Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:38 PM GMT

PDB ID	:	4M4W
Title	:	Mechanistic implications for the bacterial primosome assembly of the structure of a helicase-helicase loader complex
Authors	:	Liu, B.; Eliason, W.K.; Steitz, T.A.
Deposited on	:	2013-08-07
Resolution	:	6.10 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

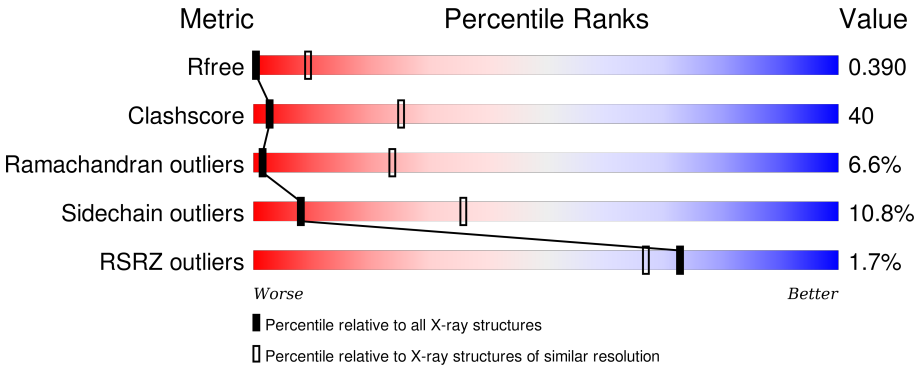
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 6.10 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}	91344	1005 (8.50-3.66)
Clashscore	102246	1053 (8.50-3.70)
Ramachandran outliers	100387	1026 (8.50-3.66)
Sidechain outliers	100360	1014 (8.50-3.64)
RSRZ outliers	91569	1004 (8.50-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	A	454	36% 35% 7% • 21%
1	B	454	41% 31% 6% 21%
1	C	454	33% 39% 6% • 21%
1	D	454	43% 30% 6% 21%
1	E	454	% 35% 35% 8% 21%

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Mol	Chain	Length	Quality of chain
1	F	454	36% 34% 8% 21%
2	G	143	49% 42% 6%
2	H	143	47% 44% 6%
2	I	143	52% 38% 6%
3	J	317	3% 36% 34% 7% 23%
3	K	317	% 40% 29% 8% 22%
3	L	317	2% 32% 38% 8% 22%
3	M	317	3% 45% 28% 5% 22%
3	N	317	3% 41% 31% 23%
3	O	317	5% 49% 26% 21%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 31981 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 Replicative helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2763	1739	473	538	13			
1	B	358	Total	C	N	O	S	0	0	0
			2763	1739	473	538	13			
1	C	358	Total	C	N	O	S	0	0	0
			2763	1739	473	538	13			
1	D	358	Total	C	N	O	S	0	0	0
			2763	1739	473	538	13			
1	E	358	Total	C	N	O	S	0	0	0
			2763	1739	473	538	13			
1	F	358	Total	C	N	O	S	0	0	0
			2763	1739	473	538	13			

- Molecule 2 is a protein called DNA primase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	138	Total	C	N	O	Se	0	0	0
			1122	712	199	205	6			
2	H	138	Total	C	N	O	Se	0	0	0
			1122	712	199	205	6			
2	I	138	Total	C	N	O	Se	0	0	0
			1122	712	199	205	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	530	GLU	ASP	CONFLICT	UNP Q9X4D0
G	531	LEU	VAL	CONFLICT	UNP Q9X4D0
H	530	GLU	ASP	CONFLICT	UNP Q9X4D0
H	531	LEU	VAL	CONFLICT	UNP Q9X4D0
I	530	GLU	ASP	CONFLICT	UNP Q9X4D0
I	531	LEU	VAL	CONFLICT	UNP Q9X4D0

- Molecule 3 is a protein called Primosomal protein DnaI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	245	Total	C	N	O	S	0	0	0
			1992	1268	332	380	12			
3	K	248	Total	C	N	O	S	0	0	0
			2013	1285	329	387	12			
3	L	247	Total	C	N	O	S	0	0	0
			2010	1280	334	383	13			
3	M	247	Total	C	N	O	S	0	0	0
			2008	1281	327	387	13			
3	N	244	Total	C	N	O	S	0	0	0
			1983	1263	331	377	12			
3	O	250	Total	C	N	O	S	0	0	0
			2031	1297	331	390	13			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	312	HIS	-	EXPRESSION TAG	UNP P06567
J	313	HIS	-	EXPRESSION TAG	UNP P06567
J	314	HIS	-	EXPRESSION TAG	UNP P06567
J	315	HIS	-	EXPRESSION TAG	UNP P06567
J	316	HIS	-	EXPRESSION TAG	UNP P06567
J	317	HIS	-	EXPRESSION TAG	UNP P06567
K	312	HIS	-	EXPRESSION TAG	UNP P06567
K	313	HIS	-	EXPRESSION TAG	UNP P06567
K	314	HIS	-	EXPRESSION TAG	UNP P06567
K	315	HIS	-	EXPRESSION TAG	UNP P06567
K	316	HIS	-	EXPRESSION TAG	UNP P06567
K	317	HIS	-	EXPRESSION TAG	UNP P06567
L	312	HIS	-	EXPRESSION TAG	UNP P06567
L	313	HIS	-	EXPRESSION TAG	UNP P06567
L	314	HIS	-	EXPRESSION TAG	UNP P06567
L	315	HIS	-	EXPRESSION TAG	UNP P06567
L	316	HIS	-	EXPRESSION TAG	UNP P06567
L	317	HIS	-	EXPRESSION TAG	UNP P06567
M	312	HIS	-	EXPRESSION TAG	UNP P06567
M	313	HIS	-	EXPRESSION TAG	UNP P06567
M	314	HIS	-	EXPRESSION TAG	UNP P06567
M	315	HIS	-	EXPRESSION TAG	UNP P06567
M	316	HIS	-	EXPRESSION TAG	UNP P06567
M	317	HIS	-	EXPRESSION TAG	UNP P06567
N	312	HIS	-	EXPRESSION TAG	UNP P06567
N	313	HIS	-	EXPRESSION TAG	UNP P06567

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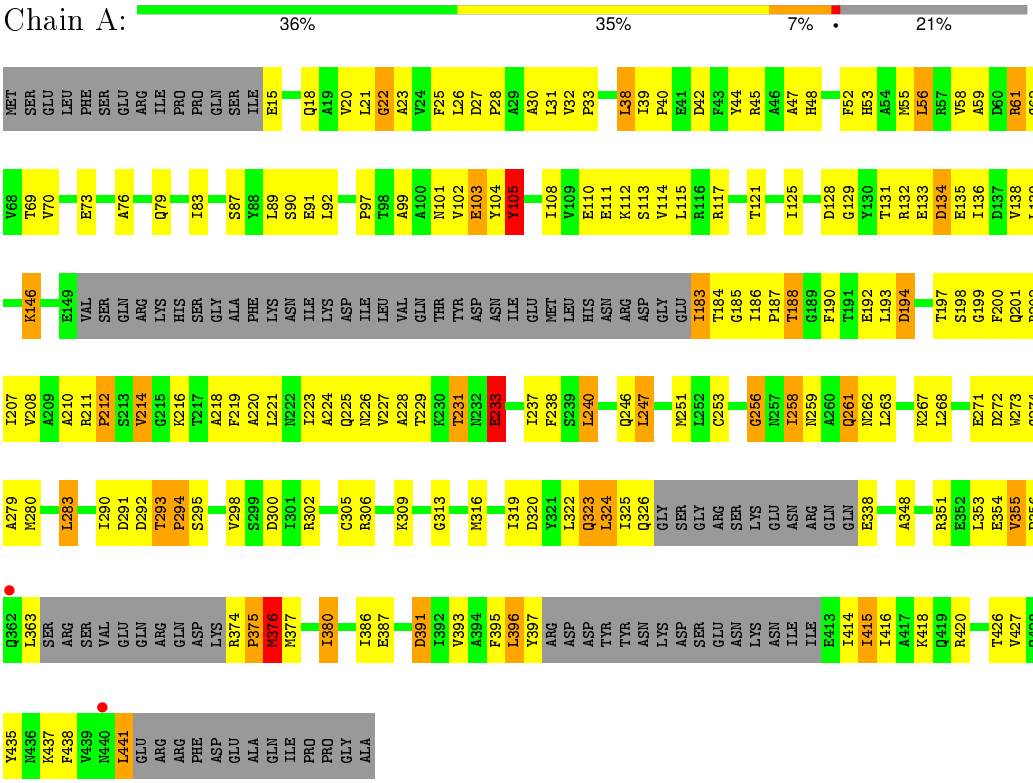
Chain	Residue	Modelled	Actual	Comment	Reference
N	314	HIS	-	EXPRESSION TAG	UNP P06567
N	315	HIS	-	EXPRESSION TAG	UNP P06567
N	316	HIS	-	EXPRESSION TAG	UNP P06567
N	317	HIS	-	EXPRESSION TAG	UNP P06567
O	312	HIS	-	EXPRESSION TAG	UNP P06567
O	313	HIS	-	EXPRESSION TAG	UNP P06567
O	314	HIS	-	EXPRESSION TAG	UNP P06567
O	315	HIS	-	EXPRESSION TAG	UNP P06567
O	316	HIS	-	EXPRESSION TAG	UNP P06567
O	317	HIS	-	EXPRESSION TAG	UNP P06567

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

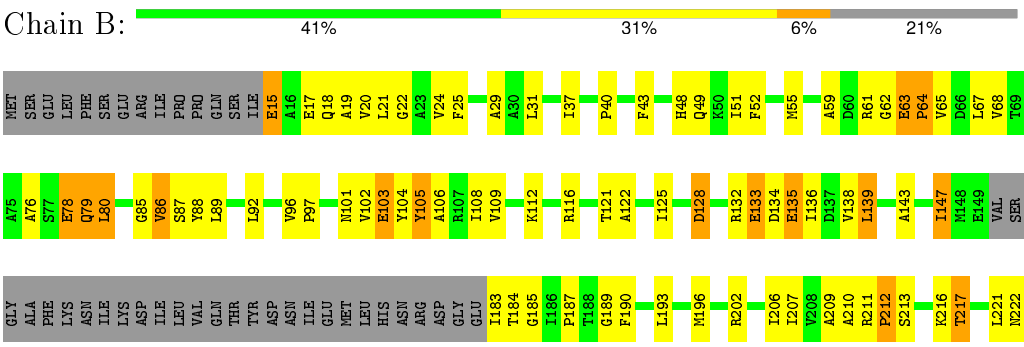
- Molecule 1: Replicative helicase

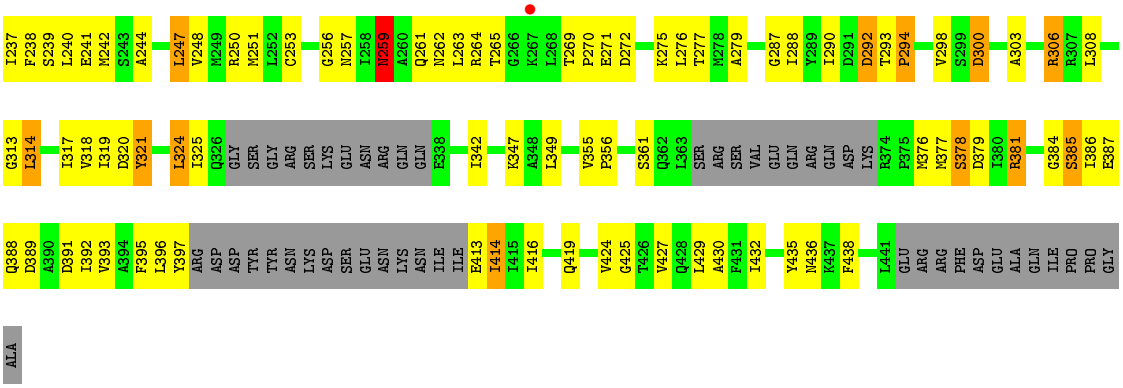
Chain A:



- Molecule 1: Replicative helicase

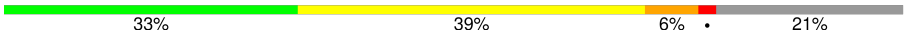
Chain B:

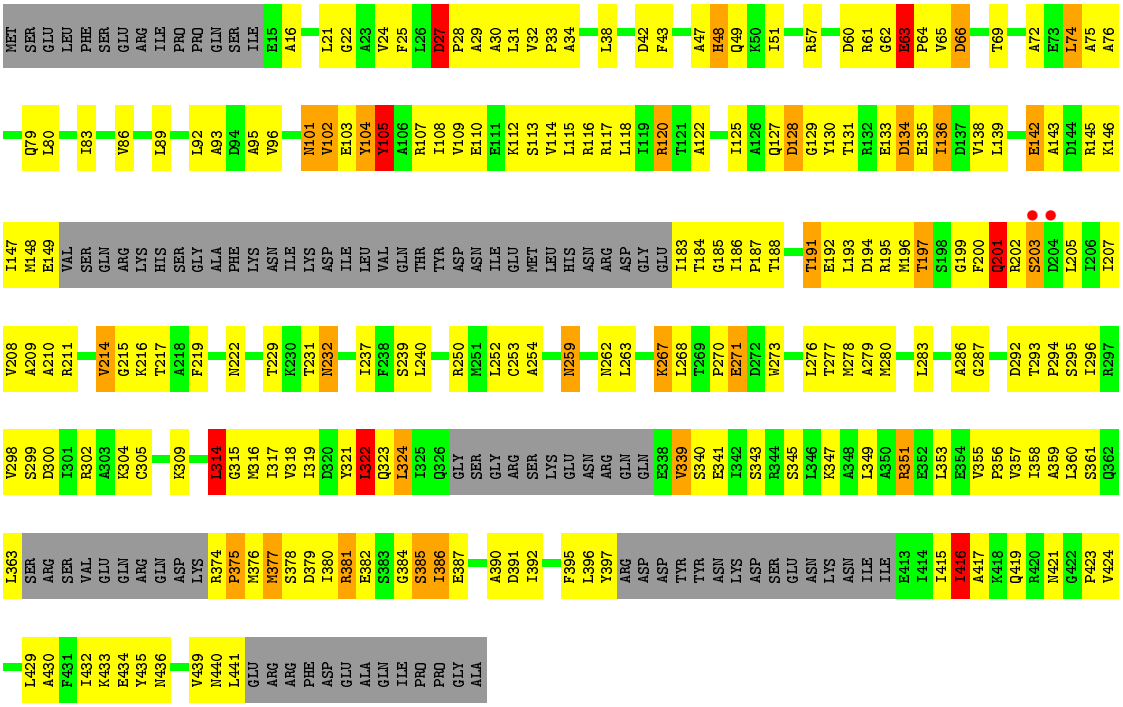




• Molecule 1: Replicative helicase

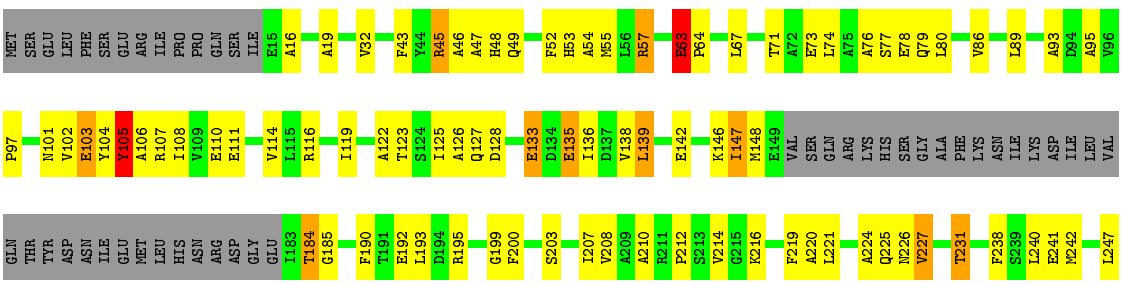
Chain C:

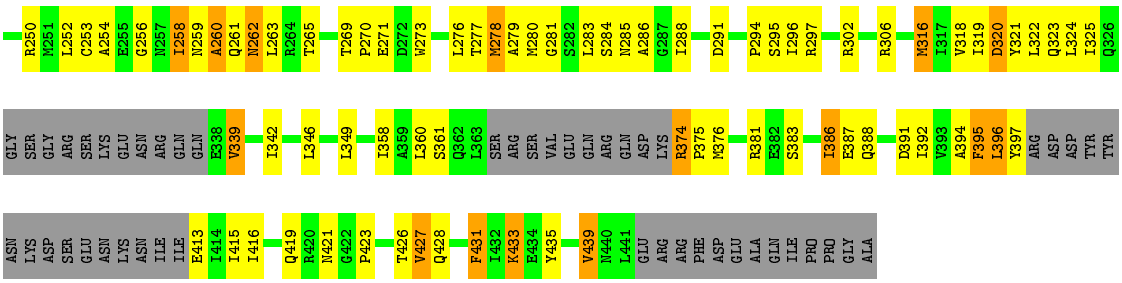




• Molecule 1: Replicative helicase

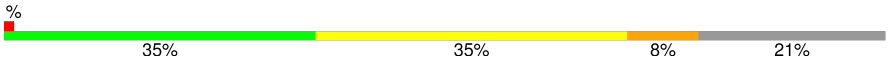
Chain D:

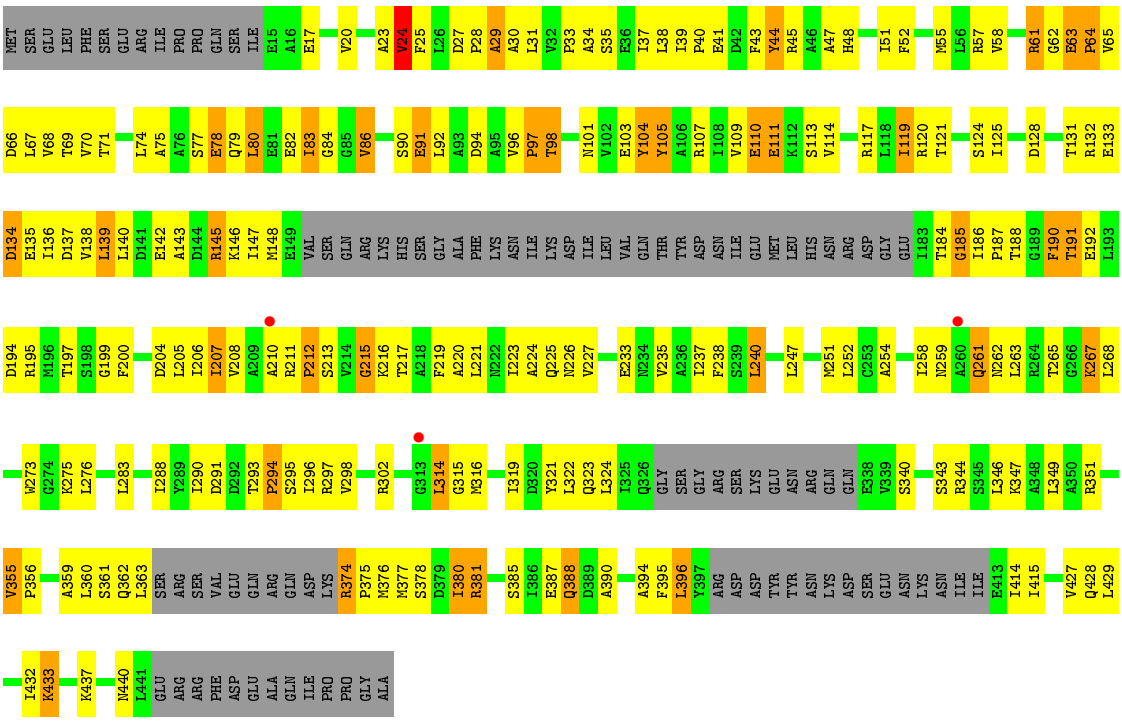




• Molecule 1: Replicative helicase

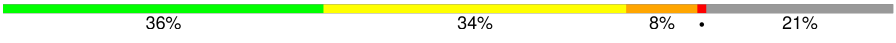
Chain E:

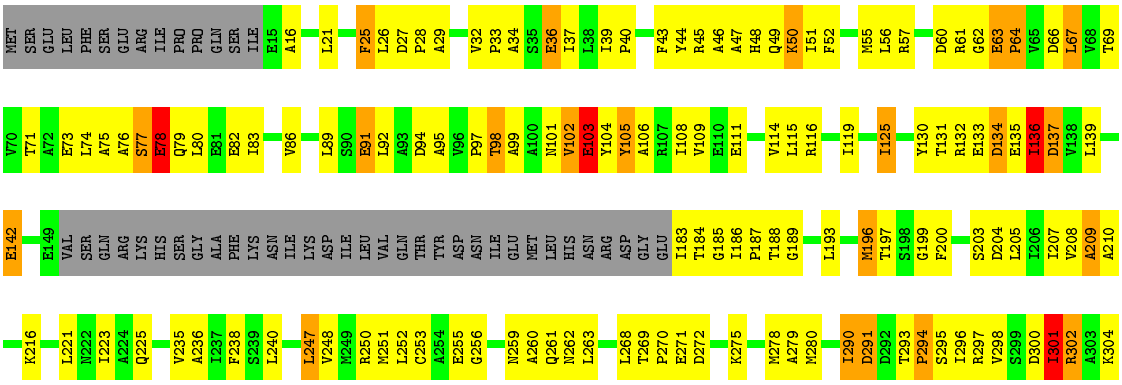


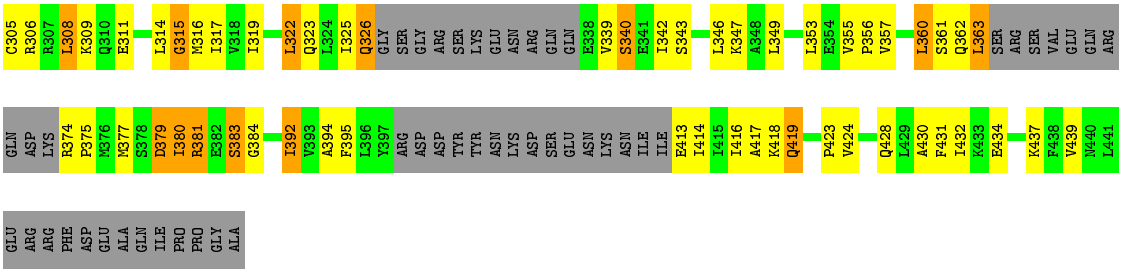


• Molecule 1: Replicative helicase

Chain F:

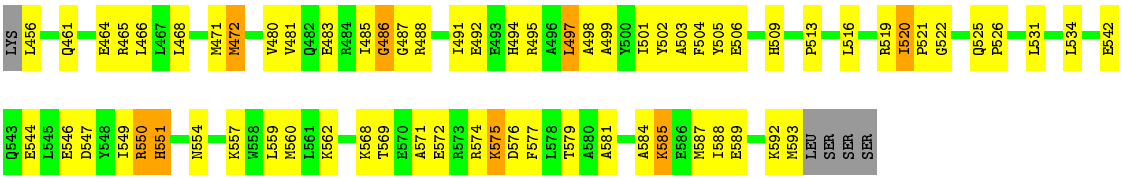






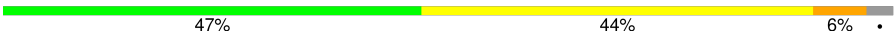
- Molecule 2: DNA primase

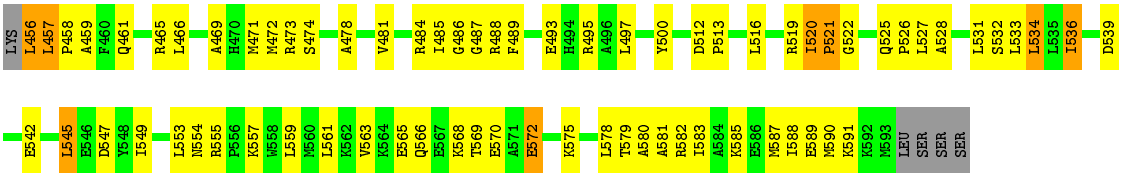
Chain G:



- Molecule 2: DNA primase

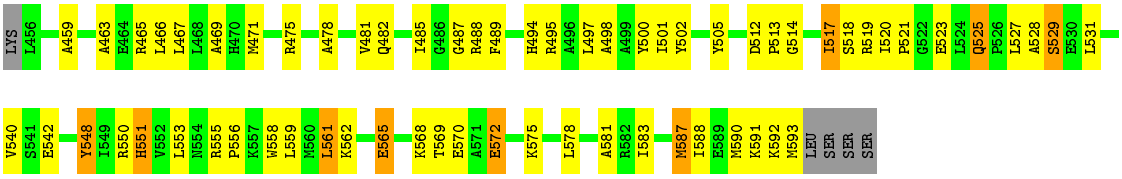
Chain H:





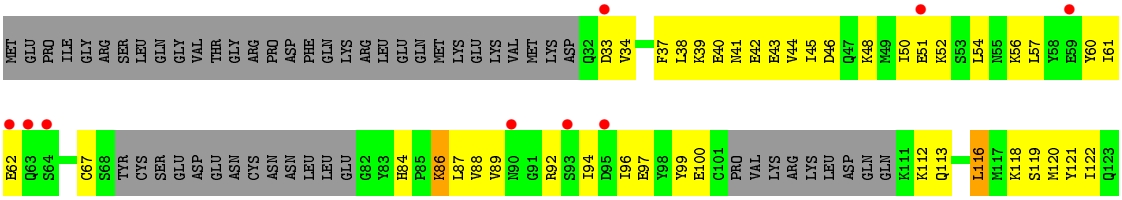
- Molecule 2: DNA primase

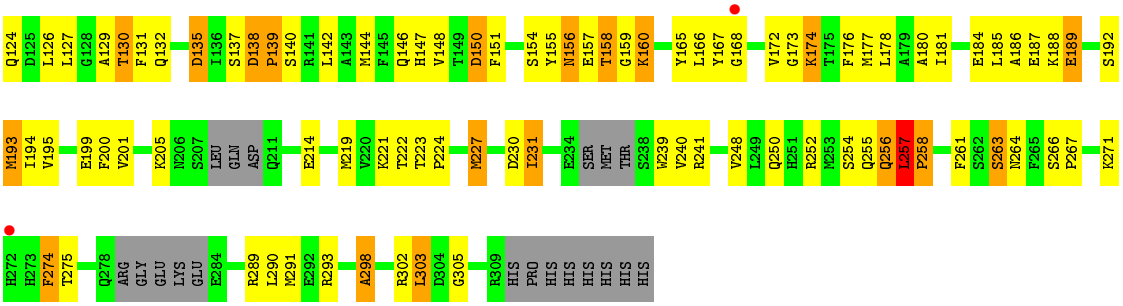
Chain I:



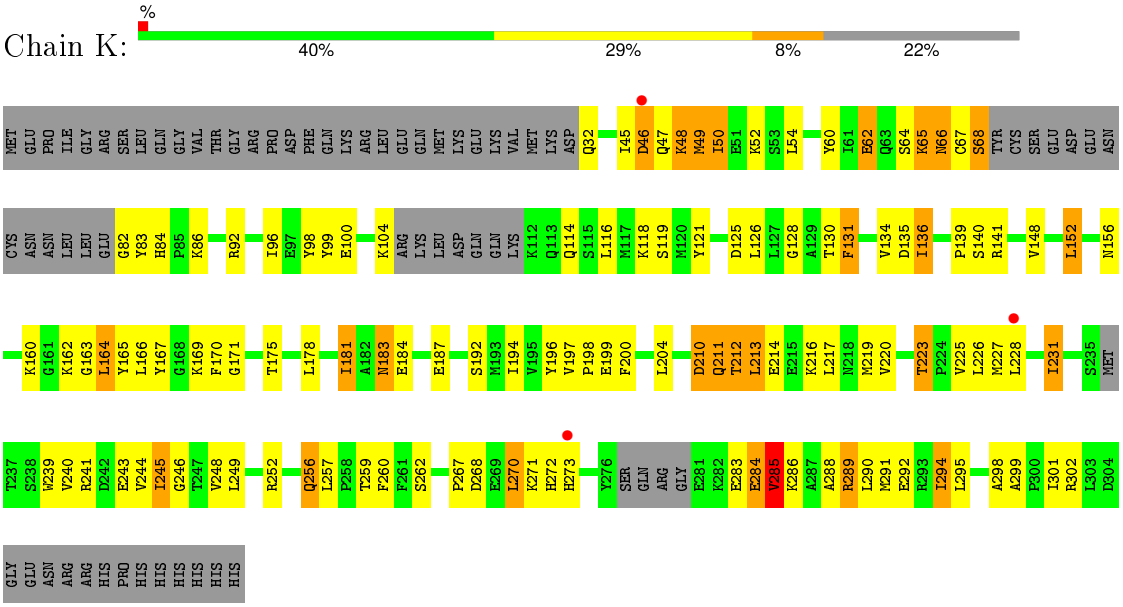
- Molecule 3: Primosomal protein DnaI

Chain J:

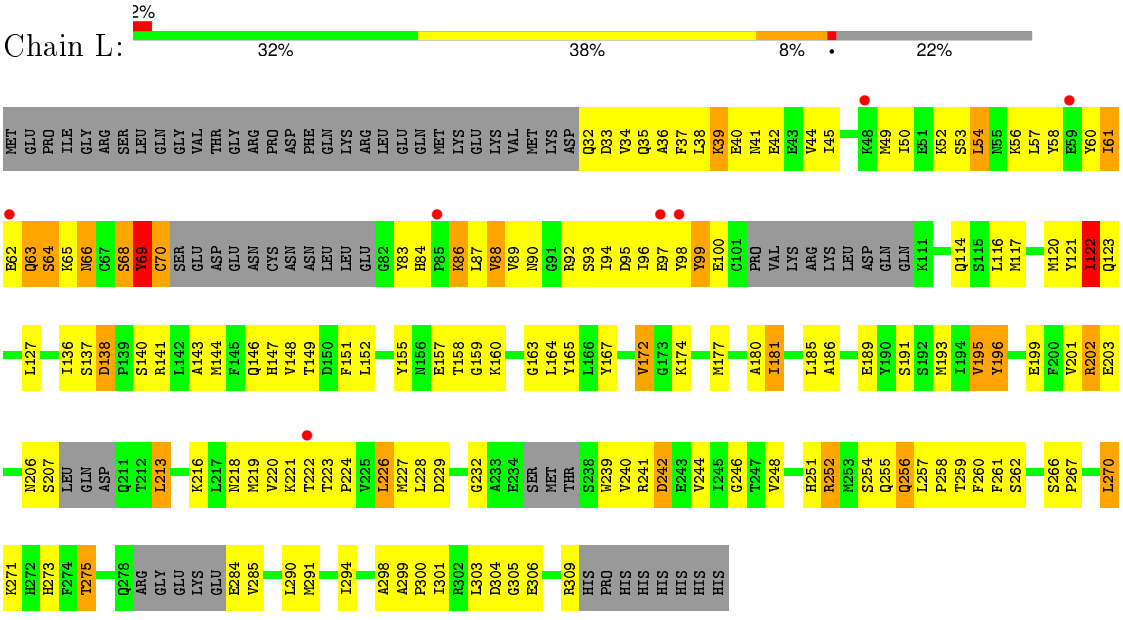




• Molecule 3: Primosomal protein DnaI

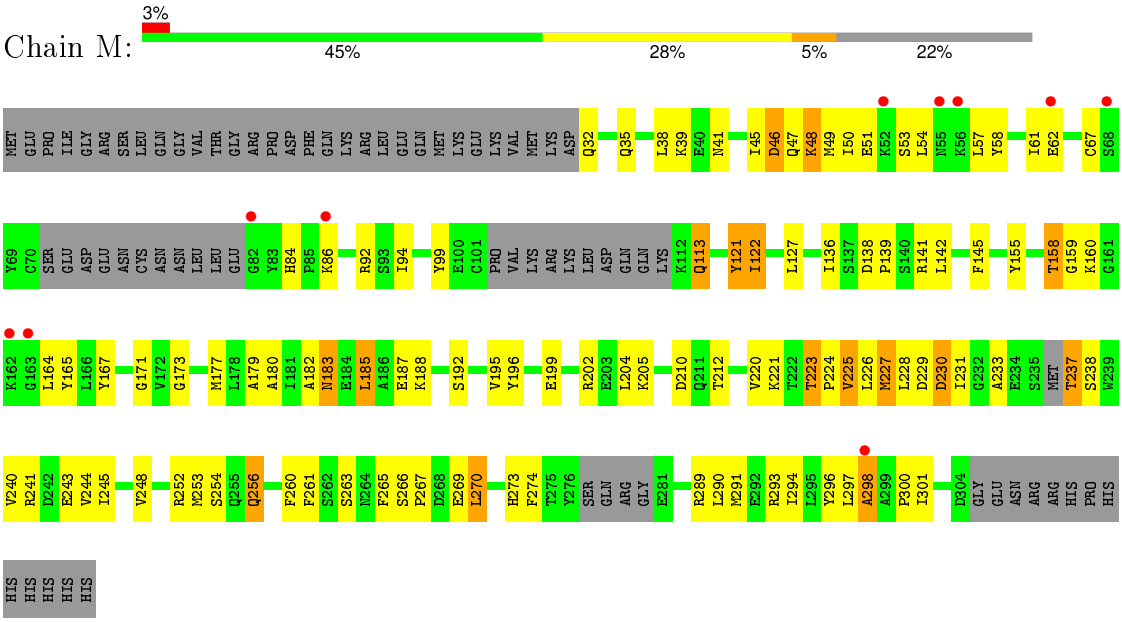


• Molecule 3: Primosomal protein DnaI



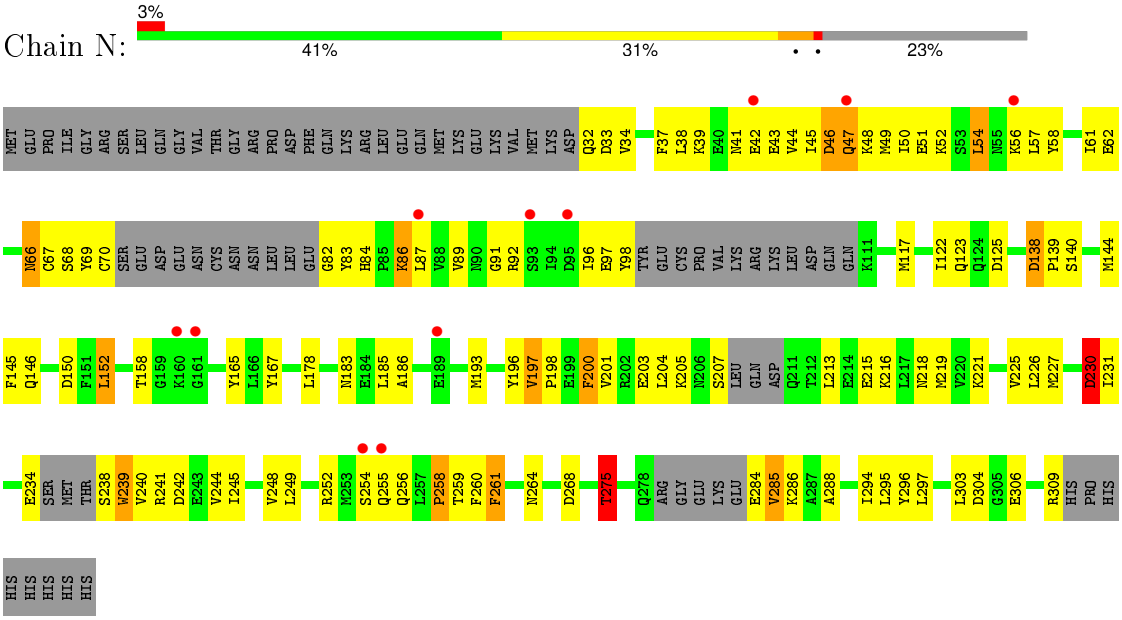
• Molecule 3: Primosomal protein DnaI

Chain M:



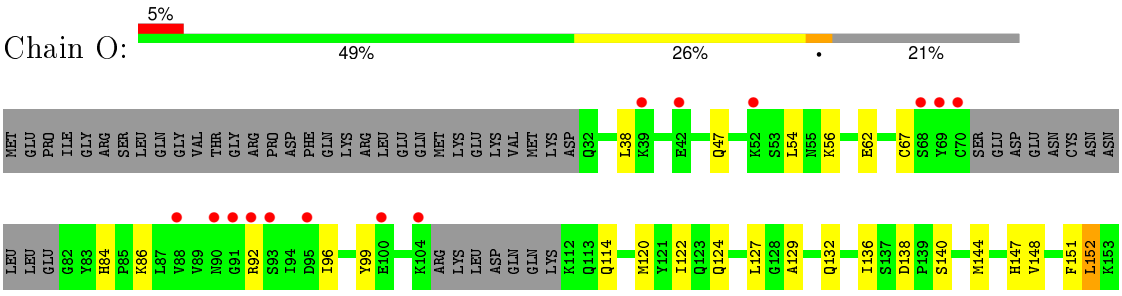
• Molecule 3: Primosomal protein DnaI

Chain N:



• Molecule 3: Primosomal protein DnaI

Chain O:




S154 Y155 N156 E157 T158 G159 K160 G161 L164 Y165 L166 Y167 V172 G173 F176 M177 L178 A179 A180 I181 E184 L185 A186 E187 K188 E189 Y190 M193 I194 V195 Y196 V197 P198 E199 P200 V201 R202 K205 N206 S207 L208 Q209 T212 L213 E214 E215 K216 L217 T223 L226 M227
L228 I231 E234 S235 MET T237 R241 D242 E243 V244 I245 L249 Q250 H251 R252 M253 S254 Q255 Q256 L257 P258 F261 S262 S266 P267 D268 E269 L270 K271 H272 H273 Y276 SER GLN ARG GLY E281 M291 E292 R293 I294 L295 Y296 L297 A298 L303 D304 GLY GLU ASN ARG
ARG HIS PRO HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	229.06Å 229.06Å 364.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 6.10 20.00 – 6.10	Depositor EDS
% Data completeness (in resolution range)	72.3 (20.00-6.10) 72.3 (20.00-6.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	0.79 (at 5.92Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.379 , 0.392 0.379 , 0.390	Depositor DCC
R_{free} test set	974 reflections (5.43%)	DCC
Wilson B-factor (Å^2)	362.7	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 941.6	EDS
Estimated twinning fraction	0.089 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.33$, $< L^2 > = 0.16$	Xtriage
Outliers	0 of 18918 reflections	Xtriage
F_o,F_c correlation	0.77	EDS
Total number of atoms	31981	wwPDB-VP
Average B, all atoms (Å^2)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.00% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.40	0/2793	0.67	1/3775 (0.0%)
1	B	0.41	0/2793	0.64	0/3775
1	C	0.42	0/2793	0.64	1/3775 (0.0%)
1	D	0.42	0/2793	0.66	0/3775
1	E	0.41	0/2793	0.64	0/3775
1	F	0.41	0/2793	0.65	0/3775
2	G	0.38	0/1134	0.60	0/1514
2	H	0.40	0/1134	0.64	0/1514
2	I	0.41	0/1134	0.62	0/1514
3	J	0.39	0/2024	0.57	0/2714
3	K	0.38	0/2047	0.57	0/2750
3	L	0.42	0/2043	0.59	0/2740
3	M	0.39	0/2042	0.54	0/2743
3	N	0.40	0/2015	0.55	0/2702
3	O	0.39	0/2066	0.56	0/2776
All	All	0.40	0/32397	0.62	2/43617 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	104	TYR	C-N-CA	5.03	134.27	121.70
1	A	38	LEU	N-CA-CB	5.02	120.44	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2763	0	2811	190	0
1	B	2763	0	2811	140	0
1	C	2763	0	2811	197	0
1	D	2763	0	2811	156	0
1	E	2763	0	2811	171	0
1	F	2763	0	2811	202	0
2	G	1122	0	1144	41	0
2	H	1122	0	1144	53	0
2	I	1122	0	1144	55	0
3	J	1992	0	1977	355	0
3	K	2013	0	2003	195	0
3	L	2010	0	1994	456	0
3	M	2008	0	1988	265	0
3	N	1983	0	1973	376	0
3	O	2031	0	2017	71	0
All	All	31981	0	32250	2589	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 40.

All (2589) 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)
3:L:33:ASP:HB3	3:L:60:TYR:CE2	1.25	1.63
3:N:45:ILE:HG21	3:N:50:ILE:CG1	1.19	1.62
3:L:86:LYS:CB	3:L:99:TYR:HE1	1.05	1.60
3:N:45:ILE:HD13	3:N:50:ILE:CD1	1.13	1.60
3:L:88:VAL:CG2	3:L:255:GLN:HB2	1.32	1.58
3:L:86:LYS:HB3	3:L:99:TYR:CE1	1.07	1.57
1:F:439:VAL:HG11	3:M:48:LYS:CE	1.29	1.57
3:L:88:VAL:CB	3:L:255:GLN:HB2	1.18	1.57
3:L:56:LYS:HD3	3:L:96:ILE:CD1	1.28	1.56
3:J:44:VAL:CG2	3:J:255:GLN:HG2	1.13	1.56
3:N:45:ILE:CD1	3:N:50:ILE:HD11	1.29	1.55
3:N:37:PHE:CE2	3:N:57:LEU:CD2	1.88	1.55
3:N:45:ILE:HG21	3:N:50:ILE:CD1	1.36	1.55
3:M:51:GLU:CG	3:N:51:GLU:CB	1.88	1.51
1:F:439:VAL:HG21	3:M:48:LYS:CE	1.37	1.51
3:N:45:ILE:CG2	3:N:50:ILE:HG12	1.41	1.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:83:TYR:CE1	3:L:219:MET:HB3	1.44	1.50
1:D:271:GLU:CB	3:J:48:LYS:HD3	1.40	1.50
3:L:86:LYS:CG	3:L:255:GLN:HE21	1.19	1.50
3:M:53:SER:HB2	3:N:48:LYS:CE	1.40	1.49
3:L:88:VAL:HG23	3:L:255:GLN:CB	1.43	1.48
3:L:98:TYR:HB3	3:L:219:MET:CE	1.02	1.48
3:L:56:LYS:HD2	3:L:96:ILE:CG1	1.40	1.48
3:L:86:LYS:CE	3:L:257:LEU:HD21	1.42	1.47
3:L:98:TYR:CB	3:L:219:MET:HE1	1.40	1.47
3:L:83:TYR:CE1	3:L:219:MET:CB	1.96	1.47
3:J:40:GLU:CA	3:J:157:GLU:HB3	1.42	1.46
3:L:98:TYR:CB	3:L:219:MET:CE	1.93	1.45
1:F:439:VAL:HG21	3:M:48:LYS:NZ	1.21	1.44
3:L:221:LYS:CE	3:L:248:VAL:HG22	1.44	1.43
1:E:104:TYR:HB3	1:E:105:TYR:CB	1.44	1.43
3:M:51:GLU:CG	3:N:51:GLU:HB3	1.45	1.43
3:M:54:LEU:CD1	3:N:52:LYS:HB2	1.46	1.42
1:F:439:VAL:CG1	3:M:48:LYS:HE3	0.94	1.41
3:L:33:ASP:HB3	3:L:60:TYR:CD2	1.53	1.41
1:D:271:GLU:HB2	3:J:48:LYS:CD	1.49	1.41
3:L:221:LYS:NZ	3:L:248:VAL:HG22	1.15	1.41
3:L:88:VAL:HB	3:L:255:GLN:CD	1.37	1.41
1:F:439:VAL:CG2	3:M:48:LYS:CE	1.96	1.41
1:F:439:VAL:CB	3:M:48:LYS:HE3	1.52	1.40
3:L:86:LYS:CD	3:L:257:LEU:HD21	1.48	1.39
3:M:54:LEU:HD13	3:N:52:LYS:CB	1.52	1.39
3:L:88:VAL:CB	3:L:255:GLN:CB	1.97	1.39
3:L:86:LYS:HG3	3:L:255:GLN:NE2	1.12	1.39
3:J:41:ASN:C	3:J:158:THR:CG2	1.80	1.38
3:J:44:VAL:HG23	3:J:255:GLN:CG	1.53	1.38
3:N:98:TYR:O	3:N:215:GLU:CB	1.71	1.38
3:L:88:VAL:CA	3:L:255:GLN:HB2	1.53	1.37
3:L:56:LYS:CD	3:L:96:ILE:CD1	2.00	1.37
3:J:40:GLU:HA	3:J:157:GLU:CG	1.53	1.35
3:J:40:GLU:C	3:J:157:GLU:HB3	1.46	1.35
3:M:57:LEU:HD13	3:N:48:LYS:CE	1.56	1.35
3:J:39:LYS:O	3:J:157:GLU:CB	1.72	1.34
3:N:37:PHE:CE2	3:N:57:LEU:HD21	1.50	1.34
3:N:67:CYS:SG	3:N:84:HIS:NE2	1.99	1.34
1:E:133:GLU:N	1:E:134:ASP:HB2	1.38	1.34
1:A:441:LEU:O	3:J:56:LYS:CE	1.77	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:88:VAL:CG2	3:L:255:GLN:CB	1.99	1.33
3:L:99:TYR:CE2	3:L:224:PRO:HD3	1.62	1.33
3:M:54:LEU:HD12	3:N:48:LYS:O	1.28	1.32
3:L:89:VAL:CB	3:L:254:SER:HB3	1.44	1.31
3:M:57:LEU:CD1	3:N:48:LYS:NZ	1.93	1.31
3:M:54:LEU:CA	3:N:48:LYS:HB2	1.60	1.30
3:J:86:LYS:HE3	3:J:222:THR:O	1.22	1.30
3:L:87:LEU:C	3:L:255:GLN:HG3	1.52	1.30
3:L:33:ASP:CB	3:L:60:TYR:CD2	2.14	1.30
3:M:54:LEU:HD13	3:N:52:LYS:CG	1.62	1.30
3:M:51:GLU:HG3	3:N:51:GLU:CB	1.54	1.30
3:M:53:SER:O	3:N:48:LYS:HD2	1.24	1.29
3:M:54:LEU:CD1	3:N:49:MET:HA	1.63	1.29
3:L:83:TYR:CE1	3:L:219:MET:HG3	1.67	1.29
3:L:56:LYS:CD	3:L:96:ILE:HG13	1.63	1.29
3:J:40:GLU:HA	3:J:157:GLU:CB	1.63	1.29
3:L:88:VAL:HB	3:L:255:GLN:OE1	1.34	1.28
3:K:62:GLU:OE2	3:L:285:VAL:HA	1.32	1.28
3:L:88:VAL:HB	3:L:255:GLN:CG	1.63	1.27
3:N:44:VAL:HG22	3:N:254:SER:CB	1.63	1.27
3:J:44:VAL:CG2	3:J:255:GLN:CG	2.06	1.27
3:K:104:LYS:CE	3:K:125:ASP:OD1	1.81	1.27
3:L:66:ASN:CB	3:L:84:HIS:CE1	2.17	1.27
1:F:439:VAL:CG2	3:M:48:LYS:NZ	1.95	1.27
3:M:51:GLU:O	3:N:52:LYS:HE3	1.27	1.27
3:M:53:SER:C	3:N:48:LYS:CD	2.03	1.27
3:J:43:GLU:CG	3:J:256:GLN:HB2	1.64	1.27
1:A:441:LEU:O	3:J:56:LYS:HE3	1.11	1.27
3:L:83:TYR:CE1	3:L:219:MET:CG	2.16	1.26
3:L:88:VAL:HA	3:L:255:GLN:CA	1.63	1.26
3:M:58:TYR:CD1	3:N:49:MET:SD	2.26	1.26
3:J:41:ASN:CA	3:J:158:THR:HG23	1.64	1.26
3:K:104:LYS:HE3	3:K:125:ASP:OD1	1.34	1.26
1:D:270:PRO:CD	3:J:51:GLU:HG3	1.65	1.26
3:L:83:TYR:HB3	3:L:219:MET:CE	1.66	1.26
3:L:33:ASP:CB	3:L:60:TYR:CE2	2.19	1.26
3:L:36:ALA:HB1	3:L:157:GLU:O	1.15	1.26
3:M:58:TYR:CE1	3:N:49:MET:SD	2.29	1.25
3:N:98:TYR:H	3:N:215:GLU:CD	1.36	1.25
3:L:99:TYR:CD1	3:L:222:THR:O	1.89	1.25
3:L:56:LYS:CD	3:L:96:ILE:CG1	2.12	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:43:GLU:HG2	3:J:256:GLN:CB	1.66	1.25
3:J:41:ASN:O	3:J:158:THR:HG21	1.07	1.24
3:L:83:TYR:CB	3:L:219:MET:HE2	1.67	1.24
3:L:86:LYS:HE2	3:L:257:LEU:CD2	1.66	1.24
3:L:88:VAL:HA	3:L:255:GLN:CB	1.68	1.24
3:J:37:PHE:CB	3:J:87:LEU:HD12	1.66	1.24
3:N:37:PHE:CD2	3:N:57:LEU:HD23	1.72	1.23
1:C:432:ILE:O	3:N:68:SER:HA	1.28	1.23
3:L:221:LYS:NZ	3:L:248:VAL:CG2	2.01	1.22
3:M:53:SER:C	3:N:48:LYS:HD2	1.53	1.22
3:L:86:LYS:CG	3:L:255:GLN:NE2	1.79	1.22
3:L:99:TYR:HD1	3:L:222:THR:O	1.18	1.22
3:L:87:LEU:O	3:L:255:GLN:CG	1.87	1.21
3:N:86:LYS:CD	3:N:218:ASN:OD1	1.87	1.21
3:M:58:TYR:HB2	3:N:46:ASP:OD2	1.05	1.21
3:N:37:PHE:CE2	3:N:57:LEU:HD23	1.60	1.21
3:M:58:TYR:HD1	3:N:46:ASP:OD1	1.21	1.21
3:M:54:LEU:HA	3:N:48:LYS:CB	1.70	1.21
3:L:86:LYS:CE	3:L:257:LEU:CD2	2.19	1.20
3:L:87:LEU:O	3:L:255:GLN:HG3	1.05	1.20
3:M:51:GLU:CD	3:N:51:GLU:HB3	1.62	1.19
3:N:45:ILE:CG2	3:N:50:ILE:CD1	2.20	1.19
3:J:38:LEU:HD21	3:J:50:ILE:CD1	1.71	1.19
1:D:261:GLN:CB	3:J:52:LYS:HZ1	1.53	1.19
3:M:57:LEU:HD13	3:N:48:LYS:NZ	1.54	1.19
3:M:54:LEU:CG	3:N:49:MET:HA	1.72	1.19
3:N:98:TYR:O	3:N:215:GLU:HB3	1.04	1.19
1:F:439:VAL:CG1	3:M:48:LYS:CE	1.90	1.18
1:F:434:GLU:OE2	3:N:58:TYR:CD1	1.96	1.18
3:J:40:GLU:CA	3:J:157:GLU:CB	2.17	1.18
3:L:86:LYS:CD	3:L:222:THR:O	1.89	1.18
3:L:66:ASN:HB2	3:L:84:HIS:CE1	1.78	1.18
3:N:44:VAL:HG23	3:N:254:SER:O	1.03	1.18
3:M:58:TYR:CB	3:N:46:ASP:OD2	1.92	1.18
3:N:86:LYS:HD3	3:N:218:ASN:OD1	1.00	1.18
1:D:270:PRO:HD3	3:J:51:GLU:CG	1.73	1.18
3:N:44:VAL:CG2	3:N:254:SER:C	2.13	1.17
3:N:44:VAL:CG2	3:N:254:SER:O	1.92	1.17
1:D:261:GLN:CG	3:J:52:LYS:HZ1	1.56	1.17
3:M:53:SER:HB2	3:N:48:LYS:CD	1.73	1.17
3:M:58:TYR:HB2	3:N:46:ASP:CG	1.63	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:43:GLU:CG	3:J:256:GLN:HE21	1.56	1.17
1:C:433:LYS:HB3	3:N:68:SER:HB2	1.20	1.17
3:L:89:VAL:HB	3:L:254:SER:CB	1.75	1.17
3:M:165:TYR:HB2	3:M:300:PRO:HA	1.18	1.17
3:M:53:SER:HB2	3:N:48:LYS:HE2	1.22	1.16
1:A:186:ILE:HG22	1:A:200:PHE:CD2	1.79	1.16
3:L:99:TYR:CD2	3:L:223:THR:OG1	1.82	1.16
3:M:58:TYR:CD1	3:N:46:ASP:OD1	1.98	1.16
3:M:54:LEU:HG	3:N:49:MET:N	1.61	1.15
3:N:44:VAL:HG23	3:N:254:SER:C	1.65	1.15
3:J:37:PHE:HB2	3:J:87:LEU:HD12	1.16	1.15
3:J:41:ASN:C	3:J:158:THR:HG21	1.35	1.15
3:L:83:TYR:CD1	3:L:219:MET:HB3	1.81	1.15
3:M:51:GLU:HG2	3:N:51:GLU:CB	1.68	1.15
3:J:40:GLU:O	3:J:157:GLU:O	1.64	1.15
3:L:86:LYS:HD2	3:L:222:THR:O	1.46	1.14
3:L:38:LEU:HD21	3:L:50:ILE:CD1	1.77	1.14
3:M:57:LEU:CD1	3:N:48:LYS:HZ1	1.57	1.14
3:J:33:ASP:HB2	3:J:61:ILE:CG2	1.76	1.14
1:F:439:VAL:HG11	3:M:48:LYS:CD	1.77	1.14
3:M:57:LEU:HD22	3:N:48:LYS:HG3	1.29	1.14
3:N:45:ILE:CG2	3:N:50:ILE:CG1	2.06	1.14
3:J:39:LYS:O	3:J:157:GLU:HB2	0.98	1.14
3:K:96:ILE:CD1	3:K:170:PHE:CB	2.26	1.14
3:L:99:TYR:CE2	3:L:224:PRO:CD	2.29	1.14
1:F:439:VAL:CB	3:M:48:LYS:CE	2.18	1.14
3:M:53:SER:CB	3:N:48:LYS:CE	2.25	1.14
3:J:99:TYR:HB3	3:J:219:MET:CE	1.77	1.13
3:J:86:LYS:HE2	3:J:223:THR:CB	1.78	1.13
3:J:34:VAL:HG22	3:J:57:LEU:HB3	1.26	1.12
3:L:88:VAL:HG23	3:L:255:GLN:HB3	1.13	1.12
1:F:439:VAL:CG2	3:M:48:LYS:HE2	1.79	1.12
3:L:88:VAL:CB	3:L:255:GLN:OE1	1.97	1.12
3:J:39:LYS:C	3:J:157:GLU:OE1	1.88	1.12
3:L:98:TYR:CB	3:L:219:MET:SD	2.38	1.12
3:L:221:LYS:CD	3:L:248:VAL:HG13	1.80	1.12
3:K:47:GLN:CG	3:K:48:LYS:HD2	1.80	1.12
3:L:36:ALA:CB	3:L:157:GLU:O	1.96	1.12
3:M:38:LEU:HG	3:N:47:GLN:HG3	1.28	1.12
3:J:44:VAL:HB	3:J:255:GLN:CB	1.79	1.12
3:L:86:LYS:HE2	3:L:257:LEU:HD21	1.18	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:GLU:CB	3:J:48:LYS:CD	2.11	1.11
3:J:38:LEU:CD2	3:J:50:ILE:HD12	1.79	1.11
3:K:96:ILE:CD1	3:K:170:PHE:HB3	1.80	1.11
3:L:83:TYR:CD1	3:L:219:MET:HE3	1.86	1.11
3:L:88:VAL:CA	3:L:255:GLN:CB	2.15	1.11
3:J:39:LYS:CB	3:J:157:GLU:OE1	1.98	1.11
3:L:83:TYR:CG	3:L:219:MET:HE2	1.85	1.10
3:J:39:LYS:HA	3:J:42:GLU:HG3	1.28	1.10
3:M:57:LEU:CD1	3:N:48:LYS:CE	2.26	1.10
3:J:86:LYS:CE	3:J:222:THR:O	2.00	1.10
1:F:133:GLU:H	1:F:134:ASP:HB2	1.01	1.10
3:L:83:TYR:CB	3:L:219:MET:CE	2.24	1.10
3:J:44:VAL:HG21	3:J:255:GLN:HG2	1.29	1.10
3:L:66:ASN:HB3	3:L:84:HIS:CE1	1.84	1.09
3:J:33:ASP:CB	3:J:61:ILE:HG22	1.80	1.09
3:K:96:ILE:HD13	3:K:170:PHE:CB	1.82	1.09
3:L:56:LYS:CD	3:L:96:ILE:HD12	1.69	1.09
3:J:86:LYS:CE	3:J:223:THR:HB	1.82	1.09
1:E:104:TYR:CB	1:E:105:TYR:HB2	1.80	1.09
1:E:104:TYR:HB3	1:E:105:TYR:HB3	1.34	1.09
3:M:50:ILE:HG22	3:N:48:LYS:HA	1.09	1.09
1:E:63:GLU:H	1:E:64:PRO:HA	1.15	1.09
3:N:37:PHE:HE2	3:N:57:LEU:CD2	1.41	1.09
1:A:426:THR:HB	1:D:265:THR:HB	1.14	1.09
3:L:83:TYR:CZ	3:L:219:MET:HG3	1.87	1.09
3:L:34:VAL:HB	3:L:57:LEU:HB2	1.22	1.09
3:J:41:ASN:HA	3:J:158:THR:HG23	1.16	1.09
3:J:43:GLU:OE2	3:J:256:GLN:NE2	1.86	1.09
3:K:104:LYS:CD	3:K:125:ASP:OD1	2.01	1.09
1:C:434:GLU:HB2	3:N:68:SER:O	1.51	1.08
3:K:104:LYS:HD3	3:K:125:ASP:CG	1.71	1.08
3:M:54:LEU:HD11	3:N:49:MET:HA	1.21	1.08
3:J:44:VAL:HA	3:J:255:GLN:HA	1.34	1.08
3:J:40:GLU:O	3:J:157:GLU:C	1.90	1.08
3:L:98:TYR:HB3	3:L:219:MET:HE2	1.28	1.08
3:L:83:TYR:CG	3:L:219:MET:CE	2.36	1.08
3:M:51:GLU:CG	3:N:51:GLU:HB2	1.63	1.08
3:J:44:VAL:HB	3:J:255:GLN:CA	1.83	1.08
1:D:261:GLN:HB3	3:J:52:LYS:HZ1	1.17	1.08
3:N:38:LEU:HD21	3:N:50:ILE:HG21	1.08	1.08
3:J:37:PHE:CD1	3:J:87:LEU:HB2	1.87	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:GLN:CG	3:J:52:LYS:NZ	2.16	1.08
3:L:98:TYR:HB2	3:L:219:MET:SD	1.95	1.07
3:M:58:TYR:CB	3:N:46:ASP:CG	2.23	1.07
3:M:54:LEU:HG	3:N:49:MET:CA	1.84	1.07
1:A:133:GLU:H	1:A:134:ASP:HB2	1.01	1.07
3:N:45:ILE:CG1	3:N:50:ILE:HD11	1.84	1.07
3:M:58:TYR:CE2	3:N:91:GLY:O	2.08	1.07
3:K:104:LYS:CD	3:K:125:ASP:CG	2.22	1.07
3:L:38:LEU:HD11	3:L:50:ILE:HD11	1.32	1.06
3:M:51:GLU:O	3:N:52:LYS:CE	2.03	1.06
1:A:184:THR:H	1:A:185:GLY:HA3	1.20	1.06
3:L:88:VAL:HA	3:L:255:GLN:HA	1.32	1.06
3:L:98:TYR:CA	3:L:219:MET:HE1	1.85	1.06
3:J:39:LYS:HA	3:J:42:GLU:CG	1.85	1.06
1:F:133:GLU:N	1:F:134:ASP:HB2	1.71	1.06
1:F:439:VAL:HG21	3:M:48:LYS:HE2	1.30	1.06
3:M:53:SER:HB3	3:N:48:LYS:NZ	1.70	1.06
3:J:86:LYS:HD3	3:J:219:MET:CE	1.85	1.06
3:J:34:VAL:HG13	3:J:57:LEU:HD23	1.09	1.06
3:L:89:VAL:HG22	3:L:94:ILE:HG12	1.11	1.05
3:L:56:LYS:HD3	3:L:96:ILE:HD11	1.34	1.05
1:D:261:GLN:HG3	3:J:52:LYS:NZ	1.70	1.05
3:L:221:LYS:HZ3	3:L:248:VAL:CG2	1.62	1.05
3:J:44:VAL:CA	3:J:255:GLN:HA	1.87	1.05
1:D:238:PHE:HA	1:D:291:ASP:HB3	1.36	1.05
2:H:484:ARG:HB3	2:H:549:ILE:HG21	1.39	1.05
3:K:83:TYR:OH	3:K:175:THR:CG2	2.04	1.05
3:M:53:SER:CA	3:N:48:LYS:HD3	1.87	1.04
3:L:41:ASN:HB2	3:L:256:GLN:HG2	1.37	1.04
3:L:221:LYS:CE	3:L:248:VAL:CG2	2.32	1.04
3:N:45:ILE:HD13	3:N:50:ILE:HD12	1.28	1.04
3:L:34:VAL:HG21	3:L:57:LEU:HD22	1.37	1.04
3:J:39:LYS:HB2	3:J:157:GLU:OE1	1.56	1.04
3:M:53:SER:C	3:N:48:LYS:HD3	1.77	1.04
3:J:43:GLU:HG3	3:J:256:GLN:HE21	1.22	1.04
1:D:271:GLU:HG3	3:J:48:LYS:HE3	1.34	1.04
1:A:20:VAL:HG22	1:A:105:TYR:O	1.56	1.04
1:E:133:GLU:H	1:E:134:ASP:CB	1.70	1.04
3:J:86:LYS:HE2	3:J:223:THR:HB	1.04	1.03
1:A:133:GLU:N	1:A:134:ASP:HB2	1.73	1.03
3:L:53:SER:CB	3:L:94:ILE:HB	1.86	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:38:LEU:CD1	3:J:50:ILE:HD11	1.87	1.03
3:J:86:LYS:HD3	3:J:219:MET:SD	1.99	1.03
3:M:50:ILE:HG22	3:N:48:LYS:CA	1.88	1.03
3:N:38:LEU:CD2	3:N:50:ILE:HG21	1.87	1.03
3:J:40:GLU:HA	3:J:157:GLU:HG2	1.11	1.03
3:J:33:ASP:HB3	3:J:60:TYR:CE2	1.93	1.03
3:K:82:GLY:HA3	3:K:126:LEU:HA	1.05	1.03
3:L:89:VAL:HB	3:L:254:SER:HB3	1.07	1.03
1:C:432:ILE:O	3:N:68:SER:CA	2.07	1.02
3:L:33:ASP:HB3	3:L:60:TYR:CZ	1.92	1.02
3:M:53:SER:CB	3:N:48:LYS:NZ	2.21	1.02
3:M:54:LEU:CD1	3:N:52:LYS:CB	2.19	1.02
3:N:44:VAL:HG22	3:N:254:SER:HB2	1.41	1.02
1:E:104:TYR:CB	1:E:105:TYR:CB	2.35	1.02
3:L:83:TYR:CD1	3:L:219:MET:HG3	1.93	1.02
3:N:98:TYR:HB2	3:N:215:GLU:OE1	1.57	1.02
3:K:62:GLU:CD	3:L:285:VAL:HA	1.80	1.02
3:L:221:LYS:CG	3:L:248:VAL:HG13	1.88	1.02
3:L:99:TYR:CD2	3:L:224:PRO:CD	2.43	1.01
1:C:433:LYS:HB3	3:N:68:SER:CB	1.88	1.01
3:L:221:LYS:HE2	3:L:248:VAL:HG22	1.41	1.01
3:N:45:ILE:HG22	3:N:50:ILE:HG12	1.40	1.01
3:J:33:ASP:HB2	3:J:61:ILE:HG22	1.05	1.01
2:I:519:ARG:H	2:I:520:ILE:HB	1.22	1.01
3:L:83:TYR:CD1	3:L:219:MET:CG	2.43	1.01
3:L:99:TYR:CD2	3:L:224:PRO:HD2	1.95	1.01
3:K:47:GLN:HG3	3:K:48:LYS:CD	1.89	1.01
3:L:41:ASN:HB2	3:L:256:GLN:CG	1.91	1.00
3:K:60:TYR:OH	3:K:65:LYS:HE2	1.61	1.00
3:K:83:TYR:CZ	3:K:175:THR:OG1	2.09	1.00
3:L:39:LYS:HG3	3:L:158:THR:O	1.61	1.00
3:K:100:GLU:OE1	3:K:125:ASP:OD2	1.77	1.00
3:L:86:LYS:CD	3:L:257:LEU:CD2	2.40	1.00
3:L:89:VAL:CB	3:L:254:SER:CB	2.37	1.00
3:L:33:ASP:HB2	3:L:60:TYR:CD2	1.97	0.99
3:N:45:ILE:CD1	3:N:50:ILE:CD1	2.03	0.99
3:J:40:GLU:CA	3:J:157:GLU:CG	2.39	0.99
1:A:104:TYR:HB3	1:A:105:TYR:HB2	1.42	0.99
3:M:54:LEU:CD1	3:N:49:MET:CA	2.39	0.99
3:M:53:SER:CB	3:N:48:LYS:CD	2.40	0.99
3:L:56:LYS:HA	3:L:96:ILE:HD11	1.41	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:67:CYS:SG	3:N:84:HIS:CD2	2.55	0.99
3:K:82:GLY:CA	3:K:126:LEU:HA	1.92	0.99
3:M:54:LEU:CD1	3:N:52:LYS:CG	2.38	0.99
1:C:133:GLU:H	1:C:134:ASP:HB2	1.28	0.99
3:N:38:LEU:HD21	3:N:50:ILE:CG2	1.92	0.98
3:L:53:SER:OG	3:L:94:ILE:HB	1.62	0.98
3:M:54:LEU:CG	3:N:49:MET:CA	2.41	0.98
3:K:83:TYR:CE2	3:K:175:THR:HG21	1.99	0.98
3:J:97:GLU:HB3	3:J:219:MET:HG2	1.45	0.98
3:L:86:LYS:HD3	3:L:257:LEU:HD21	1.45	0.98
3:M:51:GLU:OE2	3:N:51:GLU:HB3	1.63	0.98
3:K:60:TYR:HE1	3:K:65:LYS:NZ	1.59	0.98
3:L:86:LYS:HB3	3:L:99:TYR:CZ	1.95	0.98
1:B:242:MET:HA	1:E:376:MET:SD	2.04	0.98
3:K:83:TYR:HB3	3:K:126:LEU:HD22	1.42	0.98
1:F:434:GLU:OE1	3:N:54:LEU:HD22	1.63	0.98
3:J:138:ASP:HB3	3:J:139:PRO:HD2	1.44	0.98
3:L:99:TYR:CZ	3:L:224:PRO:HD3	1.99	0.98
3:J:38:LEU:HD11	3:J:50:ILE:HD11	1.44	0.97
3:N:98:TYR:N	3:N:215:GLU:CD	2.17	0.97
3:L:88:VAL:CB	3:L:255:GLN:CD	2.33	0.97
3:M:50:ILE:HA	3:N:48:LYS:HG2	1.44	0.97
3:J:43:GLU:HG2	3:J:256:GLN:HB2	0.99	0.97
3:K:83:TYR:CD1	3:K:98:TYR:CG	2.51	0.97
3:M:53:SER:HB3	3:N:48:LYS:HZ3	1.22	0.97
1:E:104:TYR:HB3	1:E:105:TYR:HB2	0.99	0.97
2:H:487:GLY:CA	2:H:488:ARG:HB2	1.94	0.97
1:F:184:THR:H	1:F:185:GLY:HA3	1.30	0.97
3:L:83:TYR:CD1	3:L:219:MET:CE	2.48	0.96
1:D:270:PRO:CD	3:J:51:GLU:CG	2.39	0.96
1:B:59:ALA:HB2	1:B:65:VAL:HG23	1.44	0.96
3:M:57:LEU:CD1	3:N:48:LYS:HE3	1.96	0.96
1:F:439:VAL:CG2	3:M:48:LYS:HZ1	1.69	0.96
1:C:432:ILE:CG2	3:N:70:CYS:C	2.34	0.96
3:L:221:LYS:HG2	3:L:248:VAL:HG13	1.46	0.96
3:L:37:PHE:HE1	3:L:255:GLN:C	1.68	0.96
3:L:89:VAL:N	3:L:254:SER:O	1.97	0.96
3:L:38:LEU:CD1	3:L:50:ILE:HD11	1.95	0.96
3:L:88:VAL:CB	3:L:255:GLN:CG	2.36	0.96
3:M:57:LEU:HD11	3:N:48:LYS:HZ1	1.28	0.96
3:M:54:LEU:HD11	3:N:52:LYS:HB2	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:104:LYS:HD2	3:K:125:ASP:CB	1.96	0.96
1:C:22:GLY:HA2	1:C:93:ALA:HA	1.48	0.96
3:L:49:MET:HG2	3:L:94:ILE:HD11	1.48	0.96
1:A:62:GLY:HA2	1:A:63:GLU:HB3	1.48	0.96
3:L:86:LYS:NZ	3:L:157:GLU:OE2	1.99	0.95
1:C:133:GLU:N	1:C:134:ASP:HB2	1.80	0.95
3:L:34:VAL:CB	3:L:57:LEU:HB2	1.96	0.95
3:J:44:VAL:HB	3:J:255:GLN:HB3	1.49	0.95
3:L:221:LYS:HE2	3:L:248:VAL:CG2	1.94	0.95
3:L:99:TYR:HD2	3:L:223:THR:OG1	1.18	0.95
3:J:34:VAL:CG2	3:J:57:LEU:HB3	1.97	0.95
3:J:40:GLU:CA	3:J:157:GLU:HG2	1.96	0.95
3:J:38:LEU:HD11	3:J:50:ILE:CD1	1.96	0.94
3:L:223:THR:OG1	3:L:224:PRO:HD2	1.67	0.94
3:L:37:PHE:HE1	3:L:255:GLN:O	1.50	0.94
3:J:44:VAL:CB	3:J:255:GLN:HA	1.97	0.94
1:D:271:GLU:CG	3:J:48:LYS:HE3	1.97	0.94
3:J:41:ASN:O	3:J:158:THR:CG2	2.00	0.94
1:D:271:GLU:HG3	3:J:48:LYS:CE	1.97	0.94
3:L:56:LYS:HD3	3:L:96:ILE:HD12	0.95	0.94
3:M:50:ILE:CG2	3:N:48:LYS:HA	1.98	0.94
3:J:99:TYR:HD2	3:J:118:LYS:NZ	1.65	0.94
2:H:513:PRO:HA	2:H:516:LEU:HB2	1.48	0.94
1:A:138:VAL:HA	1:A:141:ASP:HB2	1.49	0.94
3:K:47:GLN:HG3	3:K:48:LYS:HD2	0.96	0.93
1:D:104:TYR:HB3	1:D:105:TYR:HB2	1.49	0.93
2:H:487:GLY:HA2	2:H:488:ARG:HB2	1.50	0.93
3:K:196:TYR:HD2	3:K:199:GLU:HB2	1.33	0.93
1:D:269:THR:HG23	3:J:52:LYS:HE3	1.51	0.93
3:K:83:TYR:OH	3:K:175:THR:OG1	1.73	0.93
3:K:62:GLU:OE2	3:L:285:VAL:CA	2.16	0.93
1:D:271:GLU:HB3	3:J:48:LYS:HD3	1.49	0.93
1:E:133:GLU:H	1:E:134:ASP:HB2	0.86	0.93
3:J:37:PHE:CB	3:J:87:LEU:CD1	2.46	0.93
3:K:96:ILE:HD13	3:K:170:PHE:HB3	1.41	0.93
1:A:104:TYR:CB	1:A:105:TYR:HB2	1.98	0.92
1:D:271:GLU:HB2	3:J:48:LYS:CG	1.98	0.92
3:L:221:LYS:HD3	3:L:248:VAL:HA	1.51	0.92
3:M:54:LEU:HD11	3:N:49:MET:CA	1.97	0.92
3:K:82:GLY:HA3	3:K:126:LEU:CA	1.98	0.92
3:M:58:TYR:CA	3:N:46:ASP:CG	2.38	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:GLN:CB	3:J:52:LYS:NZ	2.30	0.92
1:C:27:ASP:HB3	1:C:29:ALA:H	1.33	0.92
3:J:41:ASN:HB3	3:J:44:VAL:CG1	1.99	0.92
1:A:186:ILE:HG22	1:A:200:PHE:HD2	1.25	0.92
3:J:116:LEU:HD13	3:J:189:GLU:HA	1.52	0.92
1:F:439:VAL:HG21	3:M:48:LYS:HZ3	1.23	0.92
3:J:39:LYS:HG3	3:J:157:GLU:CD	1.89	0.92
3:N:86:LYS:CD	3:N:218:ASN:CG	2.38	0.91
3:J:38:LEU:CD2	3:J:50:ILE:CD1	2.42	0.91
3:J:41:ASN:C	3:J:158:THR:HG23	1.68	0.91
3:N:204:LEU:HD22	3:N:216:LYS:HD3	1.52	0.91
1:A:184:THR:N	1:A:185:GLY:HA3	1.83	0.91
3:K:83:TYR:CE2	3:K:175:THR:CB	2.53	0.91
3:L:89:VAL:CG1	3:L:254:SER:HB3	2.01	0.91
3:M:54:LEU:HD13	3:N:52:LYS:HG3	1.50	0.91
3:L:83:TYR:HE1	3:L:219:MET:CB	1.59	0.91
3:J:99:TYR:HB3	3:J:219:MET:HE1	1.53	0.91
3:N:86:LYS:HD3	3:N:218:ASN:CG	1.90	0.91
3:K:83:TYR:CE1	3:K:98:TYR:CG	2.59	0.91
3:K:96:ILE:HD12	3:K:170:PHE:CG	2.06	0.91
1:C:339:VAL:HG12	1:C:384:GLY:HA3	1.51	0.91
3:K:225:VAL:HG13	3:K:259:THR:HA	1.53	0.91
3:J:37:PHE:CD1	3:J:87:LEU:CB	2.54	0.90
1:F:104:TYR:HB3	1:F:105:TYR:HB2	1.50	0.90
3:L:221:LYS:HD3	3:L:248:VAL:HG13	1.52	0.90
3:M:51:GLU:C	3:N:52:LYS:HE3	1.92	0.90
3:M:35:GLN:CD	3:N:42:GLU:HB2	1.90	0.90
3:K:96:ILE:CD1	3:K:170:PHE:CG	2.54	0.90
1:C:378:SER:HA	1:C:381:ARG:HB3	1.51	0.90
1:B:294:PRO:HB3	1:E:381:ARG:HG3	1.52	0.90
1:A:186:ILE:O	1:A:200:PHE:HB2	1.71	0.90
1:E:52:PHE:HA	1:E:55:MET:HB2	1.53	0.90
3:J:231:ILE:HD11	3:J:261:PHE:HB3	1.50	0.90
3:M:35:GLN:HG3	3:N:42:GLU:OE1	1.72	0.90
3:N:86:LYS:HE2	3:N:221:LYS:HD2	1.53	0.90
1:F:133:GLU:H	1:F:134:ASP:CB	1.85	0.90
3:L:70:CYS:SG	3:L:70:CYS:O	2.30	0.90
3:N:41:ASN:OD1	3:N:255:GLN:CG	2.20	0.89
1:C:27:ASP:CB	1:C:29:ALA:H	1.84	0.89
3:M:54:LEU:CA	3:N:48:LYS:CB	2.40	0.89
3:N:37:PHE:HE2	3:N:57:LEU:HD21	0.78	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:163:GLY:N	3:K:298:ALA:HA	1.88	0.89
3:J:39:LYS:HG3	3:J:157:GLU:OE2	1.72	0.89
3:K:96:ILE:HD12	3:K:170:PHE:HB3	1.54	0.89
3:K:83:TYR:CZ	3:K:175:THR:HG21	2.07	0.89
3:M:58:TYR:HA	3:N:46:ASP:HB3	1.54	0.89
3:J:40:GLU:C	3:J:157:GLU:CB	2.39	0.89
3:L:144:MET:HB3	3:L:177:MET:HE2	1.55	0.89
3:L:86:LYS:CG	3:L:222:THR:O	2.21	0.89
3:M:32:GLN:HE22	3:N:43:GLU:HG2	1.37	0.89
1:F:104:TYR:H	1:F:106:ALA:N	1.70	0.89
1:E:355:VAL:HG22	1:E:356:PRO:HD2	1.54	0.89
3:L:172:VAL:HG21	3:L:304:ASP:HA	1.54	0.89
1:E:221:LEU:HB3	1:E:251:MET:HB3	1.53	0.89
1:D:240:LEU:HB3	1:D:324:LEU:HD12	1.53	0.89
3:L:98:TYR:C	3:L:219:MET:HE1	1.92	0.89
3:M:50:ILE:CA	3:N:48:LYS:HG2	2.02	0.88
1:F:104:TYR:H	1:F:106:ALA:H	1.17	0.88
3:J:43:GLU:CG	3:J:256:GLN:NE2	2.35	0.88
1:D:261:GLN:HG3	3:J:52:LYS:HZ2	1.32	0.88
3:M:35:GLN:OE1	3:N:42:GLU:HB2	1.72	0.88
3:M:53:SER:HB2	3:N:48:LYS:HD3	1.53	0.88
3:M:53:SER:CB	3:N:48:LYS:HD3	2.01	0.88
3:N:45:ILE:CG2	3:N:50:ILE:HD11	1.97	0.88
1:E:66:ASP:O	1:E:69:THR:HG22	1.73	0.88
3:L:66:ASN:HB2	3:L:84:HIS:NE2	1.89	0.88
3:L:88:VAL:CG2	3:L:251:HIS:O	2.21	0.88
1:F:434:GLU:OE1	3:N:54:LEU:CD2	2.21	0.88
3:M:57:LEU:HD13	3:N:48:LYS:CD	2.03	0.88
3:M:54:LEU:CD1	3:N:48:LYS:O	2.18	0.88
1:D:261:GLN:HB3	3:J:52:LYS:NZ	1.89	0.88
3:L:98:TYR:O	3:L:219:MET:HA	1.72	0.88
3:M:51:GLU:HG2	3:N:51:GLU:HB2	1.34	0.88
3:N:37:PHE:CE1	3:N:87:LEU:CD1	2.56	0.88
1:D:276:LEU:HG	1:D:280:MET:HB2	1.54	0.88
3:M:53:SER:CB	3:N:48:LYS:HZ3	1.84	0.87
3:K:60:TYR:CE1	3:K:65:LYS:NZ	2.38	0.87
3:J:39:LYS:CA	3:J:42:GLU:HG3	2.03	0.87
1:E:43:PHE:HB3	1:E:48:HIS:HB2	1.55	0.87
1:B:240:LEU:HB2	1:B:320:ASP:HB3	1.53	0.87
1:F:104:TYR:HB3	1:F:105:TYR:CB	2.04	0.87
1:F:105:TYR:H	1:F:108:ILE:HB	1.38	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:TYR:H	1:B:106:ALA:H	1.23	0.87
3:J:86:LYS:CE	3:J:223:THR:CB	2.48	0.87
3:L:88:VAL:HB	3:L:255:GLN:CB	1.85	0.87
3:L:98:TYR:HB3	3:L:219:MET:SD	2.07	0.86
3:J:41:ASN:CA	3:J:158:THR:CG2	2.39	0.86
3:N:138:ASP:HB3	3:N:139:PRO:HD2	1.55	0.86
3:N:45:ILE:HG21	3:N:50:ILE:HG12	0.97	0.86
3:J:38:LEU:HD21	3:J:50:ILE:HD12	0.88	0.86
3:K:83:TYR:CE1	3:K:98:TYR:CD1	2.63	0.86
3:L:86:LYS:CG	3:L:99:TYR:HE1	1.89	0.86
3:J:39:LYS:C	3:J:157:GLU:CB	2.44	0.86
1:E:128:ASP:HB3	1:E:139:LEU:HD11	1.55	0.86
3:J:40:GLU:O	3:J:157:GLU:CA	2.24	0.86
3:L:122:ILE:HG12	3:L:196:TYR:HB2	1.58	0.86
3:M:58:TYR:N	3:N:46:ASP:CB	2.39	0.86
3:J:37:PHE:CE2	3:J:94:ILE:HG21	2.10	0.85
3:J:34:VAL:HG13	3:J:57:LEU:CD2	2.02	0.85
3:J:39:LYS:O	3:J:157:GLU:OE1	1.92	0.85
3:L:68:SER:O	3:L:69:TYR:HB3	1.75	0.85
3:L:83:TYR:HB3	3:L:219:MET:HE3	1.56	0.85
1:C:381:ARG:HD2	1:C:387:GLU:HB2	1.58	0.85
3:O:152:LEU:HG	3:O:184:GLU:HB2	1.57	0.85
3:L:221:LYS:HZ3	3:L:248:VAL:HG22	1.04	0.85
3:M:51:GLU:HG2	3:N:51:GLU:C	1.96	0.85
3:N:98:TYR:N	3:N:215:GLU:OE1	2.09	0.85
3:N:140:SER:HB3	3:N:304:ASP:H	1.41	0.85
3:N:44:VAL:CG2	3:N:254:SER:HB2	2.07	0.84
3:K:83:TYR:HB3	3:K:126:LEU:CD2	2.07	0.84
3:L:86:LYS:CG	3:L:99:TYR:CE1	2.60	0.84
1:F:434:GLU:OE2	3:N:58:TYR:CG	2.30	0.84
1:A:426:THR:HB	1:D:265:THR:CB	2.05	0.84
3:M:35:GLN:CB	3:N:42:GLU:OE1	2.25	0.84
3:J:37:PHE:HE2	3:J:94:ILE:HD13	1.43	0.84
3:L:32:GLN:N	3:L:61:ILE:HG21	1.91	0.84
3:L:40:GLU:OE1	3:L:160:LYS:HA	1.77	0.84
3:N:41:ASN:OD1	3:N:255:GLN:HG3	1.76	0.84
3:N:45:ILE:CB	3:N:50:ILE:HD11	2.07	0.84
1:D:76:ALA:O	1:F:133:GLU:HB3	1.77	0.84
3:L:89:VAL:HB	3:L:254:SER:CA	2.07	0.84
2:I:487:GLY:CA	2:I:488:ARG:HB2	2.08	0.84
3:L:38:LEU:CG	3:L:50:ILE:HD11	2.06	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:54:LEU:HD13	3:N:52:LYS:HB2	1.11	0.84
3:J:97:GLU:HB3	3:J:219:MET:CG	2.08	0.83
3:J:38:LEU:HD11	3:J:50:ILE:CG1	2.08	0.83
1:E:68:VAL:HA	1:E:71:THR:OG1	1.78	0.83
3:N:44:VAL:CG2	3:N:254:SER:CB	2.54	0.83
3:J:33:ASP:HB3	3:J:60:TYR:CD2	2.12	0.83
1:F:32:VAL:HG23	1:F:33:PRO:HD3	1.60	0.83
3:N:37:PHE:CZ	3:N:87:LEU:HD13	2.13	0.83
3:L:53:SER:HB3	3:L:94:ILE:HB	1.58	0.83
3:M:58:TYR:HE2	3:N:91:GLY:O	1.58	0.83
3:J:40:GLU:O	3:J:157:GLU:HB3	1.77	0.83
1:B:132:ARG:O	1:B:133:GLU:HB2	1.79	0.83
3:K:65:LYS:HG2	3:K:66:ASN:H	1.43	0.83
3:L:89:VAL:HA	3:L:94:ILE:HA	1.58	0.83
3:M:51:GLU:HG3	3:N:51:GLU:HB3	1.25	0.83
1:A:104:TYR:CA	1:A:105:TYR:HB2	2.09	0.83
3:L:140:SER:HB2	3:L:303:LEU:HD23	1.58	0.83
2:H:519:ARG:N	2:H:520:ILE:HB	1.92	0.83
1:D:269:THR:HG21	3:J:52:LYS:HG2	1.59	0.83
1:F:260:ALA:O	3:N:32:GLN:HB2	1.79	0.83
2:I:463:ALA:HA	2:I:466:LEU:HD12	1.61	0.83
1:F:434:GLU:HG2	3:N:34:VAL:HG21	1.61	0.82
1:A:261:GLN:H	1:A:262:ASN:HA	1.42	0.82
3:L:88:VAL:O	3:L:88:VAL:HG13	1.80	0.82
3:N:98:TYR:C	3:N:218:ASN:ND2	2.33	0.82
1:D:374:ARG:N	1:D:375:PRO:HA	1.94	0.82
3:O:173:GLY:HA3	3:O:303:LEU:HD13	1.60	0.82
3:L:38:LEU:CD2	3:L:50:ILE:CD1	2.57	0.82
1:D:16:ALA:HA	1:D:105:TYR:HE2	1.44	0.82
3:N:44:VAL:HG22	3:N:254:SER:OG	1.79	0.82
3:N:38:LEU:CD1	3:N:50:ILE:HG13	2.09	0.82
3:M:50:ILE:CG2	3:N:47:GLN:C	2.48	0.82
3:M:58:TYR:OH	3:N:89:VAL:HB	1.80	0.82
3:J:86:LYS:HZ3	3:J:223:THR:CB	1.93	0.82
3:K:100:GLU:CD	3:K:125:ASP:OD2	2.17	0.82
1:A:200:PHE:CE2	1:A:227:VAL:HG11	2.15	0.82
3:J:34:VAL:CG1	3:J:57:LEU:HD23	2.02	0.82
3:J:44:VAL:HG21	3:J:89:VAL:HG11	1.61	0.81
3:L:37:PHE:CE1	3:L:255:GLN:C	2.54	0.81
3:N:41:ASN:ND2	3:N:45:ILE:HG13	1.95	0.81
3:K:104:LYS:HD2	3:K:125:ASP:HB3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLU:HB3	1:A:18:GLN:HB2	1.63	0.81
1:F:52:PHE:HA	1:F:55:MET:HB2	1.61	0.81
3:N:98:TYR:O	3:N:215:GLU:HB2	1.78	0.81
1:E:63:GLU:N	1:E:64:PRO:HA	1.95	0.81
3:L:86:LYS:HG2	3:L:255:GLN:NE2	1.95	0.81
3:L:32:GLN:N	3:L:61:ILE:CG2	2.43	0.81
1:F:439:VAL:HG13	3:M:48:LYS:HE3	1.53	0.81
1:D:271:GLU:CG	3:J:48:LYS:HG2	2.09	0.81
3:K:169:LYS:HG2	3:K:170:PHE:CD2	2.15	0.81
3:K:83:TYR:CE2	3:K:175:THR:CG2	2.63	0.81
3:M:136:ILE:HG21	3:M:142:LEU:HD12	1.62	0.81
3:J:86:LYS:HD3	3:J:219:MET:HE3	1.62	0.81
3:K:160:LYS:HG2	3:K:256:GLN:HB3	1.61	0.81
3:L:37:PHE:CE1	3:L:255:GLN:O	2.33	0.81
1:F:439:VAL:CB	3:M:48:LYS:HZ1	1.93	0.81
3:N:37:PHE:CE1	3:N:87:LEU:HD12	2.16	0.81
3:K:83:TYR:HE1	3:K:98:TYR:CE1	1.99	0.81
1:B:216:LYS:HG3	1:B:217:THR:N	1.94	0.81
3:L:33:ASP:H	3:L:61:ILE:HG22	1.46	0.81
3:L:86:LYS:CB	3:L:99:TYR:CE1	1.98	0.81
3:J:44:VAL:HG12	3:J:158:THR:CG2	2.10	0.81
3:K:96:ILE:HD13	3:K:170:PHE:HB2	1.60	0.81
1:A:104:TYR:HB3	1:A:105:TYR:CB	2.11	0.81
3:L:39:LYS:HG3	3:L:158:THR:C	2.00	0.80
3:K:83:TYR:CE1	3:K:98:TYR:CD2	2.70	0.80
3:L:56:LYS:CA	3:L:96:ILE:HD11	2.12	0.80
1:A:238:PHE:HD1	1:A:291:ASP:CB	1.95	0.80
3:L:90:ASN:N	3:L:93:SER:O	2.13	0.80
3:N:46:ASP:CG	3:N:49:MET:HB2	2.01	0.80
3:J:33:ASP:HB3	3:J:60:TYR:HE2	1.43	0.80
3:K:60:TYR:CZ	3:K:65:LYS:HE2	2.15	0.80
3:K:240:VAL:HG13	3:K:244:VAL:HB	1.62	0.80
3:L:53:SER:OG	3:L:94:ILE:CB	2.29	0.80
1:E:58:VAL:HG13	1:E:63:GLU:HG2	1.62	0.80
3:K:291:MET:O	3:K:295:LEU:HG	1.81	0.80
1:D:392:ILE:HA	1:D:419:GLN:HA	1.64	0.80
3:M:50:ILE:CG2	3:N:48:LYS:CA	2.60	0.80
3:J:44:VAL:CB	3:J:255:GLN:CB	2.58	0.80
1:F:261:GLN:H	1:F:262:ASN:HA	1.45	0.80
3:L:86:LYS:HG2	3:L:222:THR:O	1.81	0.80
3:J:99:TYR:CD2	3:J:118:LYS:NZ	2.49	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:165:TYR:CZ	3:K:298:ALA:HB3	2.17	0.80
3:L:86:LYS:CD	3:L:255:GLN:NE2	2.44	0.79
3:M:54:LEU:CG	3:N:49:MET:N	2.44	0.79
3:M:51:GLU:HG3	3:N:51:GLU:HB2	1.28	0.79
1:C:434:GLU:CB	3:N:68:SER:O	2.31	0.79
1:A:441:LEU:O	3:J:56:LYS:NZ	2.15	0.79
3:K:83:TYR:HE2	3:K:175:THR:CB	1.91	0.79
2:I:519:ARG:N	2:I:520:ILE:HB	1.97	0.79
1:D:184:THR:H	1:D:185:GLY:HA3	1.47	0.79
3:N:44:VAL:HG22	3:N:254:SER:CA	2.12	0.79
3:M:57:LEU:C	3:N:46:ASP:CB	2.50	0.79
3:L:83:TYR:CD1	3:L:219:MET:CB	2.47	0.79
3:M:53:SER:O	3:N:48:LYS:CD	2.14	0.79
3:J:86:LYS:CD	3:J:219:MET:CE	2.59	0.79
3:J:34:VAL:HG22	3:J:57:LEU:CB	2.10	0.79
1:F:63:GLU:H	1:F:64:PRO:HA	1.48	0.79
3:L:99:TYR:CD2	3:L:224:PRO:HD3	2.13	0.79
3:M:57:LEU:HD13	3:N:48:LYS:HZ2	1.47	0.79
1:C:432:ILE:HG21	3:N:70:CYS:O	1.83	0.79
3:L:99:TYR:CD1	3:L:222:THR:C	2.53	0.79
3:N:45:ILE:HD13	3:N:50:ILE:HD13	1.57	0.79
3:N:67:CYS:HB3	3:N:83:TYR:O	1.82	0.79
3:K:104:LYS:CE	3:K:125:ASP:HA	2.13	0.79
3:L:165:TYR:HD1	3:L:261:PHE:HB2	1.46	0.79
3:J:257:LEU:HB3	3:J:258:PRO:CD	2.13	0.78
3:L:49:MET:HG2	3:L:94:ILE:CD1	2.12	0.78
3:M:51:GLU:HG2	3:N:51:GLU:CA	2.14	0.78
3:M:58:TYR:HA	3:N:46:ASP:CB	2.13	0.78
3:J:39:LYS:CA	3:J:157:GLU:OE1	2.31	0.78
3:K:83:TYR:OH	3:K:175:THR:CB	2.30	0.78
2:I:548:TYR:HA	2:I:551:HIS:HD2	1.46	0.78
3:J:44:VAL:CB	3:J:255:GLN:CA	2.57	0.78
1:C:340:SER:HA	1:C:385:SER:HB2	1.65	0.78
3:J:89:VAL:HG13	3:J:255:GLN:NE2	1.98	0.78
3:K:83:TYR:CZ	3:K:175:THR:CG2	2.66	0.78
1:C:103:GLU:HG2	1:C:104:TYR:CD2	2.18	0.78
3:L:98:TYR:C	3:L:219:MET:CE	2.51	0.78
3:N:97:GLU:HB3	3:N:215:GLU:HG2	1.64	0.78
1:D:270:PRO:HD3	3:J:51:GLU:HG3	0.81	0.78
1:B:261:GLN:N	1:B:262:ASN:HA	1.99	0.78
1:B:190:PHE:HZ	1:B:222:ASN:HB3	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:THR:HG21	1:A:283:LEU:HD12	1.66	0.78
3:L:99:TYR:HD1	3:L:222:THR:C	1.87	0.78
3:N:98:TYR:C	3:N:218:ASN:HD22	1.87	0.78
3:K:163:GLY:H	3:K:298:ALA:HA	1.47	0.78
3:M:58:TYR:CA	3:N:46:ASP:CB	2.61	0.78
3:K:62:GLU:OE2	3:L:284:GLU:O	2.01	0.78
3:K:104:LYS:HD3	3:K:125:ASP:OD1	1.69	0.78
3:K:83:TYR:CD1	3:K:98:TYR:CD1	2.72	0.78
1:D:269:THR:CG2	3:J:52:LYS:HG2	2.15	0.77
2:I:525:GLN:O	2:I:529:SER:HB3	1.85	0.77
3:L:40:GLU:OE1	3:L:159:GLY:O	2.03	0.77
3:M:35:GLN:CG	3:N:42:GLU:OE1	2.31	0.77
1:B:61:ARG:HB2	1:B:62:GLY:HA3	1.65	0.77
1:D:271:GLU:CB	3:J:48:LYS:CE	2.62	0.77
1:B:125:ILE:HG23	1:B:143:ALA:HB1	1.65	0.77
3:L:88:VAL:HG23	3:L:251:HIS:O	1.85	0.77
3:L:36:ALA:O	3:L:158:THR:HA	1.85	0.77
3:K:96:ILE:HD12	3:K:170:PHE:CB	2.06	0.77
1:B:133:GLU:N	1:B:134:ASP:HB2	1.98	0.77
1:A:302:ARG:HA	1:A:305:CYS:HB2	1.66	0.77
3:L:218:ASN:O	3:L:219:MET:SD	2.43	0.77
3:K:62:GLU:CD	3:L:285:VAL:CA	2.53	0.77
1:C:434:GLU:OE1	3:N:69:TYR:HA	1.84	0.77
1:C:187:PRO:HB3	1:C:194:ASP:OD1	1.84	0.77
3:L:38:LEU:HD21	3:L:50:ILE:HD11	1.65	0.77
3:M:50:ILE:CG2	3:N:48:LYS:N	2.48	0.77
3:N:38:LEU:HD11	3:N:50:ILE:HG13	1.67	0.77
1:D:271:GLU:HB2	3:J:48:LYS:HD3	0.78	0.77
1:F:205:LEU:HD13	1:F:346:LEU:HB3	1.66	0.77
3:J:86:LYS:HE2	3:J:223:THR:CA	2.15	0.76
1:C:381:ARG:CD	1:C:387:GLU:HB2	2.15	0.76
3:L:41:ASN:OD1	3:L:44:VAL:CG2	2.33	0.76
3:J:219:MET:SD	3:J:222:THR:HG23	2.24	0.76
1:E:110:GLU:HA	1:E:113:SER:HB3	1.67	0.76
1:C:22:GLY:CA	1:C:93:ALA:HA	2.14	0.76
3:N:46:ASP:O	3:N:49:MET:N	2.17	0.76
3:K:104:LYS:CD	3:K:125:ASP:CB	2.62	0.76
1:A:23:ALA:HA	1:A:26:LEU:HB2	1.67	0.76
3:N:37:PHE:CZ	3:N:87:LEU:CD1	2.68	0.76
2:I:561:LEU:HD22	2:I:591:LYS:HE2	1.66	0.76
3:N:41:ASN:OD1	3:N:255:GLN:HG2	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:37:PHE:CG	3:J:87:LEU:CD1	2.68	0.76
3:N:98:TYR:CB	3:N:215:GLU:OE1	2.31	0.76
3:K:65:LYS:HG2	3:K:66:ASN:N	1.99	0.76
2:I:548:TYR:HA	2:I:551:HIS:CD2	2.20	0.76
2:G:571:ALA:HA	2:G:574:ARG:HE	1.50	0.76
3:J:181:ILE:HG22	3:J:185:LEU:HB2	1.68	0.76
1:E:261:GLN:H	1:E:262:ASN:HA	1.50	0.76
1:B:103:GLU:HB2	1:B:104:TYR:HA	1.67	0.76
1:C:205:LEU:HD22	1:C:347:LYS:HB2	1.66	0.75
3:L:221:LYS:HZ1	3:L:248:VAL:HG22	1.45	0.75
1:B:104:TYR:HB3	1:B:105:TYR:HB2	1.68	0.75
3:M:58:TYR:CA	3:N:46:ASP:HB3	2.16	0.75
1:D:318:VAL:HG22	1:D:358:ILE:HD12	1.69	0.75
3:L:98:TYR:HB3	3:L:219:MET:HE1	0.75	0.75
3:L:99:TYR:HD2	3:L:223:THR:HG1	0.77	0.75
3:J:157:GLU:O	3:J:257:LEU:HG	1.86	0.75
1:B:216:LYS:HG3	1:B:217:THR:H	1.52	0.75
3:L:40:GLU:OE1	3:L:160:LYS:CA	2.35	0.75
3:K:83:TYR:OH	3:K:175:THR:HG23	1.85	0.75
1:F:275:LYS:HE3	1:F:278:MET:SD	2.27	0.75
1:D:253:CYS:HB3	1:D:259:ASN:HB2	1.68	0.75
3:J:193:MET:SD	3:J:223:THR:HG21	2.27	0.75
1:F:200:PHE:HB3	1:F:356:PRO:HG3	1.67	0.74
3:L:165:TYR:CE2	3:L:298:ALA:HB3	2.22	0.74
2:H:533:LEU:O	2:H:534:LEU:HB2	1.86	0.74
1:F:209:ALA:HA	1:F:361:SER:HB3	1.68	0.74
3:M:57:LEU:HD13	3:N:48:LYS:HE3	1.56	0.74
1:C:381:ARG:HG3	1:C:381:ARG:O	1.86	0.74
1:A:309:LYS:HD2	1:A:353:LEU:HG	1.69	0.74
2:H:486:GLY:H	2:H:488:ARG:HD2	1.53	0.74
2:I:488:ARG:HB3	2:I:553:LEU:HD22	1.68	0.74
1:A:103:GLU:N	1:A:104:TYR:HB2	2.02	0.74
1:F:205:LEU:HB2	1:F:347:LYS:HA	1.68	0.74
3:M:57:LEU:C	3:N:46:ASP:HB3	2.08	0.74
1:F:79:GLN:HA	1:F:82:GLU:HB3	1.69	0.74
1:F:57:ARG:HA	1:F:60:ASP:HB2	1.69	0.74
3:L:152:LEU:HA	3:L:155:TYR:HD2	1.51	0.74
3:K:196:TYR:CD2	3:K:199:GLU:HB2	2.22	0.73
1:F:261:GLN:HB2	3:N:32:GLN:HG3	1.69	0.73
3:L:83:TYR:HB2	3:L:219:MET:HE2	1.69	0.73
3:J:230:ASP:HA	3:J:263:SER:HA	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:226:LEU:HD11	3:L:248:VAL:HG12	1.70	0.73
3:J:97:GLU:CB	3:J:219:MET:HG2	2.18	0.73
1:F:413:GLU:HG2	1:F:428:GLN:HB2	1.70	0.73
3:L:61:ILE:HG13	3:L:62:GLU:H	1.52	0.73
3:L:86:LYS:CG	3:L:255:GLN:HE22	1.98	0.73
3:J:219:MET:SD	3:J:222:THR:CG2	2.77	0.73
1:F:75:ALA:HB2	1:F:80:LEU:HD12	1.71	0.73
1:B:104:TYR:H	1:B:106:ALA:N	1.86	0.73
3:L:165:TYR:CD1	3:L:261:PHE:HB2	2.23	0.73
3:J:172:VAL:HG11	3:J:305:GLY:H	1.53	0.73
3:L:58:TYR:O	3:L:61:ILE:HG12	1.89	0.73
3:M:61:ILE:CD1	3:N:44:VAL:O	2.37	0.73
3:J:43:GLU:CD	3:J:256:GLN:NE2	2.41	0.73
3:K:47:GLN:NE2	3:K:48:LYS:NZ	2.37	0.73
1:F:103:GLU:HB3	1:F:104:TYR:HA	1.69	0.73
1:C:305:CYS:HB3	1:C:314:LEU:HD11	1.71	0.73
3:M:47:GLN:O	3:M:50:ILE:HB	1.89	0.73
3:M:57:LEU:HD22	3:N:48:LYS:CG	2.16	0.73
1:D:271:GLU:CG	3:J:48:LYS:CD	2.66	0.73
1:E:133:GLU:CA	1:E:134:ASP:HB2	2.19	0.73
3:K:83:TYR:CB	3:K:126:LEU:HD22	2.17	0.73
3:J:39:LYS:CG	3:J:157:GLU:OE1	2.37	0.73
3:J:99:TYR:HD2	3:J:118:LYS:HZ1	1.37	0.73
3:K:62:GLU:OE1	3:L:285:VAL:O	2.07	0.73
3:L:206:ASN:HB2	3:M:289:ARG:HG2	1.70	0.73
1:D:271:GLU:CG	3:J:48:LYS:CG	2.66	0.73
3:L:38:LEU:O	3:L:42:GLU:N	2.22	0.72
3:N:41:ASN:OD1	3:N:44:VAL:CG2	2.36	0.72
3:J:44:VAL:H	3:J:158:THR:HG21	1.53	0.72
3:K:226:LEU:HB3	3:K:252:ARG:HH22	1.53	0.72
1:E:184:THR:H	1:E:185:GLY:HA3	1.53	0.72
1:B:49:GLN:HA	1:B:52:PHE:HB3	1.70	0.72
3:L:89:VAL:CB	3:L:254:SER:O	2.38	0.72
3:M:57:LEU:CD1	3:N:48:LYS:HZ2	1.96	0.72
3:L:163:GLY:H	3:L:298:ALA:HA	1.53	0.72
3:K:227:MET:HG2	3:K:260:PHE:HB2	1.71	0.72
1:B:259:ASN:HD21	1:B:264:ARG:CZ	2.02	0.72
1:F:61:ARG:CB	1:F:62:GLY:HA3	2.19	0.72
1:C:270:PRO:O	1:C:271:GLU:HG3	1.89	0.72
3:L:38:LEU:CD2	3:L:50:ILE:HD11	2.19	0.72
3:J:46:ASP:OD2	3:J:48:LYS:NZ	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:103:GLU:N	1:E:104:TYR:HB2	2.04	0.72
1:D:431:PHE:HB3	1:D:433:LYS:HG2	1.72	0.72
3:K:241:ARG:O	3:K:246:GLY:HA3	1.87	0.72
3:M:57:LEU:C	3:N:46:ASP:HB2	2.10	0.72
3:L:68:SER:O	3:L:69:TYR:CB	2.37	0.72
1:A:26:LEU:HD12	1:A:99:ALA:HB1	1.71	0.72
3:M:50:ILE:HG23	3:N:48:LYS:N	2.05	0.72
3:N:37:PHE:HE1	3:N:87:LEU:HD12	1.54	0.72
1:A:104:TYR:N	1:A:105:TYR:HB2	2.05	0.72
3:M:54:LEU:HD12	3:N:48:LYS:C	2.10	0.71
2:H:554:ASN:HA	2:H:557:LYS:HB2	1.70	0.71
3:L:83:TYR:HE1	3:L:219:MET:HB3	1.05	0.71
3:J:89:VAL:CG2	3:J:255:GLN:HE21	2.02	0.71
1:F:302:ARG:HH11	1:F:306:ARG:HH21	1.38	0.71
3:L:56:LYS:HD2	3:L:96:ILE:HG13	0.73	0.71
3:M:38:LEU:HG	3:N:47:GLN:CG	2.14	0.71
3:J:88:VAL:HG23	3:J:221:LYS:O	1.90	0.71
3:K:83:TYR:CD2	3:K:126:LEU:HD13	2.25	0.71
1:F:43:PHE:HB3	1:F:48:HIS:HB2	1.70	0.71
3:L:83:TYR:CG	3:L:219:MET:HE3	2.13	0.71
3:L:88:VAL:CA	3:L:255:GLN:CG	2.65	0.71
3:K:226:LEU:HB3	3:K:252:ARG:HH12	1.54	0.71
3:K:270:LEU:HA	3:K:273:HIS:HD2	1.55	0.71
1:D:319:ILE:HG22	1:D:320:ASP:H	1.56	0.71
3:N:44:VAL:HG22	3:N:254:SER:C	2.02	0.71
3:J:38:LEU:HD11	3:J:50:ILE:HG13	1.72	0.71
3:M:165:TYR:CD1	3:M:167:TYR:HE2	2.07	0.71
1:A:101:ASN:HB3	1:A:104:TYR:CD1	2.25	0.71
3:N:227:MET:HA	3:N:260:PHE:HB2	1.73	0.71
3:K:65:LYS:O	3:K:66:ASN:CB	2.39	0.71
1:A:238:PHE:CD1	1:A:291:ASP:CB	2.74	0.71
1:D:52:PHE:O	1:D:55:MET:HB2	1.91	0.71
3:J:86:LYS:NZ	3:J:223:THR:CB	2.53	0.71
3:L:33:ASP:CB	3:L:60:TYR:CG	2.74	0.71
3:L:45:ILE:HG12	3:L:89:VAL:HG21	1.73	0.71
1:A:183:ILE:HG12	1:A:194:ASP:HB3	1.72	0.71
3:L:221:LYS:HG2	3:L:248:VAL:CG1	2.20	0.70
3:J:86:LYS:CE	3:J:223:THR:CA	2.70	0.70
3:J:40:GLU:O	3:J:157:GLU:CB	2.36	0.70
1:A:253:CYS:HB3	1:A:258:ILE:O	1.90	0.70
3:L:98:TYR:O	3:L:219:MET:SD	2.49	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:35:GLN:O	3:L:39:LYS:HG2	1.91	0.70
3:M:57:LEU:HD23	3:N:47:GLN:HB2	1.72	0.70
3:J:37:PHE:CE2	3:J:45:ILE:HD11	2.25	0.70
3:K:60:TYR:HB2	3:K:169:LYS:NZ	2.06	0.70
3:K:47:GLN:CD	3:K:48:LYS:NZ	2.44	0.70
2:G:491:ILE:HB	2:G:494:HIS:HD2	1.56	0.70
3:L:89:VAL:HG23	3:L:254:SER:O	1.91	0.70
3:M:57:LEU:HD11	3:N:48:LYS:NZ	1.93	0.70
3:J:44:VAL:H	3:J:158:THR:CG2	2.04	0.70
1:D:16:ALA:HA	1:D:105:TYR:CE2	2.25	0.70
3:L:86:LYS:NZ	3:L:157:GLU:CD	2.44	0.70
3:L:34:VAL:HG21	3:L:57:LEU:CD2	2.19	0.70
3:J:39:LYS:C	3:J:157:GLU:CD	2.49	0.70
3:K:47:GLN:CD	3:K:48:LYS:CE	2.60	0.70
3:K:83:TYR:CD1	3:K:98:TYR:HB3	2.26	0.70
1:E:233:GLU:HG3	1:E:315:GLY:HA3	1.72	0.70
3:L:38:LEU:HD21	3:L:50:ILE:HD12	1.68	0.70
1:F:439:VAL:CB	3:M:48:LYS:NZ	2.42	0.70
1:C:318:VAL:HA	1:C:358:ILE:HB	1.73	0.70
1:F:238:PHE:HB2	1:F:319:ILE:HA	1.73	0.70
1:A:227:VAL:HA	1:A:231:THR:HG23	1.74	0.70
3:K:119:SER:HB3	3:K:194:ILE:HB	1.74	0.70
3:L:83:TYR:CZ	3:L:219:MET:CG	2.62	0.70
3:M:53:SER:HB2	3:N:48:LYS:NZ	1.93	0.70
3:J:41:ASN:O	3:J:44:VAL:CG1	2.40	0.70
3:N:97:GLU:HA	3:N:215:GLU:OE2	1.92	0.70
3:K:96:ILE:HD12	3:K:170:PHE:CD1	2.27	0.70
3:J:266:SER:HB2	3:J:267:PRO:HD2	1.73	0.70
3:L:83:TYR:HD1	3:L:219:MET:HE3	1.50	0.70
3:L:45:ILE:HA	3:L:49:MET:SD	2.31	0.70
1:E:133:GLU:N	1:E:134:ASP:CB	2.34	0.70
3:L:89:VAL:HG22	3:L:94:ILE:CG1	2.06	0.70
1:A:261:GLN:N	1:A:262:ASN:HA	2.06	0.70
1:F:63:GLU:HG3	1:F:64:PRO:O	1.91	0.70
3:M:58:TYR:HA	3:N:46:ASP:CG	2.12	0.69
3:L:83:TYR:CE2	3:L:219:MET:HG3	2.27	0.69
3:O:155:TYR:CE1	3:O:258:PRO:HG3	2.26	0.69
1:C:419:GLN:HB2	1:C:421:ASN:HD22	1.56	0.69
3:L:99:TYR:CE2	3:L:224:PRO:HD2	2.18	0.69
3:J:38:LEU:CD1	3:J:50:ILE:CD1	2.61	0.69
3:K:83:TYR:HE2	3:K:175:THR:HB	1.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:60:TYR:CE1	3:K:65:LYS:CE	2.74	0.69
1:B:265:THR:HA	1:E:428:GLN:HB3	1.73	0.69
3:J:89:VAL:HG22	3:J:255:GLN:HE21	1.56	0.69
1:C:254:ALA:HB2	1:C:436:ASN:HD22	1.58	0.69
1:D:271:GLU:HG2	3:J:48:LYS:HG2	1.74	0.69
3:L:37:PHE:CZ	3:L:255:GLN:HA	2.28	0.69
3:J:40:GLU:N	3:J:157:GLU:HB3	2.07	0.69
1:A:133:GLU:H	1:A:134:ASP:CB	1.92	0.69
3:M:38:LEU:CG	3:N:47:GLN:HG3	2.17	0.69
3:J:43:GLU:HG3	3:J:256:GLN:HB2	1.68	0.69
1:E:104:TYR:CB	1:E:105:TYR:HB3	2.10	0.69
3:N:67:CYS:HB3	3:N:84:HIS:CD2	2.27	0.69
1:A:187:PRO:HB2	1:A:231:THR:HB	1.74	0.69
1:A:26:LEU:HD12	1:A:99:ALA:CB	2.21	0.69
1:A:90:SER:HB3	2:G:568:LYS:HE2	1.74	0.69
1:C:268:LEU:H	1:C:273:TRP:HE1	1.39	0.69
3:M:54:LEU:HA	3:N:48:LYS:HB2	0.75	0.69
2:G:487:GLY:HA2	2:G:488:ARG:HB2	1.75	0.69
3:J:39:LYS:HA	3:J:42:GLU:CD	2.13	0.69
1:C:432:ILE:HG23	3:N:70:CYS:C	2.12	0.69
1:A:199:GLY:HA3	1:A:200:PHE:O	1.93	0.69
1:A:73:GLU:HA	1:A:76:ALA:CB	2.23	0.69
3:N:46:ASP:OD1	3:N:49:MET:HB2	1.93	0.68
3:J:43:GLU:HG2	3:J:256:GLN:HB3	1.70	0.68
3:L:88:VAL:N	3:L:255:GLN:HG3	2.08	0.68
3:J:44:VAL:HB	3:J:255:GLN:HA	1.57	0.68
1:E:377:MET:O	1:E:381:ARG:HB2	1.93	0.68
2:I:487:GLY:HA3	2:I:488:ARG:HB2	1.75	0.68
1:F:79:GLN:O	1:F:83:ILE:HB	1.93	0.68
3:M:51:GLU:OE2	3:N:51:GLU:CB	2.40	0.68
1:D:104:TYR:HB3	1:D:105:TYR:CB	2.22	0.68
1:F:16:ALA:HB1	1:F:109:VAL:HG22	1.74	0.68
1:C:62:GLY:HA2	1:C:63:GLU:HB3	1.73	0.68
1:E:192:GLU:HA	1:E:195:ARG:HD2	1.72	0.68
3:L:221:LYS:HD3	3:L:248:VAL:CG1	2.24	0.68
1:F:439:VAL:HG11	3:M:48:LYS:HE3	0.69	0.68
1:F:434:GLU:HG2	3:N:34:VAL:CG2	2.23	0.68
3:K:47:GLN:OE1	3:K:48:LYS:HE3	1.92	0.68
2:G:571:ALA:HA	2:G:574:ARG:NE	2.08	0.68
1:D:190:PHE:HB2	1:D:193:LEU:HB2	1.73	0.68
1:B:387:GLU:HG3	1:B:393:VAL:HG21	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:83:TYR:CE1	3:L:219:MET:HB2	2.20	0.68
1:F:184:THR:N	1:F:185:GLY:HA3	2.00	0.68
1:B:135:GLU:HB3	1:B:138:VAL:HB	1.74	0.68
1:B:61:ARG:CB	1:B:62:GLY:HA3	2.22	0.68
1:C:61:ARG:H	1:C:62:GLY:CA	2.07	0.68
1:C:219:PHE:HA	1:C:222:ASN:HB2	1.74	0.68
1:F:40:PRO:O	1:F:49:GLN:HG3	1.93	0.68
3:M:223:THR:O	3:M:226:LEU:HD12	1.94	0.68
3:J:41:ASN:HB3	3:J:44:VAL:HG13	1.74	0.68
1:E:61:ARG:H	1:E:62:GLY:HA3	1.58	0.68
3:L:88:VAL:CG1	3:L:255:GLN:OE1	2.41	0.68
1:C:110:GLU:HA	1:C:113:SER:HB3	1.75	0.68
1:C:127:GLN:HE22	1:C:130:TYR:HB2	1.58	0.68
3:J:44:VAL:HG23	3:J:255:GLN:HG2	0.68	0.68
2:H:487:GLY:HA3	2:H:488:ARG:HB2	1.75	0.68
1:C:24:VAL:HA	1:C:30:ALA:HB3	1.73	0.68
3:K:289:ARG:HA	3:K:292:GLU:HB2	1.76	0.68
1:D:261:GLN:N	1:D:262:ASN:HA	2.07	0.68
1:A:223:ILE:O	1:A:227:VAL:HG23	1.93	0.68
1:A:238:PHE:HD1	1:A:291:ASP:HB3	1.55	0.68
1:E:213:SER:HA	1:E:217:THR:OG1	1.93	0.68
1:C:252:LEU:HD22	1:C:279:ALA:HB1	1.75	0.68
3:L:37:PHE:HZ	3:L:254:SER:O	1.75	0.68
1:F:439:VAL:HB	3:M:48:LYS:HZ1	1.57	0.68
3:K:47:GLN:HG3	3:K:48:LYS:N	2.09	0.68
3:K:83:TYR:CZ	3:K:175:THR:CB	2.76	0.68
3:L:41:ASN:HB2	3:L:256:GLN:HG3	1.75	0.67
3:N:41:ASN:OD1	3:N:44:VAL:HB	1.94	0.67
1:C:133:GLU:CA	1:C:134:ASP:HB2	2.24	0.67
3:J:37:PHE:CE2	3:J:94:ILE:CG2	2.77	0.67
3:J:37:PHE:CG	3:J:87:LEU:HD12	2.28	0.67
3:K:271:LYS:HG2	3:K:288:ALA:HA	1.76	0.67
1:A:26:LEU:CD1	1:A:99:ALA:CB	2.71	0.67
1:A:26:LEU:CD1	1:A:99:ALA:HB2	2.23	0.67
1:C:375:PRO:HB2	1:C:395:PHE:CD2	2.29	0.67
3:L:40:GLU:HG3	3:L:256:GLN:HB3	1.76	0.67
2:I:519:ARG:H	2:I:520:ILE:CB	2.02	0.67
1:B:103:GLU:O	1:B:106:ALA:HB3	1.95	0.67
2:G:519:ARG:H	2:G:520:ILE:HB	1.59	0.67
1:A:233:GLU:HG2	1:A:316:MET:HG3	1.77	0.67
1:A:61:ARG:HB2	1:A:62:GLY:CA	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:HA	1:A:356:PRO:HD3	1.74	0.67
3:L:88:VAL:CG2	3:L:255:GLN:HB3	1.92	0.67
3:L:57:LEU:HD12	3:L:58:TYR:N	2.10	0.67
3:M:53:SER:CA	3:N:48:LYS:CD	2.55	0.67
3:J:44:VAL:HG22	3:J:89:VAL:HG21	1.76	0.67
3:J:121:TYR:HB3	3:J:199:GLU:CB	2.25	0.67
1:D:71:THR:HG22	1:D:89:LEU:HD13	1.77	0.67
3:J:41:ASN:HA	3:J:158:THR:CG2	2.08	0.67
3:K:104:LYS:HE3	3:K:125:ASP:HA	1.76	0.67
1:A:73:GLU:HA	1:A:76:ALA:HB3	1.77	0.67
2:G:557:LYS:HA	2:G:560:MSE:HB2	1.76	0.67
3:K:83:TYR:CE2	3:K:175:THR:OG1	2.37	0.67
3:J:188:LYS:O	3:J:189:GLU:HB2	1.94	0.67
3:L:140:SER:CB	3:L:303:LEU:HA	2.24	0.67
1:B:419:GLN:HE21	1:B:424:VAL:HA	1.60	0.67
3:L:116:LEU:HD12	3:L:186:ALA:HA	1.77	0.67
3:N:46:ASP:OD2	3:N:49:MET:HB2	1.95	0.67
3:J:97:GLU:HB2	3:J:222:THR:HG21	1.77	0.67
1:F:66:ASP:O	1:F:69:THR:HG22	1.95	0.67
3:L:58:TYR:CD1	3:L:61:ILE:HD11	2.30	0.66
2:H:497:LEU:HD22	2:H:520:ILE:HG12	1.76	0.66
1:A:238:PHE:CD1	1:A:291:ASP:HB2	2.30	0.66
1:A:113:SER:O	1:A:117:ARG:HG3	1.94	0.66
3:M:61:ILE:HD12	3:N:44:VAL:O	1.95	0.66
3:N:67:CYS:CB	3:N:84:HIS:CD2	2.79	0.66
1:E:63:GLU:H	1:E:64:PRO:CA	2.01	0.66
3:K:83:TYR:HH	3:K:175:THR:CB	2.08	0.66
3:K:200:PHE:O	3:K:204:LEU:HG	1.94	0.66
3:M:41:ASN:O	3:M:45:ILE:HG13	1.96	0.66
3:O:217:LEU:HD13	3:O:244:VAL:HG11	1.75	0.66
3:N:183:ASN:HA	3:N:186:ALA:HB3	1.76	0.66
1:C:358:ILE:HG22	1:C:360:LEU:HD21	1.77	0.66
3:N:245:ILE:HA	3:N:248:VAL:HB	1.77	0.66
3:L:165:TYR:CZ	3:L:298:ALA:HB3	2.31	0.66
2:I:489:PHE:HB2	2:I:495:ARG:HG2	1.76	0.66
3:K:67:CYS:O	3:K:68:SER:C	2.33	0.66
3:L:45:ILE:HG23	3:L:49:MET:SD	2.36	0.66
3:J:44:VAL:CB	3:J:255:GLN:HG2	2.16	0.66
3:N:213:LEU:HD23	3:N:216:LYS:HD2	1.78	0.66
3:J:172:VAL:HG11	3:J:305:GLY:N	2.11	0.66
1:C:375:PRO:HG2	1:C:395:PHE:HB3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:124:GLN:HG2	3:O:127:LEU:HD12	1.78	0.66
2:I:512:ASP:HB3	2:I:513:PRO:HD2	1.76	0.66
2:G:471:MSE:HB3	2:G:481:VAL:HG21	1.77	0.66
3:N:38:LEU:HD13	3:N:50:ILE:HG13	1.78	0.66
1:B:67:LEU:O	1:B:71:THR:N	2.29	0.66
3:L:100:GLU:OE2	3:L:193:MET:HE3	1.96	0.66
3:N:46:ASP:OD1	3:N:49:MET:CB	2.44	0.66
3:J:86:LYS:CD	3:J:219:MET:SD	2.82	0.66
1:B:103:GLU:CB	1:B:104:TYR:HA	2.26	0.66
3:J:121:TYR:HB3	3:J:199:GLU:HB3	1.78	0.66
1:D:125:ILE:HD11	1:D:146:LYS:CB	2.26	0.66
3:J:43:GLU:HG3	3:J:256:GLN:NE2	2.05	0.66
3:M:180:ALA:HA	3:M:183:ASN:HB2	1.78	0.66
2:I:498:ALA:HA	2:I:501:ILE:HD12	1.77	0.66
3:L:86:LYS:HD2	3:L:257:LEU:HD21	1.70	0.65
3:L:40:GLU:CG	3:L:256:GLN:HB3	2.25	0.65
3:L:86:LYS:HE2	3:L:257:LEU:CG	2.26	0.65
3:J:37:PHE:HB3	3:J:87:LEU:HD12	1.72	0.65
3:L:165:TYR:HB2	3:L:300:PRO:HB3	1.78	0.65
1:C:210:ALA:HB2	1:C:396:LEU:HB3	1.79	0.65
1:C:135:GLU:HB2	1:C:139:LEU:HD12	1.78	0.65
1:B:303:ALA:HA	1:B:306:ARG:HB3	1.78	0.65
3:L:65:LYS:O	3:L:66:ASN:HB3	1.96	0.65
2:I:487:GLY:HA2	2:I:488:ARG:HB2	1.77	0.65
3:K:204:LEU:HD22	3:K:217:LEU:HD11	1.78	0.65
1:A:387:GLU:HG3	1:A:393:VAL:HG21	1.79	0.65
1:A:200:PHE:HE2	1:A:227:VAL:HG11	1.61	0.65
1:A:432:ILE:HG21	1:A:435:TYR:HB2	1.78	0.65
3:O:200:PHE:HE1	3:O:216:LYS:HB3	1.62	0.65
3:L:45:ILE:HG12	3:L:49:MET:SD	2.37	0.65
3:M:45:ILE:O	3:M:46:ASP:CB	2.44	0.65
3:J:44:VAL:HG21	3:J:255:GLN:CG	2.00	0.65
3:L:149:THR:HG22	3:L:152:LEU:HD12	1.78	0.65
1:A:111:GLU:HA	1:A:114:VAL:HB	1.78	0.65
3:J:44:VAL:CG2	3:J:255:GLN:CB	2.75	0.65
1:D:252:LEU:HD21	1:D:280:MET:HG3	1.78	0.65
3:K:65:LYS:O	3:K:66:ASN:HB2	1.97	0.65
1:E:79:GLN:HA	1:E:82:GLU:HB3	1.78	0.65
3:L:148:VAL:HG13	3:L:181:ILE:HG23	1.78	0.65
1:E:104:TYR:CG	1:E:105:TYR:HB2	2.32	0.65
3:K:83:TYR:CE1	3:K:98:TYR:CE1	2.80	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:PHE:CD1	1:A:291:ASP:HB3	2.31	0.65
1:F:76:ALA:C	1:F:78:GLU:H	1.99	0.65
1:D:199:GLY:HA2	1:D:200:PHE:HB2	1.79	0.65
2:H:583:ILE:O	2:H:587:MSE:HG3	1.97	0.65
1:C:349:LEU:O	1:C:353:LEU:HB2	1.96	0.65
3:N:46:ASP:O	3:N:48:LYS:N	2.30	0.64
3:J:38:LEU:CD2	3:J:50:ILE:HD11	2.27	0.64
1:B:63:GLU:H	1:B:64:PRO:HA	1.62	0.64
1:E:27:ASP:HB2	1:E:30:ALA:HB2	1.79	0.64
1:F:210:ALA:HB1	1:F:216:LYS:HB3	1.78	0.64
1:C:378:SER:HA	1:C:381:ARG:CB	2.25	0.64
3:O:120:MET:HB3	3:O:200:PHE:HE2	1.62	0.64
3:K:226:LEU:CB	3:K:252:ARG:HH22	2.08	0.64
3:L:140:SER:HB3	3:L:303:LEU:HA	1.78	0.64
3:K:49:MET:O	3:K:52:LYS:N	2.29	0.64
3:N:285:VAL:HG13	3:N:288:ALA:HB3	1.80	0.64
3:L:86:LYS:HZ1	3:L:157:GLU:CD	2.01	0.64
1:C:433:LYS:CB	3:N:68:SER:HB2	2.12	0.64
1:F:104:TYR:N	1:F:106:ALA:H	1.92	0.64
3:J:154:SER:C	3:J:156:ASN:H	2.00	0.64
1:F:439:VAL:HG11	3:M:48:LYS:HD2	1.76	0.64
3:M:54:LEU:CD1	3:N:52:LYS:HG2	2.26	0.64
3:J:44:VAL:CG2	3:J:89:VAL:HG21	2.27	0.64
1:D:269:THR:CG2	3:J:52:LYS:HE3	2.25	0.64
1:C:314:LEU:HD13	1:C:355:VAL:HG21	1.78	0.64
1:D:271:GLU:HB2	3:J:48:LYS:HG2	1.79	0.64
3:M:160:LYS:HG2	3:M:256:GLN:HB3	1.79	0.64
3:K:83:TYR:CE1	3:K:98:TYR:CE2	2.86	0.64
3:K:121:TYR:HB3	3:K:199:GLU:HB3	1.80	0.64
3:L:152:LEU:HA	3:L:155:TYR:CD2	2.31	0.64
3:K:47:GLN:NE2	3:K:48:LYS:HZ2	1.94	0.64
1:D:208:VAL:HG22	1:D:394:ALA:HB3	1.79	0.64
3:L:89:VAL:HB	3:L:254:SER:O	1.98	0.64
1:D:271:GLU:CG	3:J:48:LYS:CE	2.65	0.64
1:C:185:GLY:HA2	1:C:201:GLN:HA	1.78	0.64
1:E:374:ARG:N	1:E:375:PRO:HA	2.13	0.64
1:D:108:ILE:HA	1:D:111:GLU:HB2	1.80	0.64
3:L:63:GLN:O	3:L:64:SER:C	2.36	0.64
1:C:61:ARG:N	1:C:62:GLY:CA	2.60	0.64
3:N:264:ASN:HD21	3:O:160:LYS:HD2	1.62	0.64
3:N:197:VAL:N	3:N:198:PRO:HD2	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:57:LEU:O	3:N:46:ASP:HB3	1.98	0.63
3:N:44:VAL:CA	3:N:254:SER:HB2	2.28	0.63
3:J:43:GLU:OE2	3:J:160:LYS:HE3	1.97	0.63
1:D:271:GLU:CB	3:J:48:LYS:CG	2.67	0.63
1:D:104:TYR:CB	1:D:105:TYR:HB2	2.26	0.63
2:I:494:HIS:HA	2:I:497:LEU:HD12	1.79	0.63
1:B:184:THR:N	1:B:185:GLY:HA2	2.12	0.63
1:C:104:TYR:CB	1:C:105:TYR:HB2	2.28	0.63
1:C:263:LEU:HG	1:C:268:LEU:HD21	1.79	0.63
1:E:145:ARG:HA	1:E:148:MET:HG2	1.80	0.63
2:H:489:PHE:HB2	2:H:495:ARG:HG2	1.80	0.63
1:C:32:VAL:HB	1:C:33:PRO:HD3	1.80	0.63
1:E:388:GLN:H	1:E:388:GLN:HE21	1.44	0.63
3:L:40:GLU:N	3:L:158:THR:O	2.31	0.63
3:L:68:SER:OG	3:L:69:TYR:N	2.30	0.63
1:A:89:LEU:HA	1:A:92:LEU:HD12	1.80	0.63
1:B:213:SER:H	1:B:216:LYS:HG2	1.63	0.63
3:M:54:LEU:N	3:N:48:LYS:CB	2.60	0.63
3:J:37:PHE:CZ	3:J:94:ILE:HG23	2.33	0.63
1:C:432:ILE:O	3:N:68:SER:CB	2.46	0.63
2:H:520:ILE:HD13	2:H:528:ALA:HB1	1.81	0.63
1:E:184:THR:N	1:E:185:GLY:HA3	2.12	0.63
3:L:34:VAL:CG2	3:L:57:LEU:HB2	2.29	0.63
3:L:266:SER:HB2	3:L:267:PRO:HD2	1.79	0.63
3:M:155:TYR:HD1	3:M:159:GLY:HA3	1.62	0.63
3:L:83:TYR:HE1	3:L:219:MET:HB2	1.60	0.63
1:E:315:GLY:HA2	1:E:355:VAL:HG21	1.81	0.63
1:D:45:ARG:C	1:D:47:ALA:H	2.02	0.63
1:D:43:PHE:HB2	1:D:49:GLN:HA	1.79	0.63
1:D:210:ALA:HB1	1:D:214:VAL:HB	1.81	0.63
3:J:37:PHE:CG	3:J:87:LEU:HD13	2.34	0.63
3:L:65:LYS:NZ	3:L:189:GLU:O	2.29	0.63
3:J:158:THR:HA	3:J:256:GLN:O	1.99	0.63
3:K:83:TYR:HD2	3:K:126:LEU:HD13	1.63	0.63
3:J:231:ILE:HG12	3:J:261:PHE:HD1	1.63	0.63
1:F:207:ILE:HD12	1:F:322:LEU:HD13	1.80	0.63
1:C:302:ARG:HG3	1:C:349:LEU:HD13	1.81	0.63
1:C:214:VAL:HG12	1:C:215:GLY:N	2.14	0.63
2:G:550:ARG:HG2	2:G:554:ASN:HD21	1.63	0.63
1:F:94:ASP:HA	2:I:459:ALA:HB2	1.80	0.63
2:I:467:LEU:HG	2:I:471:MSE:SE	2.49	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:THR:HA	1:E:223:ILE:HG23	1.81	0.62
3:J:219:MET:HA	3:J:222:THR:HG22	1.79	0.62
1:A:375:PRO:HG2	1:A:415:ILE:HD12	1.81	0.62
2:H:472:MSE:HG2	2:H:513:PRO:HB3	1.80	0.62
3:J:156:ASN:HB2	3:J:159:GLY:O	2.00	0.62
1:C:321:TYR:C	1:C:323:GLN:H	2.02	0.62
2:I:471:MSE:HB2	2:I:478:ALA:HB2	1.81	0.62
3:J:40:GLU:N	3:J:157:GLU:CB	2.62	0.62
1:E:104:TYR:CD1	1:E:105:TYR:HB2	2.33	0.62
1:E:51:ILE:HG22	1:E:55:MET:SD	2.39	0.62
3:L:83:TYR:CG	3:L:219:MET:HG3	2.33	0.62
3:L:86:LYS:HE2	3:L:257:LEU:HD23	1.77	0.62
3:L:88:VAL:CG2	3:L:255:GLN:OE1	2.47	0.62
3:K:60:TYR:HB2	3:K:169:LYS:HZ1	1.64	0.62
1:C:27:ASP:HB2	1:C:29:ALA:H	1.63	0.62
1:A:237:ILE:O	1:A:290:ILE:HA	1.99	0.62
3:J:41:ASN:O	3:J:44:VAL:HG12	1.99	0.62
1:A:187:PRO:HB2	1:A:231:THR:CB	2.29	0.62
3:K:47:GLN:CG	3:K:48:LYS:CD	2.61	0.62
1:E:74:LEU:HB3	1:E:79:GLN:HG3	1.80	0.62
1:C:136:ILE:HG13	1:F:111:GLU:CD	2.18	0.62
3:L:41:ASN:OD1	3:L:44:VAL:HB	1.99	0.62
3:M:54:LEU:HG	3:N:48:LYS:C	2.20	0.62
3:M:57:LEU:HD12	3:N:48:LYS:NZ	2.11	0.62
3:K:83:TYR:CD1	3:K:98:TYR:CB	2.82	0.62
2:H:473:ARG:CZ	2:H:513:PRO:HG3	2.30	0.62
1:E:31:LEU:HG	1:E:35:SER:HB3	1.81	0.62
3:L:90:ASN:ND2	3:L:95:ASP:OD2	2.28	0.62
1:E:237:ILE:HB	1:E:290:ILE:HA	1.81	0.62
1:A:190:PHE:HB3	1:A:192:GLU:HG2	1.81	0.62
1:E:86:VAL:HG21	2:I:572:GLU:HG3	1.81	0.62
1:F:221:LEU:HD22	1:F:251:MET:HB3	1.81	0.62
3:M:53:SER:CB	3:N:48:LYS:HE2	2.11	0.62
3:M:54:LEU:CD2	3:N:49:MET:HA	2.30	0.62
1:D:271:GLU:HB3	3:J:48:LYS:CE	2.30	0.62
1:A:187:PRO:HA	1:A:194:ASP:OD1	2.00	0.62
1:E:110:GLU:O	1:E:114:VAL:N	2.33	0.62
1:E:24:VAL:HA	1:E:30:ALA:HB3	1.82	0.62
3:J:37:PHE:CD2	3:J:87:LEU:HD13	2.35	0.62
3:J:43:GLU:C	3:J:255:GLN:O	2.38	0.62
3:J:44:VAL:N	3:J:255:GLN:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:57:LEU:HB3	3:N:46:ASP:HB2	1.81	0.61
3:M:51:GLU:OE2	3:N:51:GLU:O	2.17	0.61
3:J:89:VAL:CG1	3:J:255:GLN:NE2	2.63	0.61
1:D:269:THR:HB	1:D:270:PRO:HD2	1.81	0.61
1:F:238:PHE:HA	1:F:291:ASP:HB3	1.81	0.61
3:O:199:GLU:HG2	3:O:202:ARG:HD2	1.82	0.61
1:A:143:ALA:HB1	1:A:146:LYS:HE3	1.82	0.61
3:N:44:VAL:HA	3:N:254:SER:HB2	1.82	0.61
1:B:43:PHE:HE1	1:B:48:HIS:HB3	1.65	0.61
1:B:416:ILE:HB	1:B:424:VAL:HG12	1.82	0.61
1:E:283:LEU:HA	1:E:288:ILE:HD12	1.81	0.61
1:A:218:ALA:HA	1:A:221:LEU:HB2	1.82	0.61
1:E:395:PHE:HB2	1:E:415:ILE:HB	1.80	0.61
1:E:302:ARG:HH22	1:E:349:LEU:HB2	1.65	0.61
1:B:184:THR:H	1:B:185:GLY:HA2	1.66	0.61
3:L:36:ALA:CB	3:L:158:THR:HG22	2.31	0.61
3:L:89:VAL:N	3:L:254:SER:C	2.53	0.61
3:M:58:TYR:N	3:N:46:ASP:HB2	2.15	0.61
2:G:499:ALA:HA	2:G:502:TYR:CD2	2.34	0.61
1:C:430:ALA:HB3	1:C:439:VAL:HB	1.83	0.61
1:C:314:LEU:HD22	1:C:355:VAL:HG11	1.83	0.61
1:B:22:GLY:HA2	1:B:25:PHE:CD2	2.36	0.61
3:L:100:GLU:N	3:L:219:MET:O	2.32	0.61
3:J:157:GLU:O	3:J:257:LEU:CD2	2.49	0.61
1:D:271:GLU:CB	3:J:48:LYS:HE3	2.27	0.61
1:C:317:ILE:HG13	1:C:355:VAL:HG11	1.81	0.61
1:A:110:GLU:O	1:A:114:VAL:HG23	2.00	0.61
1:C:61:ARG:H	1:C:62:GLY:HA2	1.64	0.61
3:O:165:TYR:HB3	3:O:167:TYR:CE2	2.35	0.61
3:L:38:LEU:HD21	3:L:50:ILE:HD13	1.80	0.61
3:L:89:VAL:CG2	3:L:254:SER:O	2.49	0.61
3:M:57:LEU:HD11	3:N:48:LYS:HE3	1.77	0.61
3:M:35:GLN:HB3	3:N:42:GLU:OE1	2.00	0.61
3:J:43:GLU:CD	3:J:256:GLN:HE21	2.03	0.61
3:N:98:TYR:CA	3:N:215:GLU:OE1	2.49	0.61
3:K:62:GLU:CD	3:L:285:VAL:C	2.59	0.61
3:L:221:LYS:O	3:L:252:ARG:NE	2.33	0.61
3:M:57:LEU:CD2	3:N:47:GLN:HB2	2.31	0.61
3:J:138:ASP:HB3	3:J:139:PRO:CD	2.23	0.61
1:C:104:TYR:H	1:C:105:TYR:CB	2.14	0.61
2:H:457:LEU:HB3	2:H:461:GLN:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:143:ALA:HA	1:E:146:LYS:HE3	1.82	0.61
1:D:221:LEU:HD11	1:D:250:ARG:HB3	1.82	0.61
3:L:40:GLU:CD	3:L:159:GLY:O	2.39	0.60
3:L:53:SER:HB2	3:L:94:ILE:HD12	1.82	0.60
3:J:257:LEU:HB3	3:J:258:PRO:HD2	1.83	0.60
1:C:133:GLU:HB2	1:C:134:ASP:CG	2.21	0.60
3:K:162:LYS:HD3	3:K:299:ALA:HB2	1.83	0.60
3:J:39:LYS:HG3	3:J:157:GLU:OE1	1.99	0.60
3:K:62:GLU:CD	3:L:285:VAL:O	2.39	0.60
1:A:197:THR:OG1	1:A:199:GLY:O	2.19	0.60
1:E:219:PHE:CD1	1:E:396:LEU:HD21	2.36	0.60
1:C:214:VAL:HG12	1:C:215:GLY:H	1.65	0.60
1:E:205:LEU:HB3	1:E:390:ALA:HB2	1.81	0.60
3:J:44:VAL:HG12	3:J:158:THR:HG22	1.82	0.60
1:C:374:ARG:N	1:C:375:PRO:HA	2.16	0.60
1:B:239:SER:HB3	1:B:247:LEU:HD13	1.83	0.60
3:J:88:VAL:CG2	3:J:221:LYS:O	2.49	0.60
3:J:155:TYR:CE2	3:J:185:LEU:HD11	2.36	0.60
1:B:210:ALA:HB2	1:B:396:LEU:HB2	1.83	0.60
1:A:363:LEU:HD23	1:A:380:ILE:HG23	1.81	0.60
3:L:61:ILE:HG13	3:L:62:GLU:N	2.16	0.60
3:K:60:TYR:CZ	3:K:65:LYS:CE	2.83	0.60
3:L:69:TYR:CD1	3:L:69:TYR:C	2.74	0.60
3:M:121:TYR:HB2	3:M:195:VAL:HG13	1.83	0.60
3:L:87:LEU:C	3:L:255:GLN:CG	2.48	0.60
1:A:251:MET:O	1:A:251:MET:HG3	2.00	0.60
3:L:239:TRP:HE1	3:L:275:THR:H	1.50	0.60
3:L:41:ASN:CB	3:L:256:GLN:CG	2.76	0.60
3:M:54:LEU:O	3:N:46:ASP:OD2	2.19	0.60
3:J:41:ASN:O	3:J:44:VAL:HG13	2.02	0.60
3:N:67:CYS:HB3	3:N:84:HIS:HD2	1.65	0.60
1:C:104:TYR:HB3	1:C:105:TYR:HB2	1.84	0.60
1:D:125:ILE:HD11	1:D:146:LYS:HB3	1.83	0.60
1:B:184:THR:N	1:B:185:GLY:CA	2.64	0.60
1:E:31:LEU:HA	1:E:34:ALA:HB3	1.82	0.60
3:M:205:LYS:HZ1	3:M:237:THR:N	2.00	0.60
3:M:53:SER:N	3:N:48:LYS:HD3	2.17	0.60
1:F:101:ASN:CG	1:F:102:VAL:H	2.05	0.60
1:C:62:GLY:HA2	1:C:63:GLU:CB	2.32	0.60
3:K:148:VAL:HG22	3:K:181:ILE:HG12	1.84	0.60
1:F:33:PRO:HA	1:F:36:GLU:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ILE:HD13	1:C:89:LEU:HD21	1.82	0.60
3:M:39:LYS:HZ3	3:N:39:LYS:HE2	1.67	0.60
3:L:86:LYS:HD3	3:L:222:THR:O	1.98	0.59
1:F:101:ASN:O	1:F:103:GLU:N	2.35	0.59
1:F:301:ILE:HG22	1:F:305:CYS:SG	2.42	0.59
1:B:238:PHE:HD2	1:B:318:VAL:O	1.84	0.59
1:D:259:ASN:HB3	1:D:435:TYR:HA	1.84	0.59
1:A:32:VAL:HB	1:A:33:PRO:HD3	1.83	0.59
3:J:241:ARG:HH22	3:J:275:THR:HG23	1.67	0.59
3:L:37:PHE:CE2	3:L:45:ILE:HD11	2.36	0.59
3:M:61:ILE:HD11	3:N:44:VAL:O	2.01	0.59
3:N:86:LYS:HD2	3:N:218:ASN:CG	2.23	0.59
3:K:165:TYR:OH	3:K:294:ILE:O	2.16	0.59
1:C:197:THR:CB	1:C:421:ASN:HB3	2.32	0.59
1:D:53:HIS:O	1:D:57:ARG:N	2.32	0.59
3:M:54:LEU:CG	3:N:48:LYS:C	2.70	0.59
3:K:83:TYR:CE1	3:K:98:TYR:CZ	2.91	0.59
1:A:183:ILE:HA	1:A:199:GLY:H	1.67	0.59
1:F:104:TYR:CB	1:F:105:TYR:HB2	2.27	0.59
3:L:174:LYS:HB3	3:L:262:SER:HB2	1.83	0.59
3:J:86:LYS:CE	3:J:223:THR:HA	2.32	0.59
3:K:47:GLN:OE1	3:K:48:LYS:CE	2.50	0.59
1:A:62:GLY:HA2	1:A:63:GLU:CB	2.24	0.59
1:F:105:TYR:HA	1:F:109:VAL:HG23	1.85	0.59
3:M:57:LEU:CB	3:N:46:ASP:HB2	2.31	0.59
3:K:83:TYR:HE2	3:K:175:THR:CG2	2.10	0.59
1:A:18:GLN:HA	1:A:21:LEU:HD12	1.84	0.59
1:C:74:LEU:HD23	1:C:79:GLN:HG3	1.85	0.59
3:J:37:PHE:CE2	3:J:94:ILE:HD13	2.33	0.59
1:D:104:TYR:H	1:D:106:ALA:N	2.01	0.59
2:G:485:ILE:HD11	2:G:549:ILE:HA	1.85	0.59
3:O:271:LYS:HG2	3:O:291:MET:HB3	1.85	0.59
3:M:58:TYR:N	3:N:46:ASP:HB3	2.14	0.59
3:K:226:LEU:HB3	3:K:252:ARG:NH2	2.17	0.59
1:D:295:SER:HA	1:D:324:LEU:HD13	1.84	0.59
1:C:299:SER:HA	1:C:302:ARG:HD2	1.84	0.59
1:A:429:LEU:HD22	1:A:438:PHE:HD2	1.68	0.59
1:F:269:THR:O	1:F:271:GLU:N	2.35	0.59
1:D:271:GLU:CB	3:J:48:LYS:HG2	2.30	0.59
1:F:105:TYR:N	1:F:108:ILE:HB	2.15	0.59
1:F:256:GLY:HA2	1:F:278:MET:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:PHE:CB	1:A:192:GLU:HG2	2.33	0.59
1:B:21:LEU:HB2	1:B:92:LEU:HD13	1.84	0.59
3:L:221:LYS:CE	3:L:248:VAL:HG13	2.32	0.58
3:L:54:LEU:HD23	3:L:57:LEU:HD11	1.84	0.58
3:J:37:PHE:CD1	3:J:87:LEU:HB3	2.36	0.58
1:E:61:ARG:HB2	1:E:62:GLY:HA2	1.85	0.58
3:O:152:LEU:HD21	3:O:185:LEU:HG	1.85	0.58
2:H:525:GLN:H	2:H:526:PRO:HD2	1.68	0.58
3:L:221:LYS:HD3	3:L:248:VAL:CA	2.29	0.58
1:F:439:VAL:HG22	3:M:48:LYS:HE2	1.78	0.58
1:D:76:ALA:O	1:F:133:GLU:CB	2.48	0.58
1:B:419:GLN:HG2	1:B:424:VAL:HG13	1.84	0.58
3:M:199:GLU:HA	3:M:202:ARG:HB2	1.85	0.58
1:D:258:ILE:O	1:D:263:LEU:HB2	2.02	0.58
1:E:103:GLU:HB2	1:E:104:TYR:HA	1.83	0.58
3:K:169:LYS:HG2	3:K:170:PHE:HD2	1.64	0.58
1:F:325:ILE:CG2	1:F:342:ILE:HG21	2.32	0.58
1:B:298:VAL:HG21	1:B:342:ILE:HG23	1.83	0.58
2:H:542:GLU:HA	2:H:545:LEU:HD13	1.85	0.58
3:O:188:LYS:O	3:O:190:TYR:N	2.36	0.58
2:H:569:THR:HA	2:H:572:GLU:HB2	1.85	0.58
3:M:47:GLN:HB3	3:N:51:GLU:CD	2.23	0.58
1:E:363:LEU:HD23	1:E:380:ILE:HG23	1.86	0.58
3:L:86:LYS:CD	3:L:255:GLN:HE21	2.03	0.58
3:L:86:LYS:CE	3:L:257:LEU:HD23	2.27	0.58
3:K:83:TYR:HE1	3:K:98:TYR:CZ	2.22	0.58
1:D:220:ALA:HB2	1:D:360:LEU:HD11	1.85	0.58
1:F:314:LEU:CD2	1:F:353:LEU:HB3	2.33	0.58
3:N:285:VAL:HG12	3:N:285:VAL:O	2.03	0.58
3:M:182:ALA:HA	3:M:192:SER:OG	2.04	0.58
1:F:103:GLU:O	1:F:106:ALA:HB3	2.03	0.58
1:F:322:LEU:HD21	1:F:343:SER:HB2	1.86	0.58
3:N:185:LEU:HD13	3:N:225:VAL:HG11	1.85	0.58
3:J:126:LEU:HB3	3:J:176:PHE:HZ	1.68	0.58
3:M:48:LYS:O	3:M:51:GLU:N	2.37	0.58
1:A:58:VAL:HG13	1:A:62:GLY:O	2.04	0.58
1:C:184:THR:OG1	1:C:185:GLY:HA3	2.03	0.58
3:L:32:GLN:N	3:L:61:ILE:HG22	2.18	0.58
1:A:69:THR:HG23	1:A:70:VAL:HG23	1.86	0.58
3:L:88:VAL:O	3:L:88:VAL:CG1	2.52	0.57
3:N:37:PHE:CZ	3:N:57:LEU:HD21	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:487:GLY:CA	2:I:488:ARG:CB	2.82	0.57
1:B:132:ARG:O	1:B:133:GLU:CB	2.50	0.57
3:O:193:MET:HB2	3:O:226:LEU:HD23	1.85	0.57
1:C:31:LEU:HA	1:C:34:ALA:HB3	1.86	0.57
3:J:44:VAL:HG12	3:J:158:THR:HG21	1.83	0.57
3:J:37:PHE:CE2	3:J:45:ILE:CD1	2.87	0.57
3:J:86:LYS:NZ	3:J:223:THR:HA	2.18	0.57
3:J:33:ASP:OD2	3:J:61:ILE:HA	2.03	0.57
3:J:271:LYS:HE3	3:J:291:MET:HG3	1.86	0.57
1:A:240:LEU:HB2	1:A:320:ASP:HB2	1.86	0.57
3:M:231:ILE:O	3:M:270:LEU:HD21	2.05	0.57
3:L:221:LYS:HZ1	3:L:248:VAL:CG2	2.05	0.57
3:J:38:LEU:HD13	3:J:50:ILE:HD11	1.80	0.57
3:N:207:SER:C	3:N:213:LEU:HD12	2.24	0.57
3:J:165:TYR:HD2	3:J:298:ALA:HB3	1.67	0.57
3:K:197:VAL:HG13	3:K:245:ILE:HD13	1.87	0.57
3:N:165:TYR:HD1	3:N:261:PHE:HB2	1.69	0.57
3:L:271:LYS:HA	3:L:291:MET:HG3	1.87	0.57
1:B:238:PHE:HE2	1:B:317:ILE:CG2	2.17	0.57
1:B:261:GLN:H	1:B:262:ASN:HA	1.67	0.57
3:N:41:ASN:ND2	3:N:45:ILE:CG1	2.66	0.57
3:J:89:VAL:HG22	3:J:255:GLN:NE2	2.19	0.57
1:E:215:GLY:O	1:E:219:PHE:HB2	2.04	0.57
2:H:472:MSE:SE	2:H:532:SER:HB3	2.54	0.57
3:O:184:GLU:O	3:O:187:GLU:HB2	2.04	0.57
1:A:432:ILE:HD12	1:A:437:LYS:HE3	1.86	0.57
1:D:439:VAL:HB	3:O:92:ARG:HH22	1.68	0.57
1:A:227:VAL:HB	1:A:316:MET:HE1	1.87	0.57
1:A:103:GLU:HB2	1:A:104:TYR:HA	1.87	0.57
3:K:226:LEU:HB3	3:K:252:ARG:NH1	2.18	0.57
1:E:235:VAL:HG12	1:E:316:MET:HB2	1.87	0.57
2:I:466:LEU:HD13	2:I:548:TYR:CE1	2.39	0.57
3:N:178:LEU:HD22	3:N:260:PHE:HB3	1.85	0.57
3:K:49:MET:HG2	3:K:50:ILE:N	2.20	0.57
1:F:326:GLN:HA	1:F:342:ILE:HD11	1.86	0.57
1:D:110:GLU:O	1:D:114:VAL:HG23	2.05	0.57
3:L:88:VAL:HG21	3:L:251:HIS:O	2.04	0.57
3:M:54:LEU:CD1	3:N:48:LYS:C	2.71	0.57
2:I:558:TRP:O	2:I:561:LEU:HG	2.05	0.57
3:M:221:LYS:HE2	3:M:248:VAL:HG22	1.86	0.57
1:D:122:ALA:O	1:D:126:ALA:N	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:231:ILE:HD13	3:O:294:ILE:HD13	1.87	0.57
3:L:89:VAL:HG12	3:L:254:SER:HB3	1.83	0.57
3:L:41:ASN:OD1	3:L:256:GLN:NE2	2.34	0.57
3:M:54:LEU:N	3:N:48:LYS:CD	2.68	0.57
1:C:432:ILE:CG2	3:N:70:CYS:O	2.46	0.57
3:J:167:TYR:CD2	3:J:266:SER:HA	2.40	0.57
1:B:261:GLN:HG2	1:B:269:THR:OG1	2.03	0.57
2:H:566:GLN:HA	2:H:569:THR:HG22	1.87	0.57
3:L:40:GLU:OE1	3:L:160:LYS:C	2.43	0.57
1:C:104:TYR:CA	1:C:105:TYR:HB2	2.35	0.57
1:D:128:ASP:HB3	1:D:139:LEU:HD11	1.86	0.57
2:G:569:THR:HA	2:G:572:GLU:HB2	1.86	0.57
1:F:304:LYS:O	1:F:308:LEU:HB2	2.05	0.57
3:M:35:GLN:OE1	3:N:47:GLN:NE2	2.38	0.56
1:E:316:MET:SD	1:E:356:PRO:HG2	2.45	0.56
2:I:556:PRO:O	2:I:559:LEU:HB3	2.05	0.56
3:L:36:ALA:CA	3:L:158:THR:HA	2.36	0.56
3:K:164:LEU:N	3:K:298:ALA:HB1	2.20	0.56
1:B:196:MET:HB3	1:B:425:GLY:HA3	1.86	0.56
3:J:157:GLU:O	3:J:257:LEU:CG	2.53	0.56
1:A:219:PHE:O	1:A:223:ILE:HG13	2.04	0.56
1:C:75:ALA:HB2	2:H:578:LEU:HD11	1.86	0.56
2:I:528:ALA:HA	2:I:531:LEU:HB2	1.87	0.56
1:B:381:ARG:HH21	1:B:385:SER:HA	1.70	0.56
3:J:41:ASN:HB3	3:J:44:VAL:HG11	1.86	0.56
1:A:210:ALA:HB2	1:A:396:LEU:HD13	1.86	0.56
1:F:209:ALA:HB3	1:F:395:PHE:CE2	2.40	0.56
3:K:213:LEU:O	3:K:217:LEU:HG	2.06	0.56
2:I:471:MSE:HE3	2:I:478:ALA:HB1	1.87	0.56
3:J:239:TRP:CG	3:J:240:VAL:N	2.74	0.56
2:G:588:ILE:HG22	2:G:592:LYS:HE3	1.88	0.56
3:M:45:ILE:O	3:M:46:ASP:HB3	2.06	0.56
3:N:43:GLU:CD	3:N:256:GLN:HG3	2.26	0.56
1:D:125:ILE:HD11	1:D:146:LYS:HB2	1.88	0.56
1:D:258:ILE:HB	1:D:263:LEU:HD22	1.88	0.56
3:J:43:GLU:HB3	3:J:255:GLN:O	2.06	0.56
1:A:374:ARG:N	1:A:375:PRO:HA	2.21	0.56
2:H:525:GLN:N	2:H:526:PRO:HD2	2.21	0.56
3:L:241:ARG:O	3:L:246:GLY:N	2.39	0.56
3:K:166:LEU:HD12	3:K:178:LEU:HG	1.86	0.56
3:L:221:LYS:CD	3:L:248:VAL:CG1	2.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:33:ASP:CB	3:J:60:TYR:CD2	2.85	0.56
1:B:414:ILE:HG22	1:B:427:VAL:HB	1.87	0.56
1:C:127:GLN:HE21	1:C:131:THR:HG23	1.69	0.56
1:A:227:VAL:HG13	1:A:231:THR:OG1	2.06	0.56
1:B:104:TYR:CB	1:B:105:TYR:HB2	2.36	0.56
3:L:86:LYS:HD3	3:L:257:LEU:CD2	2.24	0.56
3:J:37:PHE:HB3	3:J:87:LEU:CD1	2.30	0.56
1:C:24:VAL:HA	1:C:30:ALA:CB	2.36	0.56
1:F:104:TYR:CD1	1:F:105:TYR:HB2	2.41	0.56
3:L:228:LEU:HD12	3:L:261:PHE:CZ	2.41	0.56
1:E:39:ILE:HB	1:E:40:PRO:CD	2.36	0.56
3:N:41:ASN:OD1	3:N:44:VAL:CB	2.53	0.56
3:N:41:ASN:HD22	3:N:45:ILE:CG1	2.19	0.56
3:J:239:TRP:HE1	3:J:241:ARG:HG3	1.71	0.56
1:A:320:ASP:HA	1:A:360:LEU:HD12	1.86	0.56
3:M:241:ARG:NH2	3:M:274:PHE:O	2.39	0.56
3:O:178:LEU:HD11	3:O:262:SER:HB3	1.88	0.56
1:F:293:THR:HG23	1:F:294:PRO:HD2	1.88	0.55
1:A:211:ARG:HB3	1:A:212:PRO:HD2	1.87	0.55
3:M:139:PRO:HB3	3:N:284:GLU:HG2	1.87	0.55
3:M:51:GLU:O	3:N:52:LYS:NZ	2.39	0.55
1:C:416:ILE:HG22	1:C:419:GLN:HB3	1.87	0.55
1:C:63:GLU:H	1:C:64:PRO:CA	2.19	0.55
3:M:261:PHE:CZ	3:M:294:ILE:HG12	2.41	0.55
1:D:63:GLU:H	1:D:64:PRO:HA	1.72	0.55
3:N:69:TYR:HB2	3:N:82:GLY:HA2	1.87	0.55
3:K:62:GLU:HG2	3:L:285:VAL:HG13	1.87	0.55
1:D:252:LEU:CD2	1:D:280:MET:HG3	2.36	0.55
1:B:259:ASN:HA	1:B:263:LEU:HB2	1.87	0.55
1:F:111:GLU:HA	1:F:114:VAL:HB	1.87	0.55
1:D:221:LEU:O	1:D:225:GLN:N	2.36	0.55
1:D:277:THR:HG23	1:D:278:MET:HG2	1.88	0.55
3:L:63:GLN:C	3:L:63:GLN:CD	2.65	0.55
3:J:87:LEU:C	3:J:222:THR:OG1	2.44	0.55
3:K:62:GLU:OE1	3:L:285:VAL:C	2.44	0.55
1:D:276:LEU:HA	1:D:279:ALA:HB3	1.87	0.55
1:D:220:ALA:CB	1:D:360:LEU:HD11	2.36	0.55
1:C:63:GLU:H	1:C:64:PRO:HA	1.71	0.55
3:O:120:MET:HB2	3:O:195:VAL:HA	1.89	0.55
1:A:348:ALA:HB1	1:B:29:ALA:O	2.07	0.55
1:F:252:LEU:HD22	1:F:280:MET:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:HD21	1:A:59:ALA:HB2	1.87	0.55
1:C:276:LEU:O	1:C:278:MET:N	2.38	0.55
3:N:46:ASP:OD1	3:N:49:MET:SD	2.65	0.55
3:K:165:TYR:CE1	3:K:294:ILE:HG23	2.42	0.55
2:I:485:ILE:HG23	2:I:553:LEU:HD21	1.88	0.55
1:F:260:ALA:O	3:N:32:GLN:CB	2.53	0.55
1:C:267:LYS:HA	1:C:273:TRP:HZ2	1.71	0.55
1:C:122:ALA:HA	1:C:125:ILE:HD12	1.88	0.55
3:L:242:ASP:HA	3:L:246:GLY:HA3	1.87	0.55
3:L:53:SER:OG	3:L:94:ILE:CG1	2.53	0.55
3:L:86:LYS:NZ	3:L:257:LEU:CD2	2.70	0.55
1:A:61:ARG:HB2	1:A:62:GLY:HA3	1.88	0.55
3:L:56:LYS:CE	3:L:96:ILE:HD12	2.35	0.55
3:M:58:TYR:CA	3:N:46:ASP:OD2	2.49	0.55
1:D:271:GLU:HG3	3:J:48:LYS:CG	2.36	0.55
1:A:104:TYR:HB3	1:A:105:TYR:CG	2.41	0.55
1:A:90:SER:HB3	2:G:568:LYS:CE	2.35	0.55
1:E:86:VAL:CG2	2:I:572:GLU:HG3	2.37	0.55
1:C:86:VAL:HA	1:C:89:LEU:HB2	1.88	0.55
3:N:201:VAL:HG12	3:N:205:LYS:HE3	1.89	0.55
3:L:193:MET:O	3:L:227:MET:HG3	2.07	0.55
3:L:36:ALA:HB1	3:L:157:GLU:C	2.16	0.55
3:L:138:ASP:C	3:L:140:SER:N	2.59	0.55
1:A:125:ILE:HG12	1:A:143:ALA:HB1	1.89	0.55
3:M:233:ALA:HB2	3:M:265:PHE:HE2	1.70	0.55
3:J:39:LYS:C	3:J:157:GLU:HB3	2.22	0.54
3:J:99:TYR:HB3	3:J:219:MET:HE3	1.82	0.54
3:N:67:CYS:SG	3:N:70:CYS:SG	3.03	0.54
1:F:61:ARG:HB3	1:F:62:GLY:HA3	1.89	0.54
1:F:39:ILE:HB	1:F:40:PRO:CD	2.37	0.54
3:J:194:ILE:HA	3:J:227:MET:HG2	1.88	0.54
3:J:37:PHE:CE1	3:J:87:LEU:HB3	2.42	0.54
1:B:104:TYR:N	1:B:105:TYR:HB2	2.23	0.54
3:M:57:LEU:HD13	3:N:48:LYS:HD2	1.87	0.54
3:M:165:TYR:CD1	3:M:167:TYR:CE2	2.94	0.54
3:J:138:ASP:C	3:J:140:SER:H	2.10	0.54
2:H:565:GLU:HA	2:H:587:MSE:SE	2.58	0.54
3:J:131:PHE:H	3:J:184:GLU:HG3	1.71	0.54
3:L:252:ARG:NH1	3:L:258:PRO:O	2.40	0.54
3:J:100:GLU:O	3:J:118:LYS:NZ	2.35	0.54
3:K:104:LYS:HD2	3:K:125:ASP:CA	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ALA:H	1:A:216:LYS:HD3	1.71	0.54
1:F:323:GLN:HG3	1:F:362:GLN:H	1.72	0.54
3:L:221:LYS:O	3:L:252:ARG:NH2	2.40	0.54
1:A:56:LEU:HA	1:A:59:ALA:HB3	1.89	0.54
1:B:76:ALA:HB1	1:D:133:GLU:O	2.08	0.54
1:E:23:ALA:C	1:E:25:PHE:H	2.11	0.54
2:G:525:GLN:N	2:G:526:PRO:HD2	2.22	0.54
3:L:240:VAL:HG12	3:L:244:VAL:HG23	1.89	0.54
3:L:38:LEU:CG	3:L:50:ILE:CD1	2.82	0.54
1:E:45:ARG:HB2	1:E:48:HIS:HD2	1.73	0.54
3:O:208:LEU:HA	3:O:212:THR:HG21	1.89	0.54
1:A:277:THR:HA	1:A:280:MET:HB2	1.89	0.54
1:E:395:PHE:O	1:E:414:ILE:HA	2.08	0.54
1:E:38:LEU:HD11	1:E:110:GLU:HB2	1.88	0.54
1:C:101:ASN:O	1:C:102:VAL:HB	2.07	0.54
1:A:187:PRO:O	1:A:200:PHE:CE2	2.61	0.54
1:E:111:GLU:HA	1:E:114:VAL:HB	1.90	0.54
3:L:270:LEU:HD23	3:L:273:HIS:HD2	1.72	0.54
1:A:129:GLY:HA2	1:A:139:LEU:HD11	1.90	0.54
3:L:226:LEU:HB2	3:L:252:ARG:NH1	2.23	0.54
3:L:97:GLU:HB3	3:L:222:THR:OG1	2.08	0.54
3:N:86:LYS:HG2	3:N:218:ASN:ND2	2.22	0.54
3:L:66:ASN:CB	3:L:84:HIS:HE1	2.09	0.54
1:F:434:GLU:OE1	3:N:54:LEU:HD21	2.05	0.54
3:J:112:LYS:HB3	3:J:116:LEU:HD11	1.89	0.54
1:C:381:ARG:HD2	1:C:387:GLU:CB	2.36	0.54
1:B:193:LEU:HD22	1:B:429:LEU:HD11	1.90	0.54
1:B:259:ASN:HD22	1:B:263:LEU:HB3	1.71	0.54
3:O:122:ILE:HG12	3:O:196:TYR:CD1	2.43	0.54
1:B:183:ILE:CG2	1:B:185:GLY:HA3	2.37	0.54
3:N:165:TYR:HB3	3:N:167:TYR:CE2	2.43	0.54
1:E:432:ILE:O	1:E:433:LYS:HB2	2.06	0.54
3:L:100:GLU:HG3	3:L:193:MET:HE1	1.90	0.53
3:J:252:ARG:HG2	3:J:255:GLN:HB2	1.90	0.53
3:J:39:LYS:O	3:J:157:GLU:CG	2.54	0.53
3:N:97:GLU:OE1	3:N:215:GLU:OE2	2.27	0.53
3:J:174:LYS:HB3	3:J:263:SER:O	2.08	0.53
1:D:322:LEU:H	1:D:361:SER:HA	1.73	0.53
3:L:148:VAL:HG22	3:L:181:ILE:HG12	1.91	0.53
1:A:184:THR:N	1:A:185:GLY:CA	2.67	0.53
1:E:208:VAL:HG22	1:E:394:ALA:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:PHE:HA	1:D:55:MET:SD	2.48	0.53
1:C:358:ILE:CG2	1:C:360:LEU:HD21	2.38	0.53
1:F:301:ILE:O	1:F:305:CYS:HB2	2.08	0.53
1:F:314:LEU:HD21	1:F:353:LEU:HB3	1.89	0.53
3:N:197:VAL:HB	3:N:231:ILE:HG12	1.90	0.53
1:E:388:GLN:HE21	1:E:388:GLN:N	2.06	0.53
1:A:143:ALA:CB	1:A:146:LYS:HE3	2.38	0.53
1:E:187:PRO:HG2	1:E:227:VAL:HG22	1.90	0.53
3:L:33:ASP:HB2	3:L:60:TYR:CG	2.39	0.53
1:F:104:TYR:HB3	1:F:105:TYR:HB3	1.89	0.53
1:B:238:PHE:HE2	1:B:317:ILE:HG23	1.73	0.53
1:E:132:ARG:O	1:E:139:LEU:HD12	2.08	0.53
3:L:86:LYS:CG	3:L:99:TYR:CD1	2.91	0.53
3:M:35:GLN:NE2	3:N:42:GLU:O	2.42	0.53
3:M:47:GLN:HB3	3:N:51:GLU:HG3	1.90	0.53
3:J:39:LYS:CG	3:J:157:GLU:CD	2.68	0.53
1:A:193:LEU:O	1:A:197:THR:OG1	2.20	0.53
1:A:200:PHE:CZ	1:A:227:VAL:HG11	2.43	0.53
3:L:122:ILE:HG22	3:M:254:SER:HB2	1.90	0.53
3:L:148:VAL:CG2	3:L:181:ILE:HG12	2.39	0.53
3:J:201:VAL:HG12	3:J:205:LYS:HG3	1.90	0.53
1:E:224:ALA:C	1:E:226:ASN:H	2.12	0.53
1:A:52:PHE:HA	1:A:55:MET:HB3	1.90	0.53
3:L:41:ASN:OD1	3:L:44:VAL:CB	2.56	0.53
3:M:58:TYR:CG	3:N:46:ASP:OD1	2.60	0.53
1:A:183:ILE:HA	1:A:199:GLY:N	2.23	0.53
1:F:78:GLU:C	1:F:80:LEU:H	2.11	0.53
3:L:202:ARG:HD2	3:M:293:ARG:HE	1.72	0.53
1:D:242:MET:HG3	1:D:247:LEU:HD12	1.90	0.53
1:E:101:ASN:HB3	1:E:104:TYR:CD1	2.44	0.53
1:F:102:VAL:O	1:F:103:GLU:C	2.47	0.53
1:D:146:LYS:O	1:D:147:ILE:HG12	2.08	0.53
2:I:587:MSE:HA	2:I:590:MSE:HE3	1.90	0.53
1:F:104:TYR:HD1	1:F:105:TYR:HB2	1.73	0.53
1:D:276:LEU:HD12	1:D:279:ALA:HB3	1.89	0.53
3:N:138:ASP:HB3	3:N:139:PRO:CD	2.34	0.53
1:C:321:TYR:CE1	1:C:324:LEU:HB2	2.44	0.53
3:O:144:MET:HB3	3:O:177:MET:HE2	1.91	0.53
2:I:565:GLU:HA	2:I:568:LYS:HB3	1.90	0.53
3:L:164:LEU:HA	3:L:299:ALA:H	1.73	0.53
1:B:86:VAL:HA	1:B:89:LEU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:245:ILE:HG22	3:M:245:ILE:O	2.07	0.53
3:L:41:ASN:CG	3:L:256:GLN:HE21	2.11	0.53
3:M:50:ILE:CG2	3:N:47:GLN:O	2.57	0.53
3:J:37:PHE:CG	3:J:87:LEU:CB	2.92	0.53
3:K:252:ARG:HD3	3:K:259:THR:HG21	1.91	0.53
1:F:261:GLN:HG2	1:F:272:ASP:HB2	1.89	0.53
1:F:50:LYS:HB3	1:F:79:GLN:HE22	1.72	0.53
2:H:578:LEU:HA	2:H:581:ALA:HB3	1.91	0.53
3:O:148:VAL:HG22	3:O:181:ILE:HG12	1.90	0.53
3:L:34:VAL:CG2	3:L:57:LEU:CB	2.86	0.53
3:J:99:TYR:HB3	3:J:219:MET:HE2	1.79	0.53
3:L:66:ASN:HB3	3:L:84:HIS:HE1	1.63	0.53
2:H:519:ARG:H	2:H:520:ILE:HB	1.70	0.53
1:A:38:LEU:HD21	1:A:110:GLU:HB2	1.91	0.53
1:A:267:LYS:HG3	1:A:268:LEU:N	2.23	0.53
3:L:56:LYS:HD2	3:L:96:ILE:CB	2.30	0.53
2:H:549:ILE:O	2:H:553:LEU:HG	2.09	0.53
1:B:40:PRO:HA	1:B:52:PHE:CE2	2.44	0.53
1:B:277:THR:C	1:B:279:ALA:H	2.11	0.53
3:M:46:ASP:CG	3:M:47:GLN:H	2.11	0.52
1:A:210:ALA:HA	1:A:396:LEU:HB2	1.89	0.52
1:E:199:GLY:HA2	1:E:200:PHE:HB2	1.91	0.52
1:E:128:ASP:HA	1:E:131:THR:OG1	2.08	0.52
3:O:297:LEU:O	3:O:298:ALA:HB2	2.09	0.52
3:O:271:LYS:HG2	3:O:291:MET:CB	2.39	0.52
3:J:39:LYS:O	3:J:157:GLU:HB3	1.87	0.52
3:N:37:PHE:HZ	3:N:87:LEU:HD13	1.70	0.52
1:C:317:ILE:HG22	1:C:319:ILE:HG12	1.91	0.52
2:G:487:GLY:CA	2:G:488:ARG:HB2	2.39	0.52
2:G:519:ARG:N	2:G:520:ILE:HB	2.23	0.52
1:F:186:ILE:HD13	1:F:315:GLY:HA2	1.90	0.52
1:C:38:LEU:HD21	1:C:109:VAL:HB	1.90	0.52
3:L:36:ALA:C	3:L:158:THR:HA	2.28	0.52
3:L:89:VAL:HB	3:L:254:SER:C	2.29	0.52
3:M:51:GLU:CG	3:N:51:GLU:C	2.72	0.52
2:H:487:GLY:CA	2:H:488:ARG:CB	2.73	0.52
1:B:238:PHE:HB2	1:B:319:ILE:HA	1.90	0.52
3:O:138:ASP:C	3:O:140:SER:H	2.13	0.52
1:C:183:ILE:HG12	1:C:194:ASP:HB3	1.92	0.52
1:F:322:LEU:HB2	1:F:360:LEU:O	2.10	0.52
1:E:29:ALA:HA	1:E:65:VAL:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:ALA:HB1	1:C:83:ILE:HG23	1.91	0.52
3:J:173:GLY:HA3	3:J:303:LEU:HD13	1.91	0.52
3:J:37:PHE:CZ	3:J:94:ILE:CG2	2.92	0.52
1:E:104:TYR:CA	1:E:105:TYR:CB	2.88	0.52
3:K:47:GLN:CD	3:K:48:LYS:CD	2.78	0.52
1:A:103:GLU:CB	1:A:104:TYR:HA	2.40	0.52
3:M:39:LYS:NZ	3:N:39:LYS:HE2	2.24	0.52
2:H:469:ALA:HA	2:H:472:MSE:HB2	1.91	0.52
1:F:342:ILE:HD12	1:F:342:ILE:H	1.74	0.52
3:K:83:TYR:CG	3:K:98:TYR:HB3	2.45	0.52
1:D:431:PHE:HB3	1:D:433:LYS:CG	2.38	0.52
1:C:259:ASN:HB3	1:C:435:TYR:HA	1.92	0.52
1:A:114:VAL:HG22	1:A:117:ARG:CZ	2.39	0.52
3:O:241:ARG:HA	3:O:245:ILE:HD12	1.90	0.52
3:N:294:ILE:HG22	3:N:294:ILE:O	2.09	0.52
1:E:23:ALA:HB2	1:E:96:VAL:HG11	1.90	0.52
3:L:164:LEU:H	3:L:260:PHE:HA	1.74	0.52
1:C:143:ALA:HA	1:C:146:LYS:HE3	1.91	0.52
3:N:43:GLU:OE1	3:N:256:GLN:HG3	2.09	0.52
3:J:37:PHE:CE1	3:J:87:LEU:CB	2.93	0.52
3:K:47:GLN:CD	3:K:48:LYS:HZ1	2.13	0.52
1:A:102:VAL:C	1:A:104:TYR:HB2	2.30	0.52
1:B:104:TYR:CA	1:B:105:TYR:HB2	2.40	0.52
2:G:571:ALA:CA	2:G:574:ARG:HE	2.21	0.52
3:J:119:SER:HA	3:J:194:ILE:H	1.74	0.52
1:A:132:ARG:HB3	1:A:135:GLU:HB2	1.91	0.52
1:E:204:ASP:HB3	1:E:206:ILE:HG13	1.91	0.52
3:L:41:ASN:OD1	3:L:44:VAL:HG21	2.08	0.52
3:J:40:GLU:HG2	3:J:224:PRO:HG3	1.92	0.52
1:C:252:LEU:HD21	1:C:280:MET:SD	2.50	0.52
2:I:569:THR:O	2:I:572:GLU:HB3	2.09	0.52
1:C:196:MET:O	1:C:423:PRO:HG2	2.10	0.52
3:N:33:ASP:OD1	3:N:61:ILE:HG21	2.09	0.52
3:J:147:HIS:HD1	3:J:151:PHE:HE2	1.58	0.52
2:G:492:GLU:HA	2:G:495:ARG:HD2	1.90	0.52
3:L:86:LYS:HD3	3:L:255:GLN:NE2	2.24	0.52
3:N:44:VAL:HG12	3:N:89:VAL:HG11	1.91	0.52
3:N:66:ASN:OD1	3:N:84:HIS:CE1	2.63	0.52
3:K:49:MET:O	3:K:50:ILE:C	2.47	0.52
3:N:41:ASN:CG	3:N:255:GLN:HG2	2.30	0.51
3:J:99:TYR:CB	3:J:219:MET:HE1	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:33:ASP:CG	3:J:61:ILE:HG22	2.30	0.51
1:C:104:TYR:H	1:C:105:TYR:HB3	1.75	0.51
2:G:461:GLN:HB3	2:G:465:ARG:HH21	1.75	0.51
3:L:222:THR:HA	3:L:257:LEU:HD13	1.92	0.51
3:L:86:LYS:HG2	3:L:99:TYR:CD1	2.44	0.51
3:N:46:ASP:O	3:N:47:GLN:C	2.48	0.51
1:F:208:VAL:HB	1:F:360:LEU:HG	1.92	0.51
1:D:220:ALA:HB2	1:D:360:LEU:HD21	1.92	0.51
1:A:192:GLU:OE2	1:A:427:VAL:HG12	2.10	0.51
3:K:152:LEU:HD13	3:K:184:GLU:HB3	1.90	0.51
1:C:72:ALA:HA	2:H:578:LEU:HD13	1.90	0.51
1:F:26:LEU:HD22	1:F:99:ALA:HB3	1.91	0.51
3:J:44:VAL:CB	3:J:255:GLN:CG	2.77	0.51
3:K:65:LYS:CG	3:K:66:ASN:H	2.20	0.51
3:J:165:TYR:CD2	3:J:298:ALA:HB3	2.46	0.51
3:K:148:VAL:O	3:K:152:LEU:HG	2.09	0.51
1:F:342:ILE:N	1:F:342:ILE:HD12	2.25	0.51
2:G:497:LEU:O	2:G:501:ILE:HG13	2.11	0.51
3:J:39:LYS:CG	3:J:157:GLU:OE2	2.54	0.51
3:J:44:VAL:CB	3:J:255:GLN:HB3	2.30	0.51
1:D:270:PRO:HD2	3:J:51:GLU:HB2	1.93	0.51
3:K:252:ARG:HG2	3:K:257:LEU:HD12	1.91	0.51
3:J:167:TYR:HE1	3:J:263:SER:HG	1.58	0.51
1:B:122:ALA:HA	1:B:125:ILE:HD12	1.93	0.51
3:J:156:ASN:CB	3:J:159:GLY:O	2.59	0.51
3:M:267:PRO:C	3:M:269:GLU:H	2.13	0.51
3:L:202:ARG:CD	3:M:293:ARG:HE	2.23	0.51
3:L:39:LYS:HD3	3:L:158:THR:HB	1.92	0.51
1:A:188:THR:OG1	1:A:194:ASP:HA	2.11	0.51
1:A:25:PHE:C	1:A:28:PRO:HB3	2.31	0.51
2:G:575:LYS:HA	2:G:577:PHE:CZ	2.46	0.51
3:L:45:ILE:HG23	3:L:49:MET:HB3	1.92	0.51
3:J:97:GLU:HB2	3:J:219:MET:SD	2.51	0.51
1:B:51:ILE:O	1:B:55:MET:N	2.41	0.51
1:A:322:LEU:HB2	1:A:361:SER:HA	1.92	0.51
1:C:322:LEU:HD12	1:C:359:ALA:HB1	1.93	0.51
1:A:204:ASP:O	1:A:357:VAL:N	2.40	0.51
1:D:395:PHE:CD2	1:D:397:TYR:HB2	2.46	0.51
1:C:321:TYR:O	1:C:323:GLN:N	2.42	0.51
1:C:211:ARG:O	1:C:214:VAL:HG23	2.11	0.51
1:E:28:PRO:C	1:E:30:ALA:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:290:LEU:O	3:L:294:ILE:N	2.44	0.51
3:O:197:VAL:HB	3:O:198:PRO:HD3	1.93	0.51
1:C:16:ALA:HB2	1:C:108:ILE:HB	1.92	0.51
3:L:86:LYS:HG2	3:L:255:GLN:HE22	1.69	0.51
3:N:41:ASN:CG	3:N:44:VAL:HB	2.31	0.51
1:D:271:GLU:HG3	3:J:48:LYS:CD	2.35	0.51
1:C:434:GLU:CA	3:N:68:SER:O	2.59	0.51
3:L:172:VAL:CG2	3:L:304:ASP:HA	2.33	0.51
1:C:197:THR:HB	1:C:421:ASN:HB3	1.92	0.51
1:A:211:ARG:HB2	1:A:214:VAL:HB	1.92	0.51
2:G:468:LEU:HD23	2:G:501:ILE:HD12	1.92	0.51
3:L:36:ALA:O	3:L:158:THR:O	2.28	0.51
3:L:56:LYS:CD	3:L:96:ILE:HD11	2.09	0.51
1:C:117:ARG:HB3	1:C:149:GLU:C	2.31	0.51
1:A:272:ASP:C	1:A:274:GLY:H	2.14	0.51
3:M:94:ILE:HB	3:N:48:LYS:HZ3	1.76	0.51
3:N:45:ILE:HG21	3:N:50:ILE:HD11	1.41	0.51
3:L:66:ASN:HB3	3:L:84:HIS:ND1	2.23	0.51
1:C:259:ASN:ND2	1:C:262:ASN:OD1	2.44	0.51
3:M:57:LEU:HD11	3:N:48:LYS:CE	2.22	0.50
3:L:196:TYR:HB3	3:L:199:GLU:HB2	1.93	0.50
1:E:17:GLU:HA	1:E:20:VAL:HB	1.93	0.50
3:L:58:TYR:O	3:L:61:ILE:CG1	2.59	0.50
3:K:82:GLY:C	3:K:126:LEU:CB	2.80	0.50
1:D:322:LEU:C	1:D:324:LEU:H	2.12	0.50
1:B:216:LYS:CG	1:B:217:THR:N	2.72	0.50
3:K:197:VAL:HG11	3:K:231:ILE:HG12	1.92	0.50
2:G:585:LYS:O	2:G:585:LYS:HD3	2.11	0.50
3:L:34:VAL:HG22	3:L:38:LEU:HD23	1.91	0.50
3:L:36:ALA:O	3:L:39:LYS:HG3	2.10	0.50
3:L:33:ASP:C	3:L:60:TYR:CE2	2.85	0.50
1:D:276:LEU:CG	1:D:280:MET:HB2	2.34	0.50
3:J:155:TYR:CD2	3:J:185:LEU:HD11	2.46	0.50
1:C:317:ILE:HD12	1:C:357:VAL:HG22	1.91	0.50
1:D:45:ARG:HB2	1:D:48:HIS:HB2	1.94	0.50
1:A:237:ILE:HB	1:A:290:ILE:HG12	1.93	0.50
3:N:193:MET:CE	3:N:219:MET:HB3	2.41	0.50
3:L:100:GLU:CG	3:L:193:MET:HE1	2.40	0.50
3:L:83:TYR:CB	3:L:219:MET:HE3	2.17	0.50
3:L:54:LEU:O	3:L:57:LEU:HG	2.10	0.50
1:C:353:LEU:HB3	1:C:355:VAL:HG23	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:489:PHE:CB	2:H:495:ARG:HG2	2.41	0.50
1:C:86:VAL:HG12	1:C:89:LEU:HD12	1.92	0.50
1:F:381:ARG:C	1:F:383:SER:H	2.15	0.50
1:E:340:SER:HA	1:E:343:SER:HB3	1.94	0.50
3:L:56:LYS:CB	3:L:96:ILE:HD11	2.41	0.50
3:M:51:GLU:HG2	3:N:52:LYS:N	2.26	0.50
3:M:54:LEU:HD11	3:N:49:MET:C	2.30	0.50
3:J:46:ASP:OD2	3:J:48:LYS:HG3	2.10	0.50
1:E:109:VAL:O	1:E:113:SER:N	2.44	0.50
1:B:70:VAL:C	1:B:72:ALA:H	2.13	0.50
3:O:292:GLU:C	3:O:294:ILE:H	2.13	0.50
1:A:67:LEU:HD12	2:G:581:ALA:HB1	1.92	0.50
3:L:226:LEU:HD11	3:L:248:VAL:CG1	2.39	0.50
3:J:86:LYS:HE2	3:J:222:THR:O	2.07	0.50
3:J:239:TRP:NE1	3:J:241:ARG:HG3	2.26	0.50
3:L:83:TYR:CD2	3:L:219:MET:HG3	2.46	0.50
3:L:221:LYS:HE2	3:L:248:VAL:CG1	2.42	0.50
1:D:73:GLU:O	1:D:77:SER:N	2.43	0.50
1:F:103:GLU:CB	1:F:104:TYR:HA	2.37	0.50
1:D:184:THR:N	1:D:185:GLY:HA3	2.19	0.50
3:M:122:ILE:HG22	3:M:196:TYR:CD2	2.47	0.50
2:H:456:LEU:O	2:H:458:PRO:HD3	2.12	0.50
1:A:20:VAL:CG2	1:A:105:TYR:O	2.46	0.50
1:F:184:THR:N	1:F:185:GLY:CA	2.73	0.50
2:G:574:ARG:C	2:G:576:ASP:H	2.13	0.50
1:D:210:ALA:HB2	1:D:396:LEU:HB3	1.94	0.50
1:F:325:ILE:HG21	1:F:342:ILE:HG21	1.93	0.50
3:L:201:VAL:O	3:L:202:ARG:HG3	2.11	0.50
3:N:238:SER:N	3:N:275:THR:HG1	2.10	0.50
1:D:116:ARG:HA	1:D:119:ILE:HB	1.93	0.50
3:J:39:LYS:HA	3:J:42:GLU:OE2	2.12	0.50
1:F:184:THR:H	1:F:185:GLY:CA	2.13	0.50
1:E:82:GLU:O	1:E:83:ILE:HG13	2.12	0.50
1:F:34:ALA:C	1:F:36:GLU:H	2.13	0.50
2:I:555:ARG:N	2:I:556:PRO:HD2	2.27	0.50
3:K:211:GLN:HA	3:K:214:GLU:HB2	1.93	0.50
3:J:40:GLU:N	3:J:157:GLU:CG	2.75	0.49
1:E:188:THR:HG23	1:E:194:ASP:OD1	2.11	0.49
2:H:527:LEU:O	2:H:531:LEU:HG	2.12	0.49
3:J:44:VAL:HG21	3:J:255:GLN:NE2	2.27	0.49
1:B:248:VAL:HA	1:B:251:MET:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:155:TYR:O	3:J:156:ASN:O	2.30	0.49
1:A:258:ILE:O	1:A:435:TYR:HD2	1.95	0.49
3:K:45:ILE:O	3:K:46:ASP:O	2.30	0.49
1:A:256:GLY:HA3	1:A:279:ALA:HB2	1.94	0.49
3:M:220:VAL:O	3:M:220:VAL:HG12	2.11	0.49
1:E:347:LYS:HE3	1:E:351:ARG:HH22	1.76	0.49
3:M:94:ILE:HD12	3:N:48:LYS:HE2	1.93	0.49
3:M:51:GLU:OE2	3:N:51:GLU:CA	2.61	0.49
3:M:54:LEU:HD12	3:N:52:LYS:HG2	1.94	0.49
3:K:47:GLN:NE2	3:K:48:LYS:HZ1	2.10	0.49
1:D:392:ILE:HD12	1:D:421:ASN:ND2	2.27	0.49
3:K:183:ASN:O	3:K:187:GLU:N	2.45	0.49
3:J:120:MET:HB2	3:J:195:VAL:HA	1.94	0.49
1:D:227:VAL:HG11	1:D:316:MET:HG3	1.94	0.49
3:M:58:TYR:N	3:N:46:ASP:OD2	2.45	0.49
3:J:44:VAL:HG21	3:J:89:VAL:CG1	2.39	0.49
3:K:165:TYR:CE1	3:K:298:ALA:HB3	2.47	0.49
3:L:144:MET:HE2	3:L:177:MET:HB3	1.93	0.49
1:A:47:ALA:HA	1:A:83:ILE:HG23	1.93	0.49
3:L:33:ASP:CA	3:L:60:TYR:CE2	2.93	0.49
3:M:58:TYR:CE1	3:N:49:MET:CE	2.94	0.49
1:F:301:ILE:HD13	1:F:319:ILE:HD13	1.94	0.49
3:K:162:LYS:HB3	3:K:299:ALA:HB2	1.93	0.49
3:M:50:ILE:HG23	3:N:47:GLN:C	2.27	0.49
3:J:38:LEU:O	3:J:42:GLU:HG3	2.12	0.49
1:D:270:PRO:HD2	3:J:51:GLU:CG	2.35	0.49
3:J:231:ILE:CD1	3:J:261:PHE:HB3	2.33	0.49
1:A:26:LEU:CD1	1:A:99:ALA:HB1	2.41	0.49
3:J:121:TYR:HB3	3:J:199:GLU:HB2	1.93	0.49
1:F:293:THR:O	1:F:294:PRO:O	2.29	0.49
3:L:164:LEU:O	3:L:260:PHE:HA	2.13	0.49
1:D:241:GLU:HB2	1:D:321:TYR:HD2	1.78	0.49
1:A:219:PHE:CE1	1:A:396:LEU:HD11	2.48	0.49
1:E:79:GLN:HB2	1:E:83:ILE:HG13	1.95	0.49
3:L:155:TYR:CZ	3:L:185:LEU:HD11	2.48	0.49
1:B:265:THR:HA	1:E:428:GLN:CB	2.43	0.49
1:A:146:LYS:HB2	1:A:146:LYS:HZ2	1.78	0.49
3:M:54:LEU:N	3:N:48:LYS:HB3	2.27	0.49
1:A:200:PHE:HE2	1:A:227:VAL:CG1	2.25	0.49
1:E:302:ARG:HD2	1:F:36:GLU:HG3	1.95	0.49
1:B:121:THR:O	1:B:125:ILE:HG13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:LEU:O	1:F:71:THR:HG23	2.13	0.49
3:O:165:TYR:CE2	3:O:298:ALA:HB3	2.47	0.49
1:F:432:ILE:HD12	1:F:437:LYS:HB2	1.94	0.49
1:B:241:GLU:HB2	1:B:321:TYR:CE2	2.48	0.49
3:M:127:LEU:HA	3:M:179:ALA:HB1	1.94	0.49
1:F:392:ILE:HA	1:F:418:LYS:HB3	1.94	0.49
1:E:211:ARG:HB3	1:E:212:PRO:HD2	1.94	0.49
1:A:271:GLU:OE1	3:K:239:TRP:CZ2	2.66	0.49
3:L:40:GLU:HG2	3:L:256:GLN:HB3	1.95	0.49
3:M:53:SER:HB3	3:N:48:LYS:HZ2	1.72	0.49
3:J:99:TYR:CB	3:J:219:MET:CE	2.70	0.49
3:K:104:LYS:HE3	3:K:125:ASP:CA	2.43	0.49
2:I:488:ARG:HB3	2:I:553:LEU:CD2	2.41	0.49
1:C:252:LEU:CD2	1:C:279:ALA:HB1	2.41	0.49
3:N:197:VAL:N	3:N:198:PRO:CD	2.75	0.49
2:H:555:ARG:O	2:H:559:LEU:HB2	2.12	0.49
3:L:89:VAL:CA	3:L:254:SER:O	2.60	0.49
3:L:63:GLN:O	3:L:64:SER:O	2.30	0.49
3:K:83:TYR:CE2	3:K:175:THR:HB	2.35	0.49
1:A:73:GLU:HA	1:A:76:ALA:HB2	1.95	0.49
1:C:315:GLY:O	1:C:356:PRO:HD2	2.12	0.49
3:J:44:VAL:HG13	3:J:45:ILE:HG13	1.94	0.48
3:K:83:TYR:HD2	3:K:126:LEU:HB2	1.78	0.48
3:J:112:LYS:O	3:J:187:GLU:HA	2.12	0.48
3:O:165:TYR:HE1	3:O:261:PHE:HB2	1.78	0.48
1:F:196:MET:O	1:F:423:PRO:HG2	2.13	0.48
3:L:45:ILE:HG23	3:L:49:MET:CG	2.43	0.48
1:F:63:GLU:N	1:F:64:PRO:HA	2.23	0.48
3:L:309:ARG:HB3	3:M:158:THR:HG21	1.94	0.48
3:L:86:LYS:HG3	3:L:255:GLN:HE21	0.36	0.48
3:J:37:PHE:CG	3:J:87:LEU:HB2	2.44	0.48
1:A:414:ILE:O	1:A:426:THR:HA	2.14	0.48
3:N:138:ASP:C	3:N:140:SER:H	2.16	0.48
3:L:137:SER:H	3:L:141:ARG:HB2	1.78	0.48
1:C:208:VAL:HB	1:C:360:LEU:HD22	1.95	0.48
3:M:227:MET:HA	3:M:260:PHE:HB2	1.95	0.48
1:B:377:MET:C	1:B:379:ASP:H	2.16	0.48
1:B:209:ALA:HB2	1:B:361:SER:HB3	1.95	0.48
3:L:88:VAL:HG11	3:L:255:GLN:OE1	2.13	0.48
1:C:381:ARG:HD2	1:C:387:GLU:H	1.78	0.48
1:D:374:ARG:N	1:D:375:PRO:CA	2.70	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:LYS:HA	1:C:314:LEU:HB2	1.96	0.48
3:M:266:SER:O	3:M:270:LEU:N	2.46	0.48
3:K:228:LEU:HD13	3:K:245:ILE:HG23	1.95	0.48
1:D:284:SER:C	1:D:286:ALA:H	2.16	0.48
1:F:374:ARG:N	1:F:375:PRO:HA	2.28	0.48
1:E:319:ILE:HD13	1:E:346:LEU:HD13	1.95	0.48
1:E:78:GLU:O	1:E:78:GLU:HG3	2.12	0.48
3:L:86:LYS:NZ	3:L:257:LEU:HD23	2.29	0.48
1:A:202:ARG:O	1:A:203:SER:HB2	2.13	0.48
1:F:221:LEU:HB3	1:F:225:GLN:NE2	2.28	0.48
1:B:51:ILE:HG22	1:B:55:MET:SD	2.54	0.48
1:C:229:THR:HG22	1:C:286:ALA:HB2	1.95	0.48
3:L:53:SER:CB	3:L:94:ILE:HD12	2.44	0.48
3:N:41:ASN:OD1	3:N:44:VAL:HG21	2.10	0.48
3:L:138:ASP:C	3:L:140:SER:H	2.15	0.48
1:F:260:ALA:HB3	3:N:32:GLN:N	2.28	0.48
2:I:525:GLN:C	2:I:527:LEU:H	2.17	0.48
3:N:239:TRP:C	3:N:241:ARG:H	2.17	0.48
1:F:253:CYS:HB3	1:F:259:ASN:HB2	1.95	0.48
1:C:112:LYS:O	1:C:116:ARG:NH2	2.43	0.48
3:K:210:ASP:C	3:K:212:THR:H	2.17	0.48
3:L:203:GLU:O	3:L:207:SER:HB3	2.14	0.48
3:L:221:LYS:C	3:L:252:ARG:HH21	2.16	0.48
3:L:37:PHE:O	3:L:40:GLU:HB3	2.14	0.48
3:M:47:GLN:HB3	3:N:51:GLU:CG	2.43	0.48
3:J:39:LYS:C	3:J:157:GLU:CG	2.82	0.48
1:C:432:ILE:HG22	3:N:70:CYS:C	2.31	0.48
3:J:33:ASP:HB2	3:J:61:ILE:HG23	1.86	0.48
1:A:101:ASN:HB3	1:A:104:TYR:CG	2.48	0.48
1:F:309:LYS:HB2	1:F:353:LEU:HD23	1.95	0.48
3:O:120:MET:N	3:O:194:ILE:O	2.46	0.48
1:B:76:ALA:C	1:B:78:GLU:H	2.16	0.48
3:L:83:TYR:HB3	3:L:219:MET:HE1	1.81	0.48
3:M:38:LEU:HD11	3:M:50:ILE:HD11	1.96	0.48
1:A:61:ARG:CB	1:A:62:GLY:CA	2.91	0.48
1:E:186:ILE:HG21	1:E:316:MET:SD	2.53	0.48
1:C:103:GLU:HG3	1:C:107:ARG:NH2	2.27	0.48
1:C:318:VAL:HG22	1:C:358:ILE:HD12	1.94	0.48
1:C:321:TYR:HA	1:C:360:LEU:HB2	1.96	0.48
1:E:27:ASP:HB3	1:E:28:PRO:C	2.34	0.48
3:J:241:ARG:HH12	3:J:274:PHE:C	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:33:ASP:OD1	3:N:61:ILE:HD13	2.14	0.48
1:E:293:THR:HA	1:E:294:PRO:HD3	1.77	0.48
3:K:114:GLN:O	3:K:118:LYS:HG3	2.14	0.48
3:O:269:GLU:HA	3:O:273:HIS:CD2	2.49	0.48
3:J:92:ARG:N	3:J:92:ARG:HD2	2.29	0.48
1:B:183:ILE:HG23	1:B:185:GLY:HA3	1.94	0.48
1:B:207:ILE:HD11	1:B:361:SER:HB2	1.96	0.48
1:C:209:ALA:HB1	1:C:363:LEU:HB2	1.96	0.48
3:L:37:PHE:CZ	3:L:254:SER:O	2.63	0.48
3:L:61:ILE:CG1	3:L:62:GLU:H	2.18	0.48
3:J:86:LYS:CD	3:J:219:MET:HE1	2.44	0.48
3:L:69:TYR:HA	3:L:70:CYS:HA	1.51	0.48
1:D:322:LEU:O	1:D:325:ILE:HG22	2.14	0.48
1:F:86:VAL:HG12	1:F:89:LEU:HD12	1.96	0.48
3:O:120:MET:O	3:O:196:TYR:HB2	2.13	0.48
2:H:568:LYS:HG3	2:H:583:ILE:HB	1.96	0.48
3:O:297:LEU:O	3:O:298:ALA:CB	2.62	0.48
1:B:80:LEU:HD23	1:B:85:GLY:HA2	1.96	0.48
1:E:119:ILE:C	1:E:121:THR:H	2.17	0.48
3:J:254:SER:HB3	3:O:47:GLN:OE1	2.12	0.48
1:E:233:GLU:HG3	1:E:315:GLY:CA	2.41	0.47
1:B:319:ILE:HG22	1:B:320:ASP:H	1.79	0.47
1:A:26:LEU:HD13	1:A:99:ALA:CB	2.44	0.47
3:L:148:VAL:O	3:L:152:LEU:HG	2.14	0.47
3:J:192:SER:HB2	3:J:227:MET:SD	2.54	0.47
1:E:321:TYR:CG	1:E:322:LEU:N	2.82	0.47
3:L:92:ARG:HD2	3:L:92:ARG:N	2.28	0.47
3:L:89:VAL:HG12	3:L:254:SER:CB	2.43	0.47
3:N:46:ASP:N	3:N:46:ASP:OD1	2.42	0.47
1:E:381:ARG:HD3	1:E:387:GLU:HB2	1.97	0.47
2:H:519:ARG:HA	2:H:520:ILE:O	2.14	0.47
3:N:178:LEU:HB3	3:N:227:MET:HB3	1.95	0.47
3:K:200:PHE:HD1	3:K:204:LEU:HD11	1.79	0.47
1:F:325:ILE:HG23	1:F:342:ILE:HG21	1.95	0.47
1:E:361:SER:OG	1:E:362:GLN:N	2.47	0.47
3:K:92:ARG:N	3:K:92:ARG:HD2	2.29	0.47
1:C:239:SER:O	1:C:292:ASP:HA	2.14	0.47
3:L:86:LYS:HZ3	3:L:157:GLU:CD	2.17	0.47
3:M:58:TYR:N	3:N:46:ASP:CG	2.62	0.47
3:N:97:GLU:HB3	3:N:215:GLU:CG	2.40	0.47
1:E:376:MET:HG3	1:E:378:SER:OG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:VAL:C	1:C:341:GLU:H	2.17	0.47
1:D:224:ALA:HB2	1:D:318:VAL:HG21	1.96	0.47
1:A:202:ARG:O	1:A:203:SER:CB	2.62	0.47
3:O:92:ARG:HD2	3:O:92:ARG:N	2.29	0.47
1:B:321:TYR:CE2	1:B:324:LEU:HB2	2.49	0.47
1:B:24:VAL:HG11	1:B:31:LEU:HD12	1.96	0.47
1:E:254:ALA:HA	1:E:437:LYS:HE2	1.97	0.47
3:J:86:LYS:CE	3:J:222:THR:C	2.77	0.47
3:K:62:GLU:HG2	3:L:285:VAL:CG1	2.43	0.47
1:F:32:VAL:CG2	1:F:33:PRO:HD3	2.38	0.47
1:D:253:CYS:CB	1:D:259:ASN:HB2	2.39	0.47
1:B:21:LEU:HD13	1:B:51:ILE:HG21	1.95	0.47
1:E:61:ARG:HB2	1:E:62:GLY:CA	2.44	0.47
3:J:112:LYS:HB3	3:J:116:LEU:CD1	2.44	0.47
2:I:548:TYR:CA	2:I:551:HIS:HD2	2.24	0.47
3:O:140:SER:HB2	3:O:303:LEU:HG	1.97	0.47
3:L:155:TYR:OH	3:L:185:LEU:HD11	2.14	0.47
1:A:393:VAL:HG12	1:A:395:PHE:CE1	2.50	0.47
3:M:185:LEU:HD13	3:M:192:SER:HB3	1.97	0.47
1:D:135:GLU:HB3	1:D:139:LEU:HB2	1.96	0.47
1:E:121:THR:O	1:E:125:ILE:HG13	2.14	0.47
1:C:21:LEU:HD12	1:C:92:LEU:HD22	1.96	0.47
3:N:46:ASP:CG	3:N:49:MET:CB	2.80	0.47
1:C:27:ASP:CG	1:C:30:ALA:HB2	2.35	0.47
2:H:520:ILE:HA	2:H:521:PRO:HD3	1.75	0.47
1:C:103:GLU:H	1:C:104:TYR:HD2	1.62	0.47
1:B:121:THR:HB	1:B:147:ILE:HD13	1.97	0.47
1:F:363:LEU:HD23	1:F:380:ILE:HG23	1.96	0.47
1:C:270:PRO:O	1:C:271:GLU:CG	2.59	0.47
3:M:226:LEU:HD13	3:M:252:ARG:NH2	2.30	0.47
1:C:146:LYS:HZ2	1:C:146:LYS:HB2	1.80	0.47
1:F:317:ILE:HD12	1:F:357:VAL:HG22	1.97	0.47
3:N:45:ILE:CG2	3:N:50:ILE:HD13	2.32	0.47
1:E:101:ASN:HB2	1:E:105:TYR:CD2	2.50	0.47
1:C:433:LYS:HB3	3:N:68:SER:HB3	1.88	0.47
1:D:73:GLU:HA	1:D:76:ALA:HB3	1.96	0.47
1:B:61:ARG:HB2	1:B:63:GLU:HB3	1.97	0.47
1:F:200:PHE:HB3	1:F:356:PRO:CG	2.42	0.47
3:L:146:GLN:C	3:L:148:VAL:H	2.18	0.47
3:O:200:PHE:CE1	3:O:216:LYS:HB3	2.47	0.47
3:K:148:VAL:HG13	3:K:181:ILE:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:294:ILE:HG22	3:L:294:ILE:O	2.15	0.47
1:B:377:MET:O	1:B:379:ASP:N	2.47	0.47
3:L:57:LEU:C	3:L:57:LEU:HD12	2.35	0.47
3:N:86:LYS:HE2	3:N:221:LYS:CD	2.37	0.47
2:I:519:ARG:HB2	2:I:520:ILE:HD12	1.97	0.47
1:F:51:ILE:HG22	1:F:55:MET:SD	2.55	0.47
3:L:163:GLY:N	3:L:298:ALA:HA	2.25	0.47
1:F:305:CYS:HB3	1:F:353:LEU:HD11	1.97	0.47
1:C:125:ILE:HA	1:C:128:ASP:HB2	1.96	0.47
3:M:92:ARG:N	3:M:92:ARG:HD2	2.29	0.47
1:F:208:VAL:HG22	1:F:394:ALA:HB3	1.96	0.47
1:C:237:ILE:HG23	1:C:318:VAL:HB	1.96	0.47
3:O:167:TYR:CE2	3:O:267:PRO:HD3	2.50	0.47
1:A:67:LEU:HB2	2:G:585:LYS:HG2	1.96	0.47
1:F:248:VAL:O	1:F:248:VAL:HG12	2.14	0.47
3:N:309:ARG:HB3	3:O:157:GLU:HB2	1.96	0.47
3:N:92:ARG:N	3:N:92:ARG:HD2	2.29	0.47
1:E:376:MET:O	1:E:380:ILE:HG13	2.15	0.47
1:B:212:PRO:HA	1:B:216:LYS:HB3	1.97	0.47
1:E:142:GLU:HG3	1:E:143:ALA:N	2.29	0.47
3:J:124:GLN:HA	3:J:127:LEU:HD12	1.97	0.47
1:D:95:ALA:HA	2:H:459:ALA:HB2	1.97	0.47
3:J:146:GLN:O	3:J:150:ASP:HB2	2.15	0.47
3:L:98:TYR:C	3:L:219:MET:SD	2.93	0.46
3:J:44:VAL:HB	3:J:255:GLN:C	2.34	0.46
1:E:51:ILE:HG12	1:E:74:LEU:HD13	1.96	0.46
1:C:104:TYR:N	1:C:105:TYR:HB2	2.30	0.46
1:F:76:ALA:C	1:F:78:GLU:N	2.67	0.46
3:M:291:MET:C	3:M:293:ARG:H	2.18	0.46
2:G:504:PHE:C	2:G:506:GLU:N	2.66	0.46
1:E:429:LEU:HD22	1:E:440:ASN:HA	1.97	0.46
3:L:41:ASN:N	3:L:256:GLN:HG3	2.30	0.46
3:J:165:TYR:HB3	3:J:167:TYR:CZ	2.50	0.46
1:C:358:ILE:HG22	1:C:360:LEU:CD2	2.42	0.46
1:E:195:ARG:C	1:E:197:THR:H	2.18	0.46
1:E:28:PRO:O	1:E:30:ALA:N	2.39	0.46
1:E:258:ILE:HG22	1:E:259:ASN:N	2.30	0.46
1:F:235:VAL:HG12	1:F:316:MET:H	1.79	0.46
2:G:472:MSE:HE1	2:G:531:LEU:HB3	1.97	0.46
3:L:120:MET:O	3:L:121:TYR:HB2	2.14	0.46
1:C:48:HIS:HA	1:C:51:ILE:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:36:ALA:HA	3:L:158:THR:HA	1.97	0.46
3:L:88:VAL:HG11	3:L:97:GLU:CG	2.45	0.46
3:J:88:VAL:HG23	3:J:222:THR:HA	1.50	0.46
1:E:219:PHE:CG	1:E:396:LEU:HD11	2.51	0.46
3:J:155:TYR:O	3:J:156:ASN:C	2.54	0.46
1:E:261:GLN:N	1:E:262:ASN:HA	2.22	0.46
1:C:61:ARG:N	1:C:62:GLY:HA3	2.31	0.46
1:A:111:GLU:HA	1:A:114:VAL:CB	2.44	0.46
3:N:226:LEU:HB2	3:N:259:THR:HG22	1.96	0.46
3:L:39:LYS:CG	3:L:158:THR:O	2.49	0.46
1:E:104:TYR:CA	1:E:105:TYR:HB3	2.44	0.46
1:C:27:ASP:HB3	1:C:29:ALA:N	2.16	0.46
3:J:154:SER:C	3:J:156:ASN:N	2.68	0.46
1:A:221:LEU:HD13	1:A:247:LEU:HD21	1.97	0.46
2:I:562:LYS:O	2:I:565:GLU:HG3	2.16	0.46
1:C:66:ASP:O	1:C:69:THR:HG22	2.15	0.46
3:J:289:ARG:O	3:J:293:ARG:NH1	2.48	0.46
2:G:559:LEU:HD12	2:G:562:LYS:HD2	1.97	0.46
1:C:120:ARG:O	1:C:120:ARG:HG2	2.15	0.46
3:L:45:ILE:CG1	3:L:89:VAL:HG21	2.44	0.46
1:F:430:ALA:HB3	3:M:48:LYS:NZ	2.31	0.46
3:J:221:LYS:HE2	3:J:248:VAL:HG22	1.97	0.46
3:J:43:GLU:CB	3:J:255:GLN:O	2.63	0.46
3:J:86:LYS:NZ	3:J:223:THR:CA	2.79	0.46
1:D:252:LEU:HD13	1:D:276:LEU:HD11	1.98	0.46
1:D:397:TYR:CD2	1:D:415:ILE:HD11	2.51	0.46
1:B:261:GLN:N	1:B:262:ASN:CA	2.75	0.46
1:A:220:ALA:HB2	1:A:360:LEU:HD21	1.97	0.46
3:K:45:ILE:C	3:K:46:ASP:O	2.52	0.46
1:A:128:ASP:O	1:A:131:THR:OG1	2.34	0.46
1:D:339:VAL:HA	1:D:342:ILE:HB	1.98	0.46
3:L:122:ILE:HB	3:L:123:GLN:H	1.43	0.46
1:A:18:GLN:HG3	1:A:48:HIS:CE1	2.50	0.46
2:I:465:ARG:C	2:I:467:LEU:H	2.18	0.46
3:K:245:ILE:HA	3:K:248:VAL:HG23	1.98	0.46
1:B:187:PRO:HB2	1:B:230:LYS:HD2	1.96	0.46
3:L:97:GLU:OE2	3:L:218:ASN:OD1	2.34	0.46
3:L:86:LYS:NZ	3:L:157:GLU:OE1	2.48	0.46
3:J:43:GLU:OE2	3:J:160:LYS:CE	2.63	0.46
1:E:77:SER:O	1:E:79:GLN:HG2	2.15	0.46
1:C:127:GLN:NE2	1:C:130:TYR:HB2	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:238:SER:N	3:N:286:LYS:HB2	2.30	0.46
2:H:471:MSE:HB2	2:H:478:ALA:HB2	1.97	0.46
2:H:579:THR:O	2:H:582:ARG:HB2	2.16	0.46
1:F:21:LEU:HD12	1:F:92:LEU:HD13	1.98	0.46
3:M:54:LEU:HD21	3:N:92:ARG:O	2.15	0.46
3:K:48:LYS:N	3:K:48:LYS:HD2	2.31	0.46
1:C:104:TYR:N	1:C:105:TYR:CB	2.78	0.46
1:D:320:ASP:HA	1:D:360:LEU:HD12	1.96	0.46
3:M:192:SER:HA	3:M:225:VAL:HB	1.98	0.46
1:F:247:LEU:HA	1:F:250:ARG:HD2	1.97	0.46
3:J:129:ALA:C	3:J:180:ALA:HA	2.36	0.46
3:L:213:LEU:HD23	3:L:216:LYS:HD2	1.98	0.46
2:H:561:LEU:C	2:H:563:VAL:H	2.18	0.46
1:D:322:LEU:C	1:D:324:LEU:N	2.69	0.46
1:C:302:ARG:HH21	1:C:345:SER:C	2.20	0.46
3:M:270:LEU:HD23	3:M:270:LEU:HA	1.79	0.46
1:A:87:SER:O	1:A:91:GLU:HB2	2.16	0.46
1:B:17:GLU:HG3	1:B:109:VAL:HG11	1.97	0.46
3:M:229:ASP:HB3	3:M:230:ASP:H	1.55	0.46
3:M:113:GLN:HE22	3:M:187:GLU:HG2	1.81	0.46
3:M:94:ILE:HB	3:N:48:LYS:NZ	2.30	0.46
1:A:186:ILE:O	1:A:200:PHE:CD2	2.69	0.46
3:K:83:TYR:HB2	3:K:98:TYR:HB3	1.98	0.46
3:O:147:HIS:HB3	3:O:151:PHE:CE2	2.51	0.46
3:L:167:TYR:OH	3:L:300:PRO:HB2	2.15	0.46
2:I:475:ARG:HH22	2:I:502:TYR:HA	1.81	0.46
1:C:184:THR:H	1:C:185:GLY:C	2.18	0.46
2:H:493:GLU:C	2:H:495:ARG:H	2.18	0.46
1:D:207:ILE:HD13	1:D:386:ILE:HG23	1.97	0.46
1:C:138:VAL:O	1:C:142:GLU:HG3	2.17	0.46
1:C:192:GLU:HG3	1:C:193:LEU:N	2.31	0.46
1:C:240:LEU:HD22	1:C:295:SER:HA	1.97	0.46
3:L:41:ASN:CG	3:L:44:VAL:HB	2.36	0.45
3:L:38:LEU:CD2	3:L:50:ILE:HD12	2.37	0.45
3:L:66:ASN:HD22	3:L:84:HIS:HE1	1.64	0.45
3:K:225:VAL:HA	3:K:259:THR:HG22	1.98	0.45
3:K:285:VAL:O	3:K:289:ARG:NH1	2.49	0.45
3:N:185:LEU:HD22	3:N:225:VAL:HG21	1.97	0.45
3:N:239:TRP:HB2	3:N:275:THR:HG22	1.98	0.45
1:B:237:ILE:HD12	1:B:288:ILE:HA	1.98	0.45
3:O:252:ARG:HA	3:O:255:GLN:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:167:TYR:OH	3:K:302:ARG:HA	2.16	0.45
3:J:193:MET:CE	3:J:223:THR:HG21	2.47	0.45
3:J:45:ILE:HG21	3:J:50:ILE:HD11	1.97	0.45
1:A:183:ILE:HG12	1:A:194:ASP:CB	2.44	0.45
1:F:133:GLU:CA	1:F:134:ASP:HB2	2.44	0.45
2:I:497:LEU:O	2:I:501:ILE:HG13	2.16	0.45
1:A:66:ASP:O	1:A:69:THR:HG22	2.15	0.45
3:J:119:SER:HA	3:J:194:ILE:N	2.32	0.45
1:C:202:ARG:O	1:C:203:SER:HB2	2.16	0.45
1:E:80:LEU:HD11	2:I:575:LYS:NZ	2.30	0.45
3:L:41:ASN:CB	3:L:256:GLN:HG2	2.26	0.45
3:J:43:GLU:HG2	3:J:256:GLN:HE21	1.62	0.45
1:D:375:PRO:HD2	1:D:397:TYR:CE1	2.51	0.45
1:C:63:GLU:N	1:C:64:PRO:HA	2.30	0.45
1:E:29:ALA:C	1:E:31:LEU:H	2.20	0.45
1:E:75:ALA:HA	1:E:80:LEU:HB2	1.99	0.45
3:N:258:PRO:HA	3:N:297:LEU:HD13	1.97	0.45
1:C:199:GLY:HA2	1:C:200:PHE:HB2	1.98	0.45
3:M:54:LEU:CA	3:N:48:LYS:HB3	2.42	0.45
3:J:86:LYS:CD	3:J:219:MET:HE3	2.35	0.45
1:E:380:ILE:HD11	1:E:395:PHE:HE2	1.82	0.45
3:K:164:LEU:HD22	3:K:301:ILE:HD12	1.99	0.45
1:F:209:ALA:HB1	1:F:363:LEU:HD21	1.97	0.45
1:E:190:PHE:O	1:E:192:GLU:N	2.50	0.45
1:B:68:VAL:O	1:B:72:ALA:HB2	2.16	0.45
1:D:53:HIS:CE1	1:D:57:ARG:HB2	2.52	0.45
3:K:178:LEU:HD21	3:K:262:SER:HB3	1.99	0.45
1:A:293:THR:HA	1:A:294:PRO:HD3	1.84	0.45
1:B:104:TYR:N	1:B:106:ALA:H	2.03	0.45
1:B:63:GLU:HG3	1:B:64:PRO:O	2.16	0.45
1:F:300:ASP:C	1:F:302:ARG:H	2.18	0.45
1:E:319:ILE:HB	1:E:359:ALA:HA	1.98	0.45
3:L:39:LYS:CD	3:L:158:THR:HB	2.46	0.45
3:L:62:GLU:O	3:L:63:GLN:HB3	2.16	0.45
3:L:89:VAL:CG1	3:L:254:SER:CB	2.83	0.45
1:F:360:LEU:HB3	1:F:361:SER:H	1.61	0.45
1:F:61:ARG:HB2	1:F:62:GLY:HA3	1.98	0.45
1:C:128:ASP:HB3	1:C:139:LEU:HD21	1.98	0.45
3:O:195:VAL:HB	3:O:228:LEU:HD22	1.98	0.45
3:O:266:SER:HB2	3:O:267:PRO:HD2	1.98	0.45
3:O:252:ARG:O	3:O:256:GLN:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:514:GLY:HA2	2:I:517:ILE:HG12	1.97	0.45
1:A:108:ILE:O	1:A:112:LYS:N	2.47	0.45
3:J:166:LEU:CD1	3:J:178:LEU:HG	2.46	0.45
3:L:221:LYS:CE	3:L:248:VAL:CG1	2.94	0.45
1:D:271:GLU:HB3	3:J:48:LYS:CD	2.17	0.45
1:E:48:HIS:CD2	1:E:48:HIS:H	2.35	0.45
3:N:198:PRO:HD3	3:N:230:ASP:O	2.15	0.45
3:J:166:LEU:HD13	3:J:177:MET:HB2	1.98	0.45
3:N:144:MET:C	3:N:146:GLN:H	2.20	0.45
3:J:40:GLU:CG	3:J:224:PRO:HG3	2.47	0.45
1:E:104:TYR:O	1:E:107:ARG:NH1	2.49	0.45
1:B:104:TYR:HB3	1:B:105:TYR:CB	2.44	0.45
3:O:151:PHE:O	3:O:152:LEU:HD22	2.16	0.45
1:E:68:VAL:HA	1:E:71:THR:HG1	1.79	0.45
3:K:160:LYS:HG2	3:K:256:GLN:CB	2.39	0.45
3:N:225:VAL:CG1	3:N:227:MET:SD	3.04	0.45
3:M:230:ASP:HA	3:M:263:SER:HB3	1.98	0.45
2:G:584:ALA:HA	2:G:587:MSE:HE2	1.98	0.45
3:L:221:LYS:HE2	3:L:248:VAL:HG21	1.91	0.45
3:N:43:GLU:HB2	3:N:254:SER:O	2.17	0.45
1:A:233:GLU:HB3	1:A:316:MET:HE2	1.99	0.45
1:A:61:ARG:HB2	1:A:62:GLY:HA2	1.95	0.45
1:F:261:GLN:HB2	3:N:32:GLN:CG	2.45	0.45
1:F:395:PHE:O	1:F:414:ILE:HA	2.17	0.45
3:L:206:ASN:HB2	3:M:289:ARG:CG	2.44	0.45
1:F:308:LEU:HA	1:F:311:GLU:CB	2.47	0.45
2:G:501:ILE:C	2:G:503:ALA:H	2.20	0.45
3:L:37:PHE:CE1	3:L:255:GLN:HA	2.51	0.45
3:J:97:GLU:CB	3:J:219:MET:CG	2.86	0.45
1:D:271:GLU:HB3	3:J:48:LYS:HE3	1.97	0.45
1:E:63:GLU:N	1:E:64:PRO:CA	2.71	0.45
1:D:252:LEU:HD23	1:D:283:LEU:HD13	1.98	0.45
1:A:132:ARG:HD2	1:A:139:LEU:HA	1.99	0.45
1:B:112:LYS:HB3	1:B:116:ARG:NH2	2.32	0.45
3:L:86:LYS:CE	3:L:255:GLN:HG2	2.48	0.44
3:L:86:LYS:HD2	3:L:222:THR:C	2.31	0.44
3:J:40:GLU:OE1	3:J:157:GLU:HG2	2.17	0.44
1:A:104:TYR:N	1:A:105:TYR:CB	2.77	0.44
1:C:381:ARG:HA	1:C:386:ILE:HB	1.99	0.44
1:F:268:LEU:HD13	1:F:272:ASP:HB3	1.99	0.44
1:C:205:LEU:HD23	1:C:390:ALA:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:267:LYS:HB3	1:E:273:TRP:HZ2	1.82	0.44
1:C:191:THR:O	1:C:195:ARG:NH1	2.50	0.44
3:L:221:LYS:HD3	3:L:248:VAL:CB	2.47	0.44
3:K:121:TYR:HB3	3:K:199:GLU:CB	2.46	0.44
1:F:43:PHE:CD1	1:F:48:HIS:HB3	2.52	0.44
2:I:471:MSE:HE2	2:I:501:ILE:HG21	1.99	0.44
2:G:499:ALA:HA	2:G:502:TYR:HD2	1.77	0.44
2:G:485:ILE:O	2:G:486:GLY:C	2.56	0.44
3:K:197:VAL:HB	3:K:198:PRO:HD3	1.98	0.44
3:J:130:THR:HG22	3:J:184:GLU:HG2	1.99	0.44
1:C:316:MET:HG3	1:C:356:PRO:HB2	1.98	0.44
3:M:164:LEU:HB3	3:M:301:ILE:HD11	1.98	0.44
3:L:37:PHE:CE1	3:L:255:GLN:CA	3.01	0.44
3:N:37:PHE:CE2	3:N:57:LEU:CG	2.88	0.44
1:A:186:ILE:O	1:A:199:GLY:HA2	2.17	0.44
1:A:208:VAL:HG21	1:A:219:PHE:CE2	2.52	0.44
1:E:210:ALA:HB2	1:E:396:LEU:HB2	1.99	0.44
3:J:138:ASP:C	3:J:140:SER:N	2.71	0.44
3:L:165:TYR:HE1	3:L:261:PHE:CD2	2.36	0.44
1:B:429:LEU:HD22	1:B:438:PHE:HD2	1.81	0.44
1:C:250:ARG:HA	1:C:253:CYS:SG	2.58	0.44
1:E:290:ILE:HG22	1:E:291:ASP:N	2.32	0.44
3:N:309:ARG:HB2	3:O:156:ASN:HD22	1.83	0.44
3:N:41:ASN:CB	3:N:255:GLN:HG2	2.48	0.44
3:J:86:LYS:CG	3:J:219:MET:SD	3.05	0.44
1:E:103:GLU:HB2	1:E:104:TYR:CA	2.45	0.44
1:C:377:MET:C	1:C:379:ASP:H	2.20	0.44
1:F:205:LEU:CB	1:F:347:LYS:HA	2.42	0.44
1:C:202:ARG:O	1:C:203:SER:CB	2.65	0.44
3:L:100:GLU:HG3	3:L:193:MET:CE	2.47	0.44
3:L:252:ARG:HA	3:L:257:LEU:HD12	1.99	0.44
3:M:51:GLU:CD	3:N:51:GLU:O	2.56	0.44
1:D:104:TYR:CD1	1:D:105:TYR:HB2	2.53	0.44
1:B:430:ALA:HB3	1:B:438:PHE:HA	1.99	0.44
1:C:416:ILE:CG2	1:C:419:GLN:HB3	2.47	0.44
1:F:86:VAL:HA	1:F:89:LEU:HD12	1.99	0.44
1:F:45:ARG:O	1:F:47:ALA:N	2.51	0.44
1:A:39:ILE:HB	1:A:40:PRO:HD2	1.99	0.44
3:M:58:TYR:CZ	3:N:49:MET:CE	3.00	0.44
3:N:97:GLU:CA	3:N:215:GLU:OE2	2.64	0.44
3:K:62:GLU:OE2	3:L:284:GLU:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:SER:O	1:D:79:GLN:N	2.51	0.44
1:F:260:ALA:CB	3:N:32:GLN:N	2.81	0.44
1:B:61:ARG:CB	1:B:62:GLY:CA	2.95	0.44
1:F:314:LEU:HD21	1:F:353:LEU:CB	2.48	0.44
3:K:184:GLU:HA	3:K:187:GLU:HB2	2.00	0.44
2:G:547:ASP:O	2:G:551:HIS:HB2	2.17	0.44
1:F:132:ARG:NH1	1:F:135:GLU:HB2	2.32	0.44
3:L:38:LEU:HD11	3:L:45:ILE:HG21	2.00	0.44
1:E:62:GLY:HA2	1:E:63:GLU:HA	1.74	0.44
1:B:216:LYS:CG	1:B:217:THR:H	2.27	0.44
1:E:113:SER:O	1:E:117:ARG:HG3	2.18	0.44
1:C:127:GLN:C	1:C:129:GLY:H	2.20	0.44
1:C:375:PRO:CG	1:C:395:PHE:HB3	2.47	0.44
3:M:253:MET:HA	3:M:256:GLN:HA	1.99	0.44
1:D:45:ARG:C	1:D:47:ALA:N	2.71	0.44
1:E:238:PHE:HA	1:E:291:ASP:O	2.17	0.44
1:C:231:THR:HG23	1:C:232:ASN:H	1.82	0.44
2:H:466:LEU:HD22	2:H:536:ILE:HG23	1.99	0.44
3:M:57:LEU:CD2	3:N:48:LYS:HE3	2.47	0.44
3:J:44:VAL:HG21	3:J:255:GLN:HE21	1.83	0.44
1:E:215:GLY:C	1:E:396:LEU:HD13	2.39	0.44
1:F:48:HIS:HA	1:F:51:ILE:HB	2.00	0.44
1:A:26:LEU:HD13	1:A:99:ALA:HB2	1.99	0.44
1:F:363:LEU:HD13	1:F:379:ASP:HB3	1.99	0.44
1:C:197:THR:OG1	1:C:421:ASN:HB3	2.16	0.44
3:N:264:ASN:ND2	3:O:160:LYS:HD2	2.31	0.44
1:A:27:ASP:N	1:A:28:PRO:HA	2.33	0.44
3:O:249:LEU:O	3:O:253:MET:HG2	2.17	0.44
3:M:173:GLY:O	3:M:177:MET:HG2	2.17	0.44
1:F:197:THR:HG21	1:F:416:ILE:HG21	2.00	0.44
1:B:292:ASP:OD1	1:B:292:ASP:N	2.50	0.44
1:C:378:SER:HA	1:C:381:ARG:CG	2.48	0.44
1:E:45:ARG:HB2	1:E:48:HIS:CD2	2.50	0.44
1:B:190:PHE:CD1	1:B:193:LEU:HD23	2.52	0.44
1:C:305:CYS:CB	1:C:314:LEU:HD11	2.45	0.44
1:C:253:CYS:SG	1:C:259:ASN:ND2	2.91	0.44
1:C:262:ASN:CG	1:C:263:LEU:H	2.21	0.44
1:E:240:LEU:O	1:E:321:TYR:HB3	2.18	0.44
3:J:168:GLY:HA2	3:J:302:ARG:HD3	2.00	0.44
1:B:432:ILE:O	1:B:432:ILE:HG22	2.18	0.44
3:J:37:PHE:CZ	3:J:45:ILE:HD11	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:THR:H	1:A:185:GLY:CA	2.09	0.43
1:A:306:ARG:HG3	1:A:353:LEU:HD11	2.00	0.43
2:I:512:ASP:CB	2:I:513:PRO:HD2	2.47	0.43
3:N:197:VAL:HA	3:N:200:PHE:HB2	2.00	0.43
2:H:580:ALA:C	2:H:582:ARG:H	2.20	0.43
3:L:151:PHE:N	3:L:151:PHE:CD2	2.86	0.43
3:J:86:LYS:HE2	3:J:222:THR:C	2.39	0.43
1:E:37:ILE:CD1	1:E:103:GLU:HA	2.48	0.43
3:J:139:PRO:HA	3:J:142:LEU:HB2	2.00	0.43
3:J:165:TYR:CE1	3:J:261:PHE:HB2	2.53	0.43
3:M:155:TYR:CD1	3:M:159:GLY:HA3	2.49	0.43
1:B:189:GLY:HA2	1:B:230:LYS:NZ	2.33	0.43
2:G:505:TYR:CD1	2:G:509:HIS:O	2.71	0.43
2:I:588:ILE:HG22	2:I:592:LYS:HE3	2.00	0.43
1:B:96:VAL:HA	1:B:97:PRO:HD3	1.84	0.43
3:O:129:ALA:O	3:O:180:ALA:HA	2.17	0.43
3:L:220:VAL:O	3:L:221:LYS:CG	2.66	0.43
1:E:61:ARG:NH1	1:E:63:GLU:OE2	2.51	0.43
1:E:52:PHE:HA	1:E:55:MET:CB	2.38	0.43
3:N:140:SER:HB2	3:N:303:LEU:HD23	2.00	0.43
1:B:193:LEU:HB2	1:B:427:VAL:HG13	2.00	0.43
3:L:239:TRP:HE1	3:L:275:THR:N	2.13	0.43
1:F:44:TYR:O	1:F:45:ARG:C	2.57	0.43
2:G:513:PRO:HA	2:G:516:LEU:HD12	2.00	0.43
1:B:202:ARG:HA	1:B:356:PRO:HD3	2.01	0.43
2:G:480:VAL:HA	2:G:483:GLU:HB3	2.00	0.43
3:L:65:LYS:O	3:L:66:ASN:CB	2.64	0.43
1:A:415:ILE:HA	1:A:426:THR:OG1	2.18	0.43
3:K:220:VAL:HA	3:K:226:LEU:HD13	2.00	0.43
3:M:160:LYS:CG	3:M:256:GLN:HB3	2.45	0.43
1:F:308:LEU:HA	1:F:311:GLU:HB2	2.00	0.43
2:H:588:ILE:HA	2:H:591:LYS:HD2	1.99	0.43
1:B:128:ASP:O	1:B:139:LEU:HD22	2.19	0.43
1:D:302:ARG:HH11	1:D:306:ARG:NH2	2.16	0.43
1:E:135:GLU:HB3	1:E:138:VAL:HB	2.01	0.43
1:E:91:GLU:HA	1:E:94:ASP:HB2	1.99	0.43
3:M:50:ILE:HG21	3:N:47:GLN:O	2.19	0.43
1:A:414:ILE:O	1:A:416:ILE:HG13	2.18	0.43
3:N:213:LEU:CD2	3:N:216:LYS:HD2	2.47	0.43
1:E:68:VAL:HG22	2:I:581:ALA:HB1	2.00	0.43
3:L:266:SER:HB2	3:L:267:PRO:CD	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:292:GLU:C	3:O:294:ILE:N	2.72	0.43
3:N:123:GLN:HG2	3:O:251:HIS:ND1	2.33	0.43
3:K:292:GLU:HG2	3:K:295:LEU:HD12	1.99	0.43
3:O:296:TYR:C	3:O:298:ALA:H	2.21	0.43
1:F:27:ASP:HB3	1:F:28:PRO:C	2.39	0.43
3:L:36:ALA:O	3:L:158:THR:CA	2.60	0.43
3:J:38:LEU:O	3:J:42:GLU:CG	2.66	0.43
3:L:69:TYR:HD1	3:L:69:TYR:C	2.19	0.43
1:B:105:TYR:H	1:B:108:ILE:HB	1.84	0.43
3:L:167:TYR:OH	3:L:267:PRO:HB3	2.19	0.43
1:A:387:GLU:O	1:A:420:ARG:NH2	2.51	0.43
1:A:143:ALA:CA	1:A:146:LYS:HE3	2.48	0.43
1:A:220:ALA:HB3	1:A:360:LEU:HD11	2.00	0.43
3:M:266:SER:HB2	3:M:267:PRO:HD2	1.99	0.43
1:A:322:LEU:O	1:A:324:LEU:N	2.44	0.43
1:A:294:PRO:HB2	1:A:295:SER:H	1.63	0.43
1:F:97:PRO:O	1:F:98:THR:HB	2.19	0.43
3:M:297:LEU:O	3:M:298:ALA:HB2	2.19	0.43
1:F:116:ARG:HA	1:F:119:ILE:HB	2.01	0.43
3:L:252:ARG:CZ	3:L:257:LEU:HB3	2.49	0.43
3:M:54:LEU:HD12	3:N:52:LYS:CB	2.37	0.43
3:J:56:LYS:O	3:J:96:ILE:HD11	2.18	0.43
1:B:250:ARG:HH22	1:E:376:MET:HE2	1.83	0.43
3:L:259:THR:HB	3:L:261:PHE:HE2	1.83	0.43
1:B:18:GLN:HA	1:B:48:HIS:CE1	2.53	0.43
1:B:48:HIS:O	1:B:52:PHE:N	2.40	0.43
1:F:293:THR:CG2	1:F:294:PRO:HD2	2.48	0.43
3:O:207:SER:C	3:O:209:GLN:H	2.22	0.43
1:C:43:PHE:CD2	1:C:49:GLN:HG3	2.53	0.43
1:A:206:ILE:HG22	1:A:207:ILE:N	2.33	0.43
3:L:222:THR:HB	3:L:255:GLN:NE2	2.34	0.43
3:L:223:THR:OG1	3:L:224:PRO:CD	2.54	0.43
3:L:36:ALA:HA	3:L:39:LYS:HD2	2.01	0.43
3:M:51:GLU:OE2	3:N:51:GLU:C	2.57	0.43
1:C:27:ASP:CB	1:C:29:ALA:N	2.67	0.43
1:D:322:LEU:O	1:D:324:LEU:N	2.52	0.43
1:E:258:ILE:HG23	1:E:268:LEU:HD21	2.00	0.43
3:O:249:LEU:HD13	3:O:293:ARG:HD3	2.00	0.43
3:L:100:GLU:CD	3:L:193:MET:HE3	2.39	0.43
3:J:87:LEU:O	3:J:222:THR:OG1	2.37	0.43
1:F:103:GLU:HB2	1:F:104:TYR:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:47:ALA:HB2	1:E:83:ILE:HA	1.99	0.43
3:L:148:VAL:HG11	3:L:180:ALA:O	2.18	0.43
2:I:471:MSE:HB2	2:I:478:ALA:CB	2.48	0.43
2:H:579:THR:HA	2:H:582:ARG:HD3	2.01	0.43
1:F:340:SER:HB3	1:F:384:GLY:C	2.40	0.43
1:D:67:LEU:HD11	1:D:93:ALA:HB3	2.01	0.43
1:F:188:THR:HG23	1:F:199:GLY:C	2.39	0.43
1:C:377:MET:HE3	1:C:386:ILE:HG22	2.01	0.42
1:E:381:ARG:HD2	1:E:381:ARG:HA	1.81	0.42
3:L:172:VAL:HG22	3:L:305:GLY:H	1.83	0.42
1:C:374:ARG:N	1:C:375:PRO:CA	2.81	0.42
2:I:568:LYS:HZ3	2:I:587:MSE:HE2	1.83	0.42
1:E:273:TRP:CZ3	1:E:276:LEU:HD22	2.54	0.42
1:C:207:ILE:CG1	1:C:361:SER:HB2	2.48	0.42
3:J:113:GLN:HA	3:J:186:ALA:HB1	2.01	0.42
3:O:56:LYS:O	3:O:96:ILE:HD11	2.19	0.42
3:L:33:ASP:H	3:L:61:ILE:CG2	2.22	0.42
3:M:48:LYS:O	3:M:49:MET:C	2.55	0.42
1:D:270:PRO:CD	3:J:51:GLU:CB	2.95	0.42
1:F:77:SER:O	1:F:79:GLN:N	2.52	0.42
1:C:103:GLU:CG	1:C:104:TYR:HA	2.49	0.42
1:B:43:PHE:CE1	1:B:48:HIS:HB3	2.49	0.42
3:N:183:ASN:HA	3:N:186:ALA:CB	2.45	0.42
3:O:195:VAL:HG12	3:O:196:TYR:N	2.34	0.42
1:A:247:LEU:O	1:A:251:MET:N	2.52	0.42
1:E:143:ALA:CA	1:E:146:LYS:HE3	2.49	0.42
1:E:207:ILE:HB	1:E:359:ALA:O	2.18	0.42
3:N:252:ARG:HD3	3:N:259:THR:HG21	2.00	0.42
2:H:579:THR:HG23	2:H:582:ARG:CZ	2.49	0.42
3:L:86:LYS:HD2	3:L:257:LEU:CD2	2.38	0.42
3:M:54:LEU:HD11	3:N:49:MET:O	2.20	0.42
3:J:39:LYS:O	3:J:157:GLU:CD	2.54	0.42
3:N:98:TYR:O	3:N:215:GLU:CG	2.58	0.42
3:K:65:LYS:CG	3:K:66:ASN:N	2.74	0.42
3:K:82:GLY:C	3:K:126:LEU:HB3	2.39	0.42
1:D:19:ALA:HB3	1:D:105:TYR:CZ	2.54	0.42
1:E:186:ILE:HD11	1:E:233:GLU:HG2	2.01	0.42
3:O:147:HIS:HB3	3:O:151:PHE:HE2	1.84	0.42
1:B:134:ASP:O	1:B:135:GLU:CB	2.68	0.42
1:C:419:GLN:HG2	1:C:424:VAL:HA	2.02	0.42
3:O:194:ILE:HA	3:O:227:MET:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:181:ILE:H	3:K:181:ILE:HG13	1.59	0.42
1:E:39:ILE:HB	1:E:40:PRO:HD2	2.02	0.42
3:N:239:TRP:CE3	3:N:239:TRP:HA	2.54	0.42
1:F:135:GLU:C	1:F:136:ILE:HG12	2.39	0.42
1:C:429:LEU:HA	1:C:440:ASN:HA	2.01	0.42
3:M:94:ILE:HD12	3:N:48:LYS:CE	2.49	0.42
3:K:83:TYR:OH	3:K:175:THR:HG21	1.90	0.42
1:F:74:LEU:O	1:F:79:GLN:N	2.52	0.42
1:C:270:PRO:C	1:C:271:GLU:HG3	2.39	0.42
1:F:91:GLU:O	1:F:95:ALA:HB2	2.19	0.42
1:E:90:SER:C	1:E:92:LEU:H	2.23	0.42
3:K:136:ILE:HG13	3:K:136:ILE:H	1.59	0.42
1:F:430:ALA:HB3	1:F:439:VAL:HB	2.01	0.42
3:J:112:LYS:HD3	3:J:116:LEU:HD11	2.01	0.42
1:C:377:MET:CE	1:C:386:ILE:HG22	2.50	0.42
2:I:475:ARG:HE	2:I:478:ALA:HB3	1.83	0.42
3:O:122:ILE:HG12	3:O:196:TYR:HD1	1.84	0.42
3:N:56:LYS:O	3:N:96:ILE:HD11	2.19	0.42
3:M:35:GLN:HB2	3:N:42:GLU:OE1	2.16	0.42
1:C:339:VAL:C	1:C:341:GLU:N	2.72	0.42
1:D:296:ILE:O	1:D:325:ILE:HG13	2.19	0.42
1:D:210:ALA:HB2	1:D:396:LEU:HD13	2.02	0.42
3:L:147:HIS:HB3	3:L:164:LEU:HD21	2.02	0.42
3:N:193:MET:HE2	3:N:219:MET:HB3	2.01	0.42
3:O:129:ALA:HB2	3:O:176:PHE:CD1	2.54	0.42
1:C:118:LEU:HG	1:C:147:ILE:O	2.20	0.42
2:I:583:ILE:HG13	2:I:583:ILE:H	1.72	0.42
1:E:37:ILE:HD13	1:E:103:GLU:HA	2.02	0.42
1:D:270:PRO:HD2	3:J:51:GLU:CB	2.50	0.42
3:J:137:SER:OG	3:J:140:SER:OG	2.35	0.42
3:L:122:ILE:HD11	3:L:195:VAL:HA	1.99	0.42
1:F:51:ILE:HA	1:F:74:LEU:HD21	2.01	0.42
1:F:57:ARG:O	1:F:61:ARG:NH1	2.51	0.42
2:I:512:ASP:HB3	2:I:513:PRO:CD	2.47	0.42
3:O:144:MET:HE1	3:O:181:ILE:HD11	2.01	0.42
1:F:132:ARG:HH11	1:F:135:GLU:HB2	1.85	0.42
1:A:377:MET:CE	1:A:418:LYS:HB3	2.50	0.42
1:F:290:ILE:HG13	1:F:290:ILE:H	1.67	0.42
1:E:103:GLU:CA	1:E:104:TYR:HB2	2.50	0.42
3:K:47:GLN:OE1	3:K:48:LYS:NZ	2.49	0.42
1:A:133:GLU:HG2	1:A:136:ILE:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:ARG:CG	1:C:381:ARG:O	2.64	0.42
3:L:140:SER:OG	3:L:141:ARG:N	2.52	0.42
1:B:271:GLU:OE2	3:L:52:LYS:HE2	2.19	0.42
2:G:574:ARG:HH22	2:G:579:THR:HB	1.84	0.42
1:F:71:THR:HG22	1:F:89:LEU:HD11	2.02	0.42
3:K:84:HIS:HB2	3:K:99:TYR:CZ	2.55	0.42
1:F:111:GLU:O	1:F:115:LEU:N	2.52	0.42
1:E:259:ASN:HA	1:E:263:LEU:HD13	2.00	0.42
3:K:139:PRO:C	3:K:141:ARG:H	2.23	0.42
3:L:100:GLU:CG	3:L:193:MET:CE	2.97	0.42
3:M:54:LEU:CD1	3:N:49:MET:N	2.79	0.42
1:D:76:ALA:HB1	1:F:133:GLU:O	2.19	0.42
3:K:246:GLY:HA2	3:K:249:LEU:HD12	2.02	0.42
1:C:215:GLY:O	1:C:219:PHE:N	2.49	0.42
2:H:568:LYS:HA	2:H:583:ILE:HD12	2.01	0.42
1:A:121:THR:HB	1:A:146:LYS:HZ2	1.84	0.42
1:B:277:THR:C	1:B:279:ALA:N	2.73	0.42
1:A:108:ILE:HG22	1:A:108:ILE:O	2.20	0.42
1:D:67:LEU:HD11	1:D:93:ALA:CB	2.50	0.42
1:C:186:ILE:HG13	1:C:186:ILE:H	1.59	0.42
1:A:30:ALA:HB1	1:A:102:VAL:HG13	2.01	0.42
2:G:519:ARG:H	2:G:520:ILE:CB	2.29	0.42
3:J:271:LYS:CE	3:J:291:MET:HG3	2.49	0.42
3:O:177:MET:O	3:O:181:ILE:HG13	2.19	0.42
3:L:36:ALA:HB2	3:L:158:THR:HG22	2.00	0.41
3:L:88:VAL:HG11	3:L:97:GLU:HG3	2.02	0.41
3:M:47:GLN:O	3:M:48:LYS:C	2.58	0.41
3:M:32:GLN:NE2	3:N:43:GLU:HG2	2.17	0.41
3:M:57:LEU:CD2	3:N:48:LYS:HG3	2.21	0.41
1:C:380:ILE:HB	1:C:386:ILE:HD12	2.02	0.41
1:B:238:PHE:CD2	1:B:318:VAL:O	2.69	0.41
3:K:267:PRO:O	3:K:271:LYS:HG3	2.19	0.41
1:B:67:LEU:HA	1:B:70:VAL:HB	2.02	0.41
1:F:136:ILE:HB	1:F:137:ASP:H	1.47	0.41
3:N:122:ILE:HG22	3:N:123:GLN:O	2.20	0.41
1:A:206:ILE:HG22	1:A:207:ILE:H	1.84	0.41
1:F:255:GLU:HB3	1:F:279:ALA:HA	2.02	0.41
3:O:84:HIS:HB2	3:O:99:TYR:CZ	2.55	0.41
2:H:585:LYS:O	2:H:589:GLU:HG2	2.19	0.41
1:A:226:ASN:O	1:A:231:THR:HG23	2.20	0.41
1:A:184:THR:OG1	1:A:198:SER:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:518:SER:O	2:I:519:ARG:NE	2.53	0.41
1:C:280:MET:HG2	1:C:283:LEU:HD22	2.02	0.41
2:I:467:LEU:C	2:I:469:ALA:H	2.24	0.41
2:I:467:LEU:HD21	2:I:481:VAL:HG11	2.02	0.41
1:A:143:ALA:HA	1:A:146:LYS:HE3	2.02	0.41
1:B:19:ALA:HA	1:B:92:LEU:HD21	2.02	0.41
1:D:286:ALA:HB3	1:D:288:ILE:HD12	2.03	0.41
1:C:21:LEU:HB2	1:C:92:LEU:HB3	2.02	0.41
3:J:250:GLN:HG2	3:J:293:ARG:NH1	2.35	0.41
1:B:257:ASN:ND2	1:B:435:TYR:HB3	2.35	0.41
1:E:344:ARG:HH22	1:F:56:LEU:HD22	1.85	0.41
3:L:114:GLN:HA	3:L:117:MET:HB2	2.03	0.41
3:L:88:VAL:HG21	3:L:255:GLN:OE1	2.20	0.41
3:K:104:LYS:CD	3:K:125:ASP:HA	2.50	0.41
1:B:134:ASP:O	1:B:135:GLU:HB2	2.20	0.41
1:C:347:LYS:HZ1	1:C:351:ARG:HH22	1.68	0.41
1:F:73:GLU:HA	1:F:76:ALA:HB3	2.03	0.41
3:O:226:LEU:HD13	3:O:228:LEU:HD21	2.02	0.41
1:D:53:HIS:O	1:D:54:ALA:C	2.58	0.41
3:M:293:ARG:HA	3:M:296:TYR:HB2	2.03	0.41
1:F:235:VAL:HB	1:F:236:ALA:H	1.75	0.41
3:M:141:ARG:O	3:M:145:PHE:HD2	2.03	0.41
1:E:220:ALA:HB2	1:E:360:LEU:HD11	2.02	0.41
3:L:86:LYS:HD2	3:L:99:TYR:CD1	2.54	0.41
3:N:38:LEU:CD2	3:N:50:ILE:CG2	2.72	0.41
3:J:40:GLU:CD	3:J:224:PRO:HB3	2.40	0.41
1:C:305:CYS:HB3	1:C:314:LEU:CD1	2.46	0.41
1:F:39:ILE:HB	1:F:40:PRO:HD2	2.03	0.41
2:I:475:ARG:NH1	2:I:501:ILE:O	2.54	0.41
3:N:196:TYR:C	3:N:198:PRO:HD2	2.39	0.41
1:B:272:ASP:HA	1:B:275:LYS:HD2	2.03	0.41
3:L:33:ASP:HB3	3:L:60:TYR:CG	2.32	0.41
3:L:38:LEU:HD13	3:L:45:ILE:HD12	2.02	0.41
3:J:38:LEU:CG	3:J:50:ILE:CD1	2.97	0.41
3:J:84:HIS:HB2	3:J:99:TYR:CZ	2.55	0.41
3:K:83:TYR:CZ	3:K:98:TYR:CE2	3.08	0.41
3:J:167:TYR:HE1	3:J:231:ILE:HD12	1.85	0.41
1:E:186:ILE:O	1:E:200:PHE:HB2	2.20	0.41
1:E:44:TYR:CD2	1:E:45:ARG:HG3	2.56	0.41
1:C:103:GLU:CB	1:C:104:TYR:HA	2.51	0.41
1:B:63:GLU:HG3	1:B:64:PRO:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:CYS:HB3	1:B:259:ASN:HB2	2.01	0.41
3:L:116:LEU:HD22	3:L:191:SER:HB3	2.03	0.41
1:B:306:ARG:HH11	1:B:306:ARG:HB2	1.86	0.41
1:A:322:LEU:HD22	1:A:323:GLN:NE2	2.35	0.41
3:K:45:ILE:O	3:K:46:ASP:C	2.57	0.41
1:A:376:MET:HB2	1:A:377:MET:H	1.64	0.41
1:F:417:ALA:HA	1:F:424:VAL:HG13	2.02	0.41
1:D:260:ALA:C	1:D:262:ASN:HA	2.41	0.41
1:A:258:ILE:C	1:A:435:TYR:HD2	2.24	0.41
1:B:183:ILE:HG22	1:B:185:GLY:HA3	2.01	0.41
1:A:324:LEU:O	1:A:326:GLN:N	2.54	0.41
3:J:144:MET:HE1	3:J:166:LEU:HD22	2.02	0.41
3:K:272:HIS:ND1	3:K:284:GLU:HG2	2.36	0.41
1:C:415:ILE:HG22	1:C:417:ALA:HB2	2.02	0.41
1:D:346:LEU:HD22	1:D:349:LEU:HD22	2.03	0.41
3:M:188:LYS:HD2	3:M:188:LYS:H	1.85	0.41
1:E:57:ARG:O	1:E:61:ARG:NH1	2.54	0.41
1:E:394:ALA:HB1	1:E:414:ILE:HG22	2.01	0.41
1:F:294:PRO:O	1:F:296:ILE:HG23	2.20	0.41
3:L:202:ARG:HD3	3:M:293:ARG:HG3	2.02	0.41
1:C:216:LYS:HG3	1:C:217:THR:N	2.35	0.41
3:M:84:HIS:HB2	3:M:99:TYR:CZ	2.55	0.41
3:N:44:VAL:HG21	3:N:255:GLN:HG3	2.03	0.41
1:A:374:ARG:N	1:A:375:PRO:CA	2.84	0.41
1:D:103:GLU:N	1:D:104:TYR:HB2	2.36	0.41
3:K:68:SER:HB3	3:K:84:HIS:CE1	2.56	0.41
3:J:239:TRP:CD1	3:J:241:ARG:HG3	2.55	0.41
1:D:135:GLU:HG2	1:D:138:VAL:HB	2.03	0.41
1:F:349:LEU:HG	1:F:357:VAL:HG21	2.03	0.41
1:D:413:GLU:HG2	1:D:428:GLN:HA	2.03	0.41
1:F:139:LEU:HD23	1:F:142:GLU:HG2	2.03	0.41
1:B:206:ILE:HA	1:B:392:ILE:HG23	2.03	0.41
3:L:39:LYS:H	3:L:39:LYS:HG2	1.62	0.41
3:L:220:VAL:O	3:L:221:LYS:HG3	2.21	0.41
3:J:97:GLU:CB	3:J:219:MET:SD	3.09	0.41
1:A:441:LEU:C	3:J:56:LYS:NZ	2.73	0.41
1:D:104:TYR:N	1:D:106:ALA:N	2.68	0.41
1:C:339:VAL:HG22	1:C:343:SER:HB2	2.03	0.41
1:B:132:ARG:C	1:B:134:ASP:HB2	2.41	0.41
1:F:363:LEU:HG	1:F:363:LEU:H	1.62	0.41
1:C:419:GLN:CG	1:C:424:VAL:HA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:213:LEU:HD23	3:K:216:LYS:HB2	2.03	0.41
1:A:391:ASP:HB2	1:A:420:ARG:HD2	2.02	0.41
3:O:178:LEU:HD23	3:O:181:ILE:HD12	2.03	0.41
3:N:33:ASP:CG	3:N:61:ILE:HD12	2.41	0.41
3:K:239:TRP:O	3:K:243:GLU:HB2	2.21	0.41
1:B:112:LYS:HB3	1:B:116:ARG:HH22	1.86	0.41
3:M:240:VAL:HG12	3:M:244:VAL:HB	2.01	0.41
1:B:347:LYS:C	1:B:349:LEU:H	2.24	0.41
1:D:226:ASN:C	1:D:231:THR:HG23	2.41	0.41
3:L:37:PHE:CZ	3:L:255:GLN:CA	3.01	0.41
1:F:261:GLN:H	1:F:262:ASN:CA	2.24	0.41
1:B:67:LEU:HD22	1:B:71:THR:HG23	2.03	0.41
1:B:306:ARG:HE	1:E:148:MET:HB3	1.85	0.41
1:E:96:VAL:HA	1:E:97:PRO:HD3	1.82	0.41
1:C:108:ILE:HG13	1:C:108:ILE:H	1.69	0.41
1:F:418:LYS:O	1:F:419:GLN:HB3	2.20	0.41
3:N:249:LEU:HA	3:N:252:ARG:HD2	2.02	0.41
3:O:253:MET:HA	3:O:256:GLN:HG3	2.03	0.41
3:O:136:ILE:H	3:O:136:ILE:HG13	1.66	0.41
1:B:74:LEU:O	1:B:79:GLN:N	2.54	0.41
3:L:221:LYS:HZ3	3:L:248:VAL:HG23	1.69	0.40
3:L:39:LYS:HE2	3:L:39:LYS:HB3	1.64	0.40
3:N:41:ASN:ND2	3:N:44:VAL:HB	2.36	0.40
3:K:271:LYS:CG	3:K:288:ALA:HA	2.50	0.40
1:B:269:THR:O	1:B:271:GLU:N	2.45	0.40
3:N:225:VAL:HG13	3:N:227:MET:SD	2.60	0.40
3:L:242:ASP:N	3:L:242:ASP:OD1	2.54	0.40
1:D:277:THR:O	1:D:281:GLY:HA3	2.21	0.40
3:M:245:ILE:O	3:M:245:ILE:CG2	2.69	0.40
1:B:377:MET:SD	1:B:378:SER:N	2.95	0.40
1:F:25:PHE:HA	1:F:28:PRO:HB3	2.03	0.40
1:C:28:PRO:HB2	1:C:65:VAL:HB	2.03	0.40
3:K:267:PRO:HA	3:K:291:MET:HE2	2.04	0.40
1:E:427:VAL:HG12	1:E:428:GLN:N	2.36	0.40
1:F:125:ILE:HG23	1:F:139:LEU:HD22	2.03	0.40
1:B:256:GLY:HA3	1:B:276:LEU:HD13	2.03	0.40
1:B:37:ILE:HG13	1:B:37:ILE:H	1.72	0.40
3:L:56:LYS:HB3	3:L:87:LEU:CD2	2.51	0.40
3:K:226:LEU:HB3	3:K:252:ARG:CZ	2.50	0.40
1:F:66:ASP:O	1:F:67:LEU:C	2.60	0.40
2:H:461:GLN:HA	2:H:465:ARG:HH21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:LEU:HD22	1:A:438:PHE:CD2	2.53	0.40
1:F:325:ILE:HG12	1:F:342:ILE:HG12	2.02	0.40
2:H:566:GLN:O	2:H:570:GLU:HB2	2.21	0.40
1:A:319:ILE:HG22	1:A:320:ASP:N	2.36	0.40
1:C:229:THR:HG22	1:C:286:ALA:CB	2.51	0.40
2:G:472:MSE:HB2	2:G:472:MSE:HE2	1.94	0.40
1:B:308:LEU:HD23	1:B:314:LEU:HD12	2.03	0.40
1:D:381:ARG:HA	1:D:381:ARG:HD2	1.72	0.40
3:M:50:ILE:HG21	3:N:47:GLN:C	2.36	0.40
1:B:248:VAL:C	1:B:250:ARG:H	2.24	0.40
1:E:208:VAL:HG11	1:E:219:PHE:CE2	2.56	0.40
2:H:487:GLY:HA2	2:H:488:ARG:CB	2.34	0.40
1:D:395:PHE:HB2	1:D:415:ILE:H	1.86	0.40
1:E:262:ASN:OD1	1:E:265:THR:HG22	2.21	0.40
1:B:15:GLU:N	1:B:18:GLN:HB2	2.36	0.40
3:M:269:GLU:O	3:M:273:HIS:CD2	2.74	0.40
3:M:261:PHE:CD2	3:M:294:ILE:HG23	2.57	0.40
3:O:212:THR:C	3:O:214:GLU:H	2.24	0.40
3:L:143:ALA:HB3	3:L:301:ILE:HG21	2.03	0.40
2:H:481:VAL:O	2:H:485:ILE:N	2.55	0.40
3:K:219:MET:SD	3:K:223:THR:HG23	2.61	0.40
3:K:130:THR:HB	3:K:131:PHE:H	1.65	0.40
3:L:40:GLU:C	3:L:256:GLN:HG3	2.41	0.40
1:D:74:LEU:O	1:D:79:GLN:N	2.55	0.40
1:B:221:LEU:HD22	1:B:251:MET:HB3	2.04	0.40
1:A:22:GLY:C	1:A:26:LEU:HG	2.42	0.40
3:O:144:MET:SD	3:O:164:LEU:HD22	2.61	0.40
1:A:52:PHE:HA	1:A:55:MET:CB	2.51	0.40
1:C:300:ASP:O	1:C:304:LYS:N	2.55	0.40
1:B:384:GLY:O	1:B:386:ILE:HG13	2.22	0.40
1:A:224:ALA:O	1:A:228:ALA:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	A	348/454 (77%)	243 (70%)	79 (23%)	26 (8%)	1	20
1	B	348/454 (77%)	231 (66%)	95 (27%)	22 (6%)	2	25
1	C	348/454 (77%)	228 (66%)	90 (26%)	30 (9%)	1	17
1	D	348/454 (77%)	234 (67%)	87 (25%)	27 (8%)	1	20
1	E	348/454 (77%)	238 (68%)	82 (24%)	28 (8%)	1	19
1	F	348/454 (77%)	222 (64%)	96 (28%)	30 (9%)	1	17
2	G	136/143 (95%)	100 (74%)	28 (21%)	8 (6%)	2	26
2	H	136/143 (95%)	88 (65%)	40 (29%)	8 (6%)	2	26
2	I	136/143 (95%)	99 (73%)	32 (24%)	5 (4%)	4	37
3	J	233/317 (74%)	166 (71%)	55 (24%)	12 (5%)	2	29
3	K	238/317 (75%)	175 (74%)	47 (20%)	16 (7%)	1	23
3	L	235/317 (74%)	162 (69%)	60 (26%)	13 (6%)	2	28
3	M	237/317 (75%)	172 (73%)	52 (22%)	13 (6%)	2	28
3	N	232/317 (73%)	179 (77%)	41 (18%)	12 (5%)	2	29
3	O	240/317 (76%)	176 (73%)	57 (24%)	7 (3%)	6	42
All	All	3911/5055 (77%)	2713 (69%)	941 (24%)	257 (7%)	1	24

All (257) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	PRO
1	A	203	SER
1	A	259	ASN
1	A	294	PRO
1	A	325	ILE
1	B	64	PRO
1	B	102	VAL
1	B	133	GLU
1	B	287	GLY
1	C	63	GLU
1	C	102	VAL
1	C	105	TYR
1	C	134	ASP
1	C	203	SER
1	C	277	THR

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Mol	Chain	Res	Type
1	C	294	PRO
1	C	322	LEU
1	C	382	GLU
1	C	386	ILE
1	D	63	GLU
1	D	101	ASN
1	D	135	GLU
1	D	294	PRO
1	E	63	GLU
1	E	64	PRO
1	E	97	PRO
1	E	105	TYR
1	E	134	ASP
1	F	63	GLU
1	F	64	PRO
1	F	78	GLU
1	F	187	PRO
1	F	294	PRO
1	F	383	SER
2	G	521	PRO
2	H	521	PRO
2	H	534	LEU
2	H	545	LEU
2	H	572	GLU
2	I	521	PRO
2	I	551	HIS
3	J	156	ASN
3	J	189	GLU
3	J	257	LEU
3	L	61	ILE
3	M	46	ASP
3	M	230	ASP
3	N	47	GLN
3	N	152	LEU
3	N	230	ASP
3	N	275	THR
3	O	189	GLU
3	O	298	ALA
1	A	22	GLY
1	A	105	TYR
1	A	134	ASP
1	A	212	PRO

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Mol	Chain	Res	Type
1	A	323	GLN
1	A	386	ILE
1	B	135	GLU
1	B	136	ILE
1	B	294	PRO
1	B	378	SER
1	C	27	ASP
1	C	136	ILE
1	C	214	VAL
1	C	259	ASN
1	D	78	GLU
1	D	103	GLU
1	D	136	ILE
1	D	203	SER
1	D	227	VAL
1	D	254	ALA
1	D	423	PRO
1	D	433	LYS
1	E	29	ALA
1	E	78	GLU
1	E	140	LEU
1	E	191	THR
1	F	46	ALA
1	F	67	LEU
1	F	98	THR
1	F	102	VAL
1	F	103	GLU
1	F	134	ASP
1	F	136	ILE
1	F	189	GLY
1	F	295	SER
1	F	360	LEU
2	G	486	GLY
2	H	522	GLY
2	H	547	ASP
2	H	575	LYS
3	J	160	LYS
3	J	298	ALA
3	K	66	ASN
3	K	156	ASN
3	K	192	SER
3	L	64	SER

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Mol	Chain	Res	Type
3	L	66	ASN
3	L	69	TYR
3	L	172	VAL
3	L	275	THR
3	M	48	LYS
3	M	212	THR
3	N	158	THR
3	O	154	SER
1	A	324	LEU
1	A	355	VAL
1	A	376	MET
1	B	78	GLU
1	B	86	VAL
1	B	105	TYR
1	B	212	PRO
1	B	300	ASP
1	B	385	SER
1	C	201	GLN
1	C	232	ASN
1	C	271	GLU
1	C	287	GLY
1	C	314	LEU
1	C	385	SER
1	C	391	ASP
1	D	46	ALA
1	D	105	TYR
1	D	147	ILE
1	D	195	ARG
1	D	256	GLY
1	D	260	ALA
1	D	285	ASN
1	E	84	GLY
1	E	104	TYR
1	E	185	GLY
1	E	295	SER
1	E	433	LYS
1	F	36	GLU
1	F	77	SER
1	F	196	MET
1	F	392	ILE
1	F	419	GLN
2	G	498	ALA

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Mol	Chain	Res	Type
3	J	256	GLN
3	K	46	ASP
3	K	65	LYS
3	K	210	ASP
3	K	211	GLN
3	K	212	THR
3	K	256	GLN
3	K	286	LYS
3	L	122	ILE
3	L	229	ASP
3	M	121	TYR
3	M	256	GLN
3	N	138	ASP
3	O	234	GLU
1	A	233	GLU
1	A	246	GLN
1	A	256	GLY
1	A	354	GLU
1	B	63	GLU
1	B	314	LEU
1	C	25	PHE
1	C	42	ASP
1	C	95	ALA
1	C	96	VAL
1	C	128	ASP
1	D	133	GLU
1	D	323	GLN
1	E	91	GLU
1	E	275	LYS
1	E	314	LEU
1	F	29	ALA
1	F	137	ASP
1	F	209	ALA
1	F	270	PRO
1	F	301	ILE
2	G	520	ILE
2	G	544	GLU
2	G	575	LYS
2	H	520	ILE
2	I	517	ILE
2	I	525	GLN
3	J	135	ASP

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Mol	Chain	Res	Type
3	J	138	ASP
3	J	139	PRO
3	K	140	SER
3	L	127	LEU
3	L	232	GLY
3	M	158	THR
3	M	210	ASP
3	M	238	SER
3	M	298	ALA
3	O	132	GLN
1	A	103	GLU
1	A	273	TRP
1	A	391	ASP
1	B	103	GLU
1	C	76	ALA
1	C	416	ILE
1	D	97	PRO
1	D	102	VAL
1	E	83	ILE
1	E	98	THR
1	E	294	PRO
1	F	203	SER
1	F	240	LEU
2	G	522	GLY
2	I	523	GLU
3	J	132	GLN
3	J	174	LYS
3	J	258	PRO
3	L	256	GLN
3	N	145	PHE
3	O	297	LEU
1	A	275	LYS
1	B	71	THR
1	B	244	ALA
1	B	259	ASN
1	E	24	VAL
1	E	33	PRO
1	E	119	ILE
1	E	120	ARG
1	E	323	GLN
2	G	542	GLU
3	K	171	GLY

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Mol	Chain	Res	Type
3	K	181	ILE
3	L	88	VAL
3	L	136	ILE
3	N	240	VAL
3	N	258	PRO
1	B	313	GLY
1	D	212	PRO
1	E	212	PRO
1	E	215	GLY
1	F	315	GLY
1	F	339	VAL
3	M	171	GLY
3	M	225	VAL
1	A	415	ILE
1	C	114	VAL
1	D	339	VAL
1	E	136	ILE
3	O	172	VAL
1	D	427	VAL
3	N	197	VAL
3	N	285	VAL
1	A	214	VAL
1	A	313	GLY
3	K	50	ILE
3	K	128	GLY
3	K	285	VAL
3	M	224	PRO
3	N	244	VAL
1	B	270	PRO
1	D	386	ILE
1	C	375	PRO
1	A	375	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	A	298/386 (77%)	260 (87%)	38 (13%)	5 29
1	B	298/386 (77%)	264 (89%)	34 (11%)	7 33
1	C	298/386 (77%)	263 (88%)	35 (12%)	7 32
1	D	298/386 (77%)	260 (87%)	38 (13%)	5 29
1	E	298/386 (77%)	260 (87%)	38 (13%)	5 29
1	F	298/386 (77%)	263 (88%)	35 (12%)	7 32
2	G	117/116 (101%)	105 (90%)	12 (10%)	9 37
2	H	117/116 (101%)	109 (93%)	8 (7%)	20 57
2	I	117/116 (101%)	102 (87%)	15 (13%)	5 29
3	J	221/289 (76%)	199 (90%)	22 (10%)	9 38
3	K	225/289 (78%)	197 (88%)	28 (12%)	6 30
3	L	223/289 (77%)	203 (91%)	20 (9%)	12 44
3	M	224/289 (78%)	208 (93%)	16 (7%)	18 55
3	N	220/289 (76%)	199 (90%)	21 (10%)	11 41
3	O	227/289 (78%)	210 (92%)	17 (8%)	17 54
All	All	3479/4398 (79%)	3102 (89%)	377 (11%)	8 36

All (377) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	44	TYR
1	A	45	ARG
1	A	53	HIS
1	A	56	LEU
1	A	61	ARG
1	A	67	LEU
1	A	79	GLN
1	A	105	TYR
1	A	115	LEU
1	A	140	LEU
1	A	146	LYS
1	A	183	ILE
1	A	188	THR
1	A	194	ASP
1	A	201	GLN
1	A	225	GLN
1	A	231	THR

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Mol	Chain	Res	Type
1	A	233	GLU
1	A	240	LEU
1	A	247	LEU
1	A	258	ILE
1	A	261	GLN
1	A	263	LEU
1	A	283	LEU
1	A	292	ASP
1	A	293	THR
1	A	298	VAL
1	A	300	ASP
1	A	338	GLU
1	A	351	ARG
1	A	355	VAL
1	A	376	MET
1	A	380	ILE
1	A	396	LEU
1	A	397	TYR
1	A	429	LEU
1	A	441	LEU
1	B	15	GLU
1	B	20	VAL
1	B	79	GLN
1	B	80	LEU
1	B	87	SER
1	B	88	TYR
1	B	101	ASN
1	B	128	ASP
1	B	139	LEU
1	B	147	ILE
1	B	211	ARG
1	B	217	THR
1	B	233	GLU
1	B	247	LEU
1	B	259	ASN
1	B	290	ILE
1	B	292	ASP
1	B	293	THR
1	B	300	ASP
1	B	306	ARG
1	B	321	TYR
1	B	324	LEU

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Mol	Chain	Res	Type
1	B	325	ILE
1	B	355	VAL
1	B	376	MET
1	B	381	ARG
1	B	388	GLN
1	B	389	ASP
1	B	391	ASP
1	B	395	PHE
1	B	397	TYR
1	B	413	GLU
1	B	414	ILE
1	B	436	ASN
1	C	27	ASP
1	C	48	HIS
1	C	57	ARG
1	C	60	ASP
1	C	63	GLU
1	C	66	ASP
1	C	74	LEU
1	C	80	LEU
1	C	101	ASN
1	C	105	TYR
1	C	115	LEU
1	C	120	ARG
1	C	142	GLU
1	C	145	ARG
1	C	148	MET
1	C	188	THR
1	C	191	THR
1	C	197	THR
1	C	201	GLN
1	C	267	LYS
1	C	293	THR
1	C	296	ILE
1	C	298	VAL
1	C	314	LEU
1	C	322	LEU
1	C	324	LEU
1	C	339	VAL
1	C	351	ARG
1	C	376	MET
1	C	377	MET

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Mol	Chain	Res	Type
1	C	381	ARG
1	C	392	ILE
1	C	397	TYR
1	C	416	ILE
1	C	441	LEU
1	D	32	VAL
1	D	45	ARG
1	D	57	ARG
1	D	63	GLU
1	D	80	LEU
1	D	86	VAL
1	D	105	TYR
1	D	107	ARG
1	D	123	THR
1	D	127	GLN
1	D	139	LEU
1	D	142	GLU
1	D	148	MET
1	D	184	THR
1	D	192	GLU
1	D	216	LYS
1	D	219	PHE
1	D	231	THR
1	D	258	ILE
1	D	262	ASN
1	D	273	TRP
1	D	278	MET
1	D	297	ARG
1	D	316	MET
1	D	320	ASP
1	D	374	ARG
1	D	376	MET
1	D	383	SER
1	D	387	GLU
1	D	388	GLN
1	D	391	ASP
1	D	395	PHE
1	D	396	LEU
1	D	416	ILE
1	D	426	THR
1	D	427	VAL
1	D	431	PHE

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Mol	Chain	Res	Type
1	D	439	VAL
1	E	24	VAL
1	E	41	GLU
1	E	44	TYR
1	E	61	ARG
1	E	67	LEU
1	E	70	VAL
1	E	80	LEU
1	E	86	VAL
1	E	98	THR
1	E	110	GLU
1	E	111	GLU
1	E	124	SER
1	E	137	ASP
1	E	139	LEU
1	E	145	ARG
1	E	147	ILE
1	E	190	PHE
1	E	191	THR
1	E	207	ILE
1	E	216	LYS
1	E	225	GLN
1	E	240	LEU
1	E	247	LEU
1	E	252	LEU
1	E	261	GLN
1	E	267	LYS
1	E	296	ILE
1	E	297	ARG
1	E	298	VAL
1	E	314	LEU
1	E	324	LEU
1	E	355	VAL
1	E	374	ARG
1	E	380	ILE
1	E	381	ARG
1	E	385	SER
1	E	388	GLN
1	E	396	LEU
1	F	25	PHE
1	F	37	ILE
1	F	50	LYS

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Mol	Chain	Res	Type
1	F	78	GLU
1	F	91	GLU
1	F	103	GLU
1	F	105	TYR
1	F	125	ILE
1	F	130	TYR
1	F	131	THR
1	F	136	ILE
1	F	142	GLU
1	F	183	ILE
1	F	193	LEU
1	F	204	ASP
1	F	223	ILE
1	F	247	LEU
1	F	263	LEU
1	F	290	ILE
1	F	291	ASP
1	F	297	ARG
1	F	298	VAL
1	F	301	ILE
1	F	302	ARG
1	F	308	LEU
1	F	322	LEU
1	F	326	GLN
1	F	340	SER
1	F	355	VAL
1	F	363	LEU
1	F	377	MET
1	F	379	ASP
1	F	380	ILE
1	F	381	ARG
1	F	431	PHE
2	G	456	LEU
2	G	464	GLU
2	G	466	LEU
2	G	472	MSE
2	G	497	LEU
2	G	534	LEU
2	G	546	GLU
2	G	550	ARG
2	G	551	HIS
2	G	585	LYS

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Mol	Chain	Res	Type
2	G	589	GLU
2	G	593	MSE
2	H	456	LEU
2	H	457	LEU
2	H	474	SER
2	H	500	TYR
2	H	512	ASP
2	H	536	ILE
2	H	539	ASP
2	H	590	MSE
2	I	482	GLN
2	I	500	TYR
2	I	505	TYR
2	I	529	SER
2	I	540	VAL
2	I	542	GLU
2	I	548	TYR
2	I	550	ARG
2	I	561	LEU
2	I	565	GLU
2	I	570	GLU
2	I	572	GLU
2	I	578	LEU
2	I	587	MSE
2	I	593	MSE
3	J	54	LEU
3	J	62	GLU
3	J	67	CYS
3	J	86	LYS
3	J	116	LEU
3	J	122	ILE
3	J	130	THR
3	J	135	ASP
3	J	148	VAL
3	J	150	ASP
3	J	158	THR
3	J	193	MET
3	J	200	PHE
3	J	214	GLU
3	J	227	MET
3	J	231	ILE
3	J	257	LEU

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Mol	Chain	Res	Type
3	J	263	SER
3	J	264	ASN
3	J	274	PHE
3	J	290	LEU
3	J	303	LEU
3	K	32	GLN
3	K	48	LYS
3	K	49	MET
3	K	54	LEU
3	K	62	GLU
3	K	64	SER
3	K	68	SER
3	K	86	LYS
3	K	116	LEU
3	K	131	PHE
3	K	134	VAL
3	K	135	ASP
3	K	136	ILE
3	K	152	LEU
3	K	164	LEU
3	K	183	ASN
3	K	213	LEU
3	K	223	THR
3	K	231	ILE
3	K	245	ILE
3	K	268	ASP
3	K	270	LEU
3	K	283	GLU
3	K	284	GLU
3	K	285	VAL
3	K	289	ARG
3	K	290	LEU
3	K	294	ILE
3	L	39	LYS
3	L	54	LEU
3	L	63	GLN
3	L	68	SER
3	L	69	TYR
3	L	70	CYS
3	L	86	LYS
3	L	99	TYR
3	L	122	ILE

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Mol	Chain	Res	Type
3	L	138	ASP
3	L	181	ILE
3	L	195	VAL
3	L	196	TYR
3	L	202	ARG
3	L	213	LEU
3	L	226	LEU
3	L	242	ASP
3	L	252	ARG
3	L	270	LEU
3	L	306	GLU
3	M	62	GLU
3	M	67	CYS
3	M	86	LYS
3	M	113	GLN
3	M	122	ILE
3	M	138	ASP
3	M	183	ASN
3	M	185	LEU
3	M	204	LEU
3	M	223	THR
3	M	227	MET
3	M	228	LEU
3	M	237	THR
3	M	243	GLU
3	M	270	LEU
3	M	290	LEU
3	N	46	ASP
3	N	54	LEU
3	N	62	GLU
3	N	66	ASN
3	N	86	LYS
3	N	117	MET
3	N	125	ASP
3	N	150	ASP
3	N	152	LEU
3	N	200	PHE
3	N	203	GLU
3	N	230	ASP
3	N	234	GLU
3	N	239	TRP
3	N	242	ASP

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Mol	Chain	Res	Type
3	N	261	PHE
3	N	268	ASP
3	N	275	THR
3	N	295	LEU
3	N	296	TYR
3	N	306	GLU
3	O	38	LEU
3	O	54	LEU
3	O	62	GLU
3	O	67	CYS
3	O	86	LYS
3	O	114	GLN
3	O	152	LEU
3	O	155	TYR
3	O	184	GLU
3	O	196	TYR
3	O	200	PHE
3	O	205	LYS
3	O	212	THR
3	O	231	ILE
3	O	242	ASP
3	O	292	GLU
3	O	303	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	48	HIS
1	A	79	GLN
1	A	226	ASN
1	A	246	GLN
1	A	259	ASN
1	B	222	ASN
1	B	226	ASN
1	B	259	ASN
1	B	419	GLN
1	B	421	ASN
1	C	127	GLN
1	C	222	ASN
1	C	226	ASN
1	C	259	ASN

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Mol	Chain	Res	Type
1	C	262	ASN
1	C	421	ASN
1	C	436	ASN
1	D	53	HIS
1	D	245	GLN
1	D	421	ASN
1	E	48	HIS
1	E	101	ASN
1	E	323	GLN
1	E	388	GLN
1	F	49	GLN
1	F	79	GLN
1	F	225	GLN
2	G	462	ASN
2	G	494	HIS
2	G	554	ASN
2	H	494	HIS
2	I	551	HIS
3	J	63	GLN
3	J	84	HIS
3	J	113	GLN
3	J	183	ASN
3	J	255	GLN
3	J	256	GLN
3	K	47	GLN
3	K	63	GLN
3	K	84	HIS
3	K	255	GLN
3	K	256	GLN
3	K	273	HIS
3	L	84	HIS
3	L	124	GLN
3	L	256	GLN
3	M	32	GLN
3	M	63	GLN
3	M	84	HIS
3	M	113	GLN
3	M	147	HIS
3	M	273	HIS
3	N	47	GLN
3	N	63	GLN
3	N	114	GLN

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Mol	Chain	Res	Type
3	N	133	GLN
3	N	218	ASN
3	O	63	GLN
3	O	84	HIS
3	O	156	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	A	358/454 (78%)	-0.46	2 (0%) 90 87	81, 134, 167, 169	0
1	B	358/454 (78%)	-0.50	1 (0%) 94 92	100, 138, 156, 171	0
1	C	358/454 (78%)	-0.48	2 (0%) 90 87	87, 123, 164, 174	0
1	D	358/454 (78%)	-0.46	0 100 100	81, 130, 191, 194	0
1	E	358/454 (78%)	-0.49	3 (0%) 87 83	65, 124, 160, 176	0
1	F	358/454 (78%)	-0.38	0 100 100	77, 142, 174, 175	0
2	G	132/143 (92%)	-0.61	0 100 100	106, 130, 143, 145	0
2	H	132/143 (92%)	-0.73	0 100 100	78, 120, 134, 135	0
2	I	132/143 (92%)	-0.56	0 100 100	107, 128, 149, 149	0
3	J	245/317 (77%)	0.24	11 (4%) 37 36	120, 170, 188, 195	0
3	K	248/317 (78%)	-0.02	3 (1%) 81 75	120, 171, 186, 200	0
3	L	247/317 (77%)	0.12	7 (2%) 56 52	120, 172, 201, 204	0
3	M	247/317 (77%)	0.09	10 (4%) 42 40	120, 163, 178, 182	0
3	N	244/317 (76%)	0.21	11 (4%) 37 36	120, 180, 194, 196	0
3	O	250/317 (78%)	0.08	17 (6%) 20 22	120, 160, 178, 179	0
All	All	4025/5055 (79%)	-0.26	67 (1%) 73 67	65, 140, 186, 204	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	203	SER	4.9
3	J	63	GLN	4.4
3	N	95	ASP	3.7
1	E	260	ALA	3.7
3	J	64	SER	3.6
3	O	100	GLU	3.5
3	L	97	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
3	O	39	LYS	3.2
1	A	362	GLN	3.2
3	N	255	GLN	3.2
3	N	160	LYS	3.2
3	J	95	ASP	3.1
3	N	189	GLU	3.1
3	J	272	HIS	3.1
3	O	91	GLY	3.0
3	O	159	GLY	3.0
3	L	62	GLU	2.9
3	M	68	SER	2.8
3	O	69	TYR	2.8
3	J	62	GLU	2.8
1	A	440	ASN	2.8
3	O	93	SER	2.7
3	L	59	GLU	2.7
3	O	161	GLY	2.7
3	O	88	VAL	2.6
3	L	85	PRO	2.5
3	O	104	LYS	2.5
3	N	93	SER	2.5
3	O	68	SER	2.5
3	J	93	SER	2.5
3	K	273	HIS	2.4
3	M	162	LYS	2.4
1	B	267	LYS	2.4
3	O	70	CYS	2.4
3	J	51	GLU	2.4
3	N	87	LEU	2.4
3	O	95	ASP	2.4
3	K	228	LEU	2.3
3	O	92	ARG	2.3
1	E	210	ALA	2.3
3	N	56	LYS	2.3
3	M	56	LYS	2.3
3	K	46	ASP	2.3
3	M	55	ASN	2.3
3	N	47	GLN	2.2
3	L	48	LYS	2.2
3	M	163	GLY	2.2
3	N	161	GLY	2.2
3	O	223	THR	2.2

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Mol	Chain	Res	Type	RSRZ
3	M	82	GLY	2.1
3	L	98	TYR	2.1
3	O	52	LYS	2.1
3	M	62	GLU	2.1
3	J	33	ASP	2.1
3	L	222	THR	2.1
3	N	254	SER	2.1
3	M	298	ALA	2.1
3	O	42	GLU	2.1
3	N	42	GLU	2.1
3	M	52	LYS	2.1
3	M	86	LYS	2.0
3	J	90	ASN	2.0
1	C	204	ASP	2.0
1	E	313	GLY	2.0
3	O	90	ASN	2.0
3	J	59	GLU	2.0
3	J	168	GLY	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 carbohydrates 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.