Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:00 AM GMT

PDB ID	:	3GLH
Title	:	Crystal Structure of the E. coli clamp loader bound to Psi Peptide
Authors	:	Kazmirski, S.L.; Simonetta, K.R.; Kuriyan, J.
Deposited on	:	2009-03-12
Resolution	:	3.89 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:

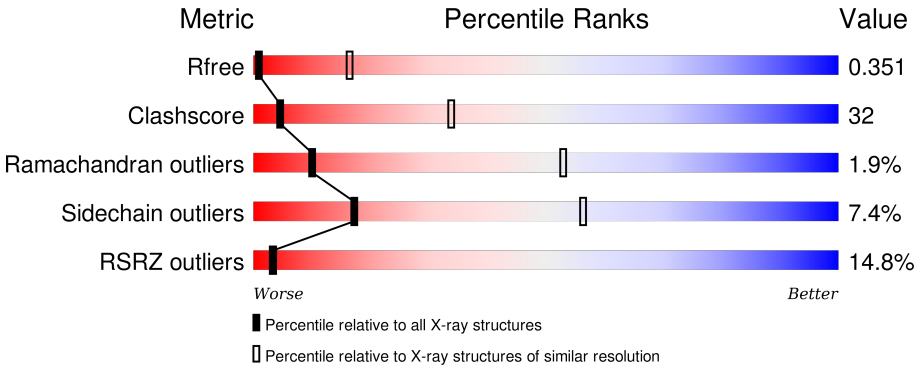
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.89 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	1014 (4.28-3.52)
Clashscore	102246	1031 (4.24-3.56)
Ramachandran outliers	100387	1012 (4.26-3.54)
Sidechain outliers	100360	1004 (4.26-3.54)
RSRZ outliers	91569	1018 (4.28-3.52)

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	343	9% 51% 41% 5%
1	F	343	50% 51% 41% 6%
1	K	343	7% 52% 39% 5%
2	B	376	10% 58% 33% 5%
2	C	376	6% 56% 39%

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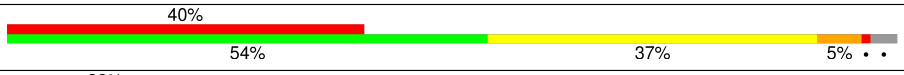
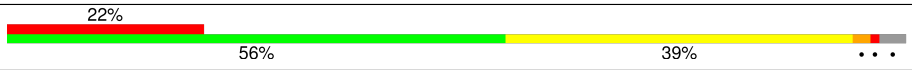
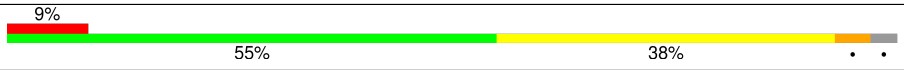
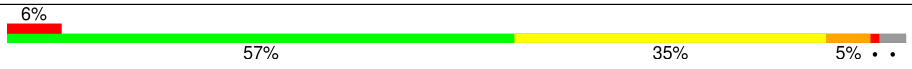
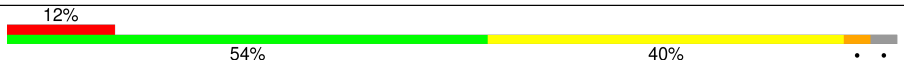
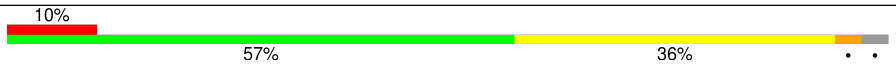
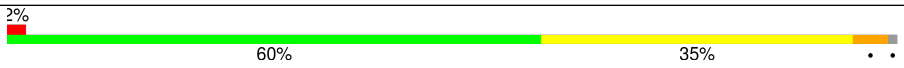
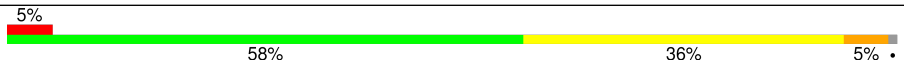
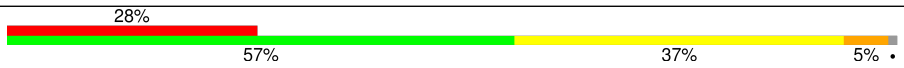
Mol	Chain	Length	Quality of chain
2	D	376	
2	G	376	
2	H	376	
2	I	376	
2	L	376	
2	M	376	
2	N	376	
3	E	334	
3	J	334	
3	O	334	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 41322 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 DNA polymerase III subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2670	1692	484	484	10			
1	F	336	Total	C	N	O	S	0	0	0
			2670	1692	484	484	10			
1	K	336	Total	C	N	O	S	0	0	0
			2670	1692	484	484	10			

- Molecule 2 is a protein called DNA polymerase III subunit tau.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	364	Total	C	N	O	S	0	0	0
			2841	1788	512	525	16			
2	C	364	Total	C	N	O	S	0	0	0
			2841	1788	512	525	16			
2	D	363	Total	C	N	O	S	0	0	0
			2829	1779	511	523	16			
2	G	364	Total	C	N	O	S	0	0	0
			2841	1788	512	525	16			
2	H	364	Total	C	N	O	S	0	0	0
			2841	1788	512	525	16			
2	I	363	Total	C	N	O	S	0	0	0
			2829	1779	511	523	16			
2	L	364	Total	C	N	O	S	0	0	0
			2841	1788	512	525	16			
2	M	364	Total	C	N	O	S	0	0	0
			2841	1788	512	525	16			
2	N	363	Total	C	N	O	S	0	0	0
			2829	1779	511	523	16			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	EXPRESSION TAG	UNP P06710

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	PRO	-	EXPRESSION TAG	UNP P06710
B	0	HIS	-	EXPRESSION TAG	UNP P06710
C	-2	GLY	-	EXPRESSION TAG	UNP P06710
C	-1	PRO	-	EXPRESSION TAG	UNP P06710
C	0	HIS	-	EXPRESSION TAG	UNP P06710
D	-2	GLY	-	EXPRESSION TAG	UNP P06710
D	-1	PRO	-	EXPRESSION TAG	UNP P06710
D	0	HIS	-	EXPRESSION TAG	UNP P06710
G	-2	GLY	-	EXPRESSION TAG	UNP P06710
G	-1	PRO	-	EXPRESSION TAG	UNP P06710
G	0	HIS	-	EXPRESSION TAG	UNP P06710
H	-2	GLY	-	EXPRESSION TAG	UNP P06710
H	-1	PRO	-	EXPRESSION TAG	UNP P06710
H	0	HIS	-	EXPRESSION TAG	UNP P06710
I	-2	GLY	-	EXPRESSION TAG	UNP P06710
I	-1	PRO	-	EXPRESSION TAG	UNP P06710
I	0	HIS	-	EXPRESSION TAG	UNP P06710
L	-2	GLY	-	EXPRESSION TAG	UNP P06710
L	-1	PRO	-	EXPRESSION TAG	UNP P06710
L	0	HIS	-	EXPRESSION TAG	UNP P06710
M	-2	GLY	-	EXPRESSION TAG	UNP P06710
M	-1	PRO	-	EXPRESSION TAG	UNP P06710
M	0	HIS	-	EXPRESSION TAG	UNP P06710
N	-2	GLY	-	EXPRESSION TAG	UNP P06710
N	-1	PRO	-	EXPRESSION TAG	UNP P06710
N	0	HIS	-	EXPRESSION TAG	UNP P06710

- Molecule 3 is a protein called DNA polymerase III subunit delta'.

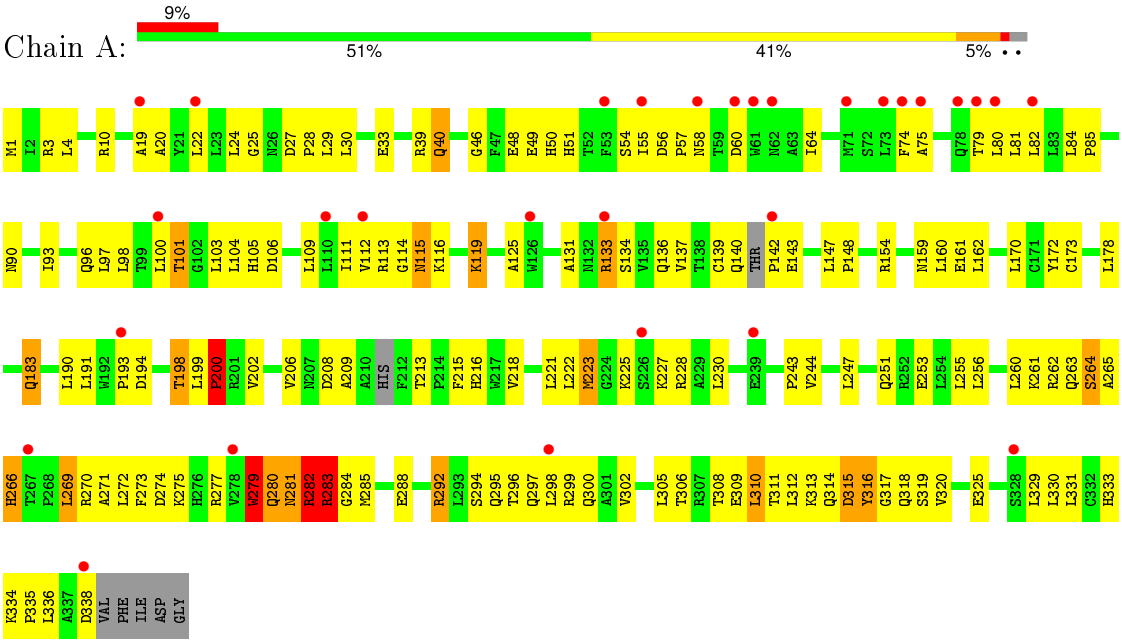
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	332	Total	C	N	O	S	0	0	0
			2593	1650	466	464	13			
3	J	332	Total	C	N	O	S	0	0	0
			2593	1650	466	464	13			
3	O	332	Total	C	N	O	S	0	0	0
			2593	1650	466	464	13			

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.

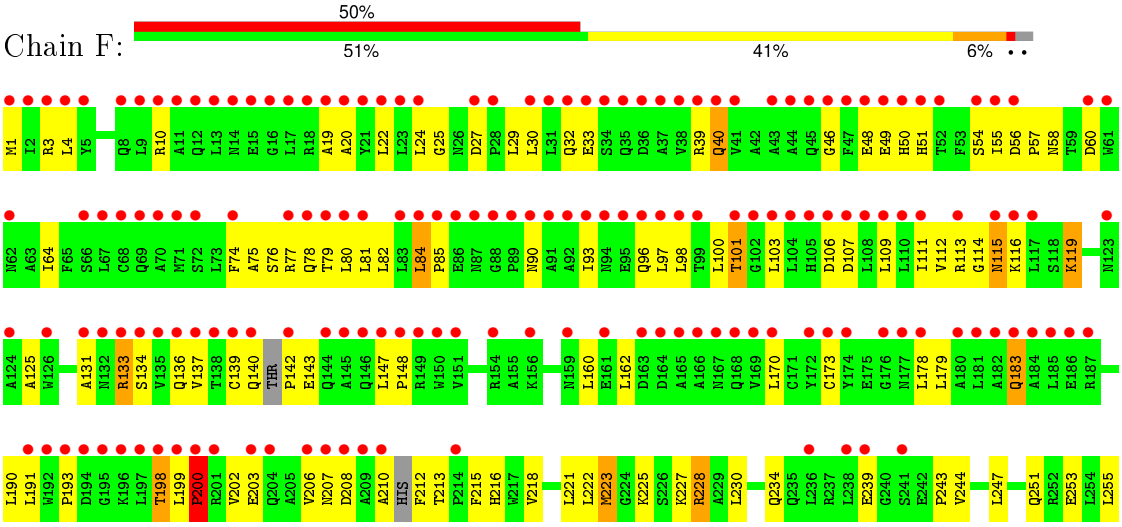
- Molecule 1: DNA polymerase III subunit delta

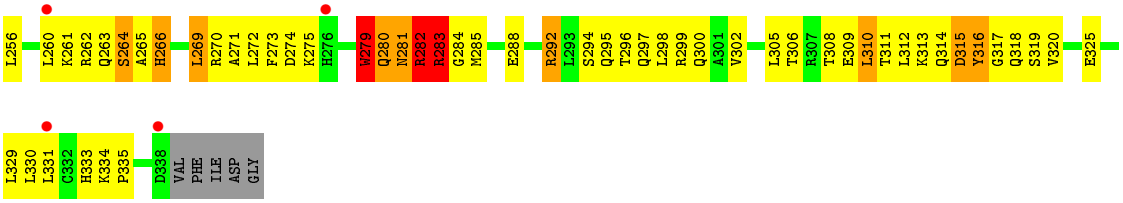
Chain A:



- Molecule 1: DNA polymerase III subunit delta

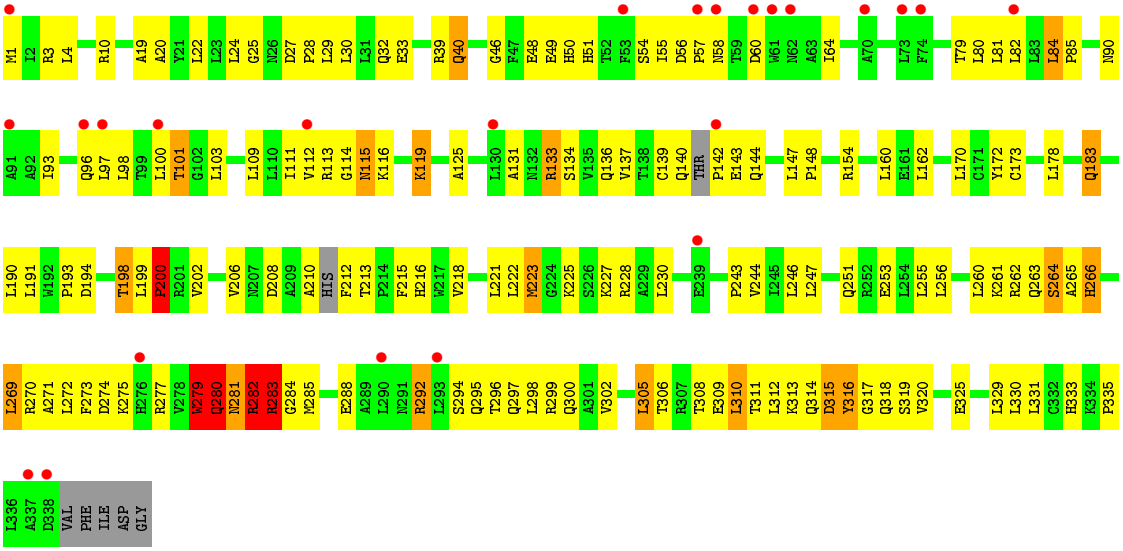
Chain F:





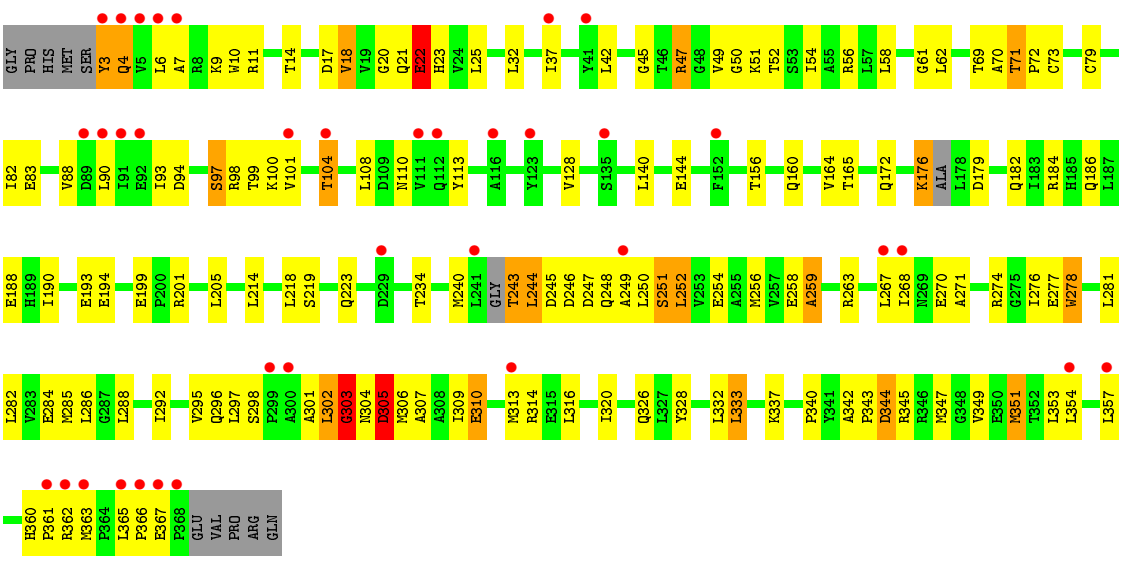
• Molecule 1: DNA polymerase III subunit delta

Chain K:



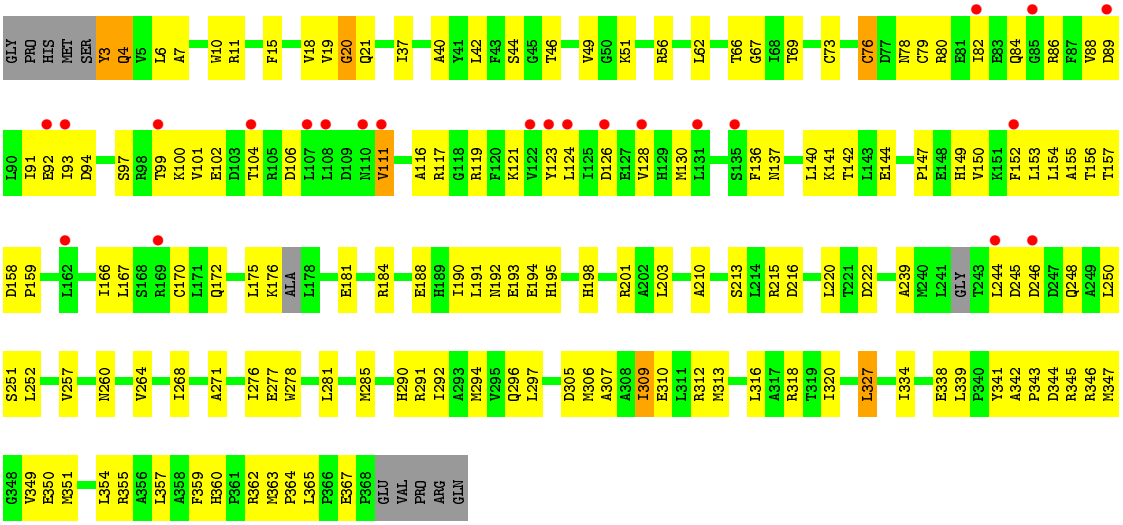
• Molecule 2: DNA polymerase III subunit tau

Chain B:

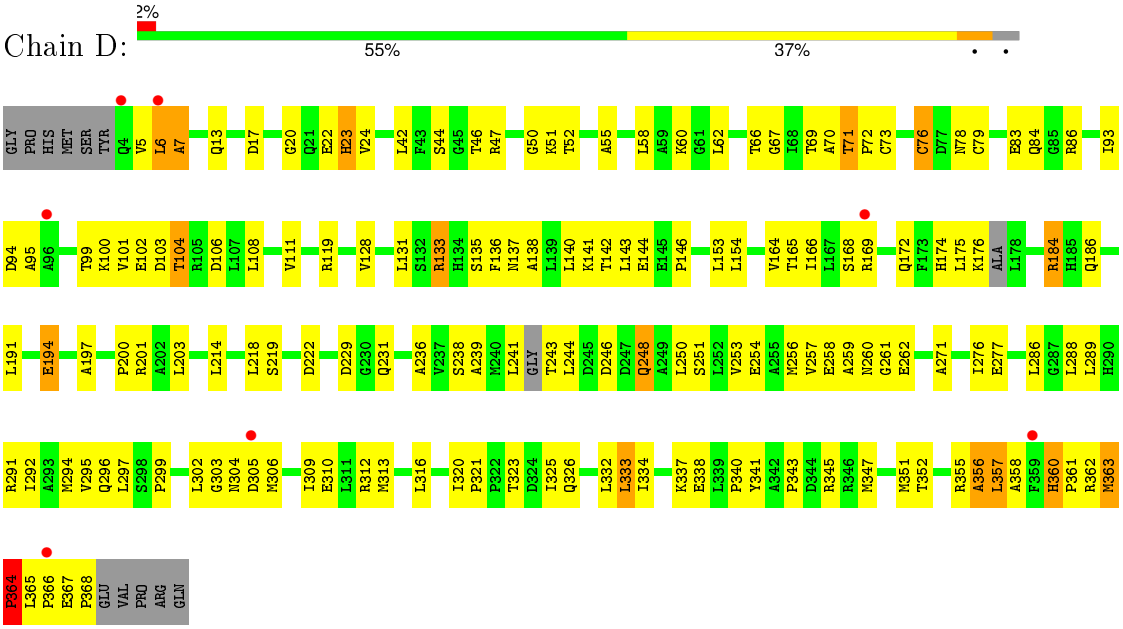


• Molecule 2: DNA polymerase III subunit tau

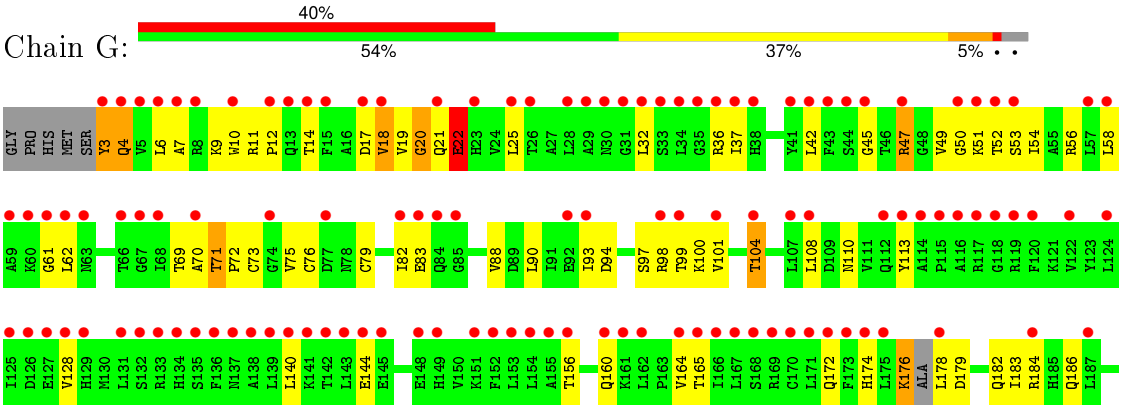
Chain C:

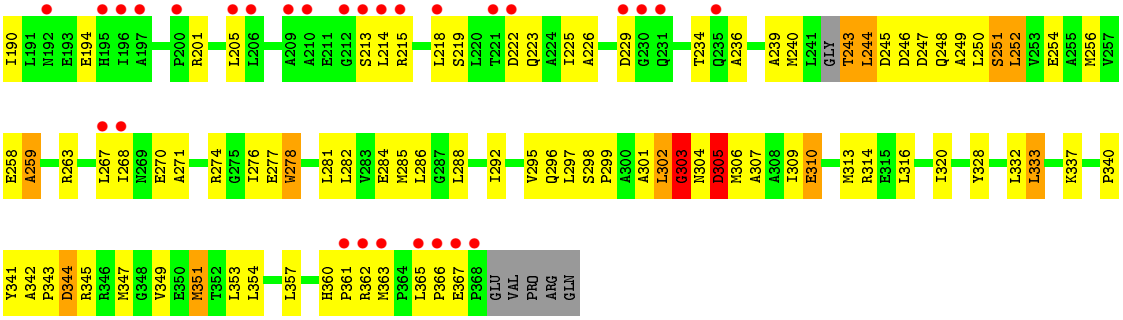


• Molecule 2: DNA polymerase III subunit tau



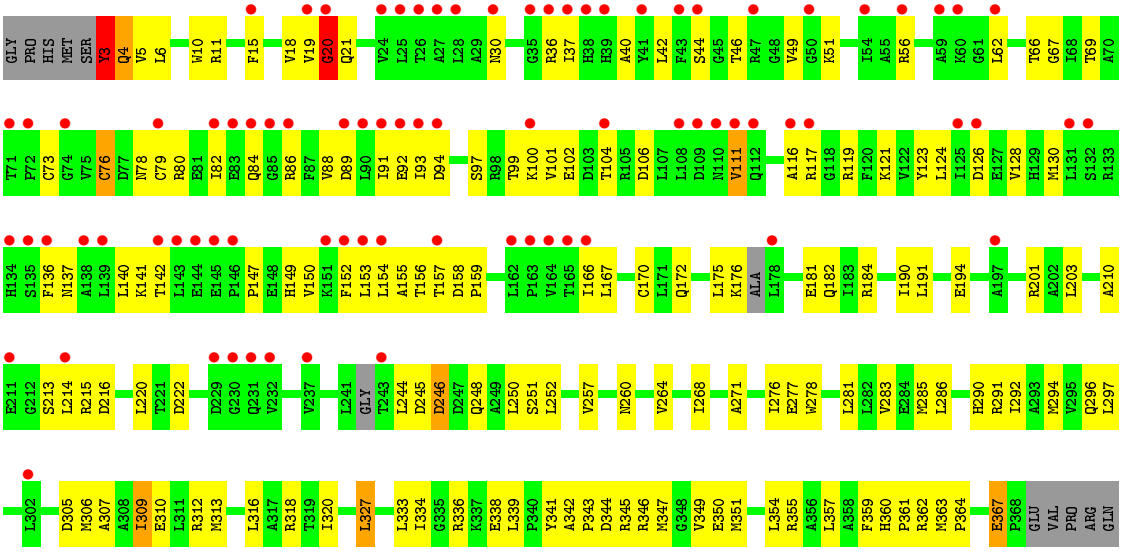
• Molecule 2: DNA polymerase III subunit tau





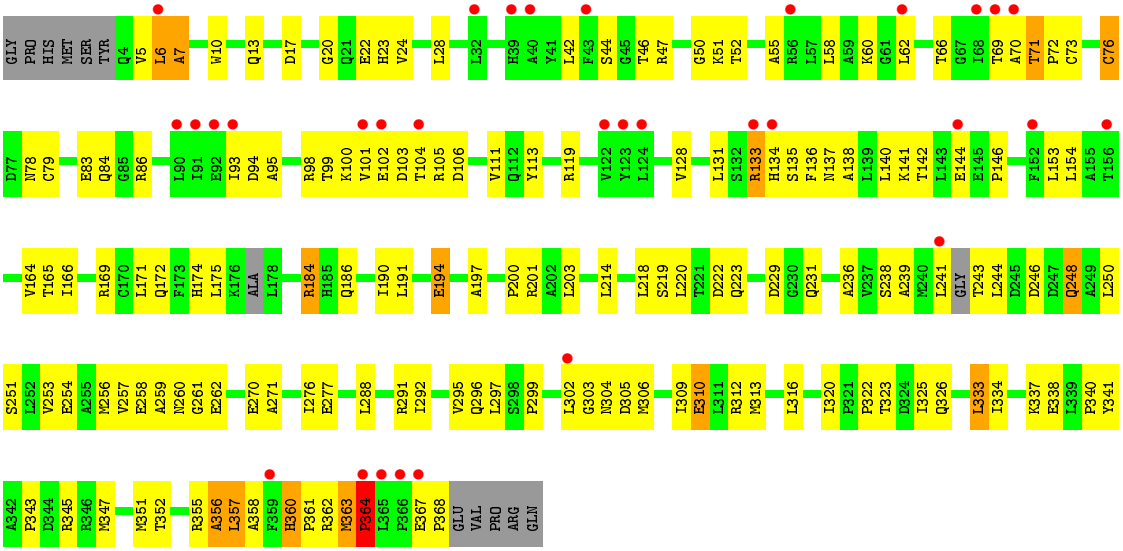
• Molecule 2: DNA polymerase III subunit tau

Chain H:



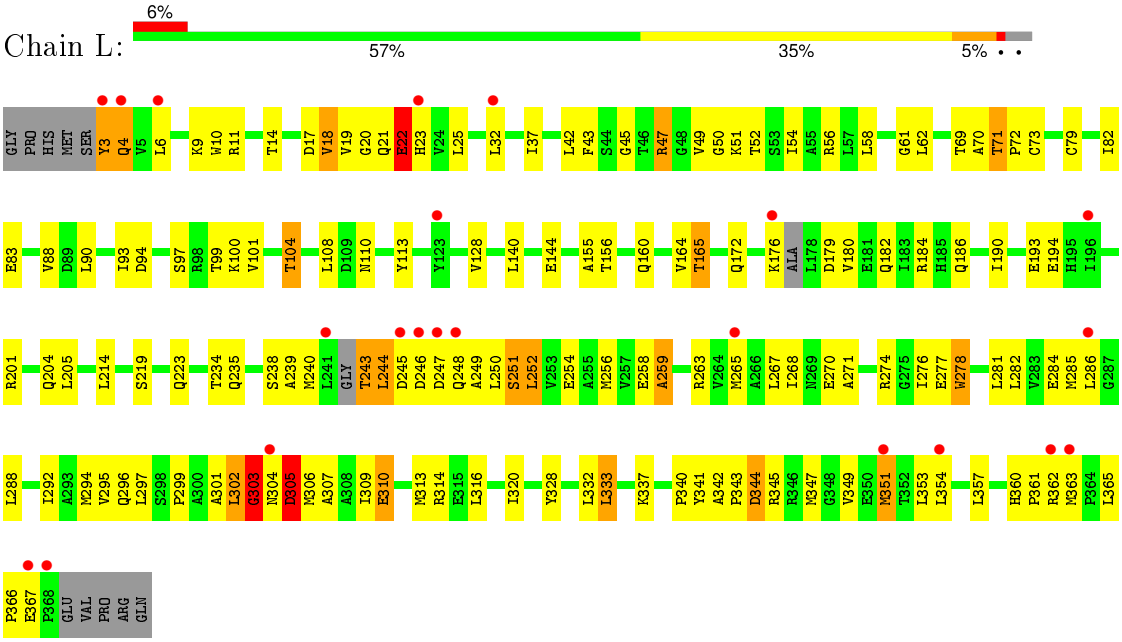
• Molecule 2: DNA polymerase III subunit tau

Chain I:



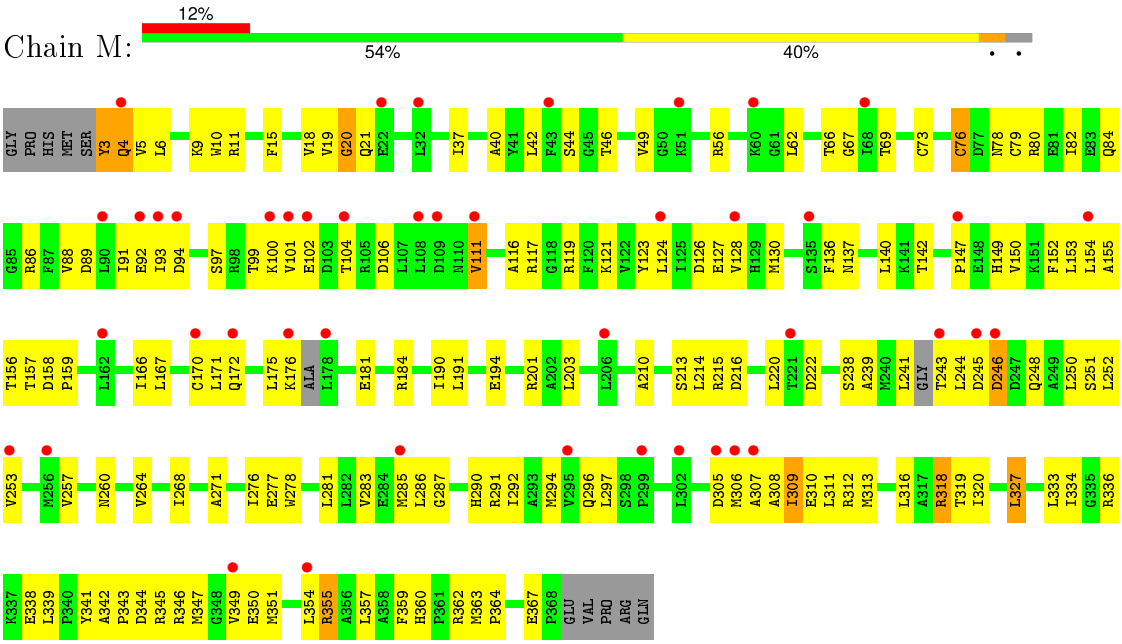
• Molecule 2: DNA polymerase III subunit tau

Chain L:



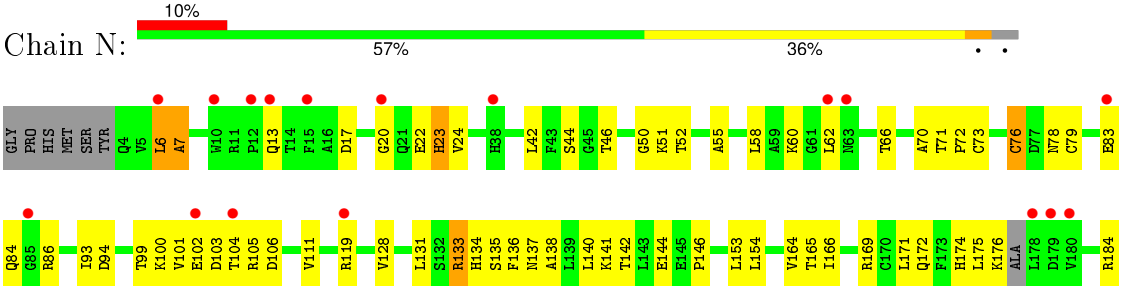
• Molecule 2: DNA polymerase III subunit tau

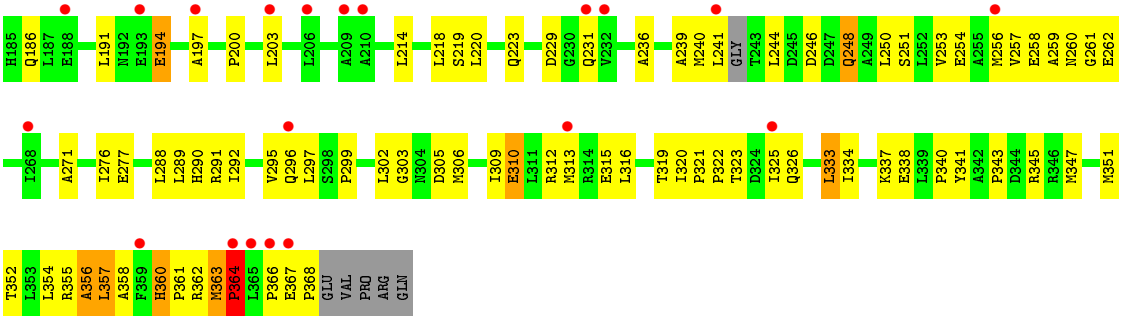
Chain M:



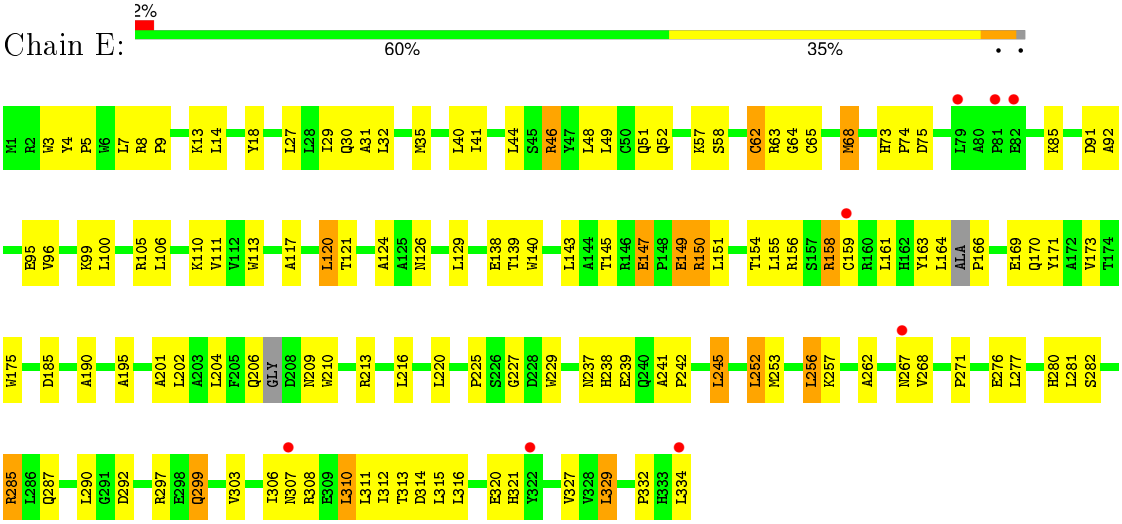
• Molecule 2: DNA polymerase III subunit tau

Chain N:

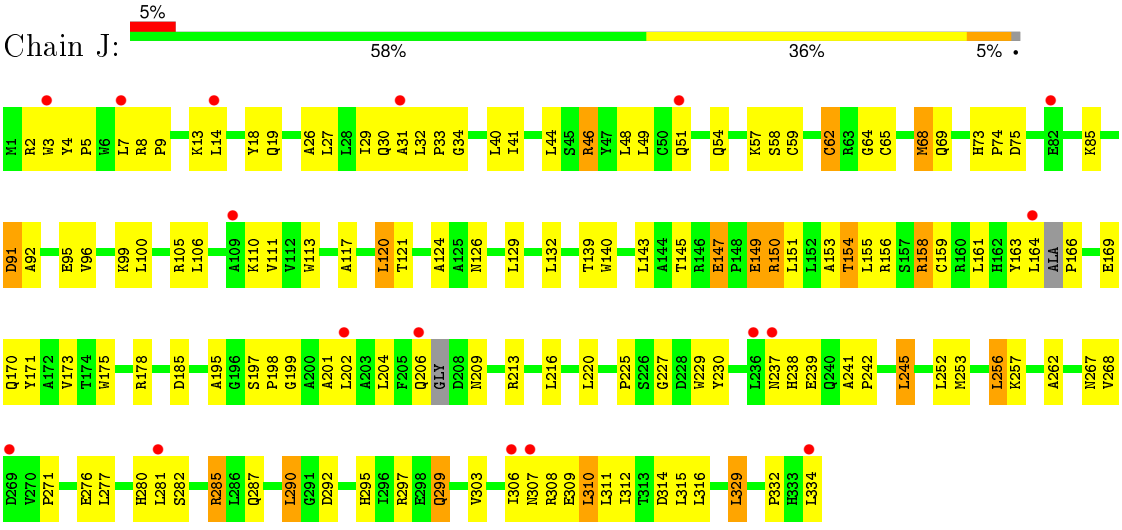




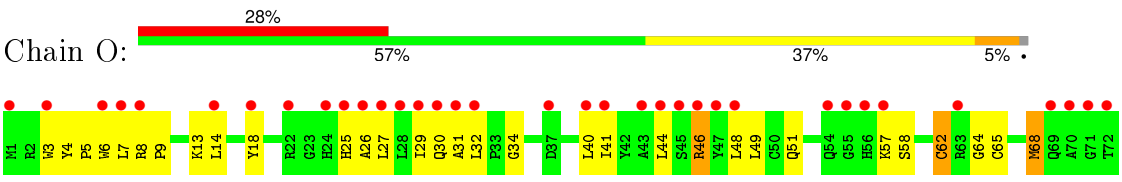
• Molecule 3: DNA polymerase III subunit delta'

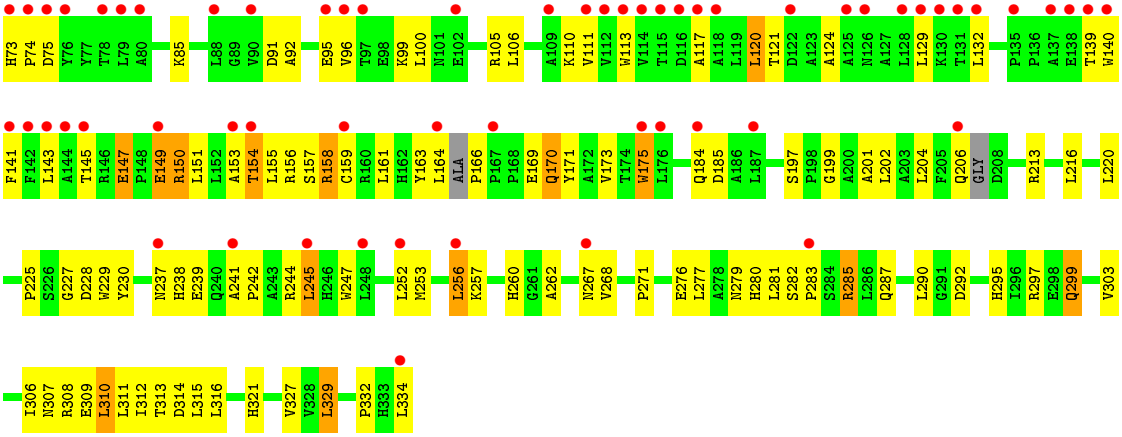


• Molecule 3: DNA polymerase III subunit delta'



• Molecule 3: DNA polymerase III subunit delta'




H73 P74 D75 Y76 Y77 T78 L79 A80 K85 Y88 G89 V90 D91 A92 E95 V96 T97 E98 K99 L100 N101 E102 R105 L106 A109 K110 V111 Y112 W113 V114 T115 D116 A117 A118 L119 L120 T121 D122 A123 A124 A125 N126 A127 L128 L129 K130 T131 L132 P135 P136 A137 E138 T139 W140
F141 F142 L143 A144 T145 R146 E147 P148 E149 R150 L151 L152 A153 T154 L155 R156 S157 R158 C159 R160 L161 H162 Y163 L164 ALA P166 P167 P168 E169 Q170 Y171 A172 V173 T174 W175 L176 Q184 D185 A186 L187 S197 P198 G199 A200 A201 L202 A203 L204 F205 Q206 GLY D208 R213 L216 L220
P225 S226 G227 D228 W229 Y230 N237 H238 E239 Q240 A241 P242 A243 R244 L245 H246 W247 L248 L252 M253 L256 K257 H260 G261 A262 N267 V268 P271 E276 L277 A278 N279 H280 L281 S282 P283 S284 R285 L286 Q287 L290 G291 D292 H295 I296 R297 E298 Q299 V303
I306 M307 R308 E309 L310 L311 I312 T313 D314 L315 L316 H321 V327 V328 L329 P332 H333 L334

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	100.16Å 228.49Å 164.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.62 – 3.89 49.62 – 3.89	Depositor EDS
% Data completeness (in resolution range)	89.9 (49.62-3.89) 94.7 (49.62-3.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 3.88Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.359 , 0.361 0.347 , 0.351	Depositor DCC
R_{free} test set	2993 reflections (4.87%)	DCC
Wilson B-factor (Å^2)	134.9	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 31.2	EDS
Estimated twinning fraction	0.030 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 128313 reflections	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	41322	wwPDB-VP
Average B, all atoms (Å^2)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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	0.86	8/2715 (0.3%)	0.93	10/3684 (0.3%)
1	F	0.86	8/2715 (0.3%)	0.93	10/3684 (0.3%)
1	K	0.86	8/2715 (0.3%)	0.93	10/3684 (0.3%)
2	B	0.57	0/2887	0.88	11/3912 (0.3%)
2	C	0.47	0/2887	0.74	2/3912 (0.1%)
2	D	0.66	7/2874 (0.2%)	0.95	14/3894 (0.4%)
2	G	0.57	0/2887	0.88	11/3912 (0.3%)
2	H	0.50	1/2887 (0.0%)	0.75	2/3912 (0.1%)
2	I	0.66	7/2874 (0.2%)	0.95	14/3894 (0.4%)
2	L	0.57	0/2887	0.88	10/3912 (0.3%)
2	M	0.47	0/2887	0.75	2/3912 (0.1%)
2	N	0.66	7/2874 (0.2%)	0.95	14/3894 (0.4%)
3	E	0.49	0/2656	0.70	0/3620
3	J	0.49	0/2656	0.70	0/3620
3	O	0.49	0/2656	0.70	0/3620
All	All	0.63	46/42057 (0.1%)	0.85	110/57066 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	F	0	4
1	K	0	4
2	D	0	1
2	H	0	1
2	I	0	1
2	N	0	1
All	All	0	16

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	315	ASP	CB-CG	29.17	2.13	1.51
1	K	315	ASP	CB-CG	29.14	2.12	1.51
1	A	315	ASP	CB-CG	29.08	2.12	1.51
2	D	133	ARG	CZ-NH2	-11.05	1.18	1.33
2	N	133	ARG	CZ-NH2	-10.98	1.18	1.33
2	I	133	ARG	CZ-NH2	-10.95	1.18	1.33
1	F	310	LEU	CG-CD2	-9.08	1.18	1.51
1	A	310	LEU	CG-CD2	-9.05	1.18	1.51
1	K	310	LEU	CG-CD2	-9.04	1.18	1.51
2	N	363	MET	CG-SD	9.02	2.04	1.81
2	I	363	MET	CG-SD	9.01	2.04	1.81
2	D	363	MET	CG-SD	8.97	2.04	1.81
2	I	363	MET	SD-CE	8.91	2.27	1.77
2	N	363	MET	SD-CE	8.90	2.27	1.77
2	D	363	MET	SD-CE	8.89	2.27	1.77
2	H	3	TYR	C-N	7.54	1.51	1.34
1	A	316	TYR	CE1-CZ	6.85	1.47	1.38
1	K	316	TYR	CE1-CZ	6.82	1.47	1.38
1	F	316	TYR	CE1-CZ	6.79	1.47	1.38
1	K	283	ARG	CB-CG	6.64	1.70	1.52
1	A	283	ARG	CB-CG	6.63	1.70	1.52
1	F	283	ARG	CB-CG	6.61	1.70	1.52
2	I	356	ALA	C-O	-5.80	1.12	1.23
2	D	360	HIS	CA-CB	5.75	1.66	1.53
2	I	360	HIS	CA-CB	5.75	1.66	1.53
2	D	356	ALA	C-O	-5.74	1.12	1.23
2	N	356	ALA	C-O	-5.73	1.12	1.23
2	N	360	HIS	CA-CB	5.67	1.66	1.53
1	A	200	PRO	N-CD	-5.67	1.40	1.47
1	F	316	TYR	CZ-OH	5.63	1.47	1.37
1	K	316	TYR	CZ-OH	5.62	1.47	1.37
1	A	316	TYR	CZ-OH	5.61	1.47	1.37
1	K	200	PRO	N-CD	-5.60	1.40	1.47
1	F	200	PRO	N-CD	-5.56	1.40	1.47
2	I	133	ARG	CZ-NH1	-5.53	1.25	1.33
2	D	133	ARG	CZ-NH1	-5.51	1.25	1.33
2	N	133	ARG	CZ-NH1	-5.48	1.25	1.33
1	K	316	TYR	CG-CD1	5.27	1.46	1.39
1	F	316	TYR	CG-CD1	5.27	1.46	1.39
1	A	316	TYR	CG-CD1	5.23	1.46	1.39
2	N	360	HIS	CG-CD2	5.16	1.44	1.35
2	D	360	HIS	CG-CD2	5.12	1.44	1.35
1	F	282	ARG	CB-CG	-5.10	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	282	ARG	CB-CG	-5.06	1.38	1.52
2	I	360	HIS	CG-CD2	5.05	1.44	1.35
1	A	282	ARG	CB-CG	-5.04	1.39	1.52

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	363	MET	CG-SD-CE	17.07	127.52	100.20
2	I	363	MET	CG-SD-CE	17.07	127.52	100.20
2	N	363	MET	CG-SD-CE	17.05	127.48	100.20
1	F	283	ARG	C-N-CA	12.41	148.35	122.30
1	A	283	ARG	C-N-CA	12.38	148.29	122.30
1	K	283	ARG	C-N-CA	12.36	148.26	122.30
2	G	244	LEU	CB-CG-CD2	-11.88	90.80	111.00
2	L	244	LEU	CB-CG-CD2	-11.88	90.80	111.00
2	B	244	LEU	CB-CG-CD2	-11.87	90.83	111.00
1	K	280	GLN	C-N-CA	11.45	150.31	121.70
1	A	280	GLN	C-N-CA	11.43	150.28	121.70
1	F	280	GLN	C-N-CA	11.43	150.27	121.70
2	N	133	ARG	NE-CZ-NH1	11.10	125.85	120.30
2	I	133	ARG	NE-CZ-NH1	10.89	125.75	120.30
2	D	133	ARG	NE-CZ-NH2	10.89	125.74	120.30
2	D	133	ARG	NE-CZ-NH1	10.82	125.71	120.30
2	I	133	ARG	NE-CZ-NH2	10.81	125.70	120.30
2	N	133	ARG	NE-CZ-NH2	10.75	125.67	120.30
1	F	315	ASP	CA-CB-CG	-10.74	89.76	113.40
1	A	315	ASP	CA-CB-CG	-10.73	89.80	113.40
1	K	315	ASP	CA-CB-CG	-10.70	89.87	113.40
2	N	133	ARG	NH1-CZ-NH2	-10.48	107.87	119.40
2	D	133	ARG	NH1-CZ-NH2	-10.41	107.95	119.40
2	I	133	ARG	NH1-CZ-NH2	-10.40	107.95	119.40
2	N	360	HIS	N-CA-CB	10.34	129.20	110.60
2	I	360	HIS	N-CA-CB	10.31	129.15	110.60
2	D	360	HIS	N-CA-CB	10.30	129.14	110.60
1	A	283	ARG	CA-C-N	-9.34	97.53	116.20
1	K	283	ARG	CA-C-N	-9.32	97.55	116.20
1	F	283	ARG	CA-C-N	-9.32	97.56	116.20
1	K	283	ARG	NE-CZ-NH1	8.43	124.51	120.30
1	A	283	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	F	283	ARG	NE-CZ-NH1	8.27	124.44	120.30
1	K	283	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	F	283	ARG	NE-CZ-NH2	-7.39	116.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	283	ARG	NE-CZ-NH2	-7.31	116.64	120.30
2	B	305	ASP	CB-CG-OD2	-6.82	112.17	118.30
2	D	363	MET	CB-CG-SD	6.79	132.77	112.40
2	N	363	MET	CB-CG-SD	6.79	132.77	112.40
2	I	363	MET	CB-CG-SD	6.78	132.75	112.40
2	G	20	GLY	N-CA-C	6.77	130.03	113.10
2	L	20	GLY	N-CA-C	6.77	130.02	113.10
2	B	20	GLY	N-CA-C	6.74	129.95	113.10
2	L	305	ASP	CB-CG-OD2	-6.65	112.31	118.30
2	G	305	ASP	CB-CG-OD2	-6.61	112.35	118.30
2	B	305	ASP	CB-CG-OD1	6.52	124.17	118.30
2	L	302	LEU	C-N-CA	6.51	135.98	122.30
2	G	302	LEU	C-N-CA	6.48	135.91	122.30
2	B	302	LEU	C-N-CA	6.46	135.86	122.30
2	L	305	ASP	CB-CG-OD1	6.45	124.10	118.30
2	L	303	GLY	N-CA-C	6.36	129.00	113.10
2	G	303	GLY	N-CA-C	6.34	128.96	113.10
2	B	303	GLY	N-CA-C	6.34	128.94	113.10
2	M	20	GLY	N-CA-C	6.32	128.90	113.10
2	G	305	ASP	CB-CG-OD1	6.32	123.99	118.30
2	C	20	GLY	N-CA-C	6.31	128.88	113.10
1	K	310	LEU	CB-CG-CD2	-6.31	100.27	111.00
1	A	310	LEU	CB-CG-CD2	-6.31	100.28	111.00
1	F	310	LEU	CB-CG-CD2	-6.29	100.30	111.00
2	H	20	GLY	N-CA-C	6.29	128.82	113.10
2	N	7	ALA	N-CA-C	-6.14	94.42	111.00
2	D	7	ALA	N-CA-C	-6.12	94.47	111.00
2	I	7	ALA	N-CA-C	-6.12	94.48	111.00
1	F	280	GLN	O-C-N	-6.06	113.01	122.70
1	K	280	GLN	O-C-N	-6.06	113.01	122.70
1	A	280	GLN	O-C-N	-6.05	113.01	122.70
2	N	360	HIS	CA-CB-CG	6.05	123.89	113.60
2	I	360	HIS	CB-CA-C	-6.00	98.39	110.40
2	D	360	HIS	CB-CA-C	-6.00	98.40	110.40
2	D	360	HIS	CA-CB-CG	6.00	123.79	113.60
2	N	360	HIS	CB-CA-C	-5.98	98.44	110.40
2	I	360	HIS	CA-CB-CG	5.97	123.76	113.60
2	I	364	PRO	CA-N-CD	-5.85	103.31	111.50
2	G	245	ASP	CB-CG-OD1	-5.85	113.04	118.30
2	L	245	ASP	CB-CG-OD1	-5.82	113.07	118.30
2	B	245	ASP	CB-CG-OD1	-5.81	113.07	118.30
2	N	364	PRO	CA-N-CD	-5.77	103.42	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	364	PRO	CA-N-CD	-5.75	103.45	111.50
2	H	327	LEU	CA-CB-CG	5.72	128.45	115.30
2	D	20	GLY	N-CA-C	5.71	127.37	113.10
2	C	327	LEU	CA-CB-CG	5.68	128.38	115.30
2	M	327	LEU	CA-CB-CG	5.68	128.35	115.30
2	N	20	GLY	N-CA-C	5.68	127.29	113.10
2	I	20	GLY	N-CA-C	5.67	127.29	113.10
2	N	360	HIS	CB-CG-ND1	5.55	137.08	123.20
2	D	360	HIS	CB-CG-ND1	5.53	137.02	123.20
2	I	360	HIS	CB-CG-ND1	5.50	136.96	123.20
2	G	259	ALA	N-CA-C	5.39	125.56	111.00
2	L	259	ALA	N-CA-C	5.37	125.51	111.00
2	B	259	ALA	N-CA-C	5.37	125.50	111.00
1	A	282	ARG	CB-CG-CD	-5.29	97.85	111.60
1	F	282	ARG	CB-CG-CD	-5.27	97.89	111.60
1	K	282	ARG	CB-CG-CD	-5.26	97.93	111.60
2	B	243	THR	N-CA-C	5.22	125.10	111.00
2	B	302	LEU	CA-C-N	-5.19	105.81	116.20
2	G	243	THR	N-CA-C	5.19	125.02	111.00
2	L	243	THR	N-CA-C	5.19	125.01	111.00
2	N	303	GLY	N-CA-C	5.18	126.05	113.10
2	D	303	GLY	N-CA-C	5.17	126.03	113.10
2	I	303	GLY	N-CA-C	5.17	126.01	113.10
2	L	302	LEU	CA-C-N	-5.16	105.88	116.20
2	G	302	LEU	CA-C-N	-5.15	105.90	116.20
2	N	133	ARG	N-CA-C	5.12	124.83	111.00
2	D	133	ARG	N-CA-C	5.11	124.79	111.00
2	I	133	ARG	N-CA-C	5.11	124.79	111.00
2	G	245	ASP	CB-CG-OD2	5.09	122.88	118.30
2	B	245	ASP	CB-CG-OD2	5.09	122.88	118.30
1	K	264	SER	N-CA-C	-5.07	97.31	111.00
1	F	264	SER	N-CA-C	-5.06	97.35	111.00
1	A	264	SER	N-CA-C	-5.04	97.39	111.00

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	280	GLN	Peptide
1	A	281	ASN	Mainchain
1	A	282	ARG	Mainchain
1	A	319	SER	Mainchain

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Mol	Chain	Res	Type	Group
2	D	23	HIS	Sidechain
1	F	280	GLN	Peptide
1	F	281	ASN	Mainchain
1	F	282	ARG	Mainchain
1	F	319	SER	Mainchain
2	H	3	TYR	Mainchain
2	I	23	HIS	Sidechain
1	K	280	GLN	Peptide
1	K	281	ASN	Mainchain
1	K	282	ARG	Mainchain
1	K	319	SER	Mainchain
2	N	23	HIS	Sidechain

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	2670	0	2724	226	5
1	F	2670	0	2719	258	36
1	K	2670	0	2726	183	5
2	B	2841	0	2890	185	15
2	C	2841	0	2888	187	36
2	D	2829	0	2878	250	5
2	G	2841	0	2887	240	5
2	H	2841	0	2889	220	13
2	I	2829	0	2880	272	7
2	L	2841	0	2888	245	7
2	M	2841	0	2886	270	1
2	N	2829	0	2876	312	3
3	E	2593	0	2598	127	14
3	J	2593	0	2598	139	21
3	O	2593	0	2598	178	1
All	All	41322	0	41925	2686	87

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 32.

All (2686) 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)
2:I:277:GLU:HB3	3:J:149:GLU:CG	1.24	1.60
2:G:10:TRP:CH2	2:G:190:ILE:HG23	1.37	1.57
2:D:277:GLU:HB3	3:E:149:GLU:CG	1.33	1.57
2:B:6:LEU:HD13	2:B:190:ILE:CG2	1.08	1.51
2:B:6:LEU:HD21	2:B:194:GLU:CG	1.37	1.50
2:I:277:GLU:CB	3:J:149:GLU:HG2	1.35	1.49
2:H:86:ARG:HH12	2:I:141:LYS:CE	1.23	1.47
2:N:345:ARG:NH2	3:O:150:ARG:HE	1.10	1.47
2:M:215:ARG:NH2	2:N:164:VAL:HG21	1.29	1.47
1:A:75:ALA:CB	1:F:207:ASN:ND2	1.76	1.45
2:N:363:MET:CG	2:N:363:MET:SD	2.04	1.45
2:I:363:MET:CG	2:I:363:MET:SD	2.04	1.45
2:D:363:MET:SD	2:D:363:MET:CG	2.04	1.45
2:L:238:SER:HB2	2:L:244:LEU:N	1.22	1.43
2:D:277:GLU:CB	3:E:149:GLU:HG2	1.48	1.42
1:A:193:PRO:CB	2:M:311:LEU:CD2	1.95	1.42
1:A:75:ALA:CB	1:F:207:ASN:HD22	1.32	1.41
2:B:6:LEU:CD1	2:B:190:ILE:HG22	1.47	1.41
2:B:6:LEU:CD1	2:B:190:ILE:CG2	1.95	1.39
2:L:6:LEU:HD21	2:L:194:GLU:CG	1.52	1.38
1:F:29:LEU:HD13	1:F:179:LEU:CB	1.51	1.38
2:G:354:LEU:HD11	2:H:294:MET:SD	1.66	1.35
2:N:345:ARG:NH2	3:O:150:ARG:NE	1.74	1.34
1:F:270:ARG:NH1	2:N:316:LEU:HD23	1.02	1.34
2:H:86:ARG:NH1	2:I:141:LYS:NZ	1.75	1.33
2:L:347:MET:HG3	2:M:290:HIS:CD2	1.63	1.32
2:H:86:ARG:NH1	2:I:141:LYS:CE	1.88	1.32
2:G:19:VAL:CG2	2:G:186:GLN:HG2	1.60	1.32
2:H:86:ARG:HH12	2:I:141:LYS:NZ	1.26	1.31
2:H:86:ARG:NH1	2:I:141:LYS:HE2	1.43	1.30
1:A:193:PRO:CB	2:M:311:LEU:HD21	1.53	1.30
1:F:29:LEU:HD22	1:F:179:LEU:CA	1.61	1.30
2:L:238:SER:CB	2:L:244:LEU:H	1.43	1.30
1:A:75:ALA:HB3	1:F:207:ASN:ND2	0.96	1.29
2:L:238:SER:CB	2:L:244:LEU:N	1.96	1.29
1:K:333:HIS:CG	2:L:297:LEU:HD21	1.66	1.28
1:A:106:ASP:CG	1:F:225:LYS:HD3	1.28	1.28
2:M:10:TRP:CZ2	2:M:190:ILE:HG23	1.70	1.27
1:A:74:PHE:HE1	1:F:203:GLU:OE1	1.15	1.27
1:F:29:LEU:HD22	1:F:179:LEU:N	1.46	1.27
2:I:277:GLU:OE1	3:J:149:GLU:HG3	1.26	1.26
1:K:333:HIS:CB	2:L:297:LEU:HD21	1.65	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:GLU:OE2	2:M:318:ARG:CD	1.74	1.25
1:F:270:ARG:NH1	2:N:316:LEU:CD2	1.97	1.25
2:G:20:GLY:C	2:G:178:LEU:CD2	2.04	1.24
3:O:163:TYR:OH	3:O:166:PRO:HD3	1.37	1.23
2:N:363:MET:CE	2:N:363:MET:SD	2.27	1.22
2:I:363:MET:SD	2:I:363:MET:CE	2.27	1.22
2:L:6:LEU:CD2	2:L:194:GLU:HG3	1.69	1.22
2:M:215:ARG:NH2	2:N:164:VAL:CG2	2.00	1.22
1:A:106:ASP:CG	1:F:225:LYS:CD	1.98	1.22
1:A:104:LEU:C	1:F:227:LYS:HZ3	1.42	1.22
2:D:363:MET:SD	2:D:363:MET:CE	2.27	1.22
1:A:193:PRO:HB3	2:M:311:LEU:CD2	1.61	1.22
2:M:351:MET:CE	2:N:326:GLN:HE22	1.53	1.21
2:G:10:TRP:CZ3	2:G:190:ILE:HG23	1.74	1.20
1:A:193:PRO:HB2	2:M:311:LEU:CD2	1.59	1.20
1:F:29:LEU:CD1	1:F:179:LEU:HB2	1.69	1.20
2:L:6:LEU:HD13	2:L:190:ILE:CG2	1.73	1.19
1:A:105:HIS:CB	1:F:227:LYS:HD2	1.71	1.19
2:L:94:ASP:H	2:L:100:LYS:NZ	1.40	1.18
2:B:94:ASP:H	2:B:100:LYS:NZ	1.40	1.18
2:H:100:LYS:HG2	2:I:133:ARG:NE	1.58	1.18
2:M:201:ARG:HB2	2:M:305:ASP:OD2	1.42	1.18
1:K:315:ASP:CG	1:K:315:ASP:CB	2.13	1.18
1:A:74:PHE:CE1	1:F:203:GLU:OE1	1.97	1.18
2:I:277:GLU:HB3	3:J:149:GLU:CB	1.73	1.17
1:F:315:ASP:CG	1:F:315:ASP:CB	2.13	1.17
2:B:6:LEU:CD2	2:B:194:GLU:HG3	1.73	1.17
1:A:315:ASP:CG	1:A:315:ASP:CB	2.12	1.17
2:L:354:LEU:HD11	2:M:294:MET:SD	1.85	1.17
1:F:29:LEU:CD1	1:F:179:LEU:HD13	1.75	1.17
2:I:345:ARG:NE	3:J:150:ARG:HH21	1.19	1.17
2:G:94:ASP:H	2:G:100:LYS:NZ	1.40	1.16
2:H:86:ARG:CZ	2:I:141:LYS:HE2	1.74	1.16
1:F:334:LYS:O	2:G:297:LEU:HD23	1.44	1.16
2:N:366:PRO:HB3	3:O:282:SER:HB2	1.26	1.16
2:G:365:LEU:CD2	2:H:297:LEU:CD1	2.24	1.15
2:C:86:ARG:HH21	2:D:138:ALA:HA	1.04	1.15
2:L:180:VAL:HG21	2:L:304:ASN:CG	1.67	1.15
2:M:351:MET:HE1	2:N:326:GLN:NE2	1.63	1.14
1:K:333:HIS:CD2	2:L:297:LEU:CD2	2.30	1.14
2:I:360:HIS:HB3	2:I:363:MET:CB	1.77	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:PRO:CB	2:M:311:LEU:HD22	1.67	1.14
1:A:106:ASP:CB	1:F:225:LYS:HD3	1.68	1.14
2:N:360:HIS:HB3	2:N:363:MET:CB	1.77	1.14
2:D:360:HIS:HB3	2:D:363:MET:CB	1.77	1.14
2:H:100:LYS:HG2	2:I:133:ARG:HE	0.98	1.13
2:L:180:VAL:HB	2:L:304:ASN:O	1.47	1.13
1:A:105:HIS:HB3	1:F:227:LYS:HD2	1.13	1.13
2:M:341:TYR:HB2	2:N:333:LEU:CD1	1.79	1.12
2:G:10:TRP:CZ3	2:G:190:ILE:HG12	1.84	1.12
2:D:277:GLU:OE1	3:E:149:GLU:HG3	1.47	1.12
1:F:270:ARG:HH12	2:N:316:LEU:CD2	1.57	1.12
2:G:354:LEU:CD1	2:H:294:MET:SD	2.38	1.12
2:I:277:GLU:CA	3:J:149:GLU:HG2	1.80	1.11
3:O:34:GLY:O	3:O:199:GLY:HA3	1.48	1.11
2:G:69:THR:HG22	2:G:71:THR:H	1.15	1.11
2:G:10:TRP:CH2	2:G:190:ILE:CG2	2.34	1.11
2:D:360:HIS:HB3	2:D:363:MET:HB2	1.11	1.11
2:G:20:GLY:HA3	2:G:178:LEU:HD22	1.30	1.10
1:F:334:LYS:CB	2:G:297:LEU:HD21	1.80	1.10
2:D:200:PRO:HB2	2:D:305:ASP:HB2	1.17	1.10
1:A:334:LYS:HB2	2:B:297:LEU:HD21	1.30	1.10
2:G:20:GLY:C	2:G:178:LEU:HD21	1.70	1.10
2:M:341:TYR:HB2	2:N:333:LEU:HD11	1.20	1.10
2:N:277:GLU:HB3	3:O:149:GLU:CG	1.82	1.10
1:F:30:LEU:CD2	1:F:178:LEU:HD12	1.83	1.09
2:D:345:ARG:NE	3:E:150:ARG:HH21	1.21	1.09
2:G:19:VAL:HG22	2:G:186:GLN:CG	1.82	1.09
2:I:277:GLU:CB	3:J:149:GLU:CG	2.05	1.09
2:N:360:HIS:HB3	2:N:363:MET:HB2	1.11	1.09
2:C:100:LYS:HG2	2:D:133:ARG:NE	1.45	1.09
2:H:351:MET:HE1	2:I:326:GLN:HE22	1.12	1.08
2:H:86:ARG:HH21	2:I:138:ALA:HA	1.12	1.08
2:D:345:ARG:HE	3:E:150:ARG:NH2	1.31	1.08
1:F:270:ARG:NH1	2:N:316:LEU:HA	1.66	1.08
2:G:20:GLY:CA	2:G:178:LEU:HD22	1.82	1.08
1:A:28:PRO:HB3	2:B:164:VAL:HG21	1.35	1.08
2:C:100:LYS:CG	2:D:133:ARG:NE	2.11	1.08
3:O:163:TYR:OH	3:O:166:PRO:CD	2.03	1.07
2:B:69:THR:HG22	2:B:71:THR:H	1.15	1.06
1:F:30:LEU:HD21	1:F:178:LEU:CD1	1.86	1.06
2:M:86:ARG:HH21	2:N:138:ALA:HA	1.19	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:360:HIS:HB3	2:I:363:MET:HB2	1.11	1.06
2:M:10:TRP:CZ3	2:M:190:ILE:HG12	1.91	1.06
2:H:100:LYS:CG	2:I:133:ARG:NE	2.18	1.06
1:F:29:LEU:HD22	1:F:179:LEU:HA	1.37	1.05
1:A:161:GLU:OE2	2:M:318:ARG:HD3	1.27	1.05
2:H:341:TYR:HB2	2:I:333:LEU:HD11	1.38	1.05
2:L:69:THR:HG22	2:L:71:THR:H	1.15	1.05
2:B:6:LEU:CD2	2:B:194:GLU:CG	2.30	1.05
2:G:365:LEU:HD22	2:H:297:LEU:CD1	1.87	1.05
2:L:246:ASP:HB3	2:L:274:ARG:HD3	1.38	1.05
2:L:238:SER:HB2	2:L:243:THR:C	1.51	1.04
2:N:277:GLU:HB3	3:O:149:GLU:HG2	1.04	1.04
2:N:200:PRO:HB2	2:N:305:ASP:HB2	1.37	1.04
2:G:365:LEU:HD21	2:H:297:LEU:CD1	1.85	1.03
1:A:193:PRO:HB2	2:M:311:LEU:HD22	1.15	1.03
2:G:19:VAL:HG12	2:G:178:LEU:HD13	1.39	1.03
2:M:201:ARG:CB	2:M:305:ASP:OD2	2.05	1.03
2:G:246:ASP:HB3	2:G:274:ARG:HD3	1.38	1.03
2:B:246:ASP:HB3	2:B:274:ARG:HD3	1.37	1.03
1:A:104:LEU:C	1:F:227:LYS:NZ	2.11	1.03
2:I:345:ARG:HE	3:J:150:ARG:NH2	1.46	1.03
2:D:277:GLU:CB	3:E:149:GLU:CG	2.20	1.02
2:B:98:ARG:NH2	2:C:137:ASN:OD1	1.92	1.02
1:F:223:MET:SD	1:F:292:ARG:HB3	1.98	1.02
1:F:25:GLY:HA3	1:F:139:CYS:O	1.59	1.02
2:G:21:GLN:HG3	2:G:178:LEU:CD2	1.88	1.02
2:I:238:SER:HB2	2:I:243:THR:HB	1.42	1.02
1:K:223:MET:SD	1:K:292:ARG:HB3	1.99	1.02
1:F:334:LYS:HB2	2:G:297:LEU:CD2	1.88	1.01
1:A:223:MET:SD	1:A:292:ARG:HB3	1.98	1.01
2:H:3:TYR:O	2:H:4:GLN:HG3	1.60	1.01
1:A:25:GLY:HA3	1:A:139:CYS:O	1.59	1.01
2:L:343:PRO:HA	2:M:283:VAL:HG13	1.40	1.01
2:G:20:GLY:O	2:G:178:LEU:CD2	2.09	1.01
2:D:363:MET:HB3	2:D:364:PRO:HD2	1.42	1.00
2:L:347:MET:SD	2:M:287:GLY:HA2	2.00	1.00
2:G:21:GLN:HG3	2:G:178:LEU:HD21	1.39	1.00
2:B:6:LEU:HD11	2:B:190:ILE:HG22	1.40	1.00
1:A:194:ASP:N	2:M:311:LEU:HD11	1.76	1.00
2:G:365:LEU:HD21	2:H:297:LEU:HD11	1.41	1.00
2:G:19:VAL:HG22	2:G:186:GLN:HG2	1.03	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:SER:CB	2:C:144:GLU:OE2	2.09	1.00
2:I:363:MET:HB3	2:I:364:PRO:HD2	1.42	1.00
1:K:333:HIS:CG	2:L:297:LEU:CD2	2.42	1.00
2:N:223:GLN:HG2	3:O:158:ARG:HH21	1.25	0.99
2:D:277:GLU:HB3	3:E:149:GLU:CB	1.92	0.99
2:G:10:TRP:CZ3	2:G:190:ILE:CG2	2.45	0.99
1:A:106:ASP:OD1	1:F:225:LYS:HD3	1.61	0.99
2:M:359:PHE:CE2	2:N:323:THR:HG23	1.97	0.99
1:F:29:LEU:HD13	1:F:179:LEU:CG	1.92	0.99
1:F:310:LEU:HD22	1:F:314:GLN:HE21	1.27	0.99
2:N:363:MET:HB3	2:N:364:PRO:HD2	1.43	0.99
2:N:366:PRO:CB	3:O:282:SER:HB2	1.92	0.98
1:K:28:PRO:HB3	2:L:164:VAL:HG21	1.42	0.98
1:A:75:ALA:HB3	1:F:207:ASN:HD21	1.26	0.98
1:K:25:GLY:HA3	1:K:139:CYS:O	1.59	0.98
2:M:201:ARG:N	2:M:305:ASP:OD2	1.96	0.98
2:D:73:CYS:SG	2:D:76:CYS:HB3	2.04	0.98
2:B:354:LEU:HD11	2:C:294:MET:SD	2.02	0.98
2:N:241:LEU:O	3:O:156:ARG:HD2	1.62	0.98
1:A:119:LYS:H	1:A:119:LYS:HD3	1.26	0.98
2:I:241:LEU:O	3:J:156:ARG:NH1	1.97	0.98
2:L:238:SER:C	2:L:243:THR:OG1	1.84	0.98
2:I:73:CYS:SG	2:I:76:CYS:HB3	2.04	0.98
1:K:310:LEU:HD22	1:K:314:GLN:HE21	1.26	0.97
2:L:180:VAL:CG2	2:L:304:ASN:CG	2.31	0.97
2:G:365:LEU:HD22	2:H:297:LEU:HD12	1.46	0.97
2:M:10:TRP:CE2	2:M:190:ILE:HG23	1.98	0.97
1:F:315:ASP:HB2	1:F:318:GLN:CG	1.94	0.97
2:N:220:LEU:HD21	3:O:154:THR:HA	1.46	0.97
2:G:12:PRO:HD3	2:G:215:ARG:HH12	1.27	0.97
2:N:345:ARG:NH2	3:O:150:ARG:CZ	2.28	0.97
2:L:354:LEU:CD1	2:M:294:MET:SD	2.53	0.97
2:G:6:LEU:HD12	2:G:222:ASP:HA	1.43	0.97
2:L:347:MET:CG	2:M:290:HIS:CD2	2.47	0.97
1:A:315:ASP:HB2	1:A:318:GLN:CG	1.94	0.97
2:B:18:VAL:HG22	2:B:25:LEU:HD11	1.47	0.97
1:F:119:LYS:H	1:F:119:LYS:HD3	1.26	0.97
1:K:315:ASP:HB2	1:K:318:GLN:CG	1.94	0.97
2:C:86:ARG:CZ	2:D:141:LYS:HB2	1.94	0.96
1:A:310:LEU:HD22	1:A:314:GLN:HE21	1.27	0.96
2:M:86:ARG:CZ	2:N:141:LYS:HB2	1.94	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:357:LEU:HA	2:D:363:MET:SD	2.05	0.96
1:K:333:HIS:HB2	2:L:297:LEU:HD21	1.45	0.96
2:L:18:VAL:HG22	2:L:25:LEU:HD11	1.47	0.96
2:N:73:CYS:SG	2:N:76:CYS:HB3	2.04	0.96
1:A:213:THR:H	1:A:216:HIS:HD2	1.13	0.96
1:F:270:ARG:HH12	2:N:316:LEU:HA	1.18	0.96
2:G:10:TRP:CZ2	2:G:190:ILE:HG23	2.01	0.96
1:A:105:HIS:HA	1:F:227:LYS:CE	1.96	0.96
2:L:6:LEU:HD13	2:L:190:ILE:HG22	1.44	0.95
2:B:98:ARG:HH12	2:C:137:ASN:CG	1.69	0.95
2:H:56:ARG:NH2	2:I:165:THR:CG2	2.28	0.95
2:I:357:LEU:HA	2:I:363:MET:SD	2.05	0.95
2:B:6:LEU:HD13	2:B:190:ILE:HG21	0.98	0.95
2:I:345:ARG:NE	3:J:150:ARG:NH2	1.92	0.95
1:K:333:HIS:CD2	2:L:297:LEU:HD21	1.98	0.95
1:K:213:THR:H	1:K:216:HIS:HD2	1.13	0.95
2:H:86:ARG:NH2	2:I:141:LYS:HE2	1.80	0.95
2:G:53:SER:OG	2:G:215:ARG:NH2	2.00	0.95
1:K:119:LYS:H	1:K:119:LYS:HD3	1.27	0.95
1:A:106:ASP:OD1	1:F:225:LYS:CD	2.14	0.95
2:N:357:LEU:HA	2:N:363:MET:SD	2.06	0.95
2:C:341:TYR:HB2	2:D:333:LEU:HD11	1.48	0.95
2:B:6:LEU:HD21	2:B:194:GLU:HG2	1.46	0.94
2:N:345:ARG:CZ	3:O:150:ARG:HE	1.81	0.94
2:N:345:ARG:HH22	3:O:150:ARG:HE	0.95	0.94
1:F:334:LYS:O	2:G:297:LEU:CD2	2.14	0.94
3:O:6:TRP:HZ3	3:O:175:TRP:CD2	1.86	0.94
2:B:6:LEU:HD21	2:B:194:GLU:HG3	0.95	0.94
2:L:6:LEU:HD13	2:L:190:ILE:HG21	1.48	0.94
2:M:351:MET:HE1	2:N:326:GLN:HE22	0.77	0.94
2:G:18:VAL:HG22	2:G:25:LEU:HD11	1.47	0.94
2:D:277:GLU:CA	3:E:149:GLU:HG2	1.98	0.93
2:L:238:SER:HB3	2:L:244:LEU:H	1.33	0.93
1:F:29:LEU:CD1	1:F:179:LEU:CD1	2.45	0.93
2:L:94:ASP:N	2:L:100:LYS:HZ3	1.65	0.93
2:L:354:LEU:CD2	2:M:297:LEU:HD22	1.97	0.93
1:F:29:LEU:HD13	1:F:179:LEU:CD1	1.98	0.93
2:L:265:MET:HE1	2:M:294:MET:HE1	1.50	0.93
1:A:105:HIS:N	1:F:227:LYS:NZ	2.16	0.93
1:A:133:ARG:NH2	1:F:227:LYS:HE3	1.82	0.93
1:F:29:LEU:HD13	1:F:179:LEU:HB2	0.95	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:100:LYS:CG	2:I:133:ARG:HE	1.77	0.92
1:F:29:LEU:CD2	1:F:179:LEU:HA	1.99	0.92
2:M:201:ARG:CA	2:M:305:ASP:OD2	2.18	0.92
2:N:345:ARG:NE	3:O:150:ARG:HH21	1.67	0.91
2:H:341:TYR:HB2	2:I:333:LEU:CD1	2.00	0.91
2:B:97:SER:HB2	2:C:144:GLU:OE2	1.69	0.91
1:F:213:THR:H	1:F:216:HIS:HD2	1.13	0.91
2:L:205:LEU:HD22	2:L:244:LEU:HD12	1.51	0.91
2:G:94:ASP:H	2:G:100:LYS:HZ3	1.09	0.91
2:H:86:ARG:NH1	2:I:141:LYS:HZ3	1.69	0.91
1:A:133:ARG:HH22	1:F:227:LYS:HE3	1.36	0.91
2:B:98:ARG:HH12	2:C:137:ASN:CB	1.83	0.91
2:M:215:ARG:HH21	2:N:164:VAL:HG21	1.30	0.91
2:N:223:GLN:HG2	3:O:158:ARG:NH2	1.84	0.91
2:G:6:LEU:HD11	2:G:225:ILE:HD12	1.53	0.91
2:G:10:TRP:HZ3	2:G:190:ILE:HG12	1.29	0.91
1:A:105:HIS:N	1:F:227:LYS:HZ2	1.68	0.91
2:N:368:PRO:C	3:O:279:ASN:O	2.09	0.91
1:F:29:LEU:CD2	1:F:179:LEU:CA	2.48	0.90
2:H:86:ARG:CZ	2:I:141:LYS:HB2	2.01	0.90
1:K:32:GLN:HE22	2:L:165:THR:CG2	1.84	0.90
2:G:20:GLY:CA	2:G:178:LEU:CD2	2.46	0.90
2:G:176:LYS:O	2:G:178:LEU:N	2.04	0.90
2:N:355:ARG:HH21	3:O:332:PRO:HD3	1.35	0.90
1:A:75:ALA:HB2	1:F:207:ASN:HD22	1.36	0.90
1:A:193:PRO:C	2:M:311:LEU:HD11	1.91	0.90
1:A:105:HIS:HA	1:F:227:LYS:NZ	1.85	0.90
2:B:94:ASP:N	2:B:100:LYS:HZ3	1.69	0.90
1:F:29:LEU:HD11	1:F:179:LEU:HD13	1.52	0.89
2:I:357:LEU:O	2:I:363:MET:SD	2.31	0.89
1:A:105:HIS:CA	1:F:227:LYS:HZ2	1.85	0.89
1:A:338:ASP:OD2	2:B:326:GLN:OE1	1.91	0.89
2:G:20:GLY:C	2:G:178:LEU:HD22	1.83	0.89
2:N:357:LEU:O	2:N:363:MET:SD	2.31	0.89
2:G:94:ASP:N	2:G:100:LYS:NZ	2.21	0.89
2:M:215:ARG:NE	2:N:164:VAL:HG11	1.88	0.88
2:D:357:LEU:O	2:D:363:MET:SD	2.31	0.88
2:B:94:ASP:N	2:B:100:LYS:NZ	2.21	0.88
2:H:351:MET:CE	2:I:326:GLN:HE22	1.85	0.88
2:G:354:LEU:CD2	2:H:297:LEU:HD22	2.03	0.88
2:D:363:MET:CB	2:D:364:PRO:HD2	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:30:LEU:HD21	1:F:178:LEU:HD12	0.92	0.88
1:F:32:GLN:HG3	2:G:164:VAL:HG11	1.53	0.88
2:D:200:PRO:HB2	2:D:305:ASP:CB	2.02	0.87
2:N:363:MET:CB	2:N:364:PRO:HD2	2.04	0.87
2:B:98:ARG:NH1	2:C:137:ASN:HB3	1.88	0.87
2:I:309:ILE:CG2	2:I:313:MET:HG2	2.05	0.87
1:F:270:ARG:CZ	2:N:316:LEU:HA	2.03	0.87
1:A:105:HIS:CA	1:F:227:LYS:NZ	2.38	0.87
1:F:334:LYS:HB2	2:G:297:LEU:HD21	0.92	0.87
2:C:86:ARG:NH2	2:D:138:ALA:HA	1.89	0.87
1:A:75:ALA:HB3	1:F:207:ASN:CG	1.95	0.86
2:M:341:TYR:CB	2:N:333:LEU:CD1	2.52	0.86
1:K:329:LEU:CD1	2:L:294:MET:SD	2.62	0.86
2:M:271:ALA:HB1	2:M:276:ILE:HD11	1.57	0.86
2:D:309:ILE:CG2	2:D:313:MET:HG2	2.05	0.86
2:L:94:ASP:N	2:L:100:LYS:NZ	2.21	0.86
2:C:215:ARG:NH2	2:D:164:VAL:CG2	2.38	0.86
2:N:345:ARG:CZ	3:O:150:ARG:HH21	1.89	0.86
2:I:363:MET:CB	2:I:364:PRO:HD2	2.04	0.86
2:I:277:GLU:CD	3:J:149:GLU:HG3	1.96	0.86
2:B:6:LEU:HD13	2:B:190:ILE:HG22	1.02	0.86
2:N:277:GLU:CB	3:O:149:GLU:HG2	1.99	0.85
2:B:179:ASP:HB3	2:B:182:GLN:HB2	1.58	0.85
2:C:271:ALA:HB1	2:C:276:ILE:HD11	1.57	0.85
2:L:347:MET:HG3	2:M:290:HIS:NE2	1.91	0.85
2:B:94:ASP:H	2:B:100:LYS:HZ3	0.88	0.85
1:F:32:GLN:HG3	2:G:164:VAL:CG1	2.07	0.85
2:L:179:ASP:HB3	2:L:182:GLN:HB2	1.58	0.85
2:M:215:ARG:CZ	2:N:164:VAL:CG2	2.55	0.85
2:C:100:LYS:HG2	2:D:133:ARG:HE	1.04	0.85
2:N:309:ILE:CG2	2:N:313:MET:HG2	2.05	0.85
2:M:359:PHE:CE2	2:N:323:THR:CG2	2.59	0.84
3:J:8:ARG:HG3	3:J:9:PRO:HD3	1.59	0.84
2:I:200:PRO:HB3	2:I:304:ASN:HB2	1.58	0.84
1:K:55:ILE:HD13	1:K:97:LEU:HD11	1.59	0.84
2:G:94:ASP:C	2:G:100:LYS:HZ1	1.80	0.84
3:E:8:ARG:HG3	3:E:9:PRO:HD3	1.60	0.84
2:G:10:TRP:CZ3	2:G:190:ILE:CG1	2.61	0.84
3:E:204:LEU:O	3:E:209:ASN:HB2	1.76	0.84
2:H:86:ARG:HH12	2:I:141:LYS:HZ1	1.21	0.84
2:H:86:ARG:NH1	2:I:141:LYS:HZ1	1.67	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:PRO:HB3	2:M:311:LEU:HD21	1.30	0.84
1:F:29:LEU:CD2	1:F:179:LEU:N	2.38	0.84
2:L:347:MET:HG3	2:M:290:HIS:CG	2.13	0.84
2:N:355:ARG:NH1	3:O:287:GLN:HB3	1.91	0.83
2:H:271:ALA:HB1	2:H:276:ILE:HD11	1.57	0.83
1:A:193:PRO:CA	2:M:311:LEU:HD21	2.07	0.83
2:G:179:ASP:HB3	2:G:182:GLN:HB2	1.58	0.83
2:L:180:VAL:HG21	2:L:304:ASN:ND2	1.92	0.83
2:C:10:TRP:CZ2	2:C:190:ILE:HG23	2.13	0.83
1:K:312:LEU:HB2	1:K:320:VAL:HG21	1.60	0.83
1:A:312:LEU:HB2	1:A:320:VAL:HG21	1.60	0.83
1:F:234:GLN:OE1	2:G:304:ASN:ND2	2.11	0.83
1:F:283:ARG:HD3	2:N:315:GLU:OE2	1.79	0.83
2:C:341:TYR:HB2	2:D:333:LEU:CD1	2.08	0.83
3:O:8:ARG:HG3	3:O:9:PRO:HD3	1.60	0.83
2:L:259:ALA:HB3	2:L:363:MET:HE3	1.60	0.83
2:L:180:VAL:CG2	2:L:304:ASN:ND2	2.41	0.83
2:N:357:LEU:HA	2:N:363:MET:CE	2.09	0.83
1:A:194:ASP:CA	2:M:311:LEU:HD11	2.08	0.83
2:C:100:LYS:CG	2:D:133:ARG:HE	1.84	0.82
2:I:345:ARG:HE	3:J:150:ARG:HH21	0.83	0.82
2:G:94:ASP:H	2:G:100:LYS:HZ1	1.23	0.82
2:I:357:LEU:HA	2:I:363:MET:CE	2.09	0.82
1:A:55:ILE:HD13	1:A:97:LEU:HD11	1.59	0.82
2:G:3:TYR:O	2:G:4:GLN:HG3	1.78	0.82
2:M:99:THR:O	2:M:99:THR:HG22	1.78	0.82
2:L:10:TRP:HH2	2:L:193:GLU:OE1	1.61	0.82
1:A:161:GLU:HG3	2:M:318:ARG:CZ	2.09	0.82
3:O:34:GLY:O	3:O:199:GLY:CA	2.26	0.82
1:F:55:ILE:HD13	1:F:97:LEU:HD11	1.59	0.82
2:B:6:LEU:HD22	2:B:190:ILE:HG23	1.60	0.82
1:F:270:ARG:HH11	2:N:316:LEU:HD23	1.02	0.82
2:L:3:TYR:O	2:L:4:GLN:HG3	1.79	0.82
2:B:94:ASP:C	2:B:100:LYS:HZ1	1.84	0.82
2:H:10:TRP:CZ2	2:H:190:ILE:HG23	2.15	0.82
2:C:99:THR:HG22	2:C:99:THR:O	1.78	0.82
2:L:6:LEU:CD1	2:L:190:ILE:HG22	2.10	0.81
1:F:283:ARG:NE	2:N:315:GLU:OE2	2.11	0.81
2:N:360:HIS:ND1	2:N:363:MET:CE	2.44	0.81
2:G:19:VAL:HG11	2:G:183:ILE:HA	1.61	0.81
1:K:333:HIS:CD2	2:L:297:LEU:HD23	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:172:TYR:OH	1:K:281:ASN:ND2	2.12	0.81
1:K:32:GLN:HE22	2:L:165:THR:HG23	1.43	0.81
2:H:309:ILE:HG13	2:H:313:MET:HG2	1.62	0.81
2:I:360:HIS:ND1	2:I:363:MET:CE	2.43	0.81
1:A:105:HIS:HA	1:F:227:LYS:HZ2	1.43	0.81
1:F:312:LEU:HB2	1:F:320:VAL:HG21	1.60	0.81
2:B:3:TYR:O	2:B:4:GLN:HG3	1.79	0.81
2:I:277:GLU:OE1	3:J:149:GLU:CG	2.21	0.81
2:M:215:ARG:CZ	2:N:164:VAL:HG21	2.10	0.81
2:N:253:VAL:O	2:N:257:VAL:HG23	1.80	0.81
2:D:253:VAL:O	2:D:257:VAL:HG23	1.80	0.81
2:D:357:LEU:HA	2:D:363:MET:CE	2.09	0.81
2:D:360:HIS:ND1	2:D:363:MET:CE	2.44	0.81
2:D:360:HIS:HB3	2:D:363:MET:CG	2.10	0.81
3:O:4:TYR:CD1	3:O:175:TRP:CH2	2.69	0.81
2:B:97:SER:HB2	2:C:144:GLU:HG2	1.61	0.81
2:I:360:HIS:HB3	2:I:363:MET:CG	2.10	0.81
1:K:315:ASP:HB2	1:K:318:GLN:HG3	1.63	0.81
2:I:277:GLU:HA	3:J:149:GLU:HG2	1.61	0.81
2:N:360:HIS:HB3	2:N:363:MET:CG	2.10	0.81
1:F:29:LEU:HD22	1:F:178:LEU:C	2.02	0.81
2:C:309:ILE:HG13	2:C:313:MET:HG2	1.62	0.81
2:C:94:ASP:O	2:C:100:LYS:HE3	1.81	0.80
2:D:99:THR:HG22	2:D:99:THR:O	1.81	0.80
2:I:277:GLU:HB3	3:J:149:GLU:HB3	1.61	0.80
2:L:94:ASP:H	2:L:100:LYS:HZ3	0.82	0.80
2:D:200:PRO:CB	2:D:305:ASP:HB2	2.08	0.80
2:H:6:LEU:HG	2:H:222:ASP:OD1	1.80	0.80
3:E:58:SER:HB3	3:E:65:CYS:SG	2.21	0.80
2:H:94:ASP:O	2:H:100:LYS:HE3	1.81	0.80
2:M:67:GLY:HA2	2:M:119:ARG:HH12	1.47	0.80
2:H:67:GLY:HA2	2:H:119:ARG:HH12	1.47	0.80
1:A:104:LEU:O	1:F:227:LYS:NZ	2.10	0.80
2:L:354:LEU:HD21	2:M:297:LEU:HD22	1.60	0.80
2:C:359:PHE:CE2	2:D:323:THR:HG23	2.15	0.80
2:M:309:ILE:HG13	2:M:313:MET:HG2	1.62	0.80
2:H:99:THR:HG22	2:H:99:THR:O	1.78	0.80
2:N:345:ARG:NH2	3:O:150:ARG:NH2	2.28	0.80
1:A:334:LYS:HB2	2:B:297:LEU:CD2	2.10	0.80
2:M:94:ASP:O	2:M:100:LYS:HE3	1.81	0.80
2:N:241:LEU:O	3:O:156:ARG:NH1	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:58:SER:HB3	3:O:65:CYS:SG	2.22	0.80
2:G:6:LEU:HD12	2:G:222:ASP:CA	2.10	0.80
2:G:10:TRP:HZ2	2:G:194:GLU:CG	1.95	0.80
2:D:259:ALA:HB2	2:D:363:MET:CG	2.12	0.80
2:G:365:LEU:CD2	2:H:297:LEU:HD11	2.04	0.80
2:N:99:THR:O	2:N:99:THR:HG22	1.81	0.80
2:D:238:SER:HB2	2:D:243:THR:HB	1.62	0.79
2:G:10:TRP:HZ2	2:G:194:GLU:HG3	1.47	0.79
2:L:265:MET:CE	2:M:294:MET:HE1	2.12	0.79
2:G:12:PRO:HD3	2:G:215:ARG:NH1	1.96	0.79
2:N:259:ALA:HB2	2:N:363:MET:CG	2.12	0.79
3:J:58:SER:HB3	3:J:65:CYS:SG	2.21	0.79
2:N:345:ARG:HE	3:O:150:ARG:HH21	1.29	0.79
2:H:56:ARG:NH2	2:I:165:THR:HG23	1.96	0.79
2:G:94:ASP:N	2:G:100:LYS:HZ1	1.81	0.79
2:M:341:TYR:CE2	2:N:337:LYS:HB2	2.17	0.79
1:K:333:HIS:CD2	2:L:297:LEU:HG	2.17	0.79
1:A:310:LEU:HD22	1:A:314:GLN:NE2	1.98	0.79
2:M:271:ALA:CB	2:M:276:ILE:HD11	2.13	0.79
2:B:365:LEU:CD2	2:C:297:LEU:CD1	2.61	0.79
1:K:329:LEU:HD11	2:L:294:MET:SD	2.22	0.79
1:F:283:ARG:CD	2:N:315:GLU:OE2	2.31	0.79
2:N:366:PRO:HB3	3:O:283:PRO:HD2	1.63	0.79
1:F:310:LEU:HD22	1:F:314:GLN:NE2	1.98	0.79
2:B:362:ARG:HE	2:B:363:MET:HE2	1.48	0.79
2:L:99:THR:HG22	2:L:99:THR:O	1.83	0.79
2:N:360:HIS:CB	2:N:363:MET:CG	2.61	0.79
2:I:253:VAL:O	2:I:257:VAL:HG23	1.80	0.79
1:A:315:ASP:HB2	1:A:318:GLN:HG3	1.63	0.79
1:K:251:GLN:OE1	3:O:307:ASN:ND2	2.16	0.79
2:I:259:ALA:HB2	2:I:363:MET:CG	2.12	0.78
2:L:6:LEU:CD2	2:L:194:GLU:CG	2.44	0.78
2:L:94:ASP:C	2:L:100:LYS:HZ1	1.86	0.78
1:A:222:LEU:O	1:A:223:MET:HB2	1.83	0.78
2:H:271:ALA:CB	2:H:276:ILE:HD11	2.13	0.78
2:I:99:THR:O	2:I:99:THR:HG22	1.81	0.78
2:H:86:ARG:HH11	2:I:141:LYS:NZ	1.81	0.78
1:F:244:VAL:HG22	1:F:312:LEU:HD21	1.64	0.78
2:G:362:ARG:HE	2:G:363:MET:HE2	1.48	0.78
2:M:80:ARG:O	2:M:84:GLN:HG3	1.82	0.78
2:D:345:ARG:NE	3:E:150:ARG:NH2	1.90	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:363:MET:HB3	2:D:364:PRO:CD	2.14	0.78
2:C:271:ALA:CB	2:C:276:ILE:HD11	2.13	0.78
2:B:248:GLN:HG3	2:B:267:LEU:HB3	1.65	0.78
1:F:270:ARG:HH12	2:N:316:LEU:CA	1.96	0.78
2:M:84:GLN:HA	2:N:144:GLU:OE1	1.84	0.78
2:C:351:MET:HE1	2:D:326:GLN:HE22	1.46	0.78
2:H:86:ARG:NH2	2:I:138:ALA:HA	1.95	0.78
2:D:360:HIS:CB	2:D:363:MET:CG	2.61	0.78
2:C:80:ARG:O	2:C:84:GLN:HG3	1.82	0.78
1:K:222:LEU:O	1:K:223:MET:HB2	1.83	0.78
2:H:56:ARG:HH21	2:I:165:THR:HG23	1.49	0.78
2:L:239:ALA:N	2:L:243:THR:OG1	2.15	0.78
2:G:351:MET:CG	2:H:290:HIS:ND1	2.46	0.78
2:D:13:GLN:HE22	2:D:83:GLU:HG2	1.49	0.78
2:D:345:ARG:NH1	3:E:150:ARG:HG3	1.98	0.78
1:F:270:ARG:HE	2:N:319:THR:HG21	1.49	0.78
2:N:244:LEU:HD21	2:N:276:ILE:HG12	1.66	0.78
1:K:310:LEU:HD22	1:K:314:GLN:NE2	1.98	0.78
3:E:204:LEU:O	3:E:209:ASN:CB	2.32	0.78
1:K:144:GLN:OE1	1:K:280:GLN:O	2.01	0.78
2:H:359:PHE:CE2	2:I:323:THR:HG23	2.18	0.78
2:H:80:ARG:O	2:H:84:GLN:HG3	1.82	0.78
2:G:45:GLY:O	2:G:51:LYS:HE2	1.84	0.78
2:B:45:GLY:O	2:B:51:LYS:HE2	1.84	0.78
1:K:333:HIS:CD2	2:L:297:LEU:CG	2.66	0.78
1:K:29:LEU:HD21	1:K:154:ARG:HH12	1.49	0.78
2:B:99:THR:O	2:B:99:THR:HG22	1.83	0.78
2:I:244:LEU:HD21	2:I:276:ILE:HG12	1.66	0.78
2:I:360:HIS:CB	2:I:363:MET:CG	2.61	0.78
2:L:4:GLN:OE1	2:L:9:LYS:HD2	1.84	0.78
2:H:97:SER:OG	2:H:100:LYS:HE3	1.83	0.78
2:H:93:ILE:CG2	2:H:100:LYS:NZ	2.47	0.78
2:L:180:VAL:CG1	2:L:305:ASP:OD2	2.31	0.78
2:M:341:TYR:CB	2:N:333:LEU:HD13	2.14	0.78
2:G:248:GLN:HG3	2:G:267:LEU:HB3	1.65	0.78
1:A:300:GLN:OE1	1:A:335:PRO:CG	2.32	0.78
1:F:315:ASP:HB2	1:F:318:GLN:HG3	1.63	0.77
1:F:270:ARG:NH2	2:N:316:LEU:HA	1.99	0.77
2:C:93:ILE:CG2	2:C:100:LYS:NZ	2.48	0.77
2:M:86:ARG:HH22	2:N:141:LYS:HE2	1.49	0.77
2:M:111:VAL:HG11	2:M:142:THR:HG21	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:99:THR:O	2:G:99:THR:HG22	1.83	0.77
1:A:75:ALA:HB2	1:F:207:ASN:ND2	1.95	0.77
2:I:363:MET:HB3	2:I:364:PRO:CD	2.14	0.77
2:B:365:LEU:HD22	2:C:297:LEU:CD1	2.14	0.77
2:C:111:VAL:HG11	2:C:142:THR:HG21	1.66	0.77
1:F:29:LEU:HB2	1:F:179:LEU:HB2	1.64	0.77
2:H:93:ILE:HG23	2:I:133:ARG:NH2	2.00	0.77
2:L:180:VAL:CG2	2:L:304:ASN:HB2	2.13	0.77
2:M:97:SER:OG	2:M:100:LYS:HE3	1.83	0.77
1:F:300:GLN:OE1	1:F:335:PRO:CG	2.32	0.77
2:N:363:MET:HB3	2:N:364:PRO:CD	2.14	0.77
1:F:29:LEU:CG	1:F:179:LEU:HB2	2.15	0.77
2:M:281:LEU:HD23	2:M:285:MET:HE2	1.66	0.77
1:K:244:VAL:HG22	1:K:312:LEU:HD21	1.64	0.77
2:B:4:GLN:OE1	2:B:9:LYS:HD2	1.84	0.77
2:M:93:ILE:CG2	2:M:100:LYS:NZ	2.47	0.77
2:C:67:GLY:HA2	2:C:119:ARG:HH12	1.47	0.77
2:C:128:VAL:HG11	2:C:154:LEU:HD22	1.67	0.77
2:D:244:LEU:HD21	2:D:276:ILE:HG12	1.66	0.77
2:N:13:GLN:HE22	2:N:83:GLU:HG2	1.49	0.77
2:L:93:ILE:HG23	2:L:100:LYS:HZ2	1.48	0.77
2:H:111:VAL:HG11	2:H:142:THR:HG21	1.67	0.77
1:F:262:ARG:NH1	3:J:230:TYR:HB3	1.99	0.77
2:C:97:SER:OG	2:C:100:LYS:HE3	1.83	0.77
1:A:336:LEU:HD12	2:B:326:GLN:NE2	2.00	0.77
2:L:45:GLY:O	2:L:51:LYS:HE2	1.84	0.77
2:C:3:TYR:O	2:C:3:TYR:CD2	2.38	0.77
1:K:300:GLN:OE1	1:K:335:PRO:CG	2.32	0.76
1:F:222:LEU:O	1:F:223:MET:HB2	1.83	0.76
2:D:360:HIS:HB2	2:D:363:MET:SD	2.26	0.76
2:H:93:ILE:CG2	2:H:100:LYS:HZ3	1.98	0.76
2:N:355:ARG:HH12	3:O:287:GLN:HB3	1.49	0.76
2:C:10:TRP:CE2	2:C:190:ILE:HG23	2.19	0.76
2:M:354:LEU:CD2	2:N:297:LEU:HD22	2.15	0.76
2:L:265:MET:CE	2:M:294:MET:CE	2.64	0.76
2:N:6:LEU:O	2:N:218:LEU:HB3	1.85	0.76
2:I:360:HIS:HB2	2:I:363:MET:SD	2.26	0.76
2:I:345:ARG:CD	3:J:150:ARG:HH21	1.98	0.76
1:A:334:LYS:CB	2:B:297:LEU:HD21	2.14	0.76
2:B:97:SER:HB3	2:C:144:GLU:OE2	1.84	0.76
1:A:244:VAL:HG22	1:A:312:LEU:HD21	1.64	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:42:LEU:HB3	2:N:172:GLN:HB3	1.67	0.76
2:L:248:GLN:HG3	2:L:267:LEU:HB3	1.66	0.76
2:I:42:LEU:HB3	2:I:172:GLN:HB3	1.67	0.76
2:M:3:TYR:O	2:M:3:TYR:CD2	2.38	0.76
2:H:281:LEU:HD23	2:H:285:MET:HE2	1.65	0.76
2:I:13:GLN:HE22	2:I:83:GLU:HG2	1.49	0.76
2:H:215:ARG:NH2	2:I:164:VAL:CG2	2.49	0.76
2:G:19:VAL:CG2	2:G:186:GLN:CG	2.50	0.76
2:G:4:GLN:OE1	2:G:9:LYS:HD2	1.84	0.76
1:F:310:LEU:HD13	1:F:314:GLN:NE2	2.01	0.76
1:A:105:HIS:HB3	1:F:227:LYS:CD	2.07	0.75
2:L:180:VAL:CG2	2:L:304:ASN:CB	2.65	0.75
2:C:281:LEU:HD23	2:C:285:MET:HE2	1.66	0.75
2:B:10:TRP:HH2	2:B:193:GLU:OE1	1.69	0.75
2:G:21:GLN:N	2:G:178:LEU:HD21	2.01	0.75
1:A:310:LEU:HD13	1:A:314:GLN:NE2	2.02	0.75
3:O:4:TYR:HD1	3:O:175:TRP:CH2	2.04	0.75
2:L:271:ALA:HB1	2:L:276:ILE:HD12	1.68	0.75
2:N:257:VAL:O	2:N:360:HIS:HE1	1.69	0.75
2:N:360:HIS:HB2	2:N:363:MET:SD	2.26	0.75
2:C:94:ASP:O	2:C:100:LYS:CE	2.35	0.75
2:G:347:MET:HG3	2:H:290:HIS:CD2	2.21	0.75
2:H:94:ASP:O	2:H:100:LYS:CE	2.35	0.75
2:L:365:LEU:CD2	2:M:297:LEU:CD1	2.64	0.75
2:G:351:MET:HG2	2:H:290:HIS:ND1	2.01	0.75
2:D:42:LEU:HB3	2:D:172:GLN:HB3	1.67	0.75
2:L:347:MET:CG	2:M:290:HIS:CG	2.68	0.75
2:G:259:ALA:HB3	2:G:363:MET:HE3	1.67	0.75
2:H:128:VAL:HG11	2:H:154:LEU:HD22	1.67	0.75
2:H:351:MET:HE1	2:I:326:GLN:NE2	1.97	0.75
2:B:98:ARG:HH12	2:C:137:ASN:HB3	1.42	0.75
2:D:257:VAL:O	2:D:360:HIS:HE1	1.69	0.75
2:M:215:ARG:NH2	2:N:164:VAL:HG22	2.02	0.75
2:N:259:ALA:CB	2:N:363:MET:HG2	2.17	0.75
2:C:215:ARG:NH2	2:D:164:VAL:HG21	2.01	0.75
2:M:94:ASP:O	2:M:100:LYS:CE	2.35	0.75
2:G:271:ALA:HB1	2:G:276:ILE:HD12	1.68	0.75
2:B:271:ALA:HB1	2:B:276:ILE:HD12	1.68	0.75
2:I:257:VAL:O	2:I:360:HIS:HE1	1.69	0.75
2:I:259:ALA:CB	2:I:363:MET:HG2	2.17	0.75
2:C:215:ARG:CZ	2:D:164:VAL:HG22	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:276:ILE:HD13	2:H:281:LEU:HD12	1.69	0.75
2:N:366:PRO:CA	3:O:283:PRO:HD2	2.16	0.74
1:K:310:LEU:HD13	1:K:314:GLN:NE2	2.01	0.74
2:I:6:LEU:O	2:I:218:LEU:HB3	1.87	0.74
2:I:200:PRO:HB3	2:I:304:ASN:CB	2.17	0.74
2:D:357:LEU:CA	2:D:363:MET:SD	2.75	0.74
2:G:365:LEU:CD2	2:H:297:LEU:HD13	2.17	0.74
3:E:5:PRO:O	3:E:8:ARG:HG2	1.87	0.74
2:L:343:PRO:CA	2:M:283:VAL:HG13	2.17	0.74
3:J:5:PRO:O	3:J:8:ARG:HG2	1.87	0.74
2:M:128:VAL:HG11	2:M:154:LEU:HD22	1.67	0.74
2:N:345:ARG:NH2	3:O:150:ARG:HH21	1.85	0.74
2:L:180:VAL:HG11	2:L:305:ASP:OD2	1.88	0.74
2:H:3:TYR:O	2:H:4:GLN:CG	2.36	0.74
2:C:276:ILE:HD13	2:C:281:LEU:HD12	1.69	0.74
2:D:345:ARG:HH12	3:E:150:ARG:HG3	1.50	0.74
2:L:180:VAL:HG23	2:L:304:ASN:HB2	1.68	0.74
2:L:204:GLN:HE21	2:L:305:ASP:HA	1.53	0.74
2:M:93:ILE:HG22	2:M:100:LYS:NZ	2.03	0.74
2:B:93:ILE:HG23	2:B:100:LYS:HZ2	1.52	0.74
2:M:276:ILE:HD13	2:M:281:LEU:HD12	1.69	0.74
2:N:360:HIS:CG	2:N:363:MET:HG3	2.23	0.74
2:N:357:LEU:CA	2:N:363:MET:SD	2.75	0.74
2:D:259:ALA:CB	2:D:363:MET:HG2	2.17	0.74
2:I:201:ARG:H	2:I:305:ASP:HB2	1.52	0.74
1:K:82:LEU:HD21	1:K:100:LEU:HD12	1.70	0.74
2:M:86:ARG:NH2	2:N:141:LYS:HE2	1.70	0.74
2:B:259:ALA:HB3	2:B:363:MET:HE3	1.68	0.74
2:C:93:ILE:HG22	2:C:100:LYS:NZ	2.03	0.73
2:N:358:ALA:HA	2:N:364:PRO:HG2	1.71	0.73
2:G:12:PRO:HD2	2:G:215:ARG:HH22	1.52	0.73
3:O:6:TRP:CZ3	3:O:175:TRP:CD2	2.74	0.73
2:C:3:TYR:O	2:C:4:GLN:HG3	1.88	0.73
2:C:156:THR:HG22	2:C:158:ASP:H	1.53	0.73
2:B:6:LEU:HD21	2:B:194:GLU:CD	2.08	0.73
2:H:93:ILE:HG22	2:H:100:LYS:NZ	2.03	0.73
2:N:366:PRO:CB	3:O:282:SER:CB	2.65	0.73
1:K:147:LEU:HB3	1:K:148:PRO:HD3	1.69	0.73
2:I:357:LEU:CA	2:I:363:MET:SD	2.75	0.73
2:M:156:THR:HG22	2:M:158:ASP:H	1.54	0.73
2:N:366:PRO:CB	3:O:283:PRO:HD2	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:7:ALA:N	2:G:222:ASP:OD2	2.18	0.73
2:D:277:GLU:HB3	3:E:149:GLU:HG2	0.76	0.73
1:F:273:PHE:HB3	1:F:279:TRP:CB	2.18	0.73
1:F:283:ARG:CZ	2:N:315:GLU:OE2	2.14	0.73
2:G:49:VAL:HA	2:G:213:SER:CB	2.18	0.73
2:I:358:ALA:HA	2:I:364:PRO:HG2	1.71	0.73
2:D:360:HIS:CG	2:D:363:MET:HG3	2.23	0.73
2:D:360:HIS:ND1	2:D:363:MET:HE2	2.02	0.73
2:H:94:ASP:C	2:H:100:LYS:HZ1	1.91	0.73
3:O:4:TYR:HD1	3:O:175:TRP:HH2	1.34	0.73
1:A:75:ALA:CB	1:F:207:ASN:CG	2.56	0.73
1:K:273:PHE:HB3	1:K:279:TRP:CB	2.18	0.73
3:E:49:LEU:HD23	3:E:68:MET:SD	2.29	0.73
2:H:10:TRP:CZ2	2:H:194:GLU:OE2	2.42	0.73
2:N:354:LEU:HD12	3:O:253:MET:HE1	1.70	0.73
1:A:82:LEU:HD21	1:A:100:LEU:HD12	1.70	0.73
2:D:271:ALA:HB1	2:D:276:ILE:CD1	2.19	0.73
3:J:49:LEU:HD23	3:J:68:MET:SD	2.29	0.73
1:A:273:PHE:HB3	1:A:279:TRP:CB	2.19	0.72
3:O:5:PRO:O	3:O:8:ARG:HG2	1.87	0.72
3:E:117:ALA:O	3:E:120:LEU:HD22	1.89	0.72
1:A:194:ASP:HA	2:M:311:LEU:CD1	2.19	0.72
2:D:337:LYS:HD3	3:E:334:LEU:HB2	1.69	0.72
2:H:215:ARG:NH2	2:I:164:VAL:HG21	2.04	0.72
2:C:56:ARG:NH2	2:D:165:THR:CG2	2.52	0.72
2:I:360:HIS:CG	2:I:363:MET:HG3	2.23	0.72
2:I:271:ALA:HB1	2:I:276:ILE:CD1	2.19	0.72
1:A:106:ASP:CB	1:F:225:LYS:CD	2.58	0.72
3:O:49:LEU:HD23	3:O:68:MET:SD	2.29	0.72
2:L:362:ARG:HE	2:L:363:MET:HE2	1.55	0.72
2:M:215:ARG:HH22	2:N:164:VAL:CG2	2.00	0.72
3:J:117:ALA:O	3:J:120:LEU:HD22	1.89	0.72
1:A:147:LEU:HB3	1:A:148:PRO:HD3	1.69	0.72
2:B:6:LEU:HD13	2:B:190:ILE:HG23	1.59	0.72
2:H:156:THR:HG22	2:H:158:ASP:H	1.54	0.72
1:F:147:LEU:HB3	1:F:148:PRO:HD3	1.70	0.72
1:F:82:LEU:HD21	1:F:100:LEU:HD12	1.70	0.72
2:H:86:ARG:HH22	2:I:141:LYS:HE2	1.54	0.72
2:M:56:ARG:NH2	2:N:165:THR:CG2	2.53	0.72
2:N:271:ALA:HB1	2:N:276:ILE:CD1	2.19	0.72
2:N:357:LEU:HA	2:N:363:MET:HE1	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:259:ALA:HB1	2:I:363:MET:HG2	1.72	0.72
2:D:259:ALA:HB1	2:D:363:MET:HG2	1.72	0.72
2:M:201:ARG:HB2	2:M:305:ASP:CG	2.11	0.72
2:I:277:GLU:HB3	3:J:149:GLU:HG2	0.74	0.71
2:I:357:LEU:HA	2:I:363:MET:HE1	1.72	0.71
2:N:356:ALA:O	2:N:363:MET:HE1	1.90	0.71
2:M:86:ARG:NH2	2:N:138:ALA:HA	2.02	0.71
1:K:223:MET:SD	1:K:292:ARG:CB	2.78	0.71
2:C:215:ARG:NH2	2:D:164:VAL:HG22	2.05	0.71
3:O:117:ALA:O	3:O:120:LEU:HD22	1.89	0.71
2:D:345:ARG:CD	3:E:150:ARG:HH21	2.02	0.71
2:N:345:ARG:HH21	3:O:150:ARG:NH2	1.87	0.71
2:D:241:LEU:O	3:E:156:ARG:NH1	2.22	0.71
2:G:12:PRO:CD	2:G:215:ARG:HH12	2.03	0.71
2:C:351:MET:HE3	2:C:351:MET:HA	1.71	0.71
2:D:6:LEU:O	2:D:218:LEU:HB3	1.90	0.71
1:F:29:LEU:CB	1:F:179:LEU:HB2	2.20	0.71
2:D:358:ALA:HA	2:D:364:PRO:HG2	1.71	0.71
2:L:6:LEU:CD1	2:L:190:ILE:CG2	2.61	0.71
2:C:351:MET:CE	2:D:326:GLN:HE22	2.04	0.71
2:M:360:HIS:HB3	2:M:363:MET:O	1.91	0.71
2:G:226:ALA:HB2	2:H:36:ARG:HH11	1.56	0.71
2:H:93:ILE:HG23	2:I:133:ARG:HH22	1.55	0.71
2:B:98:ARG:NH1	2:C:137:ASN:OD1	2.24	0.71
1:A:213:THR:H	1:A:216:HIS:CD2	2.04	0.71
2:N:354:LEU:HD12	3:O:253:MET:CE	2.20	0.71
1:A:29:LEU:HD21	1:A:154:ARG:HH12	1.56	0.71
1:F:29:LEU:CD1	1:F:179:LEU:CB	2.42	0.71
2:G:20:GLY:O	2:G:178:LEU:HD22	1.86	0.71
2:L:365:LEU:HD21	2:M:297:LEU:HD11	1.73	0.71
1:A:223:MET:SD	1:A:292:ARG:CB	2.78	0.71
2:D:355:ARG:NH1	3:E:287:GLN:HB3	2.06	0.71
2:M:276:ILE:HG22	2:M:277:GLU:H	1.56	0.71
2:N:220:LEU:CD2	3:O:154:THR:HA	2.20	0.70
2:G:20:GLY:O	2:G:178:LEU:HD23	1.91	0.70
2:M:351:MET:CE	2:N:326:GLN:NE2	2.35	0.70
1:K:32:GLN:NE2	2:L:165:THR:HG23	2.07	0.70
2:L:259:ALA:CB	2:L:363:MET:HE3	2.21	0.70
2:G:10:TRP:CZ2	2:G:194:GLU:CG	2.73	0.70
1:F:213:THR:H	1:F:216:HIS:CD2	2.04	0.70
1:F:202:VAL:O	1:F:206:VAL:HG23	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:270:ARG:HH12	2:N:316:LEU:HD23	0.87	0.70
2:I:360:HIS:ND1	2:I:363:MET:HE2	2.06	0.70
2:C:360:HIS:HB3	2:C:363:MET:O	1.91	0.70
2:N:259:ALA:HB1	2:N:363:MET:HG2	1.72	0.70
2:B:98:ARG:CZ	2:C:137:ASN:OD1	2.38	0.70
1:A:300:GLN:OE1	1:A:335:PRO:HG3	1.91	0.70
1:K:300:GLN:OE1	1:K:335:PRO:HG3	1.91	0.70
3:E:169:GLU:O	3:E:173:VAL:HG23	1.92	0.70
2:D:5:VAL:HG13	2:D:222:ASP:CG	2.12	0.70
2:G:10:TRP:CZ2	2:G:194:GLU:HG3	2.26	0.70
2:M:341:TYR:HB3	2:N:333:LEU:HD13	1.73	0.70
3:J:169:GLU:O	3:J:173:VAL:HG23	1.91	0.70
2:N:220:LEU:HD21	3:O:154:THR:CA	2.22	0.70
2:L:205:LEU:HD22	2:L:244:LEU:CD1	2.21	0.70
2:L:365:LEU:HD22	2:M:297:LEU:CD1	2.21	0.70
2:M:3:TYR:O	2:M:4:GLN:HG3	1.91	0.70
1:A:313:LYS:O	1:A:316:TYR:CZ	2.44	0.70
1:A:133:ARG:NH2	1:F:227:LYS:CE	2.55	0.70
2:H:341:TYR:CE2	2:I:337:LYS:HB2	2.27	0.70
2:H:360:HIS:HB3	2:H:363:MET:O	1.91	0.70
1:K:313:LYS:O	1:K:316:TYR:CZ	2.44	0.70
2:H:73:CYS:O	2:H:79:CYS:SG	2.50	0.70
2:B:6:LEU:CD1	2:B:190:ILE:HG21	1.92	0.69
1:A:315:ASP:CG	1:A:315:ASP:CA	2.61	0.69
2:C:341:TYR:CE2	2:D:337:LYS:HB2	2.26	0.69
2:C:67:GLY:HA2	2:C:119:ARG:NH1	2.07	0.69
1:F:306:THR:OG1	3:J:310:LEU:HD22	1.92	0.69
1:F:313:LYS:O	1:F:316:TYR:CZ	2.44	0.69
1:K:222:LEU:HD12	1:K:285:MET:HG2	1.74	0.69
2:C:276:ILE:HG22	2:C:277:GLU:H	1.56	0.69
1:F:300:GLN:OE1	1:F:335:PRO:HG3	1.91	0.69
1:A:194:ASP:HA	2:M:311:LEU:HD11	1.72	0.69
2:N:366:PRO:HB3	3:O:282:SER:CB	2.14	0.69
1:A:222:LEU:HD12	1:A:285:MET:HG2	1.74	0.69
3:O:6:TRP:CZ3	3:O:175:TRP:CE2	2.80	0.69
1:A:55:ILE:O	1:A:85:PRO:HG3	1.92	0.69
2:L:347:MET:SD	2:M:287:GLY:CA	2.80	0.69
2:G:49:VAL:HA	2:G:213:SER:HB3	1.73	0.69
2:H:94:ASP:O	2:H:100:LYS:NZ	2.25	0.69
2:L:265:MET:HE1	2:M:294:MET:CE	2.20	0.69
1:A:161:GLU:CG	2:M:318:ARG:CZ	2.67	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:32:LEU:HD11	3:E:195:ALA:O	1.91	0.69
2:N:364:PRO:HG3	3:O:260:HIS:CE1	2.26	0.69
2:C:94:ASP:O	2:C:100:LYS:NZ	2.25	0.69
2:H:67:GLY:HA2	2:H:119:ARG:NH1	2.07	0.69
2:N:345:ARG:HH22	3:O:150:ARG:NE	1.58	0.69
1:A:106:ASP:OD1	1:F:225:LYS:HD2	1.91	0.69
2:N:271:ALA:HB1	2:N:276:ILE:HD12	1.75	0.69
2:I:338:GLU:O	2:I:341:TYR:HB2	1.93	0.69
1:F:222:LEU:HD12	1:F:285:MET:HG2	1.74	0.69
2:D:334:ILE:HG21	3:E:332:PRO:HB2	1.75	0.69
2:D:338:GLU:O	2:D:341:TYR:HB2	1.93	0.69
2:H:276:ILE:HG22	2:H:277:GLU:H	1.56	0.69
1:F:308:THR:HG23	1:F:320:VAL:HG13	1.75	0.69
2:M:94:ASP:O	2:M:100:LYS:NZ	2.25	0.69
2:C:73:CYS:O	2:C:79:CYS:SG	2.50	0.69
3:O:169:GLU:O	3:O:173:VAL:HG23	1.92	0.69
1:A:202:VAL:O	1:A:206:VAL:HG23	1.92	0.69
2:L:73:CYS:O	2:L:79:CYS:SG	2.51	0.69
3:J:163:TYR:OH	3:J:166:PRO:CD	2.41	0.69
2:M:73:CYS:O	2:M:79:CYS:SG	2.50	0.69
2:L:10:TRP:CZ2	2:L:193:GLU:HB3	2.28	0.69
1:K:55:ILE:O	1:K:85:PRO:HG3	1.93	0.69
2:L:351:MET:CG	2:M:290:HIS:ND1	2.56	0.69
2:G:19:VAL:HG12	2:G:178:LEU:CD1	2.18	0.69
2:B:97:SER:HB2	2:C:144:GLU:CG	2.22	0.69
1:K:315:ASP:CG	1:K:315:ASP:CA	2.61	0.68
1:K:308:THR:HG23	1:K:320:VAL:HG13	1.75	0.68
1:A:308:THR:HG23	1:A:320:VAL:HG13	1.75	0.68
2:M:67:GLY:HA2	2:M:119:ARG:NH1	2.07	0.68
3:J:111:VAL:HG12	3:J:140:TRP:HB2	1.75	0.68
2:I:220:LEU:HD21	3:J:154:THR:HA	1.73	0.68
1:K:202:VAL:O	1:K:206:VAL:HG23	1.92	0.68
2:D:345:ARG:HH12	3:E:150:ARG:CG	2.05	0.68
2:N:259:ALA:CB	2:N:363:MET:CG	2.72	0.68
1:F:315:ASP:CA	1:F:315:ASP:CG	2.61	0.68
2:D:309:ILE:HG22	2:D:313:MET:HG2	1.74	0.68
2:I:271:ALA:HB1	2:I:276:ILE:HD12	1.75	0.68
2:D:357:LEU:HA	2:D:363:MET:HE1	1.73	0.68
2:L:180:VAL:CB	2:L:304:ASN:O	2.34	0.68
1:A:133:ARG:HG3	2:G:299:PRO:HG2	1.75	0.68
2:M:10:TRP:CH2	2:M:190:ILE:HG12	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:93:ILE:HG23	2:D:133:ARG:NH2	2.08	0.68
2:I:309:ILE:HG22	2:I:313:MET:HG2	1.74	0.68
2:B:10:TRP:CH2	2:B:193:GLU:OE1	2.45	0.68
3:E:111:VAL:HG12	3:E:140:TRP:HB2	1.75	0.68
2:G:110:ASN:HB3	2:G:113:TYR:HD1	1.58	0.68
2:B:110:ASN:HB3	2:B:113:TYR:HD1	1.58	0.68
2:B:93:ILE:HG23	2:B:100:LYS:NZ	2.09	0.68
2:H:56:ARG:NH2	2:I:165:THR:HG21	2.08	0.68
1:A:338:ASP:OD2	2:B:326:GLN:CD	2.32	0.68
2:N:338:GLU:O	2:N:341:TYR:HB2	1.93	0.68
2:I:254:GLU:OE2	2:I:312:ARG:HD3	1.93	0.68
2:N:309:ILE:HG22	2:N:313:MET:HG2	1.74	0.68
1:F:55:ILE:O	1:F:85:PRO:HG3	1.93	0.68
2:L:110:ASN:HB3	2:L:113:TYR:HD1	1.58	0.68
2:L:6:LEU:HD21	2:L:194:GLU:CD	2.12	0.68
2:G:93:ILE:HG23	2:G:100:LYS:NZ	2.09	0.68
1:F:223:MET:SD	1:F:292:ARG:CB	2.78	0.68
2:D:254:GLU:OE2	2:D:312:ARG:HD3	1.94	0.68
3:O:74:PRO:HB3	3:O:105:ARG:HD2	1.76	0.68
2:L:18:VAL:CG2	2:L:25:LEU:HD11	2.24	0.68
1:A:116:LYS:HB3	1:A:140:GLN:HE21	1.58	0.68
3:E:31:ALA:HB2	3:E:164:LEU:HB3	1.75	0.68
1:F:270:ARG:HH11	2:N:316:LEU:CD2	1.87	0.68
2:L:6:LEU:HD21	2:L:194:GLU:HG3	0.74	0.68
2:G:354:LEU:HD23	2:H:297:LEU:HD22	1.76	0.68
2:B:93:ILE:CG2	2:B:100:LYS:NZ	2.57	0.68
2:L:180:VAL:HB	2:L:304:ASN:C	2.14	0.68
2:I:200:PRO:HB2	2:I:305:ASP:N	2.09	0.68
2:B:6:LEU:CG	2:B:194:GLU:HG3	2.24	0.68
1:K:333:HIS:CG	2:L:297:LEU:CG	2.76	0.68
2:L:93:ILE:HG23	2:L:100:LYS:NZ	2.09	0.68
2:I:345:ARG:HH12	3:J:150:ARG:CG	2.07	0.68
2:G:93:ILE:CG2	2:G:100:LYS:NZ	2.57	0.68
2:C:215:ARG:CZ	2:D:164:VAL:CG2	2.72	0.68
3:J:74:PRO:HB3	3:J:105:ARG:HD2	1.76	0.68
2:G:229:ASP:HA	2:H:30:ASN:HD21	1.57	0.68
2:D:271:ALA:HB1	2:D:276:ILE:HD12	1.75	0.67
3:E:74:PRO:HB3	3:E:105:ARG:HD2	1.76	0.67
3:O:31:ALA:HB2	3:O:164:LEU:HB3	1.76	0.67
2:N:345:ARG:HH21	3:O:150:ARG:CZ	2.05	0.67
1:F:283:ARG:NH2	2:N:315:GLU:OE1	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:254:GLU:OE2	2:N:312:ARG:HD3	1.94	0.67
2:N:260:ASN:O	2:N:262:GLU:N	2.27	0.67
2:G:73:CYS:O	2:G:79:CYS:SG	2.51	0.67
2:H:341:TYR:CB	2:I:333:LEU:CD1	2.72	0.67
1:A:338:ASP:OD2	2:B:326:GLN:CG	2.42	0.67
2:B:73:CYS:O	2:B:79:CYS:SG	2.51	0.67
1:K:116:LYS:HB3	1:K:140:GLN:HE21	1.59	0.67
2:I:277:GLU:CB	3:J:149:GLU:HB3	2.25	0.67
2:D:277:GLU:HB3	3:E:149:GLU:HB3	1.76	0.67
2:L:93:ILE:CG2	2:L:100:LYS:NZ	2.57	0.67
2:H:100:LYS:CG	2:I:133:ARG:CZ	2.61	0.67
1:F:116:LYS:HB3	1:F:140:GLN:HE21	1.59	0.67
2:L:10:TRP:CH2	2:L:193:GLU:OE1	2.47	0.67
1:K:213:THR:H	1:K:216:HIS:CD2	2.04	0.67
1:K:32:GLN:NE2	2:L:165:THR:HA	2.08	0.67
2:H:10:TRP:CH2	2:H:190:ILE:HG23	2.30	0.67
2:D:260:ASN:O	2:D:262:GLU:N	2.27	0.67
3:J:31:ALA:HB2	3:J:164:LEU:HB3	1.76	0.67
2:D:259:ALA:CB	2:D:363:MET:CG	2.72	0.67
2:L:265:MET:HE2	2:M:294:MET:HE3	1.75	0.67
1:K:262:ARG:CZ	3:O:230:TYR:HB3	2.24	0.67
2:B:98:ARG:NH1	2:C:137:ASN:CB	2.51	0.67
2:N:73:CYS:O	2:N:79:CYS:SG	2.48	0.67
2:G:259:ALA:CB	2:G:363:MET:HE3	2.25	0.67
2:L:354:LEU:HD21	2:M:297:LEU:CD2	2.25	0.67
2:G:18:VAL:CG2	2:G:25:LEU:HD11	2.24	0.67
2:G:73:CYS:SG	2:G:73:CYS:O	2.53	0.67
2:C:181:GLU:HG2	2:C:184:ARG:HD2	1.77	0.67
2:N:364:PRO:HG3	3:O:260:HIS:HE1	1.60	0.67
2:D:358:ALA:HA	2:D:364:PRO:CG	2.25	0.67
2:N:93:ILE:HG22	2:N:100:LYS:NZ	2.10	0.67
1:K:28:PRO:HB3	2:L:164:VAL:CG2	2.22	0.67
2:G:351:MET:HG3	2:H:290:HIS:ND1	2.09	0.67
2:I:93:ILE:HG22	2:I:100:LYS:NZ	2.10	0.67
3:O:111:VAL:HG12	3:O:140:TRP:HB2	1.75	0.67
2:I:260:ASN:O	2:I:262:GLU:N	2.27	0.67
3:J:163:TYR:OH	3:J:166:PRO:HD2	1.94	0.66
2:I:356:ALA:O	2:I:363:MET:HE1	1.95	0.66
2:N:358:ALA:HA	2:N:364:PRO:CG	2.25	0.66
2:L:351:MET:HG2	2:M:290:HIS:ND1	2.10	0.66
2:L:73:CYS:O	2:L:73:CYS:SG	2.53	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:347:MET:O	2:N:351:MET:HG2	1.96	0.66
2:M:181:GLU:HG2	2:M:184:ARG:HD2	1.77	0.66
1:A:191:LEU:HD22	2:B:23:HIS:ND1	2.11	0.66
2:I:259:ALA:CB	2:I:363:MET:CG	2.72	0.66
2:I:73:CYS:O	2:I:79:CYS:SG	2.48	0.66
2:D:309:ILE:HG21	2:D:313:MET:HG2	1.77	0.66
3:E:64:GLY:O	3:E:68:MET:HB2	1.96	0.66
2:D:73:CYS:O	2:D:79:CYS:SG	2.48	0.66
2:D:93:ILE:HG22	2:D:100:LYS:NZ	2.10	0.66
2:D:347:MET:O	2:D:351:MET:HG2	1.96	0.66
2:B:94:ASP:H	2:B:100:LYS:HZ1	1.43	0.66
3:O:64:GLY:O	3:O:68:MET:HB2	1.96	0.66
2:I:5:VAL:HG13	2:I:222:ASP:CG	2.15	0.66
2:L:365:LEU:HD21	2:M:297:LEU:CD1	2.25	0.66
3:O:8:ARG:CG	3:O:9:PRO:HD3	2.26	0.66
1:K:329:LEU:HD12	2:L:294:MET:SD	2.36	0.66
3:J:8:ARG:CG	3:J:9:PRO:HD3	2.25	0.66
2:C:11:ARG:NH2	2:D:165:THR:HG22	2.11	0.66
2:B:73:CYS:O	2:B:73:CYS:SG	2.53	0.66
2:I:347:MET:O	2:I:351:MET:HG2	1.96	0.66
2:D:356:ALA:O	2:D:363:MET:CE	2.45	0.65
2:L:10:TRP:HZ2	2:L:193:GLU:HB3	1.61	0.65
1:A:105:HIS:CA	1:F:227:LYS:HD2	2.26	0.65
2:C:86:ARG:NE	2:D:141:LYS:HB2	2.11	0.65
2:B:259:ALA:CB	2:B:363:MET:HE3	2.26	0.65
2:H:181:GLU:HG2	2:H:184:ARG:HD2	1.77	0.65
2:D:345:ARG:NH1	3:E:150:ARG:CG	2.59	0.65
2:I:358:ALA:HA	2:I:364:PRO:CG	2.25	0.65
2:B:18:VAL:CG2	2:B:25:LEU:HD11	2.24	0.65
2:D:13:GLN:NE2	2:D:83:GLU:HG2	2.11	0.65
2:N:13:GLN:NE2	2:N:83:GLU:HG2	2.11	0.65
2:I:356:ALA:O	2:I:363:MET:CE	2.45	0.65
2:I:345:ARG:NH1	3:J:150:ARG:HG3	2.11	0.65
2:I:355:ARG:NH1	3:J:287:GLN:HB3	2.11	0.65
2:L:343:PRO:HB3	2:M:283:VAL:O	1.95	0.65
3:J:64:GLY:O	3:J:68:MET:HB2	1.96	0.65
2:N:345:ARG:CZ	3:O:150:ARG:NH2	2.60	0.65
2:N:360:HIS:ND1	2:N:363:MET:HE2	2.11	0.65
2:I:277:GLU:CG	3:J:149:GLU:CG	2.74	0.65
2:I:277:GLU:HA	3:J:149:GLU:CG	2.27	0.65
2:I:309:ILE:HG21	2:I:313:MET:HG2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:93:ILE:CG2	2:M:100:LYS:HZ3	2.10	0.65
1:A:48:GLU:HG3	1:A:49:GLU:N	2.12	0.65
1:F:274:ASP:HA	1:F:279:TRP:CE3	2.32	0.65
2:H:93:ILE:HG22	2:H:100:LYS:HZ3	1.62	0.65
2:I:13:GLN:NE2	2:I:83:GLU:HG2	2.11	0.65
2:G:98:ARG:HD2	2:H:141:LYS:HZ3	1.62	0.65
1:K:48:GLU:HG3	1:K:49:GLU:N	2.12	0.65
3:J:73:HIS:HD2	3:J:75:ASP:H	1.45	0.65
1:F:48:GLU:HG3	1:F:49:GLU:N	2.12	0.65
2:N:356:ALA:O	2:N:363:MET:CE	2.45	0.64
3:E:8:ARG:CG	3:E:9:PRO:HD3	2.26	0.64
2:N:360:HIS:CG	2:N:363:MET:CG	2.80	0.64
2:L:265:MET:HE2	2:M:294:MET:CE	2.26	0.64
1:F:239:GLU:HA	2:G:174:HIS:CE1	2.32	0.64
1:A:209:ALA:O	2:B:176:LYS:HD2	1.97	0.64
1:F:270:ARG:HH22	2:N:316:LEU:HA	1.60	0.64
2:M:201:ARG:HH21	2:M:308:ALA:HB2	1.62	0.64
1:K:255:LEU:HD22	3:O:313:THR:HG21	1.77	0.64
2:H:343:PRO:HG2	2:H:347:MET:SD	2.38	0.64
2:C:93:ILE:CG2	2:C:100:LYS:HZ2	2.11	0.64
2:I:238:SER:CB	2:I:243:THR:HB	2.25	0.64
1:A:274:ASP:HA	1:A:279:TRP:CE3	2.32	0.64
1:F:270:ARG:HE	2:N:319:THR:CG2	1.95	0.64
1:F:273:PHE:HB3	1:F:279:TRP:CG	2.33	0.64
2:G:354:LEU:HD21	2:H:297:LEU:HD22	1.76	0.64
2:M:73:CYS:SG	2:M:73:CYS:O	2.56	0.64
2:M:343:PRO:HG2	2:M:347:MET:SD	2.37	0.64
2:M:10:TRP:CE2	2:M:190:ILE:CG2	2.78	0.64
1:F:315:ASP:HB2	1:F:318:GLN:HG2	1.80	0.64
2:L:180:VAL:HG23	2:L:304:ASN:CB	2.25	0.64
2:N:337:LYS:HG3	2:N:338:GLU:N	2.12	0.64
3:O:4:TYR:CD1	3:O:175:TRP:HH2	2.11	0.64
3:O:147:GLU:HG2	3:O:147:GLU:O	1.98	0.64
2:M:6:LEU:HG	2:M:222:ASP:OD1	1.97	0.64
2:C:343:PRO:HG2	2:C:347:MET:SD	2.37	0.64
2:M:111:VAL:HG11	2:M:142:THR:CG2	2.27	0.64
2:C:73:CYS:SG	2:C:73:CYS:O	2.55	0.64
3:J:147:GLU:O	3:J:147:GLU:HG2	1.98	0.64
3:E:147:GLU:HG2	3:E:147:GLU:O	1.98	0.64
2:B:354:LEU:HD21	2:C:297:LEU:HD22	1.80	0.64
1:A:273:PHE:HB3	1:A:279:TRP:CG	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:274:ASP:HA	1:K:279:TRP:CE3	2.32	0.64
2:B:254:GLU:O	2:B:258:GLU:HG3	1.98	0.64
2:D:360:HIS:CG	2:D:363:MET:CG	2.80	0.64
2:L:354:LEU:HD23	2:M:297:LEU:HD22	1.77	0.64
2:H:10:TRP:HZ2	2:H:194:GLU:OE2	1.80	0.64
2:B:268:ILE:HD11	2:B:353:LEU:CD1	2.28	0.64
2:B:6:LEU:CD2	2:B:194:GLU:CD	2.66	0.63
1:K:273:PHE:HB3	1:K:279:TRP:CG	2.33	0.63
2:H:86:ARG:HH11	2:I:141:LYS:HZ3	1.40	0.63
2:M:215:ARG:NE	2:N:164:VAL:CG1	2.61	0.63
2:I:337:LYS:HG3	2:I:338:GLU:N	2.12	0.63
2:B:354:LEU:CD2	2:C:297:LEU:HD22	2.28	0.63
2:L:254:GLU:O	2:L:258:GLU:HG3	1.98	0.63
2:D:102:GLU:HB3	2:D:106:ASP:HB2	1.81	0.63
1:A:119:LYS:CD	1:A:119:LYS:H	2.04	0.63
2:N:309:ILE:HG21	2:N:313:MET:HG2	1.77	0.63
2:H:73:CYS:SG	2:H:73:CYS:O	2.56	0.63
3:O:329:LEU:H	3:O:329:LEU:HD23	1.63	0.63
2:D:277:GLU:HA	3:E:149:GLU:HG2	1.77	0.63
1:F:281:ASN:C	1:F:283:ARG:H	2.02	0.63
2:I:360:HIS:CG	2:I:363:MET:CG	2.81	0.63
1:K:315:ASP:HB2	1:K:318:GLN:HG2	1.80	0.63
2:B:365:LEU:HD21	2:C:297:LEU:CD1	2.29	0.63
2:G:268:ILE:HD11	2:G:353:LEU:CD1	2.28	0.63
2:M:359:PHE:CZ	2:N:323:THR:HG23	2.33	0.63
2:M:3:TYR:O	2:M:4:GLN:CB	2.46	0.63
2:I:100:LYS:HB2	2:I:103:ASP:OD1	1.99	0.63
2:I:102:GLU:HB3	2:I:106:ASP:HB2	1.80	0.63
3:E:329:LEU:HD23	3:E:329:LEU:H	1.63	0.63
3:J:161:LEU:H	3:J:161:LEU:HD12	1.64	0.63
2:N:366:PRO:HB2	3:O:282:SER:CB	2.29	0.63
2:D:100:LYS:HB2	2:D:103:ASP:OD1	1.99	0.63
3:E:73:HIS:HD2	3:E:75:ASP:H	1.45	0.63
2:N:102:GLU:HB3	2:N:106:ASP:HB2	1.81	0.63
3:O:161:LEU:H	3:O:161:LEU:HD12	1.64	0.63
1:F:333:HIS:ND1	2:G:298:SER:OG	2.32	0.63
2:I:345:ARG:HH12	3:J:150:ARG:HG3	1.62	0.63
2:D:337:LYS:HG3	2:D:338:GLU:N	2.12	0.63
1:F:222:LEU:CD1	1:F:285:MET:HG2	2.29	0.63
1:A:222:LEU:CD1	1:A:285:MET:HG2	2.29	0.63
1:A:281:ASN:C	1:A:283:ARG:H	2.02	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:111:VAL:HG11	2:H:142:THR:CG2	2.28	0.63
1:K:262:ARG:NH2	3:O:230:TYR:HB3	2.14	0.63
2:G:98:ARG:HD2	2:H:141:LYS:NZ	2.14	0.63
2:B:6:LEU:CD2	2:B:190:ILE:HG23	2.28	0.63
2:G:94:ASP:N	2:G:100:LYS:HZ3	1.89	0.63
2:M:86:ARG:NE	2:N:141:LYS:HB2	2.13	0.63
3:O:129:LEU:HD11	3:O:158:ARG:HH11	1.64	0.63
3:O:73:HIS:HD2	3:O:75:ASP:H	1.45	0.63
2:G:328:TYR:O	2:G:332:LEU:HD23	1.99	0.63
1:F:29:LEU:HD11	1:F:179:LEU:CD1	2.22	0.62
2:L:94:ASP:O	2:L:100:LYS:HE3	1.99	0.62
2:B:354:LEU:CD1	2:C:294:MET:SD	2.82	0.62
2:N:100:LYS:HB2	2:N:103:ASP:OD1	1.99	0.62
3:J:129:LEU:HD11	3:J:158:ARG:HH11	1.64	0.62
2:H:10:TRP:CE2	2:H:190:ILE:HG23	2.34	0.62
2:M:93:ILE:CG2	2:M:100:LYS:HZ2	2.12	0.62
2:G:271:ALA:HB1	2:G:276:ILE:CD1	2.30	0.62
2:L:268:ILE:HD11	2:L:353:LEU:CD1	2.28	0.62
3:J:329:LEU:HD23	3:J:329:LEU:H	1.63	0.62
2:D:345:ARG:HE	3:E:150:ARG:HH21	0.66	0.62
2:D:356:ALA:O	2:D:363:MET:HE1	1.99	0.62
2:C:111:VAL:HG11	2:C:142:THR:CG2	2.28	0.62
3:J:32:LEU:HD11	3:J:195:ALA:O	1.99	0.62
2:L:328:TYR:O	2:L:332:LEU:HD23	1.99	0.62
2:D:316:LEU:HD22	2:D:320:ILE:HD11	1.81	0.62
2:L:93:ILE:CG2	2:L:100:LYS:HZ2	2.12	0.62
2:H:84:GLN:HA	2:I:144:GLU:OE1	1.99	0.62
2:G:254:GLU:O	2:G:258:GLU:HG3	1.98	0.62
2:N:223:GLN:HE21	3:O:158:ARG:HE	1.45	0.62
1:K:24:LEU:HA	1:K:114:GLY:O	2.00	0.62
2:G:347:MET:HG3	2:H:290:HIS:NE2	2.14	0.62
1:K:222:LEU:CD1	1:K:285:MET:HG2	2.29	0.62
2:G:6:LEU:HD11	2:G:225:ILE:CD1	2.29	0.62
2:L:271:ALA:HB1	2:L:276:ILE:CD1	2.29	0.62
2:C:93:ILE:HG23	2:C:100:LYS:NZ	2.15	0.62
2:H:10:TRP:CZ3	2:H:190:ILE:HG12	2.35	0.62
2:L:223:GLN:OE1	2:M:171:LEU:CD1	2.47	0.62
2:I:316:LEU:HD22	2:I:320:ILE:HD11	1.81	0.62
2:B:94:ASP:O	2:B:100:LYS:HE3	1.99	0.62
2:H:93:ILE:HG23	2:H:100:LYS:HZ3	1.64	0.62
2:N:366:PRO:HA	3:O:283:PRO:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:ALA:HB1	2:B:276:ILE:CD1	2.30	0.62
1:A:256:LEU:O	1:A:260:LEU:HG	2.00	0.62
2:D:334:ILE:HG12	3:E:334:LEU:OXT	1.99	0.62
2:N:223:GLN:CG	3:O:158:ARG:NH2	2.60	0.62
2:G:11:ARG:HA	2:G:215:ARG:HH12	1.64	0.62
2:H:354:LEU:CD2	2:I:297:LEU:HD22	2.29	0.62
1:K:256:LEU:O	1:K:260:LEU:HG	2.00	0.62
2:H:93:ILE:HG23	2:H:100:LYS:NZ	2.14	0.61
2:G:94:ASP:O	2:G:100:LYS:HE3	2.00	0.61
2:L:180:VAL:CB	2:L:304:ASN:HB2	2.30	0.61
2:B:263:ARG:O	2:B:267:LEU:HG	2.00	0.61
1:F:256:LEU:O	1:F:260:LEU:HG	2.00	0.61
2:D:277:GLU:CD	3:E:149:GLU:HG3	2.20	0.61
2:M:351:MET:CE	2:M:351:MET:HA	2.30	0.61
2:L:180:VAL:HG23	2:L:304:ASN:ND2	2.14	0.61
2:B:97:SER:HB2	2:C:144:GLU:CD	2.21	0.61
2:B:328:TYR:O	2:B:332:LEU:HD23	1.99	0.61
2:N:316:LEU:HD22	2:N:320:ILE:HD11	1.81	0.61
3:O:163:TYR:OH	3:O:166:PRO:HD2	2.00	0.61
2:H:351:MET:HE3	2:H:351:MET:HA	1.80	0.61
2:M:250:LEU:HD22	2:M:309:ILE:HD12	1.82	0.61
3:E:73:HIS:CD2	3:E:75:ASP:H	2.18	0.61
2:D:277:GLU:CB	3:E:149:GLU:HG3	2.27	0.61
1:A:24:LEU:HA	1:A:114:GLY:O	2.00	0.61
2:I:98:ARG:NH2	3:J:91:ASP:OD1	2.33	0.61
3:E:129:LEU:HD11	3:E:158:ARG:HH11	1.64	0.61
3:E:161:LEU:HD12	3:E:161:LEU:H	1.64	0.61
2:L:343:PRO:HG3	2:M:287:GLY:CA	2.30	0.61
2:M:342:ALA:HA	2:N:333:LEU:HD21	1.82	0.61
2:M:93:ILE:HG23	2:M:100:LYS:NZ	2.14	0.61
2:H:20:GLY:HA3	2:H:182:GLN:NE2	2.15	0.61
2:B:93:ILE:CG2	2:B:100:LYS:HZ2	2.14	0.61
2:M:201:ARG:NH2	2:M:308:ALA:HB2	2.16	0.61
1:K:281:ASN:C	1:K:283:ARG:H	2.02	0.61
2:L:263:ARG:O	2:L:267:LEU:HG	2.00	0.61
2:H:351:MET:HA	2:H:351:MET:CE	2.30	0.61
2:H:250:LEU:HD22	2:H:309:ILE:HD12	1.82	0.61
2:L:223:GLN:OE1	2:M:171:LEU:HD12	2.01	0.61
2:M:215:ARG:CZ	2:N:164:VAL:CG1	2.78	0.61
2:G:263:ARG:O	2:G:267:LEU:HG	2.00	0.61
3:O:73:HIS:CD2	3:O:75:ASP:H	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:70:ALA:O	2:N:72:PRO:HD3	2.01	0.61
2:I:70:ALA:O	2:I:72:PRO:HD3	2.01	0.61
2:D:70:ALA:O	2:D:72:PRO:HD3	2.01	0.61
2:G:21:GLN:CG	2:G:178:LEU:CD2	2.73	0.61
1:A:315:ASP:HB2	1:A:318:GLN:HG2	1.80	0.61
2:I:345:ARG:NH1	3:J:150:ARG:CG	2.64	0.61
1:F:24:LEU:HA	1:F:114:GLY:O	2.00	0.61
2:H:359:PHE:CE2	2:I:323:THR:CG2	2.84	0.61
3:J:117:ALA:HB2	3:J:143:LEU:HD12	1.83	0.61
3:O:303:VAL:HB	3:O:306:ILE:HD11	1.83	0.60
2:M:359:PHE:CZ	2:N:323:THR:CG2	2.84	0.60
2:H:6:LEU:CG	2:H:222:ASP:OD1	2.50	0.60
3:E:117:ALA:HB2	3:E:143:LEU:HD12	1.83	0.60
2:B:268:ILE:HD11	2:B:353:LEU:HD12	1.83	0.60
2:I:363:MET:CG	2:I:364:PRO:HD2	2.31	0.60
1:A:161:GLU:CD	2:M:318:ARG:CD	2.67	0.60
2:I:140:LEU:HD21	2:I:166:ILE:HG12	1.83	0.60
3:O:6:TRP:HZ3	3:O:175:TRP:CE2	2.17	0.60
3:O:117:ALA:HB2	3:O:143:LEU:HD12	1.83	0.60
2:N:140:LEU:HD21	2:N:166:ILE:HG12	1.83	0.60
2:H:201:ARG:HB2	2:H:305:ASP:OD2	2.01	0.60
2:M:215:ARG:CZ	2:N:164:VAL:HG22	2.29	0.60
2:L:343:PRO:HG3	2:M:287:GLY:N	2.16	0.60
2:L:365:LEU:CD2	2:M:297:LEU:HD11	2.31	0.60
2:L:180:VAL:HB	2:L:304:ASN:HB2	1.82	0.60
2:G:12:PRO:HD2	2:G:215:ARG:NH2	2.17	0.60
2:G:10:TRP:CZ2	2:G:190:ILE:CG2	2.77	0.60
2:G:246:ASP:HB3	2:G:274:ARG:CD	2.24	0.60
2:H:362:ARG:O	2:H:363:MET:HG3	2.02	0.60
3:J:73:HIS:CD2	3:J:75:ASP:H	2.18	0.60
2:H:19:VAL:HG21	2:H:214:LEU:HD22	1.82	0.60
2:G:365:LEU:HD21	2:H:297:LEU:HD13	1.78	0.60
2:G:6:LEU:CD1	2:G:222:ASP:HA	2.26	0.60
2:C:250:LEU:HD22	2:C:309:ILE:HD12	1.82	0.60
3:O:149:GLU:C	3:O:151:LEU:H	2.05	0.60
2:N:240:MET:HB3	3:O:157:SER:HA	1.82	0.60
1:A:269:LEU:HG	1:A:273:PHE:CE1	2.37	0.60
2:L:268:ILE:HD11	2:L:353:LEU:HD12	1.83	0.60
2:H:292:ILE:O	2:H:296:GLN:HG3	2.02	0.60
3:J:149:GLU:C	3:J:151:LEU:H	2.05	0.60
2:D:363:MET:CG	2:D:364:PRO:HD2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:341:TYR:CE2	2:N:337:LYS:CB	2.84	0.60
2:M:362:ARG:O	2:M:363:MET:HG3	2.02	0.60
2:M:292:ILE:O	2:M:296:GLN:HG3	2.02	0.60
1:F:210:ALA:O	1:F:212:PHE:CE1	2.55	0.60
2:N:363:MET:CG	2:N:364:PRO:HD2	2.31	0.60
2:C:351:MET:CE	2:C:351:MET:HA	2.30	0.60
2:G:268:ILE:HD11	2:G:353:LEU:HD12	1.83	0.60
2:H:19:VAL:HG21	2:H:214:LEU:CD2	2.31	0.60
1:F:10:ARG:HH12	1:F:40:GLN:NE2	2.00	0.60
2:B:343:PRO:HG2	2:B:347:MET:SD	2.42	0.60
2:M:88:VAL:HG11	2:M:116:ALA:HB3	1.83	0.60
1:K:269:LEU:HG	1:K:273:PHE:CE1	2.37	0.59
2:H:84:GLN:CB	2:I:144:GLU:OE1	2.50	0.59
2:C:354:LEU:HD11	2:D:294:MET:SD	2.42	0.59
2:M:21:GLN:OE1	2:M:175:LEU:HD22	2.02	0.59
1:A:262:ARG:NH2	3:E:320:GLU:OE1	2.35	0.59
2:H:88:VAL:HG11	2:H:116:ALA:HB3	1.83	0.59
2:G:93:ILE:HG23	2:G:100:LYS:HZ2	1.67	0.59
3:E:303:VAL:HB	3:E:306:ILE:HD11	1.83	0.59
3:J:303:VAL:HB	3:J:306:ILE:HD11	1.83	0.59
1:K:10:ARG:HH12	1:K:40:GLN:NE2	2.00	0.59
1:A:255:LEU:HD22	3:E:313:THR:HG21	1.84	0.59
1:F:269:LEU:HG	1:F:273:PHE:CE1	2.37	0.59
2:M:10:TRP:CE3	2:M:190:ILE:HG12	2.36	0.59
3:O:6:TRP:CH2	3:O:175:TRP:CE2	2.90	0.59
2:C:11:ARG:HH22	2:D:165:THR:HG22	1.67	0.59
2:I:246:ASP:HB2	2:I:248:GLN:HG2	1.85	0.59
2:G:284:GLU:O	2:G:288:LEU:HG	2.02	0.59
2:L:343:PRO:HG2	2:L:347:MET:SD	2.43	0.59
3:E:149:GLU:C	3:E:151:LEU:H	2.05	0.59
2:C:362:ARG:O	2:C:363:MET:HG3	2.02	0.59
2:M:152:PHE:O	2:M:153:LEU:HD23	2.02	0.59
1:A:10:ARG:HH12	1:A:40:GLN:NE2	2.00	0.59
2:C:21:GLN:OE1	2:C:175:LEU:HD22	2.02	0.59
2:B:205:LEU:CD1	2:B:234:THR:HG23	2.33	0.59
2:B:302:LEU:HD13	2:B:310:GLU:HG2	1.83	0.59
2:C:88:VAL:HG11	2:C:116:ALA:HB3	1.83	0.59
2:H:21:GLN:OE1	2:H:175:LEU:HD22	2.02	0.59
2:D:140:LEU:HD21	2:D:166:ILE:HG12	1.83	0.59
2:I:47:ARG:CZ	3:J:126:ASN:OD1	2.51	0.59
2:B:284:GLU:O	2:B:288:LEU:HG	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:ARG:HG3	2:B:47:ARG:O	2.03	0.59
2:C:292:ILE:O	2:C:296:GLN:HG3	2.02	0.59
2:M:201:ARG:HG3	2:M:305:ASP:HB3	1.84	0.59
2:H:316:LEU:HD22	2:H:320:ILE:HD11	1.84	0.59
2:M:355:ARG:HG3	2:N:326:GLN:HG3	1.84	0.59
2:L:246:ASP:HB3	2:L:274:ARG:CD	2.24	0.59
2:G:259:ALA:HB3	2:G:363:MET:CE	2.33	0.59
2:G:343:PRO:HG2	2:G:347:MET:SD	2.42	0.59
2:H:215:ARG:NH2	2:I:164:VAL:HG22	2.17	0.59
3:O:46:ARG:CZ	3:O:68:MET:HG3	2.33	0.59
2:I:223:GLN:HG2	3:J:158:ARG:HH21	1.67	0.59
1:A:263:GLN:HG2	1:A:266:HIS:HD2	1.68	0.59
2:G:302:LEU:HD13	2:G:310:GLU:HG2	1.84	0.59
2:M:94:ASP:C	2:M:100:LYS:HZ1	2.06	0.58
2:B:259:ALA:HB3	2:B:363:MET:CE	2.33	0.58
3:E:46:ARG:CZ	3:E:68:MET:HG3	2.33	0.58
2:G:205:LEU:CD1	2:G:234:THR:HG23	2.33	0.58
2:I:277:GLU:CG	3:J:149:GLU:HG3	2.32	0.58
2:L:180:VAL:HG21	2:L:304:ASN:OD1	2.03	0.58
1:K:172:TYR:O	1:K:216:HIS:HE1	1.86	0.58
2:L:341:TYR:O	2:M:336:ARG:NH1	2.32	0.58
1:F:263:GLN:HG2	1:F:266:HIS:HD2	1.68	0.58
2:L:302:LEU:HD13	2:L:310:GLU:HG2	1.84	0.58
2:L:205:LEU:CD1	2:L:234:THR:HG23	2.33	0.58
1:A:105:HIS:HA	1:F:227:LYS:HE3	1.83	0.58
2:C:56:ARG:NH2	2:D:165:THR:HG21	2.18	0.58
2:M:316:LEU:HD22	2:M:320:ILE:HD11	1.84	0.58
2:H:257:VAL:HG11	2:H:320:ILE:CD1	2.34	0.58
2:B:282:LEU:CD2	2:B:332:LEU:HD12	2.34	0.58
1:F:10:ARG:HH22	1:F:40:GLN:HE22	1.51	0.58
2:B:61:GLY:HA2	2:B:72:PRO:HG3	1.86	0.58
2:C:152:PHE:O	2:C:153:LEU:HD23	2.03	0.58
2:L:284:GLU:O	2:L:288:LEU:HG	2.02	0.58
3:O:41:ILE:HG21	3:O:113:TRP:CD1	2.38	0.58
1:K:223:MET:HE1	1:K:292:ARG:HB2	1.86	0.58
2:G:6:LEU:CD1	2:G:225:ILE:HD12	2.29	0.58
2:L:259:ALA:HB3	2:L:363:MET:CE	2.33	0.58
2:D:94:ASP:O	2:D:100:LYS:HE2	2.03	0.58
1:A:10:ARG:HH22	1:A:40:GLN:HE22	1.51	0.58
2:B:304:ASN:OD1	2:B:305:ASP:N	2.37	0.58
2:I:186:GLN:HG2	2:I:214:LEU:HD21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:229:ASP:O	2:I:231:GLN:N	2.34	0.58
2:N:246:ASP:HB2	2:N:248:GLN:HG2	1.85	0.58
3:J:308:ARG:O	3:J:312:ILE:HG13	2.04	0.58
2:H:5:VAL:HG11	2:I:171:LEU:HB2	1.84	0.58
2:I:360:HIS:CB	2:I:363:MET:SD	2.92	0.58
2:L:304:ASN:OD1	2:L:305:ASP:N	2.37	0.58
2:G:304:ASN:OD1	2:G:305:ASP:N	2.37	0.58
2:C:316:LEU:HD22	2:C:320:ILE:HD11	1.84	0.58
3:E:32:LEU:CD1	3:E:195:ALA:O	2.51	0.58
2:I:367:GLU:HB3	2:I:368:PRO:HD2	1.86	0.58
2:I:58:LEU:HD23	2:I:153:LEU:HD22	1.86	0.58
1:F:221:LEU:HD13	1:F:331:LEU:HD12	1.85	0.58
2:L:47:ARG:HG3	2:L:47:ARG:O	2.03	0.58
1:F:273:PHE:CE1	1:F:283:ARG:HG3	2.39	0.58
1:A:193:PRO:C	2:M:311:LEU:HD21	2.23	0.58
1:F:222:LEU:HD12	1:F:285:MET:SD	2.44	0.58
1:K:273:PHE:CE1	1:K:283:ARG:HG3	2.39	0.58
2:I:184:ARG:HH22	2:I:304:ASN:ND2	2.02	0.58
3:J:46:ARG:CZ	3:J:68:MET:HG3	2.33	0.58
2:M:257:VAL:HG11	2:M:320:ILE:CD1	2.34	0.58
2:I:94:ASP:O	2:I:100:LYS:HE2	2.03	0.58
2:G:282:LEU:CD2	2:G:332:LEU:HD12	2.34	0.58
1:K:263:GLN:HG2	1:K:266:HIS:HD2	1.68	0.58
2:H:152:PHE:O	2:H:153:LEU:HD23	2.03	0.58
1:A:75:ALA:HB2	1:F:207:ASN:CB	2.34	0.58
2:D:360:HIS:CB	2:D:363:MET:SD	2.92	0.58
1:A:273:PHE:CE1	1:A:283:ARG:HG3	2.39	0.58
3:O:308:ARG:O	3:O:312:ILE:HG13	2.04	0.58
2:N:229:ASP:O	2:N:231:GLN:N	2.33	0.58
2:L:61:GLY:HA2	2:L:72:PRO:HG3	1.85	0.58
2:N:58:LEU:HD23	2:N:153:LEU:HD22	1.86	0.58
2:L:239:ALA:CA	2:L:243:THR:OG1	2.51	0.58
2:G:49:VAL:HA	2:G:213:SER:HB2	1.85	0.58
1:A:279:TRP:O	1:A:279:TRP:CG	2.57	0.58
2:C:10:TRP:CZ3	2:C:190:ILE:HG12	2.39	0.58
2:L:282:LEU:CD2	2:L:332:LEU:HD12	2.34	0.58
1:K:10:ARG:HH22	1:K:40:GLN:HE22	1.51	0.58
1:K:222:LEU:HD12	1:K:285:MET:CG	2.33	0.57
1:F:119:LYS:H	1:F:119:LYS:CD	2.05	0.57
2:N:94:ASP:O	2:N:100:LYS:HE2	2.03	0.57
1:F:279:TRP:O	1:F:279:TRP:CG	2.57	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:HIS:HA	1:F:227:LYS:CD	2.33	0.57
1:K:222:LEU:HD12	1:K:285:MET:SD	2.44	0.57
3:J:41:ILE:HG21	3:J:113:TRP:CD1	2.38	0.57
2:D:47:ARG:NE	3:E:126:ASN:OD1	2.37	0.57
1:F:223:MET:HE1	1:F:292:ARG:HB2	1.85	0.57
2:C:84:GLN:HA	2:D:144:GLU:OE1	2.04	0.57
1:A:221:LEU:HD13	1:A:331:LEU:HD12	1.86	0.57
2:N:360:HIS:CB	2:N:363:MET:SD	2.92	0.57
2:H:341:TYR:CB	2:I:333:LEU:HD13	2.35	0.57
2:G:246:ASP:CB	2:G:274:ARG:HD3	2.24	0.57
2:B:246:ASP:HB3	2:B:274:ARG:CD	2.24	0.57
1:F:222:LEU:HD12	1:F:285:MET:CG	2.33	0.57
1:K:279:TRP:O	1:K:279:TRP:CG	2.57	0.57
2:C:257:VAL:HG11	2:C:320:ILE:CD1	2.34	0.57
3:E:41:ILE:HG21	3:E:113:TRP:CD1	2.38	0.57
2:D:229:ASP:O	2:D:231:GLN:N	2.33	0.57
2:D:246:ASP:HB2	2:D:248:GLN:HG2	1.85	0.57
2:G:61:GLY:HA2	2:G:72:PRO:HG3	1.85	0.57
2:G:47:ARG:O	2:G:47:ARG:HG3	2.03	0.57
2:I:201:ARG:HB2	2:I:305:ASP:HB3	1.86	0.57
1:A:251:GLN:OE1	3:E:307:ASN:ND2	2.37	0.57
2:M:291:ARG:HH11	2:M:306:MET:HG3	1.69	0.57
2:H:291:ARG:HH11	2:H:306:MET:HG3	1.68	0.57
2:I:360:HIS:CB	2:I:363:MET:CB	2.68	0.57
2:C:341:TYR:CB	2:D:333:LEU:CD1	2.81	0.57
2:I:200:PRO:HB2	2:I:305:ASP:HB2	1.87	0.57
2:L:362:ARG:HH21	2:L:363:MET:HE1	1.70	0.57
1:F:270:ARG:HH22	2:N:316:LEU:CA	2.17	0.57
2:G:354:LEU:HD21	2:H:297:LEU:CD2	2.34	0.57
1:K:281:ASN:C	1:K:283:ARG:N	2.57	0.57
2:G:328:TYR:OH	2:G:361:PRO:HD2	2.05	0.57
2:D:58:LEU:HD23	2:D:153:LEU:HD22	1.86	0.57
1:K:221:LEU:HD13	1:K:331:LEU:HD12	1.86	0.57
2:L:205:LEU:HD11	2:L:234:THR:HG23	1.87	0.57
1:A:222:LEU:HD12	1:A:285:MET:SD	2.44	0.57
1:A:222:LEU:HD12	1:A:285:MET:CG	2.33	0.57
3:J:8:ARG:HG3	3:J:9:PRO:CD	2.33	0.57
2:D:194:GLU:HA	2:D:194:GLU:OE1	2.05	0.57
2:N:194:GLU:OE1	2:N:194:GLU:HA	2.05	0.57
1:F:270:ARG:NE	2:N:319:THR:HG21	2.20	0.57
1:F:281:ASN:C	1:F:283:ARG:N	2.57	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:29:LEU:CD2	1:F:178:LEU:C	2.71	0.57
1:A:281:ASN:C	1:A:283:ARG:N	2.57	0.57
2:M:3:TYR:HD2	2:M:3:TYR:O	1.86	0.57
2:D:186:GLN:HG2	2:D:214:LEU:HD21	1.86	0.57
2:L:9:LYS:HD3	2:L:194:GLU:OE2	2.04	0.57
2:L:99:THR:O	2:L:99:THR:CG2	2.53	0.57
2:D:128:VAL:HG11	2:D:154:LEU:HD22	1.87	0.57
2:D:367:GLU:HB3	2:D:368:PRO:HD2	1.86	0.57
2:C:94:ASP:C	2:C:100:LYS:HZ1	2.08	0.56
2:C:93:ILE:HG23	2:D:133:ARG:NH1	2.19	0.56
2:M:84:GLN:CA	2:N:144:GLU:OE1	2.53	0.56
2:N:128:VAL:HG11	2:N:154:LEU:HD22	1.87	0.56
2:I:93:ILE:HG22	2:I:100:LYS:HZ3	1.70	0.56
2:G:205:LEU:HD11	2:G:234:THR:HG23	1.87	0.56
1:F:270:ARG:NH1	2:N:316:LEU:CA	2.55	0.56
3:E:308:ARG:O	3:E:312:ILE:HG13	2.04	0.56
2:C:291:ARG:HH11	2:C:306:MET:HG3	1.69	0.56
1:F:270:ARG:NE	2:N:319:THR:CG2	2.68	0.56
2:I:363:MET:CB	2:I:364:PRO:CD	2.78	0.56
1:A:191:LEU:CD2	2:B:23:HIS:ND1	2.67	0.56
2:N:367:GLU:HB3	2:N:368:PRO:HD2	1.86	0.56
2:M:3:TYR:O	2:M:4:GLN:CG	2.53	0.56
2:L:328:TYR:OH	2:L:361:PRO:HD2	2.05	0.56
3:E:280:HIS:O	3:E:281:LEU:HD23	2.05	0.56
1:K:170:LEU:O	1:K:173:CYS:O	2.23	0.56
2:N:186:GLN:HG2	2:N:214:LEU:HD21	1.86	0.56
1:F:170:LEU:O	1:F:173:CYS:O	2.23	0.56
1:K:333:HIS:HD2	2:L:297:LEU:HD23	1.65	0.56
2:I:334:ILE:HG21	3:J:332:PRO:HB2	1.87	0.56
3:O:8:ARG:HG3	3:O:9:PRO:CD	2.33	0.56
2:L:362:ARG:HH21	2:L:363:MET:CE	2.19	0.56
2:C:354:LEU:CD2	2:D:297:LEU:HD22	2.35	0.56
3:O:201:ALA:O	3:O:204:LEU:HB2	2.06	0.56
2:G:362:ARG:HH21	2:G:363:MET:CE	2.19	0.56
2:B:328:TYR:OH	2:B:361:PRO:HD2	2.05	0.56
2:N:296:GLN:NE2	2:N:325:ILE:HD12	2.20	0.56
2:M:40:ALA:HB1	2:M:170:CYS:SG	2.46	0.56
3:O:280:HIS:O	3:O:281:LEU:HD23	2.05	0.56
2:L:239:ALA:HA	2:L:243:THR:OG1	2.05	0.56
2:B:69:THR:HG22	2:B:71:THR:N	2.01	0.56
2:N:223:GLN:CG	3:O:158:ARG:HH21	2.11	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:366:PRO:HA	3:O:283:PRO:CD	2.35	0.56
1:A:223:MET:HE1	1:A:292:ARG:HB2	1.87	0.56
3:O:5:PRO:CD	3:O:175:TRP:CZ3	2.89	0.56
2:M:93:ILE:HG22	2:M:100:LYS:HZ3	1.66	0.56
2:G:229:ASP:CA	2:H:30:ASN:HD21	2.19	0.56
1:F:218:VAL:HA	1:F:221:LEU:HB2	1.88	0.56
2:L:10:TRP:CH2	2:L:193:GLU:CD	2.79	0.56
2:L:246:ASP:CB	2:L:274:ARG:HD3	2.24	0.56
3:E:8:ARG:HG3	3:E:9:PRO:CD	2.33	0.56
3:E:201:ALA:O	3:E:204:LEU:HB2	2.06	0.56
2:M:99:THR:O	2:M:99:THR:CG2	2.51	0.56
1:K:262:ARG:NH1	3:O:230:TYR:HB3	2.21	0.56
2:G:341:TYR:O	2:H:336:ARG:NH1	2.35	0.56
2:H:40:ALA:HB1	2:H:170:CYS:SG	2.46	0.56
2:C:215:ARG:HH21	2:D:164:VAL:HG21	1.70	0.56
1:F:312:LEU:HB2	1:F:320:VAL:CG2	2.35	0.56
2:N:259:ALA:HB2	2:N:363:MET:SD	2.46	0.56
2:I:259:ALA:HB2	2:I:363:MET:SD	2.46	0.56
2:I:128:VAL:HG11	2:I:154:LEU:HD22	1.87	0.56
1:K:255:LEU:CD1	3:O:309:GLU:HG2	2.36	0.56
2:B:309:ILE:HG22	2:B:313:MET:HG2	1.88	0.56
2:H:97:SER:OG	2:H:100:LYS:CE	2.55	0.55
2:G:94:ASP:CA	2:G:100:LYS:HZ1	2.19	0.55
2:D:296:GLN:NE2	2:D:325:ILE:HD12	2.20	0.55
1:A:170:LEU:O	1:A:173:CYS:O	2.24	0.55
2:L:295:VAL:HG22	2:L:301:ALA:HB3	1.88	0.55
2:H:91:ILE:HD12	2:H:123:TYR:CE2	2.42	0.55
2:C:91:ILE:HD12	2:C:123:TYR:CE2	2.42	0.55
2:D:366:PRO:HB3	3:E:282:SER:HB2	1.88	0.55
2:I:296:GLN:NE2	2:I:325:ILE:HD12	2.20	0.55
1:A:308:THR:CG2	1:A:320:VAL:HG13	2.37	0.55
1:F:296:THR:HG22	1:F:299:ARG:NH1	2.22	0.55
2:D:259:ALA:HB2	2:D:363:MET:SD	2.46	0.55
2:B:365:LEU:HD21	2:C:297:LEU:HD11	1.87	0.55
1:K:308:THR:CG2	1:K:320:VAL:HG13	2.37	0.55
2:B:362:ARG:HH21	2:B:363:MET:CE	2.19	0.55
1:F:333:HIS:CG	2:G:298:SER:OG	2.59	0.55
2:C:40:ALA:HB1	2:C:170:CYS:SG	2.46	0.55
3:J:213:ARG:NH2	3:J:267:ASN:OD1	2.39	0.55
2:I:360:HIS:CG	2:I:363:MET:CE	2.90	0.55
2:L:6:LEU:CD2	2:L:194:GLU:CD	2.74	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:3:TYR:CD2	2:L:3:TYR:O	2.60	0.55
2:H:156:THR:HG22	2:H:158:ASP:N	2.21	0.55
3:O:213:ARG:NH2	3:O:267:ASN:OD1	2.39	0.55
1:A:296:THR:HG22	1:A:299:ARG:NH1	2.22	0.55
2:G:10:TRP:CZ3	2:G:190:ILE:CB	2.90	0.55
2:N:360:HIS:CG	2:N:363:MET:CE	2.90	0.55
2:G:11:ARG:HD3	2:G:83:GLU:OE2	2.07	0.55
2:D:355:ARG:HH21	3:E:332:PRO:HD3	1.72	0.55
2:M:354:LEU:HD21	2:N:297:LEU:HD22	1.88	0.55
1:A:313:LYS:O	1:A:316:TYR:CE2	2.60	0.55
3:J:201:ALA:O	3:J:204:LEU:HB2	2.06	0.55
2:D:363:MET:CB	2:D:364:PRO:CD	2.78	0.55
2:I:355:ARG:HH21	3:J:332:PRO:HD3	1.70	0.55
2:B:246:ASP:CB	2:B:274:ARG:HD3	2.23	0.55
2:B:205:LEU:HD11	2:B:234:THR:HG23	1.87	0.55
2:L:307:ALA:HA	2:L:310:GLU:HG3	1.89	0.55
1:A:218:VAL:HA	1:A:221:LEU:HB2	1.88	0.55
2:B:11:ARG:HD3	2:B:83:GLU:OE2	2.06	0.55
1:K:296:THR:HG22	1:K:299:ARG:NH1	2.22	0.55
1:K:282:ARG:O	1:K:285:MET:HB3	2.07	0.55
1:A:282:ARG:O	1:A:285:MET:HB3	2.07	0.55
3:E:4:TYR:HB3	3:E:5:PRO:HD2	1.89	0.55
2:G:351:MET:HG2	2:H:290:HIS:CE1	2.42	0.55
2:B:307:ALA:HA	2:B:310:GLU:HG3	1.89	0.55
2:I:194:GLU:OE1	2:I:194:GLU:HA	2.05	0.55
1:A:194:ASP:N	2:M:311:LEU:CD1	2.61	0.55
2:B:94:ASP:N	2:B:100:LYS:HZ1	2.01	0.55
2:H:281:LEU:HD23	2:H:285:MET:CE	2.36	0.55
2:M:91:ILE:HD12	2:M:123:TYR:CE2	2.42	0.55
2:N:259:ALA:HB2	2:N:363:MET:HG3	1.89	0.55
2:D:360:HIS:CG	2:D:363:MET:CE	2.90	0.55
2:M:97:SER:OG	2:M:100:LYS:CE	2.55	0.55
2:L:248:GLN:O	2:L:252:LEU:N	2.39	0.55
3:J:163:TYR:OH	3:J:166:PRO:HD3	2.06	0.55
3:J:280:HIS:O	3:J:281:LEU:HD23	2.05	0.55
2:G:295:VAL:HG22	2:G:301:ALA:HB3	1.88	0.55
1:A:39:ARG:NH2	1:A:50:HIS:HB3	2.21	0.55
2:C:346:ARG:O	2:C:350:GLU:HG3	2.07	0.55
2:C:97:SER:OG	2:C:100:LYS:CE	2.55	0.54
2:B:3:TYR:O	2:B:3:TYR:CD2	2.60	0.54
1:K:313:LYS:O	1:K:316:TYR:CE2	2.60	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:262:ARG:NH2	3:O:230:TYR:CB	2.70	0.54
2:B:295:VAL:HG22	2:B:301:ALA:HB3	1.88	0.54
2:M:355:ARG:HG3	2:N:326:GLN:CG	2.37	0.54
2:I:355:ARG:HH12	3:J:287:GLN:HB3	1.72	0.54
2:G:3:TYR:CD2	2:G:3:TYR:O	2.60	0.54
1:F:313:LYS:O	1:F:316:TYR:CE2	2.60	0.54
2:L:309:ILE:HG22	2:L:313:MET:HG2	1.88	0.54
2:C:307:ALA:HA	2:C:310:GLU:HB2	1.90	0.54
2:L:11:ARG:HD3	2:L:83:GLU:OE2	2.07	0.54
2:I:244:LEU:HD21	2:I:276:ILE:CG1	2.37	0.54
2:M:281:LEU:HD23	2:M:285:MET:CE	2.36	0.54
2:H:19:VAL:CG2	2:H:214:LEU:HD22	2.37	0.54
2:G:307:ALA:HA	2:G:310:GLU:HG3	1.89	0.54
1:K:39:ARG:NH2	1:K:50:HIS:HB3	2.21	0.54
1:F:39:ARG:NH2	1:F:50:HIS:HB3	2.21	0.54
2:H:346:ARG:O	2:H:350:GLU:HG3	2.08	0.54
2:N:360:HIS:HD2	2:N:361:PRO:O	1.90	0.54
2:G:21:GLN:HG3	2:G:178:LEU:HD23	1.82	0.54
1:F:308:THR:CG2	1:F:320:VAL:HG13	2.37	0.54
2:G:248:GLN:O	2:G:252:LEU:N	2.39	0.54
2:N:296:GLN:HE22	2:N:325:ILE:HD12	1.73	0.54
2:H:307:ALA:HA	2:H:310:GLU:HB2	1.90	0.54
1:F:264:SER:O	1:F:265:ALA:HB3	2.07	0.54
2:M:346:ARG:O	2:M:350:GLU:HG3	2.07	0.54
2:M:84:GLN:CB	2:N:144:GLU:OE1	2.56	0.54
1:A:48:GLU:HG3	1:A:49:GLU:H	1.72	0.54
2:G:309:ILE:HG22	2:G:313:MET:HG2	1.88	0.54
1:A:271:ALA:O	1:A:275:LYS:HG2	2.07	0.54
2:M:215:ARG:CZ	2:N:164:VAL:HG11	2.38	0.54
2:H:3:TYR:O	2:H:4:GLN:CB	2.56	0.54
2:G:104:THR:O	2:G:108:LEU:HG	2.08	0.54
1:K:218:VAL:HA	1:K:221:LEU:HB2	1.88	0.54
1:F:271:ALA:O	1:F:275:LYS:HG2	2.07	0.54
1:A:1:MET:HA	1:A:134:SER:O	2.08	0.54
2:D:360:HIS:HD2	2:D:361:PRO:O	1.90	0.54
1:F:282:ARG:O	1:F:285:MET:HB3	2.07	0.54
3:O:306:ILE:HG22	3:O:307:ASN:H	1.73	0.54
2:H:360:HIS:HD2	2:H:363:MET:H	1.56	0.54
3:J:306:ILE:HG22	3:J:307:ASN:H	1.73	0.54
3:J:238:HIS:ND1	3:J:239:GLU:N	2.56	0.54
2:D:296:GLN:HE22	2:D:325:ILE:HD12	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:255:LEU:CD1	3:J:309:GLU:HG2	2.38	0.54
1:A:264:SER:O	1:A:265:ALA:HB3	2.07	0.54
1:F:273:PHE:HB3	1:F:279:TRP:HB2	1.90	0.54
2:D:302:LEU:HD22	2:D:306:MET:HG2	1.90	0.54
2:L:104:THR:O	2:L:108:LEU:HG	2.07	0.54
3:E:213:ARG:NH2	3:E:267:ASN:OD1	2.39	0.54
1:A:161:GLU:HG3	2:M:318:ARG:NH2	2.22	0.53
2:I:241:LEU:HD22	3:J:153:ALA:HB1	1.90	0.53
1:F:48:GLU:HG3	1:F:49:GLU:H	1.72	0.53
1:K:264:SER:O	1:K:265:ALA:HB3	2.07	0.53
2:I:259:ALA:HB2	2:I:363:MET:HG3	1.89	0.53
3:O:5:PRO:HD2	3:O:175:TRP:CZ3	2.43	0.53
3:O:4:TYR:HB3	3:O:5:PRO:HD2	1.89	0.53
2:I:302:LEU:HD22	2:I:306:MET:HG2	1.91	0.53
2:C:276:ILE:HG22	2:C:277:GLU:N	2.23	0.53
3:E:306:ILE:HG22	3:E:307:ASN:H	1.73	0.53
1:K:271:ALA:O	1:K:275:LYS:HG2	2.07	0.53
2:B:104:THR:O	2:B:108:LEU:HG	2.08	0.53
2:I:360:HIS:HD2	2:I:361:PRO:O	1.90	0.53
2:G:19:VAL:HG22	2:G:186:GLN:CB	2.38	0.53
2:N:244:LEU:HD11	2:N:276:ILE:HD13	1.90	0.53
2:C:94:ASP:C	2:C:100:LYS:NZ	2.62	0.53
2:L:69:THR:HG22	2:L:71:THR:N	2.01	0.53
1:F:262:ARG:HH12	3:J:230:TYR:HB3	1.70	0.53
1:F:270:ARG:NH2	2:N:315:GLU:O	2.41	0.53
2:I:334:ILE:HG12	3:J:334:LEU:OXT	2.09	0.53
1:K:282:ARG:HG2	1:K:285:MET:HE2	1.90	0.53
3:O:6:TRP:HZ3	3:O:175:TRP:CG	2.24	0.53
3:J:4:TYR:HB3	3:J:5:PRO:HD2	1.90	0.53
2:C:360:HIS:HD2	2:C:363:MET:H	1.57	0.53
1:F:1:MET:HA	1:F:134:SER:O	2.08	0.53
2:D:271:ALA:HB1	2:D:276:ILE:HD11	1.90	0.53
1:A:25:GLY:O	1:A:115:ASN:HA	2.08	0.53
2:I:291:ARG:HD2	2:I:306:MET:SD	2.49	0.53
2:G:276:ILE:HG22	2:G:277:GLU:N	2.24	0.53
3:O:238:HIS:ND1	3:O:239:GLU:N	2.56	0.53
1:K:1:MET:HA	1:K:134:SER:O	2.08	0.53
2:G:10:TRP:CE3	2:G:190:ILE:HG12	2.40	0.53
1:A:161:GLU:CD	2:M:318:ARG:HD3	2.22	0.53
2:N:244:LEU:HD21	2:N:276:ILE:CG1	2.37	0.53
2:N:241:LEU:HD22	3:O:153:ALA:HB1	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:84:GLN:HB3	2:D:86:ARG:NH2	2.24	0.53
2:D:291:ARG:HD2	2:D:306:MET:SD	2.49	0.53
1:K:93:ILE:HG23	1:K:97:LEU:HD13	1.91	0.53
1:F:93:ILE:HG23	1:F:97:LEU:HD13	1.91	0.53
1:K:48:GLU:HG3	1:K:49:GLU:H	1.72	0.53
2:M:307:ALA:HA	2:M:310:GLU:HB2	1.90	0.53
2:D:360:HIS:O	2:D:363:MET:HB2	2.09	0.53
1:F:25:GLY:O	1:F:115:ASN:HA	2.08	0.53
3:E:268:VAL:O	3:E:271:PRO:HD3	2.09	0.53
2:D:244:LEU:HD11	2:D:276:ILE:HD13	1.90	0.53
3:O:268:VAL:O	3:O:271:PRO:HD3	2.09	0.53
2:D:244:LEU:HD21	2:D:276:ILE:CG1	2.37	0.53
2:L:351:MET:HG3	2:M:290:HIS:ND1	2.24	0.53
2:H:11:ARG:NH2	2:I:165:THR:HG22	2.23	0.53
2:B:248:GLN:O	2:B:252:LEU:N	2.39	0.53
1:F:309:GLU:O	1:F:313:LYS:HG3	2.09	0.53
2:I:296:GLN:HE22	2:I:325:ILE:HD12	1.73	0.53
2:H:334:ILE:O	2:H:338:GLU:HG3	2.09	0.53
2:C:334:ILE:O	2:C:338:GLU:HG3	2.09	0.53
2:I:244:LEU:HD11	2:I:276:ILE:HD13	1.90	0.52
2:L:354:LEU:HD12	2:M:294:MET:SD	2.44	0.52
2:M:94:ASP:C	2:M:100:LYS:NZ	2.62	0.52
2:D:238:SER:CB	2:D:243:THR:HB	2.34	0.52
1:K:309:GLU:O	1:K:313:LYS:HG3	2.09	0.52
2:M:334:ILE:O	2:M:338:GLU:HG3	2.09	0.52
2:C:278:TRP:HB3	2:C:349:VAL:HG21	1.91	0.52
2:N:259:ALA:CB	2:N:363:MET:SD	2.97	0.52
2:D:360:HIS:HB2	2:D:363:MET:CE	2.39	0.52
2:D:360:HIS:CG	2:D:363:MET:SD	3.03	0.52
2:M:10:TRP:CH2	2:M:190:ILE:HG23	2.37	0.52
2:C:93:ILE:HG23	2:D:133:ARG:HH12	1.73	0.52
2:C:281:LEU:HD23	2:C:285:MET:CE	2.36	0.52
2:M:100:LYS:CB	2:N:133:ARG:NE	2.43	0.52
2:M:156:THR:HG22	2:M:158:ASP:N	2.21	0.52
2:M:360:HIS:HD2	2:M:363:MET:H	1.57	0.52
2:N:360:HIS:CG	2:N:363:MET:SD	3.03	0.52
2:B:365:LEU:CD2	2:C:297:LEU:HD13	2.39	0.52
2:N:291:ARG:HD2	2:N:306:MET:SD	2.49	0.52
2:M:3:TYR:O	2:M:4:GLN:HB2	2.09	0.52
2:B:276:ILE:HG22	2:B:277:GLU:N	2.24	0.52
2:I:259:ALA:CB	2:I:363:MET:SD	2.98	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:365:LEU:HD22	2:C:297:LEU:HD12	1.92	0.52
2:N:240:MET:SD	3:O:157:SER:HB2	2.50	0.52
2:I:250:LEU:HD23	2:I:312:ARG:HH11	1.75	0.52
2:N:250:LEU:HD23	2:N:312:ARG:HH11	1.75	0.52
2:C:359:PHE:CE2	2:D:323:THR:CG2	2.89	0.52
2:C:156:THR:HG22	2:C:158:ASP:N	2.21	0.52
1:A:309:GLU:O	1:A:313:LYS:HG3	2.10	0.52
2:B:6:LEU:CD1	2:B:190:ILE:HG23	2.26	0.52
2:I:360:HIS:O	2:I:363:MET:HB2	2.09	0.52
2:L:94:ASP:N	2:L:100:LYS:HZ1	2.06	0.52
2:L:93:ILE:HG22	2:L:100:LYS:NZ	2.25	0.52
1:K:25:GLY:O	1:K:115:ASN:HA	2.08	0.52
1:K:10:ARG:HH22	1:K:40:GLN:NE2	2.08	0.52
2:N:360:HIS:HB2	2:N:363:MET:CE	2.39	0.52
2:I:257:VAL:HG11	2:I:320:ILE:CD1	2.40	0.52
2:I:360:HIS:CG	2:I:363:MET:SD	3.03	0.52
2:G:93:ILE:HG22	2:G:100:LYS:NZ	2.25	0.52
2:N:271:ALA:HB1	2:N:276:ILE:HD11	1.90	0.52
2:I:200:PRO:HB2	2:I:305:ASP:H	1.75	0.52
3:E:204:LEU:O	3:E:209:ASN:HB3	2.07	0.52
1:A:312:LEU:HB2	1:A:320:VAL:CG2	2.35	0.52
2:L:276:ILE:HG22	2:L:277:GLU:N	2.24	0.52
2:C:191:LEU:HD12	2:C:203:LEU:HD21	1.91	0.52
2:D:345:ARG:NH1	3:E:149:GLU:OE1	2.43	0.52
1:A:75:ALA:HB2	1:F:207:ASN:HB3	1.90	0.52
2:M:341:TYR:CB	2:N:333:LEU:HD11	2.11	0.52
2:N:302:LEU:HD22	2:N:306:MET:HG2	1.90	0.52
1:F:294:SER:H	1:F:297:GLN:NE2	2.08	0.52
3:J:268:VAL:O	3:J:271:PRO:HD3	2.09	0.52
1:A:282:ARG:HG2	1:A:285:MET:HE2	1.91	0.52
2:H:215:ARG:HH21	2:I:164:VAL:HG21	1.74	0.52
2:H:19:VAL:CG2	2:H:214:LEU:CD2	2.88	0.52
3:E:238:HIS:ND1	3:E:239:GLU:N	2.56	0.52
1:A:294:SER:H	1:A:297:GLN:NE2	2.08	0.52
2:D:259:ALA:HB2	2:D:363:MET:HG3	1.89	0.52
2:D:357:LEU:C	2:D:363:MET:SD	2.88	0.52
2:G:93:ILE:CG2	2:G:100:LYS:HZ2	2.22	0.52
2:L:180:VAL:HG11	2:L:305:ASP:HB2	1.91	0.52
2:N:223:GLN:NE2	3:O:158:ARG:HE	2.08	0.52
2:G:7:ALA:HB2	2:G:219:SER:HB3	1.90	0.52
2:N:13:GLN:HE22	2:N:83:GLU:CG	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:93:ILE:HG22	2:N:100:LYS:HZ2	1.75	0.52
1:F:10:ARG:HH22	1:F:40:GLN:NE2	2.08	0.52
2:I:360:HIS:HB2	2:I:363:MET:CE	2.39	0.52
2:D:257:VAL:HG11	2:D:320:ILE:CD1	2.40	0.52
2:D:360:HIS:CB	2:D:363:MET:CB	2.68	0.52
2:N:240:MET:O	3:O:156:ARG:HG3	2.10	0.52
2:D:352:THR:O	2:D:355:ARG:HB3	2.10	0.52
2:H:252:LEU:HD13	2:H:281:LEU:HD21	1.92	0.52
1:K:306:THR:HG21	3:O:314:ASP:OD2	2.10	0.52
2:I:357:LEU:C	2:I:363:MET:SD	2.88	0.51
2:D:259:ALA:CB	2:D:363:MET:SD	2.98	0.51
1:K:333:HIS:NE2	2:L:297:LEU:HG	2.24	0.51
2:B:99:THR:O	2:B:99:THR:CG2	2.53	0.51
3:O:27:LEU:O	3:O:143:LEU:N	2.39	0.51
1:A:10:ARG:HH22	1:A:40:GLN:NE2	2.08	0.51
3:O:311:LEU:O	3:O:314:ASP:HB3	2.11	0.51
2:H:89:ASP:HB3	2:H:121:LYS:HA	1.92	0.51
1:K:27:ASP:HB3	1:K:30:LEU:HB2	1.92	0.51
3:J:311:LEU:O	3:J:314:ASP:HB3	2.10	0.51
2:N:357:LEU:C	2:N:363:MET:SD	2.88	0.51
1:F:27:ASP:HB3	1:F:30:LEU:HB2	1.93	0.51
3:O:151:LEU:HD21	3:O:155:LEU:HD12	1.93	0.51
2:N:352:THR:O	2:N:355:ARG:HB3	2.10	0.51
2:D:250:LEU:HD23	2:D:312:ARG:HH11	1.74	0.51
2:C:252:LEU:HD13	2:C:281:LEU:HD21	1.92	0.51
2:D:13:GLN:HE22	2:D:83:GLU:CG	2.22	0.51
1:F:218:VAL:HG11	1:F:253:GLU:HG3	1.91	0.51
1:A:218:VAL:HG11	1:A:253:GLU:HG3	1.91	0.51
2:N:360:HIS:O	2:N:363:MET:HB2	2.09	0.51
1:A:310:LEU:O	1:A:314:GLN:HG3	2.11	0.51
2:M:181:GLU:HA	2:M:184:ARG:HB3	1.93	0.51
2:I:84:GLN:HB3	2:I:86:ARG:NH2	2.24	0.51
2:H:278:TRP:HB3	2:H:349:VAL:HG21	1.91	0.51
2:M:191:LEU:HD12	2:M:203:LEU:HD21	1.91	0.51
2:H:86:ARG:NE	2:I:141:LYS:HB2	2.26	0.51
2:L:347:MET:SD	2:M:290:HIS:CD2	3.03	0.51
2:H:11:ARG:HH22	2:I:165:THR:HG22	1.74	0.51
1:A:93:ILE:HG23	1:A:97:LEU:HD13	1.91	0.51
2:G:343:PRO:CG	2:G:347:MET:SD	2.99	0.51
2:D:93:ILE:HG22	2:D:100:LYS:HZ2	1.76	0.51
2:N:84:GLN:HB3	2:N:86:ARG:NH2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:213:SER:OG	2:M:216:ASP:HB2	2.11	0.51
1:A:333:HIS:CE1	2:B:298:SER:OG	2.64	0.51
2:I:271:ALA:HB1	2:I:276:ILE:HD11	1.90	0.51
2:N:257:VAL:HG11	2:N:320:ILE:CD1	2.40	0.51
2:B:93:ILE:HG22	2:B:100:LYS:NZ	2.25	0.51
2:I:352:THR:O	2:I:355:ARG:HB3	2.10	0.51
1:K:273:PHE:HB3	1:K:279:TRP:HB2	1.90	0.51
2:D:93:ILE:HG22	2:D:100:LYS:HZ3	1.74	0.51
2:H:181:GLU:HA	2:H:184:ARG:HB3	1.93	0.51
2:H:213:SER:OG	2:H:216:ASP:HB2	2.11	0.51
2:C:89:ASP:HB3	2:C:121:LYS:HA	1.92	0.51
3:J:151:LEU:HD21	3:J:155:LEU:HD12	1.92	0.51
2:B:365:LEU:CD2	2:C:297:LEU:HD11	2.38	0.51
1:K:310:LEU:O	1:K:314:GLN:HG3	2.11	0.51
1:F:262:ARG:CZ	3:J:230:TYR:HB3	2.40	0.51
1:K:262:ARG:CZ	3:O:230:TYR:HD2	2.24	0.51
2:M:278:TRP:HB3	2:M:349:VAL:HG21	1.91	0.51
2:M:89:ASP:HB3	2:M:121:LYS:HA	1.92	0.51
2:H:341:TYR:HB3	2:I:333:LEU:HD13	1.93	0.51
3:J:139:THR:HG22	3:J:140:TRP:N	2.26	0.51
2:G:302:LEU:HG	2:G:314:ARG:NH1	2.26	0.51
2:L:302:LEU:HG	2:L:314:ARG:NH1	2.26	0.51
2:G:243:THR:HG22	2:G:244:LEU:N	2.26	0.51
2:H:191:LEU:HD12	2:H:203:LEU:HD21	1.91	0.51
2:M:252:LEU:HD13	2:M:281:LEU:HD21	1.92	0.51
1:K:218:VAL:HG11	1:K:253:GLU:HG3	1.91	0.51
2:L:243:THR:HG22	2:L:244:LEU:N	2.26	0.51
1:K:300:GLN:OE1	1:K:335:PRO:HG2	2.09	0.51
3:O:139:THR:HG22	3:O:140:TRP:N	2.26	0.51
3:J:34:GLY:O	3:J:199:GLY:HA3	2.11	0.51
2:B:303:GLY:HA3	2:B:306:MET:HG2	1.93	0.51
1:K:261:LYS:HE3	1:K:295:GLN:HE21	1.76	0.51
2:L:10:TRP:CZ2	2:L:193:GLU:CB	2.94	0.51
2:G:21:GLN:CG	2:G:178:LEU:HD23	2.40	0.51
2:C:93:ILE:HG23	2:C:100:LYS:HZ2	1.75	0.51
1:F:310:LEU:O	1:F:314:GLN:HG3	2.11	0.51
2:G:362:ARG:HH21	2:G:363:MET:HE1	1.76	0.51
3:E:311:LEU:O	3:E:314:ASP:HB3	2.10	0.51
1:F:283:ARG:CZ	2:N:315:GLU:OE1	2.33	0.50
2:G:19:VAL:H	2:G:214:LEU:CD2	2.23	0.50
2:C:100:LYS:HG2	2:D:133:ARG:CD	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:60:LYS:HE3	2:I:79:CYS:HB3	1.93	0.50
1:A:300:GLN:OE1	1:A:335:PRO:HG2	2.09	0.50
2:B:201:ARG:O	2:B:205:LEU:HG	2.11	0.50
1:F:300:GLN:OE1	1:F:335:PRO:HG2	2.09	0.50
2:M:360:HIS:CD2	2:M:362:ARG:H	2.30	0.50
2:C:360:HIS:CD2	2:C:362:ARG:H	2.30	0.50
3:E:145:THR:HG22	3:E:147:GLU:N	2.27	0.50
2:C:365:LEU:HD21	2:D:297:LEU:HD13	1.92	0.50
1:K:20:ALA:O	1:K:134:SER:HB2	2.12	0.50
2:L:303:GLY:HA3	2:L:306:MET:HG2	1.93	0.50
3:E:151:LEU:HD21	3:E:155:LEU:HD12	1.93	0.50
2:M:342:ALA:CA	2:N:333:LEU:HD21	2.41	0.50
1:A:338:ASP:OD2	2:B:326:GLN:HG3	2.10	0.50
2:H:276:ILE:HG22	2:H:277:GLU:N	2.24	0.50
2:N:99:THR:CG2	2:N:99:THR:O	2.53	0.50
2:D:5:VAL:CG1	2:D:222:ASP:CG	2.80	0.50
3:J:100:LEU:HD13	3:J:139:THR:HG21	1.93	0.50
1:K:294:SER:H	1:K:297:GLN:NE2	2.08	0.50
1:A:261:LYS:HE3	1:A:295:GLN:HE21	1.76	0.50
2:H:102:GLU:HB3	2:H:106:ASP:CB	2.41	0.50
3:E:35:MET:HE1	3:E:166:PRO:HA	1.94	0.50
2:B:6:LEU:CD2	2:B:194:GLU:OE2	2.59	0.50
2:L:343:PRO:CG	2:L:347:MET:SD	2.99	0.50
2:L:180:VAL:HG11	2:L:305:ASP:CB	2.41	0.50
2:G:69:THR:HG22	2:G:71:THR:N	2.01	0.50
1:A:172:TYR:OH	1:A:281:ASN:ND2	2.44	0.50
1:A:336:LEU:CD1	2:B:326:GLN:NE2	2.72	0.50
2:M:347:MET:HG2	2:N:290:HIS:ND1	2.27	0.50
2:B:347:MET:HG3	2:C:290:HIS:CD2	2.46	0.50
2:C:213:SER:OG	2:C:216:ASP:HB2	2.11	0.50
2:B:243:THR:HG22	2:B:244:LEU:N	2.26	0.50
1:F:270:ARG:NH2	2:N:316:LEU:CA	2.72	0.50
1:K:96:GLN:O	1:K:100:LEU:HG	2.12	0.50
1:F:96:GLN:O	1:F:100:LEU:HG	2.12	0.50
2:H:360:HIS:CD2	2:H:362:ARG:H	2.30	0.50
2:H:20:GLY:HA3	2:H:182:GLN:HE21	1.76	0.50
2:B:343:PRO:CG	2:B:347:MET:SD	2.99	0.50
2:H:92:GLU:HG2	2:H:124:LEU:HD23	1.94	0.50
2:D:288:LEU:O	2:D:292:ILE:HG13	2.12	0.50
2:D:60:LYS:HE3	2:D:79:CYS:HB3	1.93	0.50
2:D:302:LEU:HD11	2:D:313:MET:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:184:ARG:HH22	2:I:304:ASN:HD22	1.59	0.50
1:A:20:ALA:O	1:A:134:SER:HB2	2.11	0.50
1:F:20:ALA:O	1:F:134:SER:HB2	2.12	0.50
2:C:102:GLU:HB3	2:C:106:ASP:CB	2.41	0.50
2:B:6:LEU:HD23	2:B:194:GLU:OE2	2.12	0.50
2:G:49:VAL:HG12	2:G:50:GLY:N	2.27	0.50
2:N:302:LEU:HD11	2:N:313:MET:HB2	1.94	0.50
2:G:343:PRO:HA	2:H:283:VAL:HG13	1.93	0.50
3:E:46:ARG:NH1	3:E:68:MET:HG3	2.27	0.50
2:C:181:GLU:HA	2:C:184:ARG:HB3	1.93	0.50
1:K:296:THR:HG22	1:K:299:ARG:HH12	1.77	0.50
2:G:303:GLY:HA3	2:G:306:MET:HG2	1.93	0.50
2:C:201:ARG:HB2	2:C:305:ASP:OD2	2.12	0.50
2:B:366:PRO:C	2:B:367:GLU:HG3	2.32	0.50
2:M:92:GLU:HG2	2:M:124:LEU:HD23	1.94	0.50
2:G:354:LEU:HD12	2:H:294:MET:SD	2.44	0.50
2:L:347:MET:HG3	2:M:290:HIS:CE1	2.47	0.50
1:F:282:ARG:HG2	1:F:285:MET:HE2	1.94	0.50
1:A:274:ASP:HA	1:A:279:TRP:CZ3	2.47	0.50
1:K:312:LEU:HB2	1:K:320:VAL:CG2	2.35	0.50
1:K:144:GLN:NE2	1:K:280:GLN:HB2	2.27	0.50
2:I:223:GLN:HG2	3:J:158:ARG:NH2	2.26	0.50
1:F:261:LYS:HE3	1:F:295:GLN:HE21	1.76	0.50
2:L:366:PRO:C	2:L:367:GLU:HG3	2.32	0.50
2:N:288:LEU:O	2:N:292:ILE:HG13	2.12	0.50
3:O:46:ARG:NH1	3:O:68:MET:HG3	2.27	0.50
3:E:139:THR:HG22	3:E:140:TRP:N	2.26	0.50
2:B:302:LEU:HG	2:B:314:ARG:NH1	2.26	0.50
1:A:306:THR:OG1	3:E:310:LEU:HD22	2.12	0.50
2:I:236:ALA:O	2:I:239:ALA:HB3	2.12	0.50
1:A:27:ASP:HB3	1:A:30:LEU:HB2	1.93	0.50
2:M:102:GLU:HB3	2:M:106:ASP:CB	2.41	0.50
1:A:273:PHE:HB3	1:A:279:TRP:HB2	1.90	0.49
2:M:277:GLU:OE2	2:N:176:LYS:HD2	2.12	0.49
3:J:46:ARG:NH1	3:J:68:MET:HG3	2.27	0.49
1:A:309:GLU:HG3	3:E:306:ILE:HG23	1.94	0.49
2:I:5:VAL:CG1	2:I:222:ASP:CG	2.80	0.49
3:J:145:THR:HG22	3:J:147:GLU:N	2.27	0.49
2:I:47:ARG:NE	3:J:126:ASN:OD1	2.45	0.49
3:O:41:ILE:HG21	3:O:113:TRP:CG	2.47	0.49
2:M:44:SER:HB2	2:M:159:PRO:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:82:ILE:HG23	2:G:90:LEU:CD2	2.42	0.49
2:D:360:HIS:HB2	2:D:363:MET:HE3	1.94	0.49
1:K:274:ASP:HA	1:K:279:TRP:CZ3	2.47	0.49
2:H:271:ALA:HB1	2:H:276:ILE:CD1	2.36	0.49
3:O:145:THR:HG22	3:O:147:GLU:N	2.27	0.49
2:C:92:GLU:HG2	2:C:124:LEU:HD23	1.94	0.49
2:C:44:SER:HB2	2:C:159:PRO:HG3	1.94	0.49
2:I:52:THR:O	2:I:55:ALA:HB3	2.13	0.49
2:N:363:MET:CB	2:N:364:PRO:CD	2.78	0.49
2:G:69:THR:HG22	2:G:70:ALA:N	2.28	0.49
2:H:351:MET:CE	2:I:326:GLN:NE2	2.63	0.49
2:L:69:THR:HG22	2:L:70:ALA:N	2.28	0.49
2:M:276:ILE:HG22	2:M:277:GLU:N	2.24	0.49
2:B:362:ARG:HH21	2:B:363:MET:HE1	1.77	0.49
2:N:93:ILE:HG22	2:N:100:LYS:HZ3	1.75	0.49
3:O:100:LEU:HD13	3:O:139:THR:HG21	1.93	0.49
1:A:296:THR:HG22	1:A:299:ARG:HH12	1.77	0.49
2:C:341:TYR:CB	2:D:333:LEU:HD13	2.41	0.49
2:D:355:ARG:HH12	3:E:287:GLN:HB3	1.74	0.49
1:K:32:GLN:HE22	2:L:165:THR:HG22	1.72	0.49
2:G:99:THR:CG2	2:G:99:THR:O	2.53	0.49
2:D:140:LEU:HD22	2:D:169:ARG:CZ	2.43	0.49
2:I:288:LEU:O	2:I:292:ILE:HG13	2.12	0.49
1:K:119:LYS:H	1:K:119:LYS:CD	2.05	0.49
2:C:56:ARG:HH21	2:D:165:THR:HG23	1.76	0.49
2:B:82:ILE:HG23	2:B:90:LEU:CD2	2.42	0.49
2:L:49:VAL:HG12	2:L:50:GLY:N	2.27	0.49
1:A:22:LEU:HD22	1:A:112:VAL:HB	1.95	0.49
2:N:257:VAL:HG11	2:N:320:ILE:HD13	1.95	0.49
2:D:356:ALA:O	2:D:363:MET:HE3	2.12	0.49
2:N:276:ILE:HG22	2:N:277:GLU:N	2.28	0.49
2:M:244:LEU:HB3	2:M:248:GLN:HB2	1.95	0.49
1:F:199:LEU:HB3	1:F:200:PRO:HD3	1.94	0.49
2:D:277:GLU:HA	3:E:149:GLU:CG	2.42	0.49
2:N:360:HIS:CG	2:N:363:MET:HE3	2.47	0.49
2:H:94:ASP:C	2:H:100:LYS:NZ	2.62	0.49
2:D:200:PRO:HB2	2:D:305:ASP:N	2.28	0.49
1:A:172:TYR:O	1:A:216:HIS:HE1	1.96	0.49
2:G:201:ARG:O	2:G:205:LEU:HG	2.12	0.49
3:J:312:ILE:O	3:J:316:LEU:HG	2.13	0.49
2:N:52:THR:O	2:N:55:ALA:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:85:LYS:NZ	3:E:85:LYS:HB3	2.28	0.49
2:I:276:ILE:HG22	2:I:277:GLU:N	2.28	0.49
2:H:342:ALA:HA	2:I:333:LEU:HD21	1.95	0.49
2:N:60:LYS:HE3	2:N:79:CYS:HB3	1.93	0.49
1:A:96:GLN:O	1:A:100:LEU:HG	2.12	0.49
1:K:48:GLU:CG	1:K:49:GLU:N	2.76	0.49
1:F:48:GLU:CG	1:F:49:GLU:N	2.76	0.49
3:O:312:ILE:O	3:O:316:LEU:HG	2.13	0.49
3:J:41:ILE:HG21	3:J:113:TRP:CG	2.47	0.49
2:D:236:ALA:O	2:D:239:ALA:HB3	2.12	0.49
2:D:276:ILE:HG22	2:D:277:GLU:N	2.28	0.49
2:L:235:GLN:HA	2:L:243:THR:HG21	1.94	0.49
2:C:84:GLN:CB	2:D:144:GLU:OE1	2.61	0.49
3:E:312:ILE:O	3:E:316:LEU:HG	2.12	0.49
1:K:183:GLN:HA	1:K:183:GLN:HE21	1.78	0.49
2:N:236:ALA:O	2:N:239:ALA:HB3	2.12	0.49
2:H:244:LEU:HB3	2:H:248:GLN:HB2	1.95	0.49
2:B:49:VAL:HG12	2:B:50:GLY:N	2.27	0.49
1:F:270:ARG:HH22	2:N:316:LEU:C	2.17	0.49
1:F:274:ASP:HA	1:F:279:TRP:CZ3	2.47	0.49
2:D:257:VAL:HG11	2:D:320:ILE:HD13	1.95	0.49
2:I:140:LEU:HD22	2:I:169:ARG:CZ	2.43	0.49
1:F:22:LEU:HD22	1:F:112:VAL:HB	1.94	0.49
2:L:201:ARG:O	2:L:205:LEU:HG	2.11	0.48
2:B:69:THR:HG22	2:B:70:ALA:N	2.28	0.48
2:G:12:PRO:CD	2:G:215:ARG:NH1	2.70	0.48
2:N:140:LEU:HD22	2:N:169:ARG:CZ	2.42	0.48
3:E:100:LEU:HD13	3:E:139:THR:HG21	1.93	0.48
3:E:41:ILE:HG21	3:E:113:TRP:CG	2.47	0.48
2:G:366:PRO:C	2:G:367:GLU:HG3	2.32	0.48
2:L:82:ILE:HG23	2:L:90:LEU:CD2	2.42	0.48
3:J:85:LYS:NZ	3:J:85:LYS:HB3	2.28	0.48
1:A:48:GLU:CG	1:A:49:GLU:N	2.76	0.48
3:O:145:THR:HG22	3:O:147:GLU:H	1.78	0.48
1:F:183:GLN:HE21	1:F:183:GLN:HA	1.78	0.48
3:E:57:LYS:HG3	3:E:58:SER:H	1.78	0.48
2:M:56:ARG:NH2	2:N:165:THR:HG21	2.27	0.48
1:F:251:GLN:OE1	3:J:307:ASN:ND2	2.46	0.48
2:I:360:HIS:HB2	2:I:363:MET:HE3	1.95	0.48
1:A:311:THR:HG23	1:A:318:GLN:CD	2.34	0.48
2:C:86:ARG:CZ	2:D:141:LYS:CB	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:338:GLU:HA	2:N:341:TYR:CD1	2.48	0.48
2:G:270:GLU:HG2	2:G:274:ARG:NH1	2.29	0.48
2:L:256:MET:CE	2:L:332:LEU:HD21	2.44	0.48
1:K:199:LEU:HB3	1:K:200:PRO:HD3	1.94	0.48
2:L:286:LEU:HD11	2:L:333:LEU:HA	1.96	0.48
2:M:19:VAL:HG21	2:M:214:LEU:HD22	1.96	0.48
3:J:241:ALA:O	3:J:245:LEU:HD22	2.14	0.48
1:K:311:THR:HG23	1:K:318:GLN:CD	2.34	0.48
2:L:365:LEU:HD22	2:M:297:LEU:HD12	1.95	0.48
2:I:337:LYS:HD3	3:J:334:LEU:HB2	1.96	0.48
2:D:302:LEU:HD11	2:D:313:MET:CB	2.44	0.48
2:N:302:LEU:HD11	2:N:313:MET:CB	2.44	0.48
2:L:362:ARG:HE	2:L:363:MET:CE	2.25	0.48
3:O:57:LYS:HG3	3:O:58:SER:H	1.78	0.48
2:H:84:GLN:HG2	2:I:144:GLU:OE1	2.13	0.48
3:J:27:LEU:O	3:J:143:LEU:N	2.39	0.48
2:G:140:LEU:O	2:G:144:GLU:HG3	2.14	0.48
2:D:52:THR:O	2:D:55:ALA:HB3	2.13	0.48
2:B:270:GLU:HG2	2:B:274:ARG:NH1	2.28	0.48
2:H:10:TRP:HZ2	2:H:194:GLU:HG2	1.78	0.48
2:H:215:ARG:CZ	2:I:164:VAL:HG22	2.43	0.48
3:E:306:ILE:HG22	3:E:307:ASN:N	2.29	0.48
3:J:145:THR:HG22	3:J:147:GLU:H	1.78	0.48
2:G:286:LEU:HD11	2:G:333:LEU:HA	1.96	0.48
1:K:210:ALA:HA	1:K:212:PHE:CE1	2.49	0.48
3:O:85:LYS:HB3	3:O:85:LYS:NZ	2.28	0.48
2:H:93:ILE:CG2	2:H:100:LYS:HZ2	2.25	0.48
2:M:271:ALA:HB1	2:M:276:ILE:CD1	2.36	0.48
3:J:57:LYS:HG3	3:J:58:SER:H	1.78	0.48
2:D:260:ASN:OD1	2:D:260:ASN:O	2.32	0.48
2:L:32:LEU:HD11	2:L:58:LEU:HD12	1.95	0.48
2:G:32:LEU:HD11	2:G:58:LEU:HD12	1.95	0.48
2:H:341:TYR:CE2	2:I:337:LYS:CB	2.95	0.48
2:G:347:MET:CG	2:H:290:HIS:CD2	2.95	0.48
2:H:316:LEU:HB3	2:H:320:ILE:HD12	1.96	0.48
1:K:191:LEU:HD22	2:L:23:HIS:ND1	2.29	0.48
2:C:239:ALA:HB1	2:D:23:HIS:CE1	2.49	0.48
2:N:24:VAL:HG11	2:N:175:LEU:HD21	1.96	0.48
2:N:360:HIS:HB2	2:N:363:MET:HE3	1.95	0.48
2:G:20:GLY:O	2:G:182:GLN:NE2	2.46	0.48
1:F:311:THR:HG23	1:F:318:GLN:CD	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:270:GLU:HG2	2:L:274:ARG:NH1	2.29	0.48
1:K:281:ASN:O	1:K:283:ARG:N	2.47	0.48
2:C:341:TYR:CE2	2:D:337:LYS:CB	2.96	0.48
2:I:302:LEU:HD11	2:I:313:MET:CB	2.44	0.48
2:I:302:LEU:HD11	2:I:313:MET:HB2	1.94	0.48
2:N:93:ILE:CG2	2:N:100:LYS:HZ2	2.26	0.48
2:D:93:ILE:CG2	2:D:100:LYS:HZ2	2.27	0.48
2:B:256:MET:CE	2:B:332:LEU:HD21	2.44	0.48
1:K:22:LEU:HD22	1:K:112:VAL:HB	1.94	0.48
2:C:66:THR:O	2:C:66:THR:HG22	2.14	0.48
2:G:19:VAL:N	2:G:214:LEU:HD22	2.21	0.48
2:I:338:GLU:HA	2:I:341:TYR:CD1	2.48	0.48
1:A:281:ASN:O	1:A:283:ARG:N	2.47	0.48
2:D:338:GLU:HA	2:D:341:TYR:CD1	2.48	0.48
2:H:84:GLN:CG	2:I:144:GLU:OE1	2.62	0.48
2:H:84:GLN:CA	2:I:144:GLU:OE1	2.62	0.48
2:I:260:ASN:O	2:I:260:ASN:OD1	2.32	0.48
1:K:10:ARG:NH2	1:K:40:GLN:HE22	2.11	0.48
1:F:296:THR:HG22	1:F:299:ARG:HH12	1.77	0.48
2:I:24:VAL:HG11	2:I:175:LEU:HD21	1.96	0.48
2:H:44:SER:HB2	2:H:159:PRO:HG3	1.94	0.48
2:N:355:ARG:NH2	3:O:332:PRO:HD3	2.18	0.47
2:H:147:PRO:HG2	2:H:150:VAL:HB	1.96	0.47
2:C:147:PRO:HG2	2:C:150:VAL:HB	1.96	0.47
1:A:199:LEU:HB3	1:A:200:PRO:HD3	1.94	0.47
3:O:306:ILE:HG22	3:O:307:ASN:N	2.29	0.47
3:J:306:ILE:HG22	3:J:307:ASN:N	2.29	0.47
1:A:10:ARG:NH2	1:A:40:GLN:HE22	2.11	0.47
2:L:140:LEU:O	2:L:144:GLU:HG3	2.14	0.47
2:B:286:LEU:HD11	2:B:333:LEU:HA	1.96	0.47
3:O:241:ALA:O	3:O:245:LEU:HD22	2.14	0.47
2:I:257:VAL:HG11	2:I:320:ILE:HD13	1.95	0.47
3:E:145:THR:HG22	3:E:147:GLU:H	1.78	0.47
2:C:354:LEU:HD22	2:D:297:LEU:HD22	1.96	0.47
2:N:316:LEU:HD22	2:N:320:ILE:CD1	2.45	0.47
2:L:244:LEU:HA	2:L:244:LEU:HD23	1.51	0.47
2:G:19:VAL:N	2:G:214:LEU:CD2	2.78	0.47
2:B:94:ASP:O	2:B:100:LYS:CE	2.62	0.47
2:H:10:TRP:HZ2	2:H:194:GLU:CG	2.28	0.47
2:M:257:VAL:HG11	2:M:320:ILE:HD13	1.97	0.47
2:L:223:GLN:HG2	2:M:171:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:241:ALA:N	3:J:242:PRO:HD2	2.29	0.47
3:O:241:ALA:N	3:O:242:PRO:HD2	2.29	0.47
2:C:126:ASP:HA	2:C:155:ALA:HB3	1.96	0.47
2:D:51:LYS:HE3	2:D:51:LYS:HB2	1.76	0.47
2:G:19:VAL:HG21	2:G:186:GLN:HG2	1.78	0.47
1:A:74:PHE:CZ	1:F:203:GLU:OE1	2.62	0.47
1:A:310:LEU:HD13	1:A:314:GLN:HE22	1.77	0.47
2:N:260:ASN:OD1	2:N:260:ASN:O	2.32	0.47
2:G:256:MET:CE	2:G:332:LEU:HD21	2.44	0.47
1:A:221:LEU:HA	1:A:221:LEU:HD23	1.47	0.47
2:D:246:ASP:HB2	2:D:248:GLN:CG	2.45	0.47
2:C:291:ARG:NH1	2:C:306:MET:HG3	2.29	0.47
2:H:216:ASP:O	2:H:220:LEU:HG	2.15	0.47
2:I:10:TRP:CE2	2:I:190:ILE:HG23	2.49	0.47
2:H:126:ASP:HA	2:H:155:ALA:HB3	1.96	0.47
2:B:292:ILE:O	2:B:296:GLN:HG3	2.14	0.47
3:E:241:ALA:O	3:E:245:LEU:HD22	2.14	0.47
2:H:66:THR:O	2:H:66:THR:HG22	2.14	0.47
2:G:10:TRP:CE3	2:G:190:ILE:CG2	2.96	0.47
2:D:244:LEU:HD11	2:D:276:ILE:CG2	2.45	0.47
1:A:105:HIS:CB	1:F:227:LYS:CD	2.66	0.47
2:C:281:LEU:CD2	2:C:285:MET:HE2	2.41	0.47
1:F:262:ARG:CZ	3:J:230:TYR:CD2	2.97	0.47
2:C:316:LEU:HB3	2:C:320:ILE:HD12	1.96	0.47
2:H:257:VAL:HG11	2:H:320:ILE:HD13	1.97	0.47
1:K:263:GLN:HB2	1:K:272:LEU:HD21	1.97	0.47
2:M:291:ARG:NH1	2:M:306:MET:HG3	2.29	0.47
2:H:101:VAL:HG12	2:H:102:GLU:HG3	1.96	0.47
1:F:98:LEU:O	1:F:101:THR:HG22	2.14	0.47
1:F:281:ASN:O	1:F:283:ARG:N	2.47	0.47
1:A:194:ASP:CA	2:M:311:LEU:CD1	2.80	0.47
2:G:50:GLY:O	2:G:54:ILE:HG13	2.15	0.47
2:N:220:LEU:HD21	3:O:154:THR:HB	1.96	0.47
1:A:60:ASP:O	1:A:64:ILE:HD12	2.15	0.47
2:M:316:LEU:HB3	2:M:320:ILE:HD12	1.96	0.47
1:A:263:GLN:HB2	1:A:272:LEU:HD21	1.97	0.47
2:N:246:ASP:HB2	2:N:248:GLN:CG	2.45	0.47
2:M:101:VAL:HG12	2:M:102:GLU:HG3	1.96	0.47
2:B:50:GLY:O	2:B:54:ILE:HG13	2.15	0.47
2:B:333:LEU:CD1	2:B:337:LYS:HE3	2.45	0.47
3:E:241:ALA:N	3:E:242:PRO:HD2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:147:PRO:HG2	2:M:150:VAL:HB	1.96	0.47
2:L:292:ILE:O	2:L:296:GLN:HG3	2.14	0.47
2:B:32:LEU:HD11	2:B:58:LEU:HD12	1.95	0.47
2:B:6:LEU:CG	2:B:190:ILE:CG2	2.86	0.47
2:G:20:GLY:HA3	2:G:182:GLN:CD	2.36	0.47
1:K:311:THR:HG23	1:K:318:GLN:OE1	2.15	0.47
1:A:311:THR:HG23	1:A:318:GLN:OE1	2.15	0.47
2:G:94:ASP:O	2:G:100:LYS:CE	2.63	0.47
2:N:244:LEU:HD11	2:N:276:ILE:CG2	2.45	0.47
1:A:119:LYS:HD3	1:A:119:LYS:N	2.11	0.47
2:H:281:LEU:CD2	2:H:285:MET:HE2	2.40	0.47
2:H:6:LEU:CB	2:H:222:ASP:OD1	2.63	0.47
1:K:262:ARG:CZ	3:O:230:TYR:CD2	2.98	0.47
2:M:216:ASP:O	2:M:220:LEU:HG	2.15	0.47
2:M:241:LEU:C	2:M:243:THR:N	2.68	0.47
2:D:24:VAL:HG11	2:D:175:LEU:HD21	1.96	0.47
2:N:334:ILE:HG12	3:O:334:LEU:OXT	2.14	0.47
2:C:244:LEU:HB3	2:C:248:GLN:HB2	1.95	0.47
2:G:292:ILE:O	2:G:296:GLN:HG3	2.14	0.47
3:E:227:GLY:O	3:E:229:TRP:HD1	1.98	0.47
2:N:256:MET:HA	2:N:357:LEU:HD11	1.97	0.47
2:C:97:SER:HG	2:C:100:LYS:HE3	1.76	0.47
2:I:200:PRO:CG	2:I:304:ASN:HB3	2.44	0.47
3:E:27:LEU:O	3:E:143:LEU:N	2.39	0.47
1:K:305:LEU:HD22	3:O:310:LEU:HD11	1.97	0.47
1:K:98:LEU:O	1:K:101:THR:HG22	2.14	0.47
2:I:44:SER:OG	2:I:174:HIS:HA	2.14	0.47
2:N:361:PRO:O	2:N:362:ARG:HB2	2.15	0.47
2:I:256:MET:HA	2:I:357:LEU:HD11	1.97	0.47
2:L:94:ASP:O	2:L:100:LYS:CE	2.63	0.47
3:O:6:TRP:CH2	3:O:175:TRP:CZ2	3.03	0.47
2:M:11:ARG:NH1	2:N:144:GLU:OE2	2.48	0.47
2:C:257:VAL:HG11	2:C:320:ILE:HD13	1.97	0.47
2:B:140:LEU:O	2:B:144:GLU:HG3	2.14	0.47
2:I:316:LEU:HD22	2:I:320:ILE:CD1	2.45	0.46
2:D:256:MET:HA	2:D:357:LEU:HD11	1.97	0.46
2:M:201:ARG:NH2	2:M:308:ALA:CB	2.78	0.46
1:K:315:ASP:HB2	1:K:318:GLN:CD	2.36	0.46
1:F:312:LEU:O	1:F:312:LEU:HG	2.15	0.46
1:K:60:ASP:O	1:K:64:ILE:HD12	2.15	0.46
2:D:165:THR:O	2:D:169:ARG:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:263:GLN:HB2	1:F:272:LEU:HD21	1.97	0.46
1:K:263:GLN:OE1	1:K:272:LEU:HD11	2.16	0.46
2:H:291:ARG:NH1	2:H:306:MET:HG3	2.29	0.46
2:C:101:VAL:HG12	2:C:102:GLU:HG3	1.96	0.46
1:A:98:LEU:O	1:A:101:THR:HG22	2.14	0.46
2:I:361:PRO:O	2:I:362:ARG:HB2	2.15	0.46
2:D:361:PRO:O	2:D:362:ARG:HB2	2.15	0.46
1:A:315:ASP:HB2	1:A:318:GLN:CD	2.36	0.46
2:C:365:LEU:HD21	2:D:297:LEU:CD1	2.45	0.46
1:F:263:GLN:OE1	1:F:272:LEU:HD11	2.15	0.46
2:G:316:LEU:HD22	2:G:320:ILE:HD11	1.97	0.46
2:M:126:ASP:HA	2:M:155:ALA:HB3	1.96	0.46
2:D:44:SER:OG	2:D:174:HIS:HA	2.15	0.46
2:B:316:LEU:HD22	2:B:320:ILE:HD11	1.97	0.46
3:O:227:GLY:O	3:O:229:TRP:HD1	1.98	0.46
2:N:44:SER:OG	2:N:174:HIS:HA	2.15	0.46
1:A:183:GLN:HA	1:A:183:GLN:HE21	1.78	0.46
2:M:66:THR:O	2:M:66:THR:HG22	2.14	0.46
2:I:165:THR:O	2:I:169:ARG:HG3	2.15	0.46
2:H:246:ASP:O	2:H:250:LEU:HB2	2.16	0.46
1:F:10:ARG:NH2	1:F:40:GLN:HE22	2.11	0.46
2:I:246:ASP:HB2	2:I:248:GLN:CG	2.45	0.46
1:F:19:ALA:CB	1:F:133:ARG:HD3	2.46	0.46
3:J:227:GLY:O	3:J:229:TRP:HD1	1.98	0.46
2:N:345:ARG:CZ	3:O:150:ARG:NE	2.55	0.46
2:L:343:PRO:HG3	2:M:287:GLY:HA2	1.97	0.46
1:A:213:THR:N	1:A:216:HIS:HD2	1.96	0.46
2:M:100:LYS:HB3	2:N:133:ARG:NE	2.26	0.46
1:K:144:GLN:HE22	1:K:280:GLN:HB2	1.80	0.46
1:A:263:GLN:OE1	1:A:272:LEU:HD11	2.15	0.46
1:F:198:THR:HB	1:F:200:PRO:HD2	1.98	0.46
2:G:93:ILE:HG23	2:G:100:LYS:HZ3	1.81	0.46
2:N:291:ARG:O	2:N:295:VAL:HG23	2.16	0.46
1:A:312:LEU:O	1:A:312:LEU:HG	2.15	0.46
2:M:246:ASP:O	2:M:250:LEU:HB2	2.16	0.46
2:I:197:ALA:HB3	2:I:231:GLN:HG2	1.98	0.46
2:L:333:LEU:CD1	2:L:337:LYS:HE3	2.45	0.46
1:A:198:THR:HB	1:A:200:PRO:HD2	1.98	0.46
1:A:284:GLY:O	1:A:288:GLU:HB2	2.16	0.46
1:K:279:TRP:O	1:K:279:TRP:CD2	2.69	0.46
3:J:27:LEU:CD2	3:J:29:ILE:HD11	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:HIS:CE1	2:B:298:SER:HG	2.33	0.46
2:L:50:GLY:O	2:L:54:ILE:HG13	2.15	0.46
2:C:149:HIS:CD2	2:C:149:HIS:H	2.34	0.46
1:K:19:ALA:CB	1:K:133:ARG:HD3	2.46	0.46
1:K:298:LEU:O	1:K:302:VAL:HG23	2.16	0.46
2:N:360:HIS:CB	2:N:363:MET:HE3	2.46	0.46
2:I:360:HIS:CG	2:I:363:MET:HE3	2.51	0.46
2:H:99:THR:O	2:H:99:THR:CG2	2.51	0.46
1:F:60:ASP:O	1:F:64:ILE:HD12	2.15	0.46
2:M:56:ARG:HH21	2:N:165:THR:HG23	1.79	0.46
2:I:343:PRO:HG3	2:I:347:MET:SD	2.56	0.46
2:D:197:ALA:HB3	2:D:231:GLN:HG2	1.98	0.46
1:F:298:LEU:O	1:F:302:VAL:HG23	2.16	0.46
2:D:316:LEU:HD22	2:D:320:ILE:CD1	2.45	0.46
2:G:19:VAL:H	2:G:214:LEU:HD22	1.81	0.46
1:K:315:ASP:HB2	1:K:318:GLN:NE2	2.31	0.46
1:F:315:ASP:HB2	1:F:318:GLN:NE2	2.31	0.46
2:L:204:GLN:HE21	2:L:305:ASP:CG	2.18	0.46
1:A:222:LEU:CD1	1:A:285:MET:SD	3.04	0.46
2:M:359:PHE:CZ	2:N:323:THR:HG22	2.50	0.46
2:I:291:ARG:O	2:I:295:VAL:HG23	2.16	0.46
2:D:302:LEU:HA	2:D:302:LEU:HD23	1.54	0.46
2:M:73:CYS:SG	2:M:76:CYS:HB3	2.56	0.46
2:I:93:ILE:HG22	2:I:100:LYS:HZ2	1.80	0.46
2:G:333:LEU:CD1	2:G:337:LYS:HE3	2.45	0.46
1:A:298:LEU:O	1:A:302:VAL:HG23	2.16	0.46
2:I:244:LEU:HD11	2:I:276:ILE:CG2	2.45	0.46
1:K:32:GLN:NE2	2:L:165:THR:CA	2.78	0.46
1:F:247:LEU:HD11	1:F:308:THR:HG22	1.98	0.46
2:D:343:PRO:HG3	2:D:347:MET:SD	2.56	0.46
1:F:221:LEU:HA	1:F:221:LEU:HD23	1.47	0.46
2:C:216:ASP:O	2:C:220:LEU:HG	2.15	0.46
2:H:149:HIS:CD2	2:H:149:HIS:H	2.34	0.46
3:J:95:GLU:O	3:J:99:LYS:HB2	2.15	0.46
2:C:7:ALA:O	2:D:168:SER:HB2	2.16	0.46
2:G:10:TRP:CE3	2:G:190:ILE:HD13	2.51	0.46
2:G:354:LEU:CD2	2:H:297:LEU:CD2	2.85	0.46
2:G:19:VAL:CG1	2:G:183:ILE:HA	2.38	0.46
1:K:247:LEU:HD11	1:K:308:THR:HG22	1.98	0.46
2:D:42:LEU:HD12	2:D:172:GLN:OE1	2.16	0.46
1:F:306:THR:OG1	3:J:310:LEU:CD2	2.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:354:LEU:HD22	2:I:297:LEU:HD22	1.96	0.46
2:B:344:ASP:O	2:B:347:MET:HB3	2.16	0.46
2:M:21:GLN:NE2	2:M:176:LYS:O	2.49	0.46
2:L:56:ARG:NH1	2:L:82:ILE:O	2.49	0.46
1:K:198:THR:HB	1:K:200:PRO:HD2	1.98	0.46
2:L:316:LEU:HD22	2:L:320:ILE:HD11	1.98	0.46
3:J:51:GLN:HB2	3:J:62:CYS:HB2	1.97	0.46
3:E:14:LEU:HD13	3:E:44:LEU:HD11	1.97	0.46
3:E:51:GLN:HB2	3:E:62:CYS:HB2	1.98	0.46
1:F:284:GLY:O	1:F:288:GLU:HB2	2.16	0.46
2:M:37:ILE:HD12	2:M:62:LEU:HD21	1.98	0.46
2:C:51:LYS:HE3	2:C:51:LYS:HB2	1.77	0.46
2:I:338:GLU:HA	2:I:341:TYR:HD1	1.81	0.45
2:C:246:ASP:O	2:C:250:LEU:HB2	2.16	0.45
2:H:215:ARG:CZ	2:I:164:VAL:CG2	2.94	0.45
2:C:21:GLN:NE2	2:C:176:LYS:O	2.49	0.45
3:E:282:SER:OG	3:E:285:ARG:HB2	2.16	0.45
1:K:284:GLY:O	1:K:288:GLU:HB2	2.16	0.45
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.61	0.45
2:N:165:THR:O	2:N:169:ARG:HG3	2.15	0.45
3:O:27:LEU:CD2	3:O:29:ILE:HD11	2.46	0.45
2:H:73:CYS:SG	2:H:76:CYS:HB3	2.56	0.45
3:J:282:SER:OG	3:J:285:ARG:HB2	2.16	0.45
2:L:19:VAL:HG21	2:L:186:GLN:CD	2.37	0.45
2:D:184:ARG:HH22	2:D:304:ASN:HD22	1.64	0.45
3:E:95:GLU:O	3:E:99:LYS:HB2	2.15	0.45
2:H:260:ASN:OD1	2:H:260:ASN:O	2.34	0.45
2:C:260:ASN:O	2:C:260:ASN:OD1	2.35	0.45
2:L:344:ASP:O	2:L:347:MET:HB3	2.16	0.45
1:F:315:ASP:HB2	1:F:318:GLN:CD	2.36	0.45
1:K:213:THR:N	1:K:216:HIS:HD2	1.96	0.45
2:D:338:GLU:HA	2:D:341:TYR:HD1	1.81	0.45
2:C:271:ALA:HB1	2:C:276:ILE:CD1	2.36	0.45
2:C:252:LEU:CD1	2:C:281:LEU:HD21	2.47	0.45
3:O:57:LYS:HA	3:O:57:LYS:HD2	1.67	0.45
2:N:42:LEU:HD12	2:N:172:GLN:OE1	2.16	0.45
2:C:73:CYS:SG	2:C:76:CYS:HB3	2.56	0.45
2:B:56:ARG:NH1	2:B:82:ILE:O	2.49	0.45
3:J:14:LEU:HD13	3:J:44:LEU:HD11	1.98	0.45
2:I:191:LEU:HD12	2:I:203:LEU:HD21	1.99	0.45
2:B:186:GLN:HG2	2:B:214:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:253:MET:O	3:J:256:LEU:N	2.50	0.45
1:F:311:THR:HG23	1:F:318:GLN:OE1	2.15	0.45
1:F:310:LEU:HD13	1:F:314:GLN:HE22	1.77	0.45
1:K:312:LEU:HG	1:K:312:LEU:O	2.15	0.45
3:O:27:LEU:HG	3:O:29:ILE:CD1	2.47	0.45
2:M:257:VAL:O	2:M:360:HIS:HE1	1.99	0.45
2:I:95:ALA:HA	2:I:100:LYS:HZ1	1.81	0.45
2:G:56:ARG:NH1	2:G:82:ILE:O	2.49	0.45
2:D:191:LEU:HD12	2:D:203:LEU:HD21	1.99	0.45
2:N:191:LEU:HD12	2:N:203:LEU:HD21	1.99	0.45
3:O:51:GLN:HB2	3:O:62:CYS:HB2	1.98	0.45
2:L:22:GLU:HG3	2:L:22:GLU:H	1.09	0.45
1:F:279:TRP:CD2	1:F:279:TRP:O	2.69	0.45
2:N:364:PRO:CG	3:O:260:HIS:CE1	2.99	0.45
2:I:258:GLU:O	2:I:259:ALA:HB3	2.17	0.45
1:A:19:ALA:CB	1:A:133:ARG:HD3	2.46	0.45
1:A:133:ARG:HG3	2:G:299:PRO:CG	2.45	0.45
2:M:351:MET:HA	2:M:351:MET:HE3	1.97	0.45
1:A:315:ASP:HB2	1:A:318:GLN:NE2	2.31	0.45
2:D:291:ARG:O	2:D:295:VAL:HG23	2.16	0.45
2:M:94:ASP:N	2:M:100:LYS:HZ3	2.14	0.45
2:M:238:SER:CB	2:M:245:ASP:OD1	2.65	0.45
2:N:142:THR:O	2:N:146:PRO:N	2.50	0.45
2:G:42:LEU:HD23	2:G:172:GLN:HG2	1.99	0.45
2:D:142:THR:O	2:D:146:PRO:N	2.50	0.45
1:F:315:ASP:CB	1:F:318:GLN:HG2	2.45	0.45
3:O:282:SER:OG	3:O:285:ARG:HB2	2.16	0.45
2:M:342:ALA:HA	2:N:333:LEU:CD2	2.46	0.45
2:D:200:PRO:HD2	2:D:305:ASP:CG	2.37	0.45
1:F:222:LEU:CD1	1:F:285:MET:SD	3.04	0.45
1:A:25:GLY:N	1:A:114:GLY:O	2.41	0.45
1:A:279:TRP:O	1:A:279:TRP:CD2	2.69	0.45
2:G:344:ASP:O	2:G:347:MET:HB3	2.16	0.45
2:I:13:GLN:HE22	2:I:83:GLU:CG	2.22	0.45
2:H:257:VAL:O	2:H:360:HIS:HE1	2.00	0.45
2:N:343:PRO:HG3	2:N:347:MET:SD	2.56	0.45
3:J:204:LEU:O	3:J:209:ASN:HB2	2.16	0.45
2:C:37:ILE:HD12	2:C:62:LEU:HD21	1.98	0.45
2:D:131:LEU:HB2	2:D:136:PHE:CD1	2.52	0.45
2:B:270:GLU:HG2	2:B:274:ARG:CZ	2.46	0.45
1:K:222:LEU:HD11	1:K:285:MET:CE	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LEU:HD11	1:A:285:MET:CE	2.47	0.45
2:G:11:ARG:HA	2:G:215:ARG:NH1	2.31	0.45
1:K:32:GLN:HE22	2:L:165:THR:HA	1.79	0.45
2:I:201:ARG:N	2:I:305:ASP:HB2	2.28	0.45
2:I:42:LEU:HD12	2:I:172:GLN:OE1	2.16	0.45
3:E:27:LEU:HG	3:E:29:ILE:CD1	2.47	0.45
2:H:102:GLU:HB3	2:H:106:ASP:HB2	1.99	0.45
3:E:257:LYS:HB3	3:E:262:ALA:HB3	1.98	0.45
2:B:219:SER:O	2:B:223:GLN:HG3	2.17	0.45
3:O:14:LEU:HD13	3:O:44:LEU:HD11	1.98	0.45
2:H:37:ILE:HD12	2:H:62:LEU:HD21	1.99	0.45
3:J:257:LYS:HB3	3:J:262:ALA:HB3	1.98	0.45
1:K:315:ASP:CB	1:K:318:GLN:HG2	2.45	0.45
1:F:315:ASP:H	1:F:318:GLN:HE21	1.65	0.45
2:H:252:LEU:CD1	2:H:281:LEU:HD21	2.47	0.45
2:D:140:LEU:HD11	2:D:165:THR:HB	1.99	0.45
1:F:48:GLU:CG	1:F:49:GLU:H	2.30	0.45
2:H:21:GLN:NE2	2:H:176:LYS:O	2.49	0.45
2:N:197:ALA:HB3	2:N:231:GLN:HG2	1.98	0.45
2:L:214:LEU:HD12	2:L:214:LEU:HA	1.85	0.45
1:K:225:LYS:HE3	1:K:227:LYS:HD2	1.99	0.45
3:O:257:LYS:HB3	3:O:262:ALA:HB3	1.97	0.45
2:I:51:LYS:HB2	2:I:51:LYS:HE3	1.76	0.45
1:A:223:MET:HB3	1:A:223:MET:HE3	1.90	0.45
2:C:99:THR:CG2	2:C:99:THR:O	2.51	0.45
2:B:248:GLN:O	2:B:252:LEU:HB2	2.17	0.45
2:L:248:GLN:HA	2:L:251:SER:OG	2.17	0.45
3:O:253:MET:O	3:O:256:LEU:N	2.49	0.45
3:E:27:LEU:CD2	3:E:29:ILE:HD11	2.46	0.45
2:I:94:ASP:O	2:I:100:LYS:CE	2.65	0.45
2:D:94:ASP:O	2:D:100:LYS:CE	2.65	0.45
2:M:5:VAL:HG11	2:N:171:LEU:HB2	1.99	0.45
2:L:223:GLN:OE1	2:M:171:LEU:HD11	2.17	0.45
2:B:360:HIS:CD2	2:B:361:PRO:HD2	2.52	0.45
2:C:21:GLN:HE22	2:C:49:VAL:HG13	1.82	0.45
2:H:21:GLN:HE22	2:H:49:VAL:HG13	1.81	0.45
2:M:149:HIS:H	2:M:149:HIS:CD2	2.34	0.45
2:I:131:LEU:HB2	2:I:136:PHE:CD1	2.52	0.45
2:L:204:GLN:NE2	2:L:305:ASP:CG	2.67	0.45
2:G:270:GLU:HG2	2:G:274:ARG:CZ	2.47	0.45
1:F:25:GLY:N	1:F:114:GLY:O	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:355:ARG:HA	3:O:287:GLN:NE2	2.32	0.45
2:M:252:LEU:CD1	2:M:281:LEU:HD21	2.47	0.45
2:N:302:LEU:HD23	2:N:302:LEU:HA	1.54	0.45
2:I:42:LEU:HB3	2:I:172:GLN:CB	2.42	0.45
2:B:351:MET:HG2	2:C:290:HIS:ND1	2.32	0.45
2:C:147:PRO:HB2	2:C:149:HIS:CD2	2.53	0.45
2:L:186:GLN:HG2	2:L:214:LEU:HD21	1.98	0.45
2:N:131:LEU:HB2	2:N:136:PHE:CD1	2.52	0.45
1:F:225:LYS:HE3	1:F:227:LYS:HD2	1.99	0.44
1:F:334:LYS:C	2:G:297:LEU:CD2	2.81	0.44
2:L:180:VAL:HB	2:L:304:ASN:CB	2.48	0.44
2:D:200:PRO:CB	2:D:305:ASP:N	2.80	0.44
2:N:277:GLU:CB	3:O:149:GLU:CG	2.75	0.44
2:L:270:GLU:HG2	2:L:274:ARG:CZ	2.46	0.44
2:G:11:ARG:HG2	2:G:215:ARG:NH2	2.32	0.44
2:I:140:LEU:HD11	2:I:165:THR:HB	1.99	0.44
1:F:234:GLN:CD	2:G:304:ASN:ND2	2.70	0.44
2:G:248:GLN:O	2:G:252:LEU:HB2	2.17	0.44
2:L:248:GLN:O	2:L:252:LEU:HB2	2.17	0.44
2:L:307:ALA:HA	2:L:310:GLU:CG	2.47	0.44
2:L:104:THR:HG22	2:L:108:LEU:HG	1.99	0.44
3:O:299:GLN:HE21	3:O:311:LEU:HD21	1.82	0.44
3:J:299:GLN:HE21	3:J:311:LEU:HD21	1.82	0.44
2:G:244:LEU:HD23	2:G:247:ASP:OD2	2.18	0.44
3:E:299:GLN:HE21	3:E:311:LEU:HD21	1.82	0.44
2:B:244:LEU:HD23	2:B:247:ASP:OD2	2.17	0.44
2:L:340:PRO:HB3	2:L:345:ARG:HH21	1.83	0.44
2:G:10:TRP:CZ2	2:G:194:GLU:OE2	2.70	0.44
2:D:258:GLU:O	2:D:259:ALA:HB3	2.17	0.44
1:K:222:LEU:CD1	1:K:285:MET:SD	3.04	0.44
2:D:355:ARG:NH1	3:E:287:GLN:CB	2.79	0.44
1:F:32:GLN:HG3	2:G:164:VAL:HG12	1.97	0.44
2:I:62:LEU:O	2:I:119:ARG:HD2	2.18	0.44
2:I:142:THR:O	2:I:146:PRO:N	2.50	0.44
3:E:253:MET:O	3:E:256:LEU:N	2.50	0.44
1:A:190:LEU:HD23	1:A:190:LEU:HA	1.84	0.44
2:I:135:SER:O	2:I:138:ALA:HB3	2.17	0.44
2:G:93:ILE:CG2	2:G:100:LYS:HZ3	2.29	0.44
2:N:338:GLU:OE2	3:O:295:HIS:NE2	2.50	0.44
2:G:248:GLN:HA	2:G:251:SER:OG	2.18	0.44
2:C:257:VAL:O	2:C:360:HIS:HE1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:360:HIS:CD2	2:G:361:PRO:HD2	2.52	0.44
2:L:219:SER:O	2:L:223:GLN:HG3	2.17	0.44
2:G:307:ALA:HA	2:G:310:GLU:CG	2.47	0.44
2:H:245:ASP:HB2	2:H:248:GLN:HG3	1.99	0.44
1:A:57:PRO:HB3	1:A:90:ASN:ND2	2.33	0.44
3:O:95:GLU:O	3:O:99:LYS:HB2	2.15	0.44
2:D:66:THR:HG22	2:D:66:THR:O	2.17	0.44
2:I:257:VAL:O	2:I:257:VAL:HG12	2.17	0.44
3:J:57:LYS:HD2	3:J:57:LYS:HA	1.67	0.44
3:J:27:LEU:HG	3:J:29:ILE:CD1	2.47	0.44
2:L:250:LEU:HD13	2:L:288:LEU:HD13	2.00	0.44
1:K:191:LEU:HA	1:K:191:LEU:HD23	1.80	0.44
1:F:325:GLU:O	1:F:329:LEU:HG	2.18	0.44
1:K:57:PRO:HB3	1:K:90:ASN:ND2	2.33	0.44
2:N:135:SER:O	2:N:138:ALA:HB3	2.17	0.44
1:F:213:THR:N	1:F:216:HIS:HD2	1.96	0.44
2:I:200:PRO:CB	2:I:304:ASN:CB	2.92	0.44
1:A:247:LEU:HD11	1:A:308:THR:HG22	1.98	0.44
3:E:57:LYS:HA	3:E:57:LYS:HD2	1.67	0.44
1:A:29:LEU:CD2	1:A:154:ARG:HH12	2.26	0.44
2:M:5:VAL:HB	2:M:222:ASP:OD2	2.17	0.44
3:E:30:GLN:HA	3:E:145:THR:O	2.17	0.44
2:G:250:LEU:HD13	2:G:288:LEU:HD13	2.00	0.44
2:B:250:LEU:HD13	2:B:288:LEU:HD13	2.00	0.44
2:M:260:ASN:O	2:M:260:ASN:OD1	2.35	0.44
2:D:135:SER:O	2:D:138:ALA:HB3	2.17	0.44
2:N:240:MET:HB3	3:O:157:SER:CA	2.48	0.44
1:K:172:TYR:O	1:K:216:HIS:CE1	2.67	0.44
2:B:248:GLN:HA	2:B:251:SER:OG	2.17	0.44
2:B:307:ALA:HA	2:B:310:GLU:CD	2.38	0.44
1:A:325:GLU:O	1:A:329:LEU:HG	2.18	0.44
3:J:7:LEU:HD22	3:J:40:LEU:HB2	2.00	0.44
2:H:167:LEU:HB3	2:H:172:GLN:NE2	2.33	0.44
1:F:191:LEU:O	1:F:193:PRO:HD3	2.18	0.44
1:F:56:ASP:HB3	1:F:58:ASN:H	1.83	0.44
2:M:9:LYS:NZ	2:M:194:GLU:OE1	2.51	0.44
3:J:33:PRO:O	3:J:197:SER:OG	2.33	0.44
2:G:10:TRP:HZ2	2:G:194:GLU:CD	2.21	0.44
2:D:360:HIS:CB	2:D:363:MET:HE3	2.48	0.44
2:L:244:LEU:HD23	2:L:247:ASP:OD2	2.17	0.44
1:K:310:LEU:HD13	1:K:314:GLN:HE22	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:219:SER:O	2:G:223:GLN:HG3	2.17	0.44
1:K:119:LYS:N	1:K:119:LYS:HD3	2.11	0.44
1:F:100:LEU:O	1:F:103:LEU:HB3	2.18	0.44
2:N:94:ASP:O	2:N:100:LYS:CE	2.65	0.44
2:M:21:GLN:HE22	2:M:49:VAL:HG13	1.82	0.44
2:G:250:LEU:HD22	2:G:309:ILE:CG2	2.48	0.44
2:M:147:PRO:HB2	2:M:149:HIS:CD2	2.52	0.44
2:C:245:ASP:HB2	2:C:248:GLN:HG3	1.99	0.44
3:J:51:GLN:HG2	3:J:62:CYS:SG	2.58	0.44
3:E:51:GLN:HG2	3:E:62:CYS:SG	2.58	0.44
2:D:62:LEU:O	2:D:119:ARG:HD2	2.18	0.44
2:B:340:PRO:HB3	2:B:345:ARG:HH21	1.83	0.44
2:B:278:TRP:CE3	2:B:349:VAL:HG21	2.53	0.44
2:I:66:THR:HG22	2:I:66:THR:O	2.18	0.44
2:N:360:HIS:CB	2:N:363:MET:CB	2.68	0.44
2:M:354:LEU:HD21	2:N:297:LEU:CD2	2.48	0.44
1:A:100:LEU:O	1:A:103:LEU:HB3	2.18	0.44
2:M:347:MET:HG3	2:N:290:HIS:CE1	2.53	0.44
3:O:30:GLN:HA	3:O:145:THR:O	2.17	0.44
2:G:307:ALA:HA	2:G:310:GLU:CD	2.38	0.44
2:B:42:LEU:HD23	2:B:172:GLN:HG2	1.99	0.44
2:G:278:TRP:CE3	2:G:349:VAL:HG21	2.53	0.44
2:C:167:LEU:HB3	2:C:172:GLN:NE2	2.33	0.44
2:D:277:GLU:CG	3:E:149:GLU:CG	2.94	0.44
2:N:257:VAL:O	2:N:360:HIS:CE1	2.60	0.44
1:A:191:LEU:O	1:A:193:PRO:HD3	2.18	0.44
1:A:315:ASP:H	1:A:318:GLN:HE21	1.65	0.44
1:F:222:LEU:HD11	1:F:285:MET:CE	2.47	0.44
2:B:104:THR:HG22	2:B:108:LEU:HG	1.99	0.44
2:H:147:PRO:HB2	2:H:149:HIS:CD2	2.52	0.44
2:M:264:VAL:O	2:M:268:ILE:HG13	2.18	0.44
2:N:258:GLU:O	2:N:259:ALA:HB3	2.17	0.43
2:N:244:LEU:CD1	2:N:276:ILE:HD13	2.48	0.43
2:M:3:TYR:N	2:M:3:TYR:CD2	2.83	0.43
3:J:30:GLN:HA	3:J:145:THR:O	2.17	0.43
2:B:243:THR:CG2	2:B:244:LEU:N	2.81	0.43
2:M:245:ASP:HB2	2:M:248:GLN:HG3	1.99	0.43
3:O:51:GLN:HG2	3:O:62:CYS:SG	2.58	0.43
1:F:57:PRO:HB3	1:F:90:ASN:ND2	2.33	0.43
2:N:66:THR:O	2:N:66:THR:HG22	2.18	0.43
2:N:356:ALA:C	2:N:363:MET:HE1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:201:ARG:HH21	2:M:308:ALA:CB	2.30	0.43
2:N:140:LEU:HD11	2:N:165:THR:HB	1.99	0.43
2:I:93:ILE:CG2	2:I:100:LYS:HZ2	2.31	0.43
2:L:250:LEU:HD22	2:L:309:ILE:CG2	2.48	0.43
2:L:42:LEU:HD23	2:L:172:GLN:HG2	1.99	0.43
1:A:183:GLN:OE1	2:B:172:GLN:HG3	2.17	0.43
2:H:264:VAL:O	2:H:268:ILE:HG13	2.18	0.43
1:A:3:ARG:HG2	1:A:136:GLN:NE2	2.33	0.43
3:J:18:TYR:HB3	3:J:48:LEU:HD21	2.01	0.43
2:G:10:TRP:CB	2:G:218:LEU:HD13	2.48	0.43
2:N:257:VAL:HG12	2:N:257:VAL:O	2.17	0.43
2:L:6:LEU:HD22	2:L:190:ILE:HG23	2.00	0.43
2:M:10:TRP:CH2	2:M:190:ILE:HA	2.53	0.43
2:H:100:LYS:CB	2:I:133:ARG:NE	2.78	0.43
2:M:86:ARG:CZ	2:N:141:LYS:CB	2.83	0.43
2:L:360:HIS:CD2	2:L:361:PRO:HD2	2.52	0.43
2:B:307:ALA:HA	2:B:310:GLU:CG	2.47	0.43
2:L:307:ALA:HA	2:L:310:GLU:CD	2.38	0.43
1:K:221:LEU:HA	1:K:221:LEU:HD23	1.47	0.43
2:C:345:ARG:O	2:C:349:VAL:HG23	2.19	0.43
2:M:102:GLU:HB3	2:M:106:ASP:HB2	1.99	0.43
1:F:191:LEU:HD23	1:F:191:LEU:HA	1.80	0.43
2:G:340:PRO:HB3	2:G:345:ARG:HH21	1.83	0.43
3:J:92:ALA:O	3:J:96:VAL:HG23	2.19	0.43
2:N:62:LEU:O	2:N:119:ARG:HD2	2.18	0.43
1:F:84:LEU:HA	1:F:84:LEU:HD12	1.84	0.43
2:D:257:VAL:O	2:D:257:VAL:HG12	2.17	0.43
3:J:117:ALA:HB2	3:J:143:LEU:CD1	2.47	0.43
3:O:73:HIS:HA	3:O:74:PRO:HD3	1.77	0.43
2:I:5:VAL:HG12	2:I:222:ASP:OD2	2.17	0.43
2:C:6:LEU:HG	2:C:222:ASP:OD1	2.18	0.43
3:E:7:LEU:HD22	3:E:40:LEU:HB2	2.00	0.43
3:E:92:ALA:O	3:E:96:VAL:HG23	2.19	0.43
2:I:360:HIS:CB	2:I:363:MET:HE3	2.47	0.43
2:M:355:ARG:CG	2:N:326:GLN:HG3	2.49	0.43
2:M:93:ILE:HG23	2:M:100:LYS:HZ2	1.77	0.43
1:K:100:LEU:O	1:K:103:LEU:HB3	2.18	0.43
2:D:347:MET:O	2:D:351:MET:CG	2.65	0.43
1:A:48:GLU:CG	1:A:49:GLU:H	2.30	0.43
2:B:250:LEU:HD22	2:B:309:ILE:CG2	2.48	0.43
1:A:50:HIS:O	1:A:51:HIS:CD2	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:104:THR:HG22	2:G:108:LEU:HG	1.99	0.43
1:K:183:GLN:OE1	2:L:172:GLN:HG3	2.18	0.43
2:L:42:LEU:HD11	2:L:156:THR:HG22	2.01	0.43
2:B:140:LEU:HA	2:B:140:LEU:HD23	1.84	0.43
1:F:270:ARG:NH2	2:N:319:THR:H	2.16	0.43
2:M:276:ILE:HG13	2:M:276:ILE:H	1.66	0.43
2:C:84:GLN:HG2	2:D:144:GLU:OE1	2.17	0.43
1:K:48:GLU:CG	1:K:49:GLU:H	2.30	0.43
3:J:30:GLN:HG3	3:J:30:GLN:O	2.18	0.43
1:F:50:HIS:O	1:F:51:HIS:CD2	2.72	0.43
2:C:102:GLU:HB3	2:C:106:ASP:HB2	1.99	0.43
2:B:21:GLN:HE22	2:B:49:VAL:CG1	2.32	0.43
2:L:278:TRP:CE3	2:L:349:VAL:HG21	2.53	0.43
1:A:225:LYS:HE3	1:A:227:LYS:HD2	1.99	0.43
3:J:149:GLU:C	3:J:151:LEU:N	2.71	0.43
1:K:315:ASP:H	1:K:318:GLN:HE21	1.65	0.43
2:N:338:GLU:HA	2:N:341:TYR:HD1	1.81	0.43
2:B:365:LEU:HD22	2:C:297:LEU:HD13	1.96	0.43
2:I:229:ASP:C	2:I:231:GLN:N	2.71	0.43
1:K:191:LEU:O	1:K:193:PRO:HD3	2.18	0.43
2:G:42:LEU:HD11	2:G:156:THR:HG22	2.00	0.43
3:O:7:LEU:HD22	3:O:40:LEU:HB2	2.00	0.43
2:C:264:VAL:O	2:C:268:ILE:HG13	2.18	0.43
1:F:3:ARG:HG2	1:F:136:GLN:NE2	2.33	0.43
2:I:338:GLU:OE2	3:J:295:HIS:NE2	2.52	0.43
2:D:337:LYS:O	2:D:340:PRO:HD2	2.19	0.43
2:H:42:LEU:HD12	2:H:154:LEU:HB2	2.00	0.43
1:A:29:LEU:O	1:A:33:GLU:HG3	2.19	0.43
2:M:333:LEU:O	2:M:336:ARG:N	2.49	0.43
3:E:18:TYR:HB3	3:E:48:LEU:HD21	2.00	0.43
3:O:92:ALA:O	3:O:96:VAL:HG23	2.19	0.43
2:D:143:LEU:HD23	2:D:143:LEU:HA	1.89	0.43
1:A:315:ASP:CB	1:A:318:GLN:HG2	2.45	0.43
2:L:204:GLN:HE21	2:L:305:ASP:CA	2.26	0.43
1:K:325:GLU:O	1:K:329:LEU:HG	2.18	0.43
3:O:117:ALA:HB2	3:O:143:LEU:CD1	2.47	0.43
1:K:50:HIS:O	1:K:51:HIS:CD2	2.72	0.43
1:F:270:ARG:HH12	2:N:316:LEU:CB	2.31	0.43
2:L:10:TRP:CZ2	2:L:193:GLU:CG	3.02	0.43
2:I:76:CYS:SG	2:I:78:ASN:HB2	2.59	0.43
1:K:29:LEU:HD21	1:K:154:ARG:NH1	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:42:LEU:HD12	2:M:154:LEU:HB2	2.00	0.43
2:M:362:ARG:C	2:M:363:MET:HG3	2.39	0.43
2:H:345:ARG:O	2:H:349:VAL:HG23	2.19	0.43
2:M:345:ARG:O	2:M:349:VAL:HG23	2.19	0.43
3:J:149:GLU:O	3:J:151:LEU:N	2.52	0.42
3:E:149:GLU:O	3:E:151:LEU:N	2.52	0.42
2:I:337:LYS:O	2:I:340:PRO:HD2	2.19	0.42
2:N:76:CYS:SG	2:N:78:ASN:HB2	2.59	0.42
2:M:100:LYS:HB3	2:N:133:ARG:HD2	2.01	0.42
2:N:347:MET:O	2:N:351:MET:CG	2.65	0.42
1:F:228:ARG:HG2	1:F:228:ARG:H	1.52	0.42
2:I:244:LEU:HD11	2:I:276:ILE:HG21	2.02	0.42
2:D:277:GLU:CG	3:E:149:GLU:HG3	2.49	0.42
2:C:42:LEU:HD12	2:C:154:LEU:HB2	2.00	0.42
2:C:156:THR:HG22	2:C:157:THR:N	2.34	0.42
2:G:243:THR:CG2	2:G:244:LEU:N	2.81	0.42
1:A:56:ASP:HB3	1:A:58:ASN:H	1.83	0.42
2:B:7:ALA:HA	2:B:218:LEU:HD13	2.01	0.42
2:L:4:GLN:OE1	2:L:9:LYS:CD	2.64	0.42
2:G:20:GLY:CA	2:G:182:GLN:NE2	2.83	0.42
2:G:362:ARG:HE	2:G:363:MET:CE	2.24	0.42
1:K:29:LEU:O	1:K:33:GLU:HG3	2.19	0.42
3:O:30:GLN:O	3:O:30:GLN:HG3	2.18	0.42
3:J:245:LEU:HB2	3:J:297:ARG:HG3	2.01	0.42
2:M:147:PRO:HB2	2:M:149:HIS:NE2	2.35	0.42
1:K:3:ARG:HG2	1:K:136:GLN:NE2	2.33	0.42
1:K:56:ASP:HB3	1:K:58:ASN:H	1.83	0.42
2:C:136:PHE:CZ	2:C:166:ILE:HD12	2.54	0.42
2:L:238:SER:HB3	2:L:244:LEU:N	2.02	0.42
2:N:277:GLU:OE1	3:O:149:GLU:HG3	2.19	0.42
2:D:76:CYS:SG	2:D:78:ASN:HB2	2.59	0.42
2:D:229:ASP:C	2:D:231:GLN:N	2.71	0.42
2:I:131:LEU:HB2	2:I:136:PHE:HD1	1.85	0.42
2:M:78:ASN:O	2:M:82:ILE:HG13	2.20	0.42
3:O:170:GLN:HG2	3:O:170:GLN:H	1.65	0.42
2:N:289:LEU:HD23	2:N:289:LEU:HA	1.81	0.42
2:N:271:ALA:O	2:N:276:ILE:HG13	2.20	0.42
1:F:310:LEU:HA	1:F:310:LEU:HD23	1.61	0.42
1:K:25:GLY:N	1:K:114:GLY:O	2.41	0.42
2:G:6:LEU:HD12	2:G:222:ASP:N	2.34	0.42
2:H:84:GLN:HB3	2:I:144:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:117:ALA:HB2	3:E:143:LEU:CD1	2.47	0.42
1:K:262:ARG:HH12	3:O:228:ASP:CG	2.23	0.42
2:D:95:ALA:HA	2:D:100:LYS:HZ1	1.85	0.42
2:I:347:MET:O	2:I:351:MET:CG	2.65	0.42
2:C:18:VAL:HG12	2:C:19:VAL:N	2.35	0.42
2:N:357:LEU:CA	2:N:363:MET:HE1	2.46	0.42
2:D:257:VAL:O	2:D:360:HIS:CE1	2.61	0.42
1:F:334:LYS:CA	2:G:297:LEU:HD21	2.47	0.42
2:N:337:LYS:O	2:N:340:PRO:HD2	2.19	0.42
2:N:220:LEU:HD21	3:O:154:THR:CB	2.48	0.42
2:G:342:ALA:HB1	2:G:343:PRO:HD2	2.01	0.42
2:M:360:HIS:CD2	2:M:363:MET:H	2.37	0.42
2:H:360:HIS:CD2	2:H:363:MET:H	2.37	0.42
2:L:21:GLN:HE22	2:L:49:VAL:CG1	2.32	0.42
2:M:167:LEU:HB3	2:M:172:GLN:NE2	2.33	0.42
2:H:136:PHE:CZ	2:H:166:ILE:HD12	2.54	0.42
1:K:79:THR:HG22	1:K:80:LEU:N	2.34	0.42
1:K:246:LEU:HA	1:K:246:LEU:HD23	1.87	0.42
2:I:244:LEU:CD1	2:I:276:ILE:HD13	2.48	0.42
1:A:28:PRO:CB	2:B:164:VAL:HG21	2.25	0.42
2:C:342:ALA:HA	2:D:333:LEU:HD21	2.01	0.42
2:B:362:ARG:HE	2:B:363:MET:CE	2.24	0.42
2:G:276:ILE:CG2	2:G:277:GLU:N	2.82	0.42
3:E:30:GLN:HG3	3:E:30:GLN:O	2.18	0.42
2:M:18:VAL:HG12	2:M:19:VAL:N	2.35	0.42
2:H:137:ASN:HA	2:H:140:LEU:HD12	2.02	0.42
3:O:225:PRO:HB3	3:O:276:GLU:OE2	2.20	0.42
1:K:190:LEU:HD23	1:K:190:LEU:HA	1.84	0.42
2:I:358:ALA:C	2:I:360:HIS:H	2.23	0.42
1:K:333:HIS:HB2	2:L:297:LEU:CD2	2.32	0.42
1:K:311:THR:O	1:K:318:GLN:NE2	2.53	0.42
1:F:243:PRO:HG2	1:F:244:VAL:H	1.85	0.42
2:B:4:GLN:OE1	2:B:9:LYS:CD	2.64	0.42
2:C:362:ARG:C	2:C:363:MET:HG3	2.40	0.42
2:H:362:ARG:C	2:H:363:MET:HG3	2.39	0.42
2:I:351:MET:SD	3:J:290:LEU:HD13	2.59	0.42
1:F:255:LEU:HD12	3:J:309:GLU:OE1	2.20	0.42
3:J:311:LEU:HA	3:J:311:LEU:HD12	1.86	0.42
3:E:35:MET:CE	3:E:166:PRO:HA	2.50	0.42
2:B:42:LEU:HD11	2:B:156:THR:HG22	2.00	0.42
3:O:18:TYR:HB3	3:O:48:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:225:PRO:HB3	3:E:276:GLU:OE2	2.20	0.42
2:D:358:ALA:C	2:D:360:HIS:H	2.23	0.42
1:F:29:LEU:O	1:F:33:GLU:HG3	2.19	0.42
3:O:149:GLU:C	3:O:151:LEU:N	2.71	0.42
3:O:149:GLU:O	3:O:151:LEU:N	2.53	0.42
3:O:5:PRO:HD3	3:O:175:TRP:CZ3	2.54	0.42
2:C:215:ARG:CZ	2:D:164:VAL:HG21	2.45	0.42
2:C:277:GLU:OE2	2:D:176:LYS:HD2	2.19	0.42
1:K:243:PRO:HG2	1:K:244:VAL:H	1.85	0.42
2:B:342:ALA:HB1	2:B:343:PRO:HD2	2.01	0.42
2:L:37:ILE:HG12	2:L:62:LEU:HD21	2.02	0.42
2:G:10:TRP:CE3	2:G:190:ILE:CG1	3.01	0.42
2:D:244:LEU:CD1	2:D:276:ILE:HD13	2.48	0.42
2:I:356:ALA:O	2:I:363:MET:HE3	2.17	0.42
1:F:142:PRO:CD	1:F:178:LEU:HD11	2.50	0.42
2:G:21:GLN:HE22	2:G:49:VAL:CG1	2.32	0.42
1:F:334:LYS:CB	2:G:297:LEU:CD2	2.71	0.42
2:H:6:LEU:HB2	2:H:222:ASP:OD1	2.19	0.42
2:D:42:LEU:HD23	2:D:154:LEU:HB2	2.02	0.42
2:C:360:HIS:CD2	2:C:363:MET:H	2.37	0.42
1:F:264:SER:O	1:F:265:ALA:CB	2.68	0.42
2:M:136:PHE:CZ	2:M:166:ILE:HD12	2.54	0.42
2:L:281:LEU:O	2:L:285:MET:HG3	2.20	0.42
2:G:37:ILE:HG12	2:G:62:LEU:HD21	2.02	0.42
1:F:4:LEU:CD1	1:F:137:VAL:HG22	2.50	0.42
2:B:281:LEU:O	2:B:285:MET:HG3	2.20	0.42
2:D:360:HIS:CG	2:D:363:MET:HE3	2.54	0.41
2:N:338:GLU:OE2	3:O:295:HIS:CE1	2.73	0.41
2:C:137:ASN:HA	2:C:140:LEU:HD12	2.02	0.41
1:K:310:LEU:HB3	1:K:314:GLN:NE2	2.35	0.41
2:N:42:LEU:HD23	2:N:154:LEU:HB2	2.02	0.41
2:G:104:THR:HG22	2:G:108:LEU:CD1	2.50	0.41
1:K:264:SER:O	1:K:265:ALA:CB	2.68	0.41
2:M:239:ALA:HB1	2:N:23:HIS:CE1	2.55	0.41
2:D:244:LEU:HD11	2:D:276:ILE:HG21	2.01	0.41
2:L:342:ALA:HB1	2:L:343:PRO:HD2	2.01	0.41
2:L:343:PRO:HD3	2:M:286:LEU:HB3	2.01	0.41
2:C:3:TYR:N	2:C:3:TYR:CD2	2.86	0.41
2:L:276:ILE:CG2	2:L:277:GLU:N	2.82	0.41
2:B:276:ILE:CG2	2:B:277:GLU:N	2.82	0.41
2:M:156:THR:HG22	2:M:157:THR:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:220:LEU:HD21	3:J:154:THR:CA	2.47	0.41
2:H:18:VAL:HG12	2:H:19:VAL:N	2.35	0.41
2:C:147:PRO:HB2	2:C:149:HIS:NE2	2.35	0.41
3:O:245:LEU:HB2	3:O:297:ARG:HG3	2.01	0.41
2:B:37:ILE:HG12	2:B:62:LEU:HD21	2.02	0.41
1:F:79:THR:HG22	1:F:80:LEU:N	2.34	0.41
1:A:79:THR:HG22	1:A:80:LEU:N	2.34	0.41
2:N:320:ILE:HA	2:N:321:PRO:HD3	1.90	0.41
2:N:358:ALA:C	2:N:360:HIS:H	2.23	0.41
1:A:310:LEU:HB3	1:A:314:GLN:NE2	2.35	0.41
2:I:302:LEU:HA	2:I:302:LEU:HD23	1.54	0.41
2:H:156:THR:HG22	2:H:157:THR:N	2.34	0.41
2:N:229:ASP:C	2:N:231:GLN:N	2.71	0.41
2:L:104:THR:HG22	2:L:108:LEU:CD1	2.50	0.41
3:J:197:SER:HA	3:J:198:PRO:HD3	1.87	0.41
2:H:78:ASN:O	2:H:82:ILE:HG13	2.20	0.41
1:A:142:PRO:CD	1:A:178:LEU:HD11	2.50	0.41
2:C:78:ASN:O	2:C:82:ILE:HG13	2.20	0.41
1:K:4:LEU:CD1	1:K:137:VAL:HG22	2.50	0.41
3:O:26:ALA:HB2	3:O:132:LEU:HD22	2.02	0.41
3:J:171:TYR:CD2	3:J:171:TYR:N	2.88	0.41
3:E:149:GLU:C	3:E:151:LEU:N	2.71	0.41
2:L:10:TRP:HZ2	2:L:193:GLU:CB	2.28	0.41
3:O:34:GLY:O	3:O:199:GLY:N	2.51	0.41
2:H:56:ARG:HH22	2:I:165:THR:HG21	1.84	0.41
2:C:341:TYR:HB3	2:D:333:LEU:HD13	2.01	0.41
1:A:243:PRO:HG2	1:A:244:VAL:H	1.85	0.41
1:F:262:ARG:HD2	3:J:230:TYR:CD2	2.55	0.41
2:C:3:TYR:O	2:C:3:TYR:HD2	2.00	0.41
1:F:64:ILE:HG12	1:F:96:GLN:HB3	2.02	0.41
3:E:329:LEU:HD23	3:E:329:LEU:N	2.34	0.41
2:G:256:MET:HE1	2:G:332:LEU:HD21	2.02	0.41
2:N:246:ASP:CB	2:N:248:GLN:HG2	2.50	0.41
3:E:245:LEU:HB2	3:E:297:ARG:HG3	2.01	0.41
3:E:171:TYR:N	3:E:171:TYR:CD2	2.88	0.41
3:O:171:TYR:CD2	3:O:171:TYR:N	2.88	0.41
2:D:320:ILE:HA	2:D:321:PRO:HD3	1.90	0.41
2:M:342:ALA:N	2:N:333:LEU:HD21	2.35	0.41
2:G:82:ILE:HG23	2:G:90:LEU:HD23	2.03	0.41
3:J:225:PRO:HB3	3:J:276:GLU:OE2	2.20	0.41
2:I:271:ALA:O	2:I:276:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:311:THR:O	1:F:318:GLN:NE2	2.53	0.41
1:A:311:THR:O	1:A:318:GLN:NE2	2.53	0.41
1:F:310:LEU:HB3	1:F:314:GLN:NE2	2.35	0.41
1:K:270:ARG:HG2	1:K:283:ARG:NH2	2.36	0.41
2:M:210:ALA:HB1	2:M:213:SER:OG	2.20	0.41
2:L:82:ILE:HG23	2:L:90:LEU:HD23	2.03	0.41
2:H:147:PRO:HB2	2:H:149:HIS:NE2	2.35	0.41
2:M:137:ASN:HA	2:M:140:LEU:HD12	2.02	0.41
3:E:121:THR:O	3:E:124:ALA:HB3	2.21	0.41
1:A:159:ASN:OD1	2:M:319:THR:HG21	2.20	0.41
1:A:81:LEU:HA	1:A:111:ILE:O	2.21	0.41
2:I:28:LEU:HD23	2:I:28:LEU:HA	1.90	0.41
2:D:271:ALA:O	2:D:276:ILE:HG13	2.20	0.41
1:F:29:LEU:HB2	1:F:179:LEU:CB	2.43	0.41
2:D:5:VAL:HG12	2:D:222:ASP:OD2	2.21	0.41
2:M:347:MET:CG	2:N:290:HIS:CE1	3.03	0.41
3:J:32:LEU:CD1	3:J:195:ALA:O	2.67	0.41
2:H:333:LEU:O	2:H:336:ARG:N	2.49	0.41
1:F:193:PRO:HA	2:G:36:ARG:HH22	1.86	0.41
2:I:69:THR:HG22	2:I:71:THR:H	1.86	0.41
1:K:81:LEU:HA	1:K:111:ILE:O	2.21	0.41
1:A:4:LEU:CD1	1:A:137:VAL:HG22	2.50	0.41
3:O:32:LEU:HD13	3:O:197:SER:HB2	2.03	0.41
2:L:43:PHE:O	2:L:155:ALA:HA	2.21	0.41
2:D:277:GLU:CB	3:E:149:GLU:HB3	2.45	0.41
1:F:270:ARG:HG2	1:F:283:ARG:NH2	2.36	0.41
2:N:119:ARG:HG3	2:N:119:ARG:H	1.65	0.41
3:O:244:ARG:O	3:O:247:TRP:HB2	2.21	0.41
3:E:252:LEU:HA	3:E:252:LEU:HD12	1.83	0.41
2:G:22:GLU:HG3	2:G:22:GLU:H	1.09	0.41
2:I:244:LEU:CD2	2:I:276:ILE:HG12	2.44	0.41
2:L:10:TRP:CD2	2:L:190:ILE:HG12	2.55	0.41
1:K:333:HIS:CB	2:L:297:LEU:CD2	2.61	0.41
1:K:333:HIS:CE1	2:L:297:LEU:HG	2.56	0.41
2:D:200:PRO:HB2	2:D:305:ASP:CA	2.51	0.41
2:B:98:ARG:HD3	2:C:141:LYS:HE2	2.03	0.41
1:A:281:ASN:OD1	1:A:281:ASN:O	2.39	0.41
2:I:140:LEU:HD21	2:I:166:ILE:CG1	2.51	0.41
2:D:42:LEU:HB3	2:D:172:GLN:CB	2.43	0.41
1:A:64:ILE:HG12	1:A:96:GLN:HB3	2.02	0.41
2:N:343:PRO:CG	2:N:347:MET:SD	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:73:HIS:CE1	3:E:106:LEU:HD22	2.56	0.41
2:H:21:GLN:HE22	2:H:49:VAL:CG1	2.34	0.41
3:O:239:GLU:HA	3:O:308:ARG:CZ	2.51	0.41
1:F:39:ARG:CZ	1:F:50:HIS:HB3	2.51	0.41
1:A:264:SER:O	1:A:265:ALA:CB	2.68	0.41
2:B:104:THR:HG22	2:B:108:LEU:CD1	2.50	0.41
2:C:210:ALA:HB1	2:C:213:SER:OG	2.20	0.41
2:D:131:LEU:HB2	2:D:136:PHE:HD1	1.85	0.41
2:N:105:ARG:HD2	2:N:134:HIS:NE2	2.36	0.41
2:D:69:THR:HG22	2:D:71:THR:H	1.86	0.41
3:J:26:ALA:HB2	3:J:132:LEU:HD22	2.03	0.41
2:N:51:LYS:HE3	2:N:51:LYS:HB2	1.76	0.41
1:K:142:PRO:CD	1:K:178:LEU:HD11	2.50	0.41
2:D:104:THR:HG22	2:D:108:LEU:CD1	2.51	0.41
2:H:367:GLU:HG3	2:I:322:PRO:HD2	2.02	0.41
1:A:105:HIS:HB2	1:F:225:LYS:HE3	0.88	0.41
2:N:240:MET:HB3	3:O:157:SER:CB	2.51	0.41
2:I:250:LEU:CD2	2:I:309:ILE:HG23	2.51	0.41
2:I:302:LEU:HD13	2:I:310:GLU:HA	2.03	0.41
2:H:283:VAL:HA	2:H:286:LEU:HD12	2.03	0.41
3:J:27:LEU:HG	3:J:29:ILE:HD11	2.03	0.41
3:J:163:TYR:HH	3:J:166:PRO:HD2	1.86	0.41
3:J:329:LEU:N	3:J:329:LEU:HD23	2.33	0.41
2:M:21:GLN:HE22	2:M:49:VAL:CG1	2.34	0.41
2:N:131:LEU:HB2	2:N:136:PHE:HD1	1.85	0.41
2:G:281:LEU:O	2:G:285:MET:HG3	2.20	0.41
3:E:190:ALA:HB2	3:E:210:TRP:CZ3	2.56	0.41
2:D:244:LEU:HD21	2:D:276:ILE:HG23	2.03	0.40
2:B:6:LEU:CD2	2:B:190:ILE:CG2	2.94	0.40
1:F:29:LEU:HD13	1:F:179:LEU:CA	2.37	0.40
1:K:310:LEU:HA	1:K:310:LEU:HD23	1.61	0.40
3:O:6:TRP:HH2	3:O:175:TRP:CZ2	2.39	0.40
2:N:302:LEU:HD13	2:N:310:GLU:HA	2.03	0.40
2:N:250:LEU:CD2	2:N:309:ILE:HG23	2.51	0.40
2:B:4:GLN:CD	2:B:9:LYS:HD2	2.42	0.40
1:K:64:ILE:HG12	1:K:96:GLN:HB3	2.02	0.40
2:I:220:LEU:CD2	3:J:154:THR:HA	2.47	0.40
2:I:343:PRO:CG	2:I:347:MET:SD	3.09	0.40
3:J:73:HIS:CE1	3:J:106:LEU:HD22	2.56	0.40
3:E:73:HIS:HE1	3:E:106:LEU:HD22	1.86	0.40
3:E:311:LEU:HA	3:E:311:LEU:HD12	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:25:HIS:O	3:O:141:PHE:HB2	2.22	0.40
2:N:345:ARG:HE	3:O:150:ARG:NH2	2.08	0.40
2:N:244:LEU:HD11	2:N:276:ILE:HG21	2.01	0.40
2:D:250:LEU:CD2	2:D:309:ILE:HG23	2.52	0.40
2:M:100:LYS:HA	2:N:133:ARG:HG3	2.02	0.40
2:G:363:MET:HE3	2:G:363:MET:HB2	1.86	0.40
2:D:343:PRO:CG	2:D:347:MET:SD	3.09	0.40
3:J:73:HIS:HE1	3:J:106:LEU:HD22	1.86	0.40
2:D:246:ASP:CB	2:D:248:GLN:HG2	2.50	0.40
2:H:210:ALA:HB1	2:H:213:SER:OG	2.20	0.40
3:J:121:THR:O	3:J:124:ALA:HB3	2.21	0.40
1:F:81:LEU:HA	1:F:111:ILE:O	2.21	0.40
1:K:84:LEU:HD12	1:K:84:LEU:HA	1.84	0.40
2:N:345:ARG:NE	3:O:150:ARG:NH2	2.50	0.40
2:M:215:ARG:CD	2:N:164:VAL:HG11	2.51	0.40
1:A:75:ALA:CB	1:F:207:ASN:CB	2.97	0.40
3:O:34:GLY:C	3:O:199:GLY:HA3	2.30	0.40
2:D:201:ARG:H	2:D:305:ASP:HB2	1.87	0.40
1:A:270:ARG:HG2	1:A:283:ARG:NH2	2.36	0.40
2:M:250:LEU:HD23	2:M:312:ARG:CZ	2.51	0.40
2:L:248:GLN:HA	2:L:251:SER:HG	1.86	0.40
2:I:42:LEU:HD23	2:I:154:LEU:HB2	2.02	0.40
2:M:253:VAL:O	2:M:257:VAL:HG23	2.22	0.40
2:M:257:VAL:O	2:M:257:VAL:HG12	2.21	0.40
3:O:73:HIS:CE1	3:O:106:LEU:HD22	2.56	0.40
3:J:239:GLU:HA	3:J:308:ARG:CZ	2.51	0.40
3:E:239:GLU:HA	3:E:308:ARG:CZ	2.51	0.40
1:K:39:ARG:CZ	1:K:50:HIS:HB3	2.51	0.40
3:E:163:TYR:OH	3:E:166:PRO:HD2	2.22	0.40
2:B:82:ILE:HG23	2:B:90:LEU:HD23	2.03	0.40
2:L:32:LEU:HD23	2:L:32:LEU:HA	1.94	0.40
2:I:105:ARG:HD2	2:I:134:HIS:NE2	2.36	0.40
3:O:321:HIS:O	3:O:327:VAL:HG21	2.21	0.40
2:H:51:LYS:HE3	2:H:51:LYS:HB2	1.77	0.40
2:N:321:PRO:HA	2:N:322:PRO:HD2	1.92	0.40
2:M:283:VAL:HA	2:M:286:LEU:HD12	2.03	0.40
2:G:214:LEU:HD12	2:G:214:LEU:HA	1.85	0.40
2:N:244:LEU:CD2	2:N:276:ILE:HG12	2.44	0.40
2:B:363:MET:HB2	2:B:363:MET:HE3	1.85	0.40
3:E:117:ALA:CB	3:E:143:LEU:HD12	2.50	0.40
2:H:257:VAL:O	2:H:257:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:40:GLN:HE21	1:F:40:GLN:HB3	1.69	0.40
2:D:365:LEU:HB3	2:D:366:PRO:HD2	2.03	0.40
1:A:275:LYS:HA	1:A:275:LYS:HD3	1.91	0.40
3:O:121:THR:O	3:O:124:ALA:HB3	2.21	0.40
3:E:321:HIS:O	3:E:327:VAL:HG21	2.21	0.40
2:D:289:LEU:HD23	2:D:289:LEU:HA	1.81	0.40
1:F:190:LEU:HA	1:F:190:LEU:HD23	1.85	0.40
2:L:6:LEU:HD23	2:L:6:LEU:HA	1.89	0.40
2:G:19:VAL:CG2	2:G:186:GLN:CB	2.99	0.40
1:A:105:HIS:HA	1:F:227:LYS:HD2	1.94	0.40
1:K:281:ASN:O	1:K:281:ASN:OD1	2.40	0.40
2:I:200:PRO:HB3	2:I:304:ASN:HB3	2.00	0.40
2:H:250:LEU:HD23	2:H:312:ARG:CZ	2.51	0.40
2:C:250:LEU:HD23	2:C:312:ARG:CZ	2.51	0.40
2:N:297:LEU:HA	2:N:297:LEU:HD12	1.90	0.40
2:B:304:ASN:OD1	2:B:304:ASN:C	2.60	0.40
2:M:126:ASP:OD1	2:M:127:GLU:HG3	2.22	0.40
2:G:236:ALA:O	2:G:239:ALA:HB3	2.22	0.40
2:D:286:LEU:HD21	2:D:332:LEU:HB2	2.03	0.40
2:B:22:GLU:H	2:B:22:GLU:HG3	1.09	0.40

All (87) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:63:ARG:NH1	2:H:361:PRO:CA[1_455]	0.61	1.59
2:C:193:GLU:O	1:F:75:ALA:CA[2_546]	0.77	1.43
3:J:19:GLN:OE1	2:L:299:PRO:CB[2_756]	0.81	1.39
2:C:195:HIS:CD2	1:F:74:PHE:O[2_546]	0.91	1.29
2:C:193:GLU:O	1:F:75:ALA:CB[2_546]	0.94	1.26
2:B:193:GLU:OE2	3:J:69:GLN:NE2[2_646]	1.02	1.18
1:A:277:ARG:NH2	2:D:66:THR:C[1_655]	1.08	1.12
2:C:193:GLU:C	1:F:75:ALA:O[2_546]	1.23	0.97
2:C:193:GLU:C	1:F:75:ALA:C[2_546]	1.24	0.96
2:B:3:TYR:CE2	3:J:54:GLN:CG[2_646]	1.33	0.87
2:C:192:ASN:ND2	1:F:77:ARG:NE[2_546]	1.33	0.87
2:B:4:GLN:NE2	3:J:59:CYS:O[2_646]	1.33	0.87
2:C:188:GLU:OE2	1:F:77:ARG:NH2[2_546]	1.37	0.83
1:K:277:ARG:NH2	2:N:66:THR:CG2[1_655]	1.40	0.80
3:E:51:GLN:OE1	2:H:362:ARG:NH1[1_455]	1.41	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:63:ARG:NH1	2:H:361:PRO:CB[1_455]	1.42	0.78
3:J:19:GLN:CD	2:L:299:PRO:CB[2_756]	1.42	0.78
1:A:277:ARG:NH2	2:D:66:THR:CA[1_655]	1.44	0.76
2:C:194:GLU:N	1:F:75:ALA:O[2_546]	1.44	0.76
1:K:277:ARG:CZ	2:N:66:THR:CG2[1_655]	1.48	0.72
3:E:63:ARG:CZ	2:H:361:PRO:CA[1_455]	1.48	0.72
2:C:192:ASN:OD1	1:F:107:ASP:OD2[2_546]	1.49	0.71
1:K:277:ARG:NH1	2:N:66:THR:CG2[1_655]	1.51	0.69
2:C:195:HIS:NE2	1:F:74:PHE:O[2_546]	1.52	0.68
2:C:193:GLU:CA	1:F:75:ALA:C[2_546]	1.53	0.67
2:C:193:GLU:CA	1:F:75:ALA:O[2_546]	1.55	0.65
2:B:3:TYR:CE2	3:J:54:GLN:CD[2_646]	1.56	0.64
2:C:193:GLU:O	1:F:75:ALA:C[2_546]	1.58	0.62
2:C:192:ASN:OD1	1:F:107:ASP:CG[2_546]	1.59	0.61
3:J:19:GLN:CD	2:L:299:PRO:CG[2_756]	1.60	0.60
3:J:19:GLN:CG	2:L:299:PRO:CG[2_756]	1.62	0.58
2:C:193:GLU:C	1:F:75:ALA:CA[2_546]	1.69	0.51
2:B:193:GLU:CD	3:J:69:GLN:NE2[2_646]	1.70	0.50
3:E:63:ARG:NH1	2:H:361:PRO:C[1_455]	1.72	0.48
2:C:193:GLU:CG	1:F:76:SER:OG[2_546]	1.74	0.46
1:A:277:ARG:NH2	2:D:67:GLY:N[1_655]	1.75	0.45
3:E:63:ARG:CD	2:H:361:PRO:O[1_455]	1.75	0.45
2:C:193:GLU:CA	1:F:76:SER:N[2_546]	1.77	0.43
2:G:76:CYS:N	2:I:270:GLU:OE2[1_455]	1.78	0.42
2:G:75:VAL:C	2:I:270:GLU:OE2[1_455]	1.80	0.40
2:C:192:ASN:O	1:F:76:SER:CA[2_546]	1.80	0.40
2:C:192:ASN:OD1	1:F:107:ASP:OD1[2_546]	1.81	0.39
2:C:188:GLU:CD	1:F:77:ARG:NH2[2_546]	1.81	0.39
2:C:193:GLU:CG	1:F:76:SER:CB[2_546]	1.83	0.37
3:E:52:GLN:NE2	2:H:363:MET:CE[1_455]	1.84	0.36
2:C:193:GLU:N	1:F:75:ALA:O[2_546]	1.85	0.35
2:C:192:ASN:ND2	1:F:77:ARG:CD[2_546]	1.85	0.35
2:C:193:GLU:C	1:F:75:ALA:CB[2_546]	1.86	0.34
2:I:113:TYR:OH	2:M:66:THR:OG1[2_656]	1.88	0.32
2:I:86:ARG:NE	1:K:194:ASP:O[2_756]	1.89	0.31
2:B:199:GLU:OE2	3:J:178:ARG:NH1[2_646]	1.90	0.30
1:A:277:ARG:NH2	2:D:66:THR:O[1_655]	1.92	0.28
2:B:188:GLU:CG	3:J:2:ARG:NH1[2_646]	1.93	0.27
2:B:3:TYR:CE2	3:J:54:GLN:CB[2_646]	1.95	0.25
2:C:192:ASN:ND2	1:F:77:ARG:CG[2_546]	1.95	0.25
3:J:19:GLN:OE1	2:L:299:PRO:CG[2_756]	1.96	0.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:TYR:CZ	3:J:54:GLN:CG[2_646]	1.96	0.24
3:E:138:GLU:OE2	2:G:367:GLU:O[1_455]	1.97	0.23
3:E:52:GLN:OE1	2:H:363:MET:SD[1_455]	1.98	0.22
3:E:63:ARG:NH1	2:H:361:PRO:N[1_455]	1.98	0.22
2:G:75:VAL:O	2:I:270:GLU:OE2[1_455]	1.98	0.22
2:B:3:TYR:CD2	3:J:54:GLN:CD[2_646]	2.01	0.19
2:G:76:CYS:CA	2:I:270:GLU:OE2[1_455]	2.01	0.19
2:C:192:ASN:C	1:F:76:SER:CA[2_546]	2.02	0.18
2:B:4:GLN:NE2	3:J:59:CYS:C[2_646]	2.02	0.18
2:C:195:HIS:CD2	1:F:74:PHE:C[2_546]	2.03	0.17
3:J:19:GLN:CG	2:L:299:PRO:CB[2_756]	2.04	0.16
2:C:193:GLU:CA	1:F:76:SER:CA[2_546]	2.05	0.15
2:C:193:GLU:O	1:F:75:ALA:N[2_546]	2.06	0.14
2:B:193:GLU:OE1	3:J:69:GLN:NE2[2_646]	2.06	0.14
2:C:195:HIS:CG	1:F:74:PHE:O[2_546]	2.06	0.14
2:B:361:PRO:O	3:O:184:GLN:CG[2_646]	2.07	0.13
1:A:277:ARG:CZ	2:D:66:THR:C[1_655]	2.07	0.13
2:C:192:ASN:O	1:F:76:SER:C[2_546]	2.07	0.13
2:C:188:GLU:CG	1:F:77:ARG:NH2[2_546]	2.08	0.12
2:B:3:TYR:OH	3:J:54:GLN:CG[2_646]	2.10	0.10
3:E:63:ARG:NH2	2:H:361:PRO:N[1_455]	2.11	0.09
2:C:193:GLU:N	1:F:76:SER:CA[2_546]	2.12	0.08
2:I:86:ARG:NH2	1:K:193:PRO:O[2_756]	2.12	0.08
3:J:19:GLN:OE1	2:L:299:PRO:CA[2_756]	2.12	0.08
3:E:63:ARG:NH2	2:H:360:HIS:C[1_455]	2.13	0.07
2:C:195:HIS:CE1	1:F:78:GLN:NE2[2_546]	2.15	0.05
3:E:63:ARG:NH2	2:H:360:HIS:O[1_455]	2.17	0.03
2:C:198:HIS:O	1:F:106:ASP:OD2[2_546]	2.17	0.03
2:B:3:TYR:CD2	3:J:54:GLN:OE1[2_646]	2.17	0.03
2:C:192:ASN:C	1:F:75:ALA:O[2_546]	2.18	0.02
3:E:63:ARG:CZ	2:H:361:PRO:N[1_455]	2.18	0.02

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	330/343 (96%)	301 (91%)	22 (7%)	7 (2%)	9 51
1	F	330/343 (96%)	301 (91%)	22 (7%)	7 (2%)	9 51
1	K	330/343 (96%)	301 (91%)	22 (7%)	7 (2%)	9 51
2	B	358/376 (95%)	327 (91%)	23 (6%)	8 (2%)	8 50
2	C	358/376 (95%)	329 (92%)	23 (6%)	6 (2%)	11 55
2	D	357/376 (95%)	320 (90%)	27 (8%)	10 (3%)	6 46
2	G	358/376 (95%)	328 (92%)	22 (6%)	8 (2%)	8 50
2	H	358/376 (95%)	329 (92%)	22 (6%)	7 (2%)	9 52
2	I	357/376 (95%)	320 (90%)	27 (8%)	10 (3%)	6 46
2	L	358/376 (95%)	327 (91%)	23 (6%)	8 (2%)	8 50
2	M	358/376 (95%)	329 (92%)	22 (6%)	7 (2%)	9 52
2	N	357/376 (95%)	320 (90%)	27 (8%)	10 (3%)	6 46
3	E	326/334 (98%)	296 (91%)	28 (9%)	2 (1%)	30 73
3	J	326/334 (98%)	296 (91%)	28 (9%)	2 (1%)	30 73
3	O	326/334 (98%)	296 (91%)	28 (9%)	2 (1%)	30 73
All	All	5187/5415 (96%)	4720 (91%)	366 (7%)	101 (2%)	10 53

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	TRP
2	B	104	THR
2	B	310	GLU
2	C	20	GLY
2	C	104	THR
2	C	111	VAL
2	C	364	PRO
2	D	22	GLU
2	D	104	THR
2	D	261	GLY
2	D	310	GLU
1	F	279	TRP
2	G	310	GLU
2	H	4	GLN
2	H	20	GLY
2	H	104	THR
2	H	111	VAL
2	H	364	PRO

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Mol	Chain	Res	Type
2	I	22	GLU
2	I	104	THR
2	I	261	GLY
2	I	310	GLU
1	K	279	TRP
2	L	104	THR
2	L	310	GLU
2	M	4	GLN
2	M	20	GLY
2	M	104	THR
2	M	111	VAL
2	M	364	PRO
2	N	22	GLU
2	N	104	THR
2	N	261	GLY
2	N	310	GLU
1	A	131	ALA
1	A	282	ARG
2	B	303	GLY
2	D	50	GLY
1	F	131	ALA
1	F	282	ARG
2	G	104	THR
2	G	303	GLY
2	I	50	GLY
1	K	131	ALA
1	K	282	ARG
2	L	303	GLY
2	N	50	GLY
1	A	46	GLY
1	A	269	LEU
2	B	4	GLN
2	D	111	VAL
3	E	62	CYS
1	F	46	GLY
1	F	269	LEU
2	G	4	GLN
2	I	111	VAL
3	J	62	CYS
1	K	46	GLY
1	K	269	LEU
2	L	4	GLN

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Mol	Chain	Res	Type
2	N	111	VAL
3	O	62	CYS
1	A	125	ALA
2	B	249	ALA
3	E	150	ARG
1	F	125	ALA
2	G	249	ALA
3	J	150	ARG
1	K	125	ALA
2	L	249	ALA
3	O	150	ARG
2	B	22	GLU
2	C	4	GLN
2	C	339	LEU
2	D	7	ALA
2	D	364	PRO
2	G	22	GLU
2	G	278	TRP
2	H	339	LEU
2	I	7	ALA
2	I	364	PRO
2	L	22	GLU
2	L	278	TRP
2	M	339	LEU
2	N	7	ALA
2	N	364	PRO
2	B	278	TRP
2	D	101	VAL
2	D	299	PRO
2	H	246	ASP
2	I	101	VAL
2	I	299	PRO
2	M	246	ASP
2	N	101	VAL
2	N	299	PRO
1	A	317	GLY
1	F	317	GLY
1	K	317	GLY
2	B	101	VAL
2	G	101	VAL
2	L	101	VAL

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	285/291 (98%)	259 (91%)	26 (9%)	12 47
1	F	285/291 (98%)	259 (91%)	26 (9%)	12 47
1	K	285/291 (98%)	259 (91%)	26 (9%)	12 47
2	B	303/312 (97%)	280 (92%)	23 (8%)	16 55
2	C	303/312 (97%)	288 (95%)	15 (5%)	30 68
2	D	302/312 (97%)	289 (96%)	13 (4%)	35 72
2	G	303/312 (97%)	280 (92%)	23 (8%)	16 55
2	H	303/312 (97%)	288 (95%)	15 (5%)	30 68
2	I	302/312 (97%)	289 (96%)	13 (4%)	35 72
2	L	303/312 (97%)	280 (92%)	23 (8%)	16 55
2	M	303/312 (97%)	288 (95%)	15 (5%)	30 68
2	N	302/312 (97%)	289 (96%)	13 (4%)	35 72
3	E	270/270 (100%)	239 (88%)	31 (12%)	7 36
3	J	270/270 (100%)	239 (88%)	31 (12%)	7 36
3	O	270/270 (100%)	239 (88%)	31 (12%)	7 36
All	All	4389/4491 (98%)	4065 (93%)	324 (7%)	17 56

All (324) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	54	SER
1	A	84	LEU
1	A	101	THR
1	A	109	LEU
1	A	113	ARG
1	A	115	ASN
1	A	119	LYS
1	A	133	ARG
1	A	143	GLU

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Mol	Chain	Res	Type
1	A	160	LEU
1	A	162	LEU
1	A	183	GLN
1	A	198	THR
1	A	200	PRO
1	A	208	ASP
1	A	215	PHE
1	A	223	MET
1	A	228	ARG
1	A	230	LEU
1	A	266	HIS
1	A	279	TRP
1	A	283	ARG
1	A	292	ARG
1	A	305	LEU
1	A	330	LEU
2	B	3	TYR
2	B	14	THR
2	B	17	ASP
2	B	18	VAL
2	B	22	GLU
2	B	47	ARG
2	B	52	THR
2	B	71	THR
2	B	88	VAL
2	B	97	SER
2	B	128	VAL
2	B	160	GLN
2	B	165	THR
2	B	176	LYS
2	B	184	ARG
2	B	240	MET
2	B	251	SER
2	B	252	LEU
2	B	305	ASP
2	B	333	LEU
2	B	344	ASP
2	B	351	MET
2	B	357	LEU
2	C	3	TYR
2	C	15	PHE
2	C	46	THR

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Mol	Chain	Res	Type
2	C	69	THR
2	C	76	CYS
2	C	117	ARG
2	C	130	MET
2	C	251	SER
2	C	309	ILE
2	C	318	ARG
2	C	327	LEU
2	C	344	ASP
2	C	355	ARG
2	C	357	LEU
2	C	367	GLU
2	D	6	LEU
2	D	17	ASP
2	D	46	THR
2	D	71	THR
2	D	76	CYS
2	D	137	ASN
2	D	184	ARG
2	D	194	GLU
2	D	219	SER
2	D	248	GLN
2	D	251	SER
2	D	333	LEU
2	D	357	LEU
3	E	3	TRP
3	E	13	LYS
3	E	46	ARG
3	E	68	MET
3	E	91	ASP
3	E	110	LYS
3	E	120	LEU
3	E	147	GLU
3	E	149	GLU
3	E	154	THR
3	E	158	ARG
3	E	159	CYS
3	E	170	GLN
3	E	175	TRP
3	E	185	ASP
3	E	202	LEU
3	E	206	GLN

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Mol	Chain	Res	Type
3	E	216	LEU
3	E	220	LEU
3	E	237	ASN
3	E	245	LEU
3	E	252	LEU
3	E	256	LEU
3	E	277	LEU
3	E	285	ARG
3	E	290	LEU
3	E	292	ASP
3	E	299	GLN
3	E	310	LEU
3	E	315	LEU
3	E	329	LEU
1	F	40	GLN
1	F	54	SER
1	F	84	LEU
1	F	101	THR
1	F	109	LEU
1	F	113	ARG
1	F	115	ASN
1	F	119	LYS
1	F	133	ARG
1	F	143	GLU
1	F	160	LEU
1	F	162	LEU
1	F	183	GLN
1	F	198	THR
1	F	200	PRO
1	F	208	ASP
1	F	215	PHE
1	F	223	MET
1	F	228	ARG
1	F	230	LEU
1	F	266	HIS
1	F	279	TRP
1	F	283	ARG
1	F	292	ARG
1	F	305	LEU
1	F	330	LEU
2	G	3	TYR
2	G	14	THR

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Mol	Chain	Res	Type
2	G	17	ASP
2	G	18	VAL
2	G	22	GLU
2	G	47	ARG
2	G	52	THR
2	G	71	THR
2	G	88	VAL
2	G	97	SER
2	G	128	VAL
2	G	160	GLN
2	G	165	THR
2	G	176	LYS
2	G	184	ARG
2	G	240	MET
2	G	251	SER
2	G	252	LEU
2	G	305	ASP
2	G	333	LEU
2	G	344	ASP
2	G	351	MET
2	G	357	LEU
2	H	3	TYR
2	H	15	PHE
2	H	46	THR
2	H	69	THR
2	H	76	CYS
2	H	117	ARG
2	H	130	MET
2	H	251	SER
2	H	309	ILE
2	H	318	ARG
2	H	327	LEU
2	H	344	ASP
2	H	355	ARG
2	H	357	LEU
2	H	367	GLU
2	I	6	LEU
2	I	17	ASP
2	I	46	THR
2	I	71	THR
2	I	76	CYS
2	I	137	ASN

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Mol	Chain	Res	Type
2	I	184	ARG
2	I	194	GLU
2	I	219	SER
2	I	248	GLN
2	I	251	SER
2	I	333	LEU
2	I	357	LEU
3	J	3	TRP
3	J	13	LYS
3	J	46	ARG
3	J	68	MET
3	J	91	ASP
3	J	110	LYS
3	J	120	LEU
3	J	147	GLU
3	J	149	GLU
3	J	154	THR
3	J	158	ARG
3	J	159	CYS
3	J	170	GLN
3	J	175	TRP
3	J	185	ASP
3	J	202	LEU
3	J	206	GLN
3	J	216	LEU
3	J	220	LEU
3	J	237	ASN
3	J	245	LEU
3	J	252	LEU
3	J	256	LEU
3	J	277	LEU
3	J	285	ARG
3	J	290	LEU
3	J	292	ASP
3	J	299	GLN
3	J	310	LEU
3	J	315	LEU
3	J	329	LEU
1	K	40	GLN
1	K	54	SER
1	K	84	LEU
1	K	101	THR

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Mol	Chain	Res	Type
1	K	109	LEU
1	K	113	ARG
1	K	115	ASN
1	K	119	LYS
1	K	133	ARG
1	K	143	GLU
1	K	160	LEU
1	K	162	LEU
1	K	183	GLN
1	K	198	THR
1	K	200	PRO
1	K	208	ASP
1	K	215	PHE
1	K	223	MET
1	K	228	ARG
1	K	230	LEU
1	K	266	HIS
1	K	279	TRP
1	K	283	ARG
1	K	292	ARG
1	K	305	LEU
1	K	330	LEU
2	L	3	TYR
2	L	14	THR
2	L	17	ASP
2	L	18	VAL
2	L	22	GLU
2	L	47	ARG
2	L	52	THR
2	L	71	THR
2	L	88	VAL
2	L	97	SER
2	L	128	VAL
2	L	160	GLN
2	L	165	THR
2	L	176	LYS
2	L	184	ARG
2	L	240	MET
2	L	251	SER
2	L	252	LEU
2	L	305	ASP
2	L	333	LEU

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Mol	Chain	Res	Type
2	L	344	ASP
2	L	351	MET
2	L	357	LEU
2	M	3	TYR
2	M	15	PHE
2	M	46	THR
2	M	69	THR
2	M	76	CYS
2	M	117	ARG
2	M	130	MET
2	M	251	SER
2	M	309	ILE
2	M	318	ARG
2	M	327	LEU
2	M	344	ASP
2	M	355	ARG
2	M	357	LEU
2	M	367	GLU
2	N	6	LEU
2	N	17	ASP
2	N	46	THR
2	N	71	THR
2	N	76	CYS
2	N	137	ASN
2	N	184	ARG
2	N	194	GLU
2	N	219	SER
2	N	248	GLN
2	N	251	SER
2	N	333	LEU
2	N	357	LEU
3	O	3	TRP
3	O	13	LYS
3	O	46	ARG
3	O	68	MET
3	O	91	ASP
3	O	110	LYS
3	O	120	LEU
3	O	147	GLU
3	O	149	GLU
3	O	154	THR
3	O	158	ARG

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Mol	Chain	Res	Type
3	O	159	CYS
3	O	170	GLN
3	O	175	TRP
3	O	185	ASP
3	O	202	LEU
3	O	206	GLN
3	O	216	LEU
3	O	220	LEU
3	O	237	ASN
3	O	245	LEU
3	O	252	LEU
3	O	256	LEU
3	O	277	LEU
3	O	285	ARG
3	O	290	LEU
3	O	292	ASP
3	O	299	GLN
3	O	310	LEU
3	O	315	LEU
3	O	329	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	51	HIS
1	A	94	ASN
1	A	105	HIS
1	A	136	GLN
1	A	216	HIS
1	A	266	HIS
1	A	276	HIS
1	A	281	ASN
1	A	295	GLN
1	A	297	GLN
1	A	314	GLN
1	A	318	GLN
2	B	172	GLN
2	B	198	HIS
2	B	360	HIS
2	C	198	HIS
2	C	360	HIS

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Mol	Chain	Res	Type
2	D	198	HIS
2	D	248	GLN
2	D	304	ASN
2	D	326	GLN
3	E	73	HIS
3	E	237	ASN
3	E	240	GLN
3	E	260	HIS
3	E	280	HIS
3	E	299	GLN
3	E	307	ASN
1	F	40	GLN
1	F	51	HIS
1	F	94	ASN
1	F	105	HIS
1	F	136	GLN
1	F	183	GLN
1	F	207	ASN
1	F	216	HIS
1	F	266	HIS
1	F	276	HIS
1	F	295	GLN
1	F	297	GLN
1	F	314	GLN
1	F	318	GLN
2	G	21	GLN
2	G	172	GLN
2	G	174	HIS
2	G	198	HIS
2	G	360	HIS
2	H	198	HIS
2	H	360	HIS
2	I	198	HIS
2	I	248	GLN
2	I	290	HIS
2	I	304	ASN
2	I	326	GLN
3	J	73	HIS
3	J	237	ASN
3	J	240	GLN
3	J	260	HIS
3	J	280	HIS

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Mol	Chain	Res	Type
3	J	299	GLN
3	J	307	ASN
1	K	32	GLN
1	K	40	GLN
1	K	51	HIS
1	K	94	ASN
1	K	105	HIS
1	K	136	GLN
1	K	183	GLN
1	K	216	HIS
1	K	266	HIS
1	K	276	HIS
1	K	281	ASN
1	K	295	GLN
1	K	297	GLN
1	K	314	GLN
1	K	318	GLN
1	K	333	HIS
2	L	172	GLN
2	L	198	HIS
2	L	204	GLN
2	L	360	HIS
2	M	198	HIS
2	M	360	HIS
2	N	198	HIS
2	N	223	GLN
2	N	248	GLN
2	N	326	GLN
3	O	73	HIS
3	O	237	ASN
3	O	240	GLN
3	O	260	HIS
3	O	299	GLN
3	O	307	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	336/343 (97%)	0.54	30 (8%) 12 8	69, 78, 90, 90	0
1	F	336/343 (97%)	2.77	172 (51%) 0 1	127, 241, 267, 267	0
1	K	336/343 (97%)	0.48	24 (7%) 19 12	56, 67, 79, 79	0
2	B	364/376 (96%)	0.68	36 (9%) 9 7	85, 90, 111, 111	0
2	C	364/376 (96%)	0.41	23 (6%) 23 15	61, 66, 76, 85	0
2	D	363/376 (96%)	0.35	7 (1%) 70 59	57, 67, 70, 70	0
2	G	364/376 (96%)	2.38	149 (40%) 0 1	84, 208, 291, 291	0
2	H	364/376 (96%)	1.20	83 (22%) 1 1	59, 171, 228, 228	0
2	I	363/376 (96%)	0.52	32 (8%) 12 8	66, 67, 151, 151	0
2	L	364/376 (96%)	0.51	22 (6%) 25 17	66, 94, 101, 101	0
2	M	364/376 (96%)	0.73	44 (12%) 6 5	79, 127, 140, 140	0
2	N	363/376 (96%)	0.62	37 (10%) 9 7	102, 107, 133, 133	0
3	E	332/334 (99%)	0.24	8 (2%) 62 50	30, 46, 62, 62	0
3	J	332/334 (99%)	0.41	17 (5%) 32 23	52, 66, 71, 71	0
3	O	332/334 (99%)	1.46	95 (28%) 1 1	75, 182, 266, 266	0
All	All	5277/5415 (97%)	0.89	779 (14%) 3 3	30, 79, 267, 291	0

All (779) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	181	LEU	20.0
3	O	55	GLY	18.4
2	G	104	THR	17.2
1	F	55	ILE	14.3
2	G	42	LEU	13.5
3	O	56	HIS	13.5
2	G	170	CYS	12.9

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Mol	Chain	Res	Type	RSRZ
2	G	139	LEU	12.8
1	F	85	PRO	12.7
2	G	50	GLY	12.6
2	G	142	THR	12.6
1	F	132	ASN	11.8
2	H	162	LEU	11.4
2	G	133	ARG	10.8
2	G	43	PHE	10.6
3	O	144	ALA	10.2
1	F	95	GLU	10.0
2	G	33	SER	9.9
1	F	17	LEU	9.8
1	F	78	GLN	9.6
1	F	91	ALA	9.6
2	G	172	GLN	9.6
2	N	366	PRO	9.6
1	F	18	ARG	9.5
1	F	110	LEU	9.4
1	F	182	ALA	9.3
1	F	51	HIS	9.1
2	G	108	LEU	9.1
1	F	46	GLY	9.1
2	G	128	VAL	9.0
1	F	80	LEU	8.9
1	F	52	THR	8.9
1	F	180	ALA	8.9
3	O	54	GLN	8.8
2	G	168	SER	8.7
1	F	12	GLN	8.7
2	H	85	GLY	8.7
1	F	198	THR	8.5
2	G	206	LEU	8.4
1	F	185	LEU	8.4
2	G	107	LEU	8.4
2	B	362	ARG	8.2
1	F	13	LEU	8.2
2	G	44	SER	8.1
2	G	116	ALA	7.9
3	O	116	ASP	7.9
2	G	61	GLY	7.9
1	F	15	GLU	7.9
2	G	137	ASN	7.8

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Mol	Chain	Res	Type	RSRZ
2	G	136	PHE	7.8
1	F	16	GLY	7.8
3	O	117	ALA	7.7
2	G	6	LEU	7.6
2	M	101	VAL	7.6
2	H	152	PHE	7.6
1	F	19	ALA	7.6
3	O	111	VAL	7.6
1	F	8	GLN	7.5
3	O	31	ALA	7.5
1	F	66	SER	7.5
2	G	12	PRO	7.4
2	G	34	LEU	7.4
2	G	153	LEU	7.4
1	F	164	ASP	7.4
2	H	39	HIS	7.3
1	F	35	GLN	7.3
2	G	93	ILE	7.3
1	F	94	ASN	7.2
2	M	299	PRO	7.2
1	F	96	GLN	7.2
2	H	153	LEU	7.2
2	H	154	LEU	7.2
1	F	34	SER	7.1
1	F	50	HIS	7.1
2	G	169	ARG	7.1
1	F	106	ASP	7.0
2	L	363	MET	7.0
1	F	79	THR	7.0
2	L	4	GLN	7.0
1	F	138	THR	7.0
2	G	135	SER	6.9
1	F	145	ALA	6.9
1	F	165	ALA	6.9
2	G	120	PHE	6.8
2	G	154	LEU	6.8
1	F	97	LEU	6.8
1	A	60	ASP	6.7
1	F	209	ALA	6.6
2	H	94	ASP	6.6
2	G	35	GLY	6.6
2	G	152	PHE	6.6

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Mol	Chain	Res	Type	RSRZ
2	H	163	PRO	6.6
3	O	69	GLN	6.6
1	F	166	ALA	6.6
1	F	88	GLY	6.6
1	F	98	LEU	6.6
1	F	161	GLU	6.6
1	F	163	ASP	6.5
2	G	171	LEU	6.5
1	F	192	TRP	6.5
1	A	74	PHE	6.5
3	O	70	ALA	6.4
2	B	5	VAL	6.4
1	F	14	ASN	6.4
2	N	364	PRO	6.3
3	O	143	LEU	6.3
3	O	79	LEU	6.3
2	G	32	LEU	6.3
2	G	132	SER	6.2
2	G	210	ALA	6.2
1	F	170	LEU	6.2
2	G	212	GLY	6.2
2	G	143	LEU	6.2
1	F	49	GLU	6.1
1	F	150	TRP	6.1
3	O	131	THR	6.1
2	I	365	LEU	6.1
1	F	92	ALA	6.0
1	F	67	LEU	6.0
2	G	205	LEU	6.0
2	I	366	PRO	6.0
2	G	131	LEU	5.9
1	F	48	GLU	5.9
3	O	26	ALA	5.9
2	G	3	TYR	5.9
2	G	29	ALA	5.9
1	F	86	GLU	5.8
3	O	141	PHE	5.8
2	G	51	LYS	5.8
2	G	141	LYS	5.7
1	F	137	VAL	5.7
1	F	133	ARG	5.7
1	F	71	MET	5.7

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Mol	Chain	Res	Type	RSRZ
2	G	74	GLY	5.6
2	G	200	PRO	5.6
2	C	85	GLY	5.6
1	F	104	LEU	5.6
2	G	151	LYS	5.6
2	H	145	GLU	5.5
2	I	123	TYR	5.5
1	F	45	GLN	5.5
2	B	361	PRO	5.5
2	B	101	VAL	5.5
2	G	112	GLN	5.4
1	F	30	LEU	5.4
2	H	41	TYR	5.4
2	L	368	PRO	5.4
2	G	156	THR	5.4
1	F	193	PRO	5.4
1	F	89	PRO	5.4
2	L	6	LEU	5.3
2	G	37	ILE	5.3
2	H	146	PRO	5.3
2	G	30	ASN	5.3
3	O	1	MET	5.3
2	B	367	GLU	5.3
1	F	196	LYS	5.2
2	G	62	LEU	5.2
2	H	93	ILE	5.2
3	O	112	VAL	5.2
1	F	28	PRO	5.2
2	G	134	HIS	5.2
1	F	184	ALA	5.2
2	G	52	THR	5.2
1	F	168	GLN	5.1
1	F	210	ALA	5.1
2	I	364	PRO	5.1
2	G	164	VAL	5.1
3	O	137	ALA	5.1
2	G	165	THR	5.1
2	I	133	ARG	5.1
2	G	7	ALA	5.1
2	B	365	LEU	5.1
1	K	58	ASN	5.1
1	F	11	ALA	5.0

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Mol	Chain	Res	Type	RSRZ
2	G	231	GLN	5.0
2	H	166	ILE	5.0
1	K	91	ALA	5.0
3	O	45	SER	5.0
3	O	118	ALA	5.0
2	H	111	VAL	5.0
3	O	96	VAL	5.0
1	F	173	CYS	5.0
2	G	53	SER	5.0
1	F	207	ASN	4.9
2	G	129	HIS	4.9
2	H	71	THR	4.9
2	G	230	GLY	4.9
2	G	26	THR	4.9
1	F	111	ILE	4.9
2	G	82	ILE	4.9
2	G	367	GLU	4.9
2	B	268	ILE	4.9
2	N	367	GLU	4.9
2	G	195	HIS	4.9
1	F	176	GLY	4.9
2	G	362	ARG	4.9
1	F	87	ASN	4.9
2	M	68	ILE	4.9
3	O	37	ASP	4.8
1	F	21	TYR	4.8
2	G	140	LEU	4.8
1	F	36	ASP	4.8
2	G	125	ILE	4.8
1	F	146	GLN	4.8
2	G	173	PHE	4.8
1	F	139	CYS	4.7
2	G	363	MET	4.7
1	F	154	ARG	4.7
1	F	136	GLN	4.7
2	G	83	GLU	4.7
1	A	338	ASP	4.7
2	L	3	TYR	4.6
2	G	60	LYS	4.6
3	O	72	THR	4.6
1	A	61	TRP	4.6
2	G	63	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	F	140	GLN	4.6
2	H	72	PRO	4.6
1	F	194	ASP	4.6
3	O	145	THR	4.6
2	M	104	THR	4.5
2	B	6	LEU	4.5
2	H	38	HIS	4.5
1	F	177	ASN	4.5
2	H	151	LYS	4.5
1	F	81	LEU	4.5
2	G	214	LEU	4.5
1	K	61	TRP	4.5
2	G	15	PHE	4.5
2	L	362	ARG	4.5
3	O	6	TRP	4.4
1	F	186	GLU	4.4
2	H	104	THR	4.4
1	F	47	PHE	4.4
2	B	363	MET	4.4
1	F	60	ASP	4.4
2	G	45	GLY	4.4
2	B	241	LEU	4.4
1	F	172	TYR	4.4
2	G	174	HIS	4.3
1	F	93	ILE	4.3
2	L	367	GLU	4.3
2	G	221	THR	4.3
2	G	178	LEU	4.3
1	F	203	GLU	4.3
2	M	93	ILE	4.3
2	H	100	LYS	4.3
2	N	232	VAL	4.3
2	H	108	LEU	4.2
2	N	365	LEU	4.2
1	F	200	PRO	4.2
2	G	25	LEU	4.2
1	F	178	LEU	4.2
2	H	302	LEU	4.2
1	F	208	ASP	4.2
2	G	5	VAL	4.2
1	F	101	THR	4.2
2	D	366	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	90	ASN	4.2
2	N	210	ALA	4.1
1	K	57	PRO	4.1
1	F	23	LEU	4.1
2	G	8	ARG	4.1
2	G	41	TYR	4.1
1	F	70	ALA	4.1
3	O	142	PHE	4.1
1	F	144	GLN	4.1
3	O	27	LEU	4.1
2	H	139	LEU	4.1
2	G	59	ALA	4.0
2	M	305	ASP	4.0
2	G	14	THR	4.0
2	G	36	ARG	4.0
2	D	305	ASP	4.0
1	F	69	GLN	4.0
3	J	3	TRP	4.0
2	H	15	PHE	4.0
2	G	161	LYS	4.0
2	G	66	THR	4.0
2	G	155	ALA	4.0
2	N	63	ASN	4.0
1	F	126	TRP	4.0
3	O	48	LEU	3.9
1	K	60	ASP	3.9
3	E	82	GLU	3.9
2	G	166	ILE	3.9
2	H	36	ARG	3.9
1	K	62	ASN	3.9
2	B	368	PRO	3.9
1	F	169	VAL	3.9
1	F	197	LEU	3.9
2	G	175	LEU	3.9
2	G	38	HIS	3.9
2	B	229	ASP	3.8
1	F	31	LEU	3.8
2	M	102	GLU	3.8
1	F	62	ASN	3.8
3	O	95	GLU	3.8
2	G	57	LEU	3.8
2	B	366	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
2	H	35	GLY	3.8
1	F	3	ARG	3.8
1	A	55	ILE	3.7
2	B	89	ASP	3.7
2	L	246	ASP	3.7
2	G	117	ARG	3.7
2	H	37	ILE	3.7
1	A	53	PHE	3.7
2	G	197	ALA	3.7
2	H	211	GLU	3.7
2	G	124	LEU	3.7
1	A	142	PRO	3.7
2	H	126	ASP	3.6
2	I	144	GLU	3.6
1	F	43	ALA	3.6
2	I	102	GLU	3.6
1	F	24	LEU	3.6
1	F	38	VAL	3.6
2	H	20	GLY	3.6
2	G	138	ALA	3.6
1	F	183	GLN	3.6
2	H	92	GLU	3.6
3	O	140	TRP	3.6
2	G	99	THR	3.6
2	G	148	GLU	3.6
3	O	40	LEU	3.6
2	M	246	ASP	3.5
2	G	85	GLY	3.5
2	G	18	VAL	3.5
1	F	44	ALA	3.5
1	F	199	LEU	3.5
2	H	28	LEU	3.5
2	G	213	SER	3.5
3	J	236	LEU	3.5
3	O	7	LEU	3.5
2	H	59	ALA	3.5
3	O	159	CYS	3.5
1	A	75	ALA	3.5
3	O	29	ILE	3.5
1	K	100	LEU	3.5
2	G	84	GLN	3.5
1	F	61	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	142	PRO	3.5
1	F	195	GLY	3.5
2	G	47	ARG	3.5
2	G	10	TRP	3.5
3	O	176	LEU	3.5
2	H	157	THR	3.4
1	F	149	ARG	3.4
2	H	232	VAL	3.4
1	F	117	LEU	3.4
1	F	99	THR	3.4
2	H	135	SER	3.4
2	N	104	THR	3.4
3	O	187	LEU	3.4
1	F	338	ASP	3.4
3	O	75	ASP	3.4
2	D	4	GLN	3.4
1	F	77	ARG	3.4
2	N	179	ASP	3.4
2	G	187	LEU	3.4
3	E	159	CYS	3.4
1	K	82	LEU	3.4
2	C	104	THR	3.4
2	D	6	LEU	3.4
2	B	249	ALA	3.4
2	H	43	PHE	3.4
2	G	126	ASP	3.4
2	L	247	ASP	3.4
2	H	19	VAL	3.4
2	H	112	GLN	3.4
2	I	359	PHE	3.4
2	I	101	VAL	3.4
2	C	99	THR	3.3
1	F	135	VAL	3.3
1	F	9	LEU	3.3
2	H	24	VAL	3.3
2	H	143	LEU	3.3
2	B	299	PRO	3.3
2	H	117	ARG	3.3
2	I	40	ALA	3.3
2	H	142	THR	3.3
2	L	248	GLN	3.3
2	I	134	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
2	M	92	GLU	3.3
3	O	28	LEU	3.3
3	O	14	LEU	3.3
3	O	125	ALA	3.3
1	F	2	ILE	3.3
3	J	334	LEU	3.2
1	F	109	LEU	3.2
2	M	302	LEU	3.2
1	F	68	CYS	3.2
1	F	33	GLU	3.2
2	H	132	SER	3.2
3	O	97	THR	3.2
2	C	123	TYR	3.2
3	O	74	PRO	3.2
1	F	174	TYR	3.2
2	C	128	VAL	3.2
2	I	69	THR	3.2
2	N	6	LEU	3.2
3	O	25	HIS	3.2
2	M	256	MET	3.2
3	O	115	THR	3.2
2	H	74	GLY	3.2
1	F	27	ASP	3.1
1	F	83	LEU	3.1
3	J	237	ASN	3.1
2	H	47	ARG	3.1
2	B	3	TYR	3.1
1	F	116	LYS	3.1
1	A	82	LEU	3.1
3	O	126	ASN	3.1
2	H	134	HIS	3.1
3	O	78	THR	3.1
1	F	10	ARG	3.1
2	L	241	LEU	3.1
3	O	114	VAL	3.1
1	F	4	LEU	3.1
2	M	354	LEU	3.1
1	K	338	ASP	3.1
2	N	188	GLU	3.1
2	M	108	LEU	3.1
2	G	4	GLN	3.0
2	N	241	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	111	VAL	3.0
1	F	84	LEU	3.0
1	K	53	PHE	3.0
2	H	131	LEU	3.0
1	K	276	HIS	3.0
1	F	241	SER	3.0
3	O	113	TRP	3.0
2	B	90	LEU	3.0
2	B	300	ALA	3.0
2	H	110	ASN	3.0
1	F	54	SER	3.0
3	O	245	LEU	3.0
3	O	267	ASN	3.0
2	D	359	PHE	3.0
3	O	3	TRP	3.0
2	H	89	ASP	3.0
3	O	153	ALA	3.0
1	A	298	LEU	3.0
2	I	152	PHE	3.0
1	F	22	LEU	3.0
2	G	192	ASN	3.0
2	M	206	LEU	3.0
2	M	349	VAL	3.0
2	H	60	LYS	3.0
1	A	62	ASN	3.0
2	I	91	ILE	3.0
2	B	92	GLU	3.0
2	G	70	ALA	2.9
1	K	337	ALA	2.9
2	H	30	ASN	2.9
3	O	46	ARG	2.9
1	F	107	ASP	2.9
2	H	229	ASP	2.9
2	L	123	TYR	2.9
3	O	256	LEU	2.9
3	O	22	ARG	2.9
3	O	63	ARG	2.9
2	G	144	GLU	2.9
2	G	58	LEU	2.9
2	H	116	ALA	2.9
3	J	109	ALA	2.9
2	H	86	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
2	G	209	ALA	2.9
3	O	47	TYR	2.9
2	H	138	ALA	2.9
1	F	191	LEU	2.9
2	L	351	MET	2.9
2	N	193	GLU	2.9
2	M	162	LEU	2.9
2	G	127	GLU	2.9
2	I	104	THR	2.9
2	H	230	GLY	2.9
2	B	37	ILE	2.9
2	I	367	GLU	2.9
2	I	122	VAL	2.9
2	M	128	VAL	2.9
3	E	267	ASN	2.9
1	F	37	ALA	2.8
1	F	124	ALA	2.8
2	G	68	ILE	2.8
2	L	196	ILE	2.8
1	K	293	LEU	2.8
1	F	167	ASN	2.8
3	O	44	LEU	2.8
2	B	116	ALA	2.8
1	F	134	SER	2.8
3	J	202	LEU	2.8
2	N	178	LEU	2.8
1	A	239	GLU	2.8
2	N	231	GLN	2.8
2	H	62	LEU	2.8
2	L	32	LEU	2.8
1	F	20	ALA	2.8
2	H	136	PHE	2.8
2	I	62	LEU	2.8
2	G	17	ASP	2.8
1	K	130	LEU	2.8
2	C	108	LEU	2.8
2	H	90	LEU	2.7
3	O	132	LEU	2.7
2	G	235	GLN	2.7
2	L	245	ASP	2.7
2	C	124	LEU	2.7
1	F	113	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
2	G	114	ALA	2.7
2	H	197	ALA	2.7
2	M	135	SER	2.7
2	H	82	ILE	2.7
2	B	4	GLN	2.7
2	G	361	PRO	2.7
2	M	32	LEU	2.7
2	N	203	LEU	2.7
2	I	156	THR	2.7
2	N	10	TRP	2.7
2	G	101	VAL	2.7
2	H	231	GLN	2.7
2	G	162	LEU	2.7
2	N	180	VAL	2.7
3	O	73	HIS	2.7
1	F	204	GLN	2.7
2	M	306	MET	2.7
2	I	93	ILE	2.7
2	N	38	HIS	2.7
3	O	241	ALA	2.7
3	O	8	ARG	2.7
2	C	135	SER	2.7
1	F	40	GLN	2.7
2	G	31	GLY	2.7
3	J	14	LEU	2.7
1	K	97	LEU	2.7
2	G	149	HIS	2.7
2	G	160	GLN	2.7
3	O	71	GLY	2.6
2	M	51	LYS	2.6
3	O	30	GLN	2.6
1	A	78	GLN	2.6
2	M	221	THR	2.6
1	F	156	LYS	2.6
3	O	88	LEU	2.6
1	K	73	LEU	2.6
2	G	13	GLN	2.6
2	M	295	VAL	2.6
2	N	20	GLY	2.6
1	A	278	VAL	2.6
2	G	222	ASP	2.6
3	J	306	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
3	O	90	VAL	2.6
2	G	118	GLY	2.6
1	A	79	THR	2.6
2	I	302	LEU	2.6
3	O	122	ASP	2.6
2	G	145	GLU	2.6
3	J	82	GLU	2.6
3	O	167	PRO	2.6
1	F	39	ARG	2.6
1	F	187	ARG	2.6
1	F	56	ASP	2.6
1	K	96	GLN	2.6
2	G	229	ASP	2.6
2	N	313	MET	2.6
3	O	334	LEU	2.6
2	G	122	VAL	2.6
2	G	23	HIS	2.6
2	H	83	GLU	2.6
2	H	164	VAL	2.5
2	H	165	THR	2.5
2	M	90	LEU	2.5
3	O	129	LEU	2.5
2	N	15	PHE	2.5
2	H	79	CYS	2.5
3	O	32	LEU	2.5
1	F	201	ARG	2.5
2	C	122	VAL	2.5
2	H	54	ILE	2.5
2	B	313	MET	2.5
2	N	206	LEU	2.5
3	O	109	ALA	2.5
3	O	18	TYR	2.5
2	C	89	ASP	2.5
1	F	41	VAL	2.5
3	J	307	ASN	2.5
3	O	184	GLN	2.5
3	E	334	LEU	2.5
3	O	237	ASN	2.5
2	I	92	GLU	2.5
2	N	325	ILE	2.5
2	G	368	PRO	2.5
2	M	100	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	G	184	ARG	2.5
2	M	307	ALA	2.5
1	F	151	VAL	2.5
2	H	109	ASP	2.5
1	F	131	ALA	2.5
2	C	111	VAL	2.5
2	B	112	GLN	2.4
2	M	43	PHE	2.4
1	A	267	THR	2.4
2	H	178	LEU	2.4
1	A	110	LEU	2.4
3	E	307	ASN	2.4
2	C	82	ILE	2.4
2	H	91	ILE	2.4
2	G	98	ARG	2.4
2	M	147	PRO	2.4
2	M	172	GLN	2.4
3	O	139	THR	2.4
2	G	28	LEU	2.4
2	B	41	TYR	2.4
2	M	176	LYS	2.4
2	N	62	LEU	2.4
2	B	104	THR	2.4
3	O	283	PRO	2.4
1	A	71	MET	2.4
2	C	126	ASP	2.4
1	F	238	LEU	2.4
3	O	252	LEU	2.4
1	A	193	PRO	2.4
3	J	51	GLN	2.4
3	O	80	ALA	2.4
3	O	135	PRO	2.4
2	M	243	THR	2.4
2	I	6	LEU	2.4
2	B	267	LEU	2.4
2	G	67	GLY	2.4
2	N	359	PHE	2.4
2	G	77	ASP	2.4
2	M	170	CYS	2.4
2	G	119	ARG	2.4
2	I	56	ARG	2.4
2	H	25	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	237	VAL	2.4
2	I	124	LEU	2.4
1	A	328	SER	2.4
2	G	196	ILE	2.4
2	M	94	ASP	2.4
1	F	102	GLY	2.3
2	M	178	LEU	2.3
2	M	285	MET	2.3
2	G	21	GLN	2.3
2	N	102	GLU	2.3
2	H	27	ALA	2.3
1	F	236	LEU	2.3
3	O	57	LYS	2.3
3	O	164	LEU	2.3
2	N	85	GLY	2.3
1	A	58	ASN	2.3
2	I	43	PHE	2.3
1	F	74	PHE	2.3
2	M	245	ASP	2.3
2	N	83	GLU	2.3
1	A	73	LEU	2.3
1	F	32	GLN	2.3
2	N	12	PRO	2.3
3	O	154	THR	2.3
1	F	103	LEU	2.3
1	F	147	LEU	2.3
1	K	239	GLU	2.3
2	N	296	GLN	2.3
1	K	74	PHE	2.3
2	C	152	PHE	2.3
2	G	167	LEU	2.3
2	G	215	ARG	2.3
2	L	23	HIS	2.3
3	O	206	GLN	2.3
1	F	72	SER	2.3
3	O	175	TRP	2.3
2	M	124	LEU	2.3
2	H	44	SER	2.3
2	H	125	ILE	2.3
2	C	169	ARG	2.3
3	O	248	LEU	2.3
3	O	128	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	I	39	HIS	2.3
1	A	80	LEU	2.2
1	F	123	ASN	2.2
2	M	60	LYS	2.2
2	M	109	ASP	2.2
1	F	5	TYR	2.2
1	F	331	LEU	2.2
1	F	148	PRO	2.2
2	C	92	GLU	2.2
3	O	130	LYS	2.2
2	H	56	ARG	2.2
2	L	265	MET	2.2
2	L	304	ASN	2.2
2	G	366	PRO	2.2
2	C	162	LEU	2.2
2	B	152	PHE	2.2
2	I	241	LEU	2.2
2	N	13	GLN	2.2
1	F	239	GLU	2.2
2	N	197	ALA	2.2
3	O	149	GLU	2.2
2	M	253	VAL	2.2
1	K	290	LEU	2.2
2	C	110	ASN	2.2
2	I	32	LEU	2.2
1	F	105	HIS	2.2
2	H	50	GLY	2.2
2	M	22	GLU	2.2
3	J	206	GLN	2.2
2	G	218	LEU	2.2
2	B	357	LEU	2.2
2	M	4	GLN	2.2
2	I	90	LEU	2.2
2	G	268	ILE	2.2
2	H	26	THR	2.2
1	K	142	PRO	2.2
2	B	135	SER	2.2
2	N	209	ALA	2.2
1	F	260	LEU	2.1
3	J	281	LEU	2.1
2	L	176	LYS	2.1
1	A	126	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
2	M	111	VAL	2.1
3	O	102	GLU	2.1
1	F	276	HIS	2.1
3	J	31	ALA	2.1
1	F	108	LEU	2.1
1	F	206	VAL	2.1
3	J	164	LEU	2.1
1	F	214	PRO	2.1
2	G	113	TYR	2.1
2	G	92	GLU	2.1
1	A	226	SER	2.1
2	G	267	LEU	2.1
3	J	7	LEU	2.1
3	E	81	PRO	2.1
1	A	19	ALA	2.1
3	E	79	LEU	2.1
2	B	354	LEU	2.1
2	L	354	LEU	2.1
1	K	1	MET	2.1
2	H	144	GLU	2.1
3	J	269	ASP	2.1
1	A	133	ARG	2.1
2	H	243	THR	2.1
3	O	24	HIS	2.1
1	A	22	LEU	2.1
3	O	76	TYR	2.1
2	B	7	ALA	2.1
3	O	138	GLU	2.1
2	C	246	ASP	2.1
3	O	43	ALA	2.1
2	C	131	LEU	2.1
2	L	286	LEU	2.1
2	I	68	ILE	2.1
3	O	41	ILE	2.1
2	D	169	ARG	2.0
1	F	115	ASN	2.0
2	G	115	PRO	2.0
2	C	93	ILE	2.0
1	A	112	VAL	2.0
1	F	1	MET	2.0
1	K	70	ALA	2.0
1	K	112	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	96	ALA	2.0
1	F	159	ASN	2.0
2	G	365	LEU	2.0
3	E	322	TYR	2.0
2	C	107	LEU	2.0
2	N	119	ARG	2.0
2	B	123	TYR	2.0
2	M	154	LEU	2.0
2	H	214	LEU	2.0
2	N	256	MET	2.0
2	B	91	ILE	2.0
2	H	84	GLN	2.0
2	N	268	ILE	2.0
1	A	100	LEU	2.0
2	C	244	LEU	2.0
2	I	70	ALA	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.