



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 08:34 pm BST

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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

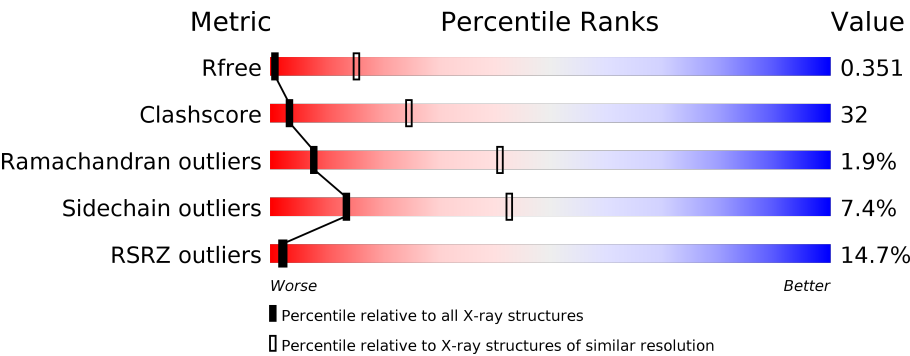
1 Overall quality at a glance i

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}	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div><div>9%</div><div><div>51%</div><div>41%</div><div>5%</div><div>..</div></div></div>
1	F	343	<div><div>50%</div><div><div>51%</div><div>41%</div><div>6%</div><div>..</div></div></div>
1	K	343	<div><div>7%</div><div><div>52%</div><div>39%</div><div>5%</div><div>..</div></div></div>
2	B	376	<div><div>9%</div><div><div>58%</div><div>33%</div><div>5%</div><div>..</div></div></div>
2	C	376	<div><div>6%</div><div><div>56%</div><div>39%</div><div>..</div></div></div>
2	D	376	<div><div>2%</div><div><div>55%</div><div>37%</div><div>..</div></div></div>

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Mol	Chain	Length	Quality of chain
2	G	376	<div><div></div><div>40%</div><div>54%</div><div>37%</div><div>5%</div><div></div></div>
2	H	376	<div><div></div><div>22%</div><div>56%</div><div>39%</div><div></div><div></div></div>
2	I	376	<div><div></div><div>9%</div><div>55%</div><div>38%</div><div></div><div></div></div>
2	L	376	<div><div></div><div>6%</div><div>57%</div><div>35%</div><div>5%</div><div></div></div>
2	M	376	<div><div></div><div>12%</div><div>54%</div><div>40%</div><div></div><div></div></div>
2	N	376	<div><div></div><div>10%</div><div>57%</div><div>36%</div><div></div><div></div></div>
3	E	334	<div><div></div><div>2%</div><div>60%</div><div>35%</div><div></div><div></div></div>
3	J	334	<div><div></div><div>5%</div><div>58%</div><div>36%</div><div>5%</div><div></div></div>
3	O	334	<div><div></div><div>29%</div><div>57%</div><div>37%</div><div>5%</div><div></div></div>

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

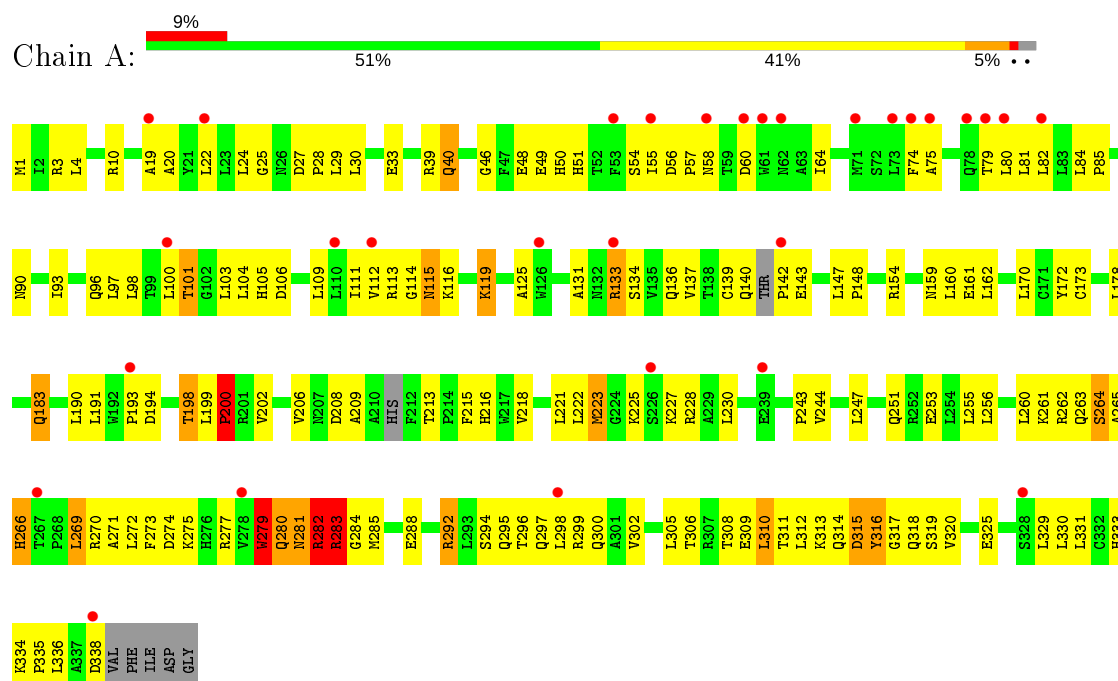
- Molecule 3 is a protein called DNA polymerase III subunit delta'.

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			

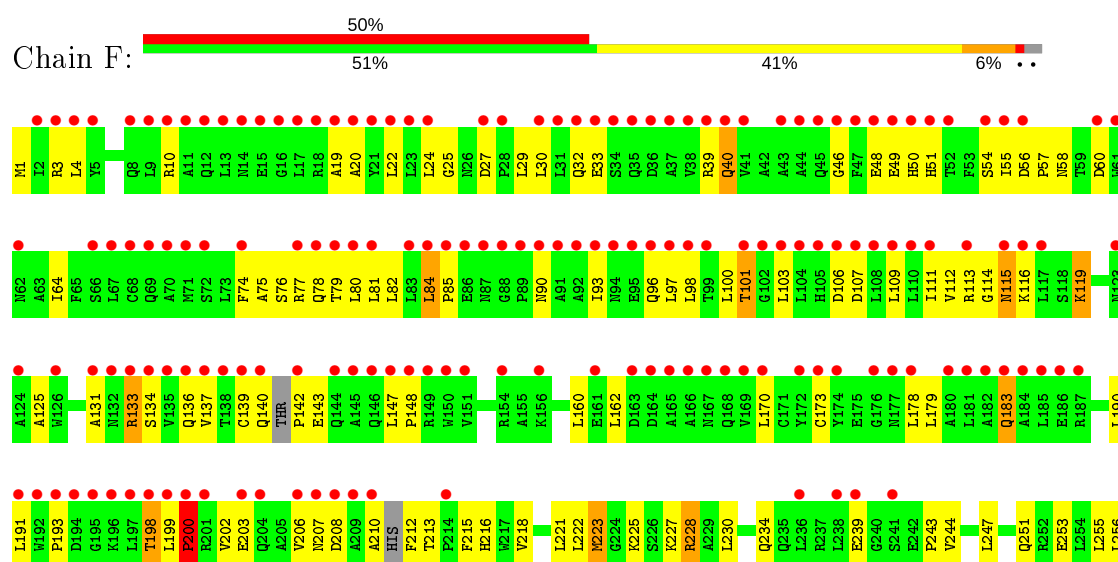
3 Residue-property plots

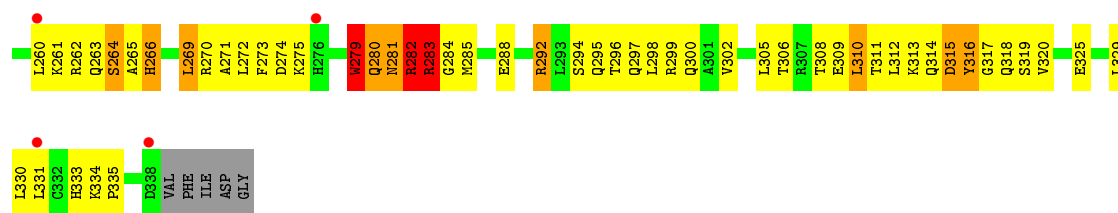
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: DNA polymerase III subunit delta

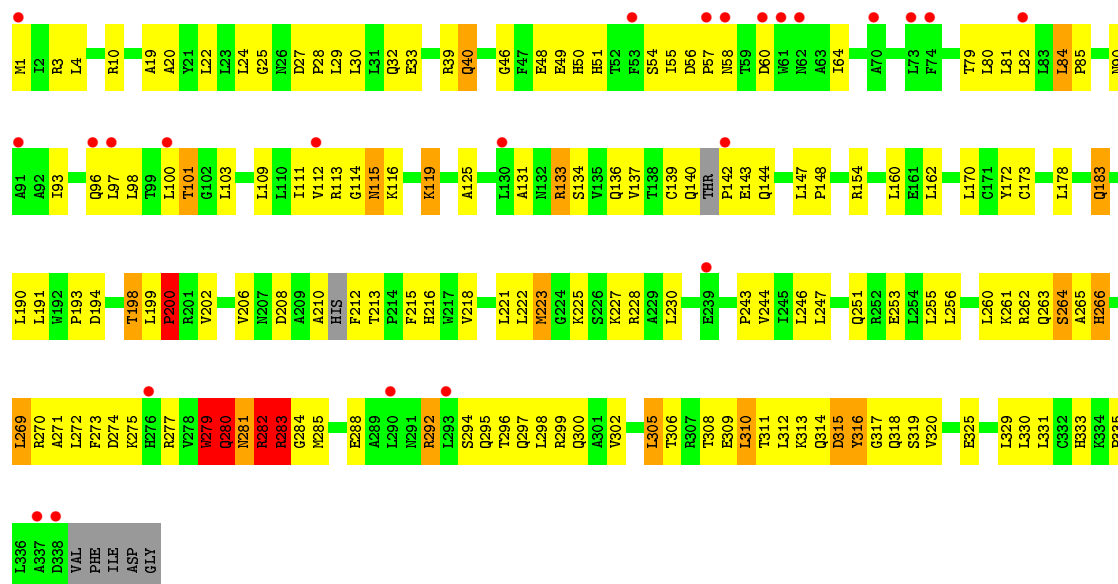


• Molecule 1: DNA polymerase III subunit delta

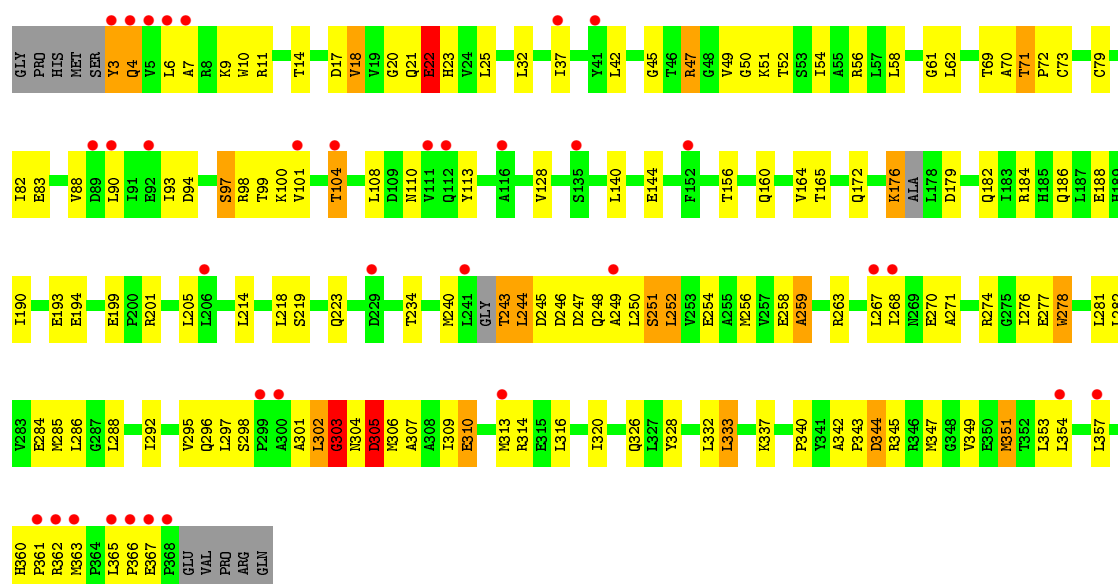




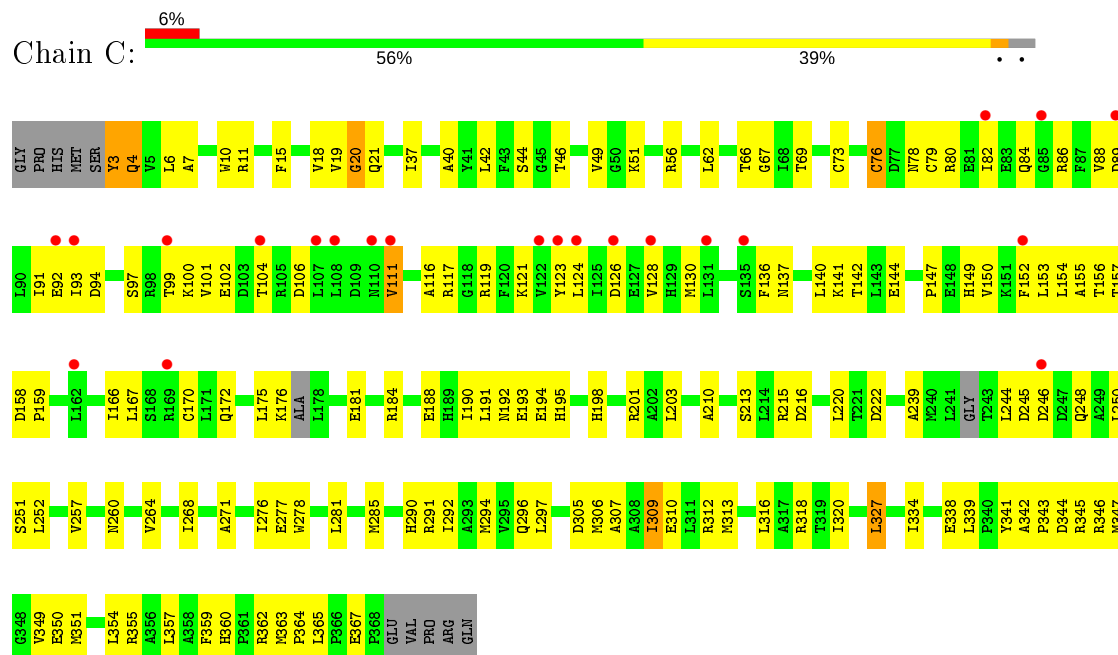
• Molecule 1: DNA polymerase III subunit delta



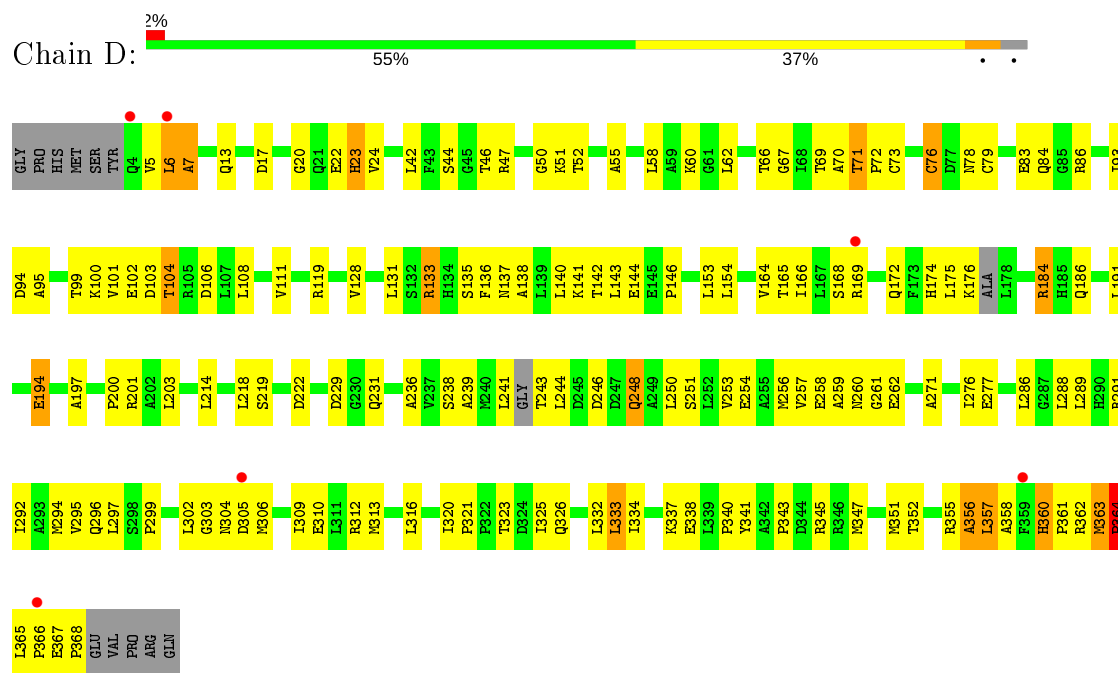
• Molecule 2: DNA polymerase III subunit tau



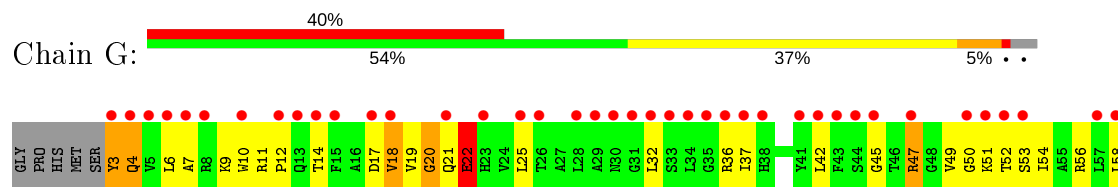
- Molecule 2: DNA polymerase III subunit tau

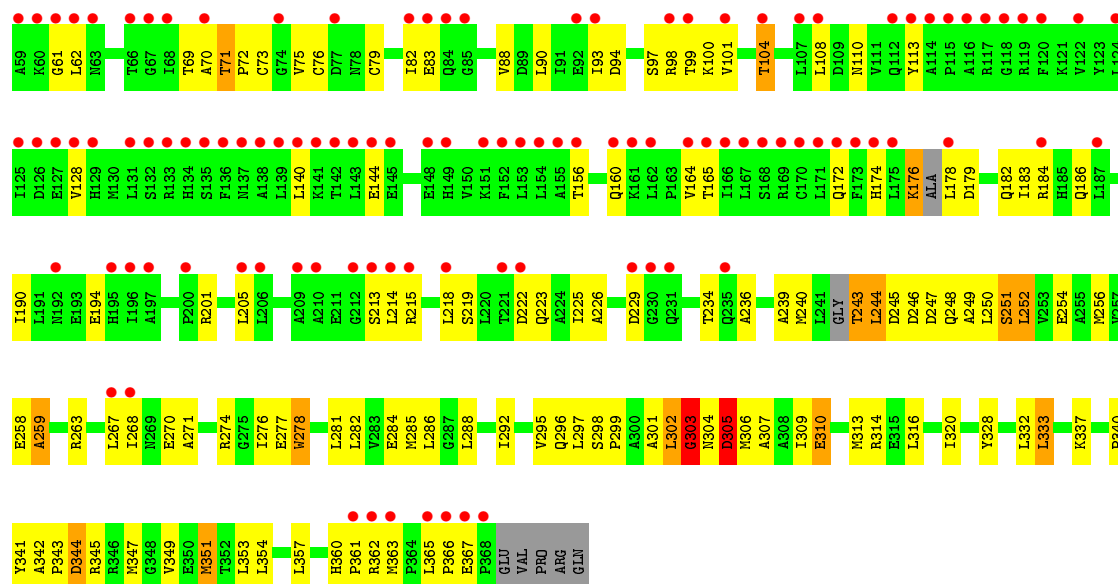


- Molecule 2: DNA polymerase III subunit tau

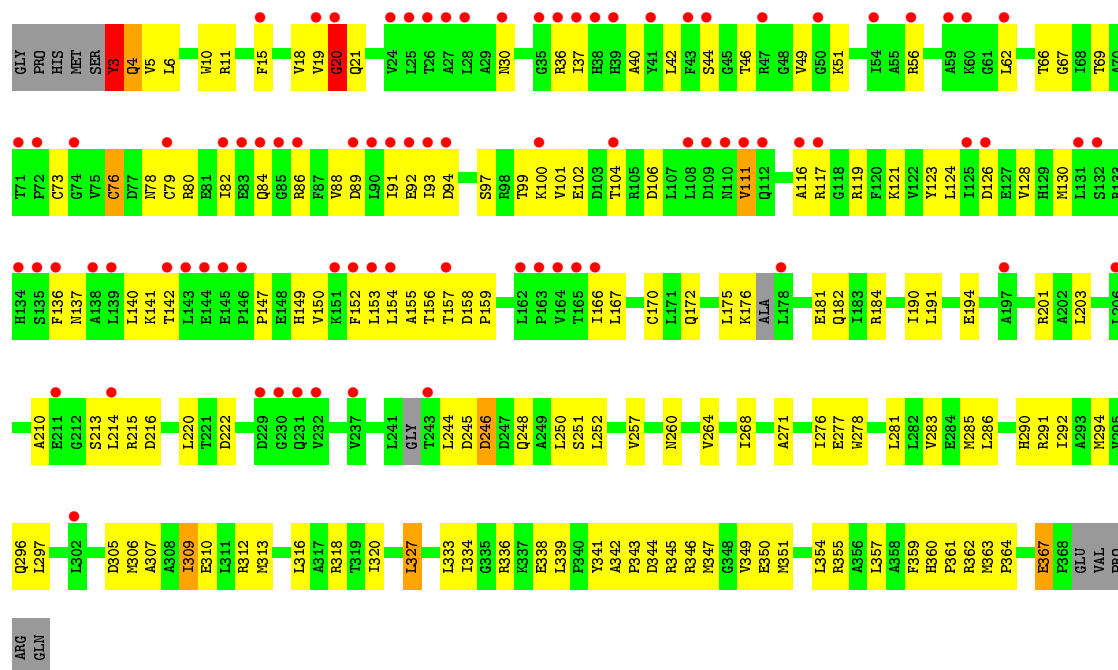


- Molecule 2: DNA polymerase III subunit tau

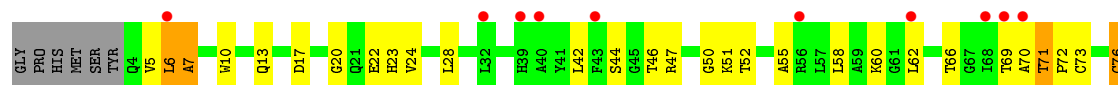


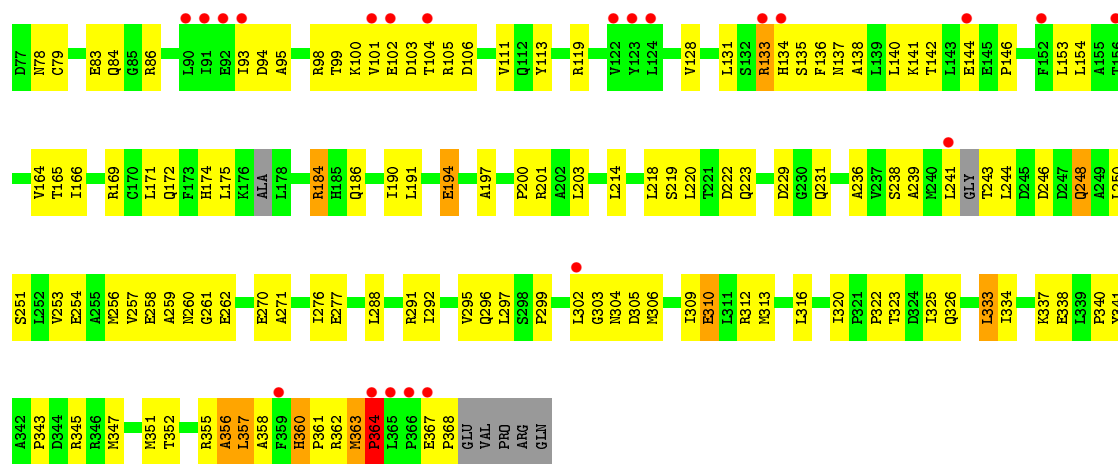


• Molecule 2: DNA polymerase III subunit tau

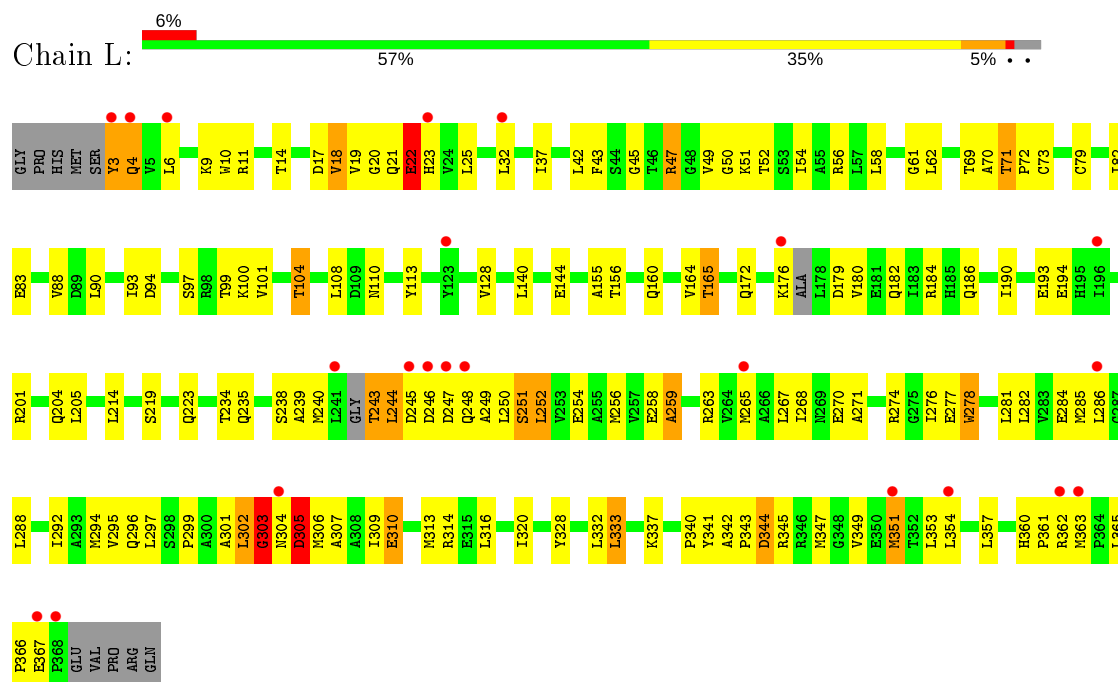


• Molecule 2: DNA polymerase III subunit tau

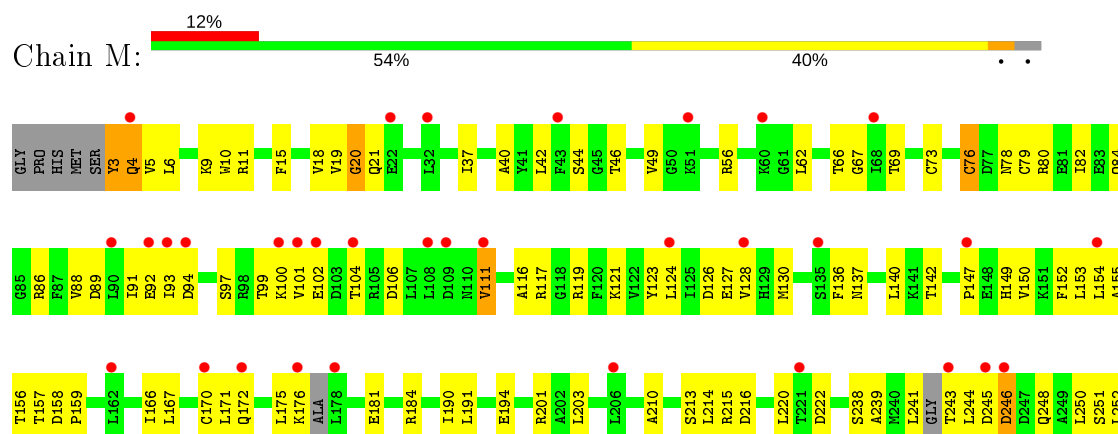


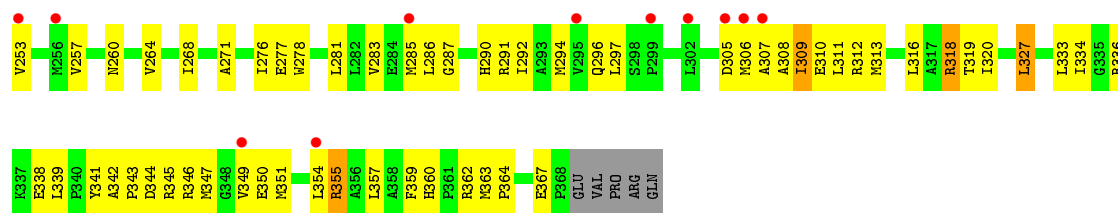


• Molecule 2: DNA polymerase III subunit tau

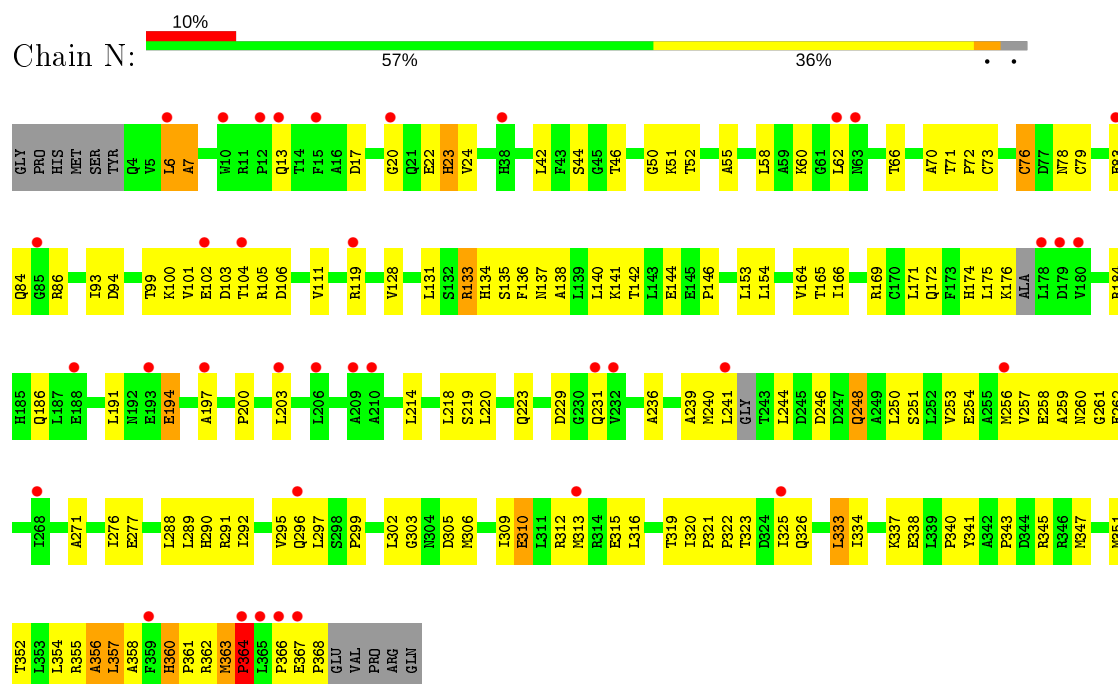


• Molecule 2: DNA polymerase III subunit tau

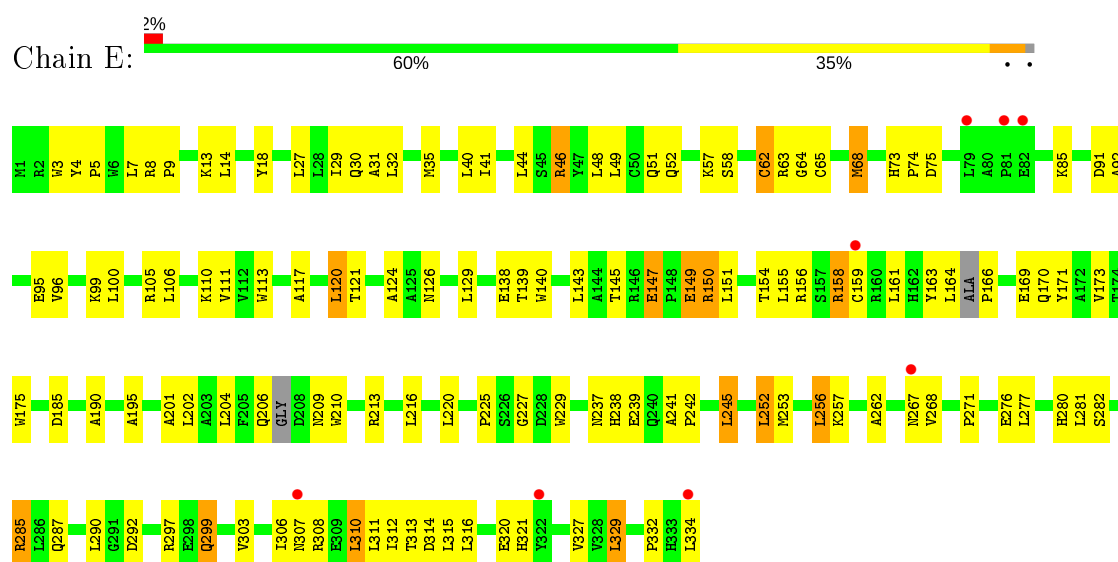




• Molecule 2: DNA polymerase III subunit tau

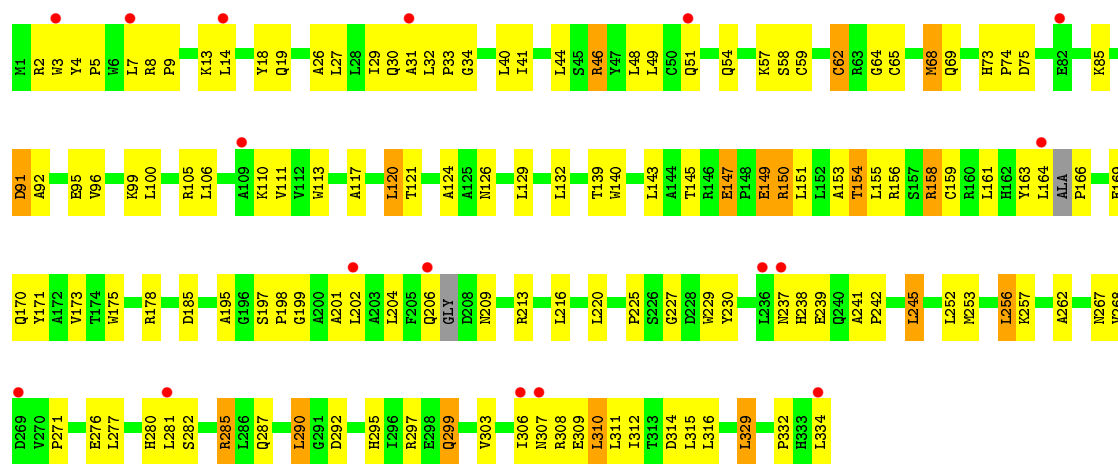


• Molecule 3: DNA polymerase III subunit delta'

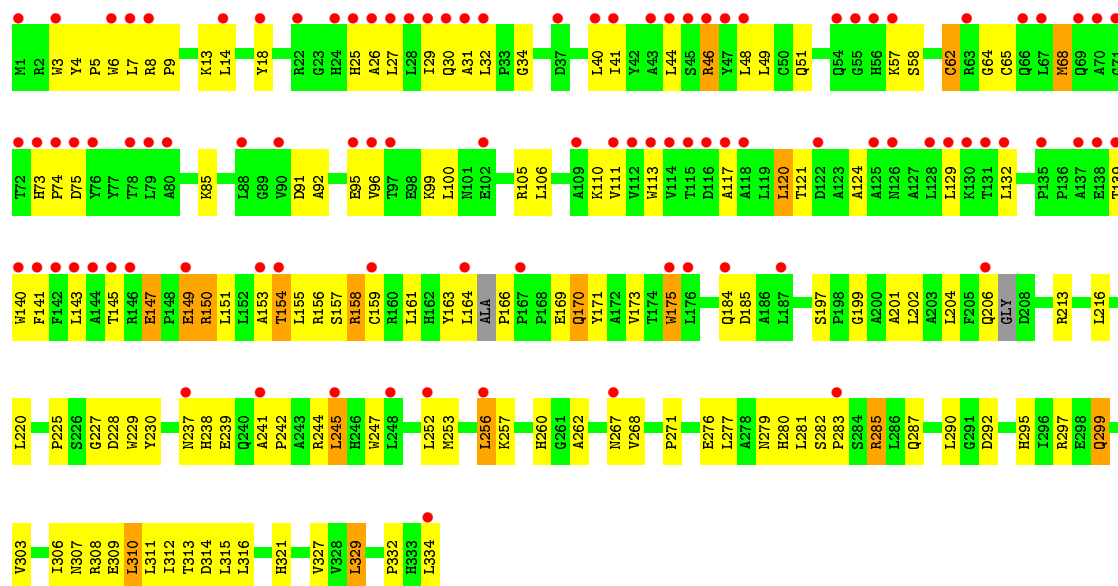


• Molecule 3: DNA polymerase III subunit delta'





• Molecule 3: DNA polymerase III subunit delta'



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.359 , 0.361 0.347 , 0.351	Depositor DCC
R_{free} test set	6264 reflections (4.88%)	wwPDB-VP
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
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-l	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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
1:A:193:PRO:CB	2:M:311:LEU:CD2	1.95	1.42
2:D:277:GLU:CB	3:E:149:GLU:HG2	1.48	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
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:H:86:ARG:NH1	2:I:141:LYS:HE2	1.43	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: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:N:363:MET:CE	2:N:363:MET:SD	2.27	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
1:A:193:PRO:HB3	2:M:311:LEU:CD2	1.61	1.22
2:D:363:MET:SD	2:D:363:MET:CE	2.27	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
1:F:315:ASP:CG	1:F:315:ASP:CB	2.13	1.17
2:I:277:GLU:HB3	3:J:149:GLU:CB	1.73	1.17
1:A:315:ASP:CG	1:A:315:ASP:CB	2.12	1.17
2:B:6:LEU:CD2	2:B:194:GLU:HG3	1.73	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
1:F:334:LYS:O	2:G:297:LEU:HD23	1.44	1.16
2:H:86:ARG:CZ	2:I:141:LYS:HE2	1.74	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:D:360:HIS:HB3	2:D:363:MET:CB	1.77	1.14
2:N:360:HIS:HB3	2:N: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
2:D:200:PRO:HB2	2:D:305:ASP:HB2	1.17	1.10
1:F:334:LYS:CB	2:G:297:LEU:HD21	1.80	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:N:277:GLU:HB3	3:O:149:GLU:CG	1.82	1.10
2:M:341:TYR:HB2	2:N:333:LEU:HD11	1.20	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
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
1:F:270:ARG:NH1	2:N:316:LEU:HA	1.66	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:H:100:LYS:CG	2:I:133:ARG:NE	2.18	1.06
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
1:A:161:GLU:OE2	2:M:318:ARG:HD3	1.27	1.05
1:F:29:LEU:HD22	1:F:179:LEU:HA	1.37	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:G:365:LEU:HD22	2:H:297:LEU:CD1	1.87	1.05
2:B:6:LEU:CD2	2:B:194:GLU:CG	2.30	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
2:M:201:ARG:CB	2:M:305:ASP:OD2	2.05	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: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:B:98:ARG:NH2	2:C:137:ASN:OD1	1.92	1.02
2:D:277:GLU:CB	3:E:149:GLU:CG	2.20	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:A:223:MET:SD	1:A:292:ARG:HB3	1.98	1.01
1:F:334:LYS:HB2	2:G:297:LEU:CD2	1.88	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:G:20:GLY:O	2:G:178:LEU:CD2	2.09	1.01
2:L:343:PRO:HA	2:M:283:VAL:HG13	1.40	1.01
2:D:363:MET:HB3	2:D:364:PRO:HD2	1.42	1.00
2:G:21:GLN:HG3	2:G:178:LEU:HD21	1.39	1.00
2:L:347:MET:SD	2:M:287:GLY:HA2	2.00	1.00
2:B:6:LEU:HD11	2:B:190:ILE:HG22	1.40	1.00
2:G:365:LEU:HD21	2:H:297:LEU:HD11	1.41	1.00
1:A:194:ASP:N	2:M:311:LEU:HD11	1.76	1.00
2:B:97:SER:CB	2:C:144:GLU:OE2	2.09	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:19:VAL:HG22	2:G:186:GLN:HG2	1.03	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
1:A:106:ASP:OD1	1:F:225:LYS:HD3	1.61	0.99
2:G:10:TRP:CZ3	2:G:190:ILE:CG2	2.45	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
1:K:28:PRO:HB3	2:L:164:VAL:HG21	1.42	0.98
2:N:366:PRO:CB	3:O:282:SER:HB2	1.92	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:B:354:LEU:HD11	2:C:294:MET:SD	2.02	0.98
2:D:73:CYS:SG	2:D:76:CYS:HB3	2.04	0.98
1:A:119:LYS:H	1:A:119:LYS:HD3	1.26	0.98
2:N:241:LEU:O	3:O:156:ARG:HD2	1.62	0.98
2:I:241:LEU:O	3:J:156:ARG:NH1	1.97	0.98
2:I:73:CYS:SG	2:I:76:CYS:HB3	2.04	0.98
2:L:238:SER:C	2:L:243:THR:OG1	1.84	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
1:F:315:ASP:HB2	1:F:318:GLN:CG	1.94	0.97
2:G:12:PRO:HD3	2:G:215:ARG:HH12	1.27	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
2:N:220:LEU:HD21	3:O:154:THR:HA	1.46	0.97
2:G:6:LEU:HD12	2:G:222:ASP:HA	1.43	0.97
2:L:354:LEU:CD1	2:M:294:MET:SD	2.53	0.97
2:N:345:ARG:NH2	3:O:150:ARG:CZ	2.28	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
2:L:347:MET:CG	2:M:290:HIS:CD2	2.47	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
1:A:310:LEU:HD22	1:A:314:GLN:HE21	1.27	0.96
2:C:86:ARG:CZ	2:D:141:LYS:HB2	1.94	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
2:L:18:VAL:HG22	2:L:25:LEU:HD11	1.47	0.96
1:K:333:HIS:HB2	2:L:297:LEU:HD21	1.45	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
1:A:105:HIS:HA	1:F:227:LYS:CE	1.96	0.96
2:G:10:TRP:CZ2	2:G:190:ILE:HG23	2.01	0.96
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:L:6:LEU:HD13	2:L:190:ILE:HG22	1.44	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:213:THR:H	1:K:216:HIS:HD2	1.13	0.95
1:K:333:HIS:CD2	2:L:297:LEU:HD21	1.98	0.95
2:G:53:SER:OG	2:G:215:ARG:NH2	2.00	0.95
2:H:86:ARG:NH2	2:I:141:LYS:HE2	1.80	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:C:341:TYR:HB2	2:D:333:LEU:HD11	1.48	0.95
2:N:357:LEU:HA	2:N:363:MET:SD	2.06	0.95
2:B:6:LEU:HD21	2:B:194:GLU:HG2	1.46	0.94
1:F:334:LYS:O	2:G:297:LEU:CD2	2.14	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
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
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:238:SER:HB3	2:L:244:LEU:H	1.33	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: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:H:341:TYR:HB2	2:I:333:LEU:CD1	2.00	0.91
2:G:94:ASP:H	2:G:100:LYS:HZ3	1.09	0.91
2:L:205:LEU:HD22	2:L:244:LEU:HD12	1.51	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:H:86:ARG:NH1	2:I:141:LYS:HZ3	1.69	0.91
2:G:6:LEU:HD11	2:G:225:ILE:HD12	1.53	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
1:A:105:HIS:N	1:F:227:LYS:HZ2	1.68	0.91
2:G:10:TRP:HZ3	2:G:190:ILE:HG12	1.29	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:105:HIS:HA	1:F:227:LYS:NZ	1.85	0.90
1:A:193:PRO:C	2:M:311:LEU:HD11	1.91	0.90
1:A:75:ALA:HB2	1:F:207:ASN:HD22	1.36	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
1:A:338:ASP:OD2	2:B:326:GLN:OE1	1.91	0.89
1:A:105:HIS:CA	1:F:227:LYS:HZ2	1.85	0.89
2:I:357:LEU:O	2:I:363:MET:SD	2.31	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:B:94:ASP:N	2:B:100:LYS:NZ	2.21	0.88
2:D:357:LEU:O	2:D:363:MET:SD	2.31	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:B:98:ARG:NH1	2:C:137:ASN:HB3	1.88	0.87
2:N:363:MET:CB	2:N:364:PRO:HD2	2.04	0.87
2:I:309:ILE:CG2	2:I:313:MET:HG2	2.05	0.87
1:A:105:HIS:CA	1:F:227:LYS:NZ	2.38	0.87
2:C:86:ARG:NH2	2:D:138:ALA:HA	1.89	0.87
1:F:270:ARG:CZ	2:N:316:LEU:HA	2.03	0.87
1:F:334:LYS:HB2	2:G:297:LEU:HD21	0.92	0.87
1:A:75:ALA:HB3	1:F:207:ASN:CG	1.95	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:M:341:TYR:CB	2:N:333:LEU:CD1	2.52	0.86
2:D:309:ILE:CG2	2:D:313:MET:HG2	2.05	0.86
2:C:215:ARG:NH2	2:D:164:VAL:CG2	2.38	0.86
2:L:94:ASP:N	2:L:100:LYS:NZ	2.21	0.86
2:I:363:MET:CB	2:I:364:PRO:HD2	2.04	0.86
2:N:345:ARG:CZ	3:O:150:ARG:HH21	1.89	0.86
2:B:6:LEU:HD13	2:B:190:ILE:HG22	1.02	0.86
2:I:277:GLU:CD	3:J:149:GLU:HG3	1.96	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:C:100:LYS:HG2	2:D:133:ARG:HE	1.04	0.85
2:M:215:ARG:CZ	2:N:164:VAL:CG2	2.55	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
3:E:204:LEU:O	3:E:209:ASN:HB2	1.76	0.84
2:G:10:TRP:CZ3	2:G:190:ILE:CG1	2.61	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:H:271:ALA:HB1	2:H:276:ILE:HD11	1.57	0.83
2:N:355:ARG:NH1	3:O:287:GLN:HB3	1.91	0.83
1:A:193:PRO:CA	2:M:311:LEU:HD21	2.07	0.83
2:C:10:TRP:CZ2	2:C:190:ILE:HG23	2.13	0.83
2:G:179:ASP:HB3	2:G:182:GLN:HB2	1.58	0.83
1:K:312:LEU:HB2	1:K:320:VAL:HG21	1.60	0.83
2:L:180:VAL:HG21	2:L:304:ASN:ND2	1.92	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
2:C:341:TYR:HB2	2:D:333:LEU:CD1	2.08	0.83
1:F:283:ARG:HD3	2:N:315:GLU:OE2	1.79	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
1:A:194:ASP:CA	2:M:311:LEU:HD11	2.08	0.83
2:N:357:LEU:HA	2:N:363:MET:CE	2.09	0.83
2:C:100:LYS:CG	2:D:133:ARG:HE	1.84	0.82
2:G:94:ASP:H	2:G:100:LYS:HZ1	1.23	0.82
2:I:345:ARG:HE	3:J:150:ARG:HH21	0.83	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:I:357:LEU:HA	2:I:363:MET:CE	2.09	0.82
2:M:99:THR:O	2:M:99:THR:HG22	1.78	0.82
1:A:161:GLU:HG3	2:M:318:ARG:CZ	2.09	0.82
2:L:10:TRP:HH2	2:L:193:GLU:OE1	1.61	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
2:L:3:TYR:O	2:L:4:GLN:HG3	1.79	0.82
1:F:270:ARG:HH11	2:N:316:LEU:HD23	1.02	0.82
2:B:94:ASP:C	2:B:100:LYS:HZ1	1.84	0.82
2:C:99:THR:HG22	2:C:99:THR:O	1.78	0.82
2:H:10:TRP:CZ2	2:H:190:ILE:HG23	2.15	0.82
2:L:6:LEU:CD1	2:L:190:ILE:HG22	2.10	0.81
2:G:19:VAL:HG11	2:G:183:ILE:HA	1.61	0.81
2:H:309:ILE:HG13	2:H:313:MET:HG2	1.62	0.81
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:K:333:HIS:CD2	2:L:297:LEU:HD23	2.14	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:I:360:HIS:ND1	2:I:363:MET:CE	2.43	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: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
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
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:C:309:ILE:HG13	2:C:313:MET:HG2	1.62	0.81
1:F:29:LEU:HD22	1:F:178:LEU:C	2.02	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
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: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
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
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:H:67:GLY:HA2	2:H:119:ARG:HH12	1.47	0.80
2:M:67:GLY:HA2	2:M:119:ARG:HH12	1.47	0.80
1:A:104:LEU:O	1:F:227:LYS:NZ	2.10	0.80
2:C:359:PHE:CE2	2:D:323:THR:HG23	2.15	0.80
2:H:99:THR:HG22	2:H:99:THR:O	1.78	0.80
2:L:354:LEU:HD21	2:M:297:LEU:HD22	1.60	0.80
2:M:309:ILE:HG13	2:M:313:MET:HG2	1.62	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:345:ARG:NH2	3:O:150:ARG:NH2	2.28	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:D:259:ALA:HB2	2:D:363:MET:CG	2.12	0.80
2:G:10:TRP:HZ2	2:G:194:GLU:CG	1.95	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:G:12:PRO:HD3	2:G:215:ARG:NH1	1.96	0.79
2:L:265:MET:CE	2:M:294:MET:HE1	2.12	0.79
3:J:58:SER:HB3	3:J:65:CYS:SG	2.21	0.79
2:N:259:ALA:HB2	2:N:363:MET:CG	2.12	0.79
2:H:56:ARG:NH2	2:I:165:THR:HG23	1.96	0.79
2:N:345:ARG:HE	3:O:150:ARG:HH21	1.29	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:A:310:LEU:HD22	1:A:314:GLN:NE2	1.98	0.79
1:K:333:HIS:CD2	2:L:297:LEU:HG	2.17	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
2:B:362:ARG:HE	2:B:363:MET:HE2	1.48	0.79
1:F:283:ARG:CD	2:N:315:GLU:OE2	2.31	0.79
1:F:310:LEU:HD22	1:F:314:GLN:NE2	1.98	0.79
2:N:366:PRO:HB3	3:O:283:PRO:HD2	1.63	0.79
2:L:99:THR:HG22	2:L:99:THR:O	1.83	0.79
1:A:315:ASP:HB2	1:A:318:GLN:HG3	1.63	0.79
2:I:253:VAL:O	2:I:257:VAL:HG23	1.80	0.79
1:K:251:GLN:OE1	3:O:307:ASN:ND2	2.16	0.79
2:N:360:HIS:CB	2:N:363:MET:CG	2.61	0.79
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:259:ALA:HB2	2:I:363:MET:CG	2.12	0.78
2:I:99:THR:O	2:I:99:THR:HG22	1.81	0.78
2:L:94:ASP:C	2:L:100:LYS:HZ1	1.86	0.78
2:L:6:LEU:CD2	2:L:194:GLU:CG	2.44	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:H:86:ARG:HH11	2:I:141:LYS:NZ	1.81	0.78
2:M:80:ARG:O	2:M:84:GLN:HG3	1.82	0.78
2:B:248:GLN:HG3	2:B:267:LEU:HB3	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:271:ALA:CB	2:C:276:ILE:HD11	2.13	0.78
2:D:363:MET:HB3	2:D:364:PRO:CD	2.14	0.78
2:D:345:ARG:NE	3:E:150:ARG:NH2	1.90	0.78
2:C:351:MET:HE1	2:D:326:GLN:HE22	1.46	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:80:ARG:O	2:C:84:GLN:HG3	1.82	0.78
2:D:360:HIS:CB	2:D:363:MET:CG	2.61	0.78
2:H:86:ARG:NH2	2:I:138:ALA:HA	1.95	0.78
2:H:56:ARG:HH21	2:I:165:THR:HG23	1.49	0.78
1:K:222:LEU:O	1:K:223:MET:HB2	1.83	0.78
2:D:13:GLN:HE22	2:D:83:GLU:HG2	1.49	0.78
2:G:351:MET:CG	2:H:290:HIS:ND1	2.46	0.78
2:L:239:ALA:N	2:L:243:THR:OG1	2.15	0.78
2:B:45:GLY:O	2:B:51:LYS:HE2	1.84	0.78
2:D:345:ARG:NH1	3:E:150:ARG:HG3	1.98	0.78
3:E:204:LEU:O	3:E:209:ASN:CB	2.32	0.78
1:F:270:ARG:HE	2:N:319:THR:HG21	1.49	0.78
2:G:45:GLY:O	2:G:51:LYS:HE2	1.84	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
1:K:144:GLN:OE1	1:K:280:GLN:O	2.01	0.78
1:K:310:LEU:HD22	1:K:314:GLN:NE2	1.98	0.78
2:N:244:LEU:HD21	2:N:276:ILE:HG12	1.66	0.78
2:B:99:THR:O	2:B:99:THR:HG22	1.83	0.78
1:K:29:LEU:HD21	1:K:154:ARG:HH12	1.49	0.78
1:K:333:HIS:CD2	2:L:297:LEU:CG	2.66	0.78
1:A:300:GLN:OE1	1:A:335:PRO:CG	2.32	0.78
2:G:248:GLN:HG3	2:G:267:LEU:HB3	1.65	0.78
2:H:93:ILE:CG2	2:H:100:LYS:NZ	2.47	0.78
2:H:97:SER:OG	2:H:100:LYS:HE3	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:180:VAL:CG1	2:L:305:ASP:OD2	2.31	0.78
2:L:4:GLN:OE1	2:L:9:LYS:HD2	1.84	0.78
2:M:341:TYR:CB	2:N:333:LEU:HD13	2.14	0.78
1:F:315:ASP:HB2	1:F:318:GLN:HG3	1.63	0.77
2:C:93:ILE:CG2	2:C:100:LYS:NZ	2.48	0.77
2:G:99:THR:O	2:G:99:THR:HG22	1.83	0.77
2:M:111:VAL:HG11	2:M:142:THR:HG21	1.66	0.77
2:M:86:ARG:HH22	2:N:141:LYS:HE2	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:270:ARG:NH2	2:N:316:LEU:HA	1.99	0.77
2:C:111:VAL:HG11	2:C:142:THR:HG21	1.66	0.77
2:B:365:LEU:HD22	2:C:297:LEU:CD1	2.14	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
1:F:29:LEU:HB2	1:F:179:LEU:HB2	1.64	0.77
1:F:300:GLN:OE1	1:F:335:PRO:CG	2.32	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:29:LEU:CG	1:F:179:LEU:HB2	2.15	0.77
1:K:244:VAL:HG22	1:K:312:LEU:HD21	1.64	0.77
2:M:281:LEU:HD23	2:M:285:MET:HE2	1.66	0.77
2:N:363:MET:HB3	2:N:364:PRO:CD	2.14	0.77
2:B:4:GLN:OE1	2:B:9:LYS:HD2	1.84	0.77
2:C:128:VAL:HG11	2:C:154:LEU:HD22	1.67	0.77
2:C:67:GLY:HA2	2:C:119:ARG:HH12	1.47	0.77
2:M:93:ILE:CG2	2:M:100:LYS:NZ	2.47	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:H:111:VAL:HG11	2:H:142:THR:HG21	1.67	0.77
2:L:93:ILE:HG23	2:L:100:LYS:HZ2	1.48	0.77
1:F:262:ARG:NH1	3:J:230:TYR:HB3	1.99	0.77
1:A:336:LEU:HD12	2:B:326:GLN:NE2	2.00	0.77
2:C:97:SER:OG	2:C:100:LYS:HE3	1.83	0.77
2:C:3:TYR:O	2:C:3:TYR:CD2	2.38	0.77
2:L:45:GLY:O	2:L:51:LYS:HE2	1.84	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:C:10:TRP:CE2	2:C:190:ILE:HG23	2.19	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:M:354:LEU:CD2	2:N:297:LEU:HD22	2.15	0.76
2:N:355:ARG:HH12	3:O:287:GLN:HB3	1.49	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:244:VAL:HG22	1:A:312:LEU:HD21	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:42:LEU:HB3	2:I:172:GLN:HB3	1.67	0.76
2:L:248:GLN:HG3	2:L:267:LEU:HB3	1.66	0.76
2:M:3:TYR:O	2:M:3:TYR:CD2	2.38	0.76
2:N:42:LEU:HB3	2:N:172:GLN:HB3	1.67	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:B:10:TRP:HH2	2:B:193:GLU:OE1	1.69	0.75
2:C:281:LEU:HD23	2:C:285:MET:HE2	1.66	0.75
2:L:180:VAL:CG2	2:L:304:ASN:CB	2.65	0.75
1:A:310:LEU:HD13	1:A:314:GLN:NE2	2.02	0.75
2:G:21:GLN:N	2:G:178:LEU:HD21	2.01	0.75
2:L:271:ALA:HB1	2:L:276:ILE:HD12	1.68	0.75
3:O:4:TYR:HD1	3:O:175:TRP:CH2	2.04	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: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:D:42:LEU:HB3	2:D:172:GLN:HB3	1.67	0.75
2:G:351:MET:HG2	2:H:290:HIS:ND1	2.01	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: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:L:347:MET:CG	2:M:290:HIS:CG	2.68	0.75
2:B:98:ARG:HH12	2:C:137:ASN:HB3	1.42	0.75
2:H:351:MET:HE1	2:I:326:GLN:NE2	1.97	0.75
2:D:257:VAL:O	2:D:360:HIS:HE1	1.69	0.75
2:B:271:ALA:HB1	2:B:276:ILE:HD12	1.68	0.75
2:C:215:ARG:NH2	2:D:164:VAL:HG21	2.01	0.75
2:G:271:ALA:HB1	2:G:276:ILE:HD12	1.68	0.75
2:M:94:ASP:O	2:M:100:LYS:CE	2.35	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:CZ	2:D:164:VAL:HG22	2.16	0.75
2:H:276:ILE:HD13	2:H:281:LEU:HD12	1.69	0.75
2:I:259:ALA:CB	2:I:363:MET:HG2	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:257:VAL:O	2:I:360:HIS:HE1	1.69	0.75
2:I:6:LEU:O	2:I:218:LEU:HB3	1.87	0.74
1:K:310:LEU:HD13	1:K:314:GLN:NE2	2.01	0.74
2:N:366:PRO:CA	3:O:283:PRO:HD2	2.16	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
3:E:5:PRO:O	3:E:8:ARG:HG2	1.87	0.74
2:G:365:LEU:CD2	2:H:297:LEU:HD13	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:L:343:PRO:CA	2:M:283:VAL:HG13	2.17	0.74
2:C:276:ILE:HD13	2:C:281:LEU:HD12	1.69	0.74
2:H:3:TYR:O	2:H:4:GLN:CG	2.36	0.74
2:L:180:VAL:HG11	2:L:305:ASP:OD2	1.88	0.74
2:N:345:ARG:NH2	3:O:150:ARG:HH21	1.85	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: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: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:B:259:ALA:HB3	2:B:363:MET:HE3	1.68	0.74
2:M:86:ARG:NH2	2:N:141:LYS:HE2	1.70	0.74
2:C:93:ILE:HG22	2:C:100:LYS:NZ	2.03	0.73
2:C:156:THR:HG22	2:C:158:ASP:H	1.53	0.73
2:C:3:TYR:O	2:C:4:GLN:HG3	1.88	0.73
2:G:12:PRO:HD2	2:G:215:ARG:HH22	1.52	0.73
2:N:358:ALA:HA	2:N:364:PRO:HG2	1.71	0.73
3:O:6:TRP:CZ3	3:O:175:TRP:CD2	2.74	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
1:K:147:LEU:HB3	1:K:148:PRO:HD3	1.69	0.73
2:N:366:PRO:CB	3:O:282:SER:CB	2.65	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:G:7:ALA:N	2:G:222:ASP:OD2	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:366:PRO:CB	3:O:283:PRO:HD2	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
2:G:49:VAL:HA	2:G:213:SER:CB	2.18	0.73
1:F:283:ARG:CZ	2:N:315:GLU:OE2	2.14	0.73
2:D:360:HIS:ND1	2:D:363:MET:HE2	2.02	0.73
2:D:360:HIS:CG	2:D:363:MET:HG3	2.23	0.73
2:H:94:ASP:C	2:H:100:LYS:HZ1	1.91	0.73
2:I:358:ALA:HA	2:I:364:PRO:HG2	1.71	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
3:E:49:LEU:HD23	3:E:68:MET:SD	2.29	0.73
1:K:273:PHE:HB3	1:K:279:TRP:CB	2.18	0.73
1:A:82:LEU:HD21	1:A:100:LEU:HD12	1.70	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
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:E:117:ALA:O	3:E:120:LEU:HD22	1.89	0.72
3:O:5:PRO:O	3:O:8:ARG:HG2	1.87	0.72
2:C:56:ARG:NH2	2:D:165:THR:CG2	2.52	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
1:A:194:ASP:HA	2:M:311:LEU:CD1	2.19	0.72
2:I:360:HIS:CG	2:I:363:MET:HG3	2.23	0.72
1:A:106:ASP:CB	1:F:225:LYS:CD	2.58	0.72
2:I:271:ALA:HB1	2:I:276:ILE:CD1	2.19	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
1:A:147:LEU:HB3	1:A:148:PRO:HD3	1.69	0.72
3:J:117:ALA:O	3:J:120:LEU:HD22	1.89	0.72
2:M:215:ARG:HH22	2:N:164:VAL:CG2	2.00	0.72
2:B:6:LEU:HD13	2:B:190:ILE:HG23	1.59	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:156:THR:HG22	2:H:158:ASP:H	1.54	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:D:259:ALA:HB1	2:D:363:MET:HG2	1.72	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:M:201:ARG:HB2	2:M:305:ASP:CG	2.11	0.72
2:N:357:LEU:HA	2:N:363:MET:HE1	1.71	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:C:215:ARG:NH2	2:D:164:VAL:HG22	2.05	0.71
1:K:223:MET:SD	1:K:292:ARG:CB	2.78	0.71
2:M:86:ARG:NH2	2:N:138:ALA:HA	2.02	0.71
2:N:356:ALA:O	2:N:363:MET:HE1	1.90	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:D:241:LEU:O	3:E:156:ARG:NH1	2.22	0.71
2:N:345:ARG:HH21	3:O:150:ARG:NH2	1.87	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
2:G:12:PRO:CD	2:G:215:ARG:HH12	2.03	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:C:351:MET:CE	2:D:326:GLN:HE22	2.04	0.71
2:G:226:ALA:HB2	2:H:36:ARG:HH11	1.56	0.71
2:L:6:LEU:CD1	2:L:190:ILE:CG2	2.61	0.71
2:M:360:HIS:HB3	2:M:363:MET:O	1.91	0.71
1:A:213:THR:H	1:A:216:HIS:CD2	2.04	0.71
1:A:29:LEU:HD21	1:A:154:ARG:HH12	1.56	0.71
2:B:98:ARG:NH1	2:C:137:ASN:OD1	2.24	0.71
2:H:93:ILE:HG23	2:I:133:ARG:HH22	1.55	0.71
2:N:354:LEU:HD12	3:O:253:MET:CE	2.20	0.71
1:F:29:LEU:CD1	1:F:179:LEU:CB	2.42	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: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
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
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:M:351:MET:CE	2:N:326:GLN:NE2	2.35	0.70
1:F:202:VAL:O	1:F:206:VAL:HG23	1.92	0.70
1:F:213:THR:H	1:F:216:HIS:CD2	2.04	0.70
2:G:10:TRP:CZ2	2:G:194:GLU:CG	2.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:360:HIS:HB3	2:C:363:MET:O	1.91	0.70
2:I:360:HIS:ND1	2:I:363:MET:HE2	2.06	0.70
1:F:270:ARG:HH12	2:N:316:LEU:HD23	0.87	0.70
1:A:300:GLN:OE1	1:A:335:PRO:HG3	1.91	0.70
2:B:98:ARG:CZ	2:C:137:ASN:OD1	2.38	0.70
2:D:5:VAL:HG13	2:D:222:ASP:CG	2.12	0.70
3:E:169:GLU:O	3:E:173:VAL:HG23	1.92	0.70
1:K:300:GLN:OE1	1:K:335:PRO:HG3	1.91	0.70
2:N:259:ALA:HB1	2:N:363:MET:HG2	1.72	0.70
2:G:10:TRP:CZ2	2:G:194:GLU:HG3	2.26	0.70
3:J:169:GLU:O	3:J:173:VAL:HG23	1.91	0.70
2:M:341:TYR:HB3	2:N:333:LEU:HD13	1.73	0.70
2:N:220:LEU:HD21	3:O:154:THR:CA	2.22	0.70
1:A:313:LYS:O	1:A:316:TYR:CZ	2.44	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: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
2:H:73:CYS:O	2:H:79:CYS:SG	2.50	0.70
1:K:313:LYS:O	1:K:316:TYR:CZ	2.44	0.70
1:A:315:ASP:CG	1:A:315:ASP:CA	2.61	0.69
2:B:6:LEU:CD1	2:B:190:ILE:HG21	1.92	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:313:LYS:O	1:F:316:TYR:CZ	2.44	0.69
1:F:306:THR:OG1	3:J:310:LEU:HD22	1.92	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:K:222:LEU:HD12	1:K:285:MET:HG2	1.74	0.69
1:A:222:LEU:HD12	1:A:285:MET:HG2	1.74	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:55:ILE:O	1:A:85:PRO:HG3	1.92	0.69
3:O:6:TRP:CZ3	3:O:175:TRP:CE2	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
2:L:347:MET:SD	2:M:287:GLY:CA	2.80	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: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:364:PRO:HG3	3:O:260:HIS:CE1	2.26	0.69
1:A:106:ASP:OD1	1:F:225:LYS:HD2	1.91	0.69
1:A:202:VAL:O	1:A:206:VAL:HG23	1.92	0.69
2:C:73:CYS:O	2:C:79:CYS:SG	2.50	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
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:N:345:ARG:HH22	3:O:150:ARG:NE	1.58	0.69
3:O:169:GLU:O	3:O:173:VAL:HG23	1.92	0.69
1:F:222:LEU:HD12	1:F:285:MET:HG2	1.74	0.69
2:H:276:ILE:HG22	2:H:277:GLU:H	1.56	0.69
2:I:338:GLU:O	2:I:341:TYR:HB2	1.93	0.69
3:J:163:TYR:OH	3:J:166:PRO:CD	2.41	0.69
2:L:73:CYS:O	2:L:79:CYS:SG	2.51	0.69
2:M:73:CYS:O	2:M:79:CYS:SG	2.50	0.69
2:N:271:ALA:HB1	2:N:276:ILE:HD12	1.75	0.69
1:K:55:ILE:O	1:K:85:PRO:HG3	1.93	0.69
2:L:10:TRP:CZ2	2:L:193:GLU:HB3	2.28	0.69
2:B:97:SER:HB2	2:C:144:GLU:CG	2.22	0.69
2:G:19:VAL:HG12	2:G:178:LEU:CD1	2.18	0.69
2:L:351:MET:CG	2:M:290:HIS:ND1	2.56	0.69
1:A:308:THR:HG23	1:A:320:VAL:HG13	1.75	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
1:K:308:THR:HG23	1:K:320:VAL:HG13	1.75	0.68
1:K:315:ASP:CG	1:K:315:ASP:CA	2.61	0.68
2:M:67:GLY:HA2	2:M:119:ARG:NH1	2.07	0.68
2:D:309:ILE:HG22	2:D:313:MET:HG2	1.74	0.68
2:D:345:ARG:HH12	3:E:150:ARG:CG	2.05	0.68
1:F:315:ASP:CA	1:F:315:ASP:CG	2.61	0.68
2:N:259:ALA:CB	2:N:363:MET:CG	2.72	0.68
2:D:357:LEU:HA	2:D:363:MET:HE1	1.73	0.68
2:I:271:ALA:HB1	2:I:276:ILE:HD12	1.75	0.68
2:L:180:VAL:CB	2:L:304:ASN:O	2.34	0.68
2:B:10:TRP:CH2	2:B:193:GLU:OE1	2.45	0.68
2:B:110:ASN:HB3	2:B:113:TYR:HD1	1.58	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
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
1:A:133:ARG:HG3	2:G:299:PRO:HG2	1.75	0.68
2:I:309:ILE:HG22	2:I:313:MET:HG2	1.74	0.68
2:M:10:TRP:CH2	2:M:190:ILE:HG12	2.28	0.68
1:A:338:ASP:OD2	2:B:326:GLN:CD	2.32	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:F:55:ILE:O	1:F:85:PRO:HG3	1.93	0.68
2:I:254:GLU:OE2	2:I:312:ARG:HD3	1.93	0.68
2:L:110:ASN:HB3	2:L:113:TYR:HD1	1.58	0.68
2:N:309:ILE:HG22	2:N:313:MET:HG2	1.74	0.68
2:N:338:GLU:O	2:N:341:TYR:HB2	1.93	0.68
2:D:254:GLU:OE2	2:D:312:ARG:HD3	1.94	0.68
1:F:223:MET:SD	1:F:292:ARG:CB	2.78	0.68
2:G:93:ILE:HG23	2:G:100:LYS:NZ	2.09	0.68
2:L:6:LEU:HD21	2:L:194:GLU:CD	2.12	0.68
3:O:74:PRO:HB3	3:O:105:ARG:HD2	1.76	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
2:L:18:VAL:CG2	2:L:25:LEU:HD11	2.24	0.68
2:B:93:ILE:CG2	2:B:100:LYS:NZ	2.57	0.68
1:F:270:ARG:HH11	2:N:316:LEU:CD2	1.87	0.68
2:G:354:LEU:HD23	2:H:297:LEU:HD22	1.76	0.68
2:I:200:PRO:HB2	2:I:305:ASP:N	2.09	0.68
2:L:180:VAL:HB	2:L:304:ASN:C	2.14	0.68
2:L:6:LEU:HD21	2:L:194:GLU:HG3	0.74	0.68
2:B:6:LEU:CG	2:B:194:GLU:HG3	2.24	0.68
2:C:215:ARG:CZ	2:D:164:VAL:CG2	2.72	0.68
2:G:93:ILE:CG2	2:G:100:LYS:NZ	2.57	0.68
2:G:229:ASP:HA	2:H:30:ASN:HD21	1.57	0.68
3:J:74:PRO:HB3	3:J:105:ARG:HD2	1.76	0.68
2:I:345:ARG:HH12	3:J:150:ARG:CG	2.07	0.68
2:L:93:ILE:HG23	2:L:100:LYS:NZ	2.09	0.68
1:K:333:HIS:CG	2:L:297:LEU:CG	2.76	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:G:73:CYS:O	2:G:79:CYS:SG	2.51	0.67
2:N:254:GLU:OE2	2:N:312:ARG:HD3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:260:ASN:O	2:N:262:GLU:N	2.27	0.67
1:F:283:ARG:NH2	2:N:315:GLU:OE1	2.26	0.67
2:N:345:ARG:HH21	3:O:150:ARG:CZ	2.05	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
2:H:341:TYR:CB	2:I:333:LEU:CD1	2.72	0.67
1:K:116:LYS:HB3	1:K:140:GLN:HE21	1.59	0.67
2:D:277:GLU:HB3	3:E:149:GLU:HB3	1.76	0.67
1:F:116:LYS:HB3	1:F:140:GLN:HE21	1.59	0.67
2:H:100:LYS:CG	2:I:133:ARG:CZ	2.61	0.67
2:I:277:GLU:CB	3:J:149:GLU:HB3	2.25	0.67
2:L:93:ILE:CG2	2:L:100:LYS:NZ	2.57	0.67
2:D:260:ASN:O	2:D:262:GLU:N	2.27	0.67
2:H:10:TRP:CH2	2:H:190:ILE:HG23	2.30	0.67
3:J:31:ALA:HB2	3:J:164:LEU:HB3	1.76	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:L:10:TRP:CH2	2:L:193:GLU:OE1	2.47	0.67
2:D:259:ALA:CB	2:D:363:MET:CG	2.72	0.67
1:K:262:ARG:CZ	3:O:230:TYR:HB3	2.24	0.67
2:L:265:MET:HE2	2:M:294:MET:HE3	1.75	0.67
2:B:98:ARG:NH1	2:C:137:ASN:CB	2.51	0.67
2:G:259:ALA:CB	2:G:363:MET:HE3	2.25	0.67
2:N:73:CYS:O	2:N:79:CYS:SG	2.48	0.67
2:C:181:GLU:HG2	2:C:184:ARG:HD2	1.77	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:L:354:LEU:HD21	2:M:297:LEU:CD2	2.25	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
2:N:364:PRO:HG3	3:O:260:HIS:HE1	1.60	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
2:I:260:ASN:O	2:I:262:GLU:N	2.27	0.67
1:K:28:PRO:HB3	2:L:164:VAL:CG2	2.22	0.67
3:O:111:VAL:HG12	3:O:140:TRP:HB2	1.75	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:L:351:MET:HG2	2:M:290:HIS:ND1	2.10	0.66
2:L:73:CYS:SG	2:L:73:CYS:O	2.53	0.66
2:M:181:GLU:HG2	2:M:184:ARG:HD2	1.77	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:N:358:ALA:HA	2:N:364:PRO:CG	2.25	0.66
1:A:191:LEU:HD22	2:B:23:HIS:ND1	2.11	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: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:347:MET:O	2:D:351:MET:HG2	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:B:94:ASP:H	2:B:100:LYS:HZ1	1.43	0.66
2:I:5:VAL:HG13	2:I:222:ASP:CG	2.15	0.66
3:O:64:GLY:O	3:O:68:MET:HB2	1.96	0.66
2:B:73:CYS:O	2:B:73:CYS:SG	2.53	0.66
2:C:11:ARG:NH2	2:D:165:THR:HG22	2.11	0.66
2:I:347:MET:O	2:I:351:MET:HG2	1.96	0.66
3:J:8:ARG:CG	3:J:9:PRO:HD3	2.25	0.66
1:K:329:LEU:HD12	2:L:294:MET:SD	2.36	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
2:B:259:ALA:CB	2:B:363:MET:HE3	2.26	0.65
2:C:86:ARG:NE	2:D:141:LYS:HB2	2.11	0.65
2:D:356:ALA:O	2:D:363:MET:CE	2.45	0.65
1:A:105:HIS:CA	1:F:227:LYS:HD2	2.26	0.65
2:H:181:GLU:HG2	2:H:184:ARG:HD2	1.77	0.65
2:L:10:TRP:HZ2	2:L:193:GLU:HB3	1.61	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: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:N:13:GLN:NE2	2:N:83:GLU:HG2	2.11	0.65
2:I:355:ARG:NH1	3:J:287:GLN:HB3	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
3:J:64:GLY:O	3:J:68:MET:HB2	1.96	0.65
2:L:343:PRO:HB3	2:M:283:VAL:O	1.95	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
1:A:48:GLU:HG3	1:A:49:GLU:N	2.12	0.65
2:I:277:GLU:HA	3:J:149:GLU:CG	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:309:ILE:HG21	2:I:313:MET:HG2	1.77	0.65
2:M:93:ILE:CG2	2:M:100:LYS:HZ3	2.10	0.65
1:F:274:ASP:HA	1:F:279:TRP:CE3	2.32	0.65
1:F:48:GLU:HG3	1:F:49:GLU:N	2.12	0.65
2:G:98:ARG:HD2	2:H:141:LYS:HZ3	1.62	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
3:J:73:HIS:HD2	3:J:75:ASP:H	1.45	0.65
1:K:48:GLU:HG3	1:K: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
1:A:209:ALA:O	2:B:176:LYS:HD2	1.97	0.64
1:F:239:GLU:HA	2:G:174:HIS:CE1	2.32	0.64
2:L:265:MET:HE2	2:M:294:MET:CE	2.26	0.64
2:N:360:HIS:CG	2:N:363:MET:CG	2.80	0.64
1:F:270:ARG:HH22	2:N:316:LEU:HA	1.60	0.64
2:H:343:PRO:HG2	2:H:347:MET:SD	2.38	0.64
1:K:255:LEU:HD22	3:O:313:THR:HG21	1.77	0.64
2:M:201:ARG:HH21	2:M:308:ALA:HB2	1.62	0.64
1:A:274:ASP:HA	1:A:279:TRP:CE3	2.32	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: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:343:PRO:HG2	2:M:347:MET:SD	2.37	0.64
2:M:73:CYS:SG	2:M:73:CYS:O	2.56	0.64
2:C:343:PRO:HG2	2:C:347:MET:SD	2.37	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:M:10:TRP:CE2	2:M:190:ILE:CG2	2.78	0.64
2:M:6:LEU:HG	2:M:222:ASP:OD1	1.97	0.64
2:N:337:LYS:HG3	2:N:338:GLU:N	2.12	0.64
3:O:147:GLU:O	3:O:147:GLU:HG2	1.98	0.64
3:O:4:TYR:CD1	3:O:175:TRP:HH2	2.11	0.64
2:C:73:CYS:SG	2:C:73:CYS:O	2.55	0.64
3:E:147:GLU:HG2	3:E:147:GLU:O	1.98	0.64
3:J:147:GLU:O	3:J:147:GLU:HG2	1.98	0.64
2:M:111:VAL:HG11	2:M:142:THR:CG2	2.27	0.64
1:A:273:PHE:HB3	1:A:279:TRP:CG	2.33	0.64
2:B:254:GLU:O	2:B:258:GLU:HG3	1.98	0.64

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:98:ARG:HD2	2:H:141:LYS:NZ	2.14	0.63
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: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:G:328:TYR:O	2:G:332:LEU:HD23	1.99	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:B:354:LEU:CD1	2:C:294:MET:SD	2.82	0.62
1:F:29:LEU:HD11	1:F:179:LEU:CD1	2.22	0.62
3:J:129:LEU:HD11	3:J:158:ARG:HH11	1.64	0.62
2:L:94:ASP:O	2:L:100:LYS:HE3	1.99	0.62
2:N:100:LYS:HB2	2:N:103:ASP:OD1	1.99	0.62
2:G:271:ALA:HB1	2:G:276:ILE:CD1	2.30	0.62
2:H:10:TRP:CE2	2:H:190:ILE:HG23	2.34	0.62
3:J:329:LEU:H	3:J:329:LEU:HD23	1.63	0.62
2:L:268:ILE:HD11	2:L:353:LEU:CD1	2.28	0.62
2:M:93:ILE:CG2	2:M:100:LYS:HZ2	2.12	0.62
2:C:111:VAL:HG11	2:C:142:THR:CG2	2.28	0.62
2:D:356:ALA:O	2:D:363:MET:HE1	1.99	0.62
2:D:345:ARG:HE	3:E:150:ARG:HH21	0.66	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:G:254:GLU:O	2:G:258:GLU:HG3	1.98	0.62
2:H:84:GLN:HA	2:I:144:GLU:OE1	1.99	0.62
2:L:93:ILE:CG2	2:L:100:LYS:HZ2	2.12	0.62
2:G:347:MET:HG3	2:H:290:HIS:NE2	2.14	0.62
1:K:24:LEU:HA	1:K:114:GLY:O	2.00	0.62
2:N:223:GLN:HE21	3:O:158:ARG:HE	1.45	0.62
2:G:6:LEU:HD11	2:G:225:ILE:CD1	2.29	0.62
1:K:222:LEU:CD1	1:K:285:MET:HG2	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
1:A:256:LEU:O	1:A:260:LEU:HG	2.00	0.62
2:B:94:ASP:O	2:B:100:LYS:HE3	1.99	0.62
2:B:271:ALA:HB1	2:B:276:ILE:CD1	2.30	0.62
2:H:93:ILE:HG23	2:H:100:LYS:HZ3	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:316:LEU:HD22	2:I:320:ILE:HD11	1.81	0.62
2:N:366:PRO:HA	3:O:283:PRO:HD2	1.81	0.62
2:D:334:ILE:HG12	3:E:334:LEU:OXT	1.99	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:N:223:GLN:CG	3:O:158:ARG:NH2	2.60	0.62
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:G:94:ASP:O	2:G:100:LYS:HE3	2.00	0.61
2:H:93:ILE:HG23	2:H:100:LYS:NZ	2.14	0.61
2:L:180:VAL:CB	2:L:304:ASN:HB2	2.30	0.61
2:B:328:TYR:O	2:B:332:LEU:HD23	1.99	0.61
2:B:97:SER:HB2	2:C:144:GLU:CD	2.21	0.61
2:D:277:GLU:CD	3:E:149:GLU:HG3	2.20	0.61
2:L:180:VAL:HG23	2:L:304:ASN:ND2	2.14	0.61
2:M:351:MET:CE	2:M:351:MET:HA	2.30	0.61
3:E:73:HIS:CD2	3:E:75:ASP:H	2.18	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
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
1:A:24:LEU:HA	1:A:114:GLY:O	2.00	0.61
2:D:277:GLU:CB	3:E:149:GLU:HG3	2.27	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:I:98:ARG:NH2	3:J:91:ASP:OD1	2.33	0.61
2:H:20:GLY:HA3	2:H:182:GLN:NE2	2.15	0.61
2:L:343:PRO:HG3	2:M:287:GLY:CA	2.30	0.61
2:M:93:ILE:HG23	2:M:100:LYS:NZ	2.14	0.61
2:M:342:ALA:HA	2:N:333:LEU:HD21	1.82	0.61
2:B:93:ILE:CG2	2:B:100:LYS:HZ2	2.14	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:M:201:ARG:NH2	2:M:308:ALA:HB2	2.16	0.61
2:H:250:LEU:HD22	2:H:309:ILE:HD12	1.82	0.61
2:H:351:MET:HA	2:H:351:MET:CE	2.30	0.61
2:L:223:GLN:OE1	2:M:171:LEU:HD12	2.01	0.61
2:G:263:ARG:O	2:G:267:LEU:HG	2.00	0.61
2:M:215:ARG:CZ	2:N:164:VAL:CG1	2.78	0.61
2:N:70:ALA:O	2:N:72:PRO:HD3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:73:HIS:CD2	3:O:75:ASP:H	2.18	0.61
2:D:70:ALA:O	2:D:72:PRO:HD3	2.01	0.61
2:I:70:ALA:O	2:I:72:PRO:HD3	2.01	0.61
1:A:315:ASP:HB2	1:A:318:GLN:HG2	1.80	0.61
1:F:24:LEU:HA	1:F:114:GLY:O	2.00	0.61
2:G:21:GLN:CG	2:G:178:LEU:CD2	2.73	0.61
2:H:359:PHE:CE2	2:I:323:THR:CG2	2.84	0.61
2:I:345:ARG:NH1	3:J:150:ARG:CG	2.64	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:B:268:ILE:HD11	2:B:353:LEU:HD12	1.83	0.60
3:E:117:ALA:HB2	3:E:143:LEU:HD12	1.83	0.60
2:H:6:LEU:CG	2:H:222:ASP:OD1	2.50	0.60
2:M:359:PHE:CZ	2:N:323:THR:CG2	2.84	0.60
2:I:140:LEU:HD21	2:I:166:ILE:HG12	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
3:O:117:ALA:HB2	3:O:143:LEU:HD12	1.83	0.60
3:O:6:TRP:HZ3	3:O:175:TRP:CE2	2.17	0.60
2:H:201:ARG:HB2	2:H:305:ASP:OD2	2.01	0.60
2:N:140:LEU:HD21	2:N:166:ILE:HG12	1.83	0.60
2:G:12:PRO:HD2	2:G:215:ARG:NH2	2.17	0.60
2:L:180:VAL:HB	2:L:304:ASN:HB2	1.82	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:M:215:ARG:CZ	2:N:164:VAL:HG22	2.29	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:19:VAL:HG21	2:H:214:LEU:HD22	1.82	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:C:250:LEU:HD22	2:C:309:ILE:HD12	1.82	0.60
2:G:6:LEU:CD1	2:G:222:ASP:HA	2.26	0.60
2:G:365:LEU:HD21	2:H:297:LEU:HD13	1.78	0.60
1:A:269:LEU:HG	1:A:273:PHE:CE1	2.37	0.60
2:H:292:ILE:O	2:H:296:GLN:HG3	2.02	0.60
2:L:268:ILE:HD11	2:L:353:LEU:HD12	1.83	0.60
2:N:240:MET:HB3	3:O:157:SER:HA	1.82	0.60
3:O:149:GLU:C	3:O:151:LEU:H	2.05	0.60
2:D:363:MET:CG	2:D:364:PRO:HD2	2.31	0.60
1:F:210:ALA:O	1:F:212:PHE:CE1	2.55	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:149:GLU:C	3:J:151:LEU:H	2.05	0.60
2:M:292:ILE:O	2:M:296:GLN:HG3	2.02	0.60
2:M:362:ARG:O	2:M:363:MET:HG3	2.02	0.60
2:M:341:TYR:CE2	2:N:337:LYS:CB	2.84	0.60
2:B:343:PRO:HG2	2:B:347:MET:SD	2.42	0.60
2:C:351:MET:CE	2:C:351:MET:HA	2.30	0.60
1:F:10:ARG:HH12	1:F:40:GLN:NE2	2.00	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
2:M:88:VAL:HG11	2:M:116:ALA:HB3	1.83	0.60
2:N:363:MET:CG	2:N:364:PRO:HD2	2.31	0.60
2:C:354:LEU:HD11	2:D:294:MET:SD	2.42	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:H:84:GLN:CB	2:I:144:GLU:OE1	2.50	0.59
1:K:269:LEU:HG	1:K:273:PHE:CE1	2.37	0.59
2:M:21:GLN:OE1	2:M:175:LEU:HD22	2.02	0.59
3:E:303:VAL:HB	3:E:306:ILE:HD11	1.83	0.59
1:A:255:LEU:HD22	3:E:313:THR:HG21	1.84	0.59
2:G:93:ILE:HG23	2:G:100:LYS:HZ2	1.67	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
2:C:11:ARG:HH22	2:D:165:THR:HG22	1.67	0.59
1:F:269:LEU:HG	1:F:273:PHE:CE1	2.37	0.59
2:G:284:GLU:O	2:G:288:LEU:HG	2.02	0.59
2:I:246:ASP:HB2	2:I:248:GLN:HG2	1.85	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:L:343:PRO:HG2	2:L:347:MET:SD	2.43	0.59
1:A:10:ARG:HH12	1:A:40:GLN:NE2	2.00	0.59
2:B:205:LEU:CD1	2:B:234:THR:HG23	2.33	0.59
2:C:21:GLN:OE1	2:C:175:LEU:HD22	2.02	0.59
2:C:362:ARG:O	2:C:363:MET:HG3	2.02	0.59
3:E:149:GLU:C	3:E:151:LEU:H	2.05	0.59
2:M:152:PHE:O	2:M:153:LEU:HD23	2.02	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:B:284:GLU:O	2:B:288:LEU:HG	2.02	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:316:LEU:HD22	2:H:320:ILE:HD11	1.84	0.59
2:M:201:ARG:HG3	2:M:305:ASP:HB3	1.84	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:G:343:PRO:HG2	2:G:347:MET:SD	2.42	0.59
2:G:259:ALA:HB3	2:G:363:MET:CE	2.33	0.59
2:H:215:ARG:NH2	2:I:164:VAL:HG22	2.17	0.59
2:I:223:GLN:HG2	3:J:158:ARG:HH21	1.67	0.59
2:L:246:ASP:HB3	2:L:274:ARG:CD	2.24	0.59
2:M:355:ARG:HG3	2:N:326:GLN:HG3	1.84	0.59
3:O:46:ARG:CZ	3:O:68:MET:HG3	2.33	0.59
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:M:94:ASP:C	2:M:100:LYS:HZ1	2.06	0.58
1:F:263:GLN:HG2	1:F:266:HIS:HD2	1.68	0.58
2:I:277:GLU:CG	3:J:149:GLU:HG3	2.32	0.58
1:K:172:TYR:O	1:K:216:HIS:HE1	1.86	0.58
2:L:180:VAL:HG21	2:L:304:ASN:OD1	2.03	0.58
2:L:302:LEU:HD13	2:L:310:GLU:HG2	1.84	0.58
2:L:341:TYR:O	2:M:336:ARG:NH1	2.32	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:B:282:LEU:CD2	2:B:332:LEU:HD12	2.34	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:C:56:ARG:NH2	2:D:165:THR:HG21	2.18	0.58
1:F:10:ARG:HH22	1:F:40:GLN:HE22	1.51	0.58
2:H:257:VAL:HG11	2:H:320:ILE:CD1	2.34	0.58
2:L:284:GLU:O	2:L:288:LEU:HG	2.02	0.58
2:M:316:LEU:HD22	2:M:320:ILE:HD11	1.84	0.58
3:O:41:ILE:HG21	3:O:113:TRP:CD1	2.38	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:D:94:ASP:O	2:D:100:LYS:HE2	2.03	0.58
2:G:6:LEU:CD1	2:G:225:ILE:HD12	2.29	0.58
2:H:5:VAL:HG11	2:I:171:LEU:HB2	1.84	0.58
2:I:186:GLN:HG2	2:I:214:LEU:HD21	1.86	0.58
2:I:229:ASP:O	2:I:231:GLN:N	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:308:ARG:O	3:J:312:ILE:HG13	2.04	0.58
1:K:223:MET:HE1	1:K:292:ARG:HB2	1.86	0.58
2:L:259:ALA:HB3	2:L:363:MET:CE	2.33	0.58
2:N:246:ASP:HB2	2:N:248:GLN:HG2	1.85	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:G:304:ASN:OD1	2:G:305:ASP:N	2.37	0.58
2:I:360:HIS:CB	2:I:363:MET:SD	2.92	0.58
2:I:367:GLU:HB3	2:I:368:PRO:HD2	1.86	0.58
2:L:304:ASN:OD1	2:L:305:ASP:N	2.37	0.58
1:F:221:LEU:HD13	1:F:331:LEU:HD12	1.85	0.58
2:I:58:LEU:HD23	2:I:153:LEU:HD22	1.86	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:F:222:LEU:HD12	1:F:285:MET:SD	2.44	0.58
2:G:282:LEU:CD2	2:G:332:LEU:HD12	2.34	0.58
2:H:152:PHE:O	2:H:153:LEU:HD23	2.03	0.58
2:I:184:ARG:HH22	2:I:304:ASN:ND2	2.02	0.58
2:I:94:ASP:O	2:I:100:LYS:HE2	2.03	0.58
3:J:46:ARG:CZ	3:J:68:MET:HG3	2.33	0.58
1:K:263:GLN:HG2	1:K:266:HIS:HD2	1.68	0.58
1:K:273:PHE:CE1	1:K:283:ARG:HG3	2.39	0.58
1:A:193:PRO:C	2:M:311:LEU:HD21	2.23	0.58
2:M:257:VAL:HG11	2:M:320:ILE:CD1	2.34	0.58
1:A:273:PHE:CE1	1:A:283:ARG:HG3	2.39	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
2:L:61:GLY:HA2	2:L:72:PRO:HG3	1.85	0.58
2:N:229:ASP:O	2:N:231:GLN:N	2.33	0.58
2:N:58:LEU:HD23	2:N:153:LEU:HD22	1.86	0.58
3:O:308:ARG:O	3:O:312:ILE:HG13	2.04	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:G:49:VAL:HA	2:G:213:SER:HB2	1.85	0.58
1:K:10:ARG:HH22	1:K:40:GLN:HE22	1.51	0.58
2:L:239:ALA:CA	2:L:243:THR:OG1	2.51	0.58
2:L:282:LEU:CD2	2:L:332:LEU:HD12	2.34	0.58
1:F:119:LYS:H	1:F:119:LYS:CD	2.05	0.57
1:K:222:LEU:HD12	1:K:285:MET:CG	2.33	0.57
2:N:94:ASP:O	2:N:100:LYS:HE2	2.03	0.57
2:D:47:ARG:NE	3:E:126:ASN:OD1	2.37	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:F:279:TRP:O	1:F:279:TRP:CG	2.57	0.57
3:J:41:ILE:HG21	3:J:113:TRP:CD1	2.38	0.57
1:K:222:LEU:HD12	1:K:285:MET:SD	2.44	0.57
1:A:221:LEU:HD13	1:A:331:LEU:HD12	1.86	0.57
2:C:84:GLN:HA	2:D:144:GLU:OE1	2.04	0.57
1:F:223:MET:HE1	1:F:292:ARG:HB2	1.85	0.57
2:B:246:ASP:HB3	2:B:274:ARG:CD	2.24	0.57
2:C:257:VAL:HG11	2:C:320:ILE:CD1	2.34	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
3:E:41:ILE:HG21	3:E:113:TRP:CD1	2.38	0.57
1:F:222:LEU:HD12	1:F:285:MET:CG	2.33	0.57
2:G:246:ASP:CB	2:G:274:ARG:HD3	2.24	0.57
2:G:47:ARG:O	2:G:47:ARG:HG3	2.03	0.57
2:G:61:GLY:HA2	2:G:72:PRO:HG3	1.85	0.57
2:H:341:TYR:CB	2:I:333:LEU:HD13	2.35	0.57
1:K:279:TRP:O	1:K:279:TRP:CG	2.57	0.57
2:N:360:HIS:CB	2:N:363:MET:SD	2.92	0.57
1:A:251:GLN:OE1	3:E:307:ASN:ND2	2.37	0.57
2:H:291:ARG:HH11	2:H:306:MET:HG3	1.68	0.57
2:I:201:ARG:HB2	2:I:305:ASP:HB3	1.86	0.57
2:M:291:ARG:HH11	2:M:306:MET:HG3	1.69	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:I:360:HIS:CB	2:I:363:MET:CB	2.68	0.57
2:L:362:ARG:HH21	2:L:363:MET:HE1	1.70	0.57
2:D:58:LEU:HD23	2:D:153:LEU:HD22	1.86	0.57
2:G:328:TYR:OH	2:G:361:PRO:HD2	2.05	0.57
2:G:354:LEU:HD21	2:H:297:LEU:CD2	2.34	0.57
1:K:221:LEU:HD13	1:K:331:LEU:HD12	1.86	0.57
1:K:281:ASN:C	1:K:283:ARG:N	2.57	0.57
1:F:270:ARG:HH22	2:N:316:LEU:CA	2.17	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
2:D:194:GLU:HA	2:D:194:GLU:OE1	2.05	0.57
3:J:8:ARG:HG3	3:J:9:PRO:CD	2.33	0.57
2:L:205:LEU:HD11	2:L:234:THR:HG23	1.87	0.57
2:N:194:GLU:OE1	2:N:194:GLU:HA	2.05	0.57
1:A:281:ASN:C	1:A:283:ARG:N	2.57	0.57
2:D:186:GLN:HG2	2:D:214:LEU:HD21	1.86	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:F:281:ASN:C	1:F:283:ARG:N	2.57	0.57
2:M:3:TYR:HD2	2:M:3:TYR:O	1.86	0.57
1:F:270:ARG:NE	2:N:319:THR:HG21	2.20	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: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: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:G:205:LEU:HD11	2:G:234:THR:HG23	1.87	0.56
2:I:93:ILE:HG22	2:I:100:LYS:HZ3	1.70	0.56
2:N:128:VAL:HG11	2:N:154:LEU:HD22	1.87	0.56
2:M:84:GLN:CA	2:N:144:GLU:OE1	2.53	0.56
2:C:291:ARG:HH11	2:C:306:MET:HG3	1.69	0.56
3:E:308:ARG:O	3:E:312:ILE:HG13	2.04	0.56
1:F:270:ARG:NH1	2:N:316:LEU:CA	2.55	0.56
3:E:280:HIS:O	3:E:281:LEU:HD23	2.05	0.56
2:I:363:MET:CB	2:I:364:PRO:CD	2.78	0.56
1:K:170:LEU:O	1:K:173:CYS:O	2.23	0.56
2:M:3:TYR:O	2:M:4:GLN:CG	2.53	0.56
2:N:367:GLU:HB3	2:N:368:PRO:HD2	1.86	0.56
1:A:191:LEU:CD2	2:B:23:HIS:ND1	2.67	0.56
1:F:170:LEU:O	1:F:173:CYS:O	2.23	0.56
2:L:328:TYR:OH	2:L:361:PRO:HD2	2.05	0.56
2:N:186:GLN:HG2	2:N:214:LEU:HD21	1.86	0.56
1:F:270:ARG:NE	2:N:319:THR:CG2	2.68	0.56
2:C:354:LEU:CD2	2:D:297:LEU:HD22	2.35	0.56
2:I:334:ILE:HG21	3:J:332:PRO:HB2	1.87	0.56
1:K:333:HIS:HD2	2:L:297:LEU:HD23	1.65	0.56
2:L:362:ARG:HH21	2:L:363:MET:CE	2.19	0.56
3:O:201:ALA:O	3:O:204:LEU:HB2	2.06	0.56
3:O:8:ARG:HG3	3:O:9:PRO:CD	2.33	0.56
2:B:328:TYR:OH	2:B:361:PRO:HD2	2.05	0.56
2:G:362:ARG:HH21	2:G:363:MET:CE	2.19	0.56
2:M:40:ALA:HB1	2:M:170:CYS:SG	2.46	0.56
2:N:296:GLN:NE2	2:N:325:ILE:HD12	2.20	0.56
3:O:280:HIS:O	3:O:281:LEU:HD23	2.05	0.56
2:B:69:THR:HG22	2:B:71:THR:N	2.01	0.56
2:L:239:ALA:HA	2:L:243:THR:OG1	2.05	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)
1:A:223:MET:HE1	1:A:292:ARG:HB2	1.87	0.56
1:F:218:VAL:HA	1:F:221:LEU:HB2	1.88	0.56
2:G:229:ASP:CA	2:H:30:ASN:HD21	2.19	0.56
2:M:93:ILE:HG22	2:M:100:LYS:HZ3	1.66	0.56
2:N:366:PRO:HA	3:O:283:PRO:CD	2.35	0.56
3:O:5:PRO:CD	3:O:175:TRP:CZ3	2.89	0.56
3:E:201:ALA:O	3:E:204:LEU:HB2	2.06	0.56
3:E:8:ARG:HG3	3:E:9:PRO:CD	2.33	0.56
2:H:40:ALA:HB1	2:H:170:CYS:SG	2.46	0.56
2:G:341:TYR:O	2:H:336:ARG:NH1	2.35	0.56
1:K:262:ARG:NH1	3:O:230:TYR:HB3	2.21	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
2:M:99:THR:O	2:M:99:THR:CG2	2.51	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:B:309:ILE:HG22	2:B:313:MET:HG2	1.88	0.56
2:I:128:VAL:HG11	2:I:154:LEU:HD22	1.87	0.56
2:I:259:ALA:HB2	2:I:363:MET:SD	2.46	0.56
2:N:259:ALA:HB2	2:N:363:MET:SD	2.46	0.56
1:K:255:LEU:CD1	3:O:309:GLU:HG2	2.36	0.56
1:A:170:LEU:O	1:A:173:CYS:O	2.24	0.55
2:D:296:GLN:NE2	2:D:325:ILE:HD12	2.20	0.55
2:G:94:ASP:CA	2:G:100:LYS:HZ1	2.19	0.55
2:H:97:SER:OG	2:H:100:LYS:CE	2.55	0.55
2:L:295:VAL:HG22	2:L:301:ALA:HB3	1.88	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:H:91:ILE:HD12	2:H:123:TYR:CE2	2.42	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:B:362:ARG:HH21	2:B:363:MET:CE	2.19	0.55
2:B:365:LEU:HD21	2:C:297:LEU:HD11	1.87	0.55
2:C:40:ALA:HB1	2:C:170:CYS:SG	2.46	0.55
2:D:259:ALA:HB2	2:D:363:MET:SD	2.46	0.55
1:F:333:HIS:CG	2:G:298:SER:OG	2.59	0.55
3:J:213:ARG:NH2	3:J:267:ASN:OD1	2.39	0.55
1:K:308:THR:CG2	1:K:320:VAL:HG13	2.37	0.55
1:A:296:THR:HG22	1:A:299:ARG:NH1	2.22	0.55
2:H:156:THR:HG22	2:H:158:ASP:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:3:TYR:CD2	2:L:3:TYR:O	2.60	0.55
3:O:213:ARG:NH2	3:O:267:ASN:OD1	2.39	0.55
1:A:313:LYS:O	1:A:316:TYR:CE2	2.60	0.55
2:D:355:ARG:HH21	3:E:332:PRO:HD3	1.72	0.55
2:G:10:TRP:CZ3	2:G:190:ILE:CB	2.90	0.55
2:G:11:ARG:HD3	2:G:83:GLU:OE2	2.07	0.55
3:J:201:ALA:O	3:J:204:LEU:HB2	2.06	0.55
2:M:354:LEU:HD21	2:N:297:LEU:HD22	1.88	0.55
2:N:360:HIS:CG	2:N:363:MET:CE	2.90	0.55
1:A:218:VAL:HA	1:A:221:LEU:HB2	1.88	0.55
2:B:205:LEU:HD11	2:B:234:THR:HG23	1.87	0.55
2:B:246:ASP:CB	2:B:274:ARG:HD3	2.23	0.55
2:B:11:ARG:HD3	2:B:83:GLU:OE2	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
1:K:296:THR:HG22	1:K:299:ARG:NH1	2.22	0.55
2:L:307:ALA:HA	2:L:310:GLU:HG3	1.89	0.55
1:A:282:ARG:O	1:A:285:MET:HB3	2.07	0.55
2:B:307:ALA:HA	2:B:310:GLU:HG3	1.89	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:I:194:GLU:OE1	2:I:194:GLU:HA	2.05	0.55
1:K:282:ARG:O	1:K:285:MET:HB3	2.07	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
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:D:360:HIS:CG	2:D:363:MET:CE	2.90	0.55
2:G:295:VAL:HG22	2:G:301:ALA:HB3	1.88	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:L:248:GLN:O	2:L:252:LEU:N	2.39	0.55
2:M:97:SER:OG	2:M:100:LYS:CE	2.55	0.55
2:N:259:ALA:HB2	2:N:363:MET:HG3	1.89	0.55
2:B:295:VAL:HG22	2:B:301:ALA:HB3	1.88	0.54
2:B:3:TYR:O	2:B:3:TYR:CD2	2.60	0.54
2:C:97:SER:OG	2:C:100:LYS:CE	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:313:LYS:O	1:K:316:TYR:CE2	2.60	0.54
1:K:262:ARG:NH2	3:O:230:TYR:CB	2.70	0.54
2:I:355:ARG:HH12	3:J:287:GLN:HB3	1.72	0.54
2:M:355:ARG:HG3	2:N:326:GLN:CG	2.37	0.54
2:C:307:ALA:HA	2:C:310:GLU:HB2	1.90	0.54
1:F:313:LYS:O	1:F:316:TYR:CE2	2.60	0.54
2:G:3:TYR:O	2:G:3:TYR:CD2	2.60	0.54
2:L:309:ILE:HG22	2:L:313:MET:HG2	1.88	0.54
2:L:11:ARG:HD3	2:L:83:GLU:OE2	2.07	0.54
1:F:39:ARG:NH2	1:F:50:HIS:HB3	2.21	0.54
2:G:307:ALA:HA	2:G:310:GLU:HG3	1.89	0.54
2:H:19:VAL:CG2	2:H:214:LEU:HD22	2.37	0.54
2:H:346:ARG:O	2:H:350:GLU:HG3	2.08	0.54
2:I:244:LEU:HD21	2:I:276:ILE:CG1	2.37	0.54
1:K:39:ARG:NH2	1:K:50:HIS:HB3	2.21	0.54
2:M:281:LEU:HD23	2:M:285:MET:CE	2.36	0.54
1:F:264:SER:O	1:F:265:ALA:HB3	2.07	0.54
1:F:308:THR:CG2	1:F:320:VAL:HG13	2.37	0.54
2:G:21:GLN:HG3	2:G:178:LEU:HD23	1.82	0.54
2:G:248:GLN:O	2:G:252:LEU:N	2.39	0.54
2:H:307:ALA:HA	2:H:310:GLU:HB2	1.90	0.54
2:M:346:ARG:O	2:M:350:GLU:HG3	2.07	0.54
2:N:296:GLN:HE22	2:N:325:ILE:HD12	1.73	0.54
2:N:360:HIS:HD2	2:N:361:PRO:O	1.90	0.54
1:A:271:ALA:O	1:A:275:LYS:HG2	2.07	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
2:M:84:GLN:CB	2:N:144:GLU:OE1	2.56	0.54
2:G:104:THR:O	2:G:108:LEU:HG	2.08	0.54
2:H:3:TYR:O	2:H:4:GLN:CB	2.56	0.54
2:M:215:ARG:CZ	2:N:164:VAL:HG11	2.38	0.54
1:A:1:MET:HA	1:A:134:SER:O	2.08	0.54
1:F:271:ALA:O	1:F:275:LYS:HG2	2.07	0.54
1:K:218:VAL:HA	1:K:221:LEU:HB2	1.88	0.54
1:A:264:SER:O	1:A:265:ALA:HB3	2.07	0.54
2:D:296:GLN:HE22	2:D:325:ILE:HD12	1.73	0.54
2:D:360:HIS:HD2	2:D:361:PRO:O	1.90	0.54
1:F:255:LEU:CD1	3:J:309:GLU:HG2	2.38	0.54
1:F:282:ARG:O	1:F:285:MET:HB3	2.07	0.54
2:H:360:HIS:HD2	2:H:363:MET:H	1.56	0.54
3:J:238:HIS:ND1	3:J:239:GLU:N	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:306:ILE:HG22	3:J:307:ASN:H	1.73	0.54
3:O:306:ILE:HG22	3:O:307:ASN:H	1.73	0.54
2:D:302:LEU:HD22	2:D:306:MET:HG2	1.90	0.54
3:E:213:ARG:NH2	3:E:267:ASN:OD1	2.39	0.54
1:F:273:PHE:HB3	1:F:279:TRP:HB2	1.90	0.54
2:L:104:THR:O	2:L:108:LEU:HG	2.07	0.54
1:A:161:GLU:HG3	2:M:318:ARG:NH2	2.22	0.53
1:F:48:GLU:HG3	1:F:49:GLU:H	1.72	0.53
2:I:241:LEU:HD22	3:J:153:ALA:HB1	1.90	0.53
1:K:264:SER:O	1:K:265:ALA:HB3	2.07	0.53
2:B:104:THR:O	2:B:108:LEU:HG	2.08	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
2:I:302:LEU:HD22	2:I:306:MET:HG2	1.91	0.53
2:I:259:ALA:HB2	2:I:363:MET:HG3	1.89	0.53
1:K:271:ALA:O	1:K:275:LYS:HG2	2.07	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:C:94:ASP:C	2:C:100:LYS:NZ	2.62	0.53
2:G:19:VAL:HG22	2:G:186:GLN:CB	2.38	0.53
2:I:360:HIS:HD2	2:I:361:PRO:O	1.90	0.53
1:F:262:ARG:HH12	3:J:230:TYR:HB3	1.70	0.53
2:L:69:THR:HG22	2:L:71:THR:N	2.01	0.53
2:N:244:LEU:HD11	2:N:276:ILE:HD13	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:I:334:ILE:HG12	3:J:334:LEU:OXT	2.09	0.53
3:J:4:TYR:HB3	3:J:5:PRO:HD2	1.90	0.53
1:K:282:ARG:HG2	1:K:285:MET:HE2	1.90	0.53
1:F:270:ARG:NH2	2:N:315:GLU:O	2.41	0.53
3:O:6:TRP:HZ3	3:O:175:TRP:CG	2.24	0.53
1:A:25:GLY:O	1:A:115:ASN:HA	2.08	0.53
2:D:271:ALA:HB1	2:D:276:ILE:HD11	1.90	0.53
2:G:276:ILE:HG22	2:G:277:GLU:N	2.24	0.53
2:I:291:ARG:HD2	2:I:306:MET:SD	2.49	0.53
1:K:1:MET:HA	1:K:134:SER:O	2.08	0.53
3:O:238:HIS:ND1	3:O:239:GLU:N	2.56	0.53
2:D:84:GLN:HB3	2:D:86:ARG:NH2	2.24	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: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:N:244:LEU:HD21	2:N:276:ILE:CG1	2.37	0.53
2:D:291:ARG:HD2	2:D:306:MET:SD	2.49	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
1:K:93:ILE:HG23	1:K:97:LEU:HD13	1.91	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
3:E:268:VAL:O	3:E:271:PRO:HD3	2.09	0.53
1:F:25:GLY:O	1:F:115:ASN:HA	2.08	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:B:248:GLN:O	2:B:252:LEU:N	2.39	0.53
2:C:334:ILE:O	2:C:338:GLU:HG3	2.09	0.53
2:D:244:LEU:HD21	2:D:276:ILE:CG1	2.37	0.53
1:F:309:GLU:O	1:F:313:LYS:HG3	2.09	0.53
2:H:11:ARG:NH2	2:I:165:THR:HG22	2.23	0.53
2:H:334:ILE:O	2:H:338:GLU:HG3	2.09	0.53
2:I:296:GLN:HE22	2:I:325:ILE:HD12	1.73	0.53
2:L:351:MET:HG3	2:M:290:HIS:ND1	2.24	0.53
2:C:278:TRP:HB3	2:C:349:VAL:HG21	1.91	0.52
2:D:238:SER:CB	2:D:243:THR:HB	2.34	0.52
2:I:244:LEU:HD11	2:I:276:ILE:HD13	1.90	0.52
1:K:309:GLU:O	1:K:313:LYS:HG3	2.09	0.52
2:L:354:LEU:HD12	2:M:294:MET:SD	2.44	0.52
2:M:334:ILE:O	2:M:338:GLU:HG3	2.09	0.52
2:M:94:ASP:C	2:M:100:LYS:NZ	2.62	0.52
2:C:281:LEU:HD23	2:C:285:MET:CE	2.36	0.52
2:C:93:ILE:HG23	2:D:133:ARG:HH12	1.73	0.52
2:D:360:HIS:CG	2:D:363:MET:SD	3.03	0.52
2:D:360:HIS:HB2	2:D:363:MET:CE	2.39	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:10:TRP:CH2	2:M:190:ILE:HG23	2.37	0.52
2:M:360:HIS:HD2	2:M:363:MET:H	1.57	0.52
2:N:259:ALA:CB	2:N:363:MET:SD	2.97	0.52
2:B:276:ILE:HG22	2:B:277:GLU:N	2.24	0.52
2:B:365:LEU:CD2	2:C:297:LEU:HD13	2.39	0.52
2:M:3:TYR:O	2:M:4:GLN:HB2	2.09	0.52
2:N:291:ARG:HD2	2:N:306:MET:SD	2.49	0.52
2:N:360:HIS:CG	2:N:363:MET:SD	3.03	0.52
1:A:309:GLU:O	1:A:313:LYS:HG3	2.10	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:C:156:THR:HG22	2:C:158:ASP:N	2.21	0.52
2:C:359:PHE:CE2	2:D:323:THR:CG2	2.89	0.52
2:I:250:LEU:HD23	2:I:312:ARG:HH11	1.75	0.52
2:I:259:ALA:CB	2:I:363:MET:SD	2.98	0.52
2:N:250:LEU:HD23	2:N:312:ARG:HH11	1.75	0.52
2:N:240:MET:SD	3:O:157:SER:HB2	2.50	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
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:L:93:ILE:HG22	2:L:100:LYS:NZ	2.25	0.52
2:L:94:ASP:N	2:L:100:LYS:HZ1	2.06	0.52
1:A:312:LEU:HB2	1:A:320:VAL:CG2	2.35	0.52
2:C:191:LEU:HD12	2:C:203:LEU:HD21	1.91	0.52
3:E:204:LEU:O	3:E:209:ASN:HB3	2.07	0.52
2:G:93:ILE:HG22	2:G:100:LYS:NZ	2.25	0.52
2:I:200:PRO:HB2	2:I:305:ASP:H	1.75	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:L:276:ILE:HG22	2:L:277:GLU:N	2.24	0.52
2:N:271:ALA:HB1	2:N:276:ILE:HD11	1.90	0.52
2:N:360:HIS:HB2	2:N:363:MET:CE	2.39	0.52
1:A:75:ALA:HB2	1:F:207:ASN:HB3	1.90	0.52
2:D:345:ARG:NH1	3:E:149:GLU:OE1	2.43	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
2:N:302:LEU:HD22	2:N:306:MET:HG2	1.90	0.52
2:M:341:TYR:CB	2:N:333:LEU:HD11	2.11	0.52
1:A:282:ARG:HG2	1:A:285:MET:HE2	1.91	0.52
1:A:294:SER:H	1:A:297:GLN:NE2	2.08	0.52
3:E:238:HIS:ND1	3:E:239:GLU:N	2.56	0.52
2:H:19:VAL:CG2	2:H:214:LEU:CD2	2.88	0.52
2:H:215:ARG:HH21	2:I:164:VAL:HG21	1.74	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
1:F:10:ARG:HH22	1:F:40:GLN:NE2	2.08	0.52
2:G:93:ILE:CG2	2:G:100:LYS:HZ2	2.22	0.52
2:G:7:ALA:HB2	2:G:219:SER:HB3	1.90	0.52
2:L:180:VAL:HG11	2:L:305:ASP:HB2	1.91	0.52
2:N:93:ILE:HG22	2:N:100:LYS:HZ2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:13:GLN:HE22	2:N:83:GLU:CG	2.22	0.52
2:N:223:GLN:NE2	3:O:158:ARG:HE	2.08	0.52
2:D:257:VAL:HG11	2:D:320:ILE:CD1	2.40	0.52
2:D:352:THR:O	2:D:355:ARG:HB3	2.10	0.52
2:D:360:HIS:CB	2:D:363:MET:CB	2.68	0.52
2:H:252:LEU:HD13	2:H:281:LEU:HD21	1.92	0.52
2:I:360:HIS:HB2	2:I:363:MET:CE	2.39	0.52
1:K:306:THR:HG21	3:O:314:ASP:OD2	2.10	0.52
2:N:240:MET:O	3:O:156:ARG:HG3	2.10	0.52
1:A:10:ARG:HH22	1:A:40:GLN:NE2	2.08	0.51
2:B:99:THR:O	2:B:99:THR:CG2	2.53	0.51
2:D:259:ALA:CB	2:D:363:MET:SD	2.98	0.51
2:H:89:ASP:HB3	2:H:121:LYS:HA	1.92	0.51
2:I:357:LEU:C	2:I:363:MET:SD	2.88	0.51
3:J:311:LEU:O	3:J:314:ASP:HB3	2.10	0.51
1:K:27:ASP:HB3	1:K:30:LEU:HB2	1.92	0.51
1:K:333:HIS:NE2	2:L:297:LEU:HG	2.24	0.51
3:O:27:LEU:O	3:O:143:LEU:N	2.39	0.51
3:O:311:LEU:O	3:O:314:ASP:HB3	2.11	0.51
1:A:218:VAL:HG11	1:A:253:GLU:HG3	1.91	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
2:D:250:LEU:HD23	2:D:312:ARG:HH11	1.74	0.51
1:F:218:VAL:HG11	1:F:253:GLU:HG3	1.91	0.51
1:F:27:ASP:HB3	1:F:30:LEU:HB2	1.93	0.51
2:N:352:THR:O	2:N:355:ARG:HB3	2.10	0.51
2:N:357:LEU:C	2:N:363:MET:SD	2.88	0.51
3:O:151:LEU:HD21	3:O:155:LEU:HD12	1.93	0.51
1:A:310:LEU:O	1:A:314:GLN:HG3	2.11	0.51
2:H:278:TRP:HB3	2:H:349:VAL:HG21	1.91	0.51
2:I:84:GLN:HB3	2:I:86:ARG:NH2	2.24	0.51
2:M:181:GLU:HA	2:M:184:ARG:HB3	1.93	0.51
2:M:191:LEU:HD12	2:M:203:LEU:HD21	1.91	0.51
2:N:360:HIS:O	2:N:363:MET:HB2	2.09	0.51
1:A:93:ILE:HG23	1:A:97:LEU:HD13	1.91	0.51
1:A:333:HIS:CE1	2:B:298:SER:OG	2.64	0.51
2:D:93:ILE:HG22	2:D:100:LYS:HZ2	1.76	0.51
2:G:343:PRO:CG	2:G:347:MET:SD	2.99	0.51
2:H:86:ARG:NE	2:I:141:LYS:HB2	2.26	0.51
2:H:11:ARG:HH22	2:I:165:THR:HG22	1.74	0.51
2:L:347:MET:SD	2:M:290:HIS:CD2	3.03	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
2:N:84:GLN:HB3	2:N:86:ARG:NH2	2.24	0.51
2:B:93:ILE:HG22	2:B:100:LYS:NZ	2.25	0.51
2:C:89:ASP:HB3	2:C:121:LYS:HA	1.92	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:I:271:ALA:HB1	2:I:276:ILE:HD11	1.90	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:N:257:VAL:HG11	2:N:320:ILE:CD1	2.40	0.51
2:B:365:LEU:CD2	2:C:297:LEU:HD11	2.38	0.51
3:J:151:LEU:HD21	3:J:155:LEU:HD12	1.92	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
1:K:310:LEU:O	1:K:314:GLN:HG3	2.11	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:G:243:THR:HG22	2:G:244:LEU:N	2.26	0.51
2:G:302:LEU:HG	2:G:314:ARG:NH1	2.26	0.51
2:H:191:LEU:HD12	2:H:203:LEU:HD21	1.91	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:L:302:LEU:HG	2:L:314:ARG:NH1	2.26	0.51
1:K:218:VAL:HG11	1:K:253:GLU:HG3	1.91	0.51
2:M:252:LEU:HD13	2:M:281:LEU:HD21	1.92	0.51
2:B:303:GLY:HA3	2:B:306:MET:HG2	1.93	0.51
3:J:34:GLY:O	3:J:199:GLY:HA3	2.11	0.51
1:K:261:LYS:HE3	1:K:295:GLN:HE21	1.76	0.51
1:K:300:GLN:OE1	1:K:335:PRO:HG2	2.09	0.51
2:L:243:THR:HG22	2:L:244:LEU:N	2.26	0.51
3:O:139:THR:HG22	3:O:140:TRP:N	2.26	0.51
2:C:93:ILE:HG23	2:C:100:LYS:HZ2	1.75	0.51
3:E:311:LEU:O	3:E:314:ASP:HB3	2.10	0.51
1:F:310:LEU:O	1:F:314:GLN:HG3	2.11	0.51
2:G:21:GLN:CG	2:G:178:LEU:HD23	2.40	0.51
2:G:362:ARG:HH21	2:G:363:MET:HE1	1.76	0.51
2:L:10:TRP:CZ2	2:L:193:GLU:CB	2.94	0.51
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
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:G:19:VAL:H	2:G:214:LEU:CD2	2.23	0.50
2:I:60:LYS:HE3	2:I:79:CYS:HB3	1.93	0.50
1:F:283:ARG:CZ	2:N:315:GLU:OE1	2.33	0.50
2:C:360:HIS:CD2	2:C:362:ARG:H	2.30	0.50
2:C:365:LEU:HD21	2:D:297:LEU:HD13	1.92	0.50
3:E:145:THR:HG22	3:E:147:GLU:N	2.27	0.50
1:F:300:GLN:OE1	1:F:335:PRO:HG2	2.09	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
2:M:360:HIS:CD2	2:M:362:ARG:H	2.30	0.50
1:A:261:LYS:HE3	1:A:295:GLN:HE21	1.76	0.50
1:A:338:ASP:OD2	2:B:326:GLN:HG3	2.10	0.50
2:D:5:VAL:CG1	2:D:222:ASP:CG	2.80	0.50
3:E:151:LEU:HD21	3:E:155:LEU:HD12	1.93	0.50
3:E:35:MET:HE1	3:E:166:PRO:HA	1.94	0.50
2:H:102:GLU:HB3	2:H:106:ASP:CB	2.41	0.50
2:H:276:ILE:HG22	2:H:277:GLU:N	2.24	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
2:M:342:ALA:CA	2:N:333:LEU:HD21	2.41	0.50
2:N:99:THR:O	2:N:99:THR:CG2	2.53	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:B:243:THR:HG22	2:B:244:LEU:N	2.26	0.50
2:B:6:LEU:CD2	2:B:194:GLU:OE2	2.59	0.50
2:C:213:SER:OG	2:C:216:ASP:HB2	2.11	0.50
2:B:347:MET:HG3	2:C:290:HIS:CD2	2.46	0.50
2:G:69:THR:HG22	2:G:71:THR:N	2.01	0.50
2:L:180:VAL:HG11	2:L:305:ASP:CB	2.41	0.50
2:L:343:PRO:CG	2:L:347:MET:SD	2.99	0.50
2:M:347:MET:HG2	2:N:290:HIS:ND1	2.27	0.50
2:B:343:PRO:CG	2:B:347:MET:SD	2.99	0.50
2:D:288:LEU:O	2:D:292:ILE:HG13	2.12	0.50
1:F:96:GLN:O	1:F:100:LEU:HG	2.12	0.50
1:F:270:ARG:NH2	2:N:316:LEU:CA	2.72	0.50
2:H:20:GLY:HA3	2:H:182:GLN:HE21	1.76	0.50
2:H:360:HIS:CD2	2:H:362:ARG:H	2.30	0.50
2:H:92:GLU:HG2	2:H:124:LEU:HD23	1.94	0.50
1:K:96:GLN:O	1:K:100:LEU:HG	2.12	0.50
1:A:20:ALA:O	1:A:134:SER:HB2	2.11	0.50
2:C:102:GLU:HB3	2:C:106:ASP:CB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:302:LEU:HD11	2:D:313:MET:HB2	1.94	0.50
2:D:60:LYS:HE3	2:D:79:CYS:HB3	1.93	0.50
1:F:20:ALA:O	1:F:134:SER:HB2	2.12	0.50
2:I:184:ARG:HH22	2:I:304:ASN:HD22	1.59	0.50
2:B:366:PRO:C	2:B:367:GLU:HG3	2.32	0.50
2:B:6:LEU:HD23	2:B:194:GLU:OE2	2.12	0.50
2:C:181:GLU:HA	2:C:184:ARG:HB3	1.93	0.50
2:C:201:ARG:HB2	2:C:305:ASP:OD2	2.12	0.50
3:E:46:ARG:NH1	3:E:68:MET:HG3	2.27	0.50
2:G:303:GLY:HA3	2:G:306:MET:HG2	1.93	0.50
2:G:49:VAL:HG12	2:G:50:GLY:N	2.27	0.50
2:G:343:PRO:HA	2:H:283:VAL:HG13	1.93	0.50
1:K:296:THR:HG22	1:K:299:ARG:HH12	1.77	0.50
2:M:92:GLU:HG2	2:M:124:LEU:HD23	1.94	0.50
2:N:302:LEU:HD11	2:N:313:MET:HB2	1.94	0.50
1:A:274:ASP:HA	1:A:279:TRP:CZ3	2.47	0.50
1:F:282:ARG:HG2	1:F:285:MET:HE2	1.94	0.50
1:F:261:LYS:HE3	1:F:295:GLN:HE21	1.76	0.50
2:G:354:LEU:HD12	2:H:294:MET:SD	2.44	0.50
2:I:223:GLN:HG2	3:J:158:ARG:NH2	2.26	0.50
1:K:144:GLN:NE2	1:K:280:GLN:HB2	2.27	0.50
1:K:312:LEU:HB2	1:K:320:VAL:CG2	2.35	0.50
2:L:347:MET:HG3	2:M:290:HIS:CE1	2.47	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
1:A:27:ASP:HB3	1:A:30:LEU:HB2	1.93	0.50
2:B:302:LEU:HG	2:B:314:ARG:NH1	2.26	0.50
3:E:139:THR:HG22	3:E:140:TRP:N	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
2:M:102:GLU:HB3	2:M:106:ASP:CB	2.41	0.50
3:O:46:ARG:NH1	3:O:68:MET:HG3	2.27	0.50
1:A:273:PHE:HB3	1:A:279:TRP:HB2	1.90	0.49
1:A:309:GLU:HG3	3:E:306:ILE:HG23	1.94	0.49
2:G:82:ILE:HG23	2:G:90:LEU:CD2	2.42	0.49
2:I:5:VAL:CG1	2:I:222:ASP:CG	2.80	0.49
2:I:47:ARG:NE	3:J:126:ASN:OD1	2.45	0.49
3:J:145:THR:HG22	3:J:147:GLU:N	2.27	0.49
3:J:46:ARG:NH1	3:J:68:MET:HG3	2.27	0.49
2:M:44:SER:HB2	2:M:159:PRO:HG3	1.94	0.49
2:M:277:GLU:OE2	2:N:176:LYS:HD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:41:ILE:HG21	3:O:113:TRP:CG	2.47	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:D:360:HIS:HB2	2:D:363:MET:HE3	1.94	0.49
2:H:271:ALA:HB1	2:H:276:ILE:CD1	2.36	0.49
2:I:52:THR:O	2:I:55:ALA:HB3	2.13	0.49
1:K:274:ASP:HA	1:K:279:TRP:CZ3	2.47	0.49
3:O:145:THR:HG22	3:O:147:GLU:N	2.27	0.49
1:A:296:THR:HG22	1:A:299:ARG:HH12	1.77	0.49
2:B:362:ARG:HH21	2:B:363:MET:HE1	1.77	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:N:363:MET:CB	2:N:364:PRO:CD	2.78	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
2:D:140:LEU:HD22	2:D:169:ARG:CZ	2.43	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
2:G:99:THR:CG2	2:G:99:THR:O	2.53	0.49
2:I:288:LEU:O	2:I:292:ILE:HG13	2.12	0.49
1:K:32:GLN:HE22	2:L:165:THR:HG22	1.72	0.49
1:A:22:LEU:HD22	1:A:112:VAL:HB	1.95	0.49
2:B:82:ILE:HG23	2:B:90:LEU:CD2	2.42	0.49
2:C:56:ARG:HH21	2:D:165:THR:HG23	1.76	0.49
1:K:119:LYS:H	1:K:119:LYS:CD	2.05	0.49
2:L:49:VAL:HG12	2:L:50:GLY:N	2.27	0.49
2:D:356:ALA:O	2:D:363:MET:HE3	2.12	0.49
1:F:199:LEU:HB3	1:F:200:PRO:HD3	1.94	0.49
2:M:244:LEU:HB3	2:M:248:GLN:HB2	1.95	0.49
2:N:276:ILE:HG22	2:N:277:GLU:N	2.28	0.49
2:N:257:VAL:HG11	2:N:320:ILE:HD13	1.95	0.49
1:A:172:TYR:O	1:A:216:HIS:HE1	1.96	0.49
2:D:277:GLU:HA	3:E:149:GLU:CG	2.42	0.49
2:D:200:PRO:HB2	2:D:305:ASP:N	2.28	0.49
3:E:85:LYS:NZ	3:E:85:LYS:HB3	2.28	0.49
2:G:201:ARG:O	2:G:205:LEU:HG	2.12	0.49
2:H:94:ASP:C	2:H:100:LYS:NZ	2.62	0.49
3:J:312:ILE:O	3:J:316:LEU:HG	2.13	0.49
2:N:360:HIS:CG	2:N:363:MET:HE3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:52:THR:O	2:N:55:ALA:HB3	2.13	0.49
1:A:96:GLN:O	1:A:100:LEU:HG	2.12	0.49
2:D:236:ALA:O	2:D:239:ALA:HB3	2.12	0.49
1:F:48:GLU:CG	1:F:49:GLU:N	2.76	0.49
2:H:342:ALA:HA	2:I:333:LEU:HD21	1.95	0.49
2:I:276:ILE:HG22	2:I:277:GLU:N	2.28	0.49
3:J:41:ILE:HG21	3:J:113:TRP:CG	2.47	0.49
1:K:48:GLU:CG	1:K:49:GLU:N	2.76	0.49
2:N:60:LYS:HE3	2:N:79:CYS:HB3	1.93	0.49
3:O:312:ILE:O	3:O:316:LEU:HG	2.13	0.49
2:B:49:VAL:HG12	2:B:50:GLY:N	2.27	0.49
2:C:84:GLN:CB	2:D:144:GLU:OE1	2.61	0.49
2:D:276:ILE:HG22	2:D:277:GLU:N	2.28	0.49
3:E:312:ILE:O	3:E:316:LEU:HG	2.12	0.49
2:H:244:LEU:HB3	2:H:248:GLN:HB2	1.95	0.49
1:K:183:GLN:HA	1:K:183:GLN:HE21	1.78	0.49
2:L:235:GLN:HA	2:L:243:THR:HG21	1.94	0.49
2:N:236:ALA:O	2:N:239:ALA:HB3	2.12	0.49
2:D:257:VAL:HG11	2:D:320:ILE:HD13	1.95	0.49
1:F:22:LEU:HD22	1:F:112:VAL:HB	1.94	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:I:140:LEU:HD22	2:I:169:ARG:CZ	2.43	0.49
2:B:69:THR:HG22	2:B:70:ALA:N	2.28	0.48
3:E:41:ILE:HG21	3:E:113:TRP:CG	2.47	0.48
3:E:100:LEU:HD13	3:E:139:THR:HG21	1.93	0.48
2:G:12:PRO:CD	2:G:215:ARG:NH1	2.70	0.48
2:G:366:PRO:C	2:G:367:GLU:HG3	2.32	0.48
3:J:85:LYS:NZ	3:J:85:LYS:HB3	2.28	0.48
2:L:201:ARG:O	2:L:205:LEU:HG	2.11	0.48
2:L:82:ILE:HG23	2:L:90:LEU:CD2	2.42	0.48
2:N:140:LEU:HD22	2:N:169:ARG:CZ	2.42	0.48
1:A:48:GLU:CG	1:A:49:GLU:N	2.76	0.48
1:F:183:GLN:HE21	1:F:183:GLN:HA	1.78	0.48
3:O:145:THR:HG22	3:O:147:GLU:H	1.78	0.48
3:E:57:LYS:HG3	3:E:58:SER:H	1.78	0.48
1:F:251:GLN:OE1	3:J:307:ASN:ND2	2.46	0.48
2:M:56:ARG:NH2	2:N:165:THR:HG21	2.27	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
2:G:270:GLU:HG2	2:G:274:ARG:NH1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:360:HIS:HB2	2:I:363:MET:HE3	1.95	0.48
3:J:241:ALA:O	3:J:245:LEU:HD22	2.14	0.48
1:K:199:LEU:HB3	1:K:200:PRO:HD3	1.94	0.48
2:L:256:MET:CE	2:L:332:LEU:HD21	2.44	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
2:N:338:GLU:HA	2:N:341:TYR:CD1	2.48	0.48
2:D:302:LEU:HD11	2:D:313:MET:CB	2.44	0.48
2:D:52:THR:O	2:D:55:ALA:HB3	2.13	0.48
2:G:140:LEU:O	2:G:144:GLU:HG3	2.14	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:I:337:LYS:HD3	3:J:334:LEU:HB2	1.96	0.48
1:K:311:THR:HG23	1:K:318:GLN:CD	2.34	0.48
2:L:362:ARG:HE	2:L:363:MET:CE	2.25	0.48
2:L:365:LEU:HD22	2:M:297:LEU:HD12	1.95	0.48
2:N:302:LEU:HD11	2:N:313:MET:CB	2.44	0.48
3:O:57:LYS:HG3	3:O:58:SER:H	1.78	0.48
2:B:270:GLU:HG2	2:B:274:ARG:NH1	2.28	0.48
3:E:306:ILE:HG22	3:E:307:ASN:N	2.29	0.48
2:G:286:LEU:HD11	2:G:333:LEU:HA	1.96	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:J:145:THR:HG22	3:J:147:GLU:H	1.78	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:D:260:ASN:OD1	2:D:260:ASN:O	2.32	0.48
2:G:32:LEU:HD11	2:G:58:LEU:HD12	1.95	0.48
2:H:93:ILE:CG2	2:H:100:LYS:HZ2	2.25	0.48
3:J:57:LYS:HG3	3:J:58:SER:H	1.78	0.48
2:L:32:LEU:HD11	2:L:58:LEU:HD12	1.95	0.48
2:M:271:ALA:HB1	2:M:276:ILE:CD1	2.36	0.48
2:C:239:ALA:HB1	2:D:23:HIS:CE1	2.49	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
2:H:341:TYR:CE2	2:I:337:LYS:CB	2.95	0.48
1:K:191:LEU:HD22	2:L:23:HIS:ND1	2.29	0.48
2:N:24:VAL:HG11	2:N:175:LEU:HD21	1.96	0.48
2:B:256:MET:CE	2:B:332:LEU:HD21	2.44	0.48
2:C:341:TYR:CE2	2:D:337:LYS:CB	2.96	0.48
2:C:66:THR:O	2:C:66:THR:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:93:ILE:CG2	2:D:100:LYS:HZ2	2.27	0.48
1:F:311:THR:HG23	1:F:318:GLN:CD	2.34	0.48
2:G:20:GLY:O	2:G:182:GLN:NE2	2.46	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
1:K:22:LEU:HD22	1:K:112:VAL:HB	1.94	0.48
1:K:281:ASN:O	1:K:283:ARG:N	2.47	0.48
2:L:270:GLU:HG2	2:L:274:ARG:NH1	2.29	0.48
2:N:360:HIS:HB2	2:N:363:MET:HE3	1.95	0.48
2:N:93:ILE:CG2	2:N:100:LYS:HZ2	2.26	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
1:F:296:THR:HG22	1:F:299:ARG:HH12	1.77	0.48
2:G:19:VAL:N	2:G:214:LEU:HD22	2.21	0.48
2:H:44:SER:HB2	2:H:159:PRO:HG3	1.94	0.48
2:H:84:GLN:CA	2:I:144:GLU:OE1	2.62	0.48
2:H:84:GLN:CG	2:I:144:GLU:OE1	2.62	0.48
2:I:24:VAL:HG11	2:I:175:LEU:HD21	1.96	0.48
2:I:260:ASN:O	2:I:260:ASN:OD1	2.32	0.48
2:I:338:GLU:HA	2:I:341:TYR:CD1	2.48	0.48
1:K:10:ARG:NH2	1:K:40:GLN:HE22	2.11	0.48
1:A:199:LEU:HB3	1:A:200:PRO:HD3	1.94	0.47
2:C:147:PRO:HG2	2:C:150:VAL:HB	1.96	0.47
2:H:147:PRO:HG2	2:H:150:VAL:HB	1.96	0.47
2:N:355:ARG:NH2	3:O:332:PRO:HD3	2.18	0.47
1:A:10:ARG:NH2	1:A:40:GLN:HE22	2.11	0.47
2:B:286:LEU:HD11	2:B:333:LEU:HA	1.96	0.47
3:J:306:ILE:HG22	3:J:307:ASN:N	2.29	0.47
2:L:140:LEU:O	2:L:144:GLU:HG3	2.14	0.47
3:O:241:ALA:O	3:O:245:LEU:HD22	2.14	0.47
3:O:306:ILE:HG22	3:O:307:ASN:N	2.29	0.47
2:C:354:LEU:HD22	2:D:297:LEU:HD22	1.96	0.47
3:E:145:THR:HG22	3:E:147:GLU:H	1.78	0.47
2:I:257:VAL:HG11	2:I:320:ILE:HD13	1.95	0.47
2:B:94:ASP:O	2:B:100:LYS:CE	2.62	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:N	2:G:214:LEU:CD2	2.78	0.47
2:H:10:TRP:HZ2	2:H:194:GLU:CG	2.28	0.47
3:J:241:ALA:N	3:J:242:PRO:HD2	2.29	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)
2:L:244:LEU:HA	2:L:244:LEU:HD23	1.51	0.47
2:M:257:VAL:HG11	2:M:320:ILE:HD13	1.97	0.47
2:N:316:LEU:HD22	2:N:320:ILE:CD1	2.45	0.47
3:O:241:ALA:N	3:O:242:PRO:HD2	2.29	0.47
1:A:221:LEU:HA	1:A:221:LEU:HD23	1.47	0.47
1:A:310:LEU:HD13	1:A:314:GLN:HE22	1.77	0.47
2:B:292:ILE:O	2:B:296:GLN:HG3	2.14	0.47
2:C:291:ARG:NH1	2:C:306:MET:HG3	2.29	0.47
2:D:246:ASP:HB2	2:D:248:GLN:CG	2.45	0.47
3:E:241:ALA:O	3:E:245:LEU:HD22	2.14	0.47
1:A:74:PHE:CZ	1:F:203:GLU:OE1	2.62	0.47
2:G:19:VAL:HG21	2:G:186:GLN:HG2	1.78	0.47
2:G:256:MET:CE	2:G:332:LEU:HD21	2.44	0.47
2:H:126:ASP:HA	2:H:155:ALA:HB3	1.96	0.47
2:H:216:ASP:O	2:H:220:LEU:HG	2.15	0.47
2:H:66:THR:O	2:H:66:THR:HG22	2.14	0.47
2:I:10:TRP:CE2	2:I:190:ILE:HG23	2.49	0.47
2:N:260:ASN:OD1	2:N:260:ASN:O	2.32	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
2:C:316:LEU:HB3	2:C:320:ILE:HD12	1.96	0.47
2:D:244:LEU:HD11	2:D:276:ILE:CG2	2.45	0.47
1:F:262:ARG:CZ	3:J:230:TYR:CD2	2.97	0.47
1:F:98:LEU:O	1:F:101:THR:HG22	2.14	0.47
2:G:10:TRP:CE3	2:G:190:ILE:CG2	2.96	0.47
2:H:101:VAL:HG12	2:H:102:GLU:HG3	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
1:A:194:ASP:CA	2:M:311:LEU:CD1	2.80	0.47
1:A:60:ASP:O	1:A:64:ILE:HD12	2.15	0.47
2:B:50:GLY:O	2:B:54:ILE:HG13	2.15	0.47
1:F:281:ASN:O	1:F:283:ARG:N	2.47	0.47
2:G:50:GLY:O	2:G:54:ILE:HG13	2.15	0.47
2:M:101:VAL:HG12	2:M:102:GLU:HG3	1.96	0.47
2:M:147:PRO:HG2	2:M:150:VAL:HB	1.96	0.47
2:N:246:ASP:HB2	2:N:248:GLN:CG	2.45	0.47
2:N:220:LEU:HD21	3:O:154:THR:HB	1.96	0.47
1:A:263:GLN:HB2	1:A:272:LEU:HD21	1.97	0.47
2:B:32:LEU:HD11	2:B:58:LEU:HD12	1.95	0.47
2:B:333:LEU:CD1	2:B:337:LYS:HE3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:241:ALA:N	3:E:242:PRO:HD2	2.29	0.47
2:L:292:ILE:O	2:L:296:GLN:HG3	2.14	0.47
2:M:316:LEU:HB3	2:M:320:ILE:HD12	1.96	0.47
1:A:119:LYS:N	1:A:119:LYS:HD3	2.11	0.47
1:A:311:THR:HG23	1:A:318:GLN:OE1	2.15	0.47
2:B:6:LEU:CG	2:B:190:ILE:CG2	2.86	0.47
2:C:244:LEU:HB3	2:C:248:GLN:HB2	1.95	0.47
2:D:24:VAL:HG11	2:D:175:LEU:HD21	1.96	0.47
3:E:227:GLY:O	3:E:229:TRP:HD1	1.98	0.47
2:G:94:ASP:O	2:G:100:LYS:CE	2.63	0.47
2:G:20:GLY:HA3	2:G:182:GLN:CD	2.36	0.47
2:G:292:ILE:O	2:G:296:GLN:HG3	2.14	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:311:THR:HG23	1:K:318:GLN:OE1	2.15	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:N:244:LEU:HD11	2:N:276:ILE:CG2	2.45	0.47
1:K:262:ARG:CZ	3:O:230:TYR:CD2	2.98	0.47
2:N:334:ILE:HG12	3:O:334:LEU:OXT	2.14	0.47
2:C:97:SER:HG	2:C:100:LYS:HE3	1.76	0.47
3:E:27:LEU:O	3:E:143:LEU:N	2.39	0.47
2:I:44:SER:OG	2:I:174:HIS:HA	2.14	0.47
2:I:200:PRO:CG	2:I:304:ASN:HB3	2.44	0.47
1:K:98:LEU:O	1:K:101:THR:HG22	2.14	0.47
1:K:305:LEU:HD22	3:O:310:LEU:HD11	1.97	0.47
2:N:256:MET:HA	2:N:357:LEU:HD11	1.97	0.47
2:B:140:LEU:O	2:B:144:GLU:HG3	2.14	0.47
2:C:257:VAL:HG11	2:C:320:ILE:HD13	1.97	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
2:M:11:ARG:NH1	2:N:144:GLU:OE2	2.48	0.47
2:N:361:PRO:O	2:N:362:ARG:HB2	2.15	0.47
3:O:6:TRP:CH2	3:O:175:TRP:CZ2	3.03	0.47
1:A:98:LEU:O	1:A:101:THR:HG22	2.14	0.46
2:C:101:VAL:HG12	2:C:102:GLU:HG3	1.96	0.46
2:D:165:THR:O	2:D:169:ARG:HG3	2.15	0.46
2:D:256:MET:HA	2:D:357:LEU:HD11	1.97	0.46
1:F:263:GLN:HB2	1:F:272:LEU:HD21	1.97	0.46
1:F:312:LEU:O	1:F:312:LEU:HG	2.15	0.46
2:H:291:ARG:NH1	2:H:306:MET:HG3	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:316:LEU:HD22	2:I:320:ILE:CD1	2.45	0.46
1:K:263:GLN:OE1	1:K:272:LEU:HD11	2.16	0.46
1:K:315:ASP:HB2	1:K:318:GLN:CD	2.36	0.46
1:K:60:ASP:O	1:K:64:ILE:HD12	2.15	0.46
2:M:201:ARG:NH2	2:M:308:ALA:CB	2.78	0.46
1:A:183:GLN:HA	1:A:183:GLN:HE21	1.78	0.46
1:A:315:ASP:HB2	1:A:318:GLN:CD	2.36	0.46
2:B:316:LEU:HD22	2:B:320:ILE:HD11	1.97	0.46
2:C:365:LEU:HD21	2:D:297:LEU:CD1	2.45	0.46
2:D:44:SER:OG	2:D:174:HIS:HA	2.15	0.46
2:D:361:PRO:O	2:D:362:ARG:HB2	2.15	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:I:361:PRO:O	2:I:362:ARG:HB2	2.15	0.46
2:M:126:ASP:HA	2:M:155:ALA:HB3	1.96	0.46
2:M:66:THR:O	2:M:66:THR:HG22	2.14	0.46
2:N:44:SER:OG	2:N:174:HIS:HA	2.15	0.46
3:O:227:GLY:O	3:O:229:TRP:HD1	1.98	0.46
1:F:19:ALA:CB	1:F:133:ARG:HD3	2.46	0.46
1:F:10:ARG:NH2	1:F:40:GLN:HE22	2.11	0.46
2:H:246:ASP:O	2:H:250:LEU:HB2	2.16	0.46
2:I:165:THR:O	2:I:169:ARG:HG3	2.15	0.46
2:I:246:ASP:HB2	2:I:248:GLN:CG	2.45	0.46
3:J:227:GLY:O	3:J:229:TRP:HD1	1.98	0.46
1:A:213:THR:N	1:A:216:HIS:HD2	1.96	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
1:K:144:GLN:HE22	1:K:280:GLN:HB2	1.80	0.46
2:L:343:PRO:HG3	2:M:287:GLY:HA2	1.97	0.46
2:M:100:LYS:HB3	2:N:133:ARG:NE	2.26	0.46
2:N:345:ARG:CZ	3:O:150:ARG:NE	2.55	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:A:312:LEU:O	1:A:312:LEU:HG	2.15	0.46
2:G:93:ILE:HG23	2:G:100:LYS:HZ3	1.81	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
2:M:246:ASP:O	2:M:250:LEU:HB2	2.16	0.46
2:N:291:ARG:O	2:N:295:VAL:HG23	2.16	0.46
1:A:333:HIS:CE1	2:B:298:SER:HG	2.33	0.46
2:C:149:HIS:CD2	2:C:149:HIS:H	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:27:LEU:CD2	3:J:29:ILE:HD11	2.46	0.46
1:K:19:ALA:CB	1:K:133:ARG:HD3	2.46	0.46
1:K:279:TRP:O	1:K:279:TRP:CD2	2.69	0.46
1:K:298:LEU:O	1:K:302:VAL:HG23	2.16	0.46
2:L:50:GLY:O	2:L:54:ILE:HG13	2.15	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
1:F:60:ASP:O	1:F:64:ILE:HD12	2.15	0.46
2:H:99:THR:O	2:H:99:THR:CG2	2.51	0.46
2:I:343:PRO:HG3	2:I:347:MET:SD	2.56	0.46
2:I:360:HIS:CG	2:I:363:MET:HE3	2.51	0.46
2:M:56:ARG:HH21	2:N:165:THR:HG23	1.79	0.46
2:N:360:HIS:CB	2:N:363:MET:HE3	2.46	0.46
1:A:222:LEU:CD1	1:A:285:MET:SD	3.04	0.46
1:A:298:LEU:O	1:A:302:VAL:HG23	2.16	0.46
2:D:302:LEU:HA	2:D:302:LEU:HD23	1.54	0.46
2:D:316:LEU:HD22	2:D:320:ILE:CD1	2.45	0.46
1:F:315:ASP:HB2	1:F:318:GLN:NE2	2.31	0.46
2:G:19:VAL:H	2:G:214:LEU:HD22	1.81	0.46
2:G:333:LEU:CD1	2:G:337:LYS:HE3	2.45	0.46
2:I:291:ARG:O	2:I:295:VAL:HG23	2.16	0.46
2:I:93:ILE:HG22	2:I:100:LYS:HZ2	1.80	0.46
1:K:315:ASP:HB2	1:K:318:GLN:NE2	2.31	0.46
2:L:204:GLN:HE21	2:L:305:ASP:CG	2.18	0.46
2:M:359:PHE:CZ	2:N:323:THR:HG22	2.50	0.46
2:M:73:CYS:SG	2:M:76:CYS:HB3	2.56	0.46
2:C:216:ASP:O	2:C:220:LEU:HG	2.15	0.46
2:C:7:ALA:O	2:D:168:SER:HB2	2.16	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
1:F:247:LEU:HD11	1:F:308:THR:HG22	1.98	0.46
2:H:149:HIS:CD2	2:H:149:HIS:H	2.34	0.46
2:I:244:LEU:HD11	2:I:276:ILE:CG2	2.45	0.46
3:J:95:GLU:O	3:J:99:LYS:HB2	2.15	0.46
1:K:32:GLN:NE2	2:L:165:THR:CA	2.78	0.46
2:B:344:ASP:O	2:B:347:MET:HB3	2.16	0.46
2:C:51:LYS:HE3	2:C:51:LYS:HB2	1.77	0.46
2:D:42:LEU:HD12	2:D:172:GLN:OE1	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:306:THR:OG1	3:J:310:LEU:CD2	2.61	0.46
2:G:10:TRP:CE3	2:G:190:ILE:HD13	2.51	0.46
2:G:19:VAL:CG1	2:G:183:ILE:HA	2.38	0.46
2:G:354:LEU:CD2	2:H:297:LEU:CD2	2.85	0.46
2:H:354:LEU:HD22	2:I:297:LEU:HD22	1.96	0.46
3:J:51:GLN:HB2	3:J:62:CYS:HB2	1.97	0.46
1:K:198:THR:HB	1:K:200:PRO:HD2	1.98	0.46
1:K:247:LEU:HD11	1:K:308:THR:HG22	1.98	0.46
2:L:316:LEU:HD22	2:L:320:ILE:HD11	1.98	0.46
2:L:56:ARG:NH1	2:L:82:ILE:O	2.49	0.46
2:M:21:GLN:NE2	2:M:176:LYS:O	2.49	0.46
2:M:37:ILE:HD12	2:M:62:LEU:HD21	1.98	0.46
2:C:21:GLN:NE2	2:C:176:LYS:O	2.49	0.45
2:C:246:ASP:O	2:C:250:LEU:HB2	2.16	0.45
3:E:282:SER:OG	3:E:285:ARG:HB2	2.16	0.45
2:H:215:ARG:CZ	2:I:164:VAL:CG2	2.94	0.45
2:I:338:GLU:HA	2:I:341:TYR:HD1	1.81	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:C:260:ASN:O	2:C:260:ASN:OD1	2.35	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:O	2:H:260:ASN:OD1	2.34	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: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:B:186:GLN:HG2	2:B:214:LEU:HD21	1.98	0.45
2:B:56:ARG:NH1	2:B:82:ILE:O	2.49	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
2:C:73:CYS:SG	2:C:76:CYS:HB3	2.56	0.45
2:D:338:GLU:HA	2:D:341:TYR:HD1	1.81	0.45
1:F:315:ASP:HB2	1:F:318:GLN:CD	2.36	0.45
2:I:191:LEU:HD12	2:I:203:LEU:HD21	1.99	0.45
3:J:253:MET:O	3:J:256:LEU:N	2.50	0.45
3:J:14:LEU:HD13	3:J:44:LEU:HD11	1.98	0.45
1:K:213:THR:N	1:K:216:HIS:HD2	1.96	0.45
2:L:344:ASP:O	2:L:347:MET:HB3	2.16	0.45
2:N:42:LEU:HD12	2:N:172:GLN:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:57:LYS:HA	3:O:57:LYS:HD2	1.67	0.45
2:D:191:LEU:HD12	2:D:203:LEU:HD21	1.99	0.45
1:F:310:LEU:HD13	1:F:314:GLN:HE22	1.77	0.45
1:F:311:THR:HG23	1:F:318:GLN:OE1	2.15	0.45
2:G:56:ARG:NH1	2:G:82:ILE:O	2.49	0.45
2:I:95:ALA:HA	2:I:100:LYS:HZ1	1.81	0.45
1:K:312:LEU:HG	1:K:312:LEU:O	2.15	0.45
2:L:22:GLU:HG3	2:L:22:GLU:H	1.09	0.45
2:M:257:VAL:O	2:M:360:HIS:HE1	1.99	0.45
2:N:191:LEU:HD12	2:N:203:LEU:HD21	1.99	0.45
3:O:27:LEU:HG	3:O:29:ILE:CD1	2.47	0.45
3:O:51:GLN:HB2	3:O:62:CYS:HB2	1.98	0.45
1:A:133:ARG:HG3	2:G:299:PRO:CG	2.45	0.45
1:A:19:ALA:CB	1:A:133:ARG:HD3	2.46	0.45
1:A:315:ASP:HB2	1:A:318:GLN:NE2	2.31	0.45
2:D:142:THR:O	2:D:146:PRO:N	2.50	0.45
2:D:291:ARG:O	2:D:295:VAL:HG23	2.16	0.45
1:F:279:TRP:CD2	1:F:279:TRP:O	2.69	0.45
2:G:42:LEU:HD23	2:G:172:GLN:HG2	1.99	0.45
2:I:258:GLU:O	2:I:259:ALA:HB3	2.17	0.45
2:M:238:SER:CB	2:M:245:ASP:OD1	2.65	0.45
2:M:351:MET:HA	2:M:351:MET:HE3	1.97	0.45
2:M:94:ASP:N	2:M:100:LYS:HZ3	2.14	0.45
2:N:142:THR:O	2:N:146:PRO:N	2.50	0.45
2:N:364:PRO:CG	3:O:260:HIS:CE1	2.99	0.45
1:A:25:GLY:N	1:A:114:GLY:O	2.41	0.45
1:A:279:TRP:CD2	1:A:279:TRP:O	2.69	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: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:F:315:ASP:CB	1:F:318:GLN:HG2	2.45	0.45
2:G:344:ASP:O	2:G:347:MET:HB3	2.16	0.45
2:H:257:VAL:O	2:H:360:HIS:HE1	2.00	0.45
2:I:13:GLN:HE22	2:I:83:GLU:CG	2.22	0.45
3:J:204:LEU:O	3:J:209:ASN:HB2	2.16	0.45
2:M:342:ALA:HA	2:N:333:LEU:CD2	2.46	0.45
2:N:343:PRO:HG3	2:N:347:MET:SD	2.56	0.45
3:O:282:SER:OG	3:O:285:ARG:HB2	2.16	0.45
1:A:222:LEU:HD11	1:A:285:MET:CE	2.47	0.45
2:B:219:SER:O	2:B:223:GLN:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:GLU:HG2	2:B:274:ARG:CZ	2.46	0.45
3:E:257:LYS:HB3	3:E:262:ALA:HB3	1.98	0.45
3:E:27:LEU:HG	3:E:29:ILE:CD1	2.47	0.45
2:G:11:ARG:HA	2:G:215:ARG:NH1	2.31	0.45
2:H:102:GLU:HB3	2:H:106:ASP:HB2	1.99	0.45
2:H:37:ILE:HD12	2:H:62:LEU:HD21	1.99	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:J:257:LYS:HB3	3:J:262:ALA:HB3	1.98	0.45
1:K:222:LEU:HD11	1:K:285:MET:CE	2.47	0.45
1:K:32:GLN:HE22	2:L:165:THR:HA	1.79	0.45
3:O:14:LEU:HD13	3:O:44:LEU:HD11	1.98	0.45
2:D:140:LEU:HD11	2:D:165:THR:HB	1.99	0.45
1:F:315:ASP:H	1:F:318:GLN:HE21	1.65	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:H:252:LEU:CD1	2:H:281:LEU:HD21	2.47	0.45
2:I:51:LYS:HB2	2:I:51:LYS:HE3	1.76	0.45
1:K:225:LYS:HE3	1:K:227:LYS:HD2	1.99	0.45
1:K:315:ASP:CB	1:K:318:GLN:HG2	2.45	0.45
2:L:214:LEU:HD12	2:L:214:LEU:HA	1.85	0.45
2:N:197:ALA:HB3	2:N:231:GLN:HG2	1.98	0.45
3:O:257:LYS:HB3	3:O:262:ALA:HB3	1.97	0.45
1:A:223:MET:HB3	1:A:223:MET:HE3	1.90	0.45
2:B:248:GLN:O	2:B:252:LEU:HB2	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:C:99:THR:CG2	2:C:99:THR:O	2.51	0.45
2:D:94:ASP:O	2:D:100:LYS:CE	2.65	0.45
3:E:27:LEU:CD2	3:E:29:ILE:HD11	2.46	0.45
2:H:21:GLN:HE22	2:H:49:VAL:HG13	1.81	0.45
2:I:131:LEU:HB2	2:I:136:PHE:CD1	2.52	0.45
2:I:94:ASP:O	2:I:100:LYS:CE	2.65	0.45
2:L:248:GLN:HA	2:L:251:SER:OG	2.17	0.45
2:M:149:HIS:H	2:M:149:HIS:CD2	2.34	0.45
2:L:223:GLN:OE1	2:M:171:LEU:HD11	2.17	0.45
2:M:5:VAL:HG11	2:N:171:LEU:HB2	1.99	0.45
3:O:253:MET:O	3:O:256:LEU:N	2.49	0.45
2:C:147:PRO:HB2	2:C:149:HIS:CD2	2.53	0.45
2:B:351:MET:HG2	2:C:290:HIS:ND1	2.32	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:G:270:GLU:HG2	2:G:274:ARG:CZ	2.47	0.45
2:I:42:LEU:HB3	2:I:172:GLN:CB	2.42	0.45
2:L:186:GLN:HG2	2:L:214:LEU:HD21	1.98	0.45
2:L:204:GLN:NE2	2:L:305:ASP:CG	2.67	0.45
2:M:252:LEU:CD1	2:M:281:LEU:HD21	2.47	0.45
2:N:131:LEU:HB2	2:N:136:PHE:CD1	2.52	0.45
2:N:302:LEU:HD23	2:N:302:LEU:HA	1.54	0.45
2:N:355:ARG:HA	3:O:287:GLN:NE2	2.32	0.45
2:B:244:LEU:HD23	2:B:247:ASP:OD2	2.17	0.44
2:D:200:PRO:CB	2:D:305:ASP:N	2.80	0.44
3:E:299:GLN:HE21	3:E:311:LEU:HD21	1.82	0.44
1:F:225:LYS:HE3	1:F:227:LYS:HD2	1.99	0.44
2:G:11:ARG:HG2	2:G:215:ARG:NH2	2.32	0.44
2:G:244:LEU:HD23	2:G:247:ASP:OD2	2.18	0.44
2:G:248:GLN:O	2:G:252:LEU:HB2	2.17	0.44
1:F:334:LYS:C	2:G:297:LEU:CD2	2.81	0.44
1:F:234:GLN:CD	2:G:304:ASN:ND2	2.70	0.44
2:I:140:LEU:HD11	2:I:165:THR:HB	1.99	0.44
3:J:299:GLN:HE21	3:J:311:LEU:HD21	1.82	0.44
2:L:104:THR:HG22	2:L:108:LEU:HG	1.99	0.44
2:L:180:VAL:HB	2:L:304:ASN:CB	2.48	0.44
2:L:248:GLN:O	2:L:252:LEU:HB2	2.17	0.44
2:L:270:GLU:HG2	2:L:274:ARG:CZ	2.46	0.44
2:L:307:ALA:HA	2:L:310:GLU:CG	2.47	0.44
2:L:340:PRO:HB3	2:L:345:ARG:HH21	1.83	0.44
2:N:277:GLU:CB	3:O:149:GLU:CG	2.75	0.44
3:O:299:GLN:HE21	3:O:311:LEU:HD21	1.82	0.44
1:A:190:LEU:HD23	1:A:190:LEU:HA	1.84	0.44
2:D:258:GLU:O	2:D:259:ALA:HB3	2.17	0.44
2:D:355:ARG:NH1	3:E:287:GLN:CB	2.79	0.44
3:E:253:MET:O	3:E:256:LEU:N	2.50	0.44
1:F:32:GLN:HG3	2:G:164:VAL:HG12	1.97	0.44
2:G:10:TRP:CZ2	2:G:194:GLU:OE2	2.70	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
1:K:222:LEU:CD1	1:K:285:MET:SD	3.04	0.44
1:A:57:PRO:HB3	1:A:90:ASN:ND2	2.33	0.44
2:C:257:VAL:O	2:C:360:HIS:HE1	2.00	0.44
2:D:66:THR:HG22	2:D:66:THR:O	2.17	0.44
2:G:248:GLN:HA	2:G:251:SER:OG	2.18	0.44
2:G:307:ALA:HA	2:G:310:GLU:CG	2.47	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:G:93:ILE:CG2	2:G:100:LYS:HZ3	2.29	0.44
2:H:245:ASP:HB2	2:H:248:GLN:HG3	1.99	0.44
2:I:135:SER:O	2:I:138:ALA:HB3	2.17	0.44
2:L:219:SER:O	2:L:223:GLN:HG3	2.17	0.44
2:N:338:GLU:OE2	3:O:295:HIS:NE2	2.50	0.44
3:O:95:GLU:O	3:O:99:LYS:HB2	2.15	0.44
1:F:325:GLU:O	1:F:329:LEU:HG	2.18	0.44
2:I:257:VAL:O	2:I:257:VAL:HG12	2.17	0.44
3:J:27:LEU:HG	3:J:29:ILE:CD1	2.47	0.44
3:J:57:LYS:HD2	3:J:57:LYS:HA	1.67	0.44
1:K:191:LEU:HA	1:K:191:LEU:HD23	1.80	0.44
1:K:57:PRO:HB3	1:K:90:ASN:ND2	2.33	0.44
2:L:250:LEU:HD13	2:L:288:LEU:HD13	2.00	0.44
1:A:29:LEU:CD2	1:A:154:ARG:HH12	2.26	0.44
1:A:247:LEU:HD11	1:A:308:THR:HG22	1.98	0.44
2:B:250:LEU:HD13	2:B:288:LEU:HD13	2.00	0.44
3:E:30:GLN:HA	3:E:145:THR:O	2.17	0.44
3:E:57:LYS:HA	3:E:57:LYS:HD2	1.67	0.44
1:F:213:THR:N	1:F:216:HIS:HD2	1.96	0.44
2:G:250:LEU:HD13	2:G:288:LEU:HD13	2.00	0.44
2:I:200:PRO:CB	2:I:304:ASN:CB	2.92	0.44
2:M:260:ASN:O	2:M:260:ASN:OD1	2.35	0.44
2:M:5:VAL:HB	2:M:222:ASP:OD2	2.17	0.44
2:N:135:SER:O	2:N:138:ALA:HB3	2.17	0.44
1:A:325:GLU:O	1:A:329:LEU:HG	2.18	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
2:D:135:SER:O	2:D:138:ALA:HB3	2.17	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:H:167:LEU:HB3	2:H:172:GLN:NE2	2.33	0.44
3:J:33:PRO:O	3:J:197:SER:OG	2.33	0.44
3:J:7:LEU:HD22	3:J:40:LEU:HB2	2.00	0.44
1:K:172:TYR:O	1:K:216:HIS:CE1	2.67	0.44
2:M:9:LYS:NZ	2:M:194:GLU:OE1	2.51	0.44
2:N:240:MET:HB3	3:O:157:SER:CA	2.48	0.44
2:B:278:TRP:CE3	2:B:349:VAL:HG21	2.53	0.44
2:B:340:PRO:HB3	2:B:345:ARG:HH21	1.83	0.44
2:C:245:ASP:HB2	2:C:248:GLN:HG3	1.99	0.44
2:D:62:LEU:O	2:D:119:ARG:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:360:HIS:CB	2:D:363:MET:HE3	2.48	0.44
3:E:51:GLN:HG2	3:E:62:CYS:SG	2.58	0.44
1:F:100:LEU:O	1:F:103:LEU:HB3	2.18	0.44
2:G:10:TRP:HZ2	2:G:194:GLU:CD	2.21	0.44
2:G:219:SER:O	2:G:223:GLN:HG3	2.17	0.44
2:G:250:LEU:HD22	2:G:309:ILE:CG2	2.48	0.44
2:I:66:THR:HG22	2:I:66:THR:O	2.18	0.44
3:J:51:GLN:HG2	3:J:62:CYS:SG	2.58	0.44
1:K:119:LYS:N	1:K:119:LYS:HD3	2.11	0.44
1:K:310:LEU:HD13	1:K:314:GLN:HE22	1.77	0.44
2:L:244:LEU:HD23	2:L:247:ASP:OD2	2.17	0.44
2:M:147:PRO:HB2	2:M:149:HIS:CD2	2.52	0.44
2:M:21:GLN:HE22	2:M:49:VAL:HG13	1.82	0.44
2:N:94:ASP:O	2:N:100:LYS:CE	2.65	0.44
1:A:100:LEU:O	1:A:103:LEU:HB3	2.18	0.44
2:B:42:LEU:HD23	2:B:172:GLN:HG2	1.99	0.44
2:C:167:LEU:HB3	2:C:172:GLN:NE2	2.33	0.44
2:G:278:TRP:CE3	2:G:349:VAL:HG21	2.53	0.44
2:G:307:ALA:HA	2:G:310:GLU:CD	2.38	0.44
2:M:347:MET:HG3	2:N:290:HIS:CE1	2.53	0.44
2:M:354:LEU:HD21	2:N:297:LEU:CD2	2.48	0.44
2:N:360:HIS:CB	2:N:363:MET:CB	2.68	0.44
3:O:30:GLN:HA	3:O:145:THR:O	2.17	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
2:B:104:THR:HG22	2:B:108:LEU:HG	1.99	0.44
2:D:277:GLU:CG	3:E:149:GLU:CG	2.94	0.44
1:F:222:LEU:HD11	1:F:285:MET:CE	2.47	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:257:VAL:O	2:N:360:HIS:CE1	2.60	0.44
2:B:243:THR:CG2	2:B:244:LEU:N	2.81	0.43
1:F:57:PRO:HB3	1:F:90:ASN:ND2	2.33	0.43
3:J:30:GLN:HA	3:J:145:THR:O	2.17	0.43
2:M:245:ASP:HB2	2:M:248:GLN:HG3	1.99	0.43
2:M:3:TYR:N	2:M:3:TYR:CD2	2.83	0.43
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:N:66:THR:O	2:N:66:THR:HG22	2.18	0.43
3:O:51:GLN:HG2	3:O:62:CYS:SG	2.58	0.43
1:A:3:ARG:HG2	1:A:136:GLN:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:I:93:ILE:CG2	2:I:100:LYS:HZ2	2.31	0.43
3:J:18:TYR:HB3	3:J:48:LEU:HD21	2.01	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
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:N:356:ALA:C	2:N:363:MET:HE1	2.37	0.43
2:B:307:ALA:HA	2:B:310:GLU:CG	2.47	0.43
2:C:345:ARG:O	2:C:349:VAL:HG23	2.19	0.43
1:F:191:LEU:HD23	1:F:191:LEU:HA	1.80	0.43
1:F:84:LEU:HA	1:F:84:LEU:HD12	1.84	0.43
2:G:10:TRP:CB	2:G:218:LEU:HD13	2.48	0.43
2:G:340:PRO:HB3	2:G:345:ARG:HH21	1.83	0.43
2:H:100:LYS:CB	2:I:133:ARG:NE	2.78	0.43
3:J:92:ALA:O	3:J:96:VAL:HG23	2.19	0.43
1:K:221:LEU:HA	1:K:221:LEU:HD23	1.47	0.43
2:L:6:LEU:HD22	2:L:190:ILE:HG23	2.00	0.43
2:L:307:ALA:HA	2:L:310:GLU:CD	2.38	0.43
2:L:360:HIS:CD2	2:L:361:PRO:HD2	2.52	0.43
2:M:102:GLU:HB3	2:M:106:ASP:HB2	1.99	0.43
2:M:10:TRP:CH2	2:M:190:ILE:HA	2.53	0.43
2:M:86:ARG:CZ	2:N:141:LYS:CB	2.83	0.43
2:N:257:VAL:HG12	2:N:257:VAL:O	2.17	0.43
2:N:62:LEU:O	2:N:119:ARG:HD2	2.18	0.43
2:C:6:LEU:HG	2:C:222:ASP:OD1	2.18	0.43
2:D:257:VAL:O	2:D:257:VAL:HG12	2.17	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:5:VAL:HG12	2:I:222:ASP:OD2	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
1:A:48:GLU:CG	1:A:49:GLU:H	2.30	0.43
1:A:50:HIS:O	1:A:51:HIS:CD2	2.72	0.43
2:B:140:LEU:HA	2:B:140:LEU:HD23	1.84	0.43
2:B:250:LEU:HD22	2:B:309:ILE:CG2	2.48	0.43
2:D:347:MET:O	2:D:351:MET:CG	2.65	0.43
2:G:104:THR:HG22	2:G:108:LEU:HG	1.99	0.43
2:I:360:HIS:CB	2:I:363:MET:HE3	2.47	0.43
1:K:100:LEU:O	1:K:103:LEU:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M:93:ILE:HG23	2:M:100:LYS:HZ2	1.77	0.43
2:M:355:ARG:CG	2:N:326:GLN:HG3	2.49	0.43
1:A:225:LYS:HE3	1:A:227:LYS:HD2	1.99	0.43
2:B:21:GLN:HE22	2:B:49:VAL:CG1	2.32	0.43
2:C:102:GLU:HB3	2:C:106:ASP:HB2	1.99	0.43
2:C:84:GLN:HG2	2:D:144:GLU:OE1	2.17	0.43
1:F:270:ARG:NH2	2:N:319:THR:H	2.16	0.43
1:F:50:HIS:O	1:F:51:HIS:CD2	2.72	0.43
3:J:30:GLN:HG3	3:J:30:GLN:O	2.18	0.43
1:K:48:GLU:CG	1:K:49:GLU:H	2.30	0.43
2:L:278:TRP:CE3	2:L:349:VAL:HG21	2.53	0.43
2:M:276:ILE:HG13	2:M:276:ILE:H	1.66	0.43
2:B:365:LEU:HD22	2:C:297:LEU:HD13	1.96	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:G:42:LEU:HD11	2:G:156:THR:HG22	2.00	0.43
2:I:229:ASP:C	2:I:231:GLN:N	2.71	0.43
3:J:149:GLU:C	3:J:151:LEU:N	2.71	0.43
1:K:191:LEU:O	1:K:193:PRO:HD3	2.18	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
3:O:7:LEU:HD22	3:O:40:LEU:HB2	2.00	0.43
1:A:29:LEU:O	1:A:33:GLU:HG3	2.19	0.43
2:D:143:LEU:HA	2:D:143:LEU:HD23	1.89	0.43
2:D:337:LYS:O	2:D:340:PRO:HD2	2.19	0.43
3:E:18:TYR:HB3	3:E:48:LEU:HD21	2.00	0.43
2:H:42:LEU:HD12	2:H:154:LEU:HB2	2.00	0.43
2:I:338:GLU:OE2	3:J:295:HIS:NE2	2.52	0.43
2:M:333:LEU:O	2:M:336:ARG:N	2.49	0.43
3:O:92:ALA:O	3:O:96:VAL:HG23	2.19	0.43
1:A:315:ASP:CB	1:A:318:GLN:HG2	2.45	0.43
1:K:325:GLU:O	1:K:329:LEU:HG	2.18	0.43
1:K:50:HIS:O	1:K:51:HIS:CD2	2.72	0.43
2:L:204:GLN:HE21	2:L:305:ASP:CA	2.26	0.43
3:O:117:ALA:HB2	3:O:143:LEU:CD1	2.47	0.43
1:F:270:ARG:HH12	2:N:316:LEU:CB	2.31	0.43
2:H:345:ARG:O	2:H:349:VAL:HG23	2.19	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:L:10:TRP:CZ2	2:L:193:GLU:CG	3.02	0.43
2:M:345:ARG:O	2:M:349:VAL:HG23	2.19	0.43
2:M:362:ARG:C	2:M:363:MET:HG3	2.39	0.43
2:M:42:LEU:HD12	2:M:154:LEU:HB2	2.00	0.43
3:E:149:GLU:O	3:E:151:LEU:N	2.52	0.42
1:F:228:ARG:HG2	1:F:228:ARG:H	1.52	0.42
2:I:337:LYS:O	2:I:340:PRO:HD2	2.19	0.42
3:J:149:GLU:O	3:J:151:LEU:N	2.52	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
2:N:76:CYS:SG	2:N:78:ASN:HB2	2.59	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:C:156:THR:HG22	2:C:157:THR:N	2.34	0.42
2:C:42:LEU:HD12	2:C:154:LEU:HB2	2.00	0.42
2:D:277:GLU:CG	3:E:149:GLU:HG3	2.49	0.42
2:G:243:THR:CG2	2:G:244:LEU:N	2.81	0.42
2:I:244:LEU:HD11	2:I:276:ILE:HG21	2.02	0.42
2:C:136:PHE:CZ	2:C:166:ILE:HD12	2.54	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
3:J:245:LEU:HB2	3:J:297:ARG:HG3	2.01	0.42
1:K:29:LEU:O	1:K:33:GLU:HG3	2.19	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:L:4:GLN:OE1	2:L:9:LYS:CD	2.64	0.42
2:M:147:PRO:HB2	2:M:149:HIS:NE2	2.35	0.42
3:O:30:GLN:O	3:O:30:GLN:HG3	2.18	0.42
2:D:229:ASP:C	2:D:231:GLN:N	2.71	0.42
2:D:76:CYS:SG	2:D:78:ASN:HB2	2.59	0.42
2:I:131:LEU:HB2	2:I:136:PHE:HD1	1.85	0.42
2:L:238:SER:HB3	2:L:244:LEU:N	2.02	0.42
2:M:78:ASN:O	2:M:82:ILE:HG13	2.20	0.42
2:N:289:LEU:HD23	2:N:289:LEU:HA	1.81	0.42
2:N:277:GLU:OE1	3:O:149:GLU:HG3	2.19	0.42
3:O:170:GLN:HG2	3:O:170:GLN:H	1.65	0.42
2:C:18:VAL:HG12	2:C:19:VAL:N	2.35	0.42
2:D:95:ALA:HA	2:D:100:LYS:HZ1	1.85	0.42
3:E:117:ALA:HB2	3:E:143:LEU:CD1	2.47	0.42
1:F:310:LEU:HA	1:F:310:LEU:HD23	1.61	0.42
2:G:6:LEU:HD12	2:G:222:ASP:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:84:GLN:HB3	2:I:144:GLU:OE1	2.20	0.42
2:I:347:MET:O	2:I:351:MET:CG	2.65	0.42
1:K:25:GLY:N	1:K:114:GLY:O	2.41	0.42
2:N:271:ALA:O	2:N:276:ILE:HG13	2.20	0.42
1:K:262:ARG:HH12	3:O:228:ASP:CG	2.23	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:G:342:ALA:HB1	2:G:343:PRO:HD2	2.01	0.42
2:H:136:PHE:CZ	2:H:166:ILE:HD12	2.54	0.42
2:H:360:HIS:CD2	2:H:363:MET:H	2.37	0.42
1:K:246:LEU:HA	1:K:246:LEU:HD23	1.87	0.42
1:K:79:THR:HG22	1:K:80:LEU:N	2.34	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:M:360:HIS:CD2	2:M:363:MET:H	2.37	0.42
2:N:220:LEU:HD21	3:O:154:THR:CB	2.48	0.42
2:N:337:LYS:O	2:N:340:PRO:HD2	2.19	0.42
2:N:357:LEU:CA	2:N:363:MET:HE1	2.46	0.42
1:A:28:PRO:CB	2:B:164:VAL:HG21	2.25	0.42
2:B:362:ARG:HE	2:B:363:MET:CE	2.24	0.42
2:C:342:ALA:HA	2:D:333:LEU:HD21	2.01	0.42
3:E:30:GLN:O	3:E:30:GLN:HG3	2.18	0.42
2:G:276:ILE:CG2	2:G:277:GLU:N	2.82	0.42
2:H:137:ASN:HA	2:H:140:LEU:HD12	2.02	0.42
2:I:244:LEU:CD1	2:I:276:ILE:HD13	2.48	0.42
1:K:190:LEU:HD23	1:K:190:LEU:HA	1.84	0.42
2:M:18:VAL:HG12	2:M:19:VAL:N	2.35	0.42
3:O:225:PRO:HB3	3:O:276:GLU:OE2	2.20	0.42
2:B:42:LEU:HD11	2:B:156:THR:HG22	2.00	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
3:E:35:MET:CE	3:E:166:PRO:HA	2.50	0.42
3:E:225:PRO:HB3	3:E:276:GLU:OE2	2.20	0.42
1:F:243:PRO:HG2	1:F:244:VAL:H	1.85	0.42
1:F:255:LEU:HD12	3:J:309:GLU:OE1	2.20	0.42
2:H:362:ARG:C	2:H:363:MET:HG3	2.39	0.42
2:I:358:ALA:C	2:I:360:HIS:H	2.23	0.42
2:I:351:MET:SD	3:J:290:LEU:HD13	2.59	0.42
3:J:311:LEU:HA	3:J:311:LEU:HD12	1.86	0.42
1:K:311:THR:O	1:K:318:GLN:NE2	2.53	0.42
1:K:333:HIS:HB2	2:L:297:LEU:CD2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:18:TYR:HB3	3:O:48:LEU:HD21	2.01	0.42
2:B:342:ALA:HB1	2:B:343:PRO:HD2	2.01	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
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
1:K:243:PRO:HG2	1:K:244:VAL:H	1.85	0.42
2:L:37:ILE:HG12	2:L:62:LEU:HD21	2.02	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:B:281:LEU:O	2:B:285:MET:HG3	2.20	0.42
2:C:360:HIS:CD2	2:C:363:MET:H	2.37	0.42
2:D:42:LEU:HD23	2:D:154:LEU:HB2	2.02	0.42
2:D:244:LEU:CD1	2:D:276:ILE:HD13	2.48	0.42
1:F:142:PRO:CD	1:F:178:LEU:HD11	2.50	0.42
1:F:264:SER:O	1:F:265:ALA:CB	2.68	0.42
1:F:334:LYS:CB	2:G:297:LEU:CD2	2.71	0.42
1:F:4:LEU:CD1	1:F:137:VAL:HG22	2.50	0.42
2:G:10:TRP:CE3	2:G:190:ILE:CG1	3.01	0.42
2:G:37:ILE:HG12	2:G:62:LEU:HD21	2.02	0.42
2:G:21:GLN:HE22	2:G:49:VAL:CG1	2.32	0.42
2:H:6:LEU:HB2	2:H:222:ASP:OD1	2.19	0.42
2:I:356:ALA:O	2:I:363:MET:HE3	2.17	0.42
2:L:281:LEU:O	2:L:285:MET:HG3	2.20	0.42
2:M:136:PHE:CZ	2:M:166:ILE:HD12	2.54	0.42
2:C:137:ASN:HA	2:C:140:LEU:HD12	2.02	0.41
2:D:360:HIS:CG	2:D:363:MET:HE3	2.54	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
1:K:310:LEU:HB3	1:K:314:GLN:NE2	2.35	0.41
2:M:239:ALA:HB1	2:N:23:HIS:CE1	2.55	0.41
2:N:42:LEU:HD23	2:N:154:LEU:HB2	2.02	0.41
2:N:338:GLU:OE2	3:O:295:HIS:CE1	2.73	0.41
1:A:79:THR:HG22	1:A:80:LEU:N	2.34	0.41
2:B:276:ILE:CG2	2:B:277:GLU:N	2.82	0.41
2:B:37:ILE:HG12	2:B:62:LEU:HD21	2.02	0.41
2:C:147:PRO:HB2	2:C:149:HIS:NE2	2.35	0.41
2:C:3:TYR:N	2:C:3:TYR:CD2	2.86	0.41
2:D:244:LEU:HD11	2:D:276:ILE:HG21	2.01	0.41
1:F:79:THR:HG22	1:F:80:LEU:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:18:VAL:HG12	2:H:19:VAL:N	2.35	0.41
2:I:220:LEU:HD21	3:J:154:THR:CA	2.47	0.41
2:L:276:ILE:CG2	2:L:277:GLU:N	2.82	0.41
2:L:342:ALA:HB1	2:L:343:PRO:HD2	2.01	0.41
2:M:156:THR:HG22	2:M:157:THR:N	2.34	0.41
2:L:343:PRO:HD3	2:M:286:LEU:HB3	2.01	0.41
3:O:245:LEU:HB2	3:O:297:ARG:HG3	2.01	0.41
1:A:142:PRO:CD	1:A:178:LEU:HD11	2.50	0.41
1:A:310:LEU:HB3	1:A:314:GLN:NE2	2.35	0.41
2:C:78:ASN:O	2:C:82:ILE:HG13	2.20	0.41
2:H:156:THR:HG22	2:H:157:THR:N	2.34	0.41
2:H:78:ASN:O	2:H:82:ILE:HG13	2.20	0.41
2:I:302:LEU:HA	2:I:302:LEU:HD23	1.54	0.41
3:J:171:TYR:CD2	3:J:171:TYR:N	2.88	0.41
3:J:197:SER:HA	3:J:198:PRO:HD3	1.87	0.41
1:K:4:LEU:CD1	1:K:137:VAL:HG22	2.50	0.41
2:L:104:THR:HG22	2:L:108:LEU:CD1	2.50	0.41
2:N:229:ASP:C	2:N:231:GLN:N	2.71	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
3:O:26:ALA:HB2	3:O:132:LEU:HD22	2.02	0.41
1:A:243:PRO:HG2	1:A:244:VAL:H	1.85	0.41
2:C:3:TYR:O	2:C:3:TYR:HD2	2.00	0.41
2:C:341:TYR:HB3	2:D:333:LEU:HD13	2.01	0.41
3:E:149:GLU:C	3:E:151:LEU:N	2.71	0.41
3:E:171:TYR:N	3:E:171:TYR:CD2	2.88	0.41
3:E:245:LEU:HB2	3:E:297:ARG:HG3	2.01	0.41
3:E:329:LEU:HD23	3:E:329:LEU:N	2.34	0.41
1:F:64:ILE:HG12	1:F:96:GLN:HB3	2.02	0.41
2:G:256:MET:HE1	2:G:332:LEU:HD21	2.02	0.41
2:H:56:ARG:HH22	2:I:165:THR:HG21	1.84	0.41
1:F:262:ARG:HD2	3:J:230:TYR:CD2	2.55	0.41
2:L:10:TRP:HZ2	2:L:193:GLU:CB	2.28	0.41
2:N:246:ASP:CB	2:N:248:GLN:HG2	2.50	0.41
3:O:171:TYR:CD2	3:O:171:TYR:N	2.88	0.41
3:O:34:GLY:O	3:O:199:GLY:N	2.51	0.41
2:D:320:ILE:HA	2:D:321:PRO:HD3	1.90	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:M:342:ALA:N	2:N:333:LEU:HD21	2.35	0.41
1:A:81:LEU:HA	1:A:111:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:THR:O	1:A:318:GLN:NE2	2.53	0.41
3:E:121:THR:O	3:E:124:ALA:HB3	2.21	0.41
1:F:310:LEU:HB3	1:F:314:GLN:NE2	2.35	0.41
1:F:311:THR:O	1:F:318:GLN:NE2	2.53	0.41
2:H:147:PRO:HB2	2:H:149:HIS:NE2	2.35	0.41
2:I:271:ALA:O	2:I:276:ILE:HG13	2.20	0.41
2:I:28:LEU:HD23	2:I:28:LEU:HA	1.90	0.41
1:K:270:ARG:HG2	1:K:283:ARG:NH2	2.36	0.41
2:L:82:ILE:HG23	2:L:90:LEU:HD23	2.03	0.41
2:M:137:ASN:HA	2:M:140:LEU:HD12	2.02	0.41
2:M:210:ALA:HB1	2:M:213:SER:OG	2.20	0.41
1:A:159:ASN:OD1	2:M:319:THR:HG21	2.20	0.41
1:A:4:LEU:CD1	1:A:137:VAL:HG22	2.50	0.41
2:D:271:ALA:O	2:D:276:ILE:HG13	2.20	0.41
2:D:5:VAL:HG12	2:D:222:ASP:OD2	2.21	0.41
1:F:29:LEU:HB2	1:F:179:LEU:CB	2.43	0.41
1:F:193:PRO:HA	2:G:36:ARG:HH22	1.86	0.41
2:H:333:LEU:O	2:H:336:ARG:N	2.49	0.41
2:I:69:THR:HG22	2:I:71:THR:H	1.86	0.41
3:J:32:LEU:CD1	3:J:195:ALA:O	2.67	0.41
1:K:81:LEU:HA	1:K:111:ILE:O	2.21	0.41
2:L:43:PHE:O	2:L:155:ALA:HA	2.21	0.41
2:M:347:MET:CG	2:N:290:HIS:CE1	3.03	0.41
3:O:32:LEU:HD13	3:O:197:SER:HB2	2.03	0.41
2:D:277:GLU:CB	3:E:149:GLU:HB3	2.45	0.41
3:E:252:LEU:HA	3:E:252:LEU:HD12	1.83	0.41
1:F:270:ARG:HG2	1:F:283:ARG:NH2	2.36	0.41
2:G:22:GLU:HG3	2:G:22:GLU:H	1.09	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
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:69:THR:HG22	2:D:71:THR:H	1.86	0.41
3:E:73:HIS:CE1	3:E:106:LEU:HD22	2.56	0.41
1:F:39:ARG:CZ	1:F:50:HIS:HB3	2.51	0.41
2:I:244:LEU:CD2	2:I:276:ILE:HG12	2.44	0.41
3:J:26:ALA:HB2	3:J:132:LEU:HD22	2.03	0.41
1:K:333:HIS:CB	2:L:297:LEU:CD2	2.61	0.41
2:L:10:TRP:CD2	2:L:190:ILE:HG12	2.55	0.41
2:N:105:ARG:HD2	2:N:134:HIS:NE2	2.36	0.41
2:N:51:LYS:HE3	2:N:51:LYS:HB2	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:SER:O	1:A:265:ALA:CB	2.68	0.41
1:A:281:ASN:OD1	1:A:281:ASN:O	2.39	0.41
1:A:64:ILE:HG12	1:A:96:GLN:HB3	2.02	0.41
2:B:98:ARG:HD3	2:C:141:LYS:HE2	2.03	0.41
2:D:104:THR:HG22	2:D:108:LEU:CD1	2.51	0.41
2:D:131:LEU:HB2	2:D:136:PHE:HD1	1.85	0.41
2:D:200:PRO:HB2	2:D:305:ASP:CA	2.51	0.41
2:D:42:LEU:HB3	2:D:172:GLN:CB	2.43	0.41
2:H:21:GLN:HE22	2:H:49:VAL:CG1	2.34	0.41
2:H:367:GLU:HG3	2:I:322:PRO:HD2	2.02	0.41
2:I:140:LEU:HD21	2:I:166:ILE:CG1	2.51	0.41
1:K:142:PRO:CD	1:K:178:LEU:HD11	2.50	0.41
1:K:333:HIS:CE1	2:L:297:LEU:HG	2.56	0.41
2:N:343:PRO:CG	2:N:347:MET:SD	3.09	0.41
3:O:239:GLU:HA	3:O:308:ARG:CZ	2.51	0.41
1:A:105:HIS:HB2	1:F:225:LYS:HE3	0.88	0.41
3:E:190:ALA:HB2	3:E:210:TRP:CZ3	2.56	0.41
2:G:281:LEU:O	2:G:285:MET:HG3	2.20	0.41
2:H:283:VAL:HA	2:H:286:LEU:HD12	2.03	0.41
2:I:302:LEU:HD13	2:I:310:GLU:HA	2.03	0.41
2:I:250:LEU:CD2	2:I:309:ILE:HG23	2.51	0.41
3:J:163:TYR:HH	3:J:166:PRO:HD2	1.86	0.41
3:J:27:LEU:HG	3:J:29:ILE:HD11	2.03	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:N:240:MET:HB3	3:O:157:SER:CB	2.51	0.41
2:B:6:LEU:CD2	2:B:190:ILE:CG2	2.94	0.40
2:B:4:GLN:CD	2:B:9:LYS:HD2	2.42	0.40
2:D:244:LEU:HD21	2:D:276:ILE:HG23	2.03	0.40
3:E:311:LEU:HA	3:E:311:LEU:HD12	1.86	0.40
3:E:73:HIS:HE1	3:E:106:LEU:HD22	1.86	0.40
1:F:29:LEU:HD13	1:F:179:LEU:CA	2.37	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
2:I:220:LEU:CD2	3:J:154:THR:HA	2.47	0.40
1:K:310:LEU:HA	1:K:310:LEU:HD23	1.61	0.40
1:K:64:ILE:HG12	1:K:96:GLN:HB3	2.02	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
3:O:25:HIS:O	3:O:141:PHE:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:6:TRP:HH2	3:O:175:TRP:CZ2	2.39	0.40
2:D:246:ASP:CB	2:D:248:GLN:HG2	2.50	0.40
2:D:250:LEU:CD2	2:D:309:ILE:HG23	2.52	0.40
2:D:343:PRO:CG	2:D:347:MET:SD	3.09	0.40
1:F:81:LEU:HA	1:F:111:ILE:O	2.21	0.40
2:G:363:MET:HE3	2:G:363:MET:HB2	1.86	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
3:J:73:HIS:HE1	3:J:106:LEU:HD22	1.86	0.40
1:K:84:LEU:HD12	1:K:84:LEU:HA	1.84	0.40
2:M:100:LYS:HA	2:N:133:ARG:HG3	2.02	0.40
2:N:244:LEU:HD11	2:N:276:ILE:HG21	2.01	0.40
2:N:345:ARG:HE	3:O:150:ARG:NH2	2.08	0.40
1:A:270:ARG:HG2	1:A:283:ARG:NH2	2.36	0.40
1:A:75:ALA:CB	1:F:207:ASN:CB	2.97	0.40
2:B:82:ILE:HG23	2:B:90:LEU:HD23	2.03	0.40
2:D:201:ARG:H	2:D:305:ASP:HB2	1.87	0.40
3:E:163:TYR:OH	3:E:166:PRO:HD2	2.22	0.40
3:E:239:GLU:HA	3:E:308:ARG:CZ	2.51	0.40
2:H:51:LYS:HE3	2:H:51:LYS:HB2	1.77	0.40
2:I:105:ARG:HD2	2:I:134:HIS:NE2	2.36	0.40
2:I:42:LEU:HD23	2:I:154:LEU:HB2	2.02	0.40
3:J:239:GLU:HA	3:J:308:ARG:CZ	2.51	0.40
1:K:39:ARG:CZ	1:K:50:HIS:HB3	2.51	0.40
2:L:248:GLN:HA	2:L:251:SER:HG	1.86	0.40
2:L:32:LEU:HD23	2:L:32:LEU:HA	1.94	0.40
2:M:250:LEU:HD23	2:M:312:ARG:CZ	2.51	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
2:M:215:ARG:CD	2:N:164:VAL:HG11	2.51	0.40
2:N:345:ARG:NE	3:O:150:ARG:NH2	2.50	0.40
3:O:73:HIS:CE1	3:O:106:LEU:HD22	2.56	0.40
3:O:34:GLY:C	3:O:199:GLY:HA3	2.30	0.40
3:O:321:HIS:O	3:O:327:VAL:HG21	2.21	0.40
1:A:275:LYS:HA	1:A:275:LYS:HD3	1.91	0.40
2:B:363:MET:HB2	2:B:363:MET:HE3	1.85	0.40
2:D:289:LEU:HD23	2:D:289:LEU:HA	1.81	0.40
2:D:365:LEU:HB3	2:D:366:PRO:HD2	2.03	0.40
3:E:117:ALA:CB	3:E:143:LEU:HD12	2.50	0.40
3:E:321:HIS:O	3:E:327:VAL:HG21	2.21	0.40
1:F:190:LEU:HA	1:F:190:LEU:HD23	1.85	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:G:214:LEU:HD12	2:G:214:LEU:HA	1.85	0.40
2:H:257:VAL:O	2:H:257:VAL:HG12	2.21	0.40
2:M:283:VAL:HA	2:M:286:LEU:HD12	2.03	0.40
2:N:244:LEU:CD2	2:N:276:ILE:HG12	2.44	0.40
2:N:321:PRO:HA	2:N:322:PRO:HD2	1.92	0.40
3:O:121:THR:O	3:O:124:ALA:HB3	2.21	0.40
2:B:22:GLU:H	2:B:22:GLU:HG3	1.09	0.40
2:B:304:ASN:C	2:B:304:ASN:OD1	2.60	0.40
2:C:250:LEU:HD23	2:C:312:ARG:CZ	2.51	0.40
2:D:286:LEU:HD21	2:D:332:LEU:HB2	2.03	0.40
1:A:105:HIS:HA	1:F:227:LYS:HD2	1.94	0.40
2:G:19:VAL:CG2	2:G:186:GLN:CB	2.99	0.40
2:G:236:ALA:O	2:G:239:ALA:HB3	2.22	0.40
2:H:250:LEU:HD23	2:H:312:ARG:CZ	2.51	0.40
2:I:200:PRO:HB3	2:I:304:ASN:HB3	2.00	0.40
1:K:281:ASN:O	1:K:281:ASN:OD1	2.40	0.40
2:L:6:LEU:HD23	2:L:6:LEU:HA	1.89	0.40
2:M:126:ASP:OD1	2:M:127:GLU:HG3	2.22	0.40
2:N:297:LEU:HA	2:N:297:LEU:HD12	1.90	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 ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	330/343 (96%)	301 (91%)	22 (7%)	7 (2%)	7	39
1	F	330/343 (96%)	301 (91%)	22 (7%)	7 (2%)	7	39
1	K	330/343 (96%)	301 (91%)	22 (7%)	7 (2%)	7	39
2	B	358/376 (95%)	327 (91%)	23 (6%)	8 (2%)	6	38
2	C	358/376 (95%)	329 (92%)	23 (6%)	6 (2%)	9	43
2	D	357/376 (95%)	320 (90%)	27 (8%)	10 (3%)	5	34
2	G	358/376 (95%)	328 (92%)	22 (6%)	8 (2%)	6	38
2	H	358/376 (95%)	329 (92%)	22 (6%)	7 (2%)	7	40
2	I	357/376 (95%)	320 (90%)	27 (8%)	10 (3%)	5	34
2	L	358/376 (95%)	327 (91%)	23 (6%)	8 (2%)	6	38
2	M	358/376 (95%)	329 (92%)	22 (6%)	7 (2%)	7	40
2	N	357/376 (95%)	320 (90%)	27 (8%)	10 (3%)	5	34
3	E	326/334 (98%)	296 (91%)	28 (9%)	2 (1%)	25	63
3	J	326/334 (98%)	296 (91%)	28 (9%)	2 (1%)	25	63
3	O	326/334 (98%)	296 (91%)	28 (9%)	2 (1%)	25	63
All	All	5187/5415 (96%)	4720 (91%)	366 (7%)	101 (2%)	8	41

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 ⓘ

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%)	9	35
1	F	285/291 (98%)	259 (91%)	26 (9%)	9	35
1	K	285/291 (98%)	259 (91%)	26 (9%)	9	35
2	B	303/312 (97%)	280 (92%)	23 (8%)	13	42
2	C	303/312 (97%)	288 (95%)	15 (5%)	24	53
2	D	302/312 (97%)	289 (96%)	13 (4%)	29	57
2	G	303/312 (97%)	280 (92%)	23 (8%)	13	42
2	H	303/312 (97%)	288 (95%)	15 (5%)	24	53
2	I	302/312 (97%)	289 (96%)	13 (4%)	29	57
2	L	303/312 (97%)	280 (92%)	23 (8%)	13	42
2	M	303/312 (97%)	288 (95%)	15 (5%)	24	53
2	N	302/312 (97%)	289 (96%)	13 (4%)	29	57
3	E	270/270 (100%)	239 (88%)	31 (12%)	5	26
3	J	270/270 (100%)	239 (88%)	31 (12%)	5	26
3	O	270/270 (100%)	239 (88%)	31 (12%)	5	26
All	All	4389/4491 (98%)	4065 (93%)	324 (7%)	13	43

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	336/343 (97%)	0.52	30 (8%) 9 7	69, 78, 90, 90	0
1	F	336/343 (97%)	2.75	170 (50%) 0 0	127, 241, 267, 267	0
1	K	336/343 (97%)	0.46	24 (7%) 16 11	56, 67, 79, 79	0
2	B	364/376 (96%)	0.66	35 (9%) 8 6	85, 90, 111, 111	0
2	C	364/376 (96%)	0.39	22 (6%) 21 16	61, 66, 76, 85	0
2	D	363/376 (96%)	0.33	6 (1%) 70 60	57, 67, 70, 70	0
2	G	364/376 (96%)	2.37	149 (40%) 0 0	84, 208, 291, 291	0
2	H	364/376 (96%)	1.18	84 (23%) 0 0	59, 171, 228, 228	0
2	I	363/376 (96%)	0.50	32 (8%) 10 7	66, 67, 151, 151	0
2	L	364/376 (96%)	0.49	22 (6%) 21 16	66, 94, 101, 101	0
2	M	364/376 (96%)	0.72	44 (12%) 4 4	79, 127, 140, 140	0
2	N	363/376 (96%)	0.60	37 (10%) 6 6	102, 107, 133, 133	0
3	E	332/334 (99%)	0.21	8 (2%) 59 48	30, 46, 62, 62	0
3	J	332/334 (99%)	0.39	17 (5%) 28 23	52, 66, 71, 71	0
3	O	332/334 (99%)	1.44	98 (29%) 0 0	75, 182, 266, 266	0
All	All	5277/5415 (97%)	0.87	778 (14%) 2 2	30, 79, 267, 291	0

All (778) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	181	LEU	20.0
3	O	55	GLY	18.9
2	G	104	THR	17.5
1	F	55	ILE	14.6
3	O	56	HIS	14.0
2	G	42	LEU	13.7
1	F	85	PRO	12.9

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Mol	Chain	Res	Type	RSRZ
2	G	139	LEU	12.8
2	G	50	GLY	12.7
2	G	142	THR	12.5
2	G	170	CYS	12.0
1	F	132	ASN	11.8
2	H	162	LEU	11.4
2	G	133	ARG	11.1
2	G	43	PHE	10.6
1	F	17	LEU	10.0
1	F	18	ARG	9.9
1	F	95	GLU	9.8
2	N	366	PRO	9.8
3	O	144	ALA	9.7
1	F	78	GLN	9.7
1	F	51	HIS	9.7
2	G	172	GLN	9.7
2	G	33	SER	9.6
1	F	91	ALA	9.5
1	F	46	GLY	9.4
1	F	110	LEU	9.3
2	G	108	LEU	9.1
1	F	182	ALA	9.0
2	H	85	GLY	9.0
2	G	128	VAL	9.0
1	F	52	THR	8.8
3	O	54	GLN	8.8
2	G	168	SER	8.8
1	F	80	LEU	8.7
1	F	12	GLN	8.6
2	B	362	ARG	8.6
2	G	206	LEU	8.6
1	F	180	ALA	8.6
1	F	198	THR	8.5
1	F	13	LEU	8.5
2	G	107	LEU	8.4
1	F	185	LEU	8.4
1	F	16	GLY	8.1
2	G	61	GLY	8.0
2	G	44	SER	8.0
1	F	15	GLU	8.0
2	G	116	ALA	8.0
2	G	12	PRO	7.9

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Mol	Chain	Res	Type	RSRZ
2	M	101	VAL	7.8
2	G	6	LEU	7.8
3	O	116	ASP	7.7
2	G	136	PHE	7.7
2	H	152	PHE	7.6
2	G	137	ASN	7.6
3	O	111	VAL	7.6
3	O	117	ALA	7.5
1	F	8	GLN	7.5
1	F	19	ALA	7.5
2	G	153	LEU	7.4
1	F	50	HIS	7.4
2	H	39	HIS	7.4
2	G	34	LEU	7.4
3	O	31	ALA	7.3
2	G	93	ILE	7.3
2	G	169	ARG	7.3
1	F	66	SER	7.3
1	F	164	ASP	7.3
1	F	35	GLN	7.2
2	M	299	PRO	7.2
1	F	94	ASN	7.2
2	L	363	MET	7.1
2	H	154	LEU	7.1
1	F	96	GLN	7.1
2	H	153	LEU	7.1
1	F	79	THR	7.0
1	F	34	SER	7.0
2	L	4	GLN	7.0
2	G	120	PHE	7.0
1	F	138	THR	7.0
1	F	106	ASP	6.9
2	G	154	LEU	6.8
1	F	145	ALA	6.8
1	F	165	ALA	6.8
2	G	171	LEU	6.8
2	G	135	SER	6.7
2	G	152	PHE	6.7
1	F	209	ALA	6.7
2	H	163	PRO	6.7
3	O	69	GLN	6.6
1	F	97	LEU	6.6

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Mol	Chain	Res	Type	RSRZ
2	G	35	GLY	6.6
1	A	60	ASP	6.5
1	F	88	GLY	6.5
1	A	74	PHE	6.5
2	B	5	VAL	6.5
2	H	94	ASP	6.5
1	F	98	LEU	6.5
1	F	166	ALA	6.5
3	O	79	LEU	6.4
1	F	192	TRP	6.4
1	F	14	ASN	6.4
1	F	163	ASP	6.4
2	N	364	PRO	6.4
3	O	70	ALA	6.3
1	F	161	GLU	6.3
2	G	212	GLY	6.3
2	G	210	ALA	6.3
3	O	143	LEU	6.3
2	G	143	LEU	6.3
1	F	170	LEU	6.3
2	G	32	LEU	6.2
3	O	131	THR	6.2
1	F	49	GLU	6.1
2	I	365	LEU	6.1
2	G	205	LEU	6.1
2	G	132	SER	6.1
2	I	366	PRO	6.0
1	F	67	LEU	6.0
1	F	150	TRP	6.0
2	G	141	LYS	6.0
2	G	131	LEU	6.0
1	F	133	ARG	5.9
1	F	92	ALA	5.9
1	F	86	GLU	5.9
2	G	3	TYR	5.9
2	G	51	LYS	5.8
1	F	48	GLU	5.8
2	C	85	GLY	5.8
3	O	141	PHE	5.8
3	O	26	ALA	5.7
2	G	29	ALA	5.7
1	F	137	VAL	5.7

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Mol	Chain	Res	Type	RSRZ
2	G	200	PRO	5.7
2	G	74	GLY	5.7
1	F	45	GLN	5.7
1	F	104	LEU	5.7
2	G	151	LYS	5.7
1	F	71	MET	5.6
3	O	1	MET	5.6
2	B	101	VAL	5.5
2	G	112	GLN	5.5
1	F	30	LEU	5.5
2	L	368	PRO	5.5
2	B	361	PRO	5.5
2	H	41	TYR	5.5
1	F	89	PRO	5.5
2	H	145	GLU	5.5
2	L	6	LEU	5.4
2	I	123	TYR	5.4
1	F	193	PRO	5.4
1	F	28	PRO	5.4
2	G	134	HIS	5.4
2	G	156	THR	5.3
2	H	146	PRO	5.3
2	G	62	LEU	5.3
2	G	37	ILE	5.3
1	F	196	LYS	5.3
2	I	133	ARG	5.2
2	G	30	ASN	5.2
2	H	93	ILE	5.2
2	G	7	ALA	5.2
3	O	137	ALA	5.2
2	I	364	PRO	5.2
1	F	168	GLN	5.1
2	G	164	VAL	5.1
2	G	82	ILE	5.1
2	B	367	GLU	5.1
1	F	210	ALA	5.1
1	F	11	ALA	5.1
2	G	129	HIS	5.1
2	G	165	THR	5.1
2	G	52	THR	5.1
2	G	195	HIS	5.1
2	G	362	ARG	5.1

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Mol	Chain	Res	Type	RSRZ
3	O	112	VAL	5.1
2	B	365	LEU	5.1
2	G	230	GLY	5.1
2	H	166	ILE	5.0
1	F	184	ALA	5.0
1	K	91	ALA	5.0
1	F	111	ILE	5.0
2	M	68	ILE	5.0
1	F	207	ASN	5.0
1	K	58	ASN	5.0
2	G	231	GLN	5.0
3	O	96	VAL	5.0
1	F	176	GLY	4.9
2	B	268	ILE	4.9
2	H	111	VAL	4.9
3	O	118	ALA	4.9
1	F	21	TYR	4.9
3	O	45	SER	4.9
2	N	367	GLU	4.9
2	H	71	THR	4.9
2	G	140	LEU	4.9
2	G	367	GLU	4.8
2	G	26	THR	4.8
2	G	363	MET	4.8
2	G	60	LYS	4.8
1	F	136	GLN	4.8
1	F	154	ARG	4.8
3	O	37	ASP	4.8
2	G	173	PHE	4.8
1	F	87	ASN	4.8
2	G	125	ILE	4.7
1	F	36	ASP	4.7
2	L	3	TYR	4.7
3	O	72	THR	4.7
1	F	146	GLN	4.7
2	L	362	ARG	4.7
2	G	53	SER	4.6
1	A	338	ASP	4.6
2	G	83	GLU	4.6
2	G	214	LEU	4.6
1	F	173	CYS	4.6
2	M	104	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	F	140	GLN	4.6
2	B	6	LEU	4.6
2	H	38	HIS	4.6
2	G	45	GLY	4.6
2	H	72	PRO	4.6
2	B	363	MET	4.6
1	A	61	TRP	4.5
2	G	174	HIS	4.5
1	F	81	LEU	4.5
1	F	194	ASP	4.5
2	H	151	LYS	4.5
1	F	139	CYS	4.5
2	G	63	ASN	4.4
2	G	15	PHE	4.4
1	K	61	TRP	4.4
3	O	145	THR	4.4
1	F	47	PHE	4.4
3	O	6	TRP	4.4
1	F	177	ASN	4.4
2	H	104	THR	4.4
2	B	241	LEU	4.4
1	F	172	TYR	4.4
1	F	93	ILE	4.3
1	F	200	PRO	4.3
2	M	93	ILE	4.3
2	G	178	LEU	4.3
1	F	60	ASP	4.3
2	N	232	VAL	4.3
2	H	100	LYS	4.3
2	H	302	LEU	4.3
2	L	367	GLU	4.3
2	G	221	THR	4.3
2	N	365	LEU	4.3
1	F	203	GLU	4.2
2	H	108	LEU	4.2
1	F	186	GLU	4.2
2	G	25	LEU	4.2
2	D	366	PRO	4.2
2	G	8	ARG	4.2
1	K	57	PRO	4.2
2	N	210	ALA	4.2
1	F	23	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
2	G	5	VAL	4.1
1	F	90	ASN	4.1
3	O	142	PHE	4.1
1	F	178	LEU	4.1
1	F	101	THR	4.1
2	G	175	LEU	4.1
2	G	59	ALA	4.1
2	G	36	ARG	4.0
1	F	208	ASP	4.0
2	H	36	ARG	4.0
2	G	41	TYR	4.0
2	G	14	THR	4.0
2	H	139	LEU	4.0
2	G	161	LYS	4.0
2	M	305	ASP	4.0
2	G	66	THR	4.0
3	O	27	LEU	4.0
2	H	15	PHE	4.0
3	J	3	TRP	4.0
3	O	48	LEU	4.0
1	F	144	GLN	4.0
1	F	169	VAL	3.9
1	F	70	ALA	3.9
2	D	305	ASP	3.9
2	G	155	ALA	3.9
2	H	35	GLY	3.9
1	F	126	TRP	3.9
1	F	3	ARG	3.9
1	K	62	ASN	3.9
2	G	117	ARG	3.9
1	F	31	LEU	3.9
2	B	368	PRO	3.9
1	F	69	GLN	3.9
2	M	102	GLU	3.9
2	G	166	ILE	3.8
1	F	62	ASN	3.8
1	F	197	LEU	3.8
3	E	82	GLU	3.8
1	K	60	ASP	3.8
1	A	55	ILE	3.8
2	G	38	HIS	3.8
2	N	63	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	366	PRO	3.8
2	H	37	ILE	3.7
2	G	57	LEU	3.7
3	O	95	GLU	3.7
1	A	142	PRO	3.7
1	A	53	PHE	3.7
2	L	246	ASP	3.7
2	B	229	ASP	3.7
2	G	99	THR	3.7
2	B	89	ASP	3.6
1	F	44	ALA	3.6
1	F	43	ALA	3.6
2	G	124	LEU	3.6
2	G	197	ALA	3.6
2	I	144	GLU	3.6
2	H	20	GLY	3.6
2	H	211	GLU	3.6
1	F	38	VAL	3.6
1	F	77	ARG	3.6
1	F	24	LEU	3.6
2	G	47	ARG	3.6
2	H	28	LEU	3.6
1	A	75	ALA	3.6
1	F	199	LEU	3.5
3	O	7	LEU	3.5
2	G	18	VAL	3.5
3	O	40	LEU	3.5
2	H	126	ASP	3.5
3	J	236	LEU	3.5
1	F	149	ARG	3.5
2	I	134	HIS	3.5
2	M	246	ASP	3.5
2	I	102	GLU	3.5
1	F	142	PRO	3.5
2	H	59	ALA	3.5
2	G	85	GLY	3.5
1	F	61	TRP	3.5
1	K	100	LEU	3.5
2	G	213	SER	3.5
3	O	176	LEU	3.5
3	O	140	TRP	3.5
3	O	187	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	H	157	THR	3.4
2	G	84	GLN	3.4
1	F	9	LEU	3.4
2	H	117	ARG	3.4
2	G	138	ALA	3.4
2	H	24	VAL	3.4
1	F	117	LEU	3.4
2	D	4	GLN	3.4
1	K	82	LEU	3.4
1	F	183	GLN	3.4
3	O	29	ILE	3.4
2	H	232	VAL	3.4
2	G	148	GLU	3.4
2	D	6	LEU	3.4
2	H	143	LEU	3.4
2	G	126	ASP	3.4
2	N	104	THR	3.4
3	O	159	CYS	3.4
1	F	195	GLY	3.4
2	H	92	GLU	3.4
2	C	104	THR	3.4
2	H	43	PHE	3.4
1	F	99	THR	3.3
2	C	99	THR	3.3
1	F	338	ASP	3.3
2	H	74	GLY	3.3
2	G	187	LEU	3.3
2	G	10	TRP	3.3
2	I	359	PHE	3.3
2	N	179	ASP	3.3
1	F	135	VAL	3.3
2	H	19	VAL	3.3
2	I	101	VAL	3.3
3	O	75	ASP	3.3
2	H	135	SER	3.3
2	B	249	ALA	3.3
2	M	302	LEU	3.3
2	L	247	ASP	3.3
2	L	248	GLN	3.3
1	F	109	LEU	3.3
2	B	299	PRO	3.3
2	I	40	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
3	O	28	LEU	3.3
3	O	25	HIS	3.3
2	H	112	GLN	3.3
3	J	334	LEU	3.2
1	F	2	ILE	3.2
2	C	123	TYR	3.2
2	H	47	ARG	3.2
3	O	14	LEU	3.2
2	M	92	GLU	3.2
1	F	10	ARG	3.2
2	I	69	THR	3.2
3	O	74	PRO	3.2
3	O	97	THR	3.2
3	O	125	ALA	3.2
1	K	276	HIS	3.2
2	H	142	THR	3.2
1	F	174	TYR	3.2
2	C	128	VAL	3.2
2	M	256	MET	3.2
2	N	6	LEU	3.2
2	B	3	TYR	3.2
3	O	78	THR	3.2
2	H	132	SER	3.1
2	N	241	LEU	3.1
1	F	33	GLU	3.1
3	E	159	CYS	3.1
1	F	4	LEU	3.1
1	F	27	ASP	3.1
2	H	134	HIS	3.1
3	O	115	THR	3.1
2	L	241	LEU	3.1
1	F	116	LYS	3.1
2	M	108	LEU	3.1
3	O	63	ARG	3.1
3	J	237	ASN	3.1
1	F	83	LEU	3.1
2	M	354	LEU	3.1
2	B	111	VAL	3.1
1	A	82	LEU	3.1
3	O	114	VAL	3.0
3	O	3	TRP	3.0
3	O	22	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
2	H	131	LEU	3.0
2	N	188	GLU	3.0
1	F	84	LEU	3.0
3	O	46	ARG	3.0
2	H	60	LYS	3.0
2	B	90	LEU	3.0
2	M	206	LEU	3.0
3	O	126	ASN	3.0
2	H	86	ARG	3.0
1	F	22	LEU	3.0
3	O	245	LEU	3.0
3	O	267	ASN	3.0
2	B	300	ALA	3.0
2	M	349	VAL	3.0
1	K	53	PHE	3.0
2	M	162	LEU	3.0
3	O	113	TRP	3.0
1	A	298	LEU	3.0
2	D	359	PHE	3.0
1	F	68	CYS	3.0
1	K	338	ASP	3.0
1	F	54	SER	2.9
1	F	191	LEU	2.9
3	O	256	LEU	2.9
2	H	30	ASN	2.9
1	F	107	ASP	2.9
2	G	4	GLN	2.9
2	G	68	ILE	2.9
2	G	209	ALA	2.9
1	A	62	ASN	2.9
2	H	229	ASP	2.9
2	G	70	ALA	2.9
3	O	153	ALA	2.9
2	G	58	LEU	2.9
2	G	192	ASN	2.9
2	H	110	ASN	2.9
2	H	116	ALA	2.9
2	I	152	PHE	2.9
2	G	144	GLU	2.9
2	L	351	MET	2.9
2	I	104	THR	2.9
1	K	337	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	37	ILE	2.9
3	O	47	TYR	2.9
1	K	293	LEU	2.9
2	I	91	ILE	2.9
2	L	123	TYR	2.9
1	F	124	ALA	2.9
3	J	109	ALA	2.9
2	M	128	VAL	2.8
2	L	196	ILE	2.8
2	H	230	GLY	2.8
2	N	193	GLU	2.8
1	F	241	SER	2.8
2	B	116	ALA	2.8
2	B	92	GLU	2.8
2	N	178	LEU	2.8
3	O	44	LEU	2.8
2	H	138	ALA	2.8
3	O	73	HIS	2.8
3	E	267	ASN	2.8
2	G	235	GLN	2.8
3	J	202	LEU	2.8
1	F	113	ARG	2.8
2	G	361	PRO	2.8
2	I	367	GLU	2.8
2	M	32	LEU	2.8
1	F	37	ALA	2.8
2	C	108	LEU	2.8
2	G	127	GLU	2.8
1	K	130	LEU	2.8
1	F	134	SER	2.8
2	L	32	LEU	2.8
1	F	167	ASN	2.8
2	G	101	VAL	2.8
2	H	62	LEU	2.8
2	I	62	LEU	2.8
2	I	122	VAL	2.8
2	I	156	THR	2.8
2	N	38	HIS	2.8
1	F	20	ALA	2.7
2	B	4	GLN	2.7
2	G	114	ALA	2.7
2	H	89	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	124	LEU	2.7
2	N	203	LEU	2.7
3	O	132	LEU	2.7
2	H	231	GLN	2.7
2	N	231	GLN	2.7
2	H	136	PHE	2.7
2	H	197	ALA	2.7
3	O	8	ARG	2.7
2	L	245	ASP	2.7
2	G	118	GLY	2.7
1	F	204	GLN	2.7
2	N	10	TRP	2.7
2	G	162	LEU	2.7
2	H	82	ILE	2.7
2	H	90	LEU	2.7
2	G	31	GLY	2.7
2	N	180	VAL	2.7
2	I	93	ILE	2.7
2	G	17	ASP	2.7
1	K	97	LEU	2.7
2	G	13	GLN	2.7
2	G	149	HIS	2.7
2	M	306	MET	2.7
1	A	239	GLU	2.7
3	J	14	LEU	2.7
2	N	20	GLY	2.7
2	M	51	LYS	2.7
2	M	295	VAL	2.7
3	O	241	ALA	2.7
2	I	302	LEU	2.6
2	G	23	HIS	2.6
2	C	135	SER	2.6
1	A	78	GLN	2.6
1	K	73	LEU	2.6
2	M	135	SER	2.6
3	O	90	VAL	2.6
2	H	83	GLU	2.6
1	A	79	THR	2.6
1	F	201	ARG	2.6
3	O	71	GLY	2.6
2	G	160	GLN	2.6
3	J	306	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
2	M	221	THR	2.6
2	N	313	MET	2.6
3	O	129	LEU	2.6
1	F	156	LYS	2.6
3	O	122	ASP	2.6
1	F	39	ARG	2.6
3	J	82	GLU	2.6
3	O	88	LEU	2.6
2	C	122	VAL	2.6
1	F	187	ARG	2.6
2	G	98	ARG	2.6
2	G	229	ASP	2.6
2	M	100	LYS	2.6
2	N	206	LEU	2.6
1	A	278	VAL	2.6
2	H	164	VAL	2.6
2	G	222	ASP	2.5
2	H	165	THR	2.5
2	M	90	LEU	2.5
1	K	96	GLN	2.5
1	F	56	ASP	2.5
3	O	30	GLN	2.5
3	O	32	LEU	2.5
2	B	313	MET	2.5
2	H	54	ILE	2.5
2	G	122	VAL	2.5
3	O	18	TYR	2.5
2	N	15	PHE	2.5
3	O	109	ALA	2.5
3	O	167	PRO	2.5
2	N	325	ILE	2.5
3	O	334	LEU	2.5
2	G	184	ARG	2.5
3	E	334	LEU	2.5
1	F	40	GLN	2.5
3	O	237	ASN	2.5
1	A	110	LEU	2.5
2	B	112	GLN	2.5
2	G	368	PRO	2.5
3	O	135	PRO	2.5
3	O	184	GLN	2.5
2	M	147	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	M	176	LYS	2.5
2	G	145	GLU	2.5
2	C	111	VAL	2.5
1	F	41	VAL	2.5
2	G	119	ARG	2.5
2	M	307	ALA	2.5
1	F	238	LEU	2.4
2	H	178	LEU	2.4
3	J	307	ASN	2.4
1	F	151	VAL	2.4
1	A	71	MET	2.4
2	M	172	GLN	2.4
2	C	82	ILE	2.4
2	B	104	THR	2.4
2	H	91	ILE	2.4
1	A	267	THR	2.4
2	M	43	PHE	2.4
2	G	196	ILE	2.4
3	E	307	ASN	2.4
1	F	131	ALA	2.4
2	G	67	GLY	2.4
2	N	62	LEU	2.4
2	I	92	GLU	2.4
2	I	6	LEU	2.4
2	C	89	ASP	2.4
2	H	25	LEU	2.4
2	H	109	ASP	2.4
2	M	243	THR	2.4
2	G	215	ARG	2.4
2	I	56	ARG	2.4
1	A	193	PRO	2.4
3	O	283	PRO	2.4
3	O	57	LYS	2.4
2	M	178	LEU	2.4
3	O	80	ALA	2.4
2	N	12	PRO	2.4
2	H	79	CYS	2.4
2	M	285	MET	2.4
2	G	28	LEU	2.4
3	O	252	LEU	2.4
2	B	41	TYR	2.4
3	J	51	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	267	LEU	2.4
3	O	139	THR	2.4
2	N	359	PHE	2.3
2	C	169	ARG	2.3
2	I	124	LEU	2.3
2	H	237	VAL	2.3
2	M	94	ASP	2.3
1	K	74	PHE	2.3
2	C	126	ASP	2.3
2	G	21	GLN	2.3
2	H	125	ILE	2.3
2	L	23	HIS	2.3
1	F	236	LEU	2.3
1	A	73	LEU	2.3
2	I	39	HIS	2.3
1	A	58	ASN	2.3
2	N	85	GLY	2.3
1	A	328	SER	2.3
2	M	245	ASP	2.3
2	H	27	ALA	2.3
2	M	170	CYS	2.3
1	F	105	HIS	2.3
3	O	130	LYS	2.3
3	O	206	GLN	2.3
3	O	154	THR	2.3
2	C	152	PHE	2.3
2	G	167	LEU	2.3
2	M	60	LYS	2.3
1	F	32	GLN	2.3
2	N	296	GLN	2.3
3	O	164	LEU	2.3
1	A	80	LEU	2.2
2	I	43	PHE	2.2
2	H	44	SER	2.2
1	F	147	LEU	2.2
2	G	218	LEU	2.2
3	O	175	TRP	2.2
3	O	248	LEU	2.2
1	F	74	PHE	2.2
2	G	77	ASP	2.2
2	L	265	MET	2.2
3	O	128	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	N	102	GLU	2.2
1	F	72	SER	2.2
2	H	50	GLY	2.2
2	M	109	ASP	2.2
2	N	13	GLN	2.2
3	J	281	LEU	2.2
1	F	103	LEU	2.2
1	K	290	LEU	2.2
2	C	162	LEU	2.2
2	I	241	LEU	2.2
2	M	124	LEU	2.2
1	A	133	ARG	2.2
3	J	206	GLN	2.2
2	H	26	THR	2.2
2	I	32	LEU	2.2
2	H	56	ARG	2.2
1	F	5	TYR	2.2
2	L	304	ASN	2.2
1	F	102	GLY	2.2
1	F	331	LEU	2.2
1	K	239	GLU	2.2
2	M	22	GLU	2.2
1	F	148	PRO	2.2
2	C	92	GLU	2.2
2	M	111	VAL	2.2
2	N	83	GLU	2.2
2	N	209	ALA	2.2
1	F	108	LEU	2.2
1	F	206	VAL	2.2
2	B	357	LEU	2.2
1	F	239	GLU	2.2
2	G	268	ILE	2.2
3	J	31	ALA	2.2
2	M	253	VAL	2.2
1	F	276	HIS	2.2
1	F	123	ASN	2.1
3	J	7	LEU	2.1
3	O	24	HIS	2.1
3	J	164	LEU	2.1
2	C	110	ASN	2.1
2	I	68	ILE	2.1
1	F	214	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	G	366	PRO	2.1
2	M	4	GLN	2.1
1	F	260	LEU	2.1
2	G	267	LEU	2.1
2	I	90	LEU	2.1
1	A	19	ALA	2.1
2	L	176	LYS	2.1
1	K	142	PRO	2.1
2	D	169	ARG	2.1
3	O	76	TYR	2.1
2	B	152	PHE	2.1
1	A	22	LEU	2.1
2	H	144	GLU	2.1
3	E	79	LEU	2.1
2	B	354	LEU	2.1
2	C	93	ILE	2.1
2	L	354	LEU	2.1
3	O	102	GLU	2.1
3	O	149	GLU	2.1
2	N	197	ALA	2.1
2	H	84	GLN	2.1
3	O	41	ILE	2.1
1	A	226	SER	2.1
2	C	131	LEU	2.1
2	G	115	PRO	2.1
3	J	269	ASP	2.1
2	N	268	ILE	2.1
2	B	135	SER	2.1
3	E	81	PRO	2.1
1	A	126	TRP	2.1
2	G	113	TYR	2.1
2	G	92	GLU	2.1
2	H	243	THR	2.1
2	G	365	LEU	2.1
2	L	286	LEU	2.1
1	K	1	MET	2.0
1	K	112	VAL	2.0
2	H	206	LEU	2.0
3	O	146	ARG	2.0
2	C	246	ASP	2.0
2	M	154	LEU	2.0
3	O	66	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	115	ASN	2.0
1	K	70	ALA	2.0
2	B	7	ALA	2.0
2	N	256	MET	2.0
2	C	107	LEU	2.0
2	H	214	LEU	2.0
2	I	70	ALA	2.0
2	B	206	LEU	2.0
2	N	119	ARG	2.0
1	A	112	VAL	2.0
3	E	322	TYR	2.0
3	O	43	ALA	2.0
1	A	100	LEU	2.0
3	O	67	LEU	2.0
3	O	138	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.