Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 04:01 AM EDT

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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

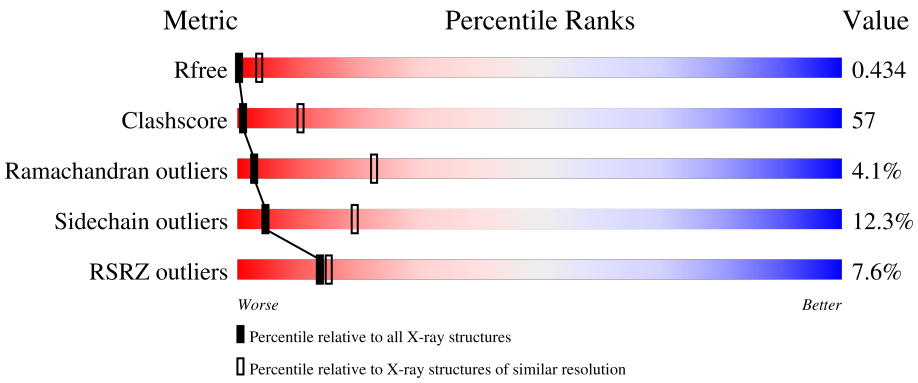
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	130704	1004 (10.00-3.90)
Clashscore	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
Sidechain outliers	138945	1002 (10.00-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	443	7%; 35%; 44%; 8%; • ; 11%
1	F	443	5%; 34%; 44%; 11%; • ; 11%
1	K	443	7%; 35%; 43%; 9%; • ; 11%
1	L	443	7%; 35%; 42%; 11%; • ; 11%
2	M	175	12%; 39%; 51%; 9%; •

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Mol	Chain	Length	Quality of chain
2	N	175	6% 38% 53% 7%
2	O	175	13% 42% 47% 10%
2	P	175	3% 35% 56% 7%

2 Entry composition (i)

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

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 SUBUNIT HSLU.

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

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

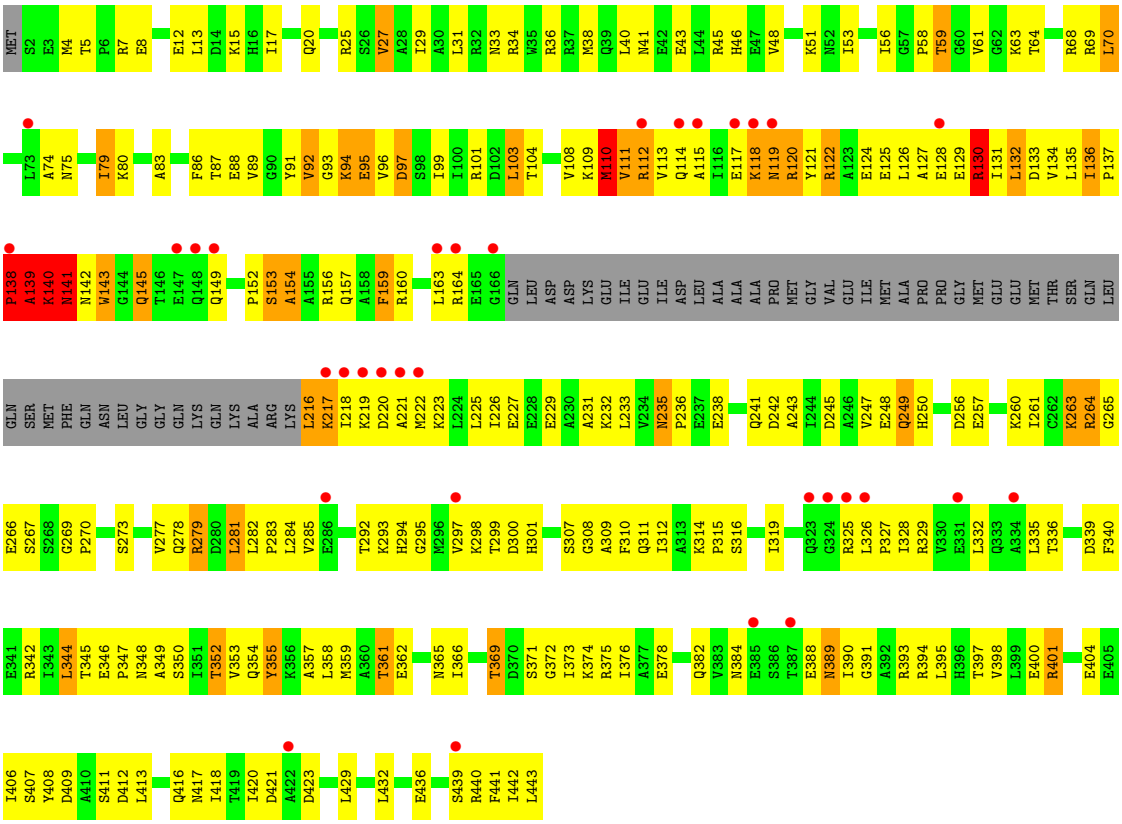
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	173	1319	828	235	252	4	0	0	0
2	N	173	1319	828	235	252	4	0	0	0
2	O	173	1319	828	235	252	4	0	0	0
2	P	173	1319	828	235	252	4	0	0	0

3 Residue-property plots (i)

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

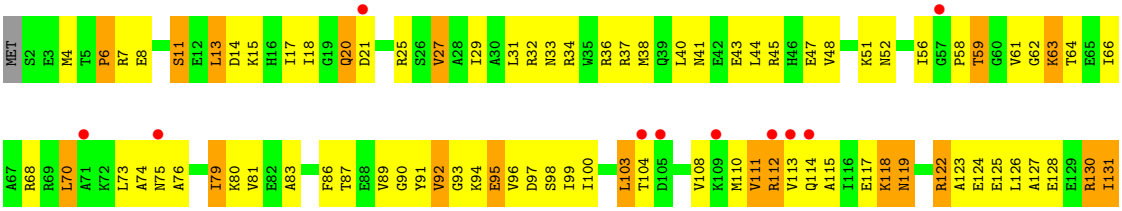
• Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU

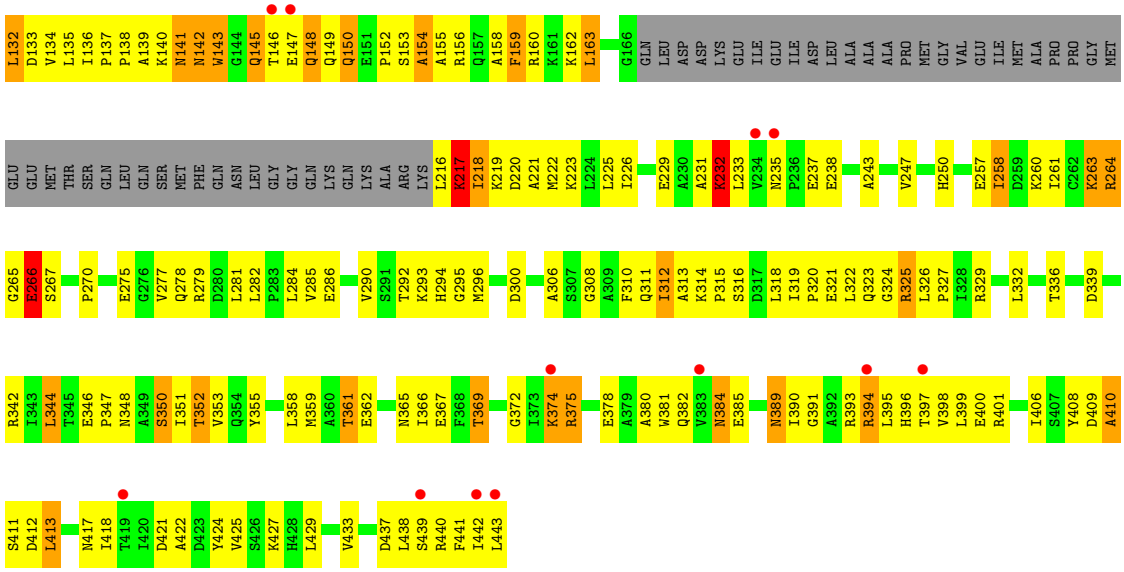
Chain E:



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

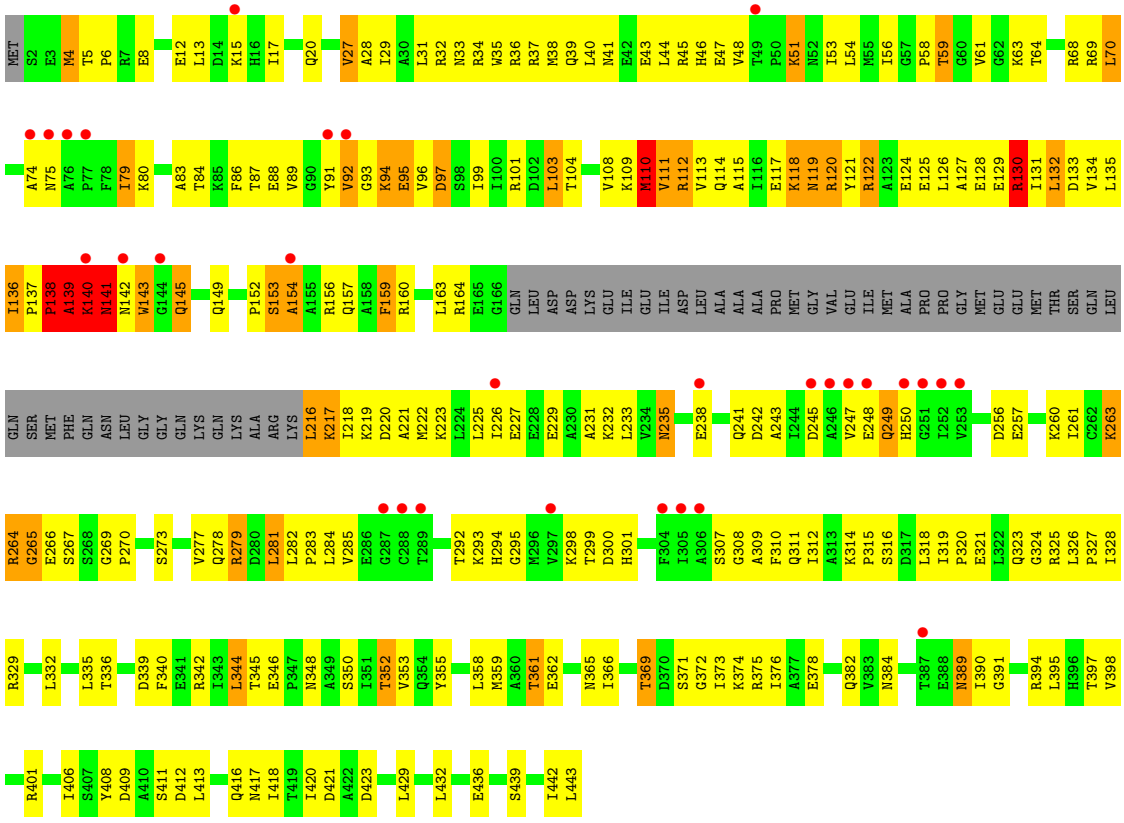
Chain F:





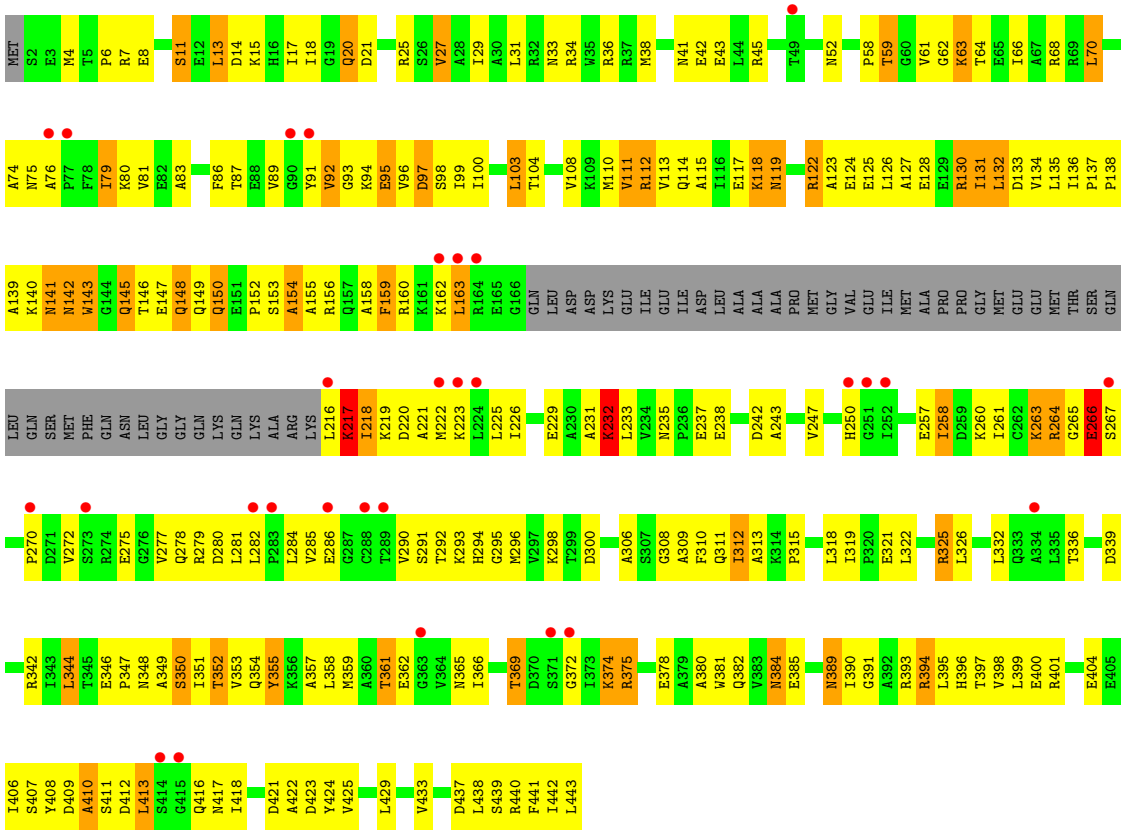
• Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU

Chain K:



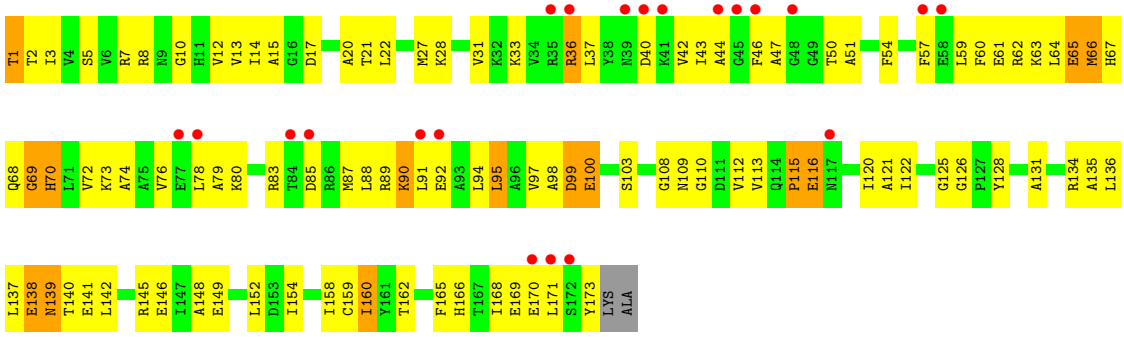
• Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU

Chain L:



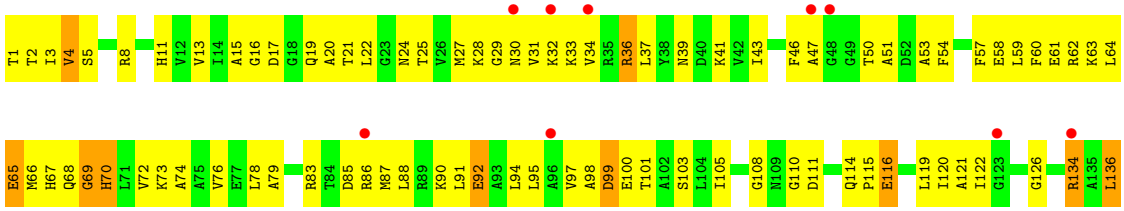
- Molecule 2: ATP-DEPENDENT PROTEASE HSLV

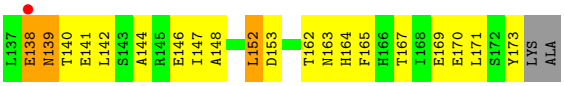
Chain M:



- Molecule 2: ATP-DEPENDENT PROTEASE HSLV

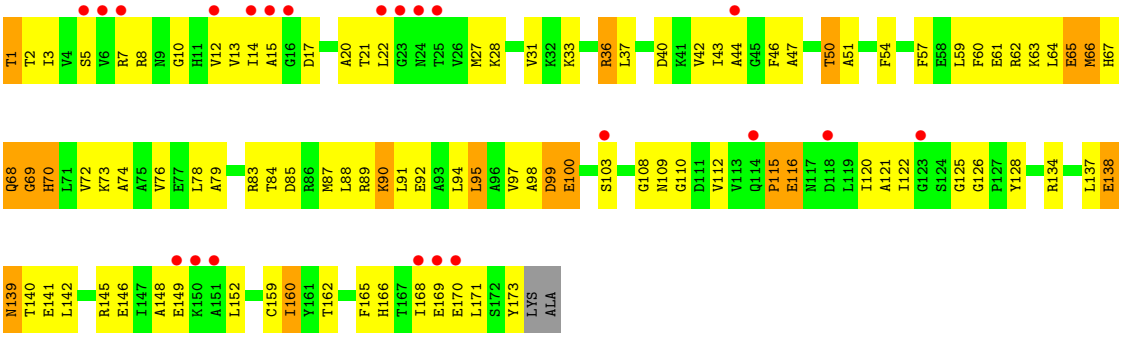
Chain N:





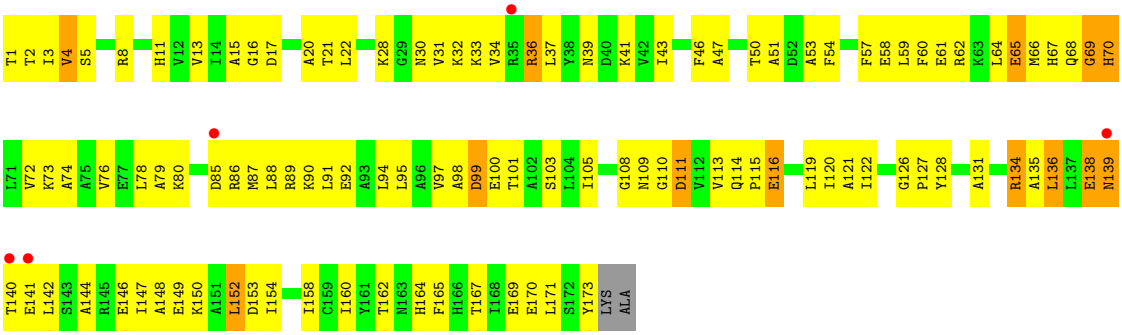
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain O:



• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain P:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.68 (at 6.72Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.401 , 0.432 0.450 , 0.434	Depositor DCC
R_{free} test set	607 reflections (9.48%)	wwPDB-VP
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 , 123.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.350 for -h,-k,l	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	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(^{o})	Ideal(^{o})
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 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 57.

All (2026) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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:CG	1:E:122:ARG:CB	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	Interatomic distance (Å)	Clash overlap (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:CG	1:K:122:ARG:CA	2.01	1.37
1:E:314:LYS:NZ	2:N:65:GLU:CG	1.70	1.36
1:E:122:ARG:CG	1:E:122:ARG:CA	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:K:293:LYS:HE3	1:L:296:MET:CE	1.60	1.30
1:L:145:GLN:CG	1:L:150:GLN:N	1.93	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
1:F:311:GLN:HG3	2:M:66:MET:CE	1.68	1.24
2:M:135:ALA:CB	2:P:154:ILE:HD13	1.66	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:E:408:TYR:OH	1:F:7:ARG:N	1.70	1.21
1:F:264:ARG:NH2	2:M:62:ARG:HB2	1.52	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:145:GLN:CB	1:F:149:GLN:HB2	1.71	1.20
1:L:264:ARG:CG	2:O:62:ARG:NH2	2.04	1.20
2:M:154:ILE:CG2	2:P:131:ALA:HB1	1.71	1.20
1:L:145:GLN:CD	1:L:145:GLN:N	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: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:L:309:ALA:CA	2:O:66:MET:SD	2.32	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:91:TYR:CD2	1:F:90:GLY:O	1.96	1.17
1:E:138:PRO:HB2	1:E:152:PRO:HB2	1.25	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:F:145:GLN:CD	1:F:145:GLN:N	1.87	1.16
1:K:145:GLN:HG3	1:K:149:GLN:CG	1.76	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:145:GLN:HG3	1:E:149:GLN:CG	1.76	1.15
1:E:407:SER:HA	1:F:36:ARG:NH1	1.38	1.15
1:E:442:ILE:HA	1:F:329:ARG:HB3	1.23	1.15
1:K:122:ARG:CG	1:K:122:ARG:HA	1.73	1.15
1:E:145:GLN:HB2	1:E:149:GLN:CB	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: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:145:GLN:HB3	1:L:149:GLN:HB2	1.15	1.13
1:L:264:ARG:NH2	2:O:59:LEU:CB	2.10	1.13
1:E:122:ARG:CG	1:E:122:ARG:HA	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:139:ALA:HB2	1:E:152:PRO:HG3	1.13	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:442:ILE:HA	1:F:329:ARG:CG	1.79	1.12
1:L:145:GLN:NE2	1:L:150:GLN:HA	1.64	1.12
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:E:408:TYR:OH	1:F:7:ARG:HA	1.36	1.12
1:K:139:ALA:HB2	1:K:152:PRO:HG3	1.12	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:86:PHE:O	1:F:89:VAL:HG22	1.51	1.11
1:F:264:ARG:NH1	2:M:62:ARG:CG	2.12	1.11
1:E:139:ALA:CB	1:E:152:PRO:CG	2.26	1.11
1:K:138:PRO:HB2	1:K:152:PRO:HB2	1.25	1.11
1:L:264:ARG:NH1	2:O:62:ARG:HB3	1.66	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
1:E:311:GLN:HE22	2:N:67:HIS:CA	1.64	1.10
2:M:135:ALA:HA	2:P:154:ILE:HD11	1.32	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:NE2	2:N:67:HIS:CA	2.16	1.09
1:E:311:GLN:HB3	2:N:66:MET:O	1.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:312:ILE:HA	2:O:62:ARG:HA	1.07	1.06
1:F:311:GLN:HG3	2:M:66:MET:HE1	1.37	1.06
1:K:311:GLN:CG	2:P:66:MET:CE	2.32	1.06
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:E:400:GLU:CD	1:F:51:LYS:CG	2.26	1.04
1:F:145:GLN:HG3	1:F:149:GLN:C	1.76	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
1:F:344:LEU:HD13	1:F:395:LEU:HD13	1.39	1.04
2:M:135:ALA:CA	2:P:154:ILE:HD11	1.85	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:K:139:ALA:HB2	1:K:152:PRO:HB3	1.35	1.03
1:L:264:ARG:CD	2:O:62:ARG:HD2	1.87	1.03
1:E:400:GLU:OE2	1:F:51:LYS:CE	2.06	1.02
1:L:309:ALA:CB	2:O:66:MET:SD	0.96	1.02
1:L:312:ILE:HA	2:O:62:ARG:CA	1.71	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:E:292:THR:HG22	1:E:294:HIS:H	1.20	1.01
1:F:311:GLN:HG3	2:M:66:MET:HE3	1.41	1.01
1:L:309:ALA:HB1	2:O:66:MET:SD	0.66	1.01
1:E:393:ARG:NE	1:F:321:GLU:HA	1.74	1.01
1:K:311:GLN:CG	2:P:66:MET:SD	2.44	1.01
1:K:408:TYR:CE2	1:L:7:ARG:CZ	2.37	1.01
1:L:313:ALA:O	2:O:65:GLU:OE2	1.79	1.01
1:E:357:ALA:HB3	1:F:44:LEU:HD13	1.39	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:400:GLU:OE2	1:F:51:LYS:NZ	1.94	1.00
1:K:163:LEU:HD11	1:K:218:ILE:HG21	1.39	1.00
1:E:354:GLN:NE2	1:F:47:GLU:C	2.14	1.00
1:E:400:GLU:OE1	1:F:51:LYS:HG2	1.57	1.00
1:K:139:ALA:CB	1:K:152:PRO:CB	2.39	1.00
1:E:408:TYR:CZ	1:F:6:PRO:C	2.34	1.00
1:F:145:GLN:CG	1:F:149:GLN:HB2	1.90	1.00
1:L:264:ARG:NH2	2:O:59:LEU:CG	0.85	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:264:ARG:HD3	2:O:62:ARG:HD2	1.02	1.00
1:K:88:GLU:OE2	1:L:280:ASP:OD2	1.79	0.99
1:L:145:GLN:CG	1:L:149:GLN:HB2	1.90	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:132:LEU:HD11	1:L:160:ARG:HB3	1.42	0.99
1:L:312:ILE:CA	2:O:62:ARG:HA	1.90	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:E:113:VAL:O	1:E:117:GLU:HG3	1.64	0.98
1:L:130:ARG:HD2	1:L:130:ARG:O	1.64	0.98
1:E:407:SER:CA	1:F:36:ARG:NH1	1.96	0.98
1:E:441:PHE:CG	1:F:56:ILE:HD13	1.97	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:O	1:F:130:ARG:HD2	1.64	0.97
1:E:92:VAL:HG11	1:F:92:VAL:HA	0.99	0.97
1:L:309:ALA:HB2	2:O:66:MET:SD	1.59	0.97
1:E:131:ILE:O	1:E:134:VAL:HG12	1.64	0.97
1:E:441:PHE:CD1	1:F:56:ILE:HG21	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:92:VAL:CG1	1:F:92:VAL:CA	2.30	0.95
1:L:311:GLN:HE22	2:O:68:GLN:C	1.69	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:141:ASN:H	1:E:141:ASN:HD22	1.14	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: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:355:TYR:HE2	1:F:51:LYS:NZ	1.64	0.94
1:E:441:PHE:O	1:F:329:ARG:CD	2.15	0.94
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:L:264:ARG:HG2	2:O:62:ARG:HH22	1.29	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:K:141:ASN:HD22	1:K:141:ASN:H	1.14	0.92
1:L:145:GLN:HB3	1:L:149:GLN:CB	1.99	0.92
1:L:309:ALA:CB	2:O:66:MET:CG	2.47	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
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
2:M:135:ALA:CA	2:P:154:ILE:CD1	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:145:GLN:CG	1:L:150:GLN:H	1.75	0.91
1:E:92:VAL:HG13	1:F:91:TYR:O	1.70	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:91:TYR:HB3	1:F:91:TYR:CA	2.00	0.91
1:E:122:ARG:CB	1:E:122:ARG:HD2	2.00	0.91
1:E:235:ASN:H	1:E:235:ASN:ND2	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:27:VAL:HG13	1:K:70:LEU:HG	1.53	0.90
1:K:264:ARG:CD	2:P:62:ARG:HH21	1.84	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:145:GLN:CG	1:E:149:GLN:CB	2.50	0.90
1:E:349:ALA:HB1	1:F:47:GLU:HG3	0.94	0.90
1:F:145:GLN:NE2	1:F:145:GLN:O	2.05	0.90
1:K:145:GLN:HB2	1:K:149:GLN:CA	2.01	0.90
1:K:235:ASN:H	1:K:235:ASN:ND2	1.67	0.90
1:E:145:GLN:HB2	1:E:149:GLN:CA	2.01	0.90
1:K:122:ARG:HA	1:K:122:ARG:HG3	1.53	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:357:ALA:HB1	1:F:40:LEU:HD22	1.55	0.89
1:E:358:LEU:HA	1:F:40:LEU:HD21	1.52	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:K:293:LYS:HE3	1:L:296:MET:SD	2.13	0.88
1:L:145:GLN:NE2	1:L:145:GLN:O	2.05	0.88
1:L:311:GLN:NE2	2:O:68:GLN:O	2.05	0.88
1:K:369:THR:HG22	1:K:372:GLY:H	1.39	0.88
1:L:264:ARG:HH11	2:O:62:ARG:CB	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2:THR:OG1	2:N:162:THR:HG21	1.73	0.87
2:N:140:THR:HG21	2:N:142:LEU:HG	1.54	0.87
1:E:358:LEU:CD1	1:F:48:VAL:HG11	2.01	0.87
1:E:393:ARG:NH2	1:F:321:GLU:HG3	1.88	0.87
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:130:ARG:NE	1:E:225:LEU:HD11	1.90	0.87
1:E:400:GLU:HG2	1:F:51:LYS:HG3	1.55	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: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:L:264:ARG:NH1	2:O:59:LEU:HA	1.90	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:130:ARG:HG3	1:F:225:LEU:CD1	2.06	0.85
1:F:264:ARG:NH2	2:M:62:ARG:CG	2.37	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:235:ASN:H	1:E:235:ASN:HD22	0.87	0.85
1:E:357:ALA:CB	1:F:40:LEU:HD22	2.07	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:H	1:K:235:ASN:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:130:ARG:HD3	1:K:225:LEU:HD12	1.60	0.84
1:K:235:ASN:HD22	1:K:235:ASN:N	1.65	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
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:HB3	2:P:134:ARG:HH11	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:E:408:TYR:HA	1:F:6:PRO:HG2	1.59	0.82
1:F:145:GLN:CG	1:F:150:GLN:H	1.75	0.82
1:E:355:TYR:CE2	1:F:51:LYS:NZ	2.46	0.82
1:F:145:GLN:CD	1:F:150:GLN:N	2.33	0.82
1:F:132:LEU:CD1	1:F:160:ARG:HB3	2.09	0.82
1:L:264:ARG:CD	2:O:62:ARG:CD	2.51	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:130:ARG:HD3	1:E:225:LEU:HD12	1.60	0.81
1:E:384:ASN:ND2	1:E:394:ARG:HD2	1.95	0.81
1:E:400:GLU:CG	1:F:51:LYS:HG3	2.10	0.81
1:L:264:ARG:HD3	2:O:62:ARG:HH21	1.44	0.81
2:M:36:ARG:HD3	2:M:40:ASP:OD1	1.80	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:F:59:THR:HG22	1:F:393:ARG:HH12	1.43	0.81
1:K:311:GLN:CG	2:P:66:MET:HE2	2.01	0.81
2:M:135:ALA:HB2	2:P:154:ILE:HD12	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:59:THR:HG22	1:L:393:ARG:HH12	1.43	0.80
1:L:136:ILE:HG22	1:L:138:PRO:HD3	1.64	0.80
1:L:141:ASN:HD22	1:L:141:ASN:H	1.30	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:K:83:ALA:HB1	1:K:261:ILE:HD12	1.64	0.78
1:L:311:GLN:NE2	2:O:68:GLN:C	2.37	0.78
1:E:400:GLU:CD	1:F:51:LYS:HG3	2.02	0.78
1:F:141:ASN:HD22	1:F:141:ASN:H	1.30	0.78
1:F:217:LYS:HB3	1:F:220:ASP:HB3	1.66	0.78
1:L:89:VAL:CG1	1:L:94:LYS:O	2.32	0.78
1:E:120:ARG:NH1	1:E:124:GLU:OE2	2.16	0.78
1:F:369:THR:HG22	1:F:372:GLY:N	1.98	0.78
1:L:264:ARG:HD3	2:O:62:ARG:HD3	1.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:89:VAL:HG12	1:E:94:LYS:H	1.48	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:407:SER:CB	1:F:36:ARG:NH1	2.47	0.77
1:E:441:PHE:HA	1:F:315:PRO:CG	2.13	0.77
1:E:389:ASN:HD22	1:E:389:ASN:C	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
1:K:5:THR:OG1	1:K:8:GLU:HG3	1.85	0.77
1:K:91:TYR:CE1	1:L:272:VAL:HG11	2.20	0.77
1:K:89:VAL:HG12	1:K:94:LYS:H	1.48	0.77
1:E:5:THR:OG1	1:E:8:GLU:HG3	1.85	0.77
1:E:94:LYS:HD2	1:E:95:GLU:H	1.50	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:F:27:VAL:HG13	1:F:70:LEU:HG	1.67	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
1:L:145:GLN:HG2	1:L:150:GLN:N	1.99	0.76
2:O:1:THR:HB	2:O:33:LYS:HZ3	1.48	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
1:L:311:GLN:HE21	2:O:67:HIS:H	1.33	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:E:257:GLU:OE1	1:F:279:ARG:HG3	1.83	0.76
1:L:145:GLN:CG	1:L:149:GLN:CA	2.64	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:C	1:K:389:ASN:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:20:GLN:HG2	1:F:332:LEU:HD23	1.68	0.75
1:K:389:ASN:ND2	1:K:391:GLY:H	1.85	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
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:K:358:LEU:O	1:K:361:THR:HG22	1.87	0.74
1:L:311:GLN:CA	2:O:65:GLU:OE1	2.31	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:118:LYS:HA	1:E:118:LYS:NZ	2.03	0.73
1:E:266:GLU:HA	2:N:85:ASP:OD1	1.88	0.73
1:F:132:LEU:CD1	1:F:156:ARG:HG2	2.17	0.73
1:F:344:LEU:CD1	1:F:395:LEU:HD13	2.17	0.73
1:E:59:THR:HG21	1:F:320:PRO:HB2	1.70	0.73
1:E:120:ARG:C	1:E:120:ARG:CD	2.56	0.73
1:E:261:ILE:O	1:E:261:ILE:HG22	1.86	0.73
1:F:258:ILE:HG13	1:F:306:ALA:HB1	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:358:LEU:HD21	1:F:37:ARG:HA	1.69	0.73
1:E:393:ARG:HH21	1:F:321:GLU:HG3	1.51	0.73
1:F:145:GLN:OE1	1:F:149:GLN:CB	2.36	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:309:ALA:HB3	2:O:66:MET:SD	1.12	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:235:ASN:HB2	1:E:238:GLU:OE2	1.89	0.73
1:E:400:GLU:CD	1:F:51:LYS:NZ	2.41	0.73
1:E:442:ILE:HD13	1:F:329:ARG:HB3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:163:LEU:CD1	1:K:218:ILE:HG21	2.18	0.73
1:L:309:ALA:CB	2:O:66:MET:CE	2.16	0.73
2:O:50:THR:HG21	2:P:111:ASP:OD1	1.89	0.73
1:E:88:GLU:HG2	1:F:89:VAL:O	1.89	0.73
1:E:411:SER:HB3	1:F:32:ARG:NH2	2.03	0.73
1:E:135:LEU:HD13	1:E:159:PHE:CE1	2.24	0.72
1:E:374:LYS:HE2	1:E:378:GLU:OE2	1.89	0.72
1:K:141:ASN:HD22	1:K:141:ASN:N	1.79	0.72
1:E:409:ASP:O	1:E:413:LEU:HD13	1.89	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:312:ILE:HD12	2:N:67:HIS:HE1	1.50	0.72
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:354:GLN:CD	1:F:47:GLU:CB	2.57	0.72
1:E:441:PHE:O	1:F:329:ARG:CB	2.37	0.72
1:F:145:GLN:CG	1:F:149:GLN:CA	2.64	0.72
1:K:120:ARG:C	1:K:120:ARG:CD	2.56	0.72
1:L:132:LEU:HD13	1:L:156:ARG:CG	2.17	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: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
1:L:264:ARG:NH1	2:O:59:LEU:CA	2.52	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: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:K:130:ARG:CD	1:K:225:LEU:HD12	2.19	0.72
1:L:311:GLN:HG2	2:O:66:MET:HE1	1.71	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:K:135:LEU:HD13	1:K:159:PHE:CE1	2.24	0.72
1:K:245:ASP:O	1:K:249:GLN:HG3	1.89	0.72
1:L:381:TRP:CH2	1:L:385:GLU:OE2	2.43	0.72
1:E:245:ASP:O	1:E:249:GLN:HG3	1.89	0.71
1:L:264:ARG:CZ	2:O:59:LEU:CB	2.42	0.71
1:E:142:ASN:O	1:E:143:TRP:HB2	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:358:LEU:O	1:F:361:THR:HB	1.90	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
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
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: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
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:F:145:GLN:HG2	1:F:150:GLN:N	1.99	0.71
1:F:389:ASN:ND2	1:F:391:GLY:H	1.88	0.71
1:K:139:ALA:HB2	1:K:152:PRO:CD	2.19	0.71
1:K:279:ARG:HH11	1:K:319:ILE:HD12	1.55	0.71
1:E:91:TYR:HB3	1:F:91:TYR:C	2.11	0.70
1:L:264:ARG:CZ	2:O:59:LEU:CA	2.69	0.70
1:L:264:ARG:C	1:L:266:GLU:H	1.94	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: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
1:K:264:ARG:CD	2:P:62:ARG:NH2	2.50	0.70
1:F:429:LEU:O	1:F:433:VAL:HG23	1.92	0.70
2:M:140:THR:CG2	2:M:142:LEU:HG	2.21	0.70
2:N:5:SER:HB3	2:N:120:ILE:HB	1.72	0.70
2:O:140:THR:CG2	2:O:142:LEU:H	2.03	0.70
1:L:389:ASN:ND2	1:L:391:GLY:H	1.88	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: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:411:SER:CB	1:F:32:ARG:NH2	2.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:441:PHE:CE1	1:F:56:ILE:HG21	2.27	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
1:E:282:LEU:HD11	1:E:319:ILE:HD11	1.74	0.70
1:F:141:ASN:H	1:F:141:ASN:ND2	1.88	0.70
1:F:263:LYS:O	1:F:264:ARG:HB3	1.92	0.70
1:K:261:ILE:HD13	1:K:277:VAL:HB	1.74	0.70
2:N:67:HIS:CD2	2:N:73:LYS:HE3	2.27	0.70
1:E:33:ASN:ND2	1:E:36:ARG:HD2	2.07	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:L:264:ARG:CZ	2:O:59:LEU:HA	2.22	0.70
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:K:139:ALA:O	1:K:140:LYS:CB	2.38	0.69
1:L:141:ASN:H	1:L:141:ASN:ND2	1.88	0.69
1:E:139:ALA:HA	1:E:152:PRO:HB3	1.74	0.69
1:E:139:ALA:O	1:E:140:LYS:CB	2.38	0.69
2:M:160:ILE:HD11	2:O:160:ILE:O	1.92	0.69
1:E:222:MET:O	1:E:226:ILE:HG13	1.93	0.69
1:E:440:ARG:CD	1:F:316:SER:OG	2.39	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: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
2:O:79:ALA:HB1	2:O:110:GLY:HA2	1.74	0.69
2:M:79:ALA:HB1	2:M:110:GLY:HA2	1.74	0.69
2:P:33:LYS:HA	2:P:46:PHE:CE1	2.27	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:E:432:LEU:H	1:E:432:LEU:HD12	1.56	0.69
1:F:92:VAL:HG23	1:F:93:GLY:N	2.08	0.69
1:L:145:GLN:N	1:L:145:GLN:OE1	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
1:K:389:ASN:HD22	1:K:390:ILE:N	1.91	0.68
1:K:432:LEU:HD12	1:K:432:LEU:H	1.56	0.68
2:N:33:LYS:HA	2:N:46:PHE:CE1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:20:ALA:HB2	2:O:31:VAL:HG21	1.75	0.68
1:E:27:VAL:CG1	1:E:70:LEU:HG	2.23	0.68
1:F:89:VAL:HG11	1:F:94:LYS:O	1.92	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:K:104:THR:HG21	1:K:292:THR:HG21	1.75	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:E:267:SER:HB3	1:E:270:PRO:HG3	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: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
2:M:20:ALA:HB2	2:M:31:VAL:HG21	1.75	0.68
2:M:160:ILE:HG23	2:O:160:ILE:HD11	1.75	0.68
1:E:163:LEU:HD11	1:E:218:ILE:CG2	2.21	0.68
1:E:261:ILE:HD13	1:E:277:VAL:HB	1.74	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: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:L:89:VAL:HG11	1:L:94:LYS:O	1.92	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
1:F:229:GLU:HA	1:F:232:LYS:HG2	1.76	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: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:229:GLU:HA	1:L:232:LYS:HG2	1.76	0.67
1:L:311:GLN:HE21	2:O:68:GLN:N	1.92	0.67
1:E:132:LEU:HD12	1:E:156:ARG:HG2	1.76	0.67
1:L:27:VAL:HG22	1:L:70:LEU:HD12	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:K:88:GLU:OE2	1:L:280:ASP:CG	2.33	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:33:ASN:HD22	1:E:36:ARG:HD2	1.58	0.67
1:E:311:GLN:NE2	2:N:66:MET:O	2.26	0.67
1:L:59:THR:HG22	1:L:393:ARG:NH1	2.10	0.67
2:N:134:ARG:HH11	2:N:134:ARG:CB	2.07	0.67
2:P:134:ARG:HH11	2:P:134:ARG:CB	2.07	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:F:319:ILE:HG22	1:F:322:LEU:HB2	1.77	0.67
1:K:163:LEU:HD11	1:K:218:ILE:CG2	2.21	0.67
1:F:125:GLU:O	1:F:128:GLU:HG2	1.95	0.67
1:L:264:ARG:NH2	2:O:59:LEU:HD22	2.00	0.67
1:L:264:ARG:NH1	2:O:62:ARG:CB	2.45	0.67
1:L:336:THR:O	1:L:339:ASP:HB2	1.95	0.67
2:O:72:VAL:O	2:O:76:VAL:HG23	1.95	0.67
2:P:94:LEU:HD13	2:P:122:ILE:HB	1.77	0.67
1:E:397:THR:OG1	1:F:327:PRO:HA	1.95	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:M:131:ALA:O	2:P:154:ILE:CG2	2.43	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:88:GLU:CG	1:F:89:VAL:O	2.44	0.66
1:E:397:THR:HA	1:F:327:PRO:CA	2.25	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:F:389:ASN:C	1:F:389:ASN:HD22	1.98	0.66
1:K:132:LEU:HD12	1:K:156:ARG:HG2	1.76	0.66
1:L:142:ASN:O	1:L:143:TRP:CB	2.42	0.66
2:O:140:THR:HG21	2:O:142:LEU:HG	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:61:GLU:O	2:P:65:GLU:HG2	1.95	0.66
1:F:145:GLN:N	1:F:145:GLN:OE1	2.12	0.65
1:K:96:VAL:HG13	1:K:99:ILE:HD12	1.78	0.65
1:L:92:VAL:CG2	1:L:93:GLY:N	2.59	0.65
1:L:311:GLN:HG2	2:O:66:MET:CE	2.26	0.65
2:P:58:GLU:O	2:P:62:ARG:HG3	1.96	0.65
1:E:20:GLN:HG3	1:E:332:LEU:HD23	1.78	0.65
1:F:362:GLU:HG3	1:F:411:SER:HA	1.78	0.65
1:L:311:GLN:HA	2:O:65:GLU:OE1	1.96	0.65
1:E:359:MET:HE3	1:F:36:ARG:HH11	1.61	0.65
1:K:20:GLN:HG3	1:K:332:LEU:HD23	1.78	0.65
1:K:293:LYS:CE	1:L:296:MET:SD	2.83	0.65
2:N:58:GLU:O	2:N:62:ARG:HG3	1.96	0.65
1:E:59:THR:CG2	1:F:321:GLU:OE1	2.43	0.65
1:E:393:ARG:HD3	1:F:321:GLU:HA	1.79	0.65
1:L:362:GLU:HG3	1:L:411:SER:HA	1.78	0.65
2:O:152:LEU:HD22	2:O:166:HIS:CE1	2.31	0.65
1:F:96:VAL:HG13	1:F:99:ILE:HD12	1.78	0.65
1:K:126:LEU:HD23	1:K:229:GLU:CD	2.17	0.65
1:E:120:ARG:C	1:E:120:ARG:HD2	2.16	0.65
1:F:92:VAL:CG2	1:F:93:GLY:N	2.59	0.65
1:K:138:PRO:CG	1:K:156:ARG:HD3	2.26	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
2:N:94:LEU:HD13	2:N:122:ILE:HB	1.77	0.65
1:E:79:ILE:HD13	1:E:80:LYS:N	2.12	0.65
1:F:59:THR:HG22	1:F:393:ARG:NH1	2.10	0.65
1:E:96:VAL:HG13	1:E:99:ILE:HD12	1.78	0.65
2:M:140:THR:HG21	2:M:142:LEU:HG	1.78	0.65
1:E:126:LEU:HD23	1:E:229:GLU:CD	2.17	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
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:CG	1:E:122:ARG:C	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:63:LYS:HG2	1:E:332:LEU:HD22	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:F:381:TRP:CZ3	1:F:385:GLU:OE2	2.50	0.64
2:N:138:GLU:HB3	2:N:139:ASN:ND2	2.12	0.64
1:E:311:GLN:HG2	2:N:66:MET:SD	2.21	0.63
1:E:359:MET:HG3	1:E:366:ILE:HG13	1.80	0.63
1:K:436:GLU:O	1:K:439:SER:HB2	1.98	0.63
2:P:138:GLU:HB3	2:P:139:ASN:ND2	2.12	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:243:ALA:O	1:E:247:VAL:HG23	1.97	0.63
1:E:358:LEU:CD2	1:F:40:LEU:HD11	2.29	0.63
1:E:442:ILE:CB	1:F:329:ARG:HB2	2.29	0.63
1:K:359:MET:HG3	1:K:366:ILE:HG13	1.80	0.63
1:L:313:ALA:N	2:O:65:GLU:HG3	2.13	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:83:ALA:HB1	1:E:261:ILE:CD1	2.29	0.63
1:E:390:ILE:HA	1:F:320:PRO:HB3	1.79	0.63
1:F:145:GLN:CB	1:F:149:GLN:CB	2.62	0.63
1:K:83:ALA:HB1	1:K:261:ILE:CD1	2.29	0.63
1:K:145:GLN:CG	1:K:149:GLN:CG	2.67	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:E:221:ALA:O	1:E:225:LEU:HD23	1.99	0.63
1:E:264:ARG:NH2	2:N:63:LYS:HZ1	1.97	0.63
1:F:261:ILE:HG22	1:F:261:ILE:O	1.99	0.63
1:E:432:LEU:H	1:E:432:LEU:CD1	2.12	0.63
1:E:436:GLU:O	1:E:439:SER:HB2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:85:ASP:HB2	2:M:88:LEU:HD23	1.81	0.63
1:E:96:VAL:HG12	1:E:284:LEU:HD11	1.81	0.63
1:E:354:GLN:OE1	1:F:47:GLU:O	2.17	0.63
1:L:130:ARG:C	1:L:130:ARG:HH11	2.01	0.63
2:M:28:LYS:HD3	2:M:31:VAL:HG22	1.81	0.63
2:O:28:LYS:HD3	2:O:31:VAL:HG22	1.81	0.63
1:E:86:PHE:O	1:E:89:VAL:HG13	1.98	0.62
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:F:141:ASN:O	1:F:142:ASN:HB2	1.98	0.62
1:K:221:ALA:O	1:K:225:LEU:HD23	1.99	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:HD22	2:M:139:ASN:N	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
1:E:108:VAL:HG21	1:E:294:HIS:ND1	2.15	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:264:ARG:HD3	2:O:62:ARG:NH2	2.12	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: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:E:109:LYS:HG2	1:F:296:MET:CB	2.30	0.62
1:E:264:ARG:NH1	2:N:63:LYS:NZ	2.46	0.62
1:E:393:ARG:CZ	1:F:321:GLU:HG3	2.30	0.62
1:K:96:VAL:HG12	1:K:284:LEU:HD11	1.81	0.62
1:K:108:VAL:HG21	1:K:294:HIS:ND1	2.15	0.62
1:L:145:GLN:HG3	1:L:149:GLN:CB	2.30	0.62
1:L:311:GLN:NE2	2:O:64:LEU:O	2.33	0.61
1:L:312:ILE:C	2:O:62:ARG:HA	2.20	0.61
2:M:17:ASP:O	2:M:33:LYS:HD3	2.00	0.61
1:F:389:ASN:HD22	1:F:391:GLY:H	1.48	0.61
1:K:432:LEU:HD12	1:K:432:LEU:N	2.15	0.61
1:L:163:LEU:C	1:L:163:LEU:HD12	2.20	0.61
2:O:54:PHE:HE2	2:P:80:LYS:CG	2.12	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:85:ASP:HB2	2:O:88:LEU:HD23	1.81	0.61
1:E:92:VAL:CG1	1:F:92:VAL:CG1	2.77	0.61
1:E:411:SER:CB	1:F:32:ARG:HH21	2.11	0.61
1:F:223:LYS:HA	1:F:226:ILE:HD12	1.81	0.61
1:F:285:VAL:HG12	1:F:325:ARG:HG2	1.83	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
2:P:28:LYS:HE2	2:P:30:ASN:OD1	1.97	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
2:O:17:ASP:O	2:O:33:LYS:HD3	2.00	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
1:F:158:ALA:O	1:F:162:LYS:HB2	2.00	0.61
2:N:11:HIS:HA	2:N:171:LEU:O	2.01	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
1:E:145:GLN:HB2	1:E:149:GLN:N	2.15	0.61
1:E:129:GLU:O	1:E:133:ASP:HB2	1.99	0.61
1:F:91:TYR:O	1:F:92:VAL:CG1	2.49	0.61
1:E:145:GLN:N	1:E:149:GLN:HB2	2.16	0.61
1:E:401:ARG:NH2	1:F:329:ARG:O	2.30	0.61
1:F:141:ASN:HD22	1:F:141:ASN:N	1.92	0.61
1:L:158:ALA:O	1:L:162:LYS:HB2	2.00	0.61
1:L:223:LYS:HA	1:L:226:ILE:HD12	1.81	0.61
2:N:20:ALA:HB2	2:N:31:VAL:HG21	1.82	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:F:286:GLU:HG2	1:F:325:ARG:NH1	2.16	0.60
1:K:145:GLN:H	1:K:149:GLN:HB2	1.63	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
1:E:432:LEU:HD12	1:E:432:LEU:N	2.15	0.60
2:P:20:ALA:HB2	2:P:31:VAL:HG21	1.82	0.60
2:P:86:ARG:HG2	2:P:87:MET:N	2.16	0.60
1:F:122:ARG:HG2	1:F:122:ARG:HH21	1.66	0.60
1:K:145:GLN:HB2	1:K:149:GLN:N	2.15	0.60
1:L:285:VAL:HG12	1:L:325:ARG:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:222:MET:O	1:F:226:ILE:HG13	2.01	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:221:ALA:O	1:F:225:LEU:HD23	2.00	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:E:264:ARG:C	1:E:266:GLU:H	2.05	0.60
1:K:92:VAL:CG2	1:K:93:GLY:H	2.14	0.60
1:K:264:ARG:C	1:K: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
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
2:P:86:ARG:CG	2:P:87:MET:N	2.64	0.60
1:F:86:PHE:HB2	1:F:277:VAL:HG13	1.84	0.60
1:K:20:GLN:CG	1:K:332:LEU:HD23	2.31	0.60
1:K:86:PHE:O	1:K:89:VAL:HG22	2.02	0.60
1:L:286:GLU:HG2	1:L:325:ARG:NH1	2.16	0.60
2:N:60:PHE:CE2	2:N:97:VAL:HG21	2.37	0.60
2:N:88:LEU:HD22	2:N:88:LEU:H	1.67	0.60
1:E:91:TYR:CB	1:F:90:GLY:C	2.71	0.60
1:F:103:LEU:HD13	1:F:247:VAL:HG13	1.84	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:E:223:LYS:HA	1:E:226:ILE:HD12	1.84	0.59
1:E:390:ILE:HD13	1:F:323:GLN:CB	2.32	0.59
1:F:384:ASN:ND2	1:F:390:ILE:H	2.00	0.59
1:K:384:ASN:HD22	1:K:394:ARG:HH11	1.49	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: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
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
2:M:60:PHE:HB2	2:M:78:LEU:HD22	1.84	0.59
1:E:34:ARG:CZ	1:E:250:HIS:HA	2.32	0.59
1:E:261:ILE:HG22	1:E:278:GLN:HG3	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:384:ASN:ND2	1:L:390:ILE:H	2.00	0.59
1:E:92:VAL:CG1	1:F:92:VAL:CB	2.75	0.59
1:E:361:THR:CG2	1:F:36:ARG:HA	2.27	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:K:34:ARG:CZ	1:K:250:HIS:HA	2.32	0.59
1:L:222:MET:O	1:L:226:ILE:HG13	2.01	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:E:109:LYS:HG2	1:F:296:MET:HB2	1.84	0.59
1:E:263:LYS:O	1:E:264:ARG:HB3	2.02	0.59
1:F:130:ARG:NH2	1:F:225:LEU:HD21	2.18	0.59
1:K:122:ARG:CA	1:K:122:ARG:HG2	2.26	0.59
1:L:86:PHE:HB2	1:L:277:VAL:HG13	1.84	0.59
1:L:264:ARG:CB	2:O:62:ARG:NH2	2.64	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
1:L:384:ASN:HD21	1:L:390:ILE:HG12	1.68	0.58
2:O:59:LEU:O	2:O:62:ARG:HB3	2.03	0.58
1:K:261:ILE:HG22	1:K:278:GLN:HG3	1.85	0.58
1:K:263:LYS:O	1:K:264:ARG:HB3	2.02	0.58
2:P:13:VAL:HG12	2:P:170:GLU:HG3	1.84	0.58
1:F:384:ASN:HD21	1:F:390:ILE:HG12	1.68	0.58
1:L:130:ARG:NH2	1:L:225:LEU:HD21	2.18	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:92:VAL:HG21	1:F:92:VAL:HA	1.84	0.58
1:E:397:THR:HA	1:F:327:PRO:HA	1.85	0.58
1:F:91:TYR:C	1:F:92:VAL:HG13	2.24	0.58
2:N:90:LYS:HD2	2:N:90:LYS:C	2.23	0.58
2:P:85:ASP:CB	2:P:88:LEU:HD23	2.34	0.58
1:E:86:PHE:O	1:E:89:VAL:HG22	2.02	0.58
1:K:59:THR:O	1:K:61:VAL:HG13	2.03	0.58
1:K:223:LYS:HA	1:K:226:ILE:HD12	1.84	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:F:63:LYS:HG2	1:F:332:LEU:HD22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:261:ILE:O	1:K:261:ILE:CG2	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
2:O:139:ASN:N	2:O:139:ASN:ND2	2.52	0.58
1:F:59:THR:O	1:F:61:VAL:HG13	2.04	0.58
1:F:41:ASN:ND2	1:F:43:GLU:HB3	2.19	0.58
2:O:47:ALA:HB3	2:O:94:LEU:HB2	1.85	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
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:131:ALA:HA	2:P:158:ILE:CD1	2.34	0.57
2:O:54:PHE:CE2	2:P:80:LYS:CD	2.85	0.57
2:P:86:ARG:HG2	2:P:87:MET:H	1.69	0.57
1:F:374:LYS:NZ	1:F:378:GLU:OE2	2.29	0.57
1:K:264:ARG:CB	2:P:62:ARG:HH22	2.17	0.57
2:M:59:LEU:O	2:M:62:ARG:HB3	2.03	0.57
2:O:1:THR:HA	2:O:162:THR:HG22	1.87	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
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:92:VAL:CG1	1:F:91:TYR:O	2.50	0.57
1:E:354:GLN:CD	1:F:47:GLU:O	2.38	0.57
1:L:63:LYS:HG2	1:L:332:LEU:HD22	1.85	0.57
2:P:79:ALA:HB1	2:P:110:GLY:HA2	1.86	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
2:O:37:LEU:HD21	2:O:57:PHE:CB	2.32	0.57
1:E:41:ASN:ND2	1:E:43:GLU:HB3	2.20	0.57
1:E:408:TYR:HE2	1:F:7:ARG:HG3	1.70	0.57
1:F:4:MET:HB3	1:F:8:GLU:HB3	1.86	0.57
1:F:264:ARG:NH2	2:M:59:LEU:HA	2.20	0.57
2:M:1:THR:HA	2:M:162:THR:HG22	1.86	0.57
2:O:3:ILE:HD11	2:O:46:PHE:O	2.05	0.57
2:O:13:VAL:HG12	2:O:170:GLU:HG3	1.86	0.57
1:F:94:LYS:HD2	1:F:95:GLU:H	1.70	0.57
1:L:4:MET:HB3	1:L:8:GLU:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:54:PHE:CE2	2:P:80:LYS:HG3	2.39	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:F:104:THR:HG21	1:F:292:THR:HG21	1.87	0.56
1:F:235:ASN:HB2	1:F:238:GLU:OE2	2.05	0.56
1:F:366:ILE:HD13	1:F:418:ILE:HB	1.87	0.56
1:K:41:ASN:ND2	1:K:43:GLU:HB3	2.20	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:L:309:ALA:C	2:O:66:MET:SD	2.84	0.56
2:M:139:ASN:N	2:M:139:ASN:ND2	2.52	0.56
1:L:145:GLN:N	1:L:145:GLN:NE2	2.51	0.56
1:L:235:ASN:HB2	1:L:238:GLU:OE2	2.05	0.56
2:N:86:ARG:HG2	2:N:87:MET:H	1.69	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
1:K:17:ILE:HD11	1:K:69:ARG:HG3	1.86	0.56
1:L:96:VAL:HG12	1:L:284:LEU:HD11	1.86	0.56
1:L:308:GLY:HA3	1:L:310:PHE:CE2	2.40	0.56
2:N:3:ILE:HD11	2:N:46:PHE:O	2.05	0.56
1:E:358:LEU:HD23	1:F:37:ARG:CA	2.29	0.56
1:E:358:LEU:HD21	1:F:37:ARG:CA	2.29	0.56
1:F:96:VAL:HG12	1:F:284:LEU:HD11	1.86	0.56
1:F:126:LEU:HD23	1:F:229:GLU:CD	2.26	0.56
1:F:308:GLY:HA3	1:F:310:PHE:CE2	2.40	0.56
1:L:104:THR:HG21	1:L:292:THR:HG21	1.88	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:N:1:THR:HB	2:N:33:LYS:NZ	2.20	0.56
2:O:57:PHE:CE1	2:O:95:LEU:HD21	2.41	0.56
2:P:3:ILE:HD11	2:P:46:PHE:O	2.05	0.56
1:E:362:GLU:OE1	1:F:36:ARG:HG2	2.06	0.56
1:E:441:PHE:CE1	1:F:56:ILE:CG2	2.89	0.56
1:F:86:PHE:O	1:F:89:VAL:CG2	2.41	0.56
1:K:91:TYR:HE1	1:L:272:VAL:HG11	1.69	0.56
2:M:3:ILE:HD11	2:M:46:PHE:O	2.05	0.56
2:M:135:ALA:CA	2:P:154:ILE:HD13	2.25	0.56
2:N:21:THR:HG22	2:N:22:LEU:N	2.21	0.56
1:K:103:LEU:HD13	1:K:247:VAL:HG13	1.88	0.56
1:E:145:GLN:CG	1:E:149:GLN:CG	2.67	0.56
1:F:33:ASN:HD22	1:F:36:ARG:HD2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:145:GLN:CA	1:K:149:GLN:HB2	2.29	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:E:17:ILE:HD11	1:E:69:ARG:HG3	1.86	0.56
1:E:118:LYS:HA	1:E:118:LYS:CE	2.36	0.56
1:F:58:PRO:HG2	1:F:61:VAL:HG11	1.88	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:91:TYR:HB3	1:F:91:TYR:HA	1.85	0.55
1:F:27:VAL:CG1	1:F:70:LEU:HG	2.35	0.55
1:F:89:VAL:HG12	1:F:94:LYS:N	2.21	0.55
1:K:153:SER:O	1:K:154:ALA:C	2.45	0.55
1:L:366:ILE:HD13	1:L:418:ILE:HB	1.88	0.55
2:P:1:THR:HB	2:P:33:LYS:NZ	2.20	0.55
1:E:89:VAL:CG1	1:E:94:LYS:O	2.53	0.55
1:E:92:VAL:HG11	1:F:92:VAL:HB	1.81	0.55
1:F:155:ALA:O	1:F:159:PHE:HB2	2.06	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
2:M:136:LEU:HD11	2:P:135:ALA:HB1	1.88	0.55
2:P:21:THR:HG22	2:P:22:LEU:N	2.21	0.55
1:E:15:LYS:HB3	1:E:348:ASN:ND2	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:F:91:TYR:O	1:F:92:VAL:HG13	2.07	0.55
1:K:64:THR:HG22	1:K:68:ARG:HD2	1.88	0.55
1:K:118:LYS:HA	1:K:118:LYS:CE	2.36	0.55
2:O:54:PHE:CE2	2:P:80:LYS:HD2	2.42	0.55
1:E:103:LEU:HD13	1:E:247:VAL:HG13	1.88	0.55
1:E:408:TYR:HB2	1:F:29:ILE:HG12	1.87	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:62:ARG:O	2:M:65:GLU:HB2	2.07	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:64:THR:HG22	1:E:68:ARG:HD2	1.88	0.55
1:E:362:GLU:OE2	1:F:32:ARG:NH2	2.40	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:L:58:PRO:HG2	1:L:61:VAL:HG11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:70:HIS:HD2	2:P:73:LYS:HB2	1.72	0.55
1:E:139:ALA:O	1:E:140:LYS:CG	2.55	0.55
1:E:292:THR:HG22	1:E:294:HIS:N	2.05	0.55
1:E:442:ILE:CG2	1:F:329:ARG:HB2	2.37	0.55
1:F:108:VAL:HA	1:F:111:VAL:HG22	1.89	0.55
1:F:397:THR:HG21	1:F:443:LEU:O	2.07	0.55
1:L:374:LYS:NZ	1:L:378:GLU:OE2	2.29	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: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
1:E:153:SER:O	1:E:154:ALA:C	2.45	0.54
1:K:15:LYS:HB3	1:K:348:ASN:ND2	2.21	0.54
2:O:62:ARG:O	2:O:65:GLU:HB2	2.07	0.54
1:K:122:ARG:HG2	1:K:122:ARG:O	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:N	2:P:139:ASN:ND2	2.48	0.54
1:E:145:GLN:CA	1:E:149:GLN:HB2	2.29	0.54
1:F:111:VAL:HG21	1:F:243:ALA:HB2	1.88	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
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:366:ILE:HD13	1:E:418:ILE:HB	1.88	0.54
1:E:394:ARG:NH2	1:F:323:GLN:OE1	2.40	0.54
1:K:91:TYR:CE1	1:L:272:VAL:HG12	2.40	0.54
1:K:132:LEU:HD12	1:K:156:ARG:CG	2.38	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
2:N:70:HIS:HD2	2:N:73:LYS:HB2	1.72	0.54
1:E:122:ARG:O	1:E:122:ARG:HG2	2.06	0.54
1:F:285:VAL:CG1	1:F:325:ARG:HB3	2.38	0.54
1:K:312:ILE:HD12	2:P:62:ARG:O	2.07	0.54
1:L:264:ARG:O	1:L:266:GLU:N	2.40	0.54
2:M:131:ALA:HA	2:P:158:ILE:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:41:ASN:HD22	1:E:43:GLU:HB3	1.73	0.54
1:F:131:ILE:O	1:F:134:VAL:HG12	2.08	0.54
1:K:139:ALA:O	1:K:140:LYS:CG	2.55	0.54
1:L:397:THR:HG21	1:L:443:LEU:O	2.07	0.54
1:K:41:ASN:HD22	1:K:43:GLU:HB3	1.73	0.53
1:L:91:TYR:O	1:L:92:VAL:HG13	2.07	0.53
1:E:91:TYR:CD2	1:F:91:TYR:HA	2.43	0.53
1:K:131:ILE:HD12	1:K:134:VAL:CG1	2.39	0.53
1:L:145:GLN:OE1	1:L:149:GLN:C	2.46	0.53
2:N:67:HIS:O	2:N:69:GLY:N	2.41	0.53
2:O:98:ALA:CB	2:O:103:SER:HB3	2.38	0.53
2:P:140:THR:HG22	2:P:141:GLU:N	2.23	0.53
1:E:92:VAL:HG13	1:F:91:TYR:C	2.28	0.53
1:K:374:LYS:O	1:K:378:GLU:HG3	2.07	0.53
1:L:20:GLN:CG	1:L:332:LEU:HD23	2.36	0.53
1:L:309:ALA:CB	2:O:66:MET:HE2	2.29	0.53
2:P:67:HIS:O	2:P:69:GLY:N	2.41	0.53
1:K:111:VAL:HG21	1:K:243:ALA:HB2	1.90	0.53
1:L:285:VAL:HG12	1:L:325:ARG:CG	2.38	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: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
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
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:K:257:GLU:OE1	1:L:279:ARG:NH2	2.42	0.53
2:O:98:ALA:HB2	2:O:103:SER:HB3	1.91	0.53
1:E:145:GLN:H	1:E:149:GLN:CB	2.22	0.53
1:E:358:LEU:HG	1:F:40:LEU:CD1	2.30	0.53
1:E:312:ILE:CD1	2:N:67:HIS:CE1	2.91	0.53
1:F:219:LYS:O	1:F:223:LYS:HD3	2.09	0.53
1:K:91:TYR:C	1:K:92:VAL:HG13	2.30	0.53
2:P:59:LEU:O	2:P:62:ARG:HB2	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:285:VAL:HG12	1:F:325:ARG:CG	2.38	0.53
1:K:382:GLN:OE1	1:K:382:GLN:HA	2.09	0.53
1:L:217:LYS:HB3	1:L:220:ASP:CB	2.38	0.53
1:L:397:THR:HG21	1:L:443:LEU:C	2.29	0.53
2:O:7:ARG:HB2	2:O:12:VAL:HG23	1.91	0.53
2:O:66:MET:O	2:O:67:HIS:ND1	2.42	0.53
1:F:217:LYS:HB3	1:F:220:ASP:CB	2.38	0.53
2:M:85:ASP:O	2:M:89:ARG:HB3	2.09	0.53
2:M:98:ALA:HB2	2:M:103:SER:HB3	1.90	0.53
2:M:140:THR:HG22	2:M:142:LEU:N	2.17	0.53
2:O:85:ASP:O	2:O:89:ARG:HB3	2.09	0.53
2:O:90:LYS:HZ1	2:P:89:ARG:HD2	1.74	0.53
1:E:122:ARG:CA	1:E:122:ARG:HG2	2.26	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
2:O:140:THR:HG21	2:O:142:LEU:CG	2.38	0.52
1:F:20:GLN:CG	1:F:332:LEU:HD23	2.36	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:27:VAL:CG1	1:L:70:LEU:HG	2.35	0.52
1:L:131:ILE:O	1:L:134:VAL:HG12	2.08	0.52
1:K:91:TYR:O	1:K:92:VAL:CG1	2.58	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:E:131:ILE:HD12	1:E:134:VAL:CG1	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:382:GLN:OE1	1:E:382:GLN:HA	2.09	0.52
1:E:443:LEU:N	1:F:329:ARG:HG3	2.21	0.52
1:F:18:ILE:HD13	1:F:347:PRO:HG3	1.92	0.52
1:F:397:THR:HG21	1:F:443:LEU:C	2.29	0.52
1:L:145:GLN:CD	1:L:150:GLN:CA	2.78	0.52
2:N:64:LEU:HD23	2:N:74:ALA:CB	2.40	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: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:L:264:ARG:C	1:L:266:GLU:N	2.62	0.52
1:E:92:VAL:HG21	1:F:92:VAL:C	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:15:LYS:HB3	1:F:348:ASN:ND2	2.25	0.51
1:L:18:ILE:HD13	1:L:347:PRO:HG3	1.92	0.51
1:L:362:GLU:HG2	1:L:411:SER:N	2.24	0.51
2:O:149:GLU:HG3	2:O:166:HIS:HD2	1.74	0.51
2:M:7:ARG:HB2	2:M:12:VAL:HG23	1.91	0.51
2:M:149:GLU:HG3	2:M:166:HIS:HD2	1.74	0.51
1:K:389:ASN:C	1:K:389:ASN:ND2	2.57	0.51
1:L:263:LYS:HE2	1:L:275:GLU:OE1	2.10	0.51
1:E:145:GLN:HB2	1:E:149:GLN:H	1.74	0.51
1:F:141:ASN:ND2	1:F:141:ASN:N	2.54	0.51
1:K:362:GLU:HG3	1:K:411:SER:HA	1.93	0.51
2:M:37:LEU:HD21	2:M:57:PHE:CB	2.32	0.51
2:O:88:LEU:HD22	2:O:88:LEU:H	1.76	0.51
1:E:91:TYR:O	1:E:92:VAL:CG1	2.58	0.51
1:E:122:ARG:C	1:E:122:ARG:HG2	2.30	0.51
1:E:216:LEU:O	1:E:220:ASP:HB3	2.10	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:K:96:VAL:CG1	1:K:99:ILE:HD12	2.40	0.51
1:K:145:GLN:HB2	1:K:149:GLN:H	1.74	0.51
1:L:145:GLN:CD	1:L:149:GLN:HB2	2.30	0.51
1:L:264:ARG:NH1	2:O:59:LEU:O	2.39	0.51
2:N:3:ILE:HB	2:N:122:ILE:HG13	1.93	0.51
2:N:98:ALA:HA	2:N:103:SER:HA	1.93	0.51
2:P:3:ILE:HB	2:P:122:ILE:HG13	1.93	0.51
1:E:440:ARG:O	1:F:315:PRO:CD	2.58	0.51
1:K:91:TYR:HE1	1:L:272:VAL:CG1	2.23	0.51
1:K:122:ARG:C	1:K:122:ARG:HG2	2.30	0.51
1:L:122:ARG:HH21	1:L:122:ARG:CG	2.24	0.51
2:M:108:GLY:C	2:M:110:GLY:H	2.14	0.51
2:N:8:ARG:NH1	2:N:142:LEU:O	2.43	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:H	2:M:88:LEU:HD22	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:E:282:LEU:CD1	1:E:319:ILE:HD11	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:235:ASN:OD1	1:F:238:GLU:OE2	2.29	0.51
1:K:139:ALA:O	1:K:140:LYS:HB2	2.11	0.51
2:M:22:LEU:HB2	2:M:27:MET:HG3	1.93	0.51
2:O:108:GLY:C	2:O:110:GLY:H	2.14	0.51
2:P:8:ARG:NH1	2:P:142:LEU:O	2.43	0.51
1:E:34:ARG:NH1	1:E:250:HIS:HA	2.25	0.51
1:E:263:LYS:O	1:E:264:ARG:CB	2.58	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:K:369:THR:O	1:K:373:ILE:HG12	2.11	0.51
1:E:96:VAL:CG1	1:E:99:ILE:HD12	2.40	0.51
1:E:131:ILE:HG23	1:E:132:LEU:N	2.26	0.51
1:F:117:GLU:C	1:F:119:ASN:H	2.13	0.51
1:F:264:ARG:HH12	2:M:62:ARG:CG	1.94	0.51
1:K:34:ARG:NH1	1:K:250:HIS:HA	2.25	0.51
1:K:350:SER:OG	1:K:353:VAL:HG23	2.11	0.51
2:M:21:THR:HG22	2:M:22:LEU:N	2.26	0.51
1:E:109:LYS:CG	1:F:296:MET:HB2	2.41	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
2:N:59:LEU:HA	2:N:62:ARG:HD2	1.93	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
1:L:15:LYS:HB3	1:L:348:ASN:ND2	2.25	0.50
2:O:15:ALA:CB	2:O:152:LEU:HD12	2.41	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
1:L:76:ALA:HB1	1:L:250:HIS:O	2.11	0.50
1:L:235:ASN:OD1	1:L:238:GLU:OE2	2.29	0.50
1:L:264:ARG:CZ	2:O:62:ARG:HD3	2.39	0.50
2:N:90:LYS:HD2	2:N:91:LEU:N	2.27	0.50
1:E:86:PHE:HB2	1:E:277:VAL:HG13	1.92	0.50
1:E:389:ASN:C	1:E:389:ASN:ND2	2.57	0.50
1:E:440:ARG:CD	1:F:314:LYS:HD2	2.41	0.50
1:K:329:ARG:HH11	1:K:329:ARG:HG3	1.77	0.50
1:E:350:SER:OG	1:E:353:VAL:HG23	2.11	0.50
1:E:440:ARG:HE	1:F:316:SER:HG	1.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:ILE:O	1:E:136:ILE:CG2	2.60	0.50
1:E:400:GLU:CD	1:F:51:LYS:CE	2.80	0.50
1:F:135:LEU:O	1:F:136:ILE:HG12	2.10	0.50
1:F:145:GLN:CD	1:F:149:GLN:HB2	2.30	0.50
1:K:278:GLN:OE1	1:K:319:ILE:HG23	2.11	0.50
1:L:135:LEU:O	1:L:136:ILE:HG12	2.11	0.50
2:M:15:ALA:CB	2:M:152:LEU:HD12	2.41	0.50
2:M:37:LEU:CD2	2:M:57:PHE:HB3	2.35	0.50
2:M:51:ALA:O	2:M:54:PHE:HB3	2.11	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:E:20:GLN:HG3	1:E:332:LEU:CD2	2.42	0.50
1:E:362:GLU:HG3	1:E:411:SER:HA	1.93	0.50
1:E:397:THR:CA	1:F:327:PRO:HA	2.42	0.50
1:K:86:PHE:HB2	1:K:277:VAL:HG13	1.92	0.50
2:M:100:GLU:HG2	2:M:173:TYR:CD2	2.47	0.50
2:O:21:THR:HG22	2:O:22:LEU:N	2.26	0.50
2:O:70:HIS:CD2	2:O:73:LYS:H	2.30	0.50
1:F:76:ALA:HB1	1:F:250:HIS:O	2.11	0.50
1:F:232:LYS:HB2	1:F:232:LYS:NZ	2.27	0.50
1:K:263:LYS:O	1:K:264:ARG:CB	2.58	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
2:P:59:LEU:HA	2:P:62:ARG:HD2	1.93	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
1:K:120:ARG:HG3	1:K:121:TYR:N	2.25	0.50
2:M:138:GLU:HB3	2:M:139:ASN:ND2	2.26	0.50
1:E:329:ARG:HG3	1:E:329:ARG:HH11	1.77	0.49
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
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:E:369:THR:O	1:E:373:ILE:HG12	2.11	0.49
1:F:94:LYS:NZ	1:F:95:GLU:OE2	2.36	0.49
1:F:264:ARG:NH1	1:F:312:ILE:HD12	2.27	0.49
1:K:141:ASN:ND2	1:K:141:ASN:N	2.42	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
1:F:286:GLU:HG2	1:F:325:ARG:HH12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:70:HIS:CD2	2:M:73:LYS:H	2.30	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:79:ILE:HD13	1:E:80:LYS:H	1.78	0.49
1:E:357:ALA:HB2	1:F:44:LEU:HD11	1.75	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: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
1:K:217:LYS:HB2	1:K:220:ASP:HB3	1.95	0.49
1:L:264:ARG:HH11	2:O:62:ARG:CG	2.25	0.49
1:L:413:LEU:HD13	1:L:413:LEU:N	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: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
1:L:311:GLN:CG	2:O:66:MET:CE	2.90	0.49
2:P:51:ALA:O	2:P:54:PHE:HB3	2.12	0.49
2:P:140:THR:HG21	2:P:142:LEU:CG	2.35	0.49
1:E:388:GLU:OE2	1:F:318:LEU:O	2.30	0.49
1:K:384:ASN:ND2	1:K:390:ILE:H	2.10	0.49
1:L:130:ARG:NH1	1:L:131:ILE:HA	2.28	0.49
1:L:285:VAL:HG11	1:L:325:ARG:HB3	1.93	0.49
1:E:217:LYS:HB2	1:E:220:ASP:HB3	1.95	0.49
1:E:359:MET:CE	1:F:36:ARG:HD3	2.40	0.49
1:E:384:ASN:ND2	1:E:390:ILE:H	2.10	0.49
1:F:123:ALA:O	1:F:127:ALA:HB2	2.13	0.49
1:K:89:VAL:HG12	1:K:94:LYS:N	2.25	0.49
1:K:136:ILE:O	1:K:136:ILE:CG2	2.60	0.49
1:K:145:GLN:CB	1:K:149:GLN:H	2.25	0.49
1:L:409:ASP:O	1:L:413:LEU:HD22	2.12	0.49
2:N:39:ASN:HD22	2:N:39:ASN:N	2.09	0.49
1:E:235:ASN:ND2	1:E:235:ASN:N	2.37	0.49
1:F:79:ILE:HD13	1:F:80:LYS:O	2.13	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
2:O:61:GLU:O	2:O:65:GLU:HG2	2.13	0.49
1:E:108:VAL:HA	1:E:111:VAL:HG22	1.95	0.48
1:E:441:PHE:CE1	1:F:310:PHE:CB	2.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:94:LYS:NZ	1:F:98:SER:HB3	2.28	0.48
1:L:286:GLU:HG2	1:L:325:ARG:HH12	1.77	0.48
2:O:5:SER:HB2	2:O:14:ILE:HG12	1.95	0.48
1:E:109:LYS:HG3	1:F:296:MET:CB	2.43	0.48
1:L:145:GLN:CD	1:L:149:GLN:CB	2.81	0.48
2:N:88:LEU:HD22	2:N:88:LEU:N	2.28	0.48
2:N:100:GLU:HG2	2:N:173:TYR:HB3	1.96	0.48
2:P:53:ALA:HB1	2:P:57:PHE:CE2	2.48	0.48
1:E:92:VAL:CG2	1:F:92:VAL:CA	2.91	0.48
1:K:79:ILE:HD13	1:K:80:LYS:H	1.78	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
2:O:51:ALA:CB	2:P:109:ASN:O	2.61	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
1:L:118:LYS:CE	1:L:118:LYS:HA	2.44	0.48
2:O:5:SER:HB3	2:O:120:ILE:HB	1.95	0.48
2:O:43:ILE:HG23	2:O:171:LEU:HD13	1.95	0.48
2:P:39:ASN:N	2:P:39:ASN:ND2	2.62	0.48
1:E:89:VAL:HG12	1:E:94:LYS:O	2.14	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
2:P:88:LEU:HD22	2:P:88:LEU:N	2.28	0.48
1:E:354:GLN:CD	1:F:48:VAL:N	2.60	0.48
1:E:441:PHE:HD1	1:F:56:ILE:CG1	2.20	0.48
1:F:217:LYS:O	1:F:221:ALA:N	2.44	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:L:232:LYS:HB2	1:L:232:LYS:NZ	2.27	0.48
2:M:8:ARG:HH21	2:M:137:LEU:HA	1.78	0.48
2:P:16:GLY:CA	2:P:152:LEU:HD11	2.44	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
1:F:145:GLN:CD	1:F:149:GLN:CB	2.81	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
1:L:263:LYS:O	1:L:264:ARG:CB	2.59	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:N:51:ALA:O	2:N:54:PHE:HB3	2.13	0.48
2:O:17:ASP:HA	2:O:165:PHE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:108:VAL:C	1:E:110:MET:N	2.66	0.48
1:E:389:ASN:HD22	1:E:391:GLY:H	1.56	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
1:L:135:LEU:HD13	1:L:159:PHE:CE1	2.49	0.48
2:M:83:ARG:HG3	2:M:108:GLY:O	2.14	0.48
2:M:128:TYR:CE1	2:P:128:TYR:CE1	3.01	0.48
2:N:28:LYS:HD3	2:N:31:VAL:HG22	1.96	0.48
2:O:15:ALA:HB1	2:O:152:LEU:HD12	1.96	0.48
2:O:83:ARG:HG3	2:O:108:GLY:O	2.14	0.48
2:P:32:LYS:HD3	2:P:34:VAL:O	2.14	0.48
1:E:358:LEU:O	1:E:361:THR:CG2	2.60	0.48
1:E:369:THR:HB	1:E:421:ASP:HA	1.96	0.48
1:L:145:GLN:CD	1:L:150:GLN:HA	2.30	0.48
1:L:309:ALA:HB3	2:O:66:MET:CG	2.28	0.48
2:N:58:GLU:HG3	2:N:62:ARG:HE	1.78	0.48
2:N:116:GLU:H	2:N:116:GLU:HG2	1.42	0.48
2:O:8:ARG:HH21	2:O:137:LEU:HA	1.78	0.48
2:O:159:CYS:HB3	2:O:162:THR:OG1	2.13	0.48
1:E:344:LEU:HD13	1:E:395:LEU:HD13	1.96	0.47
1:F:131:ILE:CG2	1:F:132:LEU:N	2.77	0.47
1:K:309:ALA:O	2:P:66:MET:HE1	2.14	0.47
1:L:94:LYS:NZ	1:L:98:SER:HB3	2.29	0.47
2:P:1:THR:HB	2:P:33:LYS:HZ2	1.79	0.47
2:P:58:GLU:HG3	2:P:62:ARG:HE	1.78	0.47
2:P:100:GLU:HG2	2:P:173:TYR:HB3	1.96	0.47
1:F:17:ILE:HD13	1:F:66:ILE:CG1	2.35	0.47
1:F:231:ALA:C	1:F:233:LEU:H	2.17	0.47
1:L:374:LYS:O	1:L:378:GLU:HG3	2.13	0.47
2:M:3:ILE:HB	2:M:122:ILE:CG1	2.44	0.47
2:N:16:GLY:CA	2:N:152:LEU:HD11	2.44	0.47
2:N:39:ASN:N	2:N:39:ASN:ND2	2.62	0.47
2:O:51:ALA:HB2	2:P:109:ASN:O	2.14	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
1:F:413:LEU:HD13	1:F:413:LEU:N	2.28	0.47
1:K:397:THR:HG21	1:K:443:LEU:HA	1.94	0.47
1:L:231:ALA:C	1:L:233:LEU:H	2.17	0.47
2:M:5:SER:HB3	2:M:120:ILE:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:32:LYS:HD3	2:N:34:VAL:O	2.14	0.47
1:K:63:LYS:HE2	1:K:307:SER:OG	2.15	0.47
1:K:235:ASN:ND2	1:K:235:ASN:N	2.37	0.47
1:L:216:LEU:O	1:L:220:ASP:HB3	2.14	0.47
1:L:312:ILE:C	2:O:62:ARG:HG3	2.33	0.47
1:E:117:GLU:C	1:E:119:ASN:H	2.16	0.47
1:E:354:GLN:HG2	1:F:47:GLU:HB2	1.95	0.47
1:F:257:GLU:HG2	1:F:260:LYS:HG3	1.96	0.47
1:F:278:GLN:OE1	1:F:319:ILE:HB	2.15	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:118:LYS:HA	1:F:118:LYS:CE	2.44	0.47
1:K:264:ARG:HD2	2:P:62:ARG:NH2	2.16	0.47
1:L:146:THR:C	1:L:150:GLN:HB2	2.35	0.47
2:M:5:SER:HB2	2:M:14:ILE:HG12	1.95	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
1:F:132:LEU:CG	1:F:160:ARG:HB3	2.44	0.47
1:K:96:VAL:HG11	1:K:281:LEU:CD1	2.44	0.47
2:M:63:LYS:CB	2:M:74:ALA:HB1	2.45	0.47
2:N:88:LEU:H	2:N:88:LEU:CD2	2.28	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
1:E:96:VAL:HG13	1:E:99:ILE:CD1	2.43	0.47
1:E:118:LYS:HA	1:E:118:LYS:HZ3	1.76	0.47
1:E:406:ILE:CD1	1:E:420:ILE:HD11	2.45	0.47
1:F:110:MET:O	1:F:112:ARG:N	2.48	0.47
1:K:344:LEU:HD13	1:K:395:LEU:HD13	1.96	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:L:257:GLU:HG2	1:L:260:LYS:HG3	1.96	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
2:N:3:ILE:O	2:N:121:ALA:HA	2.15	0.47
2:O:63:LYS:HB3	2:O:74:ALA:HB1	1.97	0.47
1:E:87:THR:HG23	1:E:273:SER:HB2	1.97	0.47
1:F:261:ILE:CG2	1:F:278:GLN:HG3	2.44	0.47
1:F:365:ASN:HB3	1:F:417:ASN:HD22	1.79	0.47
1:L:131:ILE:CG2	1:L:132:LEU:N	2.77	0.47
1:L:147:GLU:HG2	1:L:148:GLN:N	2.29	0.47
2:M:115:PRO:HG2	2:M:120:ILE:HG12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:3:ILE:HB	2:O:122:ILE:CG1	2.44	0.47
1:E:109:LYS:HG2	1:F:296:MET:CG	2.45	0.47
1:E:110:MET:O	1:E:112:ARG:N	2.49	0.47
1:F:141:ASN:C	1:F:142:ASN:HD22	2.18	0.47
1:F:153:SER:O	1:F:154:ALA:C	2.53	0.47
1:F:216:LEU:O	1:F:220:ASP:HB3	2.15	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:L:132:LEU:CG	1:L:160:ARG:HB3	2.44	0.47
2:M:154:ILE:HD11	2:P:135:ALA:HB2	1.97	0.47
2:P:3:ILE:O	2:P:121:ALA:HA	2.15	0.47
2:P:138:GLU:HB3	2:P:139:ASN:HD22	1.80	0.47
1:E:124:GLU:O	1:E:127:ALA:HB3	2.15	0.46
1:F:147:GLU:HG2	1:F:148:GLN: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:K:408:TYR:HE2	1:L:7:ARG:HH22	0.58	0.46
1:L:312:ILE:HD11	2:O:59:LEU:O	2.15	0.46
2:M:168:ILE:HG22	2:M:169:GLU:N	2.30	0.46
1:E:89:VAL:HG11	1:E:94:LYS:O	2.16	0.46
1:F:375:ARG:HB3	1:F:425:VAL:HG11	1.97	0.46
1:L:141:ASN:C	1:L:142:ASN:HD22	2.18	0.46
2:N:87:MET:O	2:N:90:LYS:HB3	2.16	0.46
1:K:110:MET:O	1:K:112:ARG:N	2.49	0.46
1:L:153:SER:O	1:L:154:ALA:C	2.53	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: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:91:TYR:C	1:L:92:VAL:CG1	2.83	0.46
1:L:145:GLN:HG2	1:L:150:GLN:H	1.64	0.46
2:O:10:GLY:HA2	2:O:173:TYR:CE1	2.50	0.46
1:E:354:GLN:CG	1:F:47:GLU:CB	2.93	0.46
1:K:124:GLU:O	1:K:127:ALA:HB3	2.15	0.46
1:K:408:TYR:OH	1:L:7:ARG:CG	2.63	0.46
1:L:278:GLN:OE1	1:L:319:ILE:HB	2.15	0.46
2:M:160:ILE:CD1	2:O:160:ILE:HG23	2.38	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:F:350:SER:OG	1:F:353:VAL:HG23	2.16	0.46
1:K:89:VAL:HG11	1:K:94:LYS:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:350:SER:OG	1:L:353:VAL:HG23	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: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:F:384:ASN:HD22	1:F:394:ARG:HH11	1.63	0.46
1:K:139:ALA:CA	1:K:152:PRO:CB	2.79	0.46
1:K:299:THR:O	1:K:301:HIS:N	2.49	0.46
2:N:17:ASP:OD1	2:N:33:LYS:NZ	2.49	0.46
2:O:134:ARG:HG3	2:O:134:ARG:HH11	1.81	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:299:THR:O	1:E:301:HIS:N	2.49	0.46
1:E:369:THR:HG22	1:E:371:SER:N	2.30	0.46
1:E:401:ARG:HH21	1:F:329:ARG:H	1.63	0.46
1:F:112:ARG:HH11	1:F:112:ARG:HG3	1.81	0.46
1:K:432:LEU:CD1	1:K:432:LEU:N	2.78	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: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:E:309:ALA:O	2:N:66:MET:SD	2.74	0.46
1:E:358:LEU:HD21	1:F:37:ARG:CB	2.46	0.46
1:E:372:GLY:O	1:E:376:ILE:HG13	2.16	0.46
1:F:11:SER:O	1:F:14:ASP:HB2	2.15	0.46
1:L:11:SER:O	1:L:14:ASP:HB2	2.15	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
2:P:99:ASP:OD1	2:P:99:ASP:C	2.55	0.46
1:F:108:VAL:HA	1:F:111:VAL:CG2	2.46	0.45
1:K:122:ARG:HD2	1:K:122:ARG:HB2	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:L:362:GLU:CG	1:L:411:SER:HA	2.45	0.45
1:L:365:ASN:HB3	1:L:417:ASN:HD22	1.80	0.45
2:M:145:ARG:NE	2:M:170:GLU:OE1	2.47	0.45
2:P:5:SER:O	2:P:119:LEU:HD12	2.15	0.45
1:E:122:ARG:HD2	1:E:122:ARG:HB2	1.92	0.45
1:E:441:PHE:HD1	1:F:56:ILE:CG2	2.24	0.45
1:F:406:ILE:HG13	1:F:424:TYR:OH	2.16	0.45
1:K:293:LYS:HG2	1:K:294:HIS:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:134:ARG:HH11	2:M:134:ARG:HG3	1.81	0.45
2:P:36:ARG:HH11	2:P:36:ARG:CB	2.21	0.45
1:K:64:THR:HG21	1:K:68:ARG:NH1	2.32	0.45
2:P:87:MET:O	2:P:90:LYS:HB3	2.16	0.45
1:F:134:VAL:O	1:F:135:LEU:HD23	2.16	0.45
1:F:267:SER:O	1:F:270:PRO:HG2	2.16	0.45
1:K:384:ASN:ND2	1:K:394:ARG:HH11	2.14	0.45
1:L:124:GLU:HG3	1:L:222:MET:HE3	1.98	0.45
2:M:99:ASP:HA	2:M:171:LEU:HD22	1.99	0.45
1:E:293:LYS:HG2	1:E:294:HIS:CD2	2.51	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:K:442:ILE:O	1:K:442:ILE:HG22	2.17	0.45
1:L:79:ILE:HD13	1:L:80:LYS:N	2.32	0.45
2:N:99:ASP:OD1	2:N:99:ASP:C	2.55	0.45
2:N:138:GLU:HB3	2:N:139:ASN:HD22	1.80	0.45
1:E:64:THR:HG21	1:E:68:ARG:NH1	2.32	0.45
1:E:92:VAL:HG11	1:F:92:VAL:HG12	1.93	0.45
1:E:269:GLY:N	1:E:270:PRO:HD2	2.32	0.45
1:E:413:LEU:O	1:E:416:GLN:HG3	2.17	0.45
1:F:25:ARG:O	1:F:29:ILE:HG13	2.17	0.45
1:F:145:GLN:OE1	1:F:149:GLN:HB2	2.16	0.45
2:P:17:ASP:OD1	2:P:33:LYS:NZ	2.49	0.45
2:P:116:GLU:H	2:P:116:GLU:HG2	1.42	0.45
1:K:372:GLY:O	1:K:376:ILE:HG13	2.16	0.45
1:L:315:PRO:O	1:L:318:LEU:HB2	2.17	0.45
2:M:36:ARG:C	2:M:37:LEU:HD12	2.37	0.45
2:O:67:HIS:O	2:O:69:GLY:N	2.49	0.45
2:P:8:ARG:HB2	2:P:144:ALA:HB2	1.98	0.45
1:E:97:ASP:HB2	1:E:101:ARG:NH2	2.32	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: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
1:F:79:ILE:HD13	1:F:80:LYS:N	2.31	0.45
1:K:248:GLU:OE1	1:K:298:LYS:N	2.46	0.45
1:K:398:VAL:HG13	1:K:429:LEU:HD13	1.99	0.45
2:O:60:PHE:CE2	2:O:97:VAL:HG21	2.52	0.45
2:P:105:ILE:CD1	2:P:120:ILE:HG23	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:119:ASN:HD22	1:F:119:ASN:HA	1.57	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
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:L:365:ASN:HB3	1:L:417:ASN:ND2	2.32	0.45
2:N:91:LEU:O	2:N:91:LEU:HD12	2.16	0.45
1:E:91:TYR:CB	1:F:91:TYR:N	2.78	0.44
1:E:390:ILE:CG2	1:F:320:PRO:HA	2.46	0.44
1:F:34:ARG:NH2	1:F:250:HIS:HA	2.32	0.44
1:K:125:GLU:O	1:K:128:GLU:HB2	2.17	0.44
1:L:112:ARG:HG3	1:L:112:ARG:HH11	1.81	0.44
2:M:60:PHE:CE2	2:M:97:VAL:HG21	2.52	0.44
2:P:148:ALA:O	2:P:152:LEU:HB2	2.17	0.44
1:E:365:ASN:HB3	1:E:417:ASN:HD22	1.81	0.44
1:K:413:LEU:O	1:K:416:GLN:HG3	2.17	0.44
1:L:134:VAL:O	1:L:135:LEU:HD23	2.16	0.44
1:L:145:GLN:HB3	1:L:149:GLN:CG	2.47	0.44
2:N:8:ARG:HB2	2:N:144:ALA:HB2	1.98	0.44
2:O:36:ARG:C	2:O:37:LEU:HD12	2.37	0.44
1:E:86:PHE:HB2	1:E:277:VAL:CG1	2.48	0.44
1:E:132:LEU:HD22	1:E:132:LEU:HA	1.83	0.44
1:F:406:ILE:O	1:F:410:ALA:N	2.48	0.44
1:K:358:LEU:O	1:K:361:THR:CG2	2.60	0.44
1:L:217:LYS:O	1:L:221:ALA:N	2.44	0.44
1:L:389:ASN:ND2	1:L:389:ASN:C	2.69	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
2:N:5:SER:HB3	2:N:120:ILE:CB	2.44	0.44
2:N:98:ALA:CB	2:N:103:SER:HB3	2.47	0.44
2:O:99:ASP:HA	2:O:171:LEU:HD22	1.98	0.44
1:E:256:ASP:O	1:E:257:GLU:HB2	2.17	0.44
1:E:398:VAL:HG13	1:E:429:LEU:HD13	1.99	0.44
1:F:141:ASN:O	1:F:142:ASN:CB	2.62	0.44
1:K:264:ARG:O	1:K:266:GLU:N	2.50	0.44
1:L:25:ARG:O	1:L:29:ILE:HG13	2.17	0.44
1:L:34:ARG:NH2	1:L:250:HIS:HA	2.32	0.44
1:E:293:LYS:HG2	1:E:294:HIS:HD2	1.83	0.44
1:E:442:ILE:O	1:E:442:ILE:HG22	2.17	0.44
1:K:86:PHE:HB2	1:K:277:VAL:CG1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:293:LYS:HG2	1:K:294:HIS:HD2	1.83	0.44
1:K:365:ASN:HB3	1:K:417:ASN:HD22	1.81	0.44
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
2:N:60:PHE:HE2	2:N:97:VAL:HG21	1.79	0.44
1:F:342:ARG:HE	1:F:346:GLU:CD	2.21	0.44
2:M:43:ILE:HG13	2:M:43:ILE:O	2.17	0.44
2:P:98:ALA:CB	2:P:103:SER:HB3	2.47	0.44
1:E:135:LEU:HD13	1:E:159:PHE:CD1	2.52	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:145:GLN:CG	1:F:150:GLN:CA	2.87	0.44
1:F:293:LYS:HG2	1:F:294:HIS:HD2	1.81	0.44
1:F:393:ARG:HA	1:F:396:HIS:CD2	2.53	0.44
1:K:145:GLN:HB2	1:K:149:GLN:C	2.38	0.44
1:K:269:GLY:N	1:K:270:PRO:HD2	2.32	0.44
1:L:100:ILE:HG13	1:L:290:VAL:HG21	1.99	0.44
1:L:264:ARG:CD	2:O:62:ARG:HD3	2.38	0.44
2:M:66:MET:C	2:M:67:HIS:ND1	2.71	0.44
2:N:46:PHE:HB3	2:N:57:PHE:CZ	2.53	0.44
2:N:148:ALA:O	2:N:152:LEU:HB2	2.17	0.44
2:O:66:MET:C	2:O:67:HIS:ND1	2.71	0.44
2:P:88:LEU:H	2:P:88:LEU:CD2	2.28	0.44
1:E:145:GLN:HB2	1:E:149:GLN:C	2.38	0.44
1:F:64:THR:HG22	1:F:68:ARG:HD2	2.00	0.44
1:F:131:ILE:HD13	1:F:134:VAL:HG12	2.00	0.44
1:K:58:PRO:HG2	1:K:61:VAL:HG11	1.99	0.44
1:L:62:GLY:O	1:L:66:ILE:HG13	2.18	0.44
1:L:282:LEU:HD21	1:L:321:GLU:HG2	2.00	0.44
2:M:44:ALA:HB2	2:M:97:VAL:HG23	2.00	0.44
2:N:21:THR:HG22	2:N:22:LEU:H	1.81	0.44
2:O:36:ARG:NH1	2:O:40:ASP:HB3	2.33	0.44
2:P:62:ARG:O	2:P:65:GLU:HB2	2.17	0.44
2:P:108:GLY:C	2:P:110:GLY:H	2.21	0.44
1:E:354:GLN:CG	1:F:47:GLU:HB2	2.48	0.44
1:K:135:LEU:HD13	1:K:159:PHE:CD1	2.52	0.44
1:L:131:ILE:HD13	1:L:134:VAL:HG12	2.00	0.44
1:L:380:ALA:HA	1:L:394:ARG:HG2	2.00	0.44
2:N:1:THR:HB	2:N:33:LYS:HZ2	1.82	0.44
2:N:36:ARG:HH11	2:N:36:ARG:CB	2.21	0.44
2:P:5:SER:HB3	2:P:120:ILE:CB	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:237:GLU:HA	1:F:237:GLU:OE2	2.18	0.43
1:F:362:GLU:CG	1:F:411:SER:HA	2.46	0.43
1:F:380:ALA:HA	1:F:394:ARG:HG2	2.00	0.43
1:K:94:LYS:HA	1:K:94:LYS:HD3	1.74	0.43
1:L:21:ASP:OD2	1:L:25:ARG:HD2	2.18	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
2:M:131:ALA:HB1	2:P:154:ILE:HG22	1.99	0.43
2:P:60:PHE:HE2	2:P:97:VAL:HG21	1.79	0.43
1:E:359:MET:HE3	1:F:36:ARG:NH1	2.31	0.43
1:K:119:ASN:HD22	1:K:119:ASN:HA	1.56	0.43
1:L:118:LYS:HA	1:L:118:LYS:HE2	2.00	0.43
1:L:237:GLU:HA	1:L:237:GLU:OE2	2.18	0.43
1:L:263:LYS:HB3	1:L:264:ARG:H	1.36	0.43
2:M:160:ILE:CG2	2:O:160:ILE:HD11	2.40	0.43
2:N:39:ASN:O	2:N:41:LYS:HG3	2.18	0.43
2:O:43:ILE:HG13	2:O:43:ILE:O	2.17	0.43
1:E:56:ILE:HA	1:E:308:GLY:O	2.18	0.43
1:F:34:ARG:CZ	1:F:250:HIS:HA	2.47	0.43
1:F:83:ALA:HB1	1:F:261:ILE:HG13	2.00	0.43
1:K:40:LEU:O	1:K:45:ARG:NH1	2.52	0.43
1:K:120:ARG:HD2	1:K:121:TYR:N	2.33	0.43
1:K:336:THR:O	1:K:339:ASP:HB2	2.19	0.43
2:N:108:GLY:C	2:N:110:GLY:H	2.21	0.43
2:O:92:GLU:HG3	2:O:92:GLU:O	2.16	0.43
2:P:46:PHE:HB3	2:P:57:PHE:CZ	2.53	0.43
1:E:89:VAL:HG12	1:E:94:LYS:N	2.25	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:F:100:ILE:HG13	1:F:290:VAL:HG21	1.99	0.43
1:K:256:ASP:O	1:K:257:GLU:HB2	2.17	0.43
1:L:131:ILE:O	1:L:135:LEU:HG	2.19	0.43
1:L:238:GLU:O	1:L:242:ASP:N	2.49	0.43
2:M:36:ARG:NH1	2:M:40:ASP:HB3	2.33	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:N:62:ARG:O	2:N:65:GLU:HB2	2.18	0.43
2:O:21:THR:CG2	2:O:22:LEU:N	2.81	0.43
2:O:44:ALA:HB2	2:O:97:VAL:HG23	2.00	0.43
1:E:119:ASN:HD22	1:E:119:ASN:HA	1.56	0.43
1:E:241:GLN:HG2	1:E:241:GLN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:442:ILE:CD1	1:F:329:ARG:CB	2.97	0.43
1:F:113:VAL:O	1:F:117:GLU:HG3	2.19	0.43
1:F:145:GLN:CD	1:F:145:GLN:O	2.57	0.43
1:L:86:PHE:HB2	1:L:277:VAL:CG1	2.47	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
1:L:275:GLU:O	1:L:278:GLN:HB2	2.19	0.43
2:M:98:ALA:HA	2:M:103:SER:HA	2.00	0.43
2:N:15:ALA:HB1	2:N:152:LEU:HD12	2.01	0.43
2:P:39:ASN:O	2:P:41:LYS:HG3	2.18	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:E:92:VAL:HG22	1:E:93:GLY:H	1.84	0.43
1:E:336:THR:O	1:E:339:ASP:HB2	2.19	0.43
1:F:282:LEU:HD21	1:F:321:GLU:HG2	2.00	0.43
2:M:87:MET:O	2:M:90:LYS:HB3	2.19	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:P:21:THR:HG22	2:P:22:LEU:H	1.82	0.43
1:E:132:LEU:HD21	1:E:160:ARG:HA	2.01	0.43
1:E:440:ARG:C	1:F:315:PRO:HD2	2.38	0.43
1:F:293:LYS:HG2	1:F:294:HIS:CD2	2.54	0.43
1:K:131:ILE:HD12	1:K:134:VAL:HG11	2.01	0.43
1:L:136:ILE:HG22	1:L:138:PRO:CD	2.42	0.43
1:L:293:LYS:HG2	1:L:294:HIS:CD2	2.54	0.43
1:L:393:ARG:HA	1:L:396:HIS:CD2	2.53	0.43
2:M:42:VAL:HG21	2:M:64:LEU:HD13	2.01	0.43
2:M:76:VAL:HA	2:M:112:VAL:HG21	2.00	0.43
1:E:40:LEU:O	1:E:45:ARG:NH1	2.51	0.42
1:E:109:LYS:HG2	1:F:296:MET:HG3	2.01	0.42
1:E:120:ARG:HD2	1:E:121:TYR:N	2.33	0.42
1:E:354:GLN:CG	1:F:47:GLU:HB3	2.49	0.42
1:E:417:ASN:HD22	1:E:417:ASN:HA	1.65	0.42
1:F:118:LYS:HA	1:F:118:LYS:HE2	2.00	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:L:34:ARG:CZ	1:L:250:HIS:HA	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:114:GLN:O	2:N:114:GLN:HG3	2.19	0.42
2:N:153:ASP:OD1	2:N:164:HIS:HD2	2.02	0.42
2:O:13:VAL:CG1	2:O:170:GLU:HG3	2.49	0.42
2:O:98:ALA:HA	2:O:103:SER:HA	2.00	0.42
2:O:125:GLY:HA2	2:O:128:TYR:CD2	2.53	0.42
1:E:91:TYR:C	1:E:92:VAL:CG1	2.88	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:F:124:GLU:HG3	1:F:222:MET:HE3	2.01	0.42
1:K:91:TYR:C	1:K:92:VAL:CG1	2.87	0.42
1:K:241:GLN:HG2	1:K:241:GLN:O	2.18	0.42
1:L:292:THR:C	1:L:294:HIS:N	2.73	0.42
1:E:335:LEU:HD22	1:E:339:ASP:HB3	2.01	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
1:F:257:GLU:OE1	1:F:260:LYS:NZ	2.53	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:L:384:ASN:HD22	1:L:384:ASN:HA	1.64	0.42
2:M:98:ALA:O	2:M:99:ASP:HB3	2.19	0.42
2:N:99:ASP:O	2:N:100:GLU:C	2.58	0.42
2:P:134:ARG:HH11	2:P:134:ARG:CG	2.33	0.42
1:F:112:ARG:O	1:F:115:ALA:N	2.53	0.42
1:F:310:PHE:HB3	1:F:313:ALA:O	2.19	0.42
1:K:132:LEU:HD21	1:K:160:ARG:HA	2.01	0.42
1:L:397:THR:HG21	1:L:443:LEU:HA	2.00	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
2:O:87:MET:O	2:O:90:LYS:HB3	2.19	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:E:248:GLU:OE1	1:E:298:LYS:N	2.46	0.42
1:F:131:ILE:O	1:F:131:ILE:HD13	2.20	0.42
1:F:397:THR:HG21	1:F:443:LEU:HA	2.00	0.42
1:F:442:ILE:O	1:F:443:LEU:HD23	2.20	0.42
1:K:91:TYR:O	1:K: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:345:THR:HG22	1:K:352:THR:HG21	2.01	0.42
2:P:3:ILE:HD11	2:P:46:PHE:C	2.39	0.42
2:P:4:VAL:CG2	2:P:152:LEU:HG	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:91:TYR:CD1	1:F:90:GLY:C	2.83	0.42
1:E:278:GLN:CD	1:E:319:ILE:HG23	2.39	0.42
1:F:130:ARG:NH1	1:F:131:ILE:CA	2.82	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:91:TYR:CE2	1:F:91:TYR:CD2	3.08	0.42
1:E:139:ALA:CA	1:E:152:PRO:CB	2.79	0.42
1:E:398:VAL:HG13	1:E:429:LEU:CD1	2.50	0.42
1:F:4:MET:HB3	1:F:8:GLU:CB	2.50	0.42
1:F:94:LYS:HZ2	1:F:98:SER:HB3	1.83	0.42
1:K:74:ALA:O	1:K:75:ASN:HB3	2.20	0.42
1:K:118:LYS:HA	1:K:118:LYS:HZ3	1.83	0.42
1:L:64:THR:HG22	1:L:68:ARG:HD2	2.00	0.42
2:M:99:ASP:O	2:M:100:GLU:C	2.58	0.42
1:E:111:VAL:CG2	1:E:243:ALA:HB2	2.49	0.42
1:E:354:GLN:OE1	1:F:48:VAL:CG2	2.67	0.42
1:F:136:ILE:O	1:F:138:PRO:HD2	2.20	0.42
1:K:111:VAL:CG2	1:K:243:ALA:HB2	2.49	0.42
1:K:340:PHE:CD2	1:K:395:LEU:HD21	2.54	0.42
1:L:398:VAL:HG13	1:L:429:LEU:HD13	2.00	0.42
1:L:442:ILE:O	1:L:443:LEU:HD23	2.20	0.42
2:N:37:LEU:HD12	2:N:37:LEU:N	2.34	0.42
2:N:169:GLU:HA	2:N:169:GLU:OE2	2.20	0.42
1:E:5:THR:HG1	1:E:8:GLU:HG3	1.82	0.42
1:E:329:ARG:HG3	1:E:329:ARG:NH1	2.35	0.42
1:E:345:THR:HG22	1:E:352:THR:HG21	2.01	0.42
1:E:441:PHE:C	1:F:329:ARG:HG3	2.40	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:L:136:ILE:O	1:L:138:PRO:HD2	2.20	0.42
1:L:257:GLU:OE1	1:L:260:LYS:NZ	2.53	0.42
2:O:42:VAL:HG21	2:O:64:LEU:HD13	2.02	0.42
2:O:99:ASP:O	2:O:100:GLU:C	2.58	0.42
2:O:140:THR:CG2	2:O:141:GLU:N	2.83	0.42
2:P:58:GLU:HG3	2:P:62:ARG:NE	2.34	0.42
1:E:74:ALA:O	1:E:75:ASN:HB3	2.20	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
1:K:227:GLU:O	1:K:227:GLU:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:112:ARG:O	1:L:115:ALA:N	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
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:E:88:GLU:CD	1:F:89:VAL:O	2.58	0.41
1:E:441:PHE:O	1:F:329:ARG:HG3	2.15	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:M:1:THR:CA	2:M:162:THR:HG22	2.50	0.41
2:M:13:VAL:CG1	2:M:170:GLU:HG3	2.49	0.41
2:O:50:THR:HG21	2:P:111:ASP:CG	2.39	0.41
2:O:121:ALA:O	2:O:126:GLY:HA3	2.20	0.41
1:E:408:TYR:C	1:F:6:PRO:HG2	2.39	0.41
1:F:15:LYS:HB3	1:F:348:ASN:HD21	1.85	0.41
1:F:229:GLU:O	1:F:232:LYS:HG2	2.20	0.41
1:F:264:ARG:HH11	1:F:312:ILE:HD12	1.85	0.41
1:L:74:ALA:O	1:L:75:ASN:HB3	2.20	0.41
1:L:91:TYR:O	1:L:92:VAL:HG12	2.20	0.41
1:L:397:THR:CG2	1:L:443:LEU:HA	2.50	0.41
2:M:148:ALA:O	2:M:152:LEU:HB2	2.19	0.41
2:N:98:ALA:HB2	2:N:103:SER:HB3	2.03	0.41
2:O:148:ALA:O	2:O:152:LEU:HB2	2.19	0.41
2:P:37:LEU:HD12	2:P:37:LEU:N	2.34	0.41
2:P:66:MET:O	2:P:67:HIS:ND1	2.53	0.41
1:E:139:ALA:CB	1:E:152:PRO:CD	2.92	0.41
1:E:440:ARG:O	1:F:315:PRO:HD2	2.20	0.41
1:F:52:ASN:HB2	1:F:325:ARG:O	2.19	0.41
1:F:74:ALA:O	1:F:75:ASN:HB3	2.20	0.41
1:K:110:MET:O	1:K:111:VAL:C	2.59	0.41
1:K:335:LEU:HD22	1:K:339:ASP:HB3	2.01	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
2:P:15:ALA:HB1	2:P:152:LEU:HD12	2.01	0.41
1:E:94:LYS:HD3	1:E:94:LYS:HA	1.74	0.41
1:E:160:ARG:O	1:E:163:LEU:HB3	2.20	0.41
1:E:257:GLU:OE1	1:F:279:ARG:CG	2.63	0.41
1:F:238:GLU:CD	1:F:238:GLU:H	2.22	0.41
1:F:398:VAL:HG13	1:F:429:LEU:HD13	2.01	0.41
1:K:108:VAL:O	1:K:110:MET:N	2.54	0.41
1:K:219:LYS:CG	1:K:220:ASP:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:99:ASP:HA	2:M:171:LEU:CD2	2.51	0.41
2:N:121:ALA:HB1	2:N:126:GLY:O	2.20	0.41
2:P:114:GLN:HG3	2:P:114:GLN:O	2.20	0.41
1:E:108:VAL:O	1:E:110:MET:N	2.54	0.41
1:E:131:ILE:HD12	1:E:134:VAL:HG12	2.03	0.41
1:F:397:THR:CG2	1:F:443:LEU:HA	2.50	0.41
1:L:91:TYR:HD2	1:L:91:TYR:HA	1.76	0.41
1:L:119:ASN:HD22	1:L:119:ASN:HA	1.57	0.41
1:L:442:ILE:O	1:L:442:ILE:HG22	2.20	0.41
2:N:136:LEU:HB3	2:N:147:ILE:HG12	2.02	0.41
2:O:99:ASP:HA	2:O:171:LEU:CD2	2.50	0.41
2:P:169:GLU:HA	2:P:169:GLU:OE2	2.20	0.41
1:E:222:MET:O	1:E:226:ILE:N	2.53	0.41
1:E:282:LEU:N	1:E:283:PRO:HD2	2.35	0.41
1:F:87:THR:HG23	1:F:277:VAL:HG21	2.02	0.41
1:K:92:VAL:HG22	1:K:93:GLY:H	1.84	0.41
1:K:97:ASP:OD1	1:K:97:ASP:N	2.52	0.41
1:K:160:ARG:O	1:K:163:LEU:HB3	2.20	0.41
1:L:87:THR:HG23	1:L:277:VAL:HG21	2.02	0.41
1:L:232:LYS:HB3	1:L:232:LYS:HE2	1.76	0.41
1:L:374:LYS:HG2	1:L:375:ARG:N	2.35	0.41
1:L:384:ASN:HD21	1:L:390:ILE:H	1.69	0.41
2:M:121:ALA:HB1	2:M:126:GLY:O	2.19	0.41
2:N:66:MET:O	2:N:67:HIS:ND1	2.53	0.41
2:N:99:ASP:HA	2:N:171:LEU:CD2	2.51	0.41
2:P:43:ILE:O	2:P:43:ILE:HG13	2.20	0.41
2:P:98:ALA:HB2	2:P:103:SER:HB3	2.03	0.41
2:P:121:ALA:HB1	2:P:126:GLY:O	2.20	0.41
1:F:13:LEU:HD12	1:F:13:LEU:HA	1.93	0.41
1:F:359:MET:HG3	1:F:366:ILE:HG13	2.03	0.41
1:K:342:ARG:HE	1:K:346:GLU:CD	2.23	0.41
1:K:417:ASN:HD22	1:K:417:ASN:HA	1.65	0.41
1:L:382:GLN:OE1	1:L:382:GLN:HA	2.20	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:E:441:PHE:C	1:F:329:ARG:CG	2.89	0.41
1:K:281:LEU:HD12	1:K:281:LEU:HA	1.83	0.41
1:L:131:ILE:O	1:L:131:ILE:HD13	2.20	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
2:M:98:ALA:O	2:M:99:ASP:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:99:ASP:O	2:P:100:GLU:C	2.58	0.41
2:P:136:LEU:HB3	2:P:147:ILE:HG12	2.02	0.41
1:E:358:LEU:HD21	1:F:37:ARG:HB2	2.01	0.41
1:E:369:THR:HG22	1:E:372:GLY:N	2.20	0.41
1:E:388:GLU:OE2	1:F:323:GLN:NE2	2.53	0.41
1:E:400:GLU:CD	1:F:51:LYS:HZ2	2.10	0.41
1:E:404:GLU:O	1:F:29:ILE:HD13	2.20	0.41
1:F:150:GLN:O	1:F:152:PRO:HD3	2.20	0.41
1:F:292:THR:C	1:F:294:HIS:N	2.73	0.41
1:L:4:MET:HB3	1:L:8:GLU:CB	2.50	0.41
1:L:13:LEU:HD12	1:L:13:LEU:HA	1.93	0.41
1:L:42:GLU:HA	1:L:45:ARG:NH2	2.36	0.41
1:L:232:LYS:HG3	1:L:232:LYS:O	2.21	0.41
1:L:384:ASN:CG	1:L:394:ARG:HD2	2.41	0.41
2:M:51:ALA:HB1	2:N:83:ARG:NH2	2.35	0.41
2:M:91:LEU:HD12	2:M:91:LEU:O	2.21	0.41
2:M:140:THR:CG2	2:M:141:GLU:N	2.83	0.41
2:M:154:ILE:HG23	2:P:131:ALA:CB	2.45	0.41
2:N:39:ASN:HB2	2:N:41:LYS:HE3	2.03	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
2:P:114:GLN:HA	2:P:115:PRO:HD2	1.84	0.41
1:E:342:ARG:NH2	1:E:346:GLU:OE2	2.50	0.41
1:E:358:LEU:HD23	1:F:36:ARG:C	2.41	0.41
1:F:232:LYS:HG3	1:F:232:LYS:O	2.21	0.41
1:K:84:THR:OG1	1:K:257:GLU:OE2	2.34	0.41
1:K:157:GLN:O	1:K:160:ARG:HB3	2.21	0.41
1:K:231:ALA:C	1:K:233:LEU:H	2.24	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: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:HG2	1:E:227:GLU:O	2.20	0.40
1:F:40:LEU:O	1:F:45:ARG:NH1	2.54	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
1:L:122:ARG:CG	1:L:122:ARG:NH2	2.82	0.40
1:L:145:GLN:CD	1:L:145:GLN:O	2.57	0.40
2:N:100:GLU:HG2	2:N:173:TYR:CG	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:ASN:ND2	1:E:75:ASN:O	2.54	0.40
1:E:157:GLN:O	1:E:160:ARG:HB3	2.21	0.40
1:E:248:GLU:HG3	1:E:297:VAL:HG13	2.04	0.40
1:E:393:ARG:CZ	1:F:321:GLU:HA	2.46	0.40
1:K:75:ASN:O	1:K:75:ASN:ND2	2.54	0.40
1:K:139:ALA:N	1:K:152:PRO:CB	2.85	0.40
1:L:309:ALA:CA	2:O:66:MET:CE	2.94	0.40
1:E:53:ILE:HG12	1:E:328:ILE:CG2	2.51	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:E:219:LYS:CG	1:E:220:ASP:N	2.84	0.40
1:E:231:ALA:C	1:E:233:LEU:H	2.24	0.40
1:K:4:MET:HB2	1:K:8:GLU:HB2	2.03	0.40
1:K:12:GLU:O	1:K:15:LYS:HB2	2.20	0.40
1:K:130:ARG:O	1:K:133:ASP:HB3	2.22	0.40
2:M:3:ILE:HD11	2:M:46:PHE:C	2.42	0.40
2:N:43:ILE:O	2:N:43:ILE:HG13	2.21	0.40
2:N:62:ARG:HA	2:N:65:GLU:HG3	2.03	0.40
2:N:105:ILE:CD1	2:N:120:ILE:HG23	2.44	0.40
1:E:346:GLU:O	1:E:347:PRO:C	2.59	0.40
1:F:264:ARG:CZ	2:M:62:ARG:HG3	2.20	0.40
1:F:382:GLN:OE1	1:F:382:GLN:HA	2.20	0.40
1:F:406:ILE:HD13	1:F:418:ILE:HG21	2.02	0.40
1:K:53:ILE:HG12	1:K:328:ILE:CG2	2.51	0.40
1:K:222:MET:O	1:K:226:ILE:N	2.53	0.40
1:L:97:ASP:OD1	1:L:97:ASP:N	2.54	0.40
1:L:359:MET:HG3	1:L:366:ILE:HG13	2.02	0.40
2:M:88:LEU:H	2:M:88:LEU:CD2	2.33	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:O:3:ILE:HD11	2:O:46:PHE:C	2.42	0.40
2:P:121:ALA:O	2:P:126:GLY:HA3	2.21	0.40
1:E:235:ASN:HA	1:E:236:PRO:HD2	1.88	0.40
1:F:374:LYS:HG2	1:F:375:ARG:N	2.35	0.40
1:F:442:ILE:O	1:F:442:ILE:HG22	2.20	0.40
1:K:131:ILE:HD12	1:K:134:VAL:HG12	2.02	0.40
1:K:217:LYS:CB	1:K:220:ASP:HB3	2.52	0.40
1:L:266:GLU:HB3	1:L:267:SER:H	1.75	0.40
1:L:421:ASP:OD2	1:L:423:ASP:HB2	2.21	0.40
2:M:88:LEU:HD22	2:M:88:LEU:N	2.36	0.40
2:N:22:LEU:HB2	2:N:27:MET:HE2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:91:LEU:HD12	2:O:91:LEU:O	2.21	0.40
2:P:62:ARG:HA	2:P:65:GLU:HG3	2.03	0.40
2:P:140:THR:HG22	2:P:142:LEU:HG	2.00	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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CD	1:L:441:PHE:CD2[3_665]	1.71	0.49
1:K:315:PRO:CB	1:L:440:ARG:C[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
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:NH2	1:L:443:LEU:C[3_665]	1.78	0.42
1:K:329:ARG:CA	1:L:401:ARG:NH2[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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CZ	1:L:442:ILE:O[3_665]	2.09	0.11
1:K:329:ARG:CG	1:L:442:ILE:CB[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:NH1	1:L:407:SER:CA[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: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:CG	1:F:441:PHE:CE1[2_655]	2.13	0.07
1:E:314:LYS:CA	1:F:441:PHE:CZ[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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG2	1:L:354:GLN:C[3_665]	2.16	0.04
1:K:48:VAL:N	1:L:354:GLN:OE1[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: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: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: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
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:CA	1:L:361:THR:OG1[3_665]	2.19	0.01
1:K:39:GLN:N	1:L:361:THR:CB[3_665]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	3 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	389/443 (88%)	329 (85%)	41 (10%)	19 (5%)	2	20
1	K	389/443 (88%)	335 (86%)	40 (10%)	14 (4%)	3	25
1	L	389/443 (88%)	329 (85%)	41 (10%)	19 (5%)	2	20
2	M	171/175 (98%)	145 (85%)	18 (10%)	8 (5%)	2	21
2	N	171/175 (98%)	143 (84%)	23 (14%)	5 (3%)	4	29
2	O	171/175 (98%)	145 (85%)	18 (10%)	8 (5%)	2	21
2	P	171/175 (98%)	143 (84%)	23 (14%)	5 (3%)	4	29
All	All	2240/2472 (91%)	1904 (85%)	244 (11%)	92 (4%)	3	22

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
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

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Mol	Chain	Res	Type
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
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

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

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	4 19
1	F	336/377 (89%)	287 (85%)	49 (15%)	3 15
1	K	336/377 (89%)	293 (87%)	43 (13%)	4 18
1	L	336/377 (89%)	288 (86%)	48 (14%)	3 16
2	M	135/136 (99%)	124 (92%)	11 (8%)	11 35
2	N	135/136 (99%)	121 (90%)	14 (10%)	7 24
2	O	135/136 (99%)	124 (92%)	11 (8%)	11 35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	P	135/136 (99%)	121 (90%)	14 (10%)	7 24
All	All	1884/2052 (92%)	1652 (88%)	232 (12%)	4 19

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

Sometimes 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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	1
1	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	139:ALA	C	140:LYS	N	0.93
1	K	139:ALA	C	140:LYS	N	0.93

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.36	33 (8%)	11	13	60, 60, 60, 60	0
1	F	393/443 (88%)	0.31	22 (5%)	24	24	60, 60, 60, 60	0
1	K	393/443 (88%)	0.50	30 (7%)	13	15	60, 60, 60, 60	0
1	L	393/443 (88%)	0.45	29 (7%)	14	15	60, 60, 60, 60	0
2	M	173/175 (98%)	0.53	21 (12%)	4	8	60, 60, 60, 60	0
2	N	173/175 (98%)	0.50	10 (5%)	23	23	60, 60, 60, 60	0
2	O	173/175 (98%)	0.59	22 (12%)	3	7	60, 60, 60, 60	0
2	P	173/175 (98%)	0.21	5 (2%)	51	44	60, 60, 60, 60	0
All	All	2264/2472 (91%)	0.42	172 (7%)	13	15	60, 60, 60, 60	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	77	PRO	7.8
1	L	289	THR	6.8
1	K	289	THR	6.5
1	K	247	VAL	6.0
1	F	443	LEU	5.6
2	N	47	ALA	5.4
1	K	76	ALA	5.4
1	L	77	PRO	5.2
2	M	40	ASP	5.0
1	K	246	ALA	4.8
2	O	23	GLY	4.7
2	M	92	GLU	4.6
2	O	24	ASN	4.6
1	E	219	LYS	4.5
1	L	288	CYS	4.5
1	E	220	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
2	O	114	GLN	4.2
2	O	16	GLY	4.1
1	L	415	GLY	4.1
1	F	397	THR	4.0
1	E	387	THR	4.0
2	N	32	LYS	4.0
1	K	251	GLY	3.9
1	K	297	VAL	3.8
1	L	250	HIS	3.7
1	K	252	ILE	3.7
1	L	163	LEU	3.5
1	K	74	ALA	3.5
2	O	6	VAL	3.5
2	M	117	ASN	3.5
1	K	305	ILE	3.4
1	K	144	GLY	3.4
1	F	439	SER	3.4
2	O	150	LYS	3.4
2	M	48	GLY	3.4
2	N	34	VAL	3.4
2	M	85	ASP	3.3
2	O	15	ALA	3.3
2	M	46	PHE	3.3
1	E	324	GLY	3.3
2	O	103	SER	3.3
1	K	288	CYS	3.3
2	N	138	GLU	3.2
1	E	148	GLN	3.2
1	L	76	ALA	3.2
1	F	109	LYS	3.2
1	L	414	SER	3.2
1	E	286	GLU	3.1
2	O	118	ASP	3.1
1	K	238	GLU	3.1
2	M	170	GLU	3.1
1	F	112	ARG	3.1
2	N	134	ARG	3.1
1	K	253	VAL	3.1
2	P	140	THR	3.1
2	O	44	ALA	3.0
2	M	57	PHE	3.0
1	F	442	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	325	ARG	3.0
1	E	118	LYS	3.0
1	E	119	ASN	3.0
1	E	297	VAL	3.0
1	F	57	GLY	3.0
1	K	75	ASN	3.0
1	L	222	MET	2.9
1	E	323	GLN	2.9
2	N	48	GLY	2.9
1	E	138	PRO	2.9
1	L	363	GLY	2.9
2	O	25	THR	2.9
1	K	245	ASP	2.9
1	L	286	GLU	2.8
1	F	146	THR	2.8
2	P	139	ASN	2.8
1	L	223	LYS	2.8
1	K	92	VAL	2.8
1	L	273	SER	2.8
2	P	35	ARG	2.8
1	K	287	GLY	2.7
1	K	304	PHE	2.7
1	F	113	VAL	2.7
2	O	151	ALA	2.7
2	O	5	SER	2.7
1	K	49	THR	2.7
2	O	169	GLU	2.7
1	L	164	ARG	2.7
1	K	248	GLU	2.7
1	F	147	GLU	2.6
2	M	45	GLY	2.6
1	L	282	LEU	2.6
2	N	30	ASN	2.6
2	M	36	ARG	2.6
2	N	86	ARG	2.6
2	O	12	VAL	2.6
1	F	234	VAL	2.6
1	L	371	SER	2.6
2	O	170	GLU	2.6
1	E	218	ILE	2.6
1	F	104	THR	2.5
1	L	90	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
2	O	149	GLU	2.5
2	M	171	LEU	2.5
1	K	142	ASN	2.5
1	F	75	ASN	2.5
1	F	235	ASN	2.5
2	M	91	LEU	2.5
1	E	128	GLU	2.5
2	M	35	ARG	2.4
1	L	372	GLY	2.4
1	E	422	ALA	2.4
2	M	39	ASN	2.4
1	F	21	ASP	2.4
1	E	114	GLN	2.4
1	E	163	LEU	2.4
2	M	77	GLU	2.4
2	M	44	ALA	2.4
1	E	221	ALA	2.4
1	E	117	GLU	2.4
1	E	147	GLU	2.3
2	M	41	LYS	2.3
1	F	114	GLN	2.3
1	E	164	ARG	2.3
1	L	267	SER	2.3
2	P	85	ASP	2.3
1	E	115	ALA	2.3
2	O	7	ARG	2.3
1	E	112	ARG	2.3
1	E	439	SER	2.3
1	E	326	LEU	2.3
1	L	252	ILE	2.2
1	K	306	ALA	2.2
1	L	162	LYS	2.2
1	L	283	PRO	2.2
1	K	250	HIS	2.2
1	F	419	THR	2.2
1	F	71	ALA	2.2
1	E	166	GLY	2.2
1	K	140	LYS	2.2
1	K	387	THR	2.2
2	O	123	GLY	2.2
1	E	217	LYS	2.2
2	M	78	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	105	ASP	2.1
1	E	222	MET	2.1
1	E	149	GLN	2.1
2	O	14	ILE	2.1
2	O	168	ILE	2.1
1	K	15	LYS	2.1
2	O	22	LEU	2.1
1	K	226	ILE	2.1
1	E	334	ALA	2.1
1	K	154	ALA	2.1
1	E	331	GLU	2.1
1	L	224	LEU	2.1
1	L	334	ALA	2.1
2	N	96	ALA	2.1
2	N	123	GLY	2.1
1	L	91	TYR	2.1
1	F	374	LYS	2.1
1	E	73	LEU	2.0
1	L	251	GLY	2.0
1	L	270	PRO	2.0
2	M	172	SER	2.0
1	K	91	TYR	2.0
2	P	141	GLU	2.0
1	F	394	ARG	2.0
1	L	49	THR	2.0
1	L	216	LEU	2.0
2	M	84	THR	2.0
1	E	385	GLU	2.0
1	F	383	VAL	2.0
2	M	58	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.