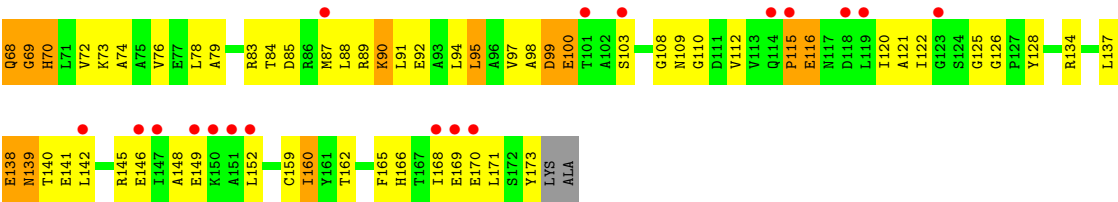
Chain N:



• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

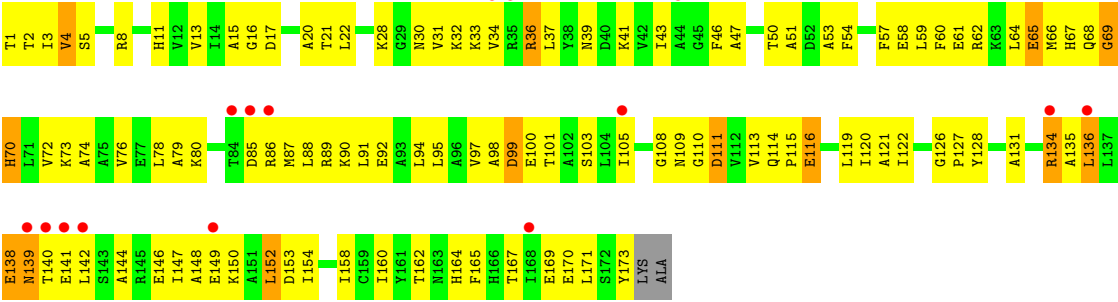
Chain O:





• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain P: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	173.38Å 173.38Å 254.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 7.00 82.06 – 7.00	Depositor EDS
% Data completeness (in resolution range)	66.0 (10.00-7.00) 81.1 (82.06-7.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 6.72Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.401 , 0.432 0.446 , 0.438	Depositor DCC
R_{free} test set	560 reflections (9.39%)	DCC
Wilson B-factor (Å ²)	101.1	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 118.1	EDS
Estimated twinning fraction	0.350 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 6405 reflections	Xtriage
F_o, F_c correlation	0.32	EDS
Total number of atoms	17660	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	E	0.61	4/3135 (0.1%)	0.96	13/4228 (0.3%)
1	F	0.46	2/3135 (0.1%)	0.70	1/4228 (0.0%)
1	K	0.61	4/3135 (0.1%)	0.96	13/4228 (0.3%)
1	L	0.46	2/3135 (0.1%)	0.70	1/4228 (0.0%)
2	M	0.37	0/1336	0.65	0/1806
2	N	0.37	0/1336	0.65	0/1806
2	O	0.37	0/1336	0.65	0/1806
2	P	0.37	0/1336	0.65	0/1806
All	All	0.50	12/17884 (0.1%)	0.79	28/24136 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	2
1	K	0	2
All	All	0	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	139	ALA	C-N	-17.84	0.93	1.34
1	K	139	ALA	C-N	-17.84	0.93	1.34
1	E	122	ARG	CB-CG	10.32	1.80	1.52
1	K	122	ARG	CB-CG	10.28	1.80	1.52
1	E	145	GLN	CG-CD	8.75	1.71	1.51
1	K	145	GLN	CG-CD	8.73	1.71	1.51
1	E	145	GLN	CA-CB	-6.33	1.40	1.53
1	K	145	GLN	CA-CB	-6.32	1.40	1.53
1	F	145	GLN	CG-CD	5.88	1.64	1.51
1	L	145	GLN	CG-CD	5.78	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	145	GLN	CA-CB	-5.24	1.42	1.53
1	L	145	GLN	CA-CB	-5.24	1.42	1.53

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	122	ARG	CA-CB-CG	-18.01	73.78	113.40
1	K	122	ARG	CA-CB-CG	-18.00	73.80	113.40
1	K	141	ASN	CA-C-N	-16.91	80.01	117.20
1	E	141	ASN	CA-C-N	-16.89	80.04	117.20
1	K	145	GLN	CA-CB-CG	-12.09	86.80	113.40
1	E	145	GLN	CA-CB-CG	-12.09	86.81	113.40
1	K	140	LYS	CG-CD-CE	11.37	146.01	111.90
1	E	140	LYS	CG-CD-CE	11.36	145.98	111.90
1	E	139	ALA	O-C-N	-11.15	104.86	122.70
1	K	139	ALA	O-C-N	-11.13	104.89	122.70
1	E	122	ARG	CB-CG-CD	-10.61	84.01	111.60
1	K	122	ARG	CB-CG-CD	-10.60	84.05	111.60
1	E	138	PRO	C-N-CA	10.45	147.83	121.70
1	E	141	ASN	O-C-N	10.43	139.39	122.70
1	K	141	ASN	O-C-N	10.42	139.38	122.70
1	K	138	PRO	C-N-CA	10.41	147.73	121.70
1	K	139	ALA	C-N-CA	9.42	145.26	121.70
1	E	139	ALA	C-N-CA	9.42	145.25	121.70
1	F	145	GLN	CA-CB-CG	-9.15	93.26	113.40
1	L	145	GLN	CA-CB-CG	-9.15	93.26	113.40
1	K	249	GLN	CA-CB-CG	8.77	132.70	113.40
1	E	249	GLN	CA-CB-CG	8.76	132.68	113.40
1	E	137	PRO	CA-N-CD	7.50	122.20	111.70
1	K	137	PRO	CA-N-CD	7.47	122.15	111.70
1	E	130	ARG	NE-CZ-NH2	6.87	123.73	120.30
1	K	130	ARG	NE-CZ-NH2	6.84	123.72	120.30
1	K	249	GLN	CB-CG-CD	6.67	128.93	111.60
1	E	249	GLN	CB-CG-CD	6.63	128.84	111.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	139	ALA	Mainchain
1	E	141	ASN	Mainchain
1	K	139	ALA	Mainchain

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Mol	Chain	Res	Type	Group
1	K	141	ASN	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3096	0	3150	570	49
1	F	3096	0	3155	585	54
1	K	3096	0	3149	320	220
1	L	3096	0	3152	385	225
2	M	1319	0	1335	172	12
2	N	1319	0	1335	141	15
2	O	1319	0	1330	197	14
2	P	1319	0	1327	178	19
All	All	17660	0	17933	2026	305

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 57.

All (2026) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:441:PHE:CD1	1:F:56:ILE:HD13	1.27	1.66
1:K:122:ARG:CB	1:K:122:ARG:CG	1.80	1.59
1:L:309:ALA:HB1	2:O:66:MET:CE	1.28	1.58
1:E:442:ILE:HA	1:F:329:ARG:CB	1.12	1.58
1:E:122:ARG:CB	1:E:122:ARG:CG	1.80	1.56
1:E:139:ALA:HB2	1:E:152:PRO:CG	1.36	1.53
1:L:264:ARG:NH2	2:O:59:LEU:CD2	1.69	1.53
1:E:407:SER:CA	1:F:36:ARG:HH12	1.11	1.50
1:K:408:TYR:CE2	1:L:7:ARG:NH2	1.79	1.50
1:K:139:ALA:HB2	1:K:152:PRO:CG	1.36	1.50
2:M:135:ALA:HB2	2:P:154:ILE:CD1	1.36	1.50
1:E:354:GLN:NE2	1:F:47:GLU:HB3	1.30	1.44
1:E:357:ALA:HB2	1:F:44:LEU:CD1	1.46	1.43
1:E:311:GLN:CB	2:N:66:MET:O	1.68	1.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:92:VAL:CG1	1:F:92:VAL:HA	1.47	1.41
1:E:139:ALA:HB2	1:E:152:PRO:CB	1.52	1.40
1:K:145:GLN:CB	1:K:149:GLN:HB2	1.52	1.39
1:E:145:GLN:CB	1:E:149:GLN:HB2	1.52	1.38
1:E:357:ALA:CB	1:F:44:LEU:HD13	1.53	1.38
1:K:139:ALA:HB2	1:K:152:PRO:CB	1.52	1.38
1:K:122:ARG:CA	1:K:122:ARG:CG	2.01	1.37
1:E:314:LYS:NZ	2:N:65:GLU:CG	1.70	1.36
1:E:122:ARG:CA	1:E:122:ARG:CG	2.01	1.36
1:F:145:GLN:CD	1:F:145:GLN:H	1.29	1.35
1:E:91:TYR:CG	1:F:90:GLY:O	1.80	1.34
1:L:264:ARG:HD3	2:O:62:ARG:CD	1.57	1.34
2:M:135:ALA:CB	2:P:154:ILE:CD1	2.06	1.34
1:F:264:ARG:HH22	2:M:62:ARG:CB	1.40	1.33
1:E:442:ILE:CA	1:F:329:ARG:CB	2.07	1.32
1:K:311:GLN:HG2	2:P:66:MET:CE	1.60	1.31
1:F:264:ARG:CZ	2:M:62:ARG:HD2	1.61	1.30
1:L:145:GLN:CG	1:L:150:GLN:N	1.93	1.30
1:K:293:LYS:HE3	1:L:296:MET:CE	1.60	1.30
1:L:264:ARG:HG2	2:O:62:ARG:NH2	1.41	1.30
1:F:145:GLN:CG	1:F:150:GLN:N	1.93	1.29
1:K:311:GLN:HG3	2:P:66:MET:SD	1.69	1.27
1:E:408:TYR:OH	1:F:7:ARG:CA	1.82	1.27
1:E:441:PHE:HD1	1:F:56:ILE:CD1	1.48	1.27
1:E:357:ALA:O	1:F:40:LEU:CD2	1.82	1.26
2:O:28:LYS:CG	2:P:113:VAL:HG11	1.58	1.26
1:L:145:GLN:H	1:L:145:GLN:CD	1.29	1.26
1:E:440:ARG:O	1:F:315:PRO:CB	1.82	1.26
1:E:92:VAL:HG11	1:F:92:VAL:CA	1.63	1.25
1:E:442:ILE:CA	1:F:329:ARG:HB2	1.67	1.25
1:L:145:GLN:HG3	1:L:150:GLN:N	1.49	1.24
2:M:135:ALA:CB	2:P:154:ILE:HD13	1.66	1.24
1:F:311:GLN:HG3	2:M:66:MET:CE	1.68	1.24
1:F:145:GLN:HG3	1:F:150:GLN:N	1.49	1.24
1:F:264:ARG:NH2	2:M:62:ARG:HD2	1.53	1.23
1:K:139:ALA:CB	1:K:152:PRO:HG3	1.68	1.22
1:E:139:ALA:CB	1:E:152:PRO:HG3	1.68	1.21
1:F:264:ARG:HH12	2:M:62:ARG:CB	1.53	1.21
1:E:357:ALA:C	1:F:40:LEU:CD2	2.07	1.21
1:F:264:ARG:NH2	2:M:62:ARG:HB2	1.52	1.21
1:E:408:TYR:OH	1:F:7:ARG:N	1.70	1.21
1:L:264:ARG:CG	2:O:62:ARG:NH2	2.04	1.20

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:145:GLN:CB	1:F:149:GLN:HB2	1.71	1.20
2:M:154:ILE:CG2	2:P:131:ALA:HB1	1.71	1.20
1:L:145:GLN:N	1:L:145:GLN:CD	1.87	1.20
1:L:145:GLN:CB	1:L:149:GLN:HB2	1.71	1.20
1:E:311:GLN:CD	2:N:66:MET:O	1.71	1.20
1:E:441:PHE:CD1	1:F:56:ILE:CD1	2.22	1.20
1:E:311:GLN:CG	2:N:66:MET:O	1.91	1.19
1:E:442:ILE:C	1:F:329:ARG:HG3	1.62	1.19
1:L:309:ALA:CA	2:O:66:MET:SD	2.32	1.18
1:E:354:GLN:NE2	1:F:47:GLU:CB	2.06	1.18
1:K:264:ARG:HG3	2:P:62:ARG:NH2	1.55	1.18
1:F:264:ARG:NH2	2:M:62:ARG:CD	2.07	1.18
1:F:264:ARG:CZ	2:M:62:ARG:HB2	1.74	1.17
1:E:138:PRO:HB2	1:E:152:PRO:HB2	1.25	1.17
1:E:91:TYR:CD2	1:F:90:GLY:O	1.96	1.17
1:F:312:ILE:HD11	2:M:62:ARG:HA	1.21	1.17
1:E:145:GLN:CG	1:E:149:GLN:HB2	1.73	1.17
1:F:264:ARG:NH2	2:M:62:ARG:CB	2.01	1.17
1:E:354:GLN:OE1	1:F:48:VAL:HA	1.46	1.16
1:K:145:GLN:CG	1:K:149:GLN:HB2	1.74	1.16
1:K:145:GLN:HG3	1:K:149:GLN:CG	1.76	1.16
1:F:145:GLN:N	1:F:145:GLN:CD	1.87	1.16
1:L:264:ARG:CG	2:O:62:ARG:HH21	1.58	1.16
1:K:122:ARG:CB	1:K:122:ARG:CD	2.24	1.15
1:E:442:ILE:HA	1:F:329:ARG:HB3	1.23	1.15
1:K:122:ARG:HA	1:K:122:ARG:CG	1.73	1.15
1:E:407:SER:HA	1:F:36:ARG:NH1	1.38	1.15
1:E:145:GLN:HG3	1:E:149:GLN:CG	1.76	1.15
1:E:440:ARG:O	1:F:315:PRO:HB2	0.98	1.15
1:K:145:GLN:HB2	1:K:149:GLN:CB	1.75	1.15
1:E:145:GLN:HB2	1:E:149:GLN:CB	1.76	1.15
1:E:441:PHE:HB3	1:F:56:ILE:HD12	1.29	1.14
1:E:122:ARG:CB	1:E:122:ARG:CD	2.24	1.14
1:F:145:GLN:NE2	1:F:150:GLN:HA	1.63	1.13
1:L:264:ARG:NH2	2:O:59:LEU:CB	2.10	1.13
1:L:145:GLN:HB3	1:L:149:GLN:HB2	1.15	1.13
1:E:122:ARG:HA	1:E:122:ARG:CG	1.73	1.13
1:L:264:ARG:CD	2:O:62:ARG:HH21	1.60	1.13
1:F:145:GLN:HB3	1:F:149:GLN:HB2	1.15	1.12
1:E:442:ILE:HA	1:F:329:ARG:CG	1.79	1.12
1:E:139:ALA:HB2	1:E:152:PRO:HG3	1.13	1.12
1:L:145:GLN:NE2	1:L:150:GLN:HA	1.64	1.12

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:264:ARG:NH1	2:M:62:ARG:HB2	1.64	1.12
1:E:311:GLN:NE2	2:N:67:HIS:HA	1.30	1.12
1:F:264:ARG:NH1	2:M:62:ARG:CB	2.11	1.12
1:K:264:ARG:HG3	2:P:62:ARG:HH22	1.04	1.12
1:K:139:ALA:HB2	1:K:152:PRO:HG3	1.12	1.12
1:E:408:TYR:OH	1:F:7:ARG:HA	1.36	1.12
1:E:442:ILE:C	1:F:329:ARG:CG	2.17	1.11
1:F:264:ARG:CZ	2:M:62:ARG:CD	2.27	1.11
1:L:86:PHE:O	1:L:89:VAL:HG22	1.51	1.11
1:F:264:ARG:NH1	2:M:62:ARG:CG	2.12	1.11
1:F:86:PHE:O	1:F:89:VAL:HG22	1.51	1.11
1:E:139:ALA:CB	1:E:152:PRO:CG	2.26	1.11
1:L:264:ARG:NH1	2:O:62:ARG:HB3	1.66	1.11
1:K:138:PRO:HB2	1:K:152:PRO:HB2	1.25	1.11
1:E:358:LEU:HD11	1:F:48:VAL:CG1	1.81	1.10
1:E:310:PHE:O	2:N:66:MET:HB2	1.29	1.10
2:M:135:ALA:HA	2:P:154:ILE:HD11	1.32	1.10
1:E:311:GLN:HE22	2:N:67:HIS:CA	1.64	1.10
1:E:441:PHE:O	1:F:329:ARG:HD2	1.50	1.10
1:L:264:ARG:NH2	2:O:59:LEU:HG	1.57	1.10
1:E:311:GLN:HB3	2:N:66:MET:O	1.25	1.09
1:E:311:GLN:NE2	2:N:67:HIS:CA	2.16	1.09
1:E:357:ALA:CB	1:F:44:LEU:CD1	2.15	1.09
1:K:311:GLN:HG2	2:P:66:MET:HE2	1.11	1.09
1:E:441:PHE:HA	1:F:315:PRO:HG2	1.28	1.08
1:F:264:ARG:CZ	2:M:62:ARG:CG	2.31	1.08
2:O:28:LYS:HG3	2:P:113:VAL:CG1	1.84	1.08
1:E:442:ILE:CA	1:F:329:ARG:CG	2.32	1.08
1:L:266:GLU:O	2:O:87:MET:SD	2.11	1.08
1:F:264:ARG:NH1	2:M:62:ARG:HG3	1.65	1.08
1:K:264:ARG:CG	2:P:62:ARG:NH2	2.16	1.08
1:F:292:THR:HG22	1:F:294:HIS:H	1.19	1.08
1:E:145:GLN:HB2	1:E:149:GLN:HB2	1.11	1.07
1:E:408:TYR:CZ	1:F:7:ARG:N	2.21	1.07
1:E:349:ALA:CB	1:F:47:GLU:HG3	1.84	1.07
1:K:292:THR:HG22	1:K:294:HIS:H	1.20	1.07
1:E:393:ARG:HB3	1:F:324:GLY:HA3	1.37	1.06
1:K:145:GLN:HB2	1:K:149:GLN:HB2	1.11	1.06
2:M:154:ILE:HG21	2:P:131:ALA:HB1	1.08	1.06
1:L:312:ILE:HA	2:O:62:ARG:HA	1.07	1.06
1:K:311:GLN:CG	2:P:66:MET:CE	2.32	1.06
1:F:311:GLN:HG3	2:M:66:MET:HE1	1.37	1.06

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:292:THR:HG22	1:L:294:HIS:H	1.19	1.06
1:E:357:ALA:C	1:F:40:LEU:HD21	1.71	1.06
1:E:354:GLN:OE1	1:F:48:VAL:CA	2.03	1.06
1:F:145:GLN:HG3	1:F:149:GLN:CA	1.86	1.06
1:E:139:ALA:HB2	1:E:152:PRO:HB3	1.35	1.05
1:E:400:GLU:CD	1:F:51:LYS:HG2	1.75	1.05
1:L:145:GLN:HG3	1:L:149:GLN:CA	1.86	1.05
1:L:344:LEU:HD13	1:L:395:LEU:HD13	1.39	1.05
1:E:349:ALA:HB1	1:F:47:GLU:CG	1.87	1.04
1:F:145:GLN:HG3	1:F:149:GLN:C	1.76	1.04
1:E:400:GLU:CD	1:F:51:LYS:CG	2.26	1.04
1:L:132:LEU:HD13	1:L:156:ARG:HG2	1.38	1.04
1:E:441:PHE:HB3	1:F:56:ILE:CD1	1.87	1.04
2:M:135:ALA:CA	2:P:154:ILE:HD11	1.85	1.04
1:F:344:LEU:HD13	1:F:395:LEU:HD13	1.39	1.04
1:K:139:ALA:CB	1:K:152:PRO:CG	2.26	1.04
1:L:145:GLN:HG3	1:L:149:GLN:C	1.76	1.04
1:K:408:TYR:HE2	1:L:7:ARG:NH2	1.28	1.04
1:L:312:ILE:C	2:O:65:GLU:HG3	1.59	1.03
1:E:357:ALA:C	1:F:40:LEU:HD22	1.75	1.03
1:E:358:LEU:HD11	1:F:48:VAL:HG11	1.08	1.03
1:E:442:ILE:CA	1:F:329:ARG:HG3	1.87	1.03
1:L:264:ARG:CD	2:O:62:ARG:HD2	1.87	1.03
1:K:139:ALA:HB2	1:K:152:PRO:HB3	1.35	1.03
1:L:312:ILE:HA	2:O:62:ARG:CA	1.71	1.02
1:L:309:ALA:CB	2:O:66:MET:SD	0.96	1.02
1:E:400:GLU:OE2	1:F:51:LYS:CE	2.06	1.02
1:E:92:VAL:HG11	1:F:92:VAL:CB	1.89	1.02
1:E:314:LYS:NZ	2:N:65:GLU:HG3	1.12	1.02
1:F:369:THR:HG22	1:F:372:GLY:H	1.22	1.02
1:L:309:ALA:HB1	2:O:66:MET:SD	0.66	1.01
1:F:311:GLN:HG3	2:M:66:MET:HE3	1.41	1.01
1:E:292:THR:HG22	1:E:294:HIS:H	1.20	1.01
1:E:393:ARG:NE	1:F:321:GLU:HA	1.74	1.01
1:L:313:ALA:O	2:O:65:GLU:OE2	1.79	1.01
1:K:408:TYR:CE2	1:L:7:ARG:CZ	2.37	1.01
1:K:311:GLN:CG	2:P:66:MET:SD	2.44	1.01
1:E:357:ALA:HB3	1:F:44:LEU:HD13	1.39	1.01
1:L:369:THR:HG22	1:L:372:GLY:H	1.22	1.01
1:E:163:LEU:HD11	1:E:218:ILE:HG21	1.39	1.01
1:E:139:ALA:CB	1:E:152:PRO:CB	2.38	1.00
1:K:163:LEU:HD11	1:K:218:ILE:HG21	1.39	1.00

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:400:GLU:OE2	1:F:51:LYS:NZ	1.94	1.00
1:E:354:GLN:NE2	1:F:47:GLU:C	2.14	1.00
1:K:139:ALA:CB	1:K:152:PRO:CB	2.39	1.00
1:E:400:GLU:OE1	1:F:51:LYS:HG2	1.57	1.00
1:F:145:GLN:CG	1:F:149:GLN:HB2	1.90	1.00
1:E:408:TYR:CZ	1:F:6:PRO:C	2.34	1.00
1:L:264:ARG:NH2	2:O:59:LEU:CG	0.85	1.00
1:L:264:ARG:HD3	2:O:62:ARG:HD2	1.02	1.00
1:E:357:ALA:O	1:F:40:LEU:HD21	1.54	1.00
1:F:132:LEU:HD13	1:F:156:ARG:HG2	1.38	1.00
1:L:145:GLN:CG	1:L:149:GLN:HB2	1.90	0.99
1:K:88:GLU:OE2	1:L:280:ASP:OD2	1.79	0.99
1:E:139:ALA:CB	1:E:152:PRO:HB3	1.91	0.99
1:K:139:ALA:CB	1:K:152:PRO:HB3	1.91	0.99
1:K:265:GLY:O	2:P:87:MET:CE	2.11	0.99
1:L:312:ILE:CA	2:O:62:ARG:HA	1.90	0.99
1:L:132:LEU:HD11	1:L:160:ARG:HB3	1.42	0.99
1:K:145:GLN:HG3	1:K:149:GLN:CB	1.92	0.99
1:K:293:LYS:HE3	1:L:296:MET:HE3	1.41	0.98
1:E:145:GLN:HG3	1:E:149:GLN:CB	1.92	0.98
1:L:130:ARG:O	1:L:130:ARG:HD2	1.64	0.98
1:E:113:VAL:O	1:E:117:GLU:HG3	1.64	0.98
1:E:441:PHE:CG	1:F:56:ILE:HD13	1.97	0.98
1:E:407:SER:CA	1:F:36:ARG:NH1	1.96	0.98
1:F:264:ARG:HH22	2:M:62:ARG:HB2	1.12	0.98
1:E:361:THR:HG21	1:F:36:ARG:HA	1.43	0.98
1:E:358:LEU:CD2	1:F:37:ARG:HA	1.94	0.98
1:E:393:ARG:CD	1:F:321:GLU:HA	1.94	0.97
1:E:354:GLN:HB3	1:F:48:VAL:HG22	1.46	0.97
1:F:130:ARG:HD2	1:F:130:ARG:O	1.64	0.97
1:L:309:ALA:HB2	2:O:66:MET:SD	1.59	0.97
1:E:92:VAL:HG11	1:F:92:VAL:HA	0.99	0.97
1:E:441:PHE:CD1	1:F:56:ILE:HG21	2.00	0.97
1:E:131:ILE:O	1:E:134:VAL:HG12	1.64	0.97
1:K:131:ILE:O	1:K:134:VAL:HG12	1.64	0.97
2:O:2:THR:OG1	2:O:162:THR:HG21	1.64	0.96
1:E:145:GLN:CB	1:E:149:GLN:CB	2.39	0.96
1:F:264:ARG:HH22	2:M:62:ARG:HB3	1.28	0.96
1:E:354:GLN:CD	1:F:47:GLU:C	2.24	0.96
2:M:154:ILE:CG2	2:P:131:ALA:CB	2.43	0.96
1:F:132:LEU:HD11	1:F:160:ARG:HB3	1.42	0.96
2:M:2:THR:OG1	2:M:162:THR:HG21	1.64	0.96

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:113:VAL:O	1:K:117:GLU:HG3	1.64	0.96
1:E:264:ARG:HH12	2:N:63:LYS:HZ3	1.12	0.96
1:L:311:GLN:HE22	2:O:68:GLN:C	1.69	0.95
1:E:92:VAL:CG1	1:F:92:VAL:CA	2.30	0.95
1:E:357:ALA:HB2	1:F:44:LEU:HD12	1.48	0.95
1:K:145:GLN:CB	1:K:149:GLN:CB	2.39	0.95
1:E:442:ILE:HA	1:F:329:ARG:HB2	0.97	0.95
1:K:264:ARG:CG	2:P:62:ARG:HH22	1.74	0.95
1:E:139:ALA:CA	1:E:152:PRO:HB3	1.97	0.94
1:E:355:TYR:HE2	1:F:51:LYS:HZ3	0.96	0.94
1:E:400:GLU:OE2	1:F:51:LYS:HE2	1.65	0.94
1:E:141:ASN:HD22	1:E:141:ASN:H	1.14	0.94
1:L:145:GLN:HG3	1:L:150:GLN:H	1.24	0.94
1:E:59:THR:HG23	1:F:321:GLU:OE1	1.67	0.94
1:K:139:ALA:CA	1:K:152:PRO:HB3	1.97	0.94
2:O:28:LYS:CG	2:P:113:VAL:CG1	2.41	0.94
1:E:441:PHE:O	1:F:329:ARG:CD	2.15	0.94
1:E:355:TYR:HE2	1:F:51:LYS:NZ	1.64	0.94
1:L:264:ARG:HG2	2:O:62:ARG:HH22	1.29	0.93
1:E:354:GLN:HA	1:F:44:LEU:HD22	1.46	0.93
1:E:408:TYR:OH	1:F:6:PRO:C	2.06	0.93
1:E:358:LEU:HG	1:F:40:LEU:HD11	1.47	0.93
2:M:135:ALA:CB	2:P:154:ILE:HD11	1.96	0.93
1:E:91:TYR:CD1	1:F:90:GLY:O	2.22	0.93
1:F:145:GLN:CD	1:F:149:GLN:C	2.28	0.93
1:L:309:ALA:CB	2:O:66:MET:CG	2.47	0.92
1:L:145:GLN:HB3	1:L:149:GLN:CB	1.99	0.92
1:K:141:ASN:HD22	1:K:141:ASN:H	1.14	0.92
1:E:440:ARG:NE	1:F:316:SER:OG	2.02	0.92
1:E:354:GLN:NE2	1:F:47:GLU:O	2.02	0.92
1:L:145:GLN:CD	1:L:149:GLN:C	2.27	0.92
2:M:135:ALA:CA	2:P:154:ILE:CD1	2.45	0.92
1:F:145:GLN:HB3	1:F:149:GLN:CB	1.99	0.92
1:F:344:LEU:HD12	1:F:351:ILE:HD11	1.50	0.92
1:L:145:GLN:CG	1:L:149:GLN:C	2.35	0.92
1:L:344:LEU:HD12	1:L:351:ILE:HD11	1.50	0.92
1:L:145:GLN:CG	1:L:150:GLN:H	1.75	0.91
1:E:354:GLN:OE1	1:F:48:VAL:N	2.03	0.91
1:E:358:LEU:CA	1:F:40:LEU:HD21	1.99	0.91
1:E:92:VAL:HG13	1:F:91:TYR:O	1.70	0.91
1:E:122:ARG:CB	1:E:122:ARG:HD2	2.00	0.91
1:E:91:TYR:HB3	1:F:91:TYR:CA	2.00	0.91

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:235:ASN:ND2	1:E:235:ASN:H	1.67	0.91
1:K:122:ARG:CB	1:K:122:ARG:HD2	2.00	0.91
1:E:122:ARG:HA	1:E:122:ARG:HG3	1.53	0.91
2:M:37:LEU:HD21	2:M:57:PHE:HB3	1.52	0.91
1:F:145:GLN:CG	1:F:149:GLN:C	2.35	0.90
1:K:264:ARG:CD	2:P:62:ARG:HH21	1.84	0.90
1:K:27:VAL:HG13	1:K:70:LEU:HG	1.53	0.90
1:E:92:VAL:HG21	1:F:92:VAL:O	1.72	0.90
1:E:235:ASN:HD22	1:E:235:ASN:N	1.65	0.90
1:E:349:ALA:HB1	1:F:47:GLU:HG3	0.94	0.90
1:K:145:GLN:HB2	1:K:149:GLN:CA	2.01	0.90
1:E:145:GLN:CG	1:E:149:GLN:CB	2.50	0.90
1:F:145:GLN:NE2	1:F:145:GLN:O	2.05	0.90
1:K:235:ASN:ND2	1:K:235:ASN:H	1.67	0.90
1:K:122:ARG:HA	1:K:122:ARG:HG3	1.53	0.90
1:E:145:GLN:HB2	1:E:149:GLN:CA	2.01	0.90
2:O:37:LEU:HD21	2:O:57:PHE:HB3	1.52	0.90
1:E:91:TYR:CG	1:F:90:GLY:C	2.44	0.89
1:E:27:VAL:HG13	1:E:70:LEU:HG	1.53	0.89
1:E:358:LEU:HA	1:F:40:LEU:HD21	1.52	0.89
1:E:357:ALA:HB1	1:F:40:LEU:HD22	1.55	0.89
1:K:145:GLN:CG	1:K:149:GLN:CB	2.50	0.89
2:M:140:THR:HG22	2:M:142:LEU:H	1.37	0.89
2:O:140:THR:HG22	2:O:142:LEU:H	1.37	0.89
1:K:264:ARG:HD2	2:P:62:ARG:HH21	1.38	0.88
1:E:441:PHE:CB	1:F:56:ILE:CD1	2.51	0.88
1:L:145:GLN:NE2	1:L:145:GLN:O	2.05	0.88
1:K:293:LYS:HE3	1:L:296:MET:SD	2.13	0.88
1:L:311:GLN:NE2	2:O:68:GLN:O	2.05	0.88
1:L:264:ARG:HH11	2:O:62:ARG:CB	1.87	0.88
1:K:369:THR:HG22	1:K:372:GLY:H	1.39	0.88
2:O:28:LYS:HG3	2:P:113:VAL:HG11	0.88	0.88
2:P:2:THR:OG1	2:P:162:THR:HG21	1.74	0.88
1:E:442:ILE:O	1:F:329:ARG:HG2	1.73	0.88
2:P:140:THR:HG21	2:P:142:LEU:HG	1.54	0.88
1:F:312:ILE:CD1	2:M:62:ARG:HA	2.04	0.87
1:L:264:ARG:NH1	2:O:62:ARG:HD3	1.89	0.87
1:F:17:ILE:HD13	1:F:66:ILE:HG12	1.57	0.87
2:N:140:THR:HG21	2:N:142:LEU:HG	1.54	0.87
2:N:2:THR:OG1	2:N:162:THR:HG21	1.73	0.87
1:E:393:ARG:NH2	1:F:321:GLU:HG3	1.88	0.87
1:E:358:LEU:CD1	1:F:48:VAL:HG11	2.01	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:145:GLN:HE21	1:F:150:GLN:HA	1.39	0.87
1:E:145:GLN:HG3	1:E:149:GLN:HG3	1.57	0.87
2:M:154:ILE:HG21	2:P:131:ALA:CB	1.98	0.87
1:E:400:GLU:HG2	1:F:51:LYS:HG3	1.55	0.87
1:E:130:ARG:NE	1:E:225:LEU:HD11	1.90	0.87
1:F:145:GLN:HG3	1:F:150:GLN:H	1.23	0.86
1:K:265:GLY:O	2:P:87:MET:HE2	1.75	0.86
1:E:354:GLN:OE1	1:F:47:GLU:C	2.13	0.86
1:E:358:LEU:HD23	1:F:37:ARG:HA	1.54	0.86
1:L:264:ARG:HH11	2:O:62:ARG:HB3	1.38	0.86
2:N:72:VAL:O	2:N:76:VAL:HG23	1.76	0.86
1:L:145:GLN:HE21	1:L:150:GLN:HA	1.39	0.86
1:L:264:ARG:NH1	2:O:59:LEU:HA	1.90	0.86
1:E:141:ASN:H	1:E:141:ASN:ND2	1.72	0.86
1:E:369:THR:HG22	1:E:372:GLY:H	1.38	0.86
1:E:407:SER:CB	1:F:36:ARG:HH12	1.89	0.85
1:E:441:PHE:O	1:F:329:ARG:CG	2.24	0.85
1:F:264:ARG:NH2	2:M:62:ARG:CG	2.37	0.85
1:F:130:ARG:HG3	1:F:225:LEU:CD1	2.06	0.85
1:L:17:ILE:HD13	1:L:66:ILE:HG12	1.57	0.85
1:K:130:ARG:NE	1:K:225:LEU:HD11	1.90	0.85
1:K:145:GLN:HG3	1:K:149:GLN:HG3	1.57	0.85
1:E:130:ARG:HD3	1:E:225:LEU:CD1	2.07	0.85
1:E:264:ARG:HH12	2:N:63:LYS:NZ	1.75	0.85
1:E:357:ALA:CB	1:F:40:LEU:HD22	2.07	0.85
1:E:235:ASN:H	1:E:235:ASN:HD22	0.87	0.85
2:P:140:THR:HG22	2:P:142:LEU:H	1.42	0.85
1:E:358:LEU:N	1:F:40:LEU:HD21	1.91	0.85
1:K:141:ASN:H	1:K:141:ASN:ND2	1.72	0.85
1:K:235:ASN:HD22	1:K:235:ASN:H	0.87	0.84
1:K:130:ARG:HD3	1:K:225:LEU:CD1	2.07	0.84
2:P:72:VAL:O	2:P:76:VAL:HG23	1.76	0.84
1:L:264:ARG:HH11	2:O:62:ARG:CD	1.91	0.84
2:P:36:ARG:HB3	2:P:36:ARG:HH11	1.43	0.84
1:K:235:ASN:N	1:K:235:ASN:HD22	1.65	0.84
1:K:130:ARG:HD3	1:K:225:LEU:HD12	1.60	0.84
1:L:130:ARG:HG3	1:L:225:LEU:CD1	2.07	0.84
1:E:312:ILE:HD12	2:N:67:HIS:CE1	2.13	0.83
1:E:145:GLN:HG3	1:E:149:GLN:HB2	1.51	0.83
1:F:145:GLN:HG3	1:F:149:GLN:N	1.92	0.83
2:N:134:ARG:HB3	2:N:134:ARG:HH11	1.43	0.83
1:L:145:GLN:HG3	1:L:149:GLN:N	1.93	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:N:140:THR:HG22	2:N:142:LEU:H	1.42	0.83
1:E:130:ARG:CD	1:E:225:LEU:CD1	2.57	0.83
2:P:134:ARG:HH11	2:P:134:ARG:HB3	1.43	0.83
1:K:109:LYS:HG3	1:L:298:LYS:HD2	1.59	0.83
1:E:442:ILE:O	1:F:329:ARG:CG	2.25	0.82
1:L:264:ARG:HG2	2:O:62:ARG:HH21	1.23	0.82
1:E:408:TYR:HH	1:F:7:ARG:HA	1.44	0.82
1:K:130:ARG:CD	1:K:225:LEU:CD1	2.57	0.82
1:F:145:GLN:CG	1:F:150:GLN:H	1.75	0.82
1:E:408:TYR:HA	1:F:6:PRO:HG2	1.59	0.82
1:F:145:GLN:CD	1:F:150:GLN:N	2.33	0.82
1:E:355:TYR:CE2	1:F:51:LYS:NZ	2.46	0.82
1:L:264:ARG:CD	2:O:62:ARG:CD	2.51	0.82
1:F:132:LEU:CD1	1:F:160:ARG:HB3	2.09	0.82
1:E:354:GLN:NE2	1:F:47:GLU:CA	2.41	0.82
1:E:407:SER:HA	1:F:36:ARG:HH12	0.65	0.82
2:N:36:ARG:HB3	2:N:36:ARG:HH11	1.43	0.82
1:E:441:PHE:O	1:F:329:ARG:HB3	1.80	0.82
2:P:139:ASN:HD22	2:P:139:ASN:N	1.78	0.82
1:K:293:LYS:CE	1:L:296:MET:CE	2.53	0.82
1:K:408:TYR:CZ	1:L:7:ARG:NH2	2.42	0.81
1:L:132:LEU:CD1	1:L:160:ARG:HB3	2.09	0.81
2:O:51:ALA:HB2	2:P:110:GLY:HA3	1.61	0.81
1:E:384:ASN:ND2	1:E:394:ARG:HD2	1.95	0.81
1:L:264:ARG:HD3	2:O:62:ARG:HH21	1.44	0.81
1:E:400:GLU:CG	1:F:51:LYS:HG3	2.10	0.81
2:M:36:ARG:HD3	2:M:40:ASP:OD1	1.80	0.81
1:E:130:ARG:HD3	1:E:225:LEU:HD12	1.60	0.81
2:O:36:ARG:HD3	2:O:40:ASP:OD1	1.80	0.81
1:E:354:GLN:HE21	1:F:47:GLU:HB3	0.91	0.81
1:K:311:GLN:CG	2:P:66:MET:HE2	2.01	0.81
1:F:59:THR:HG22	1:F:393:ARG:HH12	1.43	0.81
2:M:135:ALA:HB2	2:P:154:ILE:HD12	1.60	0.81
2:P:67:HIS:HD2	2:P:73:LYS:HE3	1.44	0.81
2:M:135:ALA:HB2	2:P:154:ILE:HD13	0.83	0.81
2:N:67:HIS:HD2	2:N:73:LYS:HE3	1.44	0.81
1:L:145:GLN:CD	1:L:150:GLN:N	2.33	0.81
1:E:92:VAL:CG1	1:F:92:VAL:HG12	2.12	0.80
2:N:139:ASN:N	2:N:139:ASN:HD22	1.78	0.80
1:E:357:ALA:CB	1:F:44:LEU:HD12	2.07	0.80
1:K:384:ASN:ND2	1:K:394:ARG:HD2	1.95	0.80
1:F:136:ILE:HG22	1:F:138:PRO:HD3	1.64	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:N:140:THR:CG2	2:N:142:LEU:HG	2.12	0.80
1:E:358:LEU:CD2	1:F:37:ARG:CA	2.60	0.80
1:L:136:ILE:HG22	1:L:138:PRO:HD3	1.64	0.80
1:L:141:ASN:H	1:L:141:ASN:HD22	1.30	0.80
1:L:59:THR:HG22	1:L:393:ARG:HH12	1.43	0.80
1:E:358:LEU:CG	1:F:40:LEU:HD11	2.11	0.80
1:E:357:ALA:HB2	1:F:44:LEU:HD13	1.15	0.79
1:E:83:ALA:HB1	1:E:261:ILE:HD12	1.64	0.79
2:M:131:ALA:O	2:P:154:ILE:HG21	1.83	0.79
1:F:312:ILE:HD11	2:M:62:ARG:CA	2.09	0.79
2:P:140:THR:CG2	2:P:142:LEU:HG	2.12	0.79
1:K:138:PRO:HG3	1:K:156:ARG:HD3	1.63	0.79
1:F:145:GLN:CG	1:F:149:GLN:CB	2.61	0.79
2:M:160:ILE:HD13	2:O:160:ILE:HG23	1.64	0.79
1:K:293:LYS:HE3	1:L:296:MET:HE1	1.63	0.79
2:M:1:THR:HB	2:M:33:LYS:HZ3	1.48	0.79
2:M:139:ASN:OD1	2:P:150:LYS:HD3	1.82	0.79
1:L:145:GLN:CG	1:L:149:GLN:CB	2.61	0.78
1:E:138:PRO:HG3	1:E:156:ARG:HD3	1.63	0.78
1:K:120:ARG:NH1	1:K:124:GLU:OE2	2.16	0.78
1:L:311:GLN:NE2	2:O:68:GLN:C	2.37	0.78
1:K:83:ALA:HB1	1:K:261:ILE:HD12	1.64	0.78
1:E:400:GLU:CD	1:F:51:LYS:HG3	2.02	0.78
1:F:217:LYS:HB3	1:F:220:ASP:HB3	1.66	0.78
1:F:141:ASN:HD22	1:F:141:ASN:H	1.30	0.78
1:L:89:VAL:CG1	1:L:94:LYS:O	2.32	0.78
1:L:264:ARG:HD3	2:O:62:ARG:HD3	1.62	0.78
1:F:369:THR:HG22	1:F:372:GLY:N	1.98	0.78
1:E:120:ARG:NH1	1:E:124:GLU:OE2	2.16	0.78
1:F:89:VAL:CG1	1:F:94:LYS:O	2.32	0.78
1:L:369:THR:HG22	1:L:372:GLY:N	1.98	0.78
1:L:217:LYS:HB3	1:L:220:ASP:HB3	1.66	0.77
1:E:130:ARG:CD	1:E:225:LEU:HD11	2.15	0.77
1:K:130:ARG:CD	1:K:225:LEU:HD11	2.15	0.77
1:E:354:GLN:CD	1:F:47:GLU:HB3	2.05	0.77
1:F:264:ARG:HH12	2:M:62:ARG:CA	1.96	0.77
1:E:89:VAL:HG12	1:E:94:LYS:H	1.48	0.77
1:E:441:PHE:HA	1:F:315:PRO:CG	2.13	0.77
1:E:407:SER:CB	1:F:36:ARG:NH1	2.47	0.77
1:E:389:ASN:C	1:E:389:ASN:HD22	1.88	0.77
1:E:397:THR:HG21	1:E:443:LEU:O	1.84	0.77
1:E:314:LYS:HZ1	2:N:65:GLU:CG	1.95	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:91:TYR:CE1	1:L:272:VAL:HG11	2.20	0.77
1:K:5:THR:OG1	1:K:8:GLU:HG3	1.85	0.77
1:K:89:VAL:HG12	1:K:94:LYS:H	1.48	0.77
1:E:94:LYS:HD2	1:E:95:GLU:H	1.50	0.77
1:E:5:THR:OG1	1:E:8:GLU:HG3	1.85	0.77
1:E:92:VAL:CB	1:F:92:VAL:HA	2.15	0.76
1:F:160:ARG:O	1:F:163:LEU:HG	1.85	0.76
1:L:145:GLN:HG2	1:L:150:GLN:N	1.99	0.76
1:F:311:GLN:CG	2:M:66:MET:CE	2.59	0.76
1:L:130:ARG:HG3	1:L:225:LEU:HD11	1.66	0.76
2:O:1:THR:HB	2:O:33:LYS:HZ3	1.48	0.76
1:F:27:VAL:HG13	1:F:70:LEU:HG	1.67	0.76
1:L:311:GLN:HE21	2:O:67:HIS:H	1.33	0.76
1:E:361:THR:HG21	1:F:36:ARG:CA	2.14	0.76
1:K:94:LYS:HD2	1:K:95:GLU:H	1.50	0.76
2:N:32:LYS:HG2	2:N:167:THR:HG21	1.67	0.76
1:L:27:VAL:HG13	1:L:70:LEU:HG	1.67	0.76
1:L:145:GLN:CG	1:L:149:GLN:CA	2.64	0.76
1:E:257:GLU:OE1	1:F:279:ARG:HG3	1.83	0.76
1:E:92:VAL:CG2	1:F:92:VAL:HA	2.15	0.76
1:E:264:ARG:NH1	2:N:63:LYS:HZ3	1.83	0.76
1:L:160:ARG:O	1:L:163:LEU:HG	1.85	0.76
1:K:397:THR:HG21	1:K:443:LEU:O	1.84	0.76
1:E:92:VAL:HG13	1:F:92:VAL:HA	1.63	0.76
1:K:91:TYR:CE1	1:L:272:VAL:CG1	2.68	0.76
1:K:389:ASN:HD22	1:K:389:ASN:C	1.88	0.76
1:E:397:THR:HG23	1:F:327:PRO:O	1.86	0.75
2:P:105:ILE:HD11	2:P:120:ILE:HG23	1.69	0.75
1:E:311:GLN:CG	2:N:66:MET:C	2.42	0.75
1:E:141:ASN:HD22	1:E:141:ASN:N	1.79	0.75
1:F:145:GLN:NE2	1:F:150:GLN:CA	2.49	0.75
1:L:145:GLN:NE2	1:L:150:GLN:CA	2.49	0.75
1:E:358:LEU:O	1:E:361:THR:HG22	1.87	0.75
1:K:389:ASN:ND2	1:K:391:GLY:H	1.85	0.75
1:F:20:GLN:HG2	1:F:332:LEU:HD23	1.68	0.75
1:K:92:VAL:HG23	1:K:93:GLY:N	2.02	0.75
1:E:389:ASN:ND2	1:E:391:GLY:H	1.85	0.74
1:K:261:ILE:HG22	1:K:261:ILE:O	1.86	0.74
1:L:20:GLN:HG2	1:L:332:LEU:HD23	1.68	0.74
1:F:132:LEU:HD13	1:F:156:ARG:CG	2.17	0.74
2:P:32:LYS:HG2	2:P:167:THR:HG21	1.68	0.74
1:L:264:ARG:HH12	2:O:62:ARG:HB3	1.50	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:130:ARG:HG3	1:F:225:LEU:HD11	1.66	0.74
1:F:264:ARG:HH12	2:M:62:ARG:HB2	1.28	0.74
1:L:311:GLN:CA	2:O:65:GLU:OE1	2.31	0.74
1:K:358:LEU:O	1:K:361:THR:HG22	1.87	0.74
1:E:163:LEU:CD1	1:E:218:ILE:HG21	2.18	0.74
2:N:105:ILE:HD11	2:N:120:ILE:HG23	1.69	0.74
1:E:92:VAL:HG23	1:E:93:GLY:N	2.02	0.74
1:L:145:GLN:OE1	1:L:149:GLN:CB	2.36	0.74
1:E:441:PHE:CE1	1:F:310:PHE:HB2	2.23	0.74
1:E:266:GLU:HA	2:N:85:ASP:OD1	1.88	0.73
1:E:118:LYS:NZ	1:E:118:LYS:HA	2.03	0.73
1:F:344:LEU:CD1	1:F:395:LEU:HD13	2.17	0.73
1:F:132:LEU:CD1	1:F:156:ARG:HG2	2.17	0.73
1:E:59:THR:HG21	1:F:320:PRO:HB2	1.70	0.73
1:L:264:ARG:CD	2:O:62:ARG:NH2	2.42	0.73
1:L:344:LEU:CD1	1:L:395:LEU:HD13	2.17	0.73
1:E:261:ILE:O	1:E:261:ILE:HG22	1.86	0.73
1:E:120:ARG:C	1:E:120:ARG:CD	2.56	0.73
1:F:258:ILE:HG13	1:F:306:ALA:HB1	1.70	0.73
1:E:393:ARG:HH21	1:F:321:GLU:HG3	1.51	0.73
1:E:358:LEU:HD21	1:F:37:ARG:HA	1.69	0.73
1:F:145:GLN:OE1	1:F:149:GLN:CB	2.36	0.73
1:L:309:ALA:HB3	2:O:66:MET:SD	1.12	0.73
1:E:357:ALA:O	1:F:40:LEU:HD23	1.83	0.73
1:L:132:LEU:CD1	1:L:156:ARG:HG2	2.17	0.73
1:L:264:ARG:HH11	2:O:62:ARG:HD3	1.50	0.73
1:L:258:ILE:HG13	1:L:306:ALA:HB1	1.70	0.73
1:E:442:ILE:HD13	1:F:329:ARG:HB3	1.71	0.73
1:L:309:ALA:CB	2:O:66:MET:CE	2.16	0.73
1:K:163:LEU:CD1	1:K:218:ILE:HG21	2.18	0.73
1:E:400:GLU:CD	1:F:51:LYS:NZ	2.41	0.73
1:E:235:ASN:HB2	1:E:238:GLU:OE2	1.89	0.73
2:O:50:THR:HG21	2:P:111:ASP:OD1	1.89	0.73
1:E:411:SER:HB3	1:F:32:ARG:NH2	2.03	0.73
1:E:88:GLU:HG2	1:F:89:VAL:O	1.89	0.73
1:K:141:ASN:N	1:K:141:ASN:HD22	1.79	0.72
1:E:374:LYS:HE2	1:E:378:GLU:OE2	1.89	0.72
1:E:135:LEU:HD13	1:E:159:PHE:CE1	2.24	0.72
1:F:264:ARG:NE	2:M:62:ARG:HD2	2.02	0.72
1:K:374:LYS:HE2	1:K:378:GLU:OE2	1.89	0.72
1:E:409:ASP:O	1:E:413:LEU:HD13	1.89	0.72
1:E:312:ILE:HD12	2:N:67:HIS:HE1	1.50	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:408:TYR:CA	1:F:6:PRO:HG2	2.19	0.72
1:K:235:ASN:HB2	1:K:238:GLU:OE2	1.89	0.72
1:K:409:ASP:O	1:K:413:LEU:HD13	1.90	0.72
1:E:441:PHE:O	1:F:329:ARG:CB	2.37	0.72
1:E:354:GLN:CD	1:F:47:GLU:CB	2.57	0.72
1:F:145:GLN:CG	1:F:149:GLN:CA	2.64	0.72
1:L:132:LEU:HD13	1:L:156:ARG:CG	2.17	0.72
1:K:120:ARG:C	1:K:120:ARG:CD	2.56	0.72
1:E:139:ALA:HB2	1:E:152:PRO:CD	2.19	0.72
1:L:264:ARG:NH2	2:O:59:LEU:HD21	1.98	0.72
2:N:36:ARG:C	2:N:37:LEU:HD12	2.10	0.72
1:L:264:ARG:NH1	2:O:59:LEU:CA	2.52	0.72
1:E:353:VAL:HG12	1:F:44:LEU:HD21	1.70	0.72
1:F:33:ASN:ND2	1:F:36:ARG:HD2	2.05	0.72
2:P:36:ARG:C	2:P:37:LEU:HD12	2.10	0.72
2:P:134:ARG:O	2:P:138:GLU:HB2	1.90	0.72
1:L:311:GLN:HG2	2:O:66:MET:HE1	1.71	0.72
1:K:130:ARG:CD	1:K:225:LEU:HD12	2.19	0.72
1:F:381:TRP:CH2	1:F:385:GLU:OE2	2.43	0.72
1:K:118:LYS:HA	1:K:118:LYS:NZ	2.03	0.72
1:L:358:LEU:O	1:L:361:THR:HB	1.90	0.72
2:N:3:ILE:HB	2:N:122:ILE:CG1	2.20	0.72
1:E:130:ARG:CD	1:E:225:LEU:HD12	2.20	0.72
1:L:381:TRP:CH2	1:L:385:GLU:OE2	2.43	0.72
1:K:245:ASP:O	1:K:249:GLN:HG3	1.89	0.72
1:K:135:LEU:HD13	1:K:159:PHE:CE1	2.24	0.72
1:L:264:ARG:CZ	2:O:59:LEU:CB	2.42	0.71
1:E:245:ASP:O	1:E:249:GLN:HG3	1.89	0.71
1:F:358:LEU:O	1:F:361:THR:HB	1.90	0.71
1:E:142:ASN:O	1:E:143:TRP:HB2	1.89	0.71
1:E:292:THR:HB	1:E:295:GLY:O	1.90	0.71
2:M:138:GLU:C	2:M:139:ASN:HD22	1.94	0.71
1:E:397:THR:HA	1:F:327:PRO:CB	2.19	0.71
2:M:140:THR:CG2	2:M:142:LEU:H	2.03	0.71
2:O:54:PHE:HE2	2:P:80:LYS:CD	2.03	0.71
1:E:279:ARG:HH11	1:E:319:ILE:HD12	1.55	0.71
1:K:142:ASN:O	1:K:143:TRP:HB2	1.89	0.71
1:F:145:GLN:OE1	1:F:149:GLN:HB3	1.90	0.71
1:L:142:ASN:O	1:L:143:TRP:HB2	1.90	0.71
1:L:384:ASN:ND2	1:L:394:ARG:HD2	2.06	0.71
1:E:357:ALA:CA	1:F:40:LEU:HD22	2.21	0.71
1:K:292:THR:HB	1:K:295:GLY:O	1.91	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:1:THR:HB	2:M:33:LYS:NZ	2.05	0.71
2:N:138:GLU:C	2:N:139:ASN:HD22	1.94	0.71
2:P:5:SER:HB3	2:P:120:ILE:HB	1.72	0.71
1:L:344:LEU:O	1:L:352:THR:HB	1.91	0.71
1:E:139:ALA:HB3	1:E:152:PRO:HG3	1.70	0.71
1:K:139:ALA:HB2	1:K:152:PRO:CD	2.19	0.71
1:F:145:GLN:HG2	1:F:150:GLN:N	1.99	0.71
1:K:279:ARG:HH11	1:K:319:ILE:HD12	1.55	0.71
1:F:389:ASN:ND2	1:F:391:GLY:H	1.88	0.71
1:L:264:ARG:C	1:L:266:GLU:H	1.94	0.70
1:L:264:ARG:CZ	2:O:59:LEU:CA	2.69	0.70
1:E:91:TYR:HB3	1:F:91:TYR:C	2.11	0.70
2:P:3:ILE:HB	2:P:122:ILE:CG1	2.20	0.70
1:E:407:SER:OG	1:F:36:ARG:NH1	2.24	0.70
1:L:33:ASN:ND2	1:L:36:ARG:HD2	2.05	0.70
1:K:264:ARG:CD	2:P:62:ARG:NH2	2.50	0.70
1:F:142:ASN:O	1:F:143:TRP:HB2	1.90	0.70
1:F:384:ASN:ND2	1:F:394:ARG:HD2	2.06	0.70
2:M:140:THR:CG2	2:M:142:LEU:HG	2.21	0.70
2:O:140:THR:CG2	2:O:142:LEU:H	2.03	0.70
2:N:5:SER:HB3	2:N:120:ILE:HB	1.72	0.70
1:F:429:LEU:O	1:F:433:VAL:HG23	1.92	0.70
2:O:1:THR:HB	2:O:33:LYS:NZ	2.05	0.70
2:O:140:THR:CG2	2:O:142:LEU:HG	2.21	0.70
1:L:389:ASN:ND2	1:L:391:GLY:H	1.88	0.70
1:K:265:GLY:O	2:P:87:MET:HE3	1.88	0.70
2:N:134:ARG:O	2:N:138:GLU:HB2	1.90	0.70
1:E:441:PHE:CE1	1:F:56:ILE:HG21	2.27	0.70
1:E:411:SER:CB	1:F:32:ARG:NH2	2.54	0.70
1:F:344:LEU:O	1:F:352:THR:HB	1.91	0.70
2:O:138:GLU:C	2:O:139:ASN:HD22	1.94	0.70
1:F:261:ILE:HG22	1:F:278:GLN:HG3	1.74	0.70
1:L:145:GLN:OE1	1:L:149:GLN:HB3	1.90	0.70
2:N:67:HIS:CD2	2:N:73:LYS:HE3	2.27	0.70
1:F:263:LYS:O	1:F:264:ARG:HB3	1.92	0.70
1:E:282:LEU:HD11	1:E:319:ILE:HD11	1.74	0.70
1:K:261:ILE:HD13	1:K:277:VAL:HB	1.74	0.70
1:F:141:ASN:ND2	1:F:141:ASN:H	1.88	0.70
1:L:264:ARG:CZ	2:O:59:LEU:HA	2.22	0.70
1:E:411:SER:OG	1:F:32:ARG:NH2	2.25	0.70
1:K:282:LEU:HD11	1:K:319:ILE:HD11	1.74	0.70
1:E:33:ASN:ND2	1:E:36:ARG:HD2	2.07	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:139:ALA:O	1:K:140:LYS:CB	2.38	0.69
1:E:92:VAL:CG2	1:E:93:GLY:N	2.55	0.69
1:K:92:VAL:CG2	1:K:93:GLY:N	2.55	0.69
1:L:141:ASN:H	1:L:141:ASN:ND2	1.88	0.69
1:E:139:ALA:O	1:E:140:LYS:CB	2.38	0.69
1:E:139:ALA:HA	1:E:152:PRO:HB3	1.74	0.69
2:M:160:ILE:HD11	2:O:160:ILE:O	1.92	0.69
1:E:440:ARG:CD	1:F:316:SER:OG	2.39	0.69
1:E:222:MET:O	1:E:226:ILE:HG13	1.93	0.69
2:N:85:ASP:HB2	2:N:88:LEU:HD23	1.73	0.69
2:O:54:PHE:HE2	2:P:80:LYS:HG3	1.57	0.69
1:K:222:MET:O	1:K:226:ILE:HG13	1.93	0.69
1:L:92:VAL:HG23	1:L:93:GLY:N	2.08	0.69
2:O:79:ALA:HB1	2:O:110:GLY:HA2	1.74	0.69
2:P:33:LYS:HA	2:P:46:PHE:CE1	2.27	0.69
2:M:79:ALA:HB1	2:M:110:GLY:HA2	1.74	0.69
1:E:311:GLN:CB	2:N:66:MET:C	2.57	0.69
1:K:92:VAL:CG1	1:L:89:VAL:O	2.40	0.69
1:E:359:MET:HE1	1:F:36:ARG:HD3	1.74	0.69
1:F:92:VAL:HG23	1:F:93:GLY:N	2.08	0.69
1:E:432:LEU:HD12	1:E:432:LEU:H	1.56	0.69
1:L:145:GLN:OE1	1:L:145:GLN:N	2.12	0.69
2:P:138:GLU:C	2:P:139:ASN:HD22	1.94	0.69
1:K:139:ALA:HB3	1:K:152:PRO:HG3	1.70	0.68
2:O:20:ALA:HB2	2:O:31:VAL:HG21	1.75	0.68
1:K:389:ASN:HD22	1:K:390:ILE:N	1.91	0.68
2:N:33:LYS:HA	2:N:46:PHE:CE1	2.27	0.68
1:K:432:LEU:H	1:K:432:LEU:HD12	1.56	0.68
1:F:89:VAL:HG11	1:F:94:LYS:O	1.92	0.68
1:E:27:VAL:CG1	1:E:70:LEU:HG	2.23	0.68
2:M:160:ILE:CG2	2:O:160:ILE:CD1	2.71	0.68
2:N:3:ILE:HD12	2:N:122:ILE:HD11	1.76	0.68
2:P:85:ASP:HB2	2:P:88:LEU:HD23	1.73	0.68
1:L:261:ILE:HG22	1:L:278:GLN:HG3	1.74	0.68
2:P:67:HIS:CD2	2:P:73:LYS:HE3	2.27	0.68
1:K:104:THR:HG21	1:K:292:THR:HG21	1.75	0.68
1:F:142:ASN:O	1:F:143:TRP:CB	2.42	0.68
1:L:429:LEU:O	1:L:433:VAL:HG23	1.92	0.68
1:E:267:SER:HB3	1:E:270:PRO:HG3	1.75	0.68
1:K:33:ASN:HD22	1:K:36:ARG:HD2	1.58	0.68
1:K:33:ASN:ND2	1:K:36:ARG:HD2	2.07	0.68
1:F:311:GLN:CG	2:M:66:MET:HE3	2.21	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:160:ILE:HG23	2:O:160:ILE:HD11	1.75	0.68
2:M:20:ALA:HB2	2:M:31:VAL:HG21	1.75	0.68
1:E:163:LEU:HD11	1:E:218:ILE:CG2	2.21	0.68
1:F:264:ARG:C	1:F:266:GLU:H	1.94	0.68
1:K:27:VAL:CG1	1:K:70:LEU:HG	2.23	0.68
1:E:261:ILE:HD13	1:E:277:VAL:HB	1.74	0.68
1:L:89:VAL:HG11	1:L:94:LYS:O	1.92	0.68
1:E:104:THR:HG21	1:E:292:THR:HG21	1.75	0.68
1:F:27:VAL:HG22	1:F:70:LEU:HD12	1.76	0.68
1:E:389:ASN:HD22	1:E:390:ILE:N	1.91	0.68
1:E:441:PHE:CA	1:F:315:PRO:HG2	2.17	0.68
2:M:160:ILE:HG23	2:O:160:ILE:CD1	2.23	0.68
2:P:3:ILE:HD12	2:P:122:ILE:HD11	1.76	0.68
1:F:229:GLU:HA	1:F:232:LYS:HG2	1.76	0.68
1:F:292:THR:HG22	1:F:294:HIS:N	2.03	0.68
1:L:292:THR:HG22	1:L:294:HIS:N	2.03	0.68
1:K:139:ALA:HA	1:K:152:PRO:HB3	1.74	0.67
1:F:336:THR:O	1:F:339:ASP:HB2	1.95	0.67
1:K:267:SER:HB3	1:K:270:PRO:HG3	1.75	0.67
1:L:311:GLN:HE21	2:O:68:GLN:N	1.92	0.67
1:L:229:GLU:HA	1:L:232:LYS:HG2	1.76	0.67
1:E:132:LEU:HD12	1:E:156:ARG:HG2	1.76	0.67
1:L:263:LYS:O	1:L:264:ARG:HB3	1.92	0.67
2:M:160:ILE:HG21	2:O:160:ILE:HD13	1.77	0.67
1:L:27:VAL:HG22	1:L:70:LEU:HD12	1.76	0.67
1:K:88:GLU:OE2	1:L:280:ASP:CG	2.33	0.67
1:E:311:GLN:NE2	2:N:66:MET:O	2.26	0.67
2:N:134:ARG:CB	2:N:134:ARG:HH11	2.07	0.67
2:P:134:ARG:HH11	2:P:134:ARG:CB	2.07	0.67
1:L:59:THR:HG22	1:L:393:ARG:NH1	2.10	0.67
1:E:33:ASN:HD22	1:E:36:ARG:HD2	1.58	0.67
1:K:163:LEU:HD11	1:K:218:ILE:CG2	2.21	0.67
1:F:319:ILE:HG22	1:F:322:LEU:HB2	1.77	0.67
1:E:400:GLU:CG	1:F:51:LYS:CG	2.72	0.67
1:F:130:ARG:HG3	1:F:225:LEU:HD12	1.77	0.67
1:L:264:ARG:NH1	2:O:62:ARG:CB	2.45	0.67
1:L:264:ARG:NH2	2:O:59:LEU:HD22	2.00	0.67
1:F:125:GLU:O	1:F:128:GLU:HG2	1.95	0.67
2:P:94:LEU:HD13	2:P:122:ILE:HB	1.77	0.67
2:O:72:VAL:O	2:O:76:VAL:HG23	1.95	0.67
1:L:336:THR:O	1:L:339:ASP:HB2	1.95	0.67
1:E:397:THR:OG1	1:F:327:PRO:HA	1.95	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:131:ALA:O	2:P:154:ILE:CG2	2.43	0.67
1:E:404:GLU:HG2	1:F:29:ILE:HD12	1.76	0.67
1:L:141:ASN:HD22	1:L:141:ASN:N	1.92	0.67
1:L:389:ASN:C	1:L:389:ASN:HD22	1.98	0.67
2:N:100:GLU:HG2	2:N:173:TYR:CD2	2.30	0.67
1:L:130:ARG:HD2	1:L:130:ARG:C	2.15	0.66
2:P:17:ASP:HA	2:P:165:PHE:O	1.95	0.66
1:E:440:ARG:O	1:F:315:PRO:CG	2.42	0.66
1:K:120:ARG:C	1:K:120:ARG:HD2	2.16	0.66
1:E:397:THR:HA	1:F:327:PRO:CA	2.25	0.66
1:E:88:GLU:CG	1:F:89:VAL:O	2.44	0.66
1:F:130:ARG:HD2	1:F:130:ARG:C	2.15	0.66
2:M:152:LEU:HD22	2:M:166:HIS:CE1	2.31	0.66
1:E:91:TYR:CE2	1:F:90:GLY:O	2.47	0.66
1:L:125:GLU:O	1:L:128:GLU:HG2	1.95	0.66
2:N:17:ASP:HA	2:N:165:PHE:O	1.95	0.66
1:L:319:ILE:HG22	1:L:322:LEU:HB2	1.77	0.66
1:K:132:LEU:HD12	1:K:156:ARG:HG2	1.76	0.66
2:O:140:THR:HG21	2:O:142:LEU:HG	1.78	0.66
1:L:142:ASN:O	1:L:143:TRP:CB	2.42	0.66
1:F:389:ASN:HD22	1:F:389:ASN:C	1.98	0.66
1:L:130:ARG:HG3	1:L:225:LEU:HD12	1.78	0.66
2:P:100:GLU:HG2	2:P:173:TYR:CD2	2.30	0.66
1:E:441:PHE:CD1	1:F:56:ILE:CG2	2.77	0.66
2:N:61:GLU:O	2:N:65:GLU:HG2	1.95	0.66
2:P:61:GLU:O	2:P:65:GLU:HG2	1.95	0.66
1:L:311:GLN:HG2	2:O:66:MET:CE	2.26	0.65
1:F:145:GLN:N	1:F:145:GLN:OE1	2.12	0.65
2:P:58:GLU:O	2:P:62:ARG:HG3	1.96	0.65
1:L:92:VAL:CG2	1:L:93:GLY:N	2.59	0.65
1:K:96:VAL:HG13	1:K:99:ILE:HD12	1.78	0.65
1:L:311:GLN:HA	2:O:65:GLU:OE1	1.96	0.65
1:F:362:GLU:HG3	1:F:411:SER:HA	1.78	0.65
1:E:20:GLN:HG3	1:E:332:LEU:HD23	1.78	0.65
1:E:359:MET:HE3	1:F:36:ARG:HH11	1.61	0.65
2:N:58:GLU:O	2:N:62:ARG:HG3	1.96	0.65
1:K:293:LYS:CE	1:L:296:MET:SD	2.83	0.65
1:K:20:GLN:HG3	1:K:332:LEU:HD23	1.78	0.65
1:E:393:ARG:HD3	1:F:321:GLU:HA	1.79	0.65
1:E:59:THR:CG2	1:F:321:GLU:OE1	2.43	0.65
2:O:152:LEU:HD22	2:O:166:HIS:CE1	2.31	0.65
1:L:362:GLU:HG3	1:L:411:SER:HA	1.78	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:126:LEU:HD23	1:K:229:GLU:CD	2.17	0.65
1:F:96:VAL:HG13	1:F:99:ILE:HD12	1.78	0.65
1:K:138:PRO:CG	1:K:156:ARG:HD3	2.26	0.65
1:F:92:VAL:CG2	1:F:93:GLY:N	2.59	0.65
1:E:120:ARG:HD2	1:E:120:ARG:C	2.16	0.65
2:N:94:LEU:HD13	2:N:122:ILE:HB	1.77	0.65
1:L:96:VAL:HG13	1:L:99:ILE:HD12	1.77	0.65
2:M:72:VAL:O	2:M:76:VAL:HG23	1.96	0.65
1:F:59:THR:HG22	1:F:393:ARG:NH1	2.10	0.65
1:E:79:ILE:HD13	1:E:80:LYS:N	2.12	0.65
2:M:140:THR:HG21	2:M:142:LEU:HG	1.78	0.65
1:E:96:VAL:HG13	1:E:99:ILE:HD12	1.78	0.65
1:K:79:ILE:HD13	1:K:80:LYS:N	2.12	0.65
2:M:14:ILE:HD12	2:M:43:ILE:HG13	1.78	0.65
1:E:126:LEU:HD23	1:E:229:GLU:CD	2.17	0.65
2:N:28:LYS:HE2	2:N:30:ASN:OD1	1.97	0.64
1:E:138:PRO:CG	1:E:156:ARG:HD3	2.26	0.64
1:E:354:GLN:HB3	1:F:48:VAL:CG2	2.24	0.64
1:L:145:GLN:CB	1:L:149:GLN:CB	2.62	0.64
1:E:122:ARG:C	1:E:122:ARG:CG	2.66	0.64
1:K:92:VAL:HG11	1:L:89:VAL:HB	1.80	0.64
2:O:14:ILE:HD12	2:O:43:ILE:HG13	1.78	0.64
1:F:292:THR:HB	1:F:295:GLY:O	1.98	0.64
1:E:354:GLN:HE22	1:F:47:GLU:C	1.87	0.64
1:L:141:ASN:O	1:L:142:ASN:HB2	1.98	0.64
1:L:381:TRP:CZ3	1:L:385:GLU:OE2	2.50	0.64
1:E:63:LYS:HG2	1:E:332:LEU:HD22	1.80	0.64
1:K:122:ARG:CG	1:K:122:ARG:C	2.66	0.64
1:E:91:TYR:HB3	1:F:91:TYR:N	2.11	0.64
1:K:86:PHE:O	1:K:89:VAL:HG13	1.98	0.64
1:K:243:ALA:O	1:K:247:VAL:HG23	1.97	0.64
1:L:344:LEU:CD1	1:L:351:ILE:HD11	2.25	0.64
1:E:401:ARG:NH2	1:F:329:ARG:H	1.95	0.64
2:N:138:GLU:HB3	2:N:139:ASN:ND2	2.12	0.64
1:F:381:TRP:CZ3	1:F:385:GLU:OE2	2.50	0.64
1:E:359:MET:HG3	1:E:366:ILE:HG13	1.80	0.63
1:E:311:GLN:HG2	2:N:66:MET:SD	2.21	0.63
2:P:138:GLU:HB3	2:P:139:ASN:ND2	2.12	0.63
1:K:436:GLU:O	1:K:439:SER:HB2	1.98	0.63
1:F:130:ARG:C	1:F:130:ARG:HH11	2.01	0.63
1:K:63:LYS:HG2	1:K:332:LEU:HD22	1.80	0.63
1:E:442:ILE:CB	1:F:329:ARG:HB2	2.29	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:313:ALA:N	2:O:65:GLU:HG3	2.13	0.63
1:E:358:LEU:CD2	1:F:40:LEU:HD11	2.29	0.63
1:E:243:ALA:O	1:E:247:VAL:HG23	1.97	0.63
1:K:359:MET:HG3	1:K:366:ILE:HG13	1.80	0.63
1:E:145:GLN:H	1:E:149:GLN:HB2	1.63	0.63
1:F:108:VAL:HG21	1:F:294:HIS:ND1	2.13	0.63
1:F:163:LEU:HD13	1:F:218:ILE:HG21	1.80	0.63
1:E:308:GLY:HA3	1:E:310:PHE:CE2	2.33	0.63
1:L:108:VAL:HG21	1:L:294:HIS:ND1	2.13	0.63
1:E:390:ILE:HA	1:F:320:PRO:HB3	1.79	0.63
1:K:145:GLN:CG	1:K:149:GLN:CG	2.67	0.63
1:F:145:GLN:CB	1:F:149:GLN:CB	2.62	0.63
1:E:83:ALA:HB1	1:E:261:ILE:CD1	2.29	0.63
1:K:83:ALA:HB1	1:K:261:ILE:CD1	2.29	0.63
1:K:432:LEU:H	1:K:432:LEU:CD1	2.12	0.63
1:E:91:TYR:CE2	1:F:91:TYR:CE2	2.87	0.63
1:F:261:ILE:HG22	1:F:261:ILE:O	1.99	0.63
1:E:264:ARG:NH2	2:N:63:LYS:HZ1	1.97	0.63
1:E:221:ALA:O	1:E:225:LEU:HD23	1.99	0.63
1:F:344:LEU:CD1	1:F:351:ILE:HD11	2.25	0.63
2:M:2:THR:HG1	2:M:162:THR:HG21	1.61	0.63
1:E:432:LEU:CD1	1:E:432:LEU:H	2.12	0.63
2:M:85:ASP:HB2	2:M:88:LEU:HD23	1.81	0.63
1:E:436:GLU:O	1:E:439:SER:HB2	1.98	0.63
1:E:354:GLN:OE1	1:F:47:GLU:O	2.17	0.63
2:O:28:LYS:HD3	2:O:31:VAL:HG22	1.81	0.63
1:L:130:ARG:HH11	1:L:130:ARG:C	2.01	0.63
2:M:28:LYS:HD3	2:M:31:VAL:HG22	1.81	0.63
1:E:96:VAL:HG12	1:E:284:LEU:HD11	1.81	0.63
1:E:393:ARG:HB3	1:F:324:GLY:CA	2.23	0.62
1:E:441:PHE:HE1	1:F:310:PHE:HB2	1.64	0.62
1:F:89:VAL:HG12	1:F:94:LYS:H	1.64	0.62
1:K:221:ALA:O	1:K:225:LEU:HD23	1.99	0.62
1:E:86:PHE:O	1:E:89:VAL:HG13	1.98	0.62
1:F:141:ASN:O	1:F:142:ASN:HB2	1.98	0.62
1:E:397:THR:CB	1:F:327:PRO:HA	2.29	0.62
1:L:292:THR:HB	1:L:295:GLY:O	1.98	0.62
1:E:311:GLN:HE22	2:N:67:HIS:HA	0.69	0.62
1:L:163:LEU:HD13	1:L:218:ILE:HG21	1.80	0.62
2:M:139:ASN:N	2:M:139:ASN:HD22	1.98	0.62
2:O:70:HIS:HD2	2:O:73:LYS:HB2	1.65	0.62
2:M:70:HIS:HD2	2:M:73:LYS:HB2	1.65	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:108:VAL:HG21	1:E:294:HIS:ND1	2.15	0.62
1:L:264:ARG:HD3	2:O:62:ARG:NH2	2.12	0.62
1:E:91:TYR:CD2	1:F:91:TYR:CD2	2.88	0.62
1:K:129:GLU:O	1:K:133:ASP:HB2	1.99	0.62
1:L:261:ILE:HG22	1:L:261:ILE:O	1.99	0.62
1:L:311:GLN:NE2	2:O:68:GLN:N	2.47	0.62
1:F:163:LEU:HD12	1:F:163:LEU:C	2.20	0.62
1:F:384:ASN:ND2	1:F:394:ARG:HH11	1.98	0.62
1:K:308:GLY:HA3	1:K:310:PHE:CE2	2.34	0.62
1:E:393:ARG:CZ	1:F:321:GLU:HG3	2.30	0.62
1:E:264:ARG:NH1	2:N:63:LYS:NZ	2.46	0.62
1:E:109:LYS:HG2	1:F:296:MET:CB	2.30	0.62
1:L:145:GLN:HG3	1:L:149:GLN:CB	2.30	0.62
1:K:108:VAL:HG21	1:K:294:HIS:ND1	2.15	0.62
1:K:96:VAL:HG12	1:K:284:LEU:HD11	1.81	0.62
1:L:312:ILE:C	2:O:62:ARG:HA	2.20	0.61
1:L:311:GLN:NE2	2:O:64:LEU:O	2.33	0.61
2:M:17:ASP:O	2:M:33:LYS:HD3	2.00	0.61
1:L:163:LEU:HD12	1:L:163:LEU:C	2.20	0.61
2:O:54:PHE:HE2	2:P:80:LYS:CG	2.12	0.61
1:F:389:ASN:HD22	1:F:391:GLY:H	1.48	0.61
1:K:432:LEU:N	1:K:432:LEU:HD12	2.15	0.61
2:O:85:ASP:HB2	2:O:88:LEU:HD23	1.81	0.61
1:E:411:SER:CB	1:F:32:ARG:HH21	2.11	0.61
1:E:92:VAL:CG1	1:F:92:VAL:CG1	2.77	0.61
1:F:223:LYS:HA	1:F:226:ILE:HD12	1.81	0.61
1:L:221:ALA:O	1:L:225:LEU:HD23	2.00	0.61
1:L:384:ASN:ND2	1:L:394:ARG:HH11	1.98	0.61
2:N:86:ARG:CG	2:N:87:MET:N	2.64	0.61
2:N:86:ARG:HG2	2:N:87:MET:N	2.16	0.61
1:F:285:VAL:HG12	1:F:325:ARG:HG2	1.83	0.61
2:P:28:LYS:HE2	2:P:30:ASN:OD1	1.97	0.61
2:O:17:ASP:O	2:O:33:LYS:HD3	2.00	0.61
1:E:141:ASN:ND2	1:E:141:ASN:N	2.42	0.61
1:E:344:LEU:O	1:E:352:THR:HB	2.01	0.61
1:E:92:VAL:HG11	1:F:92:VAL:CG1	2.30	0.61
1:F:311:GLN:HB2	2:M:66:MET:SD	2.40	0.61
1:E:92:VAL:CG2	1:E:93:GLY:H	2.14	0.61
2:N:47:ALA:HB3	2:N:94:LEU:HB2	1.83	0.61
2:O:139:ASN:HD22	2:O:139:ASN:N	1.98	0.61
2:N:11:HIS:HA	2:N:171:LEU:O	2.01	0.61
1:F:158:ALA:O	1:F:162:LYS:HB2	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:145:GLN:HB2	1:E:149:GLN:N	2.15	0.61
1:F:91:TYR:O	1:F:92:VAL:CG1	2.49	0.61
1:E:129:GLU:O	1:E:133:ASP:HB2	1.99	0.61
1:E:401:ARG:NH2	1:F:329:ARG:O	2.30	0.61
1:E:145:GLN:N	1:E:149:GLN:HB2	2.16	0.61
1:F:141:ASN:HD22	1:F:141:ASN:N	1.92	0.61
2:N:20:ALA:HB2	2:N:31:VAL:HG21	1.82	0.61
1:L:223:LYS:HA	1:L:226:ILE:HD12	1.81	0.61
1:L:158:ALA:O	1:L:162:LYS:HB2	2.00	0.61
1:E:136:ILE:O	1:E:138:PRO:HD3	2.00	0.60
1:K:145:GLN:N	1:K:149:GLN:HB2	2.16	0.60
1:K:145:GLN:H	1:K:149:GLN:HB2	1.63	0.60
1:F:286:GLU:HG2	1:F:325:ARG:NH1	2.16	0.60
1:L:122:ARG:HG2	1:L:122:ARG:HH21	1.66	0.60
1:E:400:GLU:HG2	1:F:51:LYS:CG	2.30	0.60
2:P:86:ARG:HG2	2:P:87:MET:N	2.16	0.60
1:E:432:LEU:N	1:E:432:LEU:HD12	2.15	0.60
2:P:20:ALA:HB2	2:P:31:VAL:HG21	1.82	0.60
1:K:145:GLN:HB2	1:K:149:GLN:N	2.15	0.60
1:F:122:ARG:HG2	1:F:122:ARG:HH21	1.66	0.60
1:L:285:VAL:HG12	1:L:325:ARG:HG2	1.83	0.60
1:L:312:ILE:O	2:O:62:ARG:HA	2.02	0.60
2:P:47:ALA:HB3	2:P:94:LEU:HB2	1.83	0.60
1:F:222:MET:O	1:F:226:ILE:HG13	2.01	0.60
1:K:136:ILE:O	1:K:138:PRO:HD3	2.01	0.60
1:L:89:VAL:HG12	1:L:94:LYS:H	1.64	0.60
1:F:221:ALA:O	1:F:225:LEU:HD23	2.00	0.60
1:K:264:ARG:C	1:K:266:GLU:H	2.05	0.60
1:K:92:VAL:CG2	1:K:93:GLY:H	2.14	0.60
1:E:264:ARG:C	1:E:266:GLU:H	2.05	0.60
1:K:344:LEU:O	1:K:352:THR:HB	2.01	0.60
2:P:11:HIS:HA	2:P:171:LEU:O	2.01	0.60
1:E:384:ASN:HD22	1:E:394:ARG:HH11	1.48	0.60
1:L:291:SER:HA	1:L:296:MET:HE2	1.83	0.60
2:P:86:ARG:CG	2:P:87:MET:N	2.64	0.60
1:L:389:ASN:HD22	1:L:391:GLY:H	1.48	0.60
2:N:13:VAL:HG12	2:N:170:GLU:HG3	1.84	0.60
1:F:86:PHE:HB2	1:F:277:VAL:HG13	1.84	0.60
2:N:88:LEU:H	2:N:88:LEU:HD22	1.67	0.60
1:K:86:PHE:O	1:K:89:VAL:HG22	2.02	0.60
1:K:20:GLN:CG	1:K:332:LEU:HD23	2.31	0.60
1:L:286:GLU:HG2	1:L:325:ARG:NH1	2.16	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:N:60:PHE:CE2	2:N:97:VAL:HG21	2.37	0.60
1:E:91:TYR:CB	1:F:90:GLY:C	2.71	0.60
1:F:160:ARG:HA	1:F:163:LEU:HD23	1.84	0.60
2:O:60:PHE:HB2	2:O:78:LEU:HD22	1.84	0.60
1:F:103:LEU:HD13	1:F:247:VAL:HG13	1.84	0.60
1:E:390:ILE:HD13	1:F:323:GLN:CB	2.32	0.59
1:K:384:ASN:HD22	1:K:394:ARG:HH11	1.49	0.59
1:F:384:ASN:ND2	1:F:390:ILE:H	2.00	0.59
1:E:223:LYS:HA	1:E:226:ILE:HD12	1.84	0.59
1:L:91:TYR:O	1:L:92:VAL:CG1	2.49	0.59
2:P:88:LEU:H	2:P:88:LEU:HD22	1.67	0.59
1:E:310:PHE:O	2:N:66:MET:CB	2.11	0.59
1:L:86:PHE:O	1:L:89:VAL:CG2	2.41	0.59
1:E:20:GLN:CG	1:E:332:LEU:HD23	2.31	0.59
1:E:109:LYS:CG	1:F:296:MET:CB	2.80	0.59
2:M:60:PHE:HB2	2:M:78:LEU:HD22	1.84	0.59
1:E:390:ILE:HD13	1:F:323:GLN:HB2	1.83	0.59
1:F:264:ARG:HH12	2:M:62:ARG:HA	1.68	0.59
1:E:261:ILE:HG22	1:E:278:GLN:HG3	1.85	0.59
1:L:384:ASN:ND2	1:L:390:ILE:H	2.00	0.59
1:E:34:ARG:CZ	1:E:250:HIS:HA	2.32	0.59
1:E:361:THR:CG2	1:F:36:ARG:HA	2.27	0.59
1:E:92:VAL:CG1	1:F:92:VAL:CB	2.75	0.59
1:E:400:GLU:OE1	1:F:51:LYS:NZ	2.36	0.59
2:N:3:ILE:HB	2:N:122:ILE:HG12	1.85	0.59
2:P:60:PHE:CE2	2:P:97:VAL:HG21	2.37	0.59
1:L:222:MET:O	1:L:226:ILE:HG13	2.01	0.59
1:K:34:ARG:CZ	1:K:250:HIS:HA	2.32	0.59
1:E:92:VAL:HG13	1:F:92:VAL:CA	2.28	0.59
2:P:90:LYS:HD2	2:P:90:LYS:C	2.23	0.59
1:K:122:ARG:CA	1:K:122:ARG:HG2	2.26	0.59
1:L:264:ARG:CB	2:O:62:ARG:NH2	2.64	0.59
1:L:86:PHE:HB2	1:L:277:VAL:HG13	1.84	0.59
1:F:130:ARG:NH2	1:F:225:LEU:HD21	2.18	0.59
1:E:263:LYS:O	1:E:264:ARG:HB3	2.02	0.59
1:E:109:LYS:HG2	1:F:296:MET:HB2	1.84	0.59
1:F:145:GLN:HG3	1:F:149:GLN:CB	2.30	0.59
2:P:3:ILE:HB	2:P:122:ILE:HG12	1.85	0.59
1:E:59:THR:O	1:E:61:VAL:HG13	2.03	0.59
1:F:128:GLU:O	1:F:132:LEU:HB2	2.03	0.59
2:O:59:LEU:O	2:O:62:ARG:HB3	2.03	0.58
1:L:384:ASN:HD21	1:L:390:ILE:HG12	1.68	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:263:LYS:O	1:K:264:ARG:HB3	2.02	0.58
1:K:261:ILE:HG22	1:K:278:GLN:HG3	1.85	0.58
2:P:13:VAL:HG12	2:P:170:GLU:HG3	1.84	0.58
1:L:130:ARG:NH2	1:L:225:LEU:HD21	2.18	0.58
1:F:384:ASN:HD21	1:F:390:ILE:HG12	1.68	0.58
1:L:128:GLU:O	1:L:132:LEU:HB2	2.03	0.58
1:L:160:ARG:HA	1:L:163:LEU:HD23	1.84	0.58
1:E:397:THR:HA	1:F:327:PRO:HA	1.85	0.58
1:E:92:VAL:HG21	1:F:92:VAL:HA	1.84	0.58
1:F:91:TYR:C	1:F:92:VAL:HG13	2.24	0.58
2:P:85:ASP:CB	2:P:88:LEU:HD23	2.34	0.58
2:N:90:LYS:HD2	2:N:90:LYS:C	2.23	0.58
1:E:86:PHE:O	1:E:89:VAL:HG22	2.02	0.58
1:K:223:LYS:HA	1:K:226:ILE:HD12	1.84	0.58
1:K:59:THR:O	1:K:61:VAL:HG13	2.03	0.58
2:M:47:ALA:HB3	2:M:94:LEU:HB2	1.85	0.58
1:E:145:GLN:HG3	1:E:149:GLN:HG2	1.78	0.58
1:E:261:ILE:O	1:E:261:ILE:CG2	2.52	0.58
1:K:261:ILE:O	1:K:261:ILE:CG2	2.52	0.58
1:F:63:LYS:HG2	1:F:332:LEU:HD22	1.85	0.58
2:O:139:ASN:ND2	2:O:139:ASN:N	2.52	0.58
1:L:91:TYR:C	1:L:92:VAL:HG13	2.24	0.58
1:L:103:LEU:HD13	1:L:247:VAL:HG13	1.84	0.58
1:F:59:THR:O	1:F:61:VAL:HG13	2.04	0.58
2:O:47:ALA:HB3	2:O:94:LEU:HB2	1.85	0.58
1:F:41:ASN:ND2	1:F:43:GLU:HB3	2.19	0.58
2:N:85:ASP:CB	2:N:88:LEU:HD23	2.34	0.57
1:E:408:TYR:O	1:F:6:PRO:HG2	2.03	0.57
1:K:267:SER:HB3	1:K:270:PRO:CG	2.34	0.57
1:K:285:VAL:CG1	1:K:325:ARG:HB3	2.34	0.57
2:M:131:ALA:HA	2:P:158:ILE:CD1	2.34	0.57
2:P:86:ARG:HG2	2:P:87:MET:H	1.69	0.57
2:O:54:PHE:CE2	2:P:80:LYS:CD	2.85	0.57
1:E:109:LYS:HG3	1:F:296:MET:HB3	1.86	0.57
1:E:285:VAL:CG1	1:E:325:ARG:HB3	2.34	0.57
1:L:41:ASN:ND2	1:L:43:GLU:HB3	2.19	0.57
2:M:59:LEU:O	2:M:62:ARG:HB3	2.03	0.57
1:K:264:ARG:CB	2:P:62:ARG:HH22	2.17	0.57
2:O:1:THR:HA	2:O:162:THR:HG22	1.87	0.57
1:F:374:LYS:NZ	1:F:378:GLU:OE2	2.29	0.57
1:E:358:LEU:N	1:F:40:LEU:CD2	2.59	0.57
1:L:59:THR:O	1:L:61:VAL:HG13	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:128:GLU:O	1:E:131:ILE:HG22	2.04	0.57
1:K:128:GLU:O	1:K:131:ILE:HG22	2.04	0.57
1:E:354:GLN:CD	1:F:47:GLU:O	2.38	0.57
1:E:92:VAL:CG1	1:F:91:TYR:O	2.50	0.57
2:P:79:ALA:HB1	2:P:110:GLY:HA2	1.86	0.57
1:L:63:LYS:HG2	1:L:332:LEU:HD22	1.85	0.57
2:O:37:LEU:HD21	2:O:57:PHE:CB	2.32	0.57
1:E:267:SER:HB3	1:E:270:PRO:CG	2.34	0.57
2:M:13:VAL:HG12	2:M:170:GLU:HG3	1.86	0.57
1:F:264:ARG:NH2	2:M:59:LEU:HA	2.20	0.57
1:E:408:TYR:HE2	1:F:7:ARG:HG3	1.70	0.57
2:M:1:THR:HA	2:M:162:THR:HG22	1.86	0.57
1:E:41:ASN:ND2	1:E:43:GLU:HB3	2.20	0.57
1:F:4:MET:HB3	1:F:8:GLU:HB3	1.86	0.57
2:O:13:VAL:HG12	2:O:170:GLU:HG3	1.86	0.57
2:O:3:ILE:HD11	2:O:46:PHE:O	2.05	0.57
1:F:94:LYS:HD2	1:F:95:GLU:H	1.70	0.57
2:O:54:PHE:CE2	2:P:80:LYS:HG3	2.39	0.57
1:L:4:MET:HB3	1:L:8:GLU:HB3	1.86	0.57
1:F:145:GLN:N	1:F:145:GLN:NE2	2.51	0.56
1:K:92:VAL:HG11	1:L:89:VAL:O	2.05	0.56
1:L:309:ALA:C	2:O:66:MET:SD	2.84	0.56
1:F:104:THR:HG21	1:F:292:THR:HG21	1.87	0.56
2:M:139:ASN:N	2:M:139:ASN:ND2	2.52	0.56
1:K:89:VAL:CG1	1:K:94:LYS:O	2.53	0.56
1:K:142:ASN:O	1:K:143:TRP:CB	2.53	0.56
1:K:41:ASN:ND2	1:K:43:GLU:HB3	2.20	0.56
1:F:366:ILE:HD13	1:F:418:ILE:HB	1.87	0.56
1:F:235:ASN:HB2	1:F:238:GLU:OE2	2.05	0.56
1:L:145:GLN:N	1:L:145:GLN:NE2	2.51	0.56
2:N:86:ARG:HG2	2:N:87:MET:H	1.69	0.56
1:L:235:ASN:HB2	1:L:238:GLU:OE2	2.05	0.56
1:L:308:GLY:HA3	1:L:310:PHE:CE2	2.40	0.56
1:E:411:SER:OG	1:F:32:ARG:CZ	2.54	0.56
1:F:145:GLN:HG2	1:F:150:GLN:H	1.64	0.56
2:N:3:ILE:HD11	2:N:46:PHE:O	2.05	0.56
1:L:96:VAL:HG12	1:L:284:LEU:HD11	1.86	0.56
1:K:17:ILE:HD11	1:K:69:ARG:HG3	1.86	0.56
1:F:308:GLY:HA3	1:F:310:PHE:CE2	2.40	0.56
1:E:358:LEU:HD21	1:F:37:ARG:CA	2.29	0.56
1:E:358:LEU:HD23	1:F:37:ARG:CA	2.29	0.56
1:L:104:THR:HG21	1:L:292:THR:HG21	1.88	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:126:LEU:HD23	1:F:229:GLU:CD	2.26	0.56
1:F:96:VAL:HG12	1:F:284:LEU:HD11	1.86	0.56
2:N:79:ALA:HB1	2:N:110:GLY:HA2	1.86	0.56
1:K:311:GLN:HG2	2:P:66:MET:HE3	1.74	0.56
2:O:57:PHE:CE1	2:O:95:LEU:HD21	2.41	0.56
2:N:1:THR:HB	2:N:33:LYS:NZ	2.20	0.56
2:P:3:ILE:HD11	2:P:46:PHE:O	2.05	0.56
1:E:441:PHE:CE1	1:F:56:ILE:CG2	2.89	0.56
1:E:362:GLU:OE1	1:F:36:ARG:HG2	2.06	0.56
2:M:135:ALA:CA	2:P:154:ILE:HD13	2.25	0.56
1:K:91:TYR:HE1	1:L:272:VAL:HG11	1.69	0.56
1:F:86:PHE:O	1:F:89:VAL:CG2	2.41	0.56
2:N:21:THR:HG22	2:N:22:LEU:N	2.21	0.56
2:M:3:ILE:HD11	2:M:46:PHE:O	2.05	0.56
1:K:103:LEU:HD13	1:K:247:VAL:HG13	1.88	0.56
1:F:33:ASN:HD22	1:F:36:ARG:HD2	1.71	0.56
1:K:145:GLN:CA	1:K:149:GLN:HB2	2.29	0.56
1:E:145:GLN:CG	1:E:149:GLN:CG	2.67	0.56
1:L:89:VAL:HG12	1:L:94:LYS:N	2.21	0.56
1:L:155:ALA:O	1:L:159:PHE:HB2	2.06	0.56
1:F:58:PRO:HG2	1:F:61:VAL:HG11	1.88	0.56
1:E:118:LYS:HA	1:E:118:LYS:CE	2.36	0.56
1:L:33:ASN:HD22	1:L:36:ARG:HD2	1.71	0.56
1:L:126:LEU:HD23	1:L:229:GLU:CD	2.26	0.56
1:E:17:ILE:HD11	1:E:69:ARG:HG3	1.86	0.56
1:E:91:TYR:HB3	1:F:91:TYR:HA	1.85	0.55
1:F:89:VAL:HG12	1:F:94:LYS:N	2.21	0.55
1:F:27:VAL:CG1	1:F:70:LEU:HG	2.35	0.55
2:P:1:THR:HB	2:P:33:LYS:NZ	2.20	0.55
1:L:366:ILE:HD13	1:L:418:ILE:HB	1.88	0.55
1:K:153:SER:O	1:K:154:ALA:C	2.45	0.55
1:E:92:VAL:HG11	1:F:92:VAL:HB	1.81	0.55
2:M:136:LEU:HD11	2:P:135:ALA:HB1	1.88	0.55
1:L:94:LYS:HD2	1:L:95:GLU:H	1.70	0.55
1:L:111:VAL:HG21	1:L:243:ALA:HB2	1.88	0.55
1:L:128:GLU:O	1:L:131:ILE:HG22	2.06	0.55
1:F:155:ALA:O	1:F:159:PHE:HB2	2.06	0.55
1:E:89:VAL:CG1	1:E:94:LYS:O	2.53	0.55
2:P:21:THR:HG22	2:P:22:LEU:N	2.21	0.55
1:E:257:GLU:HG2	1:E:260:LYS:HG3	1.88	0.55
1:K:366:ILE:HD13	1:K:418:ILE:HB	1.88	0.55
1:E:15:LYS:HB3	1:E:348:ASN:ND2	2.21	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:91:TYR:O	1:F:92:VAL:HG13	2.07	0.55
2:O:54:PHE:CE2	2:P:80:LYS:HD2	2.42	0.55
1:K:118:LYS:HA	1:K:118:LYS:CE	2.36	0.55
1:K:64:THR:HG22	1:K:68:ARG:HD2	1.88	0.55
2:M:62:ARG:O	2:M:65:GLU:HB2	2.07	0.55
1:E:408:TYR:HB2	1:F:29:ILE:HG12	1.87	0.55
1:E:103:LEU:HD13	1:E:247:VAL:HG13	1.88	0.55
1:F:128:GLU:O	1:F:131:ILE:HG22	2.06	0.55
2:M:57:PHE:CE1	2:M:95:LEU:HD21	2.41	0.55
2:M:160:ILE:CG2	2:O:160:ILE:HD13	2.36	0.55
2:N:17:ASP:O	2:N:33:LYS:HD2	2.07	0.55
1:E:440:ARG:HD3	1:F:314:LYS:HB3	1.89	0.55
1:E:441:PHE:C	1:F:329:ARG:HB3	2.27	0.55
1:E:362:GLU:OE2	1:F:32:ARG:NH2	2.40	0.55
2:P:70:HIS:HD2	2:P:73:LYS:HB2	1.72	0.55
1:L:58:PRO:HG2	1:L:61:VAL:HG11	1.88	0.55
1:E:64:THR:HG22	1:E:68:ARG:HD2	1.88	0.55
1:E:442:ILE:CG2	1:F:329:ARG:HB2	2.37	0.55
1:E:139:ALA:O	1:E:140:LYS:CG	2.55	0.55
1:F:108:VAL:HA	1:F:111:VAL:HG22	1.89	0.55
1:E:292:THR:HG22	1:E:294:HIS:N	2.05	0.55
2:M:85:ASP:CB	2:M:88:LEU:HD23	2.36	0.55
2:O:85:ASP:CB	2:O:88:LEU:HD23	2.36	0.55
1:L:374:LYS:NZ	1:L:378:GLU:OE2	2.29	0.55
1:F:397:THR:HG21	1:F:443:LEU:O	2.07	0.55
1:E:442:ILE:HD13	1:F:329:ARG:CB	2.35	0.55
2:N:139:ASN:N	2:N:139:ASN:ND2	2.48	0.55
2:P:17:ASP:O	2:P:33:LYS:HD2	2.07	0.55
1:F:264:ARG:O	1:F:266:GLU:N	2.40	0.54
1:K:309:ALA:HB1	2:P:66:MET:HG2	1.88	0.54
1:L:108:VAL:HA	1:L:111:VAL:HG22	1.89	0.54
2:O:62:ARG:O	2:O:65:GLU:HB2	2.07	0.54
1:K:15:LYS:HB3	1:K:348:ASN:ND2	2.21	0.54
1:E:153:SER:O	1:E:154:ALA:C	2.45	0.54
1:K:122:ARG:O	1:K:122:ARG:HG2	2.06	0.54
1:K:264:ARG:CB	2:P:62:ARG:NH2	2.69	0.54
1:E:132:LEU:HD12	1:E:156:ARG:CG	2.38	0.54
1:K:293:LYS:CE	1:L:296:MET:HE1	2.30	0.54
2:P:139:ASN:ND2	2:P:139:ASN:N	2.48	0.54
1:E:145:GLN:CA	1:E:149:GLN:HB2	2.29	0.54
1:F:264:ARG:HH21	2:M:62:ARG:HD2	1.65	0.54
1:F:311:GLN:CG	2:M:66:MET:HE1	2.25	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:111:VAL:HG21	1:F:243:ALA:HB2	1.88	0.54
1:K:257:GLU:HG2	1:K:260:LYS:HG3	1.88	0.54
2:M:128:TYR:CD1	2:P:128:TYR:CE1	2.95	0.54
1:E:394:ARG:NH2	1:F:323:GLN:OE1	2.40	0.54
1:E:366:ILE:HD13	1:E:418:ILE:HB	1.88	0.54
1:K:132:LEU:HD12	1:K:156:ARG:CG	2.38	0.54
2:N:70:HIS:HD2	2:N:73:LYS:HB2	1.72	0.54
1:K:91:TYR:CE1	1:L:272:VAL:HG12	2.40	0.54
1:L:285:VAL:CG1	1:L:325:ARG:HB3	2.38	0.54
2:M:158:ILE:HG21	2:P:127:PRO:HB3	1.90	0.54
1:L:264:ARG:O	1:L:266:GLU:N	2.40	0.54
1:E:122:ARG:HG2	1:E:122:ARG:O	2.06	0.54
2:M:131:ALA:HA	2:P:158:ILE:HD11	1.88	0.54
1:K:312:ILE:HD12	2:P:62:ARG:O	2.07	0.54
1:F:285:VAL:CG1	1:F:325:ARG:HB3	2.38	0.54
1:E:142:ASN:O	1:E:143:TRP:CB	2.53	0.54
2:N:60:PHE:HB2	2:N:78:LEU:HD22	1.90	0.54
2:P:60:PHE:HB2	2:P:78:LEU:HD22	1.90	0.54
1:K:139:ALA:O	1:K:140:LYS:CG	2.55	0.54
1:F:131:ILE:O	1:F:134:VAL:HG12	2.08	0.54
1:E:41:ASN:HD22	1:E:43:GLU:HB3	1.73	0.54
1:L:397:THR:HG21	1:L:443:LEU:O	2.07	0.54
1:L:91:TYR:O	1:L:92:VAL:HG13	2.07	0.53
1:K:41:ASN:HD22	1:K:43:GLU:HB3	1.73	0.53
1:K:131:ILE:HD12	1:K:134:VAL:CG1	2.39	0.53
2:N:67:HIS:O	2:N:69:GLY:N	2.41	0.53
1:E:91:TYR:CD2	1:F:91:TYR:HA	2.43	0.53
1:L:145:GLN:OE1	1:L:149:GLN:C	2.46	0.53
2:P:140:THR:HG22	2:P:141:GLU:N	2.23	0.53
2:O:98:ALA:CB	2:O:103:SER:HB3	2.38	0.53
1:L:309:ALA:CB	2:O:66:MET:HE2	2.29	0.53
1:E:92:VAL:HG13	1:F:91:TYR:C	2.28	0.53
2:P:67:HIS:O	2:P:69:GLY:N	2.41	0.53
1:L:20:GLN:CG	1:L:332:LEU:HD23	2.36	0.53
1:K:374:LYS:O	1:K:378:GLU:HG3	2.07	0.53
1:K:111:VAL:HG21	1:K:243:ALA:HB2	1.90	0.53
2:M:140:THR:HG21	2:M:142:LEU:CG	2.38	0.53
2:N:140:THR:HG22	2:N:141:GLU:N	2.23	0.53
1:L:285:VAL:HG12	1:L:325:ARG:CG	2.38	0.53
1:E:442:ILE:HG23	1:F:329:ARG:HB2	1.90	0.53
1:K:145:GLN:H	1:K:149:GLN:CB	2.22	0.53
2:M:98:ALA:CB	2:M:103:SER:HB3	2.38	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:390:ILE:CD1	1:F:323:GLN:HB2	2.39	0.53
1:E:411:SER:OG	1:F:32:ARG:NE	2.40	0.53
1:E:111:VAL:HG21	1:E:243:ALA:HB2	1.90	0.53
1:E:374:LYS:O	1:E:378:GLU:HG3	2.07	0.53
2:O:98:ALA:HB2	2:O:103:SER:HB3	1.91	0.53
1:K:257:GLU:OE1	1:L:279:ARG:NH2	2.42	0.53
1:E:358:LEU:HG	1:F:40:LEU:CD1	2.30	0.53
1:E:145:GLN:H	1:E:149:GLN:CB	2.22	0.53
1:E:312:ILE:CD1	2:N:67:HIS:CE1	2.91	0.53
2:P:59:LEU:O	2:P:62:ARG:HB2	2.09	0.53
1:K:91:TYR:C	1:K:92:VAL:HG13	2.30	0.53
1:F:219:LYS:O	1:F:223:LYS:HD3	2.09	0.53
2:O:66:MET:O	2:O:67:HIS:ND1	2.42	0.53
1:E:358:LEU:CD2	1:F:37:ARG:N	2.71	0.53
1:F:145:GLN:OE1	1:F:149:GLN:C	2.46	0.53
1:L:217:LYS:HB3	1:L:220:ASP:CB	2.38	0.53
1:F:285:VAL:HG12	1:F:325:ARG:CG	2.38	0.53
1:L:397:THR:HG21	1:L:443:LEU:C	2.29	0.53
1:K:382:GLN:OE1	1:K:382:GLN:HA	2.09	0.53
2:O:7:ARG:HB2	2:O:12:VAL:HG23	1.91	0.53
2:O:90:LYS:HZ1	2:P:89:ARG:HD2	1.74	0.53
1:F:217:LYS:HB3	1:F:220:ASP:CB	2.38	0.53
2:M:140:THR:HG22	2:M:142:LEU:N	2.17	0.53
2:M:98:ALA:HB2	2:M:103:SER:HB3	1.90	0.53
2:M:85:ASP:O	2:M:89:ARG:HB3	2.09	0.53
2:O:85:ASP:O	2:O:89:ARG:HB3	2.09	0.53
1:E:122:ARG:HG2	1:E:122:ARG:CA	2.26	0.52
2:O:140:THR:HG21	2:O:142:LEU:CG	2.38	0.52
1:K:282:LEU:CD1	1:K:319:ILE:HD11	2.39	0.52
1:L:219:LYS:O	1:L:223:LYS:HD3	2.09	0.52
1:F:92:VAL:CG2	1:F:93:GLY:H	2.21	0.52
1:K:292:THR:HG22	1:K:294:HIS:N	2.05	0.52
1:L:131:ILE:O	1:L:134:VAL:HG12	2.08	0.52
1:L:27:VAL:CG1	1:L:70:LEU:HG	2.35	0.52
1:F:20:GLN:CG	1:F:332:LEU:HD23	2.36	0.52
1:K:91:TYR:O	1:K:92:VAL:CG1	2.58	0.52
1:E:131:ILE:HD12	1:E:134:VAL:CG1	2.39	0.52
1:E:91:TYR:C	1:E:92:VAL:HG13	2.30	0.52
1:E:92:VAL:HG21	1:F:92:VAL:CA	2.39	0.52
1:K:145:GLN:HG3	1:K:149:GLN:HG2	1.78	0.52
2:M:66:MET:O	2:M:67:HIS:ND1	2.42	0.52
1:E:443:LEU:N	1:F:329:ARG:HG3	2.21	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:145:GLN:CD	1:L:150:GLN:CA	2.78	0.52
1:F:397:THR:HG21	1:F:443:LEU:C	2.29	0.52
2:N:64:LEU:HD23	2:N:74:ALA:CB	2.40	0.52
1:E:382:GLN:HA	1:E:382:GLN:OE1	2.09	0.52
1:F:18:ILE:HD13	1:F:347:PRO:HG3	1.92	0.52
1:L:17:ILE:HD13	1:L:66:ILE:CG1	2.36	0.52
1:L:92:VAL:CG2	1:L:93:GLY:H	2.22	0.52
2:N:59:LEU:O	2:N:62:ARG:HB2	2.09	0.52
1:L:264:ARG:C	1:L:266:GLU:N	2.62	0.52
1:F:362:GLU:HG2	1:F:411:SER:N	2.24	0.52
1:K:216:LEU:O	1:K:220:ASP:HB3	2.10	0.52
1:L:117:GLU:C	1:L:119:ASN:H	2.13	0.52
1:E:92:VAL:HG21	1:F:92:VAL:C	2.29	0.52
2:P:64:LEU:HD23	2:P:74:ALA:CB	2.40	0.52
1:E:92:VAL:HG12	1:F:92:VAL:HG12	1.90	0.52
1:F:263:LYS:HE2	1:F:275:GLU:OE1	2.10	0.52
1:F:264:ARG:C	1:F:266:GLU:N	2.62	0.52
2:O:149:GLU:HG3	2:O:166:HIS:HD2	1.74	0.51
1:L:362:GLU:HG2	1:L:411:SER:N	2.24	0.51
1:L:18:ILE:HD13	1:L:347:PRO:HG3	1.92	0.51
1:F:15:LYS:HB3	1:F:348:ASN:ND2	2.25	0.51
2:M:149:GLU:HG3	2:M:166:HIS:HD2	1.74	0.51
2:M:7:ARG:HB2	2:M:12:VAL:HG23	1.91	0.51
1:L:263:LYS:HE2	1:L:275:GLU:OE1	2.10	0.51
1:K:389:ASN:ND2	1:K:389:ASN:C	2.57	0.51
1:E:145:GLN:HB2	1:E:149:GLN:H	1.74	0.51
2:M:37:LEU:HD21	2:M:57:PHE:CB	2.32	0.51
1:F:141:ASN:ND2	1:F:141:ASN:N	2.54	0.51
2:O:88:LEU:H	2:O:88:LEU:HD22	1.76	0.51
1:K:362:GLU:HG3	1:K:411:SER:HA	1.93	0.51
1:L:264:ARG:NH1	2:O:59:LEU:O	2.39	0.51
1:E:122:ARG:HG2	1:E:122:ARG:C	2.30	0.51
1:E:91:TYR:O	1:E:92:VAL:CG1	2.58	0.51
1:K:145:GLN:HB2	1:K:149:GLN:H	1.74	0.51
1:F:145:GLN:CD	1:F:150:GLN:CA	2.78	0.51
1:F:263:LYS:O	1:F:264:ARG:CB	2.59	0.51
1:L:145:GLN:CD	1:L:149:GLN:HB2	2.30	0.51
2:N:3:ILE:HB	2:N:122:ILE:HG13	1.93	0.51
2:P:3:ILE:HB	2:P:122:ILE:HG13	1.93	0.51
1:K:96:VAL:CG1	1:K:99:ILE:HD12	2.40	0.51
1:E:216:LEU:O	1:E:220:ASP:HB3	2.10	0.51
2:N:98:ALA:HA	2:N:103:SER:HA	1.93	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:440:ARG:O	1:F:315:PRO:CD	2.58	0.51
1:K:122:ARG:C	1:K:122:ARG:HG2	2.30	0.51
1:K:91:TYR:HE1	1:L:272:VAL:CG1	2.23	0.51
2:N:8:ARG:NH1	2:N:142:LEU:O	2.43	0.51
2:M:108:GLY:C	2:M:110:GLY:H	2.14	0.51
1:L:122:ARG:CG	1:L:122:ARG:HH21	2.24	0.51
1:L:311:GLN:NE2	2:O:68:GLN:CA	2.73	0.51
1:L:313:ALA:C	2:O:65:GLU:OE2	2.49	0.51
2:M:88:LEU:HD22	2:M:88:LEU:H	1.76	0.51
2:O:22:LEU:HB2	2:O:27:MET:HG3	1.93	0.51
1:E:139:ALA:O	1:E:140:LYS:HB2	2.11	0.51
1:K:139:ALA:O	1:K:140:LYS:HB2	2.11	0.51
2:P:8:ARG:NH1	2:P:142:LEU:O	2.43	0.51
1:E:282:LEU:CD1	1:E:319:ILE:HD11	2.39	0.51
2:O:108:GLY:C	2:O:110:GLY:H	2.14	0.51
1:F:235:ASN:OD1	1:F:238:GLU:OE2	2.29	0.51
2:M:22:LEU:HB2	2:M:27:MET:HG3	1.93	0.51
1:E:263:LYS:O	1:E:264:ARG:CB	2.58	0.51
1:K:369:THR:O	1:K:373:ILE:HG12	2.11	0.51
1:E:278:GLN:OE1	1:E:319:ILE:HG23	2.10	0.51
1:F:285:VAL:HG11	1:F:325:ARG:HB3	1.93	0.51
1:E:34:ARG:NH1	1:E:250:HIS:HA	2.25	0.51
1:E:131:ILE:HG23	1:E:132:LEU:N	2.26	0.51
1:F:264:ARG:HH12	2:M:62:ARG:CG	1.94	0.51
1:E:96:VAL:CG1	1:E:99:ILE:HD12	2.40	0.51
1:K:34:ARG:NH1	1:K:250:HIS:HA	2.25	0.51
2:M:21:THR:HG22	2:M:22:LEU:N	2.26	0.51
1:F:117:GLU:C	1:F:119:ASN:H	2.13	0.51
1:K:350:SER:OG	1:K:353:VAL:HG23	2.11	0.51
2:N:59:LEU:HA	2:N:62:ARG:HD2	1.93	0.50
1:L:94:LYS:NZ	1:L:95:GLU:OE2	2.37	0.50
1:L:389:ASN:HD22	1:L:390:ILE:N	2.09	0.50
1:E:109:LYS:CG	1:F:296:MET:HB2	2.41	0.50
2:P:98:ALA:HA	2:P:103:SER:HA	1.93	0.50
1:E:145:GLN:CB	1:E:149:GLN:H	2.25	0.50
1:F:389:ASN:HD22	1:F:390:ILE:N	2.09	0.50
2:O:15:ALA:CB	2:O:152:LEU:HD12	2.41	0.50
1:L:15:LYS:HB3	1:L:348:ASN:ND2	2.25	0.50
1:L:264:ARG:CZ	2:O:62:ARG:HD3	2.39	0.50
1:E:120:ARG:HG3	1:E:121:TYR:N	2.25	0.50
1:K:20:GLN:HG3	1:K:332:LEU:CD2	2.42	0.50
2:N:90:LYS:HD2	2:N:91:LEU:N	2.27	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:235:ASN:OD1	1:L:238:GLU:OE2	2.29	0.50
1:L:76:ALA:HB1	1:L:250:HIS:O	2.11	0.50
1:E:389:ASN:ND2	1:E:389:ASN:C	2.57	0.50
1:E:440:ARG:CD	1:F:314:LYS:HD2	2.41	0.50
1:E:86:PHE:HB2	1:E:277:VAL:HG13	1.92	0.50
1:K:329:ARG:HG3	1:K:329:ARG:HH11	1.77	0.50
1:E:440:ARG:HE	1:F:316:SER:HG	1.53	0.50
1:E:350:SER:OG	1:E:353:VAL:HG23	2.11	0.50
1:K:128:GLU:HA	1:K:131:ILE:HG22	1.92	0.50
1:K:131:ILE:HG23	1:K:132:LEU:N	2.26	0.50
2:P:90:LYS:HD2	2:P:91:LEU:N	2.27	0.50
1:E:136:ILE:CG2	1:E:136:ILE:O	2.60	0.50
1:F:145:GLN:CD	1:F:149:GLN:HB2	2.30	0.50
1:E:400:GLU:CD	1:F:51:LYS:CE	2.80	0.50
1:L:135:LEU:O	1:L:136:ILE:HG12	2.11	0.50
1:F:135:LEU:O	1:F:136:ILE:HG12	2.10	0.50
2:M:37:LEU:CD2	2:M:57:PHE:HB3	2.35	0.50
2:N:140:THR:HG21	2:N:142:LEU:CG	2.35	0.50
2:O:51:ALA:O	2:O:54:PHE:HB3	2.11	0.50
1:K:278:GLN:OE1	1:K:319:ILE:HG23	2.11	0.50
2:M:15:ALA:CB	2:M:152:LEU:HD12	2.41	0.50
2:M:51:ALA:O	2:M:54:PHE:HB3	2.11	0.50
1:E:397:THR:CA	1:F:327:PRO:HA	2.42	0.50
1:E:362:GLU:HG3	1:E:411:SER:HA	1.93	0.50
1:K:86:PHE:HB2	1:K:277:VAL:HG13	1.92	0.50
1:E:20:GLN:HG3	1:E:332:LEU:CD2	2.42	0.50
2:M:100:GLU:HG2	2:M:173:TYR:CD2	2.47	0.50
2:O:70:HIS:CD2	2:O:73:LYS:H	2.30	0.50
2:O:21:THR:HG22	2:O:22:LEU:N	2.26	0.50
1:K:263:LYS:O	1:K:264:ARG:CB	2.58	0.50
2:P:59:LEU:HA	2:P:62:ARG:HD2	1.93	0.50
1:L:369:THR:HB	1:L:421:ASP:HA	1.94	0.50
2:O:37:LEU:CD2	2:O:57:PHE:HB3	2.35	0.50
2:O:140:THR:HG22	2:O:142:LEU:N	2.17	0.50
1:F:232:LYS:NZ	1:F:232:LYS:HB2	2.27	0.50
1:F:76:ALA:HB1	1:F:250:HIS:O	2.11	0.50
1:E:440:ARG:HD2	1:F:314:LYS:HD2	1.94	0.50
1:F:369:THR:HB	1:F:421:ASP:HA	1.94	0.50
2:M:138:GLU:HB3	2:M:139:ASN:ND2	2.26	0.50
1:K:120:ARG:HG3	1:K:121:TYR:N	2.25	0.50
1:F:130:ARG:HH11	1:F:131:ILE:N	2.10	0.49
2:O:138:GLU:HB3	2:O:139:ASN:ND2	2.26	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:329:ARG:HG3	1:E:329:ARG:HH11	1.77	0.49
2:P:39:ASN:HD22	2:P:39:ASN:N	2.09	0.49
1:F:122:ARG:HH21	1:F:122:ARG:CG	2.24	0.49
1:F:264:ARG:NH1	1:F:312:ILE:HD12	2.27	0.49
1:F:94:LYS:NZ	1:F:95:GLU:OE2	2.36	0.49
1:K:141:ASN:N	1:K:141:ASN:ND2	2.42	0.49
1:E:369:THR:O	1:E:373:ILE:HG12	2.11	0.49
2:O:100:GLU:HG2	2:O:173:TYR:CD2	2.47	0.49
1:E:128:GLU:HA	1:E:131:ILE:HG22	1.92	0.49
2:M:70:HIS:CD2	2:M:73:LYS:H	2.30	0.49
1:F:286:GLU:HG2	1:F:325:ARG:HH12	1.77	0.49
1:E:441:PHE:CG	1:F:56:ILE:CD1	2.69	0.49
1:F:131:ILE:C	1:F:133:ASP:H	2.15	0.49
1:F:409:ASP:O	1:F:413:LEU:HD22	2.12	0.49
1:E:397:THR:HG21	1:E:443:LEU:HA	1.94	0.49
1:E:397:THR:HG23	1:F:327:PRO:C	2.32	0.49
1:L:264:ARG:HH11	2:O:62:ARG:CG	2.25	0.49
1:E:357:ALA:HB2	1:F:44:LEU:HD11	1.75	0.49
1:F:89:VAL:CG1	1:F:94:LYS:H	2.26	0.49
1:F:130:ARG:NH1	1:F:131:ILE:HA	2.28	0.49
2:M:159:CYS:HB3	2:M:162:THR:OG1	2.13	0.49
2:N:53:ALA:HB1	2:N:57:PHE:CE2	2.48	0.49
1:E:79:ILE:HD13	1:E:80:LYS:H	1.78	0.49
1:K:217:LYS:HB2	1:K:220:ASP:HB3	1.95	0.49
1:L:413:LEU:HD13	1:L:413:LEU:N	2.28	0.49
1:L:311:GLN:CG	2:O:66:MET:CE	2.90	0.49
1:E:91:TYR:CD2	1:F:91:TYR:HD2	2.31	0.49
1:K:108:VAL:HA	1:K:111:VAL:HG22	1.95	0.49
1:L:131:ILE:C	1:L:133:ASP:H	2.15	0.49
2:P:140:THR:HG21	2:P:142:LEU:CG	2.35	0.49
2:P:51:ALA:O	2:P:54:PHE:HB3	2.12	0.49
1:E:388:GLU:OE2	1:F:318:LEU:O	2.30	0.49
1:L:130:ARG:NH1	1:L:131:ILE:HA	2.28	0.49
1:K:384:ASN:ND2	1:K:390:ILE:H	2.10	0.49
1:L:285:VAL:HG11	1:L:325:ARG:HB3	1.93	0.49
1:E:384:ASN:ND2	1:E:390:ILE:H	2.10	0.49
1:E:359:MET:CE	1:F:36:ARG:HD3	2.40	0.49
1:K:136:ILE:CG2	1:K:136:ILE:O	2.60	0.49
1:K:145:GLN:CB	1:K:149:GLN:H	2.25	0.49
1:K:89:VAL:HG12	1:K:94:LYS:N	2.25	0.49
1:E:217:LYS:HB2	1:E:220:ASP:HB3	1.95	0.49
1:L:409:ASP:O	1:L:413:LEU:HD22	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:N:39:ASN:N	2:N:39:ASN:HD22	2.09	0.49
1:F:123:ALA:O	1:F:127:ALA:HB2	2.13	0.49
2:O:61:GLU:O	2:O:65:GLU:HG2	2.13	0.49
1:E:235:ASN:ND2	1:E:235:ASN:N	2.37	0.49
1:K:389:ASN:HD22	1:K:391:GLY:H	1.56	0.49
1:L:79:ILE:HD13	1:L:80:LYS:O	2.13	0.49
1:F:79:ILE:HD13	1:F:80:LYS:O	2.13	0.49
1:E:441:PHE:CE1	1:F:310:PHE:CB	2.95	0.48
1:F:94:LYS:NZ	1:F:98:SER:HB3	2.28	0.48
1:E:108:VAL:HA	1:E:111:VAL:HG22	1.95	0.48
2:O:5:SER:HB2	2:O:14:ILE:HG12	1.95	0.48
1:L:286:GLU:HG2	1:L:325:ARG:HH12	1.77	0.48
1:L:145:GLN:CD	1:L:149:GLN:CB	2.81	0.48
2:N:88:LEU:N	2:N:88:LEU:HD22	2.28	0.48
2:P:53:ALA:HB1	2:P:57:PHE:CE2	2.48	0.48
2:N:100:GLU:HG2	2:N:173:TYR:HB3	1.96	0.48
1:E:109:LYS:HG3	1:F:296:MET:CB	2.43	0.48
1:E:92:VAL:CG2	1:F:92:VAL:CA	2.91	0.48
2:O:51:ALA:CB	2:P:109:ASN:O	2.61	0.48
1:K:89:VAL:HG12	1:K:94:LYS:O	2.14	0.48
1:K:96:VAL:HG13	1:K:99:ILE:CD1	2.43	0.48
1:K:79:ILE:HD13	1:K:80:LYS:H	1.78	0.48
2:O:70:HIS:HD2	2:O:73:LYS:CB	2.25	0.48
1:L:89:VAL:CG1	1:L:94:LYS:H	2.26	0.48
2:O:43:ILE:HG23	2:O:171:LEU:HD13	1.95	0.48
2:O:5:SER:HB3	2:O:120:ILE:HB	1.95	0.48
2:P:39:ASN:ND2	2:P:39:ASN:N	2.62	0.48
1:L:118:LYS:CE	1:L:118:LYS:HA	2.44	0.48
1:E:442:ILE:N	1:F:329:ARG:HG3	2.29	0.48
1:L:130:ARG:HH11	1:L:131:ILE:N	2.10	0.48
1:E:89:VAL:HG12	1:E:94:LYS:O	2.14	0.48
2:P:88:LEU:N	2:P:88:LEU:HD22	2.28	0.48
1:E:441:PHE:HD1	1:F:56:ILE:CG1	2.20	0.48
1:E:354:GLN:CD	1:F:48:VAL:N	2.60	0.48
1:K:108:VAL:C	1:K:110:MET:N	2.66	0.48
1:L:94:LYS:HZ2	1:L:98:SER:HB3	1.77	0.48
1:F:217:LYS:O	1:F:221:ALA:N	2.44	0.48
1:L:232:LYS:NZ	1:L:232:LYS:HB2	2.27	0.48
2:P:16:GLY:CA	2:P:152:LEU:HD11	2.44	0.48
2:M:8:ARG:HH21	2:M:137:LEU:HA	1.78	0.48
2:M:61:GLU:O	2:M:65:GLU:HG2	2.14	0.48
2:M:70:HIS:HD2	2:M:73:LYS:CB	2.25	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:263:LYS:O	1:L:264:ARG:CB	2.59	0.48
1:F:145:GLN:CD	1:F:149:GLN:CB	2.81	0.48
2:O:17:ASP:HA	2:O:165:PHE:O	2.13	0.48
2:M:17:ASP:HA	2:M:165:PHE:O	2.13	0.48
2:M:134:ARG:O	2:M:138:GLU:HB2	2.14	0.48
2:O:134:ARG:O	2:O:138:GLU:HB2	2.14	0.48
2:P:28:LYS:HD3	2:P:31:VAL:HG22	1.96	0.48
1:F:374:LYS:O	1:F:378:GLU:HG3	2.13	0.48
1:L:123:ALA:O	1:L:127:ALA:HB2	2.13	0.48
2:N:51:ALA:O	2:N:54:PHE:HB3	2.13	0.48
1:E:389:ASN:HD22	1:E:391:GLY:H	1.56	0.48
1:L:135:LEU:HD13	1:L:159:PHE:CE1	2.49	0.48
1:E:108:VAL:C	1:E:110:MET:N	2.66	0.48
1:F:135:LEU:HD13	1:F:159:PHE:CE1	2.49	0.48
1:K:117:GLU:C	1:K:119:ASN:H	2.16	0.48
2:P:32:LYS:HD3	2:P:34:VAL:O	2.14	0.48
2:O:83:ARG:HG3	2:O:108:GLY:O	2.14	0.48
2:M:83:ARG:HG3	2:M:108:GLY:O	2.14	0.48
2:O:15:ALA:HB1	2:O:152:LEU:HD12	1.96	0.48
2:N:28:LYS:HD3	2:N:31:VAL:HG22	1.96	0.48
2:M:128:TYR:CE1	2:P:128:TYR:CE1	3.01	0.48
1:L:309:ALA:HB3	2:O:66:MET:CG	2.28	0.48
1:E:358:LEU:O	1:E:361:THR:CG2	2.60	0.48
2:N:58:GLU:HG3	2:N:62:ARG:HE	1.78	0.48
1:L:145:GLN:CD	1:L:150:GLN:HA	2.30	0.48
2:O:159:CYS:HB3	2:O:162:THR:OG1	2.13	0.48
1:E:369:THR:HB	1:E:421:ASP:HA	1.96	0.48
2:O:8:ARG:HH21	2:O:137:LEU:HA	1.78	0.48
2:N:116:GLU:HG2	2:N:116:GLU:H	1.42	0.48
1:K:309:ALA:O	2:P:66:MET:HE1	2.14	0.47
2:P:58:GLU:HG3	2:P:62:ARG:HE	1.78	0.47
1:L:94:LYS:NZ	1:L:98:SER:HB3	2.29	0.47
1:F:131:ILE:CG2	1:F:132:LEU:N	2.77	0.47
2:P:1:THR:HB	2:P:33:LYS:HZ2	1.79	0.47
2:P:100:GLU:HG2	2:P:173:TYR:HB3	1.96	0.47
1:E:344:LEU:HD13	1:E:395:LEU:HD13	1.96	0.47
1:F:17:ILE:HD13	1:F:66:ILE:CG1	2.35	0.47
2:O:51:ALA:HB2	2:P:109:ASN:O	2.14	0.47
2:M:3:ILE:HB	2:M:122:ILE:CG1	2.44	0.47
1:L:374:LYS:O	1:L:378:GLU:HG3	2.13	0.47
2:N:39:ASN:N	2:N:39:ASN:ND2	2.62	0.47
2:N:16:GLY:CA	2:N:152:LEU:HD11	2.44	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:231:ALA:C	1:F:233:LEU:H	2.17	0.47
1:F:146:THR:C	1:F:150:GLN:HB2	2.35	0.47
1:F:312:ILE:HG12	2:M:65:GLU:HB3	0.83	0.47
2:N:32:LYS:HD3	2:N:34:VAL:O	2.14	0.47
1:K:397:THR:HG21	1:K:443:LEU:HA	1.94	0.47
2:M:5:SER:HB3	2:M:120:ILE:HB	1.95	0.47
1:F:413:LEU:HD13	1:F:413:LEU:N	2.28	0.47
1:L:231:ALA:C	1:L:233:LEU:H	2.17	0.47
1:L:312:ILE:C	2:O:62:ARG:HG3	2.33	0.47
1:L:216:LEU:O	1:L:220:ASP:HB3	2.14	0.47
1:K:235:ASN:ND2	1:K:235:ASN:N	2.37	0.47
1:K:63:LYS:HE2	1:K:307:SER:OG	2.15	0.47
1:E:354:GLN:HG2	1:F:47:GLU:HB2	1.95	0.47
1:F:278:GLN:OE1	1:F:319:ILE:HB	2.15	0.47
1:E:117:GLU:C	1:E:119:ASN:H	2.16	0.47
1:K:369:THR:HB	1:K:421:ASP:HA	1.96	0.47
2:M:15:ALA:HB1	2:M:152:LEU:HD12	1.96	0.47
1:F:257:GLU:HG2	1:F:260:LYS:HG3	1.96	0.47
1:L:146:THR:C	1:L:150:GLN:HB2	2.35	0.47
1:K:264:ARG:HD2	2:P:62:ARG:NH2	2.16	0.47
2:M:5:SER:HB2	2:M:14:ILE:HG12	1.95	0.47
1:F:118:LYS:CE	1:F:118:LYS:HA	2.44	0.47
1:F:132:LEU:CG	1:F:160:ARG:HB3	2.44	0.47
2:N:88:LEU:CD2	2:N:88:LEU:H	2.28	0.47
1:K:96:VAL:HG11	1:K:281:LEU:CD1	2.44	0.47
1:E:63:LYS:HE2	1:E:307:SER:OG	2.15	0.47
1:E:96:VAL:HG11	1:E:281:LEU:CD1	2.44	0.47
2:O:115:PRO:HG2	2:O:120:ILE:HG12	1.95	0.47
2:O:145:ARG:NE	2:O:170:GLU:OE1	2.47	0.47
2:M:63:LYS:CB	2:M:74:ALA:HB1	2.45	0.47
1:K:369:THR:HG22	1:K:371:SER:N	2.30	0.47
1:L:141:ASN:ND2	1:L:141:ASN:N	2.53	0.47
1:E:118:LYS:HZ3	1:E:118:LYS:HA	1.76	0.47
2:N:3:ILE:O	2:N:121:ALA:HA	2.15	0.47
1:E:96:VAL:HG13	1:E:99:ILE:CD1	2.43	0.47
2:M:10:GLY:HA2	2:M:173:TYR:CE1	2.50	0.47
2:M:43:ILE:HG23	2:M:171:LEU:HD13	1.95	0.47
1:K:344:LEU:HD13	1:K:395:LEU:HD13	1.96	0.47
1:L:257:GLU:HG2	1:L:260:LYS:HG3	1.96	0.47
1:F:110:MET:O	1:F:112:ARG:N	2.48	0.47
1:E:406:ILE:CD1	1:E:420:ILE:HD11	2.45	0.47
2:O:63:LYS:HB3	2:O:74:ALA:HB1	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:261:ILE:CG2	1:F:278:GLN:HG3	2.44	0.47
1:L:131:ILE:CG2	1:L:132:LEU:N	2.77	0.47
2:M:115:PRO:HG2	2:M:120:ILE:HG12	1.95	0.47
2:O:3:ILE:HB	2:O:122:ILE:CG1	2.44	0.47
1:F:365:ASN:HB3	1:F:417:ASN:HD22	1.79	0.47
1:L:147:GLU:HG2	1:L:148:GLN:N	2.29	0.47
1:E:87:THR:HG23	1:E:273:SER:HB2	1.97	0.47
2:M:154:ILE:HD11	2:P:135:ALA:HB2	1.97	0.47
1:L:132:LEU:CG	1:L:160:ARG:HB3	2.44	0.47
1:E:110:MET:O	1:E:112:ARG:N	2.49	0.47
1:F:216:LEU:O	1:F:220:ASP:HB3	2.15	0.47
2:P:138:GLU:HB3	2:P:139:ASN:HD22	1.80	0.47
1:F:141:ASN:C	1:F:142:ASN:HD22	2.18	0.47
2:P:3:ILE:O	2:P:121:ALA:HA	2.15	0.47
1:E:109:LYS:HG2	1:F:296:MET:CG	2.45	0.47
1:K:257:GLU:OE1	1:L:279:ARG:NH1	2.49	0.47
1:L:110:MET:O	1:L:112:ARG:N	2.48	0.47
1:F:153:SER:O	1:F:154:ALA:C	2.53	0.47
1:L:312:ILE:HD11	2:O:59:LEU:O	2.15	0.46
1:K:408:TYR:HE2	1:L:7:ARG:HH22	0.58	0.46
1:E:124:GLU:O	1:E:127:ALA:HB3	2.15	0.46
2:M:168:ILE:HG22	2:M:169:GLU:N	2.30	0.46
1:K:87:THR:HG23	1:K:273:SER:HB2	1.97	0.46
1:K:406:ILE:CD1	1:K:420:ILE:HD11	2.45	0.46
1:F:147:GLU:HG2	1:F:148:GLN:N	2.30	0.46
1:L:141:ASN:C	1:L:142:ASN:HD22	2.18	0.46
1:E:89:VAL:HG11	1:E:94:LYS:O	2.16	0.46
2:N:87:MET:O	2:N:90:LYS:HB3	2.16	0.46
1:F:375:ARG:HB3	1:F:425:VAL:HG11	1.97	0.46
1:L:267:SER:O	1:L:270:PRO:HG2	2.16	0.46
1:L:312:ILE:CA	2:O:62:ARG:CA	2.55	0.46
1:K:110:MET:O	1:K:112:ARG:N	2.49	0.46
1:L:375:ARG:HB3	1:L:425:VAL:HG11	1.97	0.46
2:O:168:ILE:HG22	2:O:169:GLU:N	2.30	0.46
1:L:153:SER:O	1:L:154:ALA:C	2.53	0.46
1:L:145:GLN:HG2	1:L:150:GLN:H	1.64	0.46
1:L:91:TYR:C	1:L:92:VAL:CG1	2.83	0.46
2:O:10:GLY:HA2	2:O:173:TYR:CE1	2.50	0.46
1:L:278:GLN:OE1	1:L:319:ILE:HB	2.15	0.46
1:E:354:GLN:CG	1:F:47:GLU:CB	2.93	0.46
1:K:408:TYR:OH	1:L:7:ARG:CG	2.63	0.46
2:M:160:ILE:CD1	2:O:160:ILE:HG23	2.38	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:124:GLU:O	1:K:127:ALA:HB3	2.15	0.46
2:N:5:SER:O	2:N:119:LEU:HD12	2.15	0.46
1:E:361:THR:HG21	1:F:36:ARG:O	2.15	0.46
1:K:89:VAL:HG11	1:K:94:LYS:O	2.16	0.46
1:L:384:ASN:HD22	1:L:394:ARG:HH11	1.63	0.46
2:M:63:LYS:HB3	2:M:74:ALA:HB1	1.97	0.46
1:L:350:SER:OG	1:L:353:VAL:HG23	2.16	0.46
1:F:350:SER:OG	1:F:353:VAL:HG23	2.16	0.46
1:E:384:ASN:ND2	1:E:394:ARG:HH11	2.13	0.46
1:E:440:ARG:HG2	1:F:316:SER:HB3	1.97	0.46
1:K:139:ALA:CA	1:K:152:PRO:CB	2.79	0.46
2:N:17:ASP:OD1	2:N:33:LYS:NZ	2.49	0.46
1:F:384:ASN:HD22	1:F:394:ARG:HH11	1.63	0.46
2:O:134:ARG:HG3	2:O:134:ARG:HH11	1.81	0.46
1:K:299:THR:O	1:K:301:HIS:N	2.49	0.46
1:F:91:TYR:C	1:F:92:VAL:CG1	2.83	0.46
2:O:63:LYS:CB	2:O:74:ALA:HB1	2.45	0.46
1:E:401:ARG:HH21	1:F:329:ARG:H	1.63	0.46
1:L:319:ILE:HD12	1:L:319:ILE:HA	1.79	0.46
2:M:135:ALA:CB	2:P:154:ILE:HD12	2.30	0.46
1:L:108:VAL:HA	1:L:111:VAL:CG2	2.46	0.46
1:L:293:LYS:HG2	1:L:294:HIS:HD2	1.81	0.46
1:E:369:THR:HG22	1:E:371:SER:N	2.30	0.46
1:K:432:LEU:N	1:K:432:LEU:CD1	2.78	0.46
1:F:112:ARG:HG3	1:F:112:ARG:HH11	1.81	0.46
1:E:299:THR:O	1:E:301:HIS:N	2.49	0.46
1:E:358:LEU:HD21	1:F:37:ARG:CB	2.46	0.46
1:E:309:ALA:O	2:N:66:MET:SD	2.74	0.46
2:M:67:HIS:O	2:M:69:GLY:N	2.49	0.46
2:P:91:LEU:HD12	2:P:91:LEU:O	2.16	0.46
1:E:372:GLY:O	1:E:376:ILE:HG13	2.16	0.46
2:P:99:ASP:OD1	2:P:99:ASP:C	2.55	0.46
1:L:11:SER:O	1:L:14:ASP:HB2	2.15	0.46
1:F:11:SER:O	1:F:14:ASP:HB2	2.15	0.46
1:K:122:ARG:HB2	1:K:122:ARG:HD2	1.92	0.45
1:K:311:GLN:N	2:P:66:MET:HE3	2.31	0.45
1:L:89:VAL:HG12	1:L:94:LYS:O	2.15	0.45
1:F:108:VAL:HA	1:F:111:VAL:CG2	2.46	0.45
2:P:5:SER:O	2:P:119:LEU:HD12	2.15	0.45
1:L:362:GLU:CG	1:L:411:SER:HA	2.45	0.45
2:M:145:ARG:NE	2:M:170:GLU:OE1	2.47	0.45
1:L:365:ASN:HB3	1:L:417:ASN:HD22	1.80	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:441:PHE:HD1	1:F:56:ILE:CG2	2.24	0.45
1:E:122:ARG:HB2	1:E:122:ARG:HD2	1.92	0.45
1:K:293:LYS:HG2	1:K:294:HIS:CD2	2.51	0.45
2:P:36:ARG:CB	2:P:36:ARG:HH11	2.21	0.45
2:M:134:ARG:HH11	2:M:134:ARG:HG3	1.81	0.45
1:F:406:ILE:HG13	1:F:424:TYR:OH	2.16	0.45
2:P:87:MET:O	2:P:90:LYS:HB3	2.16	0.45
1:K:64:THR:HG21	1:K:68:ARG:NH1	2.32	0.45
1:F:134:VAL:O	1:F:135:LEU:HD23	2.16	0.45
1:K:384:ASN:ND2	1:K:394:ARG:HH11	2.14	0.45
2:M:99:ASP:HA	2:M:171:LEU:HD22	1.99	0.45
1:L:124:GLU:HG3	1:L:222:MET:HE3	1.98	0.45
1:F:267:SER:O	1:F:270:PRO:HG2	2.16	0.45
1:E:397:THR:HG23	1:F:327:PRO:HA	1.98	0.45
1:K:293:LYS:CD	1:L:296:MET:HE1	2.47	0.45
1:E:293:LYS:HG2	1:E:294:HIS:CD2	2.51	0.45
2:N:138:GLU:HB3	2:N:139:ASN:HD22	1.80	0.45
2:N:99:ASP:OD1	2:N:99:ASP:C	2.55	0.45
1:L:79:ILE:HD13	1:L:80:LYS:N	2.32	0.45
1:K:442:ILE:O	1:K:442:ILE:HG22	2.17	0.45
1:E:92:VAL:HG11	1:F:92:VAL:HG12	1.93	0.45
1:F:145:GLN:OE1	1:F:149:GLN:HB2	2.16	0.45
1:F:25:ARG:O	1:F:29:ILE:HG13	2.17	0.45
1:E:413:LEU:O	1:E:416:GLN:HG3	2.17	0.45
2:P:17:ASP:OD1	2:P:33:LYS:NZ	2.49	0.45
1:E:269:GLY:N	1:E:270:PRO:HD2	2.32	0.45
1:E:64:THR:HG21	1:E:68:ARG:NH1	2.32	0.45
2:P:116:GLU:HG2	2:P:116:GLU:H	1.42	0.45
2:O:67:HIS:O	2:O:69:GLY:N	2.49	0.45
2:M:36:ARG:C	2:M:37:LEU:HD12	2.37	0.45
1:K:372:GLY:O	1:K:376:ILE:HG13	2.16	0.45
2:P:8:ARG:HB2	2:P:144:ALA:HB2	1.98	0.45
1:L:315:PRO:O	1:L:318:LEU:HB2	2.17	0.45
1:E:125:GLU:O	1:E:128:GLU:HB2	2.17	0.45
1:E:358:LEU:HD23	1:F:40:LEU:HD11	1.98	0.45
1:E:408:TYR:CE2	1:F:7:ARG:HG3	2.51	0.45
1:F:365:ASN:HB3	1:F:417:ASN:ND2	2.32	0.45
1:E:97:ASP:HB2	1:E:101:ARG:NH2	2.32	0.45
1:E:58:PRO:HG2	1:E:61:VAL:HG11	1.99	0.45
1:E:390:ILE:HD13	1:F:323:GLN:HB3	1.99	0.45
2:P:105:ILE:CD1	2:P:120:ILE:HG23	2.44	0.45
2:O:60:PHE:CE2	2:O:97:VAL:HG21	2.52	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:79:ILE:HD13	1:F:80:LYS:N	2.31	0.45
1:K:398:VAL:HG13	1:K:429:LEU:HD13	1.99	0.45
1:K:248:GLU:OE1	1:K:298:LYS:N	2.46	0.45
1:F:315:PRO:O	1:F:318:LEU:HB2	2.17	0.45
1:K:91:TYR:CZ	1:L:272:VAL:HG11	2.52	0.45
2:N:91:LEU:O	2:N:91:LEU:HD12	2.16	0.45
1:F:119:ASN:HD22	1:F:119:ASN:HA	1.57	0.45
1:L:365:ASN:HB3	1:L:417:ASN:ND2	2.32	0.45
1:K:97:ASP:HB2	1:K:101:ARG:NH2	2.31	0.45
1:L:342:ARG:HE	1:L:346:GLU:CD	2.21	0.45
1:E:390:ILE:CG2	1:F:320:PRO:HA	2.46	0.44
1:K:125:GLU:O	1:K:128:GLU:HB2	2.17	0.44
1:E:91:TYR:CB	1:F:91:TYR:N	2.78	0.44
2:M:60:PHE:CE2	2:M:97:VAL:HG21	2.52	0.44
1:F:34:ARG:NH2	1:F:250:HIS:HA	2.32	0.44
2:P:148:ALA:O	2:P:152:LEU:HB2	2.17	0.44
1:L:112:ARG:HH11	1:L:112:ARG:HG3	1.81	0.44
1:L:145:GLN:HB3	1:L:149:GLN:CG	2.47	0.44
1:L:134:VAL:O	1:L:135:LEU:HD23	2.16	0.44
2:O:36:ARG:C	2:O:37:LEU:HD12	2.37	0.44
2:N:8:ARG:HB2	2:N:144:ALA:HB2	1.98	0.44
1:K:413:LEU:O	1:K:416:GLN:HG3	2.17	0.44
1:E:365:ASN:HB3	1:E:417:ASN:HD22	1.81	0.44
1:E:132:LEU:HD22	1:E:132:LEU:HA	1.83	0.44
1:L:217:LYS:O	1:L:221:ALA:N	2.44	0.44
1:E:86:PHE:HB2	1:E:277:VAL:CG1	2.48	0.44
1:K:358:LEU:O	1:K:361:THR:CG2	2.60	0.44
2:N:5:SER:HB3	2:N:120:ILE:CB	2.44	0.44
1:L:389:ASN:C	1:L:389:ASN:ND2	2.69	0.44
2:O:99:ASP:HA	2:O:171:LEU:HD22	1.98	0.44
1:F:406:ILE:O	1:F:410:ALA:N	2.48	0.44
2:N:98:ALA:CB	2:N:103:SER:HB3	2.47	0.44
1:L:406:ILE:HG13	1:L:424:TYR:OH	2.16	0.44
1:L:406:ILE:O	1:L:410:ALA:N	2.48	0.44
2:M:92:GLU:HG3	2:M:92:GLU:O	2.16	0.44
1:K:264:ARG:O	1:K:266:GLU:N	2.50	0.44
1:F:141:ASN:O	1:F:142:ASN:CB	2.62	0.44
1:E:256:ASP:O	1:E:257:GLU:HB2	2.17	0.44
1:L:34:ARG:NH2	1:L:250:HIS:HA	2.32	0.44
1:L:25:ARG:O	1:L:29:ILE:HG13	2.17	0.44
1:E:398:VAL:HG13	1:E:429:LEU:HD13	1.99	0.44
1:E:442:ILE:O	1:E:442:ILE:HG22	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:83:ALA:HB1	1:L:261:ILE:HG13	2.00	0.44
1:L:145:GLN:CG	1:L:150:GLN:CA	2.87	0.44
1:K:293:LYS:HG2	1:K:294:HIS:HD2	1.83	0.44
1:E:293:LYS:HG2	1:E:294:HIS:HD2	1.83	0.44
1:K:86:PHE:HB2	1:K:277:VAL:CG1	2.48	0.44
2:N:60:PHE:HE2	2:N:97:VAL:HG21	1.79	0.44
1:K:365:ASN:HB3	1:K:417:ASN:HD22	1.81	0.44
2:M:43:ILE:O	2:M:43:ILE:HG13	2.17	0.44
2:P:98:ALA:CB	2:P:103:SER:HB3	2.47	0.44
1:F:342:ARG:HE	1:F:346:GLU:CD	2.21	0.44
1:L:264:ARG:CD	2:O:62:ARG:HD3	2.38	0.44
2:O:66:MET:C	2:O:67:HIS:ND1	2.71	0.44
1:K:145:GLN:HB2	1:K:149:GLN:C	2.38	0.44
1:F:145:GLN:CG	1:F:150:GLN:CA	2.87	0.44
2:M:66:MET:C	2:M:67:HIS:ND1	2.71	0.44
1:F:293:LYS:HG2	1:F:294:HIS:HD2	1.81	0.44
1:E:264:ARG:O	1:E:266:GLU:N	2.50	0.44
1:F:62:GLY:O	1:F:66:ILE:HG13	2.18	0.44
1:F:393:ARG:HA	1:F:396:HIS:CD2	2.53	0.44
1:E:135:LEU:HD13	1:E:159:PHE:CD1	2.52	0.44
2:N:46:PHE:HB3	2:N:57:PHE:CZ	2.53	0.44
2:P:88:LEU:H	2:P:88:LEU:CD2	2.28	0.44
1:K:269:GLY:N	1:K:270:PRO:HD2	2.32	0.44
2:N:148:ALA:O	2:N:152:LEU:HB2	2.17	0.44
1:L:100:ILE:HG13	1:L:290:VAL:HG21	1.99	0.44
1:E:145:GLN:HB2	1:E:149:GLN:C	2.38	0.44
2:P:62:ARG:O	2:P:65:GLU:HB2	2.17	0.44
1:F:131:ILE:HD13	1:F:134:VAL:HG12	2.00	0.44
2:O:36:ARG:NH1	2:O:40:ASP:HB3	2.33	0.44
1:L:62:GLY:O	1:L:66:ILE:HG13	2.18	0.44
2:P:108:GLY:C	2:P:110:GLY:H	2.21	0.44
2:M:44:ALA:HB2	2:M:97:VAL:HG23	2.00	0.44
1:K:58:PRO:HG2	1:K:61:VAL:HG11	1.99	0.44
2:N:21:THR:HG22	2:N:22:LEU:H	1.81	0.44
1:L:282:LEU:HD21	1:L:321:GLU:HG2	2.00	0.44
1:F:64:THR:HG22	1:F:68:ARG:HD2	2.00	0.44
1:E:354:GLN:CG	1:F:47:GLU:HB2	2.48	0.44
1:L:131:ILE:HD13	1:L:134:VAL:HG12	2.00	0.44
2:N:36:ARG:CB	2:N:36:ARG:HH11	2.21	0.44
2:P:5:SER:HB3	2:P:120:ILE:CB	2.45	0.44
2:N:1:THR:HB	2:N:33:LYS:HZ2	1.82	0.44
1:K:135:LEU:HD13	1:K:159:PHE:CD1	2.52	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:380:ALA:HA	1:L:394:ARG:HG2	2.00	0.44
2:M:131:ALA:HB1	2:P:154:ILE:HG22	1.99	0.43
1:K:94:LYS:HD3	1:K:94:LYS:HA	1.74	0.43
1:F:380:ALA:HA	1:F:394:ARG:HG2	2.00	0.43
1:F:362:GLU:CG	1:F:411:SER:HA	2.46	0.43
2:P:60:PHE:HE2	2:P:97:VAL:HG21	1.79	0.43
1:L:113:VAL:O	1:L:117:GLU:HG3	2.18	0.43
2:M:21:THR:CG2	2:M:22:LEU:N	2.81	0.43
1:L:21:ASP:OD2	1:L:25:ARG:HD2	2.18	0.43
1:F:237:GLU:OE2	1:F:237:GLU:HA	2.18	0.43
1:L:263:LYS:HB3	1:L:264:ARG:H	1.36	0.43
1:E:359:MET:HE3	1:F:36:ARG:NH1	2.31	0.43
1:K:119:ASN:HA	1:K:119:ASN:HD22	1.56	0.43
2:M:160:ILE:CG2	2:O:160:ILE:HD11	2.40	0.43
2:O:43:ILE:O	2:O:43:ILE:HG13	2.17	0.43
2:N:39:ASN:O	2:N:41:LYS:HG3	2.18	0.43
1:L:118:LYS:HA	1:L:118:LYS:HE2	2.00	0.43
1:L:237:GLU:OE2	1:L:237:GLU:HA	2.18	0.43
1:E:56:ILE:HA	1:E:308:GLY:O	2.18	0.43
1:F:83:ALA:HB1	1:F:261:ILE:HG13	2.00	0.43
1:K:120:ARG:HD2	1:K:121:TYR:N	2.33	0.43
2:P:46:PHE:HB3	2:P:57:PHE:CZ	2.53	0.43
2:N:108:GLY:C	2:N:110:GLY:H	2.21	0.43
1:F:34:ARG:CZ	1:F:250:HIS:HA	2.47	0.43
1:K:40:LEU:O	1:K:45:ARG:NH1	2.52	0.43
1:K:336:THR:O	1:K:339:ASP:HB2	2.19	0.43
2:O:92:GLU:O	2:O:92:GLU:HG3	2.16	0.43
1:F:21:ASP:OD2	1:F:25:ARG:HD2	2.18	0.43
1:F:89:VAL:HG12	1:F:94:LYS:O	2.15	0.43
1:L:131:ILE:O	1:L:135:LEU:HG	2.19	0.43
2:M:36:ARG:NH1	2:M:40:ASP:HB3	2.33	0.43
1:E:89:VAL:HG12	1:E:94:LYS:N	2.25	0.43
1:L:238:GLU:O	1:L:242:ASP:N	2.49	0.43
1:K:256:ASP:O	1:K:257:GLU:HB2	2.17	0.43
1:F:100:ILE:HG13	1:F:290:VAL:HG21	1.99	0.43
2:N:62:ARG:O	2:N:65:GLU:HB2	2.18	0.43
1:E:112:ARG:O	1:E:115:ALA:N	2.51	0.43
1:K:56:ILE:HA	1:K:308:GLY:O	2.18	0.43
2:O:44:ALA:HB2	2:O:97:VAL:HG23	2.00	0.43
2:O:21:THR:CG2	2:O:22:LEU:N	2.81	0.43
1:E:442:ILE:CD1	1:F:329:ARG:CB	2.97	0.43
1:F:145:GLN:CD	1:F:145:GLN:O	2.57	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:86:PHE:HB2	1:L:277:VAL:CG1	2.47	0.43
1:E:119:ASN:HD22	1:E:119:ASN:HA	1.56	0.43
1:F:113:VAL:O	1:F:117:GLU:HG3	2.19	0.43
1:E:241:GLN:O	1:E:241:GLN:HG2	2.18	0.43
1:L:275:GLU:O	1:L:278:GLN:HB2	2.19	0.43
1:F:145:GLN:HB3	1:F:149:GLN:CG	2.47	0.43
1:F:275:GLU:O	1:F:278:GLN:HB2	2.19	0.43
1:K:278:GLN:CD	1:K:319:ILE:HG23	2.39	0.43
2:M:98:ALA:HA	2:M:103:SER:HA	2.00	0.43
2:P:39:ASN:O	2:P:41:LYS:HG3	2.18	0.43
2:N:15:ALA:HB1	2:N:152:LEU:HD12	2.01	0.43
1:E:139:ALA:N	1:E:152:PRO:HB3	2.32	0.43
1:E:349:ALA:CB	1:F:47:GLU:CG	2.69	0.43
1:F:86:PHE:HB2	1:F:277:VAL:CG1	2.47	0.43
2:N:3:ILE:HD11	2:N:46:PHE:C	2.39	0.43
2:N:114:GLN:HA	2:N:115:PRO:HD2	1.84	0.43
1:F:282:LEU:HD21	1:F:321:GLU:HG2	2.00	0.43
1:E:92:VAL:HG22	1:E:93:GLY:H	1.84	0.43
2:P:21:THR:HG22	2:P:22:LEU:H	1.82	0.43
2:M:125:GLY:HA2	2:M:128:TYR:CD2	2.53	0.43
2:N:4:VAL:CG2	2:N:152:LEU:HG	2.49	0.43
2:M:87:MET:O	2:M:90:LYS:HB3	2.19	0.43
1:E:336:THR:O	1:E:339:ASP:HB2	2.19	0.43
1:E:440:ARG:C	1:F:315:PRO:HD2	2.38	0.43
1:E:132:LEU:HD21	1:E:160:ARG:HA	2.01	0.43
1:K:131:ILE:HD12	1:K:134:VAL:HG11	2.01	0.43
1:F:293:LYS:HG2	1:F:294:HIS:CD2	2.54	0.43
1:L:293:LYS:HG2	1:L:294:HIS:CD2	2.54	0.43
1:L:136:ILE:HG22	1:L:138:PRO:CD	2.42	0.43
1:L:393:ARG:HA	1:L:396:HIS:CD2	2.53	0.43
2:M:76:VAL:HA	2:M:112:VAL:HG21	2.00	0.43
2:M:42:VAL:HG21	2:M:64:LEU:HD13	2.01	0.43
1:E:354:GLN:CG	1:F:47:GLU:HB3	2.49	0.42
1:K:139:ALA:N	1:K:152:PRO:HB3	2.32	0.42
1:K:264:ARG:C	1:K:266:GLU:N	2.72	0.42
1:E:120:ARG:HD2	1:E:121:TYR:N	2.33	0.42
2:O:98:ALA:HA	2:O:103:SER:HA	2.00	0.42
1:E:109:LYS:HG2	1:F:296:MET:HG3	2.01	0.42
2:O:13:VAL:CG1	2:O:170:GLU:HG3	2.49	0.42
1:L:34:ARG:CZ	1:L:250:HIS:HA	2.47	0.42
1:F:118:LYS:HE2	1:F:118:LYS:HA	2.00	0.42
1:E:417:ASN:HA	1:E:417:ASN:HD22	1.65	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:N:114:GLN:HG3	2:N:114:GLN:O	2.19	0.42
2:O:125:GLY:HA2	2:O:128:TYR:CD2	2.53	0.42
1:E:40:LEU:O	1:E:45:ARG:NH1	2.51	0.42
2:N:153:ASP:OD1	2:N:164:HIS:HD2	2.02	0.42
1:E:91:TYR:C	1:E:92:VAL:CG1	2.88	0.42
1:K:91:TYR:C	1:K:92:VAL:CG1	2.87	0.42
1:L:292:THR:C	1:L:294:HIS:N	2.73	0.42
1:F:124:GLU:HG3	1:F:222:MET:HE3	2.01	0.42
1:E:340:PHE:CD2	1:E:395:LEU:HD21	2.54	0.42
1:F:4:MET:HE3	1:F:73:LEU:HG	2.02	0.42
1:K:241:GLN:HG2	1:K:241:GLN:O	2.18	0.42
1:E:384:ASN:HD22	1:E:394:ARG:NH1	2.16	0.42
1:F:131:ILE:O	1:F:135:LEU:HG	2.19	0.42
2:P:134:ARG:HH11	2:P:134:ARG:CG	2.33	0.42
1:L:384:ASN:HA	1:L:384:ASN:HD22	1.64	0.42
2:N:99:ASP:O	2:N:100:GLU:C	2.58	0.42
2:M:98:ALA:O	2:M:99:ASP:HB3	2.19	0.42
1:F:375:ARG:CZ	1:F:422:ALA:HB1	2.50	0.42
1:L:18:ILE:CD1	1:L:347:PRO:HG3	2.49	0.42
1:F:257:GLU:OE1	1:F:260:LYS:NZ	2.53	0.42
1:E:335:LEU:HD22	1:E:339:ASP:HB3	2.01	0.42
1:F:310:PHE:HB3	1:F:313:ALA:O	2.19	0.42
2:O:87:MET:O	2:O:90:LYS:HB3	2.19	0.42
1:K:132:LEU:HD21	1:K:160:ARG:HA	2.01	0.42
2:N:58:GLU:HG3	2:N:62:ARG:NE	2.34	0.42
2:N:134:ARG:HH11	2:N:134:ARG:CG	2.33	0.42
1:L:397:THR:HG21	1:L:443:LEU:HA	2.00	0.42
1:F:112:ARG:O	1:F:115:ALA:N	2.53	0.42
2:P:153:ASP:OD1	2:P:164:HIS:HD2	2.02	0.42
1:E:91:TYR:O	1:E:92:VAL:HG13	2.19	0.42
1:K:112:ARG:O	1:K:115:ALA:N	2.51	0.42
1:K:264:ARG:HA	2:P:62:ARG:HH22	1.84	0.42
1:K:91:TYR:O	1:K:92:VAL:HG13	2.19	0.42
1:F:131:ILE:HD13	1:F:131:ILE:O	2.20	0.42
2:P:3:ILE:HD11	2:P:46:PHE:C	2.39	0.42
1:K:345:THR:HG22	1:K:352:THR:HG21	2.01	0.42
1:F:442:ILE:O	1:F:443:LEU:HD23	2.20	0.42
1:F:397:THR:HG21	1:F:443:LEU:HA	2.00	0.42
2:P:4:VAL:CG2	2:P:152:LEU:HG	2.49	0.42
1:E:248:GLU:OE1	1:E:298:LYS:N	2.46	0.42
1:E:91:TYR:CD1	1:F:90:GLY:C	2.83	0.42
1:F:130:ARG:NH1	1:F:131:ILE:CA	2.82	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:278:GLN:CD	1:E:319:ILE:HG23	2.39	0.42
1:L:52:ASN:HB2	1:L:325:ARG:O	2.19	0.42
1:L:375:ARG:CZ	1:L:422:ALA:HB1	2.50	0.42
1:E:139:ALA:CA	1:E:152:PRO:CB	2.79	0.42
1:E:91:TYR:CE2	1:F:91:TYR:CD2	3.08	0.42
1:F:94:LYS:HZ2	1:F:98:SER:HB3	1.83	0.42
1:K:118:LYS:HZ3	1:K:118:LYS:HA	1.83	0.42
2:M:99:ASP:O	2:M:100:GLU:C	2.58	0.42
1:F:4:MET:HB3	1:F:8:GLU:CB	2.50	0.42
1:E:398:VAL:HG13	1:E:429:LEU:CD1	2.50	0.42
1:K:74:ALA:O	1:K:75:ASN:HB3	2.20	0.42
1:L:64:THR:HG22	1:L:68:ARG:HD2	2.00	0.42
1:E:354:GLN:OE1	1:F:48:VAL:CG2	2.67	0.42
1:K:111:VAL:CG2	1:K:243:ALA:HB2	2.49	0.42
1:E:111:VAL:CG2	1:E:243:ALA:HB2	2.49	0.42
1:F:136:ILE:O	1:F:138:PRO:HD2	2.20	0.42
2:N:37:LEU:N	2:N:37:LEU:HD12	2.34	0.42
1:L:398:VAL:HG13	1:L:429:LEU:HD13	2.00	0.42
1:K:340:PHE:CD2	1:K:395:LEU:HD21	2.54	0.42
1:L:442:ILE:O	1:L:443:LEU:HD23	2.20	0.42
2:N:169:GLU:OE2	2:N:169:GLU:HA	2.20	0.42
1:E:441:PHE:C	1:F:329:ARG:HG3	2.40	0.42
2:O:42:VAL:HG21	2:O:64:LEU:HD13	2.02	0.42
2:P:58:GLU:HG3	2:P:62:ARG:NE	2.34	0.42
1:L:136:ILE:O	1:L:138:PRO:HD2	2.20	0.42
2:O:140:THR:CG2	2:O:141:GLU:N	2.83	0.42
1:E:5:THR:HG1	1:E:8:GLU:HG3	1.82	0.42
2:O:99:ASP:O	2:O:100:GLU:C	2.58	0.42
1:E:345:THR:HG22	1:E:352:THR:HG21	2.01	0.42
1:F:18:ILE:CD1	1:F:347:PRO:HG3	2.49	0.42
1:L:15:LYS:HB3	1:L:348:ASN:HD21	1.85	0.42
1:E:329:ARG:HG3	1:E:329:ARG:NH1	2.35	0.42
1:L:257:GLU:OE1	1:L:260:LYS:NZ	2.53	0.42
1:L:261:ILE:CG2	1:L:278:GLN:HG3	2.44	0.42
1:L:310:PHE:HB3	1:L:313:ALA:O	2.19	0.42
1:E:131:ILE:HD12	1:E:134:VAL:HG11	2.01	0.42
1:E:411:SER:HB3	1:F:32:ARG:HH21	1.75	0.42
1:F:263:LYS:HB3	1:F:264:ARG:H	1.36	0.42
1:F:351:ILE:HG13	1:F:399:LEU:HD22	2.02	0.42
2:O:2:THR:HG1	2:O:162:THR:HG21	1.76	0.42
2:O:76:VAL:HA	2:O:112:VAL:HG21	2.00	0.42
1:L:112:ARG:O	1:L:115:ALA:N	2.53	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:74:ALA:O	1:E:75:ASN:HB3	2.20	0.42
1:K:227:GLU:HG2	1:K:227:GLU:O	2.20	0.42
1:E:441:PHE:O	1:F:329:ARG:HG3	2.15	0.41
1:E:88:GLU:CD	1:F:89:VAL:O	2.58	0.41
2:M:1:THR:CA	2:M:162:THR:HG22	2.50	0.41
2:O:50:THR:HG21	2:P:111:ASP:CG	2.39	0.41
2:M:13:VAL:CG1	2:M:170:GLU:HG3	2.49	0.41
1:K:329:ARG:HG3	1:K:329:ARG:NH1	2.35	0.41
1:K:398:VAL:HG13	1:K:429:LEU:CD1	2.50	0.41
2:O:121:ALA:O	2:O:126:GLY:HA3	2.20	0.41
1:F:264:ARG:HH11	1:F:312:ILE:HD12	1.85	0.41
2:P:66:MET:O	2:P:67:HIS:ND1	2.53	0.41
1:E:408:TYR:C	1:F:6:PRO:HG2	2.39	0.41
2:P:37:LEU:HD12	2:P:37:LEU:N	2.34	0.41
1:L:91:TYR:O	1:L:92:VAL:HG12	2.20	0.41
1:F:229:GLU:O	1:F:232:LYS:HG2	2.20	0.41
2:M:148:ALA:O	2:M:152:LEU:HB2	2.19	0.41
2:O:148:ALA:O	2:O:152:LEU:HB2	2.19	0.41
1:L:397:THR:CG2	1:L:443:LEU:HA	2.50	0.41
1:F:15:LYS:HB3	1:F:348:ASN:HD21	1.85	0.41
2:N:98:ALA:HB2	2:N:103:SER:HB3	2.03	0.41
1:L:74:ALA:O	1:L:75:ASN:HB3	2.20	0.41
1:E:440:ARG:O	1:F:315:PRO:HD2	2.20	0.41
1:E:139:ALA:CB	1:E:152:PRO:CD	2.92	0.41
1:K:110:MET:O	1:K:111:VAL:C	2.59	0.41
1:L:130:ARG:NH1	1:L:131:ILE:CA	2.83	0.41
1:L:229:GLU:O	1:L:232:LYS:HG2	2.20	0.41
1:F:52:ASN:HB2	1:F:325:ARG:O	2.19	0.41
2:P:15:ALA:HB1	2:P:152:LEU:HD12	2.01	0.41
1:K:335:LEU:HD22	1:K:339:ASP:HB3	2.01	0.41
1:F:74:ALA:O	1:F:75:ASN:HB3	2.20	0.41
1:E:160:ARG:O	1:E:163:LEU:HB3	2.20	0.41
1:K:108:VAL:O	1:K:110:MET:N	2.54	0.41
1:E:94:LYS:HD3	1:E:94:LYS:HA	1.74	0.41
1:E:257:GLU:OE1	1:F:279:ARG:CG	2.63	0.41
2:N:121:ALA:HB1	2:N:126:GLY:O	2.20	0.41
1:F:398:VAL:HG13	1:F:429:LEU:HD13	2.01	0.41
2:M:99:ASP:HA	2:M:171:LEU:CD2	2.51	0.41
1:F:238:GLU:CD	1:F:238:GLU:H	2.22	0.41
1:K:219:LYS:CG	1:K:220:ASP:N	2.84	0.41
2:P:114:GLN:HG3	2:P:114:GLN:O	2.20	0.41
1:E:131:ILE:HD12	1:E:134:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:108:VAL:O	1:E:110:MET:N	2.54	0.41
1:L:91:TYR:HD2	1:L:91:TYR:HA	1.76	0.41
2:O:99:ASP:HA	2:O:171:LEU:CD2	2.50	0.41
1:F:397:THR:CG2	1:F:443:LEU:HA	2.50	0.41
1:L:442:ILE:O	1:L:442:ILE:HG22	2.20	0.41
1:L:119:ASN:HA	1:L:119:ASN:HD22	1.57	0.41
2:N:136:LEU:HB3	2:N:147:ILE:HG12	2.02	0.41
2:P:169:GLU:HA	2:P:169:GLU:OE2	2.20	0.41
1:K:160:ARG:O	1:K:163:LEU:HB3	2.20	0.41
2:N:66:MET:O	2:N:67:HIS:ND1	2.53	0.41
1:K:92:VAL:HG22	1:K:93:GLY:H	1.84	0.41
1:L:87:THR:HG23	1:L:277:VAL:HG21	2.02	0.41
1:F:87:THR:HG23	1:F:277:VAL:HG21	2.02	0.41
1:E:282:LEU:N	1:E:283:PRO:HD2	2.35	0.41
1:L:384:ASN:HD21	1:L:390:ILE:H	1.69	0.41
2:P:121:ALA:HB1	2:P:126:GLY:O	2.20	0.41
1:E:222:MET:O	1:E:226:ILE:N	2.53	0.41
1:L:232:LYS:HB3	1:L:232:LYS:HE2	1.76	0.41
2:N:99:ASP:HA	2:N:171:LEU:CD2	2.51	0.41
1:L:374:LYS:HG2	1:L:375:ARG:N	2.35	0.41
2:P:98:ALA:HB2	2:P:103:SER:HB3	2.03	0.41
1:K:97:ASP:OD1	1:K:97:ASP:N	2.52	0.41
2:M:121:ALA:HB1	2:M:126:GLY:O	2.19	0.41
2:P:43:ILE:O	2:P:43:ILE:HG13	2.20	0.41
1:F:359:MET:HG3	1:F:366:ILE:HG13	2.03	0.41
1:K:417:ASN:HD22	1:K:417:ASN:HA	1.65	0.41
2:M:121:ALA:O	2:M:126:GLY:HA3	2.20	0.41
2:N:19:GLN:HB2	2:N:163:ASN:ND2	2.36	0.41
1:K:342:ARG:HE	1:K:346:GLU:CD	2.23	0.41
1:F:13:LEU:HD12	1:F:13:LEU:HA	1.93	0.41
1:L:382:GLN:HA	1:L:382:GLN:OE1	2.20	0.41
1:E:441:PHE:C	1:F:329:ARG:CG	2.89	0.41
1:L:150:GLN:O	1:L:152:PRO:HD3	2.21	0.41
1:L:351:ILE:HG13	1:L:399:LEU:HD22	2.02	0.41
1:L:131:ILE:HD13	1:L:131:ILE:O	2.20	0.41
2:P:99:ASP:O	2:P:100:GLU:C	2.58	0.41
1:K:281:LEU:HA	1:K:281:LEU:HD12	1.83	0.41
2:M:98:ALA:O	2:M:99:ASP:CB	2.68	0.41
2:O:88:LEU:H	2:O:88:LEU:CD2	2.34	0.41
2:O:121:ALA:HB1	2:O:126:GLY:O	2.20	0.41
2:P:136:LEU:HB3	2:P:147:ILE:HG12	2.02	0.41
1:E:388:GLU:OE2	1:F:323:GLN:NE2	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:358:LEU:HD21	1:F:37:ARG:HB2	2.01	0.41
1:F:150:GLN:O	1:F:152:PRO:HD3	2.20	0.41
1:E:404:GLU:O	1:F:29:ILE:HD13	2.20	0.41
2:M:154:ILE:HG23	2:P:131:ALA:CB	2.45	0.41
1:F:292:THR:C	1:F:294:HIS:N	2.73	0.41
1:E:400:GLU:CD	1:F:51:LYS:HZ2	2.10	0.41
2:M:140:THR:CG2	2:M:141:GLU:N	2.83	0.41
1:E:369:THR:HG22	1:E:372:GLY:N	2.20	0.41
1:L:384:ASN:CG	1:L:394:ARG:HD2	2.41	0.41
1:L:232:LYS:O	1:L:232:LYS:HG3	2.21	0.41
2:O:98:ALA:O	2:O:99:ASP:CB	2.68	0.41
2:O:98:ALA:O	2:O:99:ASP:HB3	2.19	0.41
1:L:4:MET:HB3	1:L:8:GLU:CB	2.50	0.41
2:M:51:ALA:HB1	2:N:83:ARG:NH2	2.35	0.41
2:N:39:ASN:HB2	2:N:41:LYS:HE3	2.03	0.41
2:P:114:GLN:HA	2:P:115:PRO:HD2	1.84	0.41
1:L:13:LEU:HA	1:L:13:LEU:HD12	1.93	0.41
1:L:42:GLU:HA	1:L:45:ARG:NH2	2.36	0.41
2:M:91:LEU:O	2:M:91:LEU:HD12	2.21	0.41
1:E:358:LEU:HD23	1:F:36:ARG:C	2.41	0.41
1:K:157:GLN:O	1:K:160:ARG:HB3	2.21	0.41
1:K:261:ILE:HD13	1:K:277:VAL:CB	2.49	0.41
1:K:282:LEU:N	1:K:283:PRO:HD2	2.35	0.41
1:F:232:LYS:O	1:F:232:LYS:HG3	2.21	0.41
1:K:84:THR:OG1	1:K:257:GLU:OE2	2.34	0.41
1:K:231:ALA:C	1:K:233:LEU:H	2.24	0.41
1:E:342:ARG:NH2	1:E:346:GLU:OE2	2.50	0.41
1:F:40:LEU:O	1:F:45:ARG:NH1	2.54	0.40
1:L:145:GLN:CD	1:L:145:GLN:O	2.57	0.40
1:F:136:ILE:HG22	1:F:138:PRO:CD	2.42	0.40
1:K:384:ASN:HD22	1:K:394:ARG:NH1	2.17	0.40
2:N:100:GLU:HG2	2:N:173:TYR:CG	2.56	0.40
1:L:122:ARG:CG	1:L:122:ARG:NH2	2.82	0.40
1:E:12:GLU:O	1:E:15:LYS:HB2	2.20	0.40
1:E:97:ASP:OD1	1:E:97:ASP:N	2.52	0.40
1:E:227:GLU:O	1:E:227:GLU:HG2	2.20	0.40
1:E:393:ARG:CZ	1:F:321:GLU:HA	2.46	0.40
1:L:309:ALA:CA	2:O:66:MET:CE	2.94	0.40
1:E:157:GLN:O	1:E:160:ARG:HB3	2.21	0.40
1:K:139:ALA:N	1:K:152:PRO:CB	2.85	0.40
1:E:248:GLU:HG3	1:E:297:VAL:HG13	2.04	0.40
1:K:75:ASN:ND2	1:K:75:ASN:O	2.54	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:75:ASN:ND2	1:E:75:ASN:O	2.54	0.40
2:N:62:ARG:HA	2:N:65:GLU:HG3	2.03	0.40
1:E:110:MET:O	1:E:111:VAL:C	2.59	0.40
1:E:130:ARG:O	1:E:133:ASP:HB3	2.22	0.40
1:K:130:ARG:O	1:K:133:ASP:HB3	2.22	0.40
1:K:4:MET:HB2	1:K:8:GLU:HB2	2.03	0.40
2:N:105:ILE:CD1	2:N:120:ILE:HG23	2.44	0.40
2:M:3:ILE:HD11	2:M:46:PHE:C	2.42	0.40
1:K:12:GLU:O	1:K:15:LYS:HB2	2.20	0.40
1:E:219:LYS:CG	1:E:220:ASP:N	2.84	0.40
1:E:53:ILE:HG12	1:E:328:ILE:CG2	2.51	0.40
1:E:231:ALA:C	1:E:233:LEU:H	2.24	0.40
2:N:43:ILE:HG13	2:N:43:ILE:O	2.21	0.40
1:F:264:ARG:CZ	2:M:62:ARG:HG3	2.20	0.40
2:M:154:ILE:HD13	2:P:131:ALA:O	2.21	0.40
2:N:121:ALA:O	2:N:126:GLY:HA3	2.21	0.40
2:P:121:ALA:O	2:P:126:GLY:HA3	2.21	0.40
1:K:222:MET:O	1:K:226:ILE:N	2.53	0.40
2:M:88:LEU:CD2	2:M:88:LEU:H	2.33	0.40
2:O:3:ILE:HD11	2:O:46:PHE:C	2.42	0.40
1:F:406:ILE:HD13	1:F:418:ILE:HG21	2.02	0.40
1:L:359:MET:HG3	1:L:366:ILE:HG13	2.02	0.40
1:E:346:GLU:O	1:E:347:PRO:C	2.59	0.40
1:K:53:ILE:HG12	1:K:328:ILE:CG2	2.51	0.40
1:L:97:ASP:N	1:L:97:ASP:OD1	2.54	0.40
1:F:382:GLN:OE1	1:F:382:GLN:HA	2.20	0.40
1:L:266:GLU:HB3	1:L:267:SER:H	1.75	0.40
1:K:131:ILE:HD12	1:K:134:VAL:HG12	2.02	0.40
2:P:62:ARG:HA	2:P:65:GLU:HG3	2.03	0.40
1:L:421:ASP:OD2	1:L:423:ASP:HB2	2.21	0.40
1:E:235:ASN:HA	1:E:236:PRO:HD2	1.88	0.40
2:P:140:THR:HG22	2:P:142:LEU:HG	2.00	0.40
2:M:88:LEU:N	2:M:88:LEU:HD22	2.36	0.40
1:F:374:LYS:HG2	1:F:375:ARG:N	2.35	0.40
2:N:22:LEU:HB2	2:N:27:MET:HE2	2.02	0.40
1:F:442:ILE:HG22	1:F:442:ILE:O	2.20	0.40
1:K:217:LYS:CB	1:K:220:ASP:HB3	2.52	0.40
2:O:91:LEU:O	2:O:91:LEU:HD12	2.21	0.40

All (305) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:51:LYS:CG	1:L:400:GLU:OE1[3_665]	0.41	1.79
1:K:35:TRP:CE3	1:L:362:GLU:OE2[3_665]	0.55	1.65
1:K:47:GLU:O	1:L:354:GLN:OE1[3_665]	0.59	1.61
1:E:316:SER:CB	1:F:440:ARG:O[2_655]	0.62	1.58
1:K:315:PRO:CA	1:L:440:ARG:O[3_665]	0.66	1.54
1:K:32:ARG:NE	1:L:411:SER:OG[3_665]	0.69	1.51
1:K:33:ASN:OD1	1:L:407:SER:OG[3_665]	0.73	1.47
1:K:36:ARG:NE	1:L:410:ALA:CB[3_665]	0.74	1.46
1:K:35:TRP:CE3	1:L:362:GLU:CD[3_665]	0.75	1.45
1:E:36:ARG:NE	1:F:362:GLU:OE1[2_655]	0.76	1.44
1:E:314:LYS:CG	1:F:441:PHE:CZ[2_655]	0.78	1.42
1:K:32:ARG:CZ	1:L:411:SER:CB[3_665]	0.80	1.40
1:K:51:LYS:NZ	1:L:355:TYR:CZ[3_665]	0.81	1.39
1:K:48:VAL:CG1	1:L:358:LEU:CD1[3_665]	0.82	1.38
1:K:36:ARG:NH2	1:L:410:ALA:N[3_665]	0.85	1.35
1:K:316:SER:OG	1:L:440:ARG:CG[3_665]	0.88	1.32
1:E:314:LYS:CD	1:F:441:PHE:CE2[2_655]	0.89	1.31
2:O:83:ARG:NE	2:P:90:LYS:CD[2_655]	0.93	1.27
1:F:427:LYS:NZ	1:L:149:GLN:OE1[4_545]	0.97	1.23
1:K:329:ARG:NH1	1:L:443:LEU:N[3_665]	0.97	1.23
1:K:323:GLN:OE1	1:L:394:ARG:NH2[3_665]	0.99	1.21
1:K:40:LEU:CD2	1:L:357:ALA:O[3_665]	1.00	1.20
1:K:32:ARG:NH2	1:L:411:SER:CB[3_665]	1.02	1.18
1:K:47:GLU:C	1:L:354:GLN:OE1[3_665]	1.02	1.18
1:K:28:ALA:CB	1:L:408:TYR:CE1[3_665]	1.04	1.16
1:K:315:PRO:CG	1:L:441:PHE:CA[3_665]	1.09	1.11
1:K:329:ARG:N	1:L:401:ARG:NH2[3_665]	1.09	1.11
1:K:35:TRP:CD2	1:L:362:GLU:OE2[3_665]	1.10	1.10
1:K:315:PRO:C	1:L:440:ARG:O[3_665]	1.11	1.09
1:F:149:GLN:OE1	1:F:367:GLU:OE1[5_556]	1.12	1.08
1:E:314:LYS:CG	1:F:441:PHE:CE2[2_655]	1.13	1.07
1:K:51:LYS:NZ	1:L:355:TYR:CE2[3_665]	1.15	1.05
1:E:316:SER:CB	1:F:440:ARG:C[2_655]	1.17	1.03
1:K:310:PHE:CG	1:L:441:PHE:CE1[3_665]	1.18	1.02
1:K:40:LEU:CG	1:L:357:ALA:O[3_665]	1.19	1.01
1:K:320:PRO:CB	1:L:390:ILE:CB[3_665]	1.19	1.01
1:K:320:PRO:CB	1:L:390:ILE:CG2[3_665]	1.19	1.01
1:K:37:ARG:CG	1:L:358:LEU:CD2[3_665]	1.20	1.00
1:K:47:GLU:O	1:L:354:GLN:CD[3_665]	1.21	0.99
1:K:47:GLU:OE1	1:L:349:ALA:O[3_665]	1.22	0.98
1:K:6:PRO:CG	1:L:408:TYR:O[3_665]	1.23	0.97
1:K:310:PHE:CB	1:L:441:PHE:CE1[3_665]	1.24	0.96
1:K:328:ILE:CG2	1:L:404:GLU:OE1[3_665]	1.24	0.96

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:316:SER:CA	1:F:440:ARG:O[2_655]	1.26	0.94
1:K:36:ARG:CZ	1:L:410:ALA:CB[3_665]	1.26	0.94
1:K:323:GLN:O	1:L:397:THR:OG1[3_665]	1.27	0.93
1:K:315:PRO:CB	1:L:441:PHE:CA[3_665]	1.28	0.92
1:K:39:GLN:CB	1:L:361:THR:O[3_665]	1.30	0.90
1:K:310:PHE:CB	1:L:441:PHE:CZ[3_665]	1.30	0.90
2:O:83:ARG:CD	2:P:90:LYS:NZ[2_655]	1.30	0.90
1:K:32:ARG:NE	1:L:411:SER:CB[3_665]	1.31	0.89
1:K:51:LYS:CB	1:L:400:GLU:OE1[3_665]	1.31	0.89
1:K:316:SER:OG	1:L:440:ARG:CD[3_665]	1.32	0.88
1:F:427:LYS:CE	1:L:149:GLN:OE1[4_545]	1.34	0.86
1:K:47:GLU:CB	1:L:354:GLN:CG[3_665]	1.34	0.86
1:K:39:GLN:CB	1:L:361:THR:C[3_665]	1.36	0.84
1:K:329:ARG:NH1	1:L:442:ILE:C[3_665]	1.36	0.84
1:K:35:TRP:CZ3	1:L:362:GLU:OE2[3_665]	1.37	0.83
1:K:36:ARG:O	1:L:361:THR:CB[3_665]	1.37	0.83
1:K:51:LYS:CG	1:L:400:GLU:CD[3_665]	1.37	0.83
1:K:40:LEU:CD1	1:L:357:ALA:C[3_665]	1.38	0.82
1:E:29:ILE:CD1	1:F:408:TYR:CA[2_655]	1.39	0.81
1:K:44:LEU:CB	1:L:357:ALA:CB[3_665]	1.40	0.80
1:E:316:SER:OG	1:F:440:ARG:O[2_655]	1.41	0.79
1:K:51:LYS:NZ	1:L:355:TYR:OH[3_665]	1.42	0.78
1:K:329:ARG:CB	1:L:442:ILE:CG2[3_665]	1.42	0.78
2:M:116:GLU:OE1	2:N:29:GLY:N[3_665]	1.42	0.78
1:K:32:ARG:CZ	1:L:411:SER:OG[3_665]	1.43	0.77
1:K:329:ARG:O	1:L:401:ARG:NH1[3_665]	1.43	0.77
1:E:314:LYS:CB	1:F:441:PHE:CZ[2_655]	1.44	0.76
1:K:48:VAL:CG2	1:L:354:GLN:O[3_665]	1.44	0.76
1:K:320:PRO:CG	1:L:390:ILE:CG2[3_665]	1.44	0.76
2:M:116:GLU:OE1	2:N:28:LYS:CA[3_665]	1.44	0.76
1:K:40:LEU:CD1	1:L:358:LEU:N[3_665]	1.45	0.75
1:E:36:ARG:NE	1:F:362:GLU:CD[2_655]	1.46	0.74
1:K:315:PRO:CG	1:L:441:PHE:CB[3_665]	1.47	0.73
2:M:116:GLU:OE1	2:N:28:LYS:C[3_665]	1.47	0.73
1:K:47:GLU:C	1:L:354:GLN:CD[3_665]	1.48	0.72
2:O:83:ARG:CZ	2:P:90:LYS:CD[2_655]	1.48	0.72
1:K:33:ASN:CG	1:L:407:SER:OG[3_665]	1.49	0.71
1:K:329:ARG:CG	1:L:442:ILE:O[3_665]	1.52	0.68
1:E:36:ARG:CZ	1:F:362:GLU:OE1[2_655]	1.54	0.66
1:K:320:PRO:CA	1:L:390:ILE:CG2[3_665]	1.54	0.66
2:O:83:ARG:CD	2:P:90:LYS:CE[2_655]	1.54	0.66
1:K:35:TRP:CZ3	1:L:362:GLU:CG[3_665]	1.55	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:39:GLN:CG	1:L:361:THR:O[3_665]	1.55	0.65
1:K:48:VAL:CG1	1:L:358:LEU:CG[3_665]	1.55	0.65
1:K:51:LYS:CE	1:L:355:TYR:CE2[3_665]	1.55	0.65
1:K:315:PRO:CB	1:L:441:PHE:N[3_665]	1.55	0.65
1:E:314:LYS:CA	1:F:441:PHE:CE1[2_655]	1.56	0.64
1:K:35:TRP:CZ3	1:L:362:GLU:CD[3_665]	1.56	0.64
2:O:116:GLU:OE1	2:P:28:LYS:CE[2_655]	1.57	0.63
1:K:6:PRO:O	1:L:408:TYR:OH[3_665]	1.58	0.62
1:K:36:ARG:NH2	1:L:410:ALA:CA[3_665]	1.58	0.62
1:K:316:SER:N	1:L:440:ARG:CA[3_665]	1.58	0.62
1:K:328:ILE:CB	1:L:404:GLU:OE1[3_665]	1.58	0.62
1:E:7:ARG:NE	1:F:412:ASP:OD2[2_655]	1.59	0.61
1:K:40:LEU:CD1	1:L:357:ALA:O[3_665]	1.60	0.60
1:K:314:LYS:CD	1:L:437:ASP:OD2[3_665]	1.60	0.60
1:K:315:PRO:CB	1:L:440:ARG:O[3_665]	1.60	0.60
1:K:327:PRO:CB	1:L:400:GLU:CB[3_665]	1.60	0.60
1:K:29:ILE:CG1	1:L:408:TYR:CB[3_665]	1.62	0.58
1:K:39:GLN:CB	1:L:361:THR:CA[3_665]	1.62	0.58
1:K:320:PRO:O	1:L:390:ILE:CD1[3_665]	1.62	0.58
1:E:25:ARG:CB	1:F:408:TYR:CZ[2_655]	1.63	0.57
1:F:149:GLN:CD	1:F:367:GLU:OE1[5_556]	1.64	0.56
1:K:321:GLU:CG	1:L:393:ARG:NH1[3_665]	1.65	0.55
1:K:328:ILE:CG1	1:L:404:GLU:OE1[3_665]	1.66	0.54
1:E:315:PRO:CD	1:F:441:PHE:CD1[2_655]	1.67	0.53
1:K:5:THR:CG2	1:L:412:ASP:OD1[3_665]	1.67	0.53
1:K:316:SER:CB	1:L:440:ARG:CG[3_665]	1.67	0.53
1:K:329:ARG:CG	1:L:442:ILE:CA[3_665]	1.67	0.53
1:E:25:ARG:CA	1:F:408:TYR:CE1[2_655]	1.68	0.52
1:K:36:ARG:O	1:L:358:LEU:O[3_665]	1.69	0.51
1:K:39:GLN:N	1:L:361:THR:OG1[3_665]	1.69	0.51
1:K:315:PRO:N	1:L:440:ARG:O[3_665]	1.69	0.51
1:E:25:ARG:C	1:F:408:TYR:CE1[2_655]	1.70	0.50
1:K:315:PRO:CB	1:L:440:ARG:C[3_665]	1.71	0.49
1:K:315:PRO:CD	1:L:441:PHE:CD2[3_665]	1.71	0.49
1:L:416:GLN:NE2	2:P:149:GLU:OE1[4_655]	1.71	0.49
1:K:35:TRP:CE3	1:L:362:GLU:OE1[3_665]	1.72	0.48
1:K:315:PRO:CG	1:L:441:PHE:CG[3_665]	1.72	0.48
1:E:29:ILE:CD1	1:F:408:TYR:CB[2_655]	1.73	0.47
1:K:32:ARG:CD	1:L:411:SER:OG[3_665]	1.74	0.46
1:K:315:PRO:CA	1:L:440:ARG:C[3_665]	1.74	0.46
1:K:316:SER:OG	1:L:440:ARG:CB[3_665]	1.74	0.46
1:E:36:ARG:CB	1:F:361:THR:CG2[2_655]	1.75	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:316:SER:OG	1:F:440:ARG:C[2_655]	1.75	0.45
1:K:32:ARG:NH2	1:L:411:SER:CA[3_665]	1.75	0.45
2:O:83:ARG:CD	2:P:90:LYS:CD[2_655]	1.75	0.45
1:E:314:LYS:CB	1:F:441:PHE:CE1[2_655]	1.76	0.44
1:K:329:ARG:CG	1:L:442:ILE:C[3_665]	1.76	0.44
1:E:25:ARG:O	1:F:408:TYR:CE1[2_655]	1.77	0.43
1:K:321:GLU:CG	1:L:393:ARG:CZ[3_665]	1.78	0.42
1:K:329:ARG:CA	1:L:401:ARG:NH2[3_665]	1.78	0.42
1:K:329:ARG:NH2	1:L:443:LEU:C[3_665]	1.78	0.42
1:K:36:ARG:O	1:L:361:THR:CG2[3_665]	1.79	0.41
1:K:47:GLU:CA	1:L:354:GLN:CD[3_665]	1.79	0.41
1:K:323:GLN:OE1	1:L:394:ARG:CZ[3_665]	1.79	0.41
1:E:314:LYS:CB	1:F:441:PHE:CE2[2_655]	1.80	0.40
1:K:316:SER:N	1:L:440:ARG:CB[3_665]	1.80	0.40
1:K:328:ILE:CD1	1:L:404:GLU:CG[3_665]	1.80	0.40
1:K:328:ILE:CD1	1:L:404:GLU:OE1[3_665]	1.80	0.40
2:M:116:GLU:CD	2:N:29:GLY:N[3_665]	1.80	0.40
1:K:44:LEU:CD2	1:L:353:VAL:O[3_665]	1.81	0.39
1:K:47:GLU:OE2	1:L:349:ALA:CB[3_665]	1.81	0.39
1:E:7:ARG:CZ	1:F:412:ASP:OD2[2_655]	1.82	0.38
1:K:33:ASN:OD1	1:L:407:SER:CB[3_665]	1.83	0.37
1:K:329:ARG:CG	1:L:442:ILE:CG2[3_665]	1.83	0.37
2:M:80:LYS:CE	2:N:87:MET:CE[3_665]	1.83	0.37
2:M:116:GLU:OE2	2:N:29:GLY:N[3_665]	1.83	0.37
1:E:36:ARG:O	1:F:361:THR:OG1[2_655]	1.84	0.36
1:E:316:SER:N	1:F:440:ARG:O[2_655]	1.84	0.36
1:K:6:PRO:CB	1:L:408:TYR:CD2[3_665]	1.84	0.36
1:K:37:ARG:CB	1:L:358:LEU:CD2[3_665]	1.84	0.36
1:K:40:LEU:CD1	1:L:358:LEU:CA[3_665]	1.84	0.36
1:K:28:ALA:C	1:L:408:TYR:CD1[3_665]	1.85	0.35
1:K:329:ARG:NH2	1:L:443:LEU:OXT[3_665]	1.85	0.35
1:K:37:ARG:O	1:L:361:THR:OG1[3_665]	1.86	0.34
1:K:51:LYS:CD	1:L:400:GLU:OE1[3_665]	1.86	0.34
1:K:329:ARG:C	1:L:401:ARG:NH2[3_665]	1.86	0.34
1:K:51:LYS:CD	1:L:400:GLU:OE2[3_665]	1.87	0.33
1:E:25:ARG:CG	1:F:408:TYR:OH[2_655]	1.88	0.32
1:K:5:THR:CB	1:L:412:ASP:OD1[3_665]	1.88	0.32
1:K:51:LYS:CE	1:L:400:GLU:OE2[3_665]	1.88	0.32
1:K:315:PRO:CG	1:L:441:PHE:N[3_665]	1.88	0.32
1:K:316:SER:OG	1:L:440:ARG:NE[3_665]	1.88	0.32
1:K:321:GLU:CA	1:L:393:ARG:CD[3_665]	1.88	0.32
1:K:329:ARG:N	1:L:401:ARG:CZ[3_665]	1.88	0.32

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:329:ARG:CB	1:L:442:ILE:CB[3.665]	1.88	0.32
2:M:80:LYS:CE	2:N:87:MET:SD[3.665]	1.88	0.32
1:K:47:GLU:CA	1:L:354:GLN:CG[3.665]	1.89	0.31
1:K:47:GLU:CD	1:L:349:ALA:CB[3.665]	1.89	0.31
1:K:316:SER:N	1:L:440:ARG:O[3.665]	1.89	0.31
2:O:83:ARG:NE	2:P:90:LYS:CE[2.655]	1.89	0.31
1:K:40:LEU:N	1:L:361:THR:OG1[3.665]	1.90	0.30
1:K:47:GLU:C	1:L:354:GLN:CG[3.665]	1.90	0.30
1:K:315:PRO:C	1:L:440:ARG:C[3.665]	1.90	0.30
1:K:328:ILE:CG1	1:L:404:GLU:CD[3.665]	1.90	0.30
1:K:329:ARG:O	1:L:401:ARG:CZ[3.665]	1.90	0.30
1:E:314:LYS:CD	1:F:441:PHE:CD2[2.655]	1.92	0.28
1:K:36:ARG:NH1	1:L:406:ILE:O[3.665]	1.92	0.28
1:K:321:GLU:CB	1:L:393:ARG:CD[3.665]	1.92	0.28
1:K:323:GLN:CD	1:L:394:ARG:NH2[3.665]	1.92	0.28
2:M:83:ARG:NH1	2:N:92:GLU:OE2[3.665]	1.92	0.28
1:K:29:ILE:N	1:L:408:TYR:CD1[3.665]	1.93	0.27
1:K:44:LEU:CG	1:L:357:ALA:CB[3.665]	1.93	0.27
1:K:329:ARG:CZ	1:L:442:ILE:C[3.665]	1.93	0.27
2:O:84:THR:CG2	2:P:86:ARG:NH1[2.655]	1.93	0.27
1:E:7:ARG:NH2	1:F:412:ASP:OD2[2.655]	1.94	0.26
1:K:35:TRP:CE2	1:L:362:GLU:OE2[3.665]	1.94	0.26
1:K:329:ARG:O	1:L:401:ARG:NH2[3.665]	1.94	0.26
1:K:329:ARG:NE	1:L:442:ILE:O[3.665]	1.94	0.26
2:N:24:ASN:CA	2:P:160:ILE:CD1[2.655]	1.94	0.26
1:E:25:ARG:CB	1:F:408:TYR:CE1[2.655]	1.95	0.25
1:E:316:SER:CB	1:F:440:ARG:CA[2.655]	1.95	0.25
1:K:320:PRO:CA	1:L:390:ILE:CB[3.665]	1.95	0.25
1:E:25:ARG:CA	1:F:408:TYR:OH[2.655]	1.96	0.24
1:E:25:ARG:CA	1:F:408:TYR:CZ[2.655]	1.96	0.24
1:K:36:ARG:NH2	1:L:410:ALA:CB[3.665]	1.96	0.24
1:K:315:PRO:CD	1:L:441:PHE:CG[3.665]	1.96	0.24
1:K:316:SER:N	1:L:440:ARG:C[3.665]	1.96	0.24
1:K:327:PRO:O	1:L:401:ARG:CB[3.665]	1.96	0.24
2:O:83:ARG:NH2	2:P:90:LYS:CE[2.655]	1.96	0.24
2:O:116:GLU:OE2	2:P:30:ASN:ND2[2.655]	1.96	0.24
1:K:36:ARG:C	1:L:361:THR:CG2[3.665]	1.97	0.23
1:K:36:ARG:CZ	1:L:410:ALA:CA[3.665]	1.97	0.23
1:K:323:GLN:C	1:L:397:THR:OG1[3.665]	1.97	0.23
2:N:25:THR:CG2	2:P:158:ILE:O[2.655]	1.97	0.23
1:K:6:PRO:CG	1:L:408:TYR:C[3.665]	1.98	0.22
1:K:28:ALA:CB	1:L:408:TYR:CZ[3.665]	1.98	0.22

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:O:84:THR:CG2	2:P:86:ARG:NE[2.655]	1.98	0.22
1:K:327:PRO:CG	1:L:400:GLU:CG[3.665]	1.99	0.21
1:K:6:PRO:CB	1:L:408:TYR:CE2[3.665]	2.00	0.20
1:K:44:LEU:CD1	1:L:357:ALA:CB[3.665]	2.00	0.20
1:K:328:ILE:C	1:L:401:ARG:NH2[3.665]	2.00	0.20
1:K:329:ARG:NH1	1:L:443:LEU:CA[3.665]	2.00	0.20
1:E:36:ARG:CD	1:F:362:GLU:OE1[2.655]	2.01	0.19
1:K:35:TRP:CE3	1:L:362:GLU:CG[3.665]	2.01	0.19
1:K:329:ARG:CZ	1:L:443:LEU:N[3.665]	2.01	0.19
1:E:314:LYS:CD	1:F:441:PHE:CZ[2.655]	2.02	0.18
1:K:28:ALA:CA	1:L:408:TYR:CE1[3.665]	2.02	0.18
1:K:28:ALA:CB	1:L:408:TYR:CD1[3.665]	2.02	0.18
1:K:36:ARG:CD	1:L:410:ALA:CB[3.665]	2.02	0.18
1:K:310:PHE:CD2	1:L:441:PHE:CE1[3.665]	2.02	0.18
1:E:314:LYS:CE	1:F:437:ASP:OD2[2.655]	2.03	0.17
1:K:29:ILE:CD1	1:L:404:GLU:O[3.665]	2.03	0.17
1:K:39:GLN:C	1:L:361:THR:CA[3.665]	2.03	0.17
1:K:321:GLU:CG	1:L:393:ARG:NE[3.665]	2.03	0.17
1:F:427:LYS:NZ	1:L:149:GLN:CD[4.545]	2.04	0.16
1:K:320:PRO:CB	1:L:390:ILE:CA[3.665]	2.04	0.16
1:K:321:GLU:CB	1:L:393:ARG:NE[3.665]	2.04	0.16
1:K:327:PRO:CG	1:L:400:GLU:CB[3.665]	2.04	0.16
1:L:416:GLN:OE1	2:P:149:GLU:OE2[4.655]	2.04	0.16
1:K:40:LEU:CG	1:L:357:ALA:C[3.665]	2.05	0.15
1:K:47:GLU:CA	1:L:354:GLN:OE1[3.665]	2.05	0.15
1:K:47:GLU:CD	1:L:349:ALA:O[3.665]	2.05	0.15
1:K:51:LYS:CD	1:L:400:GLU:CD[3.665]	2.05	0.15
1:K:54:LEU:CD2	1:L:441:PHE:O[3.665]	2.05	0.15
1:K:328:ILE:CD1	1:L:404:GLU:CD[3.665]	2.05	0.15
1:E:25:ARG:CB	1:F:408:TYR:OH[2.655]	2.06	0.14
2:M:83:ARG:NH1	2:N:92:GLU:CD[3.665]	2.06	0.14
2:M:113:VAL:CG1	2:N:27:MET:SD[3.665]	2.06	0.14
1:E:327:PRO:CB	1:F:400:GLU:CG[2.655]	2.07	0.13
1:K:329:ARG:CB	1:L:442:ILE:CD1[3.665]	2.07	0.13
1:K:329:ARG:CD	1:L:442:ILE:O[3.665]	2.07	0.13
1:K:36:ARG:NH2	1:L:406:ILE:O[3.665]	2.08	0.12
1:K:51:LYS:NZ	1:L:355:TYR:CE1[3.665]	2.08	0.12
1:K:315:PRO:N	1:L:440:ARG:C[3.665]	2.08	0.12
1:K:35:TRP:CD2	1:L:362:GLU:CD[3.665]	2.09	0.11
1:K:48:VAL:CB	1:L:358:LEU:CG[3.665]	2.09	0.11
1:K:310:PHE:CG	1:L:441:PHE:CZ[3.665]	2.09	0.11
1:K:329:ARG:CG	1:L:442:ILE:CB[3.665]	2.09	0.11

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:329:ARG:CZ	1:L:442:ILE:O[3.665]	2.09	0.11
1:K:36:ARG:C	1:L:358:LEU:O[3.665]	2.10	0.10
2:M:116:GLU:CD	2:N:28:LYS:C[3.665]	2.10	0.10
1:E:36:ARG:CA	1:F:361:THR:CG2[2.655]	2.11	0.09
1:K:35:TRP:O	1:L:361:THR:CG2[3.665]	2.11	0.09
1:K:36:ARG:CZ	1:L:410:ALA:N[3.665]	2.11	0.09
1:K:36:ARG:NH1	1:L:407:SER:CA[3.665]	2.11	0.09
1:K:36:ARG:NH2	1:L:409:ASP:C[3.665]	2.11	0.09
1:K:47:GLU:OE1	1:L:349:ALA:C[3.665]	2.11	0.09
1:K:51:LYS:CG	1:L:400:GLU:OE2[3.665]	2.11	0.09
2:O:83:ARG:CZ	2:P:90:LYS:CE[2.655]	2.11	0.09
1:K:32:ARG:NH1	1:L:411:SER:CB[3.665]	2.12	0.08
1:K:35:TRP:CH2	1:L:362:GLU:OE2[3.665]	2.12	0.08
1:K:40:LEU:CD2	1:L:357:ALA:C[3.665]	2.12	0.08
1:K:314:LYS:CG	1:L:437:ASP:OD2[3.665]	2.12	0.08
1:K:315:PRO:CD	1:L:441:PHE:N[3.665]	2.12	0.08
1:E:25:ARG:O	1:F:408:TYR:CD1[2.655]	2.13	0.07
1:E:314:LYS:CA	1:F:441:PHE:CZ[2.655]	2.13	0.07
1:E:314:LYS:CG	1:F:441:PHE:CE1[2.655]	2.13	0.07
1:K:39:GLN:CA	1:L:361:THR:CA[3.665]	2.13	0.07
1:K:324:GLY:CA	1:L:397:THR:OG1[3.665]	2.13	0.07
1:K:329:ARG:CD	1:L:442:ILE:CA[3.665]	2.13	0.07
2:M:83:ARG:NH1	2:N:92:GLU:CG[3.665]	2.13	0.07
2:N:24:ASN:CA	2:P:160:ILE:CG1[2.655]	2.13	0.07
2:O:83:ARG:CG	2:P:90:LYS:NZ[2.655]	2.13	0.07
1:E:36:ARG:NH2	1:F:362:GLU:OE1[2.655]	2.14	0.06
1:K:310:PHE:CD1	1:L:441:PHE:CE1[3.665]	2.14	0.06
1:K:328:ILE:CG2	1:L:404:GLU:CD[3.665]	2.14	0.06
1:K:310:PHE:CG	1:L:441:PHE:CD1[3.665]	2.15	0.05
1:E:25:ARG:CG	1:F:408:TYR:CZ[2.655]	2.16	0.04
1:E:36:ARG:CZ	1:F:362:GLU:CD[2.655]	2.16	0.04
1:K:44:LEU:CD1	1:L:357:ALA:CA[3.665]	2.16	0.04
1:K:48:VAL:N	1:L:354:GLN:OE1[3.665]	2.16	0.04
1:K:48:VAL:CG2	1:L:354:GLN:C[3.665]	2.16	0.04
1:K:316:SER:CB	1:L:440:ARG:CB[3.665]	2.16	0.04
1:K:39:GLN:N	1:L:361:THR:CG2[3.665]	2.17	0.03
1:K:39:GLN:C	1:L:361:THR:OG1[3.665]	2.17	0.03
1:K:39:GLN:O	1:L:361:THR:CA[3.665]	2.17	0.03
1:K:39:GLN:CG	1:L:361:THR:C[3.665]	2.17	0.03
1:K:39:GLN:CD	1:L:361:THR:O[3.665]	2.17	0.03
1:K:315:PRO:O	1:L:440:ARG:O[3.665]	2.17	0.03
1:K:323:GLN:OE1	1:L:394:ARG:NH1[3.665]	2.17	0.03

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:O:83:ARG:NE	2:P:90:LYS:CG[2_655]	2.17	0.03
1:E:29:ILE:CD1	1:F:408:TYR:N[2_655]	2.18	0.02
1:K:6:PRO:CD	1:L:408:TYR:O[3_665]	2.18	0.02
1:K:33:ASN:ND2	1:L:359:MET:CE[3_665]	2.18	0.02
1:K:328:ILE:CG1	1:L:404:GLU:CG[3_665]	2.18	0.02
1:E:36:ARG:NE	1:F:362:GLU:CG[2_655]	2.19	0.01
1:E:48:VAL:CG1	1:F:358:LEU:CD2[2_655]	2.19	0.01
1:K:32:ARG:NH2	1:L:411:SER:C[3_665]	2.19	0.01
1:K:39:GLN:N	1:L:361:THR:CB[3_665]	2.19	0.01
1:K:39:GLN:CA	1:L:361:THR:OG1[3_665]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. 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	E	389/443 (88%)	335 (86%)	40 (10%)	14 (4%)	5	52
1	F	389/443 (88%)	329 (85%)	41 (10%)	19 (5%)	3	43
1	K	389/443 (88%)	335 (86%)	40 (10%)	14 (4%)	5	52
1	L	389/443 (88%)	329 (85%)	41 (10%)	19 (5%)	3	43
2	M	171/175 (98%)	145 (85%)	18 (10%)	8 (5%)	4	44
2	N	171/175 (98%)	143 (84%)	23 (14%)	5 (3%)	7	58
2	O	171/175 (98%)	145 (85%)	18 (10%)	8 (5%)	4	44
2	P	171/175 (98%)	143 (84%)	23 (14%)	5 (3%)	7	58
All	All	2240/2472 (91%)	1904 (85%)	244 (11%)	92 (4%)	4	48

All (92) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	92	VAL
1	E	140	LYS
1	E	154	ALA
1	E	300	ASP

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Mol	Chain	Res	Type
1	F	92	VAL
1	F	139	ALA
1	F	142	ASN
1	F	154	ALA
1	F	263	LYS
1	F	266	GLU
1	K	92	VAL
1	K	140	LYS
1	K	154	ALA
1	K	300	ASP
1	L	92	VAL
1	L	139	ALA
1	L	142	ASN
1	L	154	ALA
1	L	263	LYS
1	L	266	GLU
2	M	116	GLU
2	O	116	GLU
1	E	143	TRP
1	F	143	TRP
1	F	265	GLY
1	F	350	SER
1	K	143	TRP
1	L	143	TRP
1	L	265	GLY
1	L	350	SER
1	E	111	VAL
1	E	264	ARG
1	F	217	LYS
1	F	264	ARG
1	F	300	ASP
1	F	410	ALA
1	K	111	VAL
1	K	264	ARG
1	L	217	LYS
1	L	264	ARG
1	L	300	ASP
1	L	410	ALA
2	M	65	GLU
2	M	68	GLN
2	M	69	GLY
2	M	100	GLU

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Mol	Chain	Res	Type
2	M	109	ASN
2	N	65	GLU
2	N	68	GLN
2	N	69	GLY
2	O	65	GLU
2	O	68	GLN
2	O	69	GLY
2	O	100	GLU
2	O	109	ASN
2	P	65	GLU
2	P	68	GLN
2	P	69	GLY
1	E	110	MET
1	K	110	MET
2	M	70	HIS
2	N	101	THR
2	O	70	HIS
2	P	101	THR
1	E	138	PRO
1	E	153	SER
1	E	217	LYS
1	E	263	LYS
1	F	111	VAL
1	F	112	ARG
1	F	218	ILE
1	F	232	LYS
1	K	138	PRO
1	K	153	SER
1	K	217	LYS
1	K	263	LYS
1	L	111	VAL
1	L	112	ARG
1	L	218	ILE
1	L	232	LYS
2	M	115	PRO
2	N	70	HIS
2	O	115	PRO
2	P	70	HIS
1	E	112	ARG
1	F	63	LYS
1	K	112	ARG
1	L	63	LYS

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Mol	Chain	Res	Type
1	E	265	GLY
1	K	265	GLY
1	L	137	PRO
1	F	137	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. 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	E	336/377 (89%)	294 (88%)	42 (12%)	7	38
1	F	336/377 (89%)	287 (85%)	49 (15%)	5	30
1	K	336/377 (89%)	293 (87%)	43 (13%)	6	37
1	L	336/377 (89%)	288 (86%)	48 (14%)	5	31
2	M	135/136 (99%)	124 (92%)	11 (8%)	17	61
2	N	135/136 (99%)	121 (90%)	14 (10%)	10	48
2	O	135/136 (99%)	124 (92%)	11 (8%)	17	61
2	P	135/136 (99%)	121 (90%)	14 (10%)	10	48
All	All	1884/2052 (92%)	1652 (88%)	232 (12%)	7	39

All (232) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	4	MET
1	E	13	LEU
1	E	27	VAL
1	E	31	LEU
1	E	38	MET
1	E	46	HIS
1	E	51	LYS
1	E	59	THR
1	E	70	LEU
1	E	79	ILE
1	E	94	LYS
1	E	95	GLU
1	E	97	ASP

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Mol	Chain	Res	Type
1	E	103	LEU
1	E	110	MET
1	E	114	GLN
1	E	118	LYS
1	E	119	ASN
1	E	120	ARG
1	E	130	ARG
1	E	132	LEU
1	E	136	ILE
1	E	141	ASN
1	E	159	PHE
1	E	164	ARG
1	E	216	LEU
1	E	232	LYS
1	E	235	ASN
1	E	242	ASP
1	E	279	ARG
1	E	281	LEU
1	E	326	LEU
1	E	344	LEU
1	E	352	THR
1	E	355	TYR
1	E	361	THR
1	E	369	THR
1	E	375	ARG
1	E	389	ASN
1	E	401	ARG
1	E	412	ASP
1	E	423	ASP
1	F	6	PRO
1	F	11	SER
1	F	13	LEU
1	F	20	GLN
1	F	27	VAL
1	F	31	LEU
1	F	38	MET
1	F	59	THR
1	F	70	LEU
1	F	79	ILE
1	F	81	VAL
1	F	95	GLU
1	F	97	ASP

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Mol	Chain	Res	Type
1	F	103	LEU
1	F	114	GLN
1	F	118	LYS
1	F	119	ASN
1	F	122	ARG
1	F	130	ARG
1	F	131	ILE
1	F	132	LEU
1	F	140	LYS
1	F	141	ASN
1	F	148	GLN
1	F	150	GLN
1	F	159	PHE
1	F	163	LEU
1	F	217	LYS
1	F	232	LYS
1	F	258	ILE
1	F	266	GLU
1	F	281	LEU
1	F	312	ILE
1	F	325	ARG
1	F	326	LEU
1	F	344	LEU
1	F	352	THR
1	F	355	TYR
1	F	361	THR
1	F	369	THR
1	F	374	LYS
1	F	375	ARG
1	F	384	ASN
1	F	389	ASN
1	F	394	ARG
1	F	401	ARG
1	F	413	LEU
1	F	438	LEU
1	F	439	SER
1	K	4	MET
1	K	13	LEU
1	K	27	VAL
1	K	31	LEU
1	K	38	MET
1	K	46	HIS

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Mol	Chain	Res	Type
1	K	51	LYS
1	K	59	THR
1	K	70	LEU
1	K	79	ILE
1	K	94	LYS
1	K	95	GLU
1	K	97	ASP
1	K	103	LEU
1	K	110	MET
1	K	114	GLN
1	K	118	LYS
1	K	119	ASN
1	K	120	ARG
1	K	130	ARG
1	K	132	LEU
1	K	136	ILE
1	K	141	ASN
1	K	159	PHE
1	K	164	ARG
1	K	216	LEU
1	K	232	LYS
1	K	235	ASN
1	K	242	ASP
1	K	279	ARG
1	K	281	LEU
1	K	318	LEU
1	K	326	LEU
1	K	344	LEU
1	K	352	THR
1	K	355	TYR
1	K	361	THR
1	K	369	THR
1	K	375	ARG
1	K	389	ASN
1	K	401	ARG
1	K	412	ASP
1	K	423	ASP
1	L	6	PRO
1	L	11	SER
1	L	13	LEU
1	L	20	GLN
1	L	27	VAL

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Mol	Chain	Res	Type
1	L	31	LEU
1	L	38	MET
1	L	59	THR
1	L	70	LEU
1	L	79	ILE
1	L	81	VAL
1	L	95	GLU
1	L	97	ASP
1	L	103	LEU
1	L	114	GLN
1	L	118	LYS
1	L	119	ASN
1	L	122	ARG
1	L	130	ARG
1	L	131	ILE
1	L	132	LEU
1	L	140	LYS
1	L	141	ASN
1	L	148	GLN
1	L	150	GLN
1	L	159	PHE
1	L	163	LEU
1	L	217	LYS
1	L	232	LYS
1	L	258	ILE
1	L	266	GLU
1	L	281	LEU
1	L	312	ILE
1	L	325	ARG
1	L	326	LEU
1	L	344	LEU
1	L	352	THR
1	L	355	TYR
1	L	361	THR
1	L	369	THR
1	L	374	LYS
1	L	375	ARG
1	L	384	ASN
1	L	389	ASN
1	L	394	ARG
1	L	413	LEU
1	L	438	LEU

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Mol	Chain	Res	Type
1	L	439	SER
2	M	1	THR
2	M	36	ARG
2	M	50	THR
2	M	66	MET
2	M	90	LYS
2	M	95	LEU
2	M	99	ASP
2	M	138	GLU
2	M	139	ASN
2	M	146	GLU
2	M	160	ILE
2	N	4	VAL
2	N	36	ARG
2	N	50	THR
2	N	92	GLU
2	N	95	LEU
2	N	99	ASP
2	N	111	ASP
2	N	116	GLU
2	N	134	ARG
2	N	136	LEU
2	N	138	GLU
2	N	139	ASN
2	N	146	GLU
2	N	152	LEU
2	O	1	THR
2	O	36	ARG
2	O	50	THR
2	O	66	MET
2	O	90	LYS
2	O	95	LEU
2	O	99	ASP
2	O	138	GLU
2	O	139	ASN
2	O	146	GLU
2	O	160	ILE
2	P	4	VAL
2	P	36	ARG
2	P	50	THR
2	P	92	GLU
2	P	95	LEU

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Mol	Chain	Res	Type
2	P	99	ASP
2	P	111	ASP
2	P	116	GLU
2	P	134	ARG
2	P	136	LEU
2	P	138	GLU
2	P	139	ASN
2	P	146	GLU
2	P	152	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	22	ASN
1	E	33	ASN
1	E	75	ASN
1	E	119	ASN
1	E	141	ASN
1	E	148	GLN
1	E	157	GLN
1	E	235	ASN
1	E	241	GLN
1	E	294	HIS
1	E	333	GLN
1	E	384	ASN
1	E	389	ASN
1	E	396	HIS
1	E	416	GLN
1	E	417	ASN
1	F	22	ASN
1	F	33	ASN
1	F	75	ASN
1	F	119	ASN
1	F	141	ASN
1	F	142	ASN
1	F	148	GLN
1	F	157	GLN
1	F	235	ASN
1	F	241	GLN
1	F	249	GLN
1	F	384	ASN
1	F	389	ASN

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Mol	Chain	Res	Type
1	F	396	HIS
1	F	416	GLN
1	F	417	ASN
1	K	22	ASN
1	K	33	ASN
1	K	75	ASN
1	K	119	ASN
1	K	141	ASN
1	K	148	GLN
1	K	157	GLN
1	K	235	ASN
1	K	241	GLN
1	K	333	GLN
1	K	384	ASN
1	K	389	ASN
1	K	396	HIS
1	K	416	GLN
1	K	417	ASN
1	L	22	ASN
1	L	33	ASN
1	L	75	ASN
1	L	119	ASN
1	L	141	ASN
1	L	142	ASN
1	L	148	GLN
1	L	157	GLN
1	L	235	ASN
1	L	241	GLN
1	L	249	GLN
1	L	311	GLN
1	L	384	ASN
1	L	389	ASN
1	L	396	HIS
1	L	416	GLN
1	L	417	ASN
2	M	70	HIS
2	M	114	GLN
2	M	139	ASN
2	M	166	HIS
2	N	39	ASN
2	N	70	HIS
2	N	139	ASN

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Mol	Chain	Res	Type
2	O	70	HIS
2	O	114	GLN
2	O	139	ASN
2	O	166	HIS
2	P	39	ASN
2	P	70	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	E	393/443 (88%)	0.90	53 (13%) 4 10	60, 60, 60, 60	0
1	F	393/443 (88%)	0.83	43 (10%) 6 14	60, 60, 60, 60	0
1	K	393/443 (88%)	1.03	64 (16%) 2 8	60, 60, 60, 60	0
1	L	393/443 (88%)	0.98	56 (14%) 3 9	60, 60, 60, 60	0
2	M	173/175 (98%)	1.05	32 (18%) 2 6	60, 60, 60, 60	0
2	N	173/175 (98%)	1.05	28 (16%) 2 8	60, 60, 60, 60	0
2	O	173/175 (98%)	1.13	31 (17%) 2 7	60, 60, 60, 60	0
2	P	173/175 (98%)	0.71	15 (8%) 10 19	60, 60, 60, 60	0
All	All	2264/2472 (91%)	0.95	322 (14%) 3 9	60, 60, 60, 60	0

All (322) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	77	PRO	8.8
1	F	443	LEU	7.5
1	L	288	CYS	7.3
1	L	289	THR	7.2
1	K	289	THR	6.9
2	N	47	ALA	6.6
1	K	76	ALA	6.4
1	K	247	VAL	6.4
1	L	77	PRO	6.0
1	K	246	ALA	5.7
1	K	288	CYS	5.5
1	E	219	LYS	5.4
2	M	92	GLU	5.4
2	O	114	GLN	5.0
1	L	163	LEU	5.0
2	M	40	ASP	5.0

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Mol	Chain	Res	Type	RSRZ
2	O	23	GLY	4.9
1	L	250	HIS	4.9
1	K	252	ILE	4.8
2	N	32	LYS	4.8
1	K	305	ILE	4.5
1	L	222	MET	4.5
1	F	397	THR	4.5
2	O	16	GLY	4.4
1	K	74	ALA	4.4
1	L	415	GLY	4.4
1	E	387	THR	4.4
1	K	297	VAL	4.4
1	E	220	ASP	4.3
2	O	150	LYS	4.3
2	O	15	ALA	4.2
1	K	251	GLY	4.2
2	N	138	GLU	4.2
1	L	76	ALA	4.1
1	E	148	GLN	4.1
2	O	24	ASN	4.1
1	E	286	GLU	4.0
1	F	442	ILE	4.0
2	M	46	PHE	4.0
2	O	44	ALA	4.0
1	F	109	LYS	4.0
1	K	238	GLU	4.0
2	N	134	ARG	4.0
2	O	6	VAL	3.9
1	L	282	LEU	3.9
1	F	112	ARG	3.9
2	N	34	VAL	3.8
1	K	144	GLY	3.8
2	M	170	GLU	3.8
1	E	325	ARG	3.8
1	E	118	LYS	3.7
2	M	48	GLY	3.7
1	E	138	PRO	3.7
1	E	323	GLN	3.7
1	E	163	LEU	3.6
1	E	324	GLY	3.6
2	O	151	ALA	3.6
1	L	286	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	218	ILE	3.6
2	M	57	PHE	3.6
1	K	253	VAL	3.6
1	E	222	MET	3.6
2	O	169	GLU	3.6
2	M	91	LEU	3.6
2	M	171	LEU	3.5
2	P	140	THR	3.5
1	E	297	VAL	3.5
1	L	91	TYR	3.5
1	E	326	LEU	3.5
2	M	36	ARG	3.4
2	P	35	ARG	3.4
1	L	164	ARG	3.4
1	L	223	LYS	3.4
2	M	85	ASP	3.4
1	K	91	TYR	3.4
1	K	248	GLU	3.4
1	K	304	PHE	3.4
2	O	170	GLU	3.4
2	O	149	GLU	3.3
2	M	78	LEU	3.3
1	F	113	VAL	3.3
1	E	296	MET	3.3
1	F	147	GLU	3.3
1	K	92	VAL	3.3
2	N	86	ARG	3.3
1	F	57	GLY	3.3
2	O	25	THR	3.3
1	L	252	ILE	3.2
1	F	146	THR	3.2
2	N	48	GLY	3.2
2	O	22	LEU	3.2
1	L	216	LEU	3.2
2	M	117	ASN	3.2
1	E	114	GLN	3.2
2	M	35	ARG	3.2
1	E	422	ALA	3.2
1	L	363	GLY	3.2
1	E	73	LEU	3.2
2	O	118	ASP	3.2
2	O	168	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	128	GLU	3.1
1	L	224	LEU	3.1
1	K	250	HIS	3.1
1	K	287	GLY	3.1
1	E	115	ALA	3.1
2	N	94	LEU	3.1
1	E	117	GLU	3.1
1	F	216	LEU	3.1
1	F	234	VAL	3.1
1	E	221	ALA	3.1
1	K	49	THR	3.1
2	M	44	ALA	3.1
1	E	112	ARG	3.1
1	E	147	GLU	3.1
2	M	77	GLU	3.1
1	F	104	THR	3.1
1	E	164	ARG	3.1
2	O	14	ILE	3.0
1	F	71	ALA	3.0
1	K	226	ILE	3.0
2	M	41	LYS	3.0
1	F	114	GLN	3.0
2	O	12	VAL	3.0
2	O	7	ARG	3.0
2	M	45	GLY	3.0
1	K	245	ASP	3.0
1	K	306	ALA	3.0
1	E	149	GLN	2.9
2	N	95	LEU	2.9
1	F	439	SER	2.9
1	L	90	GLY	2.9
1	K	140	LYS	2.9
2	O	103	SER	2.9
1	E	281	LEU	2.8
1	L	283	PRO	2.8
1	K	154	ALA	2.8
1	L	79	ILE	2.8
1	E	119	ASN	2.8
1	L	162	LYS	2.8
1	L	334	ALA	2.8
1	E	334	ALA	2.8
2	N	96	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	331	GLU	2.8
1	K	75	ASN	2.8
1	E	216	LEU	2.8
1	F	394	ARG	2.8
2	N	151	ALA	2.8
1	L	414	SER	2.7
1	K	15	LYS	2.7
1	L	372	GLY	2.7
1	L	270	PRO	2.7
2	P	141	GLU	2.7
1	F	302	ILE	2.7
2	O	152	LEU	2.7
1	F	335	LEU	2.7
2	N	133	ALA	2.7
1	E	217	LYS	2.7
1	F	374	LYS	2.7
2	P	139	ASN	2.7
2	P	136	LEU	2.7
1	L	135	LEU	2.7
1	F	419	THR	2.7
2	M	58	GLU	2.6
1	E	385	GLU	2.6
2	N	89	ARG	2.6
2	N	132	ALA	2.6
1	E	318	LEU	2.6
1	K	394	ARG	2.6
1	E	165	GLU	2.6
2	N	30	ASN	2.6
1	L	6	PRO	2.6
1	F	21	ASP	2.6
2	M	56	LEU	2.6
1	F	110	MET	2.6
1	F	383	VAL	2.5
1	E	166	GLY	2.5
2	M	59	LEU	2.5
1	L	49	THR	2.5
2	P	86	ARG	2.5
1	L	221	ALA	2.5
1	K	95	GLU	2.5
1	K	139	ALA	2.5
1	K	387	THR	2.5
1	K	393	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	50	PRO	2.5
1	E	116	ILE	2.5
2	O	123	GLY	2.5
1	K	244	ILE	2.5
1	L	284	LEU	2.5
1	L	50	PRO	2.5
2	M	84	THR	2.5
1	L	273	SER	2.5
2	P	85	ASP	2.5
2	N	112	VAL	2.5
1	K	298	LYS	2.5
2	M	39	ASN	2.5
1	K	142	ASN	2.4
2	N	135	ALA	2.4
1	L	251	GLY	2.4
1	K	143	TRP	2.4
1	L	335	LEU	2.4
1	F	235	ASN	2.4
2	M	169	GLU	2.4
1	L	281	LEU	2.4
1	L	385	GLU	2.4
2	O	147	ILE	2.4
1	E	329	ARG	2.4
1	F	75	ASN	2.4
1	K	78	PHE	2.4
1	F	217	LYS	2.4
2	M	173	TYR	2.4
1	E	432	LEU	2.4
2	P	84	THR	2.4
2	N	123	GLY	2.4
1	K	388	GLU	2.4
2	N	129	ALA	2.4
1	F	292	THR	2.4
1	K	285	VAL	2.4
1	K	286	GLU	2.4
2	M	37	LEU	2.4
1	E	137	PRO	2.4
1	F	396	HIS	2.4
1	K	134	VAL	2.4
1	F	105	ASP	2.4
2	O	5	SER	2.4
1	L	152	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	K	157	GLN	2.4
1	L	80	LYS	2.4
1	K	222	MET	2.3
1	E	289	THR	2.3
1	F	74	ALA	2.3
2	P	149	GLU	2.3
1	K	294	HIS	2.3
1	L	285	VAL	2.3
2	P	44	ALA	2.3
1	L	96	VAL	2.3
1	L	160	ARG	2.3
1	L	321	GLU	2.3
1	L	78	PHE	2.3
1	L	416	GLN	2.3
1	F	387	THR	2.3
1	L	371	SER	2.3
2	N	169	GLU	2.3
2	M	33	LYS	2.3
2	P	105	ILE	2.3
2	O	13	VAL	2.3
2	P	142	LEU	2.2
1	K	402	LEU	2.2
2	N	97	VAL	2.2
2	O	115	PRO	2.2
1	E	388	GLU	2.2
1	L	40	LEU	2.2
1	F	108	VAL	2.2
2	M	82	TRP	2.2
1	L	272	VAL	2.2
1	L	53	ILE	2.2
2	M	89	ARG	2.2
2	N	137	LEU	2.2
1	F	139	ALA	2.2
1	L	128	GLU	2.2
1	L	266	GLU	2.2
2	N	149	GLU	2.2
1	F	19	GLY	2.2
2	O	87	MET	2.2
1	L	122	ARG	2.2
1	K	299	THR	2.2
2	O	101	THR	2.2
1	E	322	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	395	LEU	2.2
2	M	50	THR	2.2
2	N	114	GLN	2.2
1	K	398	VAL	2.2
2	O	146	GLU	2.2
1	E	233	LEU	2.2
1	L	269	GLY	2.2
2	O	119	LEU	2.2
1	F	68	ARG	2.2
1	K	431	ALA	2.2
1	L	267	SER	2.2
1	F	305	ILE	2.2
1	K	293	LYS	2.2
1	F	252	ILE	2.1
1	K	333	GLN	2.1
2	P	134	ARG	2.1
1	E	129	GLU	2.1
1	E	237	GLU	2.1
1	E	265	GLY	2.1
2	M	135	ALA	2.1
1	K	296	MET	2.1
2	P	34	VAL	2.1
1	L	112	ARG	2.1
1	K	100	ILE	2.1
1	K	135	LEU	2.1
1	E	440	ARG	2.1
2	N	131	ALA	2.1
1	E	49	THR	2.1
2	N	111	ASP	2.1
2	P	168	ILE	2.1
1	K	249	GLN	2.1
1	K	94	LYS	2.1
2	N	130	GLN	2.1
1	F	255	ILE	2.1
1	L	38	MET	2.1
1	K	432	LEU	2.1
1	L	294	HIS	2.1
1	K	441	PHE	2.1
1	F	304	PHE	2.1
2	M	140	THR	2.1
1	K	380	ALA	2.0
2	O	142	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	K	440	ARG	2.0
1	F	425	VAL	2.0
2	N	122	ILE	2.0
1	F	101	ARG	2.0
2	M	49	GLY	2.0
1	K	302	ILE	2.0
1	E	144	GLY	2.0
1	E	439	SER	2.0
1	K	243	ALA	2.0
1	E	113	VAL	2.0
1	F	83	ALA	2.0
1	K	237	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.