



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:32 PM UTC

PDB ID : 3GLH / pdb_00003glh
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

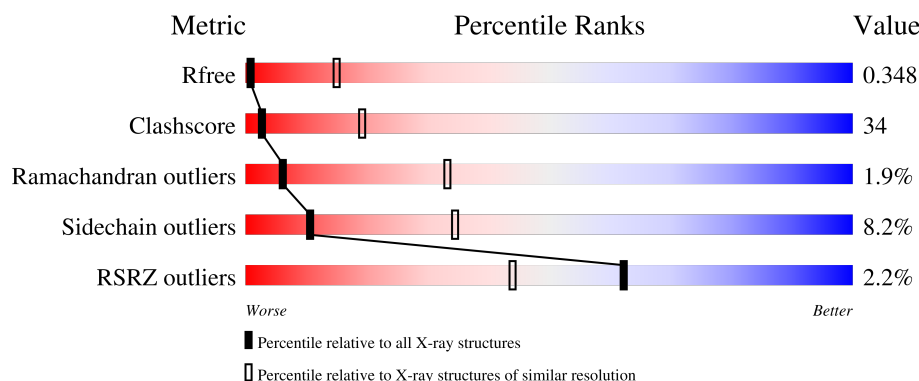
1 Overall quality at a glance i

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}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	3% 48% 38% 11% ..
1	F	343	5% 47% 38% 11% ..
1	K	343	% 49% 37% 10% ..
2	B	376	4% 53% 34% 9% ..
2	C	376	% 53% 38% 6% .

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

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 41322 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA polymerase III subunit delta.

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

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

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

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P06710

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

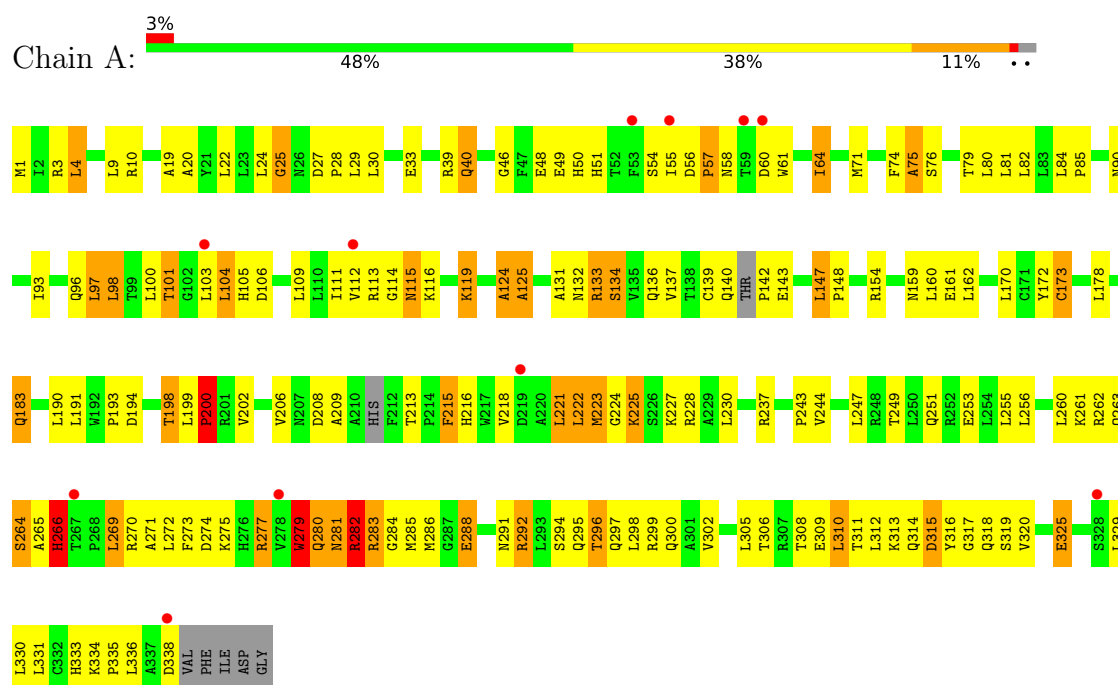
- Molecule 3 is a protein called DNA polymerase III subunit delta'.

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

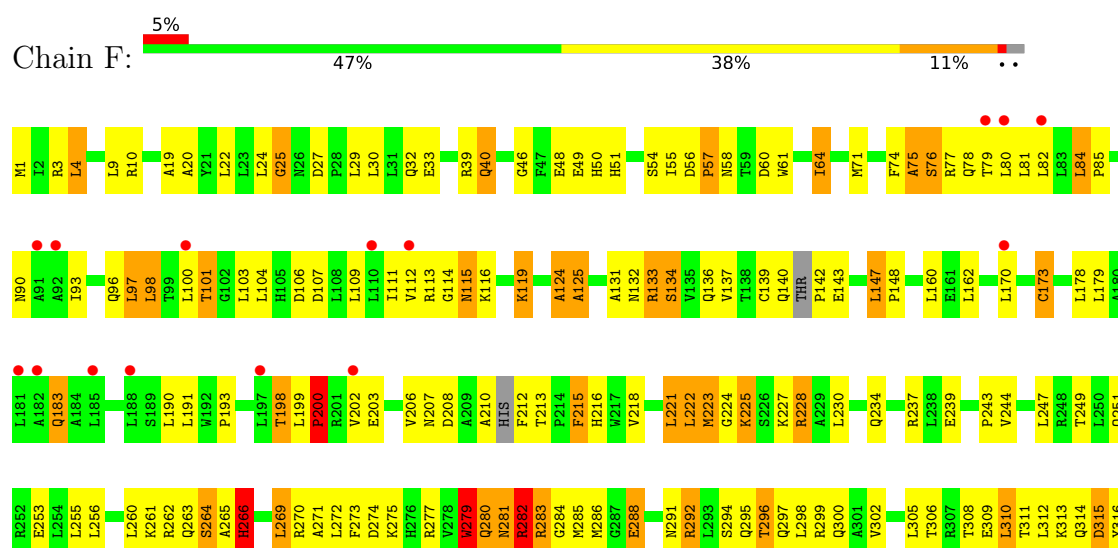
3 Residue-property plots

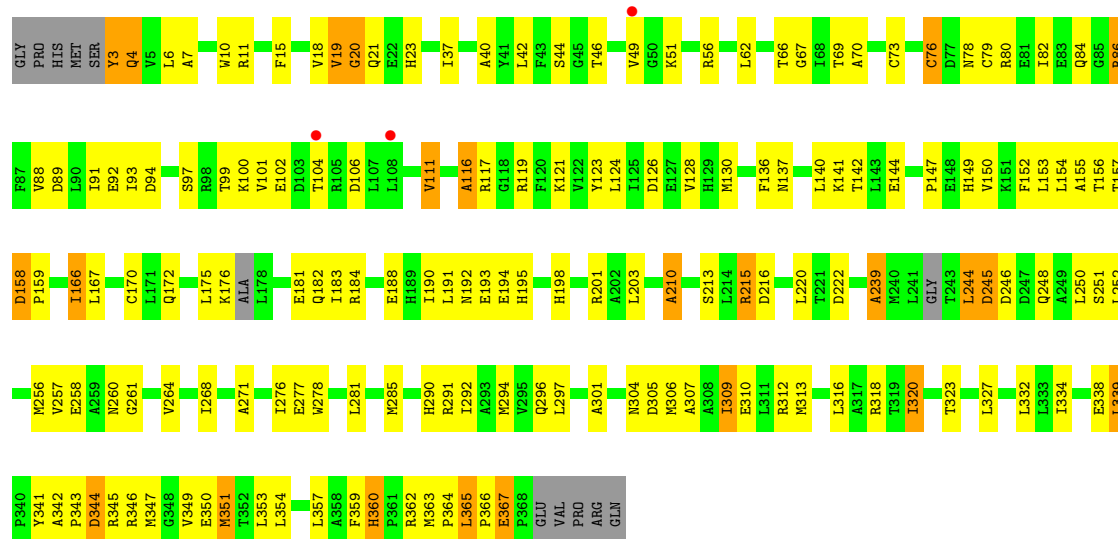
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: DNA polymerase III subunit delta

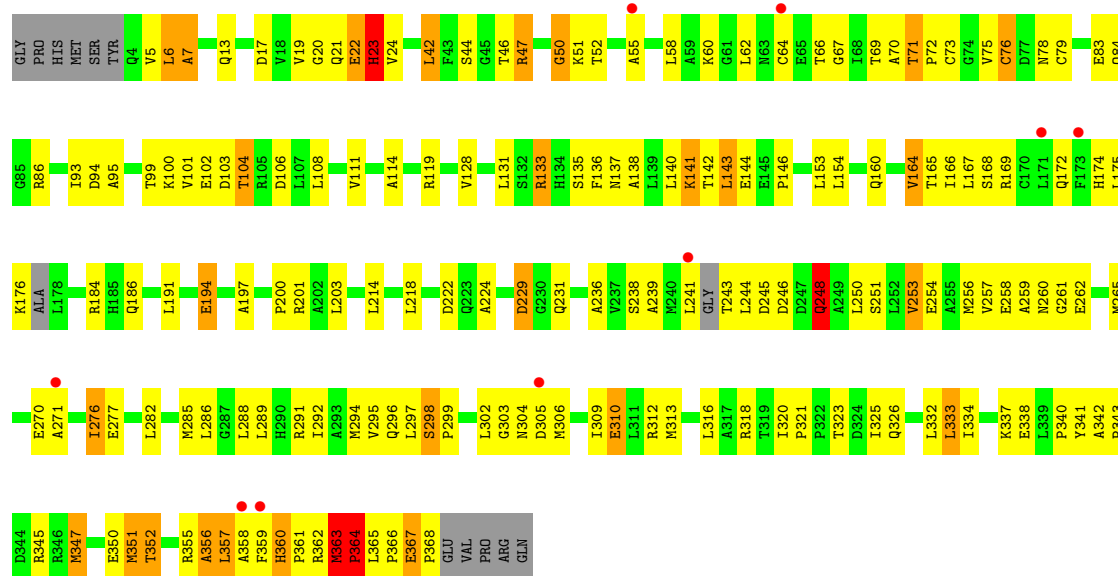


• Molecule 1: DNA polymerase III subunit delta

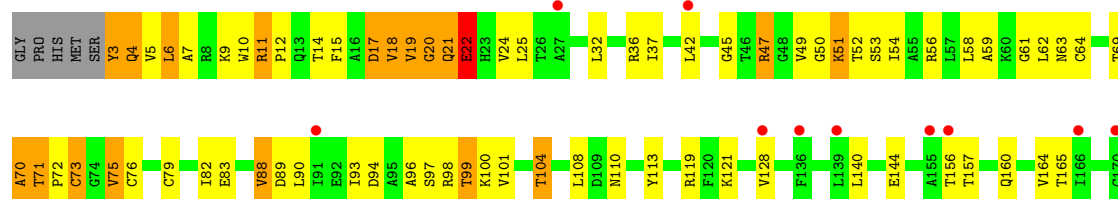


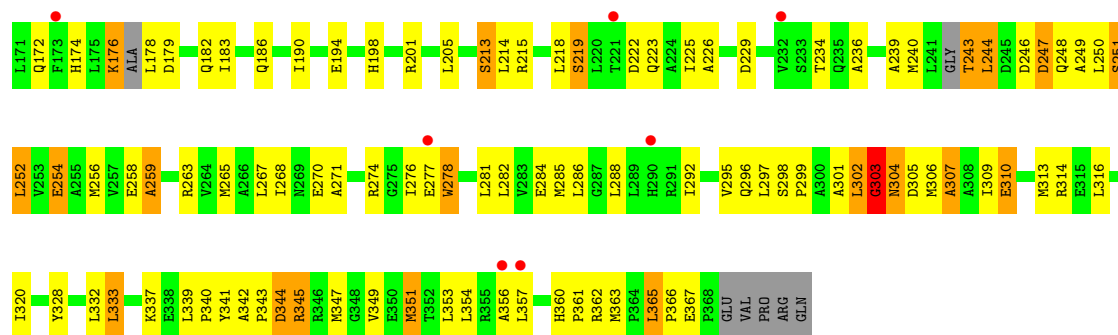


• Molecule 2: DNA polymerase III subunit tau

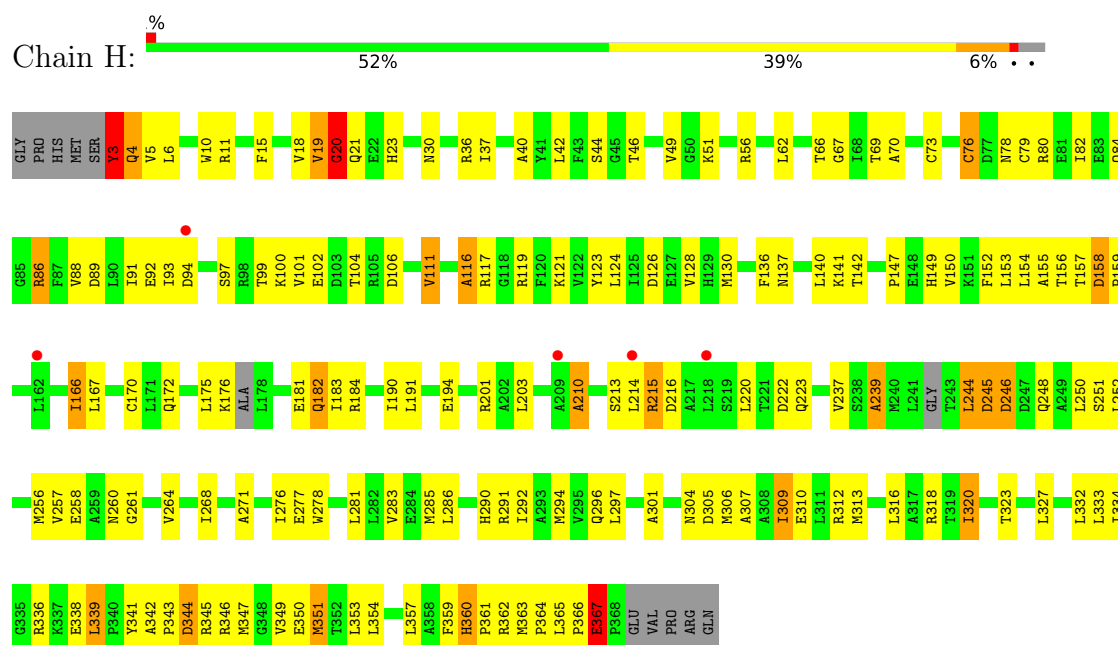


• Molecule 2: DNA polymerase III subunit tau

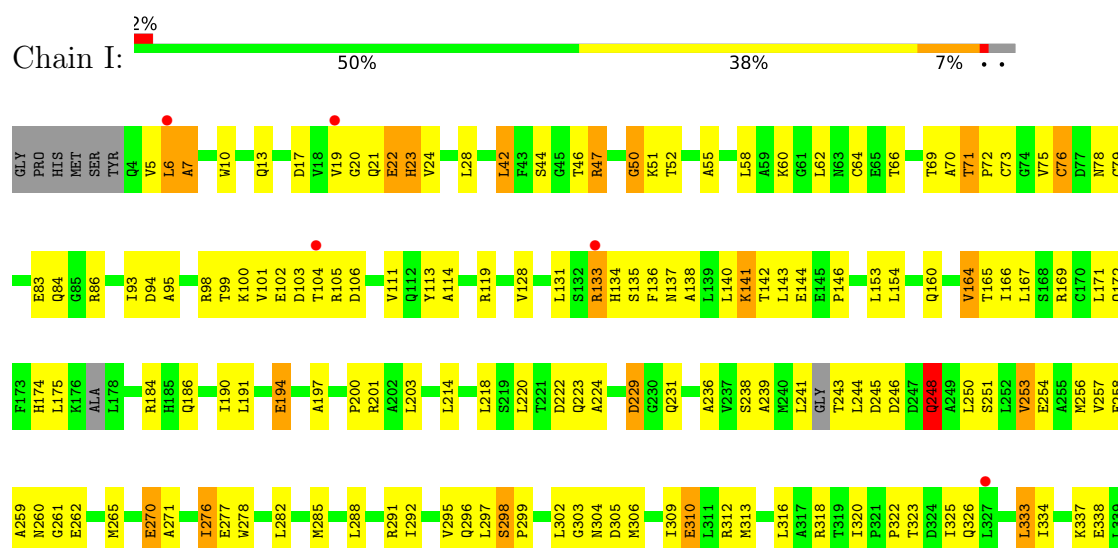


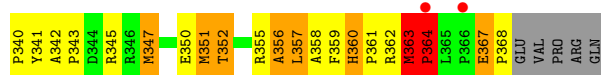


• Molecule 2: DNA polymerase III subunit tau

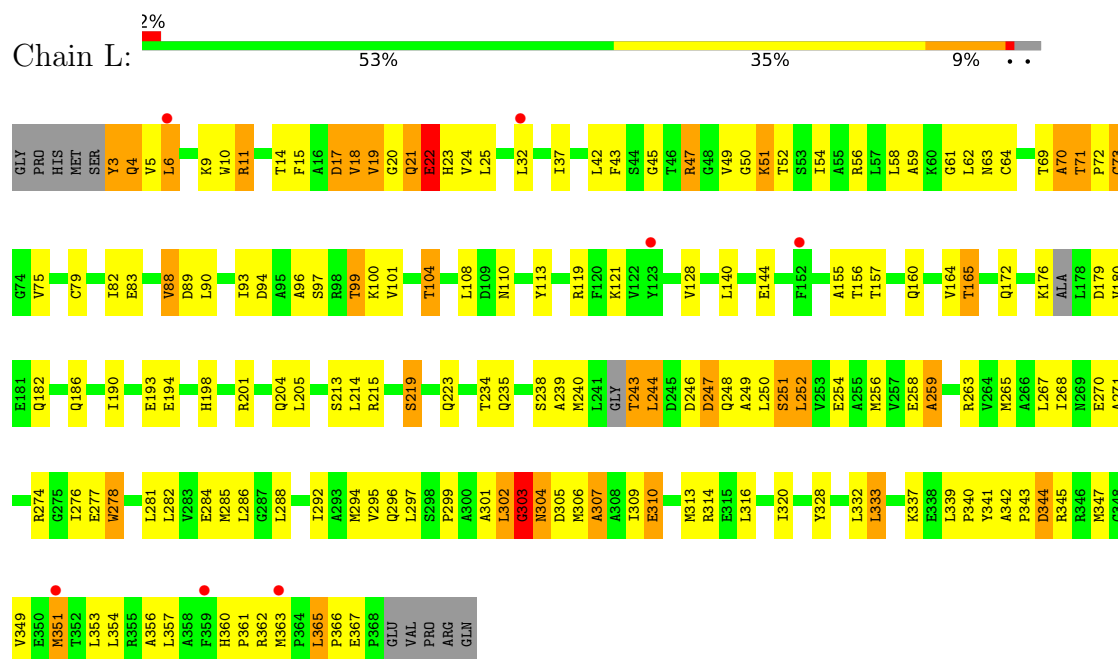


• Molecule 2: DNA polymerase III subunit tau

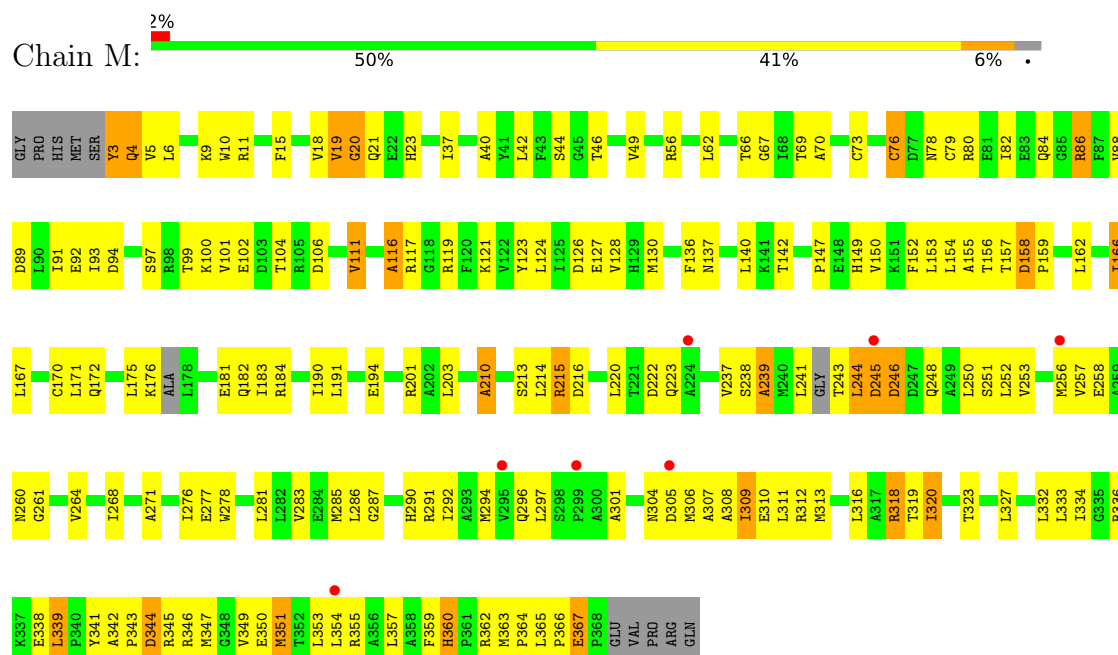




• Molecule 2: DNA polymerase III subunit tau

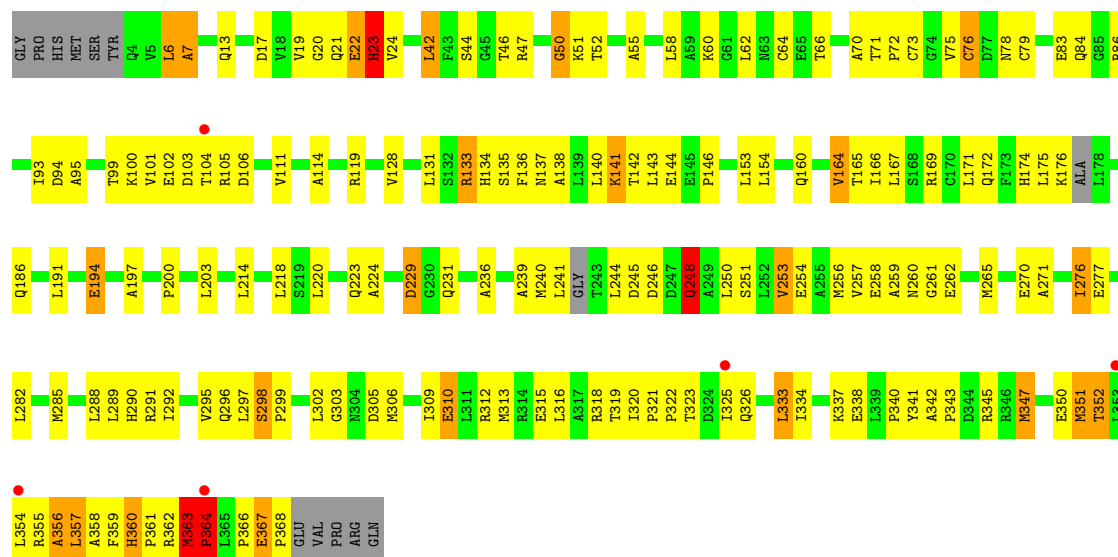


• Molecule 2: DNA polymerase III subunit tau

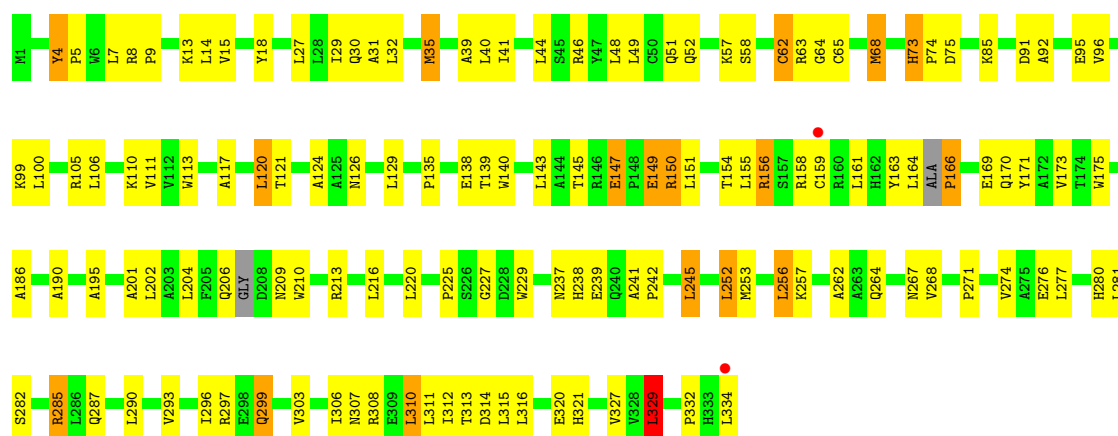


• Molecule 2: DNA polymerase III subunit tau

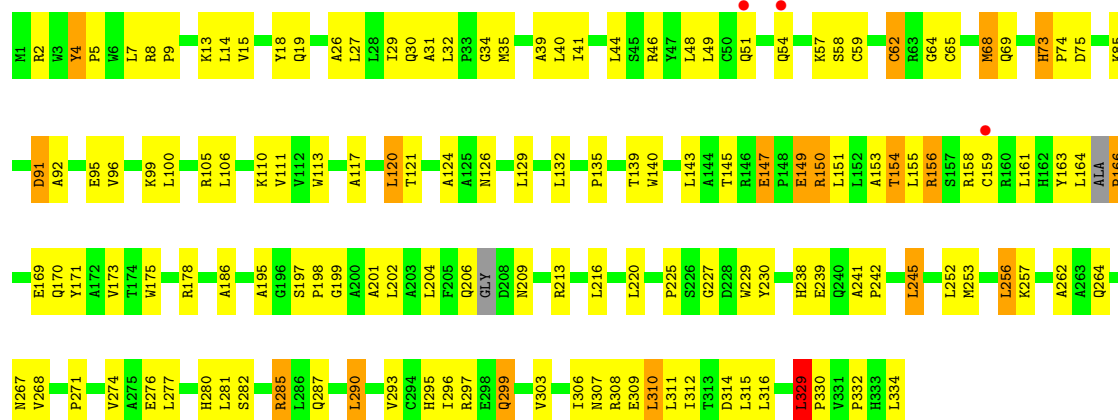




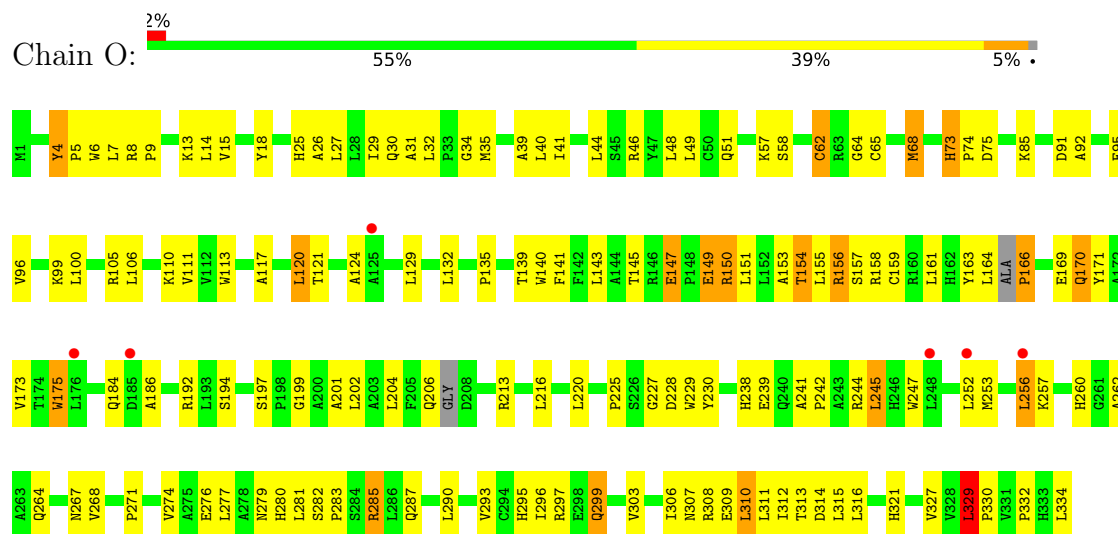
• Molecule 3: DNA polymerase III subunit delta'



• 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) 90.5 (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 , 0.348	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)	0.32 , 40.9	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	0.86	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	0.91	5/2715 (0.2%)	1.38	36/3684 (1.0%)
1	F	0.91	5/2715 (0.2%)	1.38	36/3684 (1.0%)
1	K	0.91	5/2715 (0.2%)	1.38	36/3684 (1.0%)
2	B	0.76	4/2887 (0.1%)	1.27	36/3912 (0.9%)
2	C	0.65	2/2887 (0.1%)	1.19	29/3912 (0.7%)
2	D	0.94	11/2874 (0.4%)	1.32	39/3894 (1.0%)
2	G	0.76	4/2887 (0.1%)	1.27	38/3912 (1.0%)
2	H	0.69	3/2887 (0.1%)	1.20	32/3912 (0.8%)
2	I	0.94	11/2874 (0.4%)	1.32	40/3894 (1.0%)
2	L	0.76	4/2887 (0.1%)	1.27	36/3912 (0.9%)
2	M	0.64	2/2887 (0.1%)	1.19	32/3912 (0.8%)
2	N	0.93	10/2874 (0.3%)	1.32	39/3894 (1.0%)
3	E	0.68	0/2656	1.10	13/3620 (0.4%)
3	J	0.68	0/2656	1.11	14/3620 (0.4%)
3	O	0.68	0/2656	1.11	14/3620 (0.4%)
All	All	0.80	66/42057 (0.2%)	1.26	470/57066 (0.8%)

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 (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	315	ASP	CB-CG	24.38	2.13	1.52
1	K	315	ASP	CB-CG	24.36	2.12	1.52
1	A	315	ASP	CB-CG	24.31	2.12	1.52
2	I	363	MET	SD-CE	19.28	2.27	1.79
2	N	363	MET	SD-CE	19.26	2.27	1.79
2	D	363	MET	SD-CE	19.23	2.27	1.79
2	H	3	TYR	C-N	12.65	1.51	1.33
2	I	360	HIS	ND1-CE1	11.42	1.44	1.32
2	D	360	HIS	ND1-CE1	11.41	1.44	1.32
2	D	133	ARG	CZ-NH2	-11.35	1.18	1.33
2	N	360	HIS	ND1-CE1	11.32	1.43	1.32
2	N	133	ARG	CZ-NH2	-11.29	1.18	1.33
2	I	133	ARG	CZ-NH2	-11.26	1.18	1.33
2	D	360	HIS	CA-CB	10.55	1.66	1.53
2	I	360	HIS	CA-CB	10.55	1.66	1.53
1	F	310	LEU	CG-CD2	-10.39	1.18	1.52
1	A	310	LEU	CG-CD2	-10.36	1.18	1.52
1	K	310	LEU	CG-CD2	-10.34	1.18	1.52
2	D	360	HIS	CD2-NE2	9.73	1.48	1.37
2	N	360	HIS	CD2-NE2	9.67	1.48	1.37
2	I	360	HIS	CD2-NE2	9.60	1.48	1.37
2	N	363	MET	CG-SD	9.54	2.04	1.80
2	I	363	MET	CG-SD	9.53	2.04	1.80
2	D	363	MET	CG-SD	9.49	2.04	1.80
2	N	360	HIS	CA-CB	9.43	1.66	1.53
2	I	356	ALA	C-O	-9.05	1.12	1.24
2	D	356	ALA	C-O	-8.97	1.12	1.24
2	N	356	ALA	C-O	-8.95	1.12	1.24
2	N	360	HIS	CA-C	-7.89	1.43	1.52
2	N	360	HIS	CG-CD2	7.89	1.44	1.35
2	D	360	HIS	CG-CD2	7.82	1.44	1.35
2	I	360	HIS	CG-CD2	7.71	1.44	1.35
2	I	360	HIS	CA-C	-7.36	1.42	1.52
2	D	360	HIS	CA-C	-7.34	1.42	1.52
2	D	360	HIS	C-O	-6.79	1.18	1.25
2	B	304	ASN	C-O	6.63	1.32	1.24
2	G	304	ASN	C-O	6.59	1.32	1.24
2	I	360	HIS	C-O	-6.58	1.19	1.25
2	H	239	ALA	CA-CB	-6.52	1.43	1.53
2	L	304	ASN	C-O	6.51	1.32	1.24
2	M	239	ALA	CA-CB	-6.50	1.43	1.53
2	C	239	ALA	CA-CB	-6.48	1.43	1.53
1	K	283	ARG	CB-CG	6.01	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	283	ARG	CB-CG	6.00	1.70	1.52
1	F	283	ARG	CB-CG	5.99	1.70	1.52
1	F	315	ASP	CG-OD2	5.85	1.36	1.25
1	A	315	ASP	CG-OD2	5.72	1.36	1.25
1	K	315	ASP	CG-OD2	5.65	1.36	1.25
1	A	200	PRO	N-CD	-5.59	1.40	1.47
1	K	200	PRO	N-CD	-5.53	1.40	1.47
2	B	5	VAL	CA-CB	-5.51	1.47	1.54
1	F	200	PRO	N-CD	-5.49	1.40	1.47
2	I	23	HIS	CA-C	-5.45	1.46	1.52
2	L	5	VAL	CA-CB	-5.44	1.47	1.54
2	G	5	VAL	CA-CB	-5.41	1.47	1.54
2	D	23	HIS	CA-C	-5.39	1.46	1.52
2	N	23	HIS	CA-C	-5.34	1.46	1.52
2	B	304	ASN	CA-CB	-5.28	1.44	1.53
2	B	304	ASN	CG-ND2	-5.28	1.22	1.33
2	G	304	ASN	CG-ND2	-5.28	1.22	1.33
2	L	304	ASN	CG-ND2	-5.27	1.22	1.33
2	C	351	MET	SD-CE	-5.25	1.66	1.79
2	G	304	ASN	CA-CB	-5.24	1.44	1.53
2	H	351	MET	SD-CE	-5.23	1.66	1.79
2	M	351	MET	SD-CE	-5.20	1.66	1.79
2	L	304	ASN	CA-CB	-5.17	1.44	1.53

All (470) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	315	ASP	CA-CB-CG	-22.84	89.76	112.60
1	A	315	ASP	CA-CB-CG	-22.80	89.80	112.60
1	K	315	ASP	CA-CB-CG	-22.73	89.87	112.60
1	K	280	GLN	CA-C-N	15.02	150.31	121.63
1	K	280	GLN	C-N-CA	15.02	150.31	121.63
1	A	280	GLN	CA-C-N	15.00	150.28	121.63
1	A	280	GLN	C-N-CA	15.00	150.28	121.63
1	F	280	GLN	CA-C-N	14.99	150.27	121.63
1	F	280	GLN	C-N-CA	14.99	150.27	121.63
1	F	283	ARG	CA-C-N	13.75	148.35	121.41
1	F	283	ARG	C-N-CA	13.75	148.35	121.41
1	A	283	ARG	CA-C-N	13.71	148.29	121.41
1	A	283	ARG	C-N-CA	13.71	148.29	121.41
1	K	283	ARG	CA-C-N	13.70	148.26	121.41
1	K	283	ARG	C-N-CA	13.70	148.26	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	363	MET	CG-SD-CE	12.10	127.52	100.90
2	I	363	MET	CG-SD-CE	12.10	127.52	100.90
2	N	363	MET	CG-SD-CE	12.08	127.48	100.90
2	N	360	HIS	N-CA-CB	11.27	129.20	110.05
2	L	75	VAL	N-CA-C	11.13	121.38	111.81
2	G	75	VAL	N-CA-C	11.09	121.34	111.81
2	B	75	VAL	N-CA-C	11.09	121.34	111.81
2	M	367	GLU	N-CA-C	11.01	118.12	108.22
2	H	367	GLU	N-CA-C	10.97	118.09	108.22
2	C	367	GLU	N-CA-C	10.89	118.03	108.22
2	N	360	HIS	CB-CA-C	-10.56	98.44	110.17
2	I	360	HIS	N-CA-CB	10.21	129.15	110.17
2	D	360	HIS	N-CA-CB	10.20	129.14	110.17
2	N	360	HIS	CA-CB-CG	10.09	123.89	113.80
2	D	360	HIS	CA-CB-CG	9.99	123.79	113.80
2	I	360	HIS	CA-CB-CG	9.96	123.76	113.80
2	N	360	HIS	CA-C-O	-9.95	110.44	119.59
2	D	360	HIS	CA-C-O	-9.74	110.46	119.62
2	I	360	HIS	CA-C-O	-9.68	110.52	119.62
2	N	360	HIS	CB-CG-ND1	9.59	137.08	122.70
2	D	360	HIS	CB-CG-ND1	9.54	137.02	122.70
2	I	360	HIS	CB-CG-ND1	9.51	136.96	122.70
2	G	24	VAL	N-CA-C	-9.30	102.80	111.45
2	L	24	VAL	N-CA-C	-9.21	102.89	111.45
2	B	24	VAL	N-CA-C	-9.18	102.91	111.45
2	M	301	ALA	N-CA-C	9.16	122.42	111.33
2	C	301	ALA	N-CA-C	9.16	122.41	111.33
2	H	301	ALA	N-CA-C	9.12	122.36	111.33
2	D	20	GLY	N-CA-C	9.09	127.37	115.47
2	I	20	GLY	N-CA-C	9.02	127.29	115.47
2	N	20	GLY	N-CA-C	9.02	127.29	115.47
1	F	283	ARG	CA-C-O	8.86	130.41	120.84
1	A	283	ARG	CA-C-O	8.83	130.37	120.84
1	K	283	ARG	CA-C-O	8.82	130.37	120.84
2	N	133	ARG	NH1-CZ-NH2	-8.79	107.87	119.30
2	D	133	ARG	NH1-CZ-NH2	-8.73	107.95	119.30
2	I	133	ARG	NH1-CZ-NH2	-8.73	107.95	119.30
1	K	75	ALA	N-CA-C	8.64	123.08	112.54
2	G	259	ALA	N-CA-C	8.63	125.56	113.56
1	F	75	ALA	N-CA-C	8.61	123.05	112.54
2	L	259	ALA	N-CA-C	8.60	125.51	113.56
2	B	259	ALA	N-CA-C	8.59	125.50	113.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	ALA	N-CA-C	8.57	123.00	112.54
2	I	360	HIS	CB-CA-C	-8.38	98.39	110.13
2	D	360	HIS	CB-CA-C	-8.38	98.40	110.13
3	E	4	TYR	CA-C-N	8.25	127.93	119.19
3	E	4	TYR	C-N-CA	8.25	127.93	119.19
3	O	4	TYR	CA-C-N	8.22	127.90	119.19
3	O	4	TYR	C-N-CA	8.22	127.90	119.19
3	J	4	TYR	CA-C-N	8.21	127.89	119.19
3	J	4	TYR	C-N-CA	8.21	127.89	119.19
2	N	229	ASP	N-CA-C	-8.19	99.97	110.53
2	I	229	ASP	N-CA-C	-8.17	99.99	110.53
2	N	133	ARG	N-CA-C	8.16	124.83	111.37
2	D	133	ARG	N-CA-C	8.13	124.79	111.37
2	D	229	ASP	N-CA-C	-8.13	100.04	110.53
2	I	133	ARG	N-CA-C	8.13	124.79	111.37
2	I	360	HIS	CE1-NE2-CD2	-8.03	100.97	109.00
2	N	360	HIS	CE1-NE2-CD2	-8.02	100.98	109.00
2	I	276	ILE	CB-CA-C	-8.00	102.79	111.59
1	K	280	GLN	O-C-N	-7.99	113.01	122.27
1	F	280	GLN	O-C-N	-7.98	113.01	122.27
1	A	280	GLN	O-C-N	-7.98	113.01	122.27
2	D	360	HIS	CE1-NE2-CD2	-7.96	101.04	109.00
2	D	276	ILE	CB-CA-C	-7.92	102.88	111.59
2	N	276	ILE	CB-CA-C	-7.92	102.88	111.59
2	C	70	ALA	N-CA-C	-7.84	103.73	113.38
2	L	244	LEU	N-CA-C	7.82	123.12	113.50
2	G	244	LEU	N-CA-C	7.79	123.08	113.50
2	B	244	LEU	N-CA-C	7.78	123.07	113.50
2	M	70	ALA	N-CA-C	-7.78	103.81	113.38
2	H	70	ALA	N-CA-C	-7.77	103.83	113.38
2	G	19	VAL	N-CA-C	7.76	120.03	108.54
2	L	19	VAL	N-CA-C	7.74	119.99	108.54
2	B	19	VAL	N-CA-C	7.73	119.98	108.54
2	N	360	HIS	CB-CG-CD2	-7.72	121.16	131.20
2	N	7	ALA	N-CA-C	-7.69	94.42	110.80
2	D	360	HIS	CB-CG-CD2	-7.69	121.21	131.20
2	C	182	GLN	N-CA-C	-7.68	104.13	113.97
2	D	7	ALA	N-CA-C	-7.67	94.47	110.80
2	M	182	GLN	N-CA-C	-7.66	104.16	113.97
2	I	7	ALA	N-CA-C	-7.66	94.48	110.80
2	H	182	GLN	N-CA-C	-7.66	104.17	113.97
2	B	59	ALA	N-CA-C	-7.65	103.02	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	59	ALA	N-CA-C	-7.61	103.06	111.36
2	G	59	ALA	N-CA-C	-7.61	103.07	111.36
2	I	360	HIS	CB-CG-CD2	-7.61	121.31	131.20
2	L	302	LEU	CA-C-N	7.43	135.98	121.41
2	L	302	LEU	C-N-CA	7.43	135.98	121.41
2	G	302	LEU	CA-C-N	7.40	135.91	121.41
2	G	302	LEU	C-N-CA	7.40	135.91	121.41
2	B	302	LEU	CA-C-N	7.37	135.86	121.41
2	B	302	LEU	C-N-CA	7.37	135.86	121.41
2	D	133	ARG	NE-CZ-NH2	7.27	125.74	119.20
2	I	133	ARG	NE-CZ-NH2	7.22	125.70	119.20
2	D	359	PHE	CA-C-N	7.21	133.38	122.42
2	D	359	PHE	C-N-CA	7.21	133.38	122.42
2	N	133	ARG	NE-CZ-NH2	7.19	125.67	119.20
2	D	141	LYS	N-CA-C	-7.19	103.52	111.36
2	N	141	LYS	N-CA-C	-7.19	103.53	111.36
3	J	329	LEU	CA-C-N	7.17	127.13	120.03
3	J	329	LEU	C-N-CA	7.17	127.13	120.03
2	I	359	PHE	CA-C-N	7.15	133.29	122.42
2	I	359	PHE	C-N-CA	7.15	133.29	122.42
2	I	141	LYS	N-CA-C	-7.15	103.57	111.36
2	G	20	GLY	N-CA-C	7.11	130.03	113.18
2	L	20	GLY	N-CA-C	7.11	130.02	113.18
2	B	20	GLY	N-CA-C	7.08	129.95	113.18
2	L	356	ALA	N-CA-C	-7.07	103.65	111.36
3	E	329	LEU	CA-C-N	7.07	127.03	120.03
3	E	329	LEU	C-N-CA	7.07	127.03	120.03
1	K	57	PRO	N-CA-C	-7.07	104.73	114.27
1	F	57	PRO	N-CA-C	-7.04	104.76	114.27
3	O	329	LEU	CA-C-N	7.04	127.00	120.03
3	O	329	LEU	C-N-CA	7.04	127.00	120.03
2	H	116	ALA	N-CA-C	7.00	119.76	111.71
2	G	356	ALA	N-CA-C	-6.99	103.74	111.36
1	A	57	PRO	N-CA-C	-6.98	104.84	114.27
2	B	356	ALA	N-CA-C	-6.98	103.75	111.36
1	A	283	ARG	O-C-N	6.96	131.43	122.87
1	K	283	ARG	O-C-N	6.92	131.39	122.87
2	M	116	ALA	N-CA-C	6.89	119.63	111.71
1	F	283	ARG	O-C-N	6.88	131.34	122.87
2	C	86	ARG	N-CA-C	6.87	120.08	107.99
3	J	186	ALA	N-CA-C	-6.86	103.41	111.03
2	D	360	HIS	ND1-CE1-NE2	6.84	115.25	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	360	HIS	ND1-CE1-NE2	6.84	115.25	108.40
2	C	116	ALA	N-CA-C	6.83	119.57	111.71
2	I	64	CYS	N-CA-C	6.83	119.91	110.35
3	E	186	ALA	N-CA-C	-6.82	103.46	111.03
1	F	249	THR	N-CA-C	-6.82	104.59	113.12
2	H	86	ARG	N-CA-C	6.82	119.98	107.99
1	K	264	SER	N-CA-C	-6.81	97.31	108.41
3	O	186	ALA	N-CA-C	-6.79	103.49	111.03
2	I	360	HIS	ND1-CE1-NE2	6.79	115.19	108.40
1	A	249	THR	N-CA-C	-6.79	104.64	113.12
1	F	264	SER	N-CA-C	-6.79	97.35	108.41
2	M	86	ARG	N-CA-C	6.78	119.93	107.99
1	K	249	THR	N-CA-C	-6.78	104.65	113.12
2	D	64	CYS	N-CA-C	6.77	119.82	110.35
1	A	264	SER	N-CA-C	-6.76	97.39	108.41
2	I	298	SER	CA-C-N	6.76	128.29	119.84
2	I	298	SER	C-N-CA	6.76	128.29	119.84
2	N	64	CYS	N-CA-C	6.75	119.80	110.35
2	N	298	SER	CA-C-N	6.70	128.22	119.84
2	N	298	SER	C-N-CA	6.70	128.22	119.84
2	D	298	SER	CA-C-N	6.69	128.20	119.84
2	D	298	SER	C-N-CA	6.69	128.20	119.84
2	D	363	MET	CB-CG-SD	6.69	132.77	112.70
2	N	363	MET	CB-CG-SD	6.69	132.77	112.70
2	I	363	MET	CB-CG-SD	6.68	132.75	112.70
2	L	303	GLY	N-CA-C	6.68	129.00	113.18
2	G	303	GLY	N-CA-C	6.66	128.96	113.18
2	B	303	GLY	N-CA-C	6.65	128.94	113.18
1	A	134	SER	N-CA-C	6.64	120.66	110.36
2	G	244	LEU	CB-CG-CD2	-6.63	90.80	110.70
1	K	134	SER	N-CA-C	6.63	120.64	110.36
2	M	20	GLY	N-CA-C	6.63	128.90	113.18
2	L	244	LEU	CB-CG-CD2	-6.63	90.80	110.70
2	B	244	LEU	CB-CG-CD2	-6.62	90.83	110.70
2	C	20	GLY	N-CA-C	6.62	128.88	113.18
2	C	244	LEU	N-CA-C	6.62	119.35	110.35
1	F	134	SER	N-CA-C	6.62	120.62	110.36
1	F	277	ARG	N-CA-C	6.60	120.62	111.90
2	H	20	GLY	N-CA-C	6.60	128.82	113.18
1	K	277	ARG	N-CA-C	6.59	120.60	111.90
2	H	304	ASN	N-CA-C	6.58	118.25	111.14
3	J	39	ALA	N-CA-C	6.57	119.26	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	88	VAL	CB-CA-C	-6.56	103.49	111.88
1	A	277	ARG	N-CA-C	6.55	120.55	111.90
2	M	304	ASN	N-CA-C	6.54	118.20	111.14
2	C	304	ASN	N-CA-C	6.54	118.20	111.14
2	L	88	VAL	CB-CA-C	-6.54	103.52	111.88
3	O	166	PRO	CA-C-N	6.52	124.36	119.66
3	O	166	PRO	C-N-CA	6.52	124.36	119.66
1	A	237	ARG	N-CA-C	-6.51	105.37	113.38
3	E	39	ALA	N-CA-C	6.51	119.20	111.71
2	B	88	VAL	CB-CA-C	-6.50	103.56	111.88
3	E	166	PRO	CA-C-N	6.50	124.34	119.66
3	E	166	PRO	C-N-CA	6.50	124.34	119.66
2	L	304	ASN	N-CA-C	6.50	120.47	112.54
1	F	237	ARG	N-CA-C	-6.49	105.40	113.38
1	K	237	ARG	N-CA-C	-6.48	105.41	113.38
2	B	304	ASN	N-CA-C	6.47	120.44	112.54
1	A	124	ALA	N-CA-C	6.46	120.21	110.64
3	O	39	ALA	N-CA-C	6.46	119.14	111.71
2	G	304	ASN	N-CA-C	6.44	120.40	112.54
2	H	261	GLY	N-CA-C	6.44	119.97	112.50
3	J	166	PRO	CA-C-N	6.44	124.30	119.66
3	J	166	PRO	C-N-CA	6.44	124.30	119.66
1	A	224	GLY	N-CA-C	-6.42	103.38	112.37
2	C	261	GLY	N-CA-C	6.42	119.94	112.50
1	F	224	GLY	N-CA-C	-6.41	103.39	112.37
1	F	124	ALA	N-CA-C	6.40	120.11	110.64
1	K	124	ALA	N-CA-C	6.39	120.09	110.64
1	K	224	GLY	N-CA-C	-6.38	103.44	112.37
2	N	359	PHE	CA-C-N	6.34	133.34	122.06
2	N	359	PHE	C-N-CA	6.34	133.34	122.06
2	B	213	SER	N-CA-C	6.33	119.72	109.40
2	B	89	ASP	N-CA-C	6.33	120.84	113.18
2	L	89	ASP	N-CA-C	6.33	120.84	113.18
1	F	9	LEU	N-CA-C	6.32	117.84	111.07
2	M	261	GLY	N-CA-C	6.31	119.82	112.50
2	B	70	ALA	N-CA-C	-6.31	105.58	113.28
2	L	119	ARG	N-CA-C	6.30	118.96	111.33
2	G	17	ASP	N-CA-C	6.30	120.58	112.26
1	K	9	LEU	N-CA-C	6.29	117.80	111.07
2	L	213	SER	N-CA-C	6.28	119.63	109.40
2	G	213	SER	N-CA-C	6.28	119.63	109.40
2	C	215	ARG	CB-CA-C	-6.27	100.94	110.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	LEU	N-CA-C	6.27	117.78	111.07
2	L	198	HIS	N-CA-C	6.27	118.70	108.55
2	G	119	ARG	N-CA-C	6.26	118.91	111.33
2	B	17	ASP	N-CA-C	6.26	120.52	112.26
2	G	89	ASP	N-CA-C	6.24	120.73	113.18
2	G	70	ALA	N-CA-C	-6.24	105.67	113.28
2	M	215	ARG	CB-CA-C	-6.24	101.01	110.92
2	G	198	HIS	N-CA-C	6.23	118.65	108.55
2	M	244	LEU	N-CA-C	6.23	119.27	110.23
2	I	364	PRO	CA-N-CD	-6.21	103.31	112.00
2	L	17	ASP	N-CA-C	6.21	120.46	112.26
2	B	198	HIS	N-CA-C	6.20	118.59	108.55
2	L	70	ALA	N-CA-C	-6.20	105.72	113.28
2	H	215	ARG	CB-CA-C	-6.20	101.07	110.92
2	B	119	ARG	N-CA-C	6.19	118.82	111.33
2	H	244	LEU	N-CA-C	6.19	119.21	110.23
2	I	143	LEU	N-CA-C	6.18	118.81	111.33
1	A	4	LEU	N-CA-C	6.17	118.45	109.07
1	F	4	LEU	N-CA-C	6.16	118.44	109.07
1	K	4	LEU	N-CA-C	6.16	118.43	109.07
2	N	364	PRO	CA-N-CD	-6.13	103.42	112.00
2	D	143	LEU	N-CA-C	6.12	118.74	111.33
1	A	76	SER	N-CA-C	6.12	118.50	109.69
2	D	364	PRO	CA-N-CD	-6.11	103.45	112.00
1	K	76	SER	N-CA-C	6.10	118.48	109.69
1	F	76	SER	N-CA-C	6.10	118.47	109.69
2	N	143	LEU	N-CA-C	6.10	118.71	111.33
2	G	339	LEU	N-CA-C	6.07	123.23	109.81
2	H	158	ASP	CA-C-N	6.07	125.76	119.56
2	H	158	ASP	C-N-CA	6.07	125.76	119.56
2	B	339	LEU	N-CA-C	6.07	123.23	109.81
1	K	288	GLU	N-CA-C	-6.07	104.74	111.36
1	F	288	GLU	N-CA-C	-6.07	104.75	111.36
2	L	339	LEU	N-CA-C	6.06	123.21	109.81
1	A	288	GLU	N-CA-C	-6.06	104.76	111.36
2	M	258	GLU	N-CA-C	-6.00	105.92	113.18
2	I	75	VAL	N-CA-C	5.98	118.94	112.96
2	C	258	GLU	N-CA-C	-5.97	105.95	113.18
3	E	135	PRO	N-CA-C	5.96	117.97	110.70
2	H	258	GLU	N-CA-C	-5.96	105.97	113.18
3	O	135	PRO	N-CA-C	5.96	117.97	110.70
3	J	135	PRO	N-CA-C	5.94	117.94	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	19	VAL	N-CA-C	5.93	116.41	108.11
2	M	158	ASP	CA-C-N	5.92	125.60	119.56
2	M	158	ASP	C-N-CA	5.92	125.60	119.56
2	D	75	VAL	N-CA-C	5.92	118.88	112.96
2	I	367	GLU	N-CA-C	5.90	113.32	108.07
2	N	75	VAL	N-CA-C	5.90	118.86	112.96
2	I	19	VAL	N-CA-C	5.89	116.36	108.11
2	N	19	VAL	N-CA-C	5.88	116.35	108.11
2	N	367	GLU	N-CA-C	5.87	113.29	108.07
2	C	158	ASP	CA-C-N	5.86	125.54	119.56
2	C	158	ASP	C-N-CA	5.86	125.54	119.56
2	B	365	LEU	CA-C-N	5.86	127.04	120.66
2	B	365	LEU	C-N-CA	5.86	127.04	120.66
1	A	282	ARG	CB-CG-CD	-5.85	97.85	111.30
2	D	367	GLU	N-CA-C	5.85	113.27	108.07
1	F	282	ARG	CB-CG-CD	-5.83	97.89	111.30
2	M	365	LEU	CA-C-N	5.83	127.15	120.85
2	M	365	LEU	C-N-CA	5.83	127.15	120.85
2	C	365	LEU	CA-C-N	5.81	127.13	120.85
2	C	365	LEU	C-N-CA	5.81	127.13	120.85
1	K	282	ARG	CB-CG-CD	-5.81	97.93	111.30
3	J	264	GLN	N-CA-C	5.81	119.00	109.76
2	I	360	HIS	CG-CD2-NE2	5.81	113.01	107.20
2	H	365	LEU	CA-C-N	5.80	127.12	120.85
2	H	365	LEU	C-N-CA	5.80	127.12	120.85
2	C	360	HIS	CA-C-N	5.80	125.17	118.85
2	C	360	HIS	C-N-CA	5.80	125.17	118.85
2	L	365	LEU	CA-C-N	5.80	126.98	120.66
2	L	365	LEU	C-N-CA	5.80	126.98	120.66
2	G	365	LEU	CA-C-N	5.79	126.97	120.66
2	G	365	LEU	C-N-CA	5.79	126.97	120.66
2	H	360	HIS	CA-C-N	5.78	125.15	118.85
2	H	360	HIS	C-N-CA	5.78	125.15	118.85
1	A	147	LEU	N-CA-C	-5.78	104.89	112.75
2	I	224	ALA	N-CA-C	-5.76	105.35	112.90
2	N	224	ALA	N-CA-C	-5.75	105.37	112.90
2	D	224	ALA	N-CA-C	-5.74	105.38	112.90
2	G	96	ALA	N-CA-C	5.74	117.54	111.28
3	E	264	GLN	N-CA-C	5.74	118.89	109.76
2	M	360	HIS	CA-C-N	5.74	125.11	118.85
2	M	360	HIS	C-N-CA	5.74	125.11	118.85
3	O	264	GLN	N-CA-C	5.74	118.89	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	96	ALA	N-CA-C	5.74	117.53	111.28
2	B	99	THR	N-CA-C	5.74	119.59	112.59
2	B	121	LYS	N-CA-C	-5.73	98.40	108.20
2	G	247	ASP	N-CA-C	5.73	117.55	108.67
2	G	121	LYS	N-CA-C	-5.72	98.41	108.20
2	L	247	ASP	N-CA-C	5.71	117.53	108.67
2	H	215	ARG	N-CA-C	-5.71	104.05	111.02
2	C	215	ARG	N-CA-C	-5.71	104.06	111.02
2	B	247	ASP	N-CA-C	5.71	117.51	108.67
2	G	99	THR	N-CA-C	5.70	119.54	112.59
2	L	121	LYS	N-CA-C	-5.70	98.46	108.20
2	M	215	ARG	N-CA-C	-5.69	104.08	111.02
1	F	147	LEU	N-CA-C	-5.69	105.02	112.75
1	K	147	LEU	N-CA-C	-5.69	105.02	112.75
1	F	61	TRP	N-CA-C	-5.65	105.27	111.82
2	N	360	HIS	CG-CD2-NE2	5.65	112.85	107.20
2	L	96	ALA	N-CA-C	5.65	117.43	111.28
1	A	61	TRP	N-CA-C	-5.64	105.28	111.82
2	D	360	HIS	CG-CD2-NE2	5.63	112.83	107.20
2	I	248	GLN	N-CA-C	5.62	117.86	111.11
1	K	61	TRP	N-CA-C	-5.62	105.30	111.82
2	H	339	LEU	N-CA-C	5.61	122.21	109.81
2	D	248	GLN	N-CA-C	5.61	117.84	111.11
2	N	248	GLN	N-CA-C	5.61	117.84	111.11
2	G	21	GLN	CA-C-N	5.60	132.23	121.54
2	G	21	GLN	C-N-CA	5.60	132.23	121.54
2	C	339	LEU	N-CA-C	5.60	122.18	109.81
2	M	339	LEU	N-CA-C	5.59	122.17	109.81
2	H	3	TYR	CA-C-N	-5.58	110.89	121.54
2	H	3	TYR	C-N-CA	-5.58	110.89	121.54
2	C	19	VAL	N-CA-C	5.56	116.99	108.71
2	L	21	GLN	CA-C-N	5.56	132.15	121.54
2	L	21	GLN	C-N-CA	5.56	132.15	121.54
2	B	21	GLN	CA-C-N	5.55	132.15	121.54
2	B	21	GLN	C-N-CA	5.55	132.15	121.54
2	H	23	HIS	N-CA-C	5.53	119.12	112.38
1	A	173	CYS	N-CA-C	-5.52	101.28	110.17
2	M	19	VAL	N-CA-C	5.51	116.92	108.71
1	K	173	CYS	N-CA-C	-5.50	101.31	110.17
2	L	99	THR	N-CA-C	5.49	119.51	112.26
2	D	352	THR	N-CA-C	5.49	117.12	111.03
2	H	19	VAL	N-CA-C	5.48	116.87	108.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	352	THR	N-CA-C	5.47	117.10	111.03
1	A	291	ASN	N-CA-C	5.47	119.21	112.54
2	I	278	TRP	N-CA-C	5.47	117.95	111.33
2	C	245	ASP	N-CA-C	-5.46	102.19	110.28
2	B	15	PHE	N-CA-C	-5.46	105.33	111.28
2	M	23	HIS	N-CA-C	5.45	119.03	112.38
2	N	352	THR	N-CA-C	5.44	117.07	111.03
2	C	23	HIS	N-CA-C	5.44	119.02	112.38
1	F	173	CYS	N-CA-C	-5.44	101.41	110.17
3	J	293	VAL	N-CA-C	-5.43	105.08	110.62
2	N	303	GLY	N-CA-C	5.43	126.05	113.18
2	C	320	ILE	CA-C-N	5.43	125.97	120.38
2	C	320	ILE	C-N-CA	5.43	125.97	120.38
2	H	245	ASP	N-CA-C	-5.42	102.25	110.28
2	D	303	GLY	N-CA-C	5.42	126.03	113.18
2	I	303	GLY	N-CA-C	5.42	126.01	113.18
2	C	320	ILE	N-CA-C	5.41	113.83	107.77
2	H	320	ILE	N-CA-C	5.41	113.83	107.77
3	O	293	VAL	N-CA-C	-5.41	105.10	110.62
1	F	291	ASN	N-CA-C	5.41	119.14	112.54
2	G	15	PHE	N-CA-C	-5.41	105.39	111.28
2	L	15	PHE	N-CA-C	-5.40	105.39	111.28
1	K	291	ASN	N-CA-C	5.39	119.12	112.54
2	M	245	ASP	N-CA-C	-5.39	102.30	110.28
2	H	366	PRO	N-CA-C	5.39	120.62	111.03
2	H	320	ILE	CA-C-N	5.38	125.93	120.38
2	H	320	ILE	C-N-CA	5.38	125.93	120.38
2	G	307	ALA	N-CA-C	5.37	120.24	111.37
2	M	366	PRO	N-CA-C	5.37	120.59	111.03
2	M	183	ILE	N-CA-C	-5.36	105.90	111.58
2	C	366	PRO	N-CA-C	5.36	120.56	111.03
2	I	270	GLU	N-CA-C	-5.34	105.45	111.28
2	M	320	ILE	N-CA-C	5.34	113.75	107.77
2	B	307	ALA	N-CA-C	5.33	120.17	111.37
3	E	293	VAL	N-CA-C	-5.33	105.18	110.62
2	L	307	ALA	N-CA-C	5.32	120.15	111.37
2	N	270	GLU	N-CA-C	-5.30	105.50	111.28
2	M	320	ILE	CA-C-N	5.30	125.84	120.38
2	M	320	ILE	C-N-CA	5.30	125.84	120.38
2	G	11	ARG	N-CA-C	-5.30	103.06	109.57
2	N	114	ALA	N-CA-C	5.29	117.19	109.84
2	H	183	ILE	N-CA-C	-5.28	105.98	111.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	114	ALA	N-CA-C	5.28	117.17	109.84
2	I	245	ASP	N-CA-C	-5.27	106.80	113.23
1	F	283	ARG	N-CA-C	5.27	117.56	107.75
2	N	245	ASP	N-CA-C	-5.27	106.80	113.23
2	D	270	GLU	N-CA-C	-5.27	105.54	111.28
2	B	11	ARG	N-CA-C	-5.27	103.09	109.57
1	A	225	LYS	N-CA-C	5.26	117.97	110.24
1	F	225	LYS	N-CA-C	5.25	117.96	110.24
1	K	283	ARG	N-CA-C	5.25	117.52	107.75
2	C	210	ALA	N-CA-C	-5.25	101.91	110.20
2	B	6	LEU	N-CA-C	5.25	117.41	111.11
1	K	225	LYS	N-CA-C	5.25	117.96	110.24
2	L	365	LEU	N-CA-C	5.25	115.64	109.60
2	D	114	ALA	N-CA-C	5.25	117.13	109.84
1	K	222	LEU	CB-CA-C	-5.24	104.72	111.22
2	C	183	ILE	N-CA-C	-5.24	106.03	111.58
2	B	73	CYS	N-CA-C	-5.23	101.94	110.20
1	A	222	LEU	CB-CA-C	-5.22	104.74	111.22
2	L	73	CYS	N-CA-C	-5.22	101.94	110.20
2	D	245	ASP	N-CA-C	-5.22	106.86	113.23
1	A	283	ARG	N-CA-C	5.21	117.44	107.75
2	G	365	LEU	N-CA-C	5.21	115.59	109.60
2	H	210	ALA	N-CA-C	-5.21	101.97	110.20
2	M	210	ALA	N-CA-C	-5.21	101.97	110.20
1	K	282	ARG	CA-CB-CG	-5.20	103.70	114.10
1	A	282	ARG	CA-CB-CG	-5.20	103.70	114.10
2	G	73	CYS	N-CA-C	-5.20	101.99	110.20
3	O	73	HIS	CA-C-N	5.20	126.22	120.45
3	O	73	HIS	C-N-CA	5.20	126.22	120.45
1	F	222	LEU	CB-CA-C	-5.20	104.78	111.22
2	L	11	ARG	N-CA-C	-5.18	103.20	109.57
2	B	365	LEU	N-CA-C	5.18	115.55	109.60
2	L	6	LEU	N-CA-C	5.17	117.31	111.11
3	E	73	HIS	CA-C-N	5.16	126.18	120.45
3	E	73	HIS	C-N-CA	5.16	126.18	120.45
1	F	282	ARG	CA-CB-CG	-5.16	103.77	114.10
2	D	347	MET	N-CA-C	-5.15	106.10	112.38
2	G	6	LEU	N-CA-C	5.13	117.27	111.11
1	K	132	ASN	N-CA-C	-5.13	108.05	114.56
2	N	347	MET	N-CA-C	-5.13	106.13	112.38
1	F	104	LEU	N-CA-C	5.12	117.13	110.53
2	I	342	ALA	CA-C-N	5.11	125.40	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	342	ALA	C-N-CA	5.11	125.40	119.47
1	A	132	ASN	N-CA-C	-5.11	108.08	114.56
3	J	73	HIS	CA-C-N	5.09	126.11	120.45
3	J	73	HIS	C-N-CA	5.09	126.11	120.45
1	K	25	GLY	N-CA-C	5.09	117.47	110.69
1	K	97	LEU	N-CA-C	-5.09	105.64	111.14
1	A	104	LEU	N-CA-C	5.09	117.09	110.53
2	N	342	ALA	CA-C-N	5.08	125.36	119.47
2	N	342	ALA	C-N-CA	5.08	125.36	119.47
1	F	325	GLU	N-CA-C	-5.07	105.66	111.14
2	M	223	GLN	N-CA-C	-5.06	105.67	111.14
3	O	330	PRO	N-CA-C	5.06	119.00	111.41
1	F	132	ASN	N-CA-C	-5.06	108.14	114.56
1	A	266	HIS	N-CA-C	-5.05	105.42	112.45
1	K	104	LEU	N-CA-C	5.05	117.04	110.53
2	D	342	ALA	CA-C-N	5.04	125.32	119.47
2	D	342	ALA	C-N-CA	5.04	125.32	119.47
1	F	25	GLY	N-CA-C	5.04	117.39	110.69
2	H	223	GLN	N-CA-C	-5.04	105.68	111.07
2	B	243	THR	N-CA-C	5.03	125.10	111.00
1	A	25	GLY	N-CA-C	5.03	117.38	110.69
2	I	347	MET	N-CA-C	-5.03	106.25	112.38
1	A	97	LEU	N-CA-C	-5.03	105.71	111.14
3	J	330	PRO	N-CA-C	5.03	118.95	111.41
1	K	266	HIS	N-CA-C	-5.03	105.47	112.45
2	G	254	GLU	N-CA-C	-5.02	105.50	110.97
1	A	325	GLU	N-CA-C	-5.01	105.72	111.14
1	F	266	HIS	N-CA-C	-5.01	105.48	112.45
2	G	345	ARG	N-CA-C	5.01	117.39	111.33
2	M	162	LEU	CA-C-N	5.01	124.92	119.76
2	M	162	LEU	C-N-CA	5.01	124.92	119.76
1	F	97	LEU	N-CA-C	-5.01	105.73	111.14
2	G	243	THR	N-CA-C	5.01	125.02	111.00
1	K	325	GLU	N-CA-C	-5.01	105.73	111.14
2	L	243	THR	N-CA-C	5.00	125.01	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

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Mol	Chain	Res	Type	Group
1	A	282	ARG	Mainchain
1	A	319	SER	Mainchain
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	2726	233	5
1	F	2670	0	2721	265	36
1	K	2670	0	2728	189	5
2	B	2841	0	2890	200	15
2	C	2841	0	2888	199	36
2	D	2829	0	2878	253	5
2	G	2841	0	2887	251	5
2	H	2841	0	2889	234	13
2	I	2829	0	2880	280	7
2	L	2841	0	2888	258	7
2	M	2841	0	2886	284	1
2	N	2829	0	2876	318	3
3	E	2593	0	2598	129	14
3	J	2593	0	2598	138	21
3	O	2593	0	2598	181	1
All	All	41322	0	41931	2789	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 34.

All (2789) 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:SD	2:N:363:MET:CG	2.04	1.45
2:I:363:MET:SD	2:I:363:MET:CG	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
1:A:106:ASP:CG	1:F:225:LYS:HD3	1.28	1.32
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
2:G:20:GLY:C	2:G:178:LEU:CD2	2.04	1.28
1:A:74:PHE:HE1	1:F:203:GLU:OE1	1.15	1.27
2:M:10:TRP:CZ2	2:M:190:ILE:HG23	1.70	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:29:LEU:HD22	1:F:179:LEU:N	1.46	1.27
1:A:104:LEU:C	1:F:227:LYS:HZ3	1.42	1.26
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
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:L:265:MET:CE	2:M:294:MET:HE1	1.67	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
1:K:315:ASP:CB	1:K:315:ASP:CG	2.13	1.22
2:L:6:LEU:CD2	2:L:194:GLU:HG3	1.69	1.22
2:N:363:MET:SD	2:N:363:MET:CE	2.27	1.22
1:F:315:ASP:CB	1:F:315:ASP:CG	2.13	1.22
2:M:215:ARG:NH2	2:N:164:VAL:CG2	2.00	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
1:A:315:ASP:CG	1:A:315:ASP:CB	2.12	1.21
1:A:193:PRO:HB2	2:M:311:LEU:CD2	1.59	1.20
2:G:10:TRP:CZ3	2:G:190:ILE:HG23	1.74	1.20
1:F:29:LEU:CD1	1:F:179:LEU:HB2	1.69	1.20
2:L:180:VAL:HG21	2:L:304:ASN:CG	1.67	1.19
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
1:A:106:ASP:CG	1:F:225:LYS:CD	1.98	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:A:74:PHE:CE1	1:F:203:GLU:OE1	1.97	1.18
2:I:277:GLU:HB3	3:J:149:GLU:CB	1.73	1.17
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:20:GLY:C	2:G:178:LEU:HD21	1.70	1.14
1:K:333:HIS:CD2	2:L:297:LEU:CD2	2.30	1.14
2:M:351:MET:HE2	2:N:326:GLN:HE22	1.11	1.14
1:A:106:ASP:CB	1:F:225:LYS:HD3	1.68	1.14
1:A:193:PRO:CB	2:M:311:LEU:HD22	1.67	1.14
2:I:360:HIS:HB3	2:I:363:MET:CB	1.77	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: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:10:TRP:CZ3	2:G:190:ILE:HG12	1.84	1.12
2:G:354:LEU:CD1	2:H:294:MET:SD	2.38	1.12
2:I:277:GLU:CA	3:J:149:GLU:HG2	1.80	1.11
3:O:34:GLY:O	3:O:199:GLY:HA3	1.48	1.11
2:G:69:THR:HG22	2:G:71:THR:H	1.15	1.11
2:G:10:TRP:CH2	2:G:190:ILE:CG2	2.34	1.11
2:D:360:HIS:HB3	2:D:363:MET:HB2	1.11	1.11
2:G:20:GLY:HA3	2:G:178:LEU:HD22	1.30	1.10
1:A:334:LYS:HB2	2:B:297:LEU:HD21	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
2:M:341:TYR:HB2	2:N:333:LEU:HD11	1.20	1.10
2:N:277:GLU:HB3	3:O:149:GLU:CG	1.82	1.10
1:F:30:LEU:CD2	1:F:178:LEU:HD12	1.83	1.09
2:D:345:ARG:NE	3:E:150:ARG:HH21	1.21	1.09
2:L:238:SER:HB2	2:L:243:THR:C	1.51	1.09
2:G:19:VAL:HG22	2:G:186:GLN:CG	1.82	1.09
2:C:100:LYS:HG2	2:D:133:ARG:NE	1.45	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:H:86:ARG:HH21	2:I:138:ALA:HA	1.12	1.08
1:A:28:PRO:HB3	2:B:164:VAL:HG21	1.35	1.08
2:D:345:ARG:HE	3:E:150:ARG:NH2	1.31	1.08
1:F:270:ARG:NH1	2:N:316:LEU:HA	1.66	1.08
2:G:20:GLY:CA	2:G:178:LEU:HD22	1.82	1.08
2:C:100:LYS:CG	2:D:133:ARG:NE	2.11	1.08
1:A:104:LEU:C	1:F:227:LYS:NZ	2.11	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:L:265:MET:HE2	2:M:294:MET:HE1	1.09	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:B:6:LEU:CD2	2:B:194:GLU:CG	2.30	1.05
2:G:365:LEU:HD22	2:H:297:LEU:CD1	1.87	1.05
2:L:246:ASP:HB3	2:L:274:ARG:HD3	1.38	1.05
2:N:200:PRO:HB2	2:N:305:ASP:HB2	1.37	1.04
2:N:277:GLU:HB3	3:O:149:GLU:HG2	1.04	1.04
2:G:365:LEU:HD21	2:H:297:LEU:CD1	1.85	1.03
1:A:193:PRO:HB2	2:M:311:LEU:HD22	1.15	1.03
2:G:19:VAL:HG12	2:G:178:LEU:HD13	1.39	1.03
2:G:246:ASP:HB3	2:G:274:ARG:HD3	1.38	1.03
2:M:201:ARG:CB	2:M:305:ASP:OD2	2.05	1.03
2:B:246:ASP:HB3	2:B:274:ARG:HD3	1.37	1.03
2:I:360:HIS:ND1	2:I:363:MET:HE2	1.74	1.03
2:D:360:HIS:ND1	2:D:363:MET:HE2	1.74	1.03
2:I:345:ARG:HE	3:J:150:ARG:NH2	1.46	1.03
2:M:351:MET:HE2	2:N:326:GLN:NE2	1.71	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
2:L:238:SER:C	2:L:243:THR:OG1	1.84	1.02
2:N:360:HIS:ND1	2:N:363:MET:HE2	1.74	1.02
1:F:25:GLY:HA3	1:F:139:CYS:O	1.59	1.02
2:L:180:VAL:CG2	2:L:304:ASN:CG	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:98:ARG:HH12	2:C:137:ASN:CG	1.69	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
1:A:194:ASP:N	2:M:311:LEU:HD11	1.76	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
2:B:97:SER:CB	2:C:144:GLU:OE2	2.09	1.00
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
2:G:20:GLY:C	2:G:178:LEU:HD22	1.83	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:HD3	1:A:119:LYS:H	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:B:265:MET:HE2	2:C:294:MET:HE1	1.44	0.97
1:K:310:LEU:HD22	1:K:314:GLN:HE21	1.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:351:MET:HA	2:C:351:MET:HE3	1.46	0.97
1:F:119:LYS:HD3	1:F:119:LYS:H	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
2:D:357:LEU:HA	2:D:363:MET:SD	2.05	0.96
2:H:351:MET:HA	2:H:351:MET:HE3	1.46	0.96
1:K:333:HIS:HB2	2:L:297:LEU:HD21	1.45	0.96
2:L:18:VAL:HG22	2:L:25:LEU:HD11	1.47	0.96
2:N:73:CYS:SG	2:N:76:CYS:HB3	2.04	0.96
1:A:213:THR:H	1:A:216:HIS:HD2	1.13	0.96
1:F:270:ARG:HH12	2:N:316:LEU:HA	1.18	0.96
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: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
2:N:368:PRO:C	3:O:279:ASN:O	2.09	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:G:265:MET:HE2	2:H:294:MET:HE1	1.49	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
1:A:193:PRO:C	2:M:311:LEU:HD11	1.91	0.94
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:238:SER:HB3	2:L:244:LEU:H	1.33	0.93
2:L:265:MET:HE2	2:M:294:MET:CE	1.96	0.93
2:L:354:LEU:CD2	2:M:297:LEU:HD22	1.97	0.93
2:M:351:MET:HA	2:M:351:MET:HE3	1.46	0.93
1:F:29:LEU:HD13	1:F:179:LEU:CD1	1.98	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
2:G:94:ASP:H	2:G:100:LYS:HZ3	1.01	0.93
1:F:29:LEU:HD13	1:F:179:LEU:HB2	0.95	0.93
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
1:A:75:ALA:HB3	1:F:207:ASN:CG	1.95	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
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
2:I:277:GLU:CD	3:J:149:GLU:HG3	1.96	0.90
1:K:32:GLN:HE22	2:L:165:THR:CG2	1.84	0.90
2:G:176:LYS:O	2:G:178:LEU:N	2.04	0.90
2:N:355:ARG:HH21	3:O:332:PRO:HD3	1.35	0.90
1:A:75:ALA:HB2	1:F:207:ASN:HD22	1.36	0.90
1:A:105:HIS:HA	1:F:227:LYS:NZ	1.85	0.90
2:B:94:ASP:N	2:B:100:LYS:HZ3	1.69	0.90
2:L:94:ASP:C	2:L:100:LYS:HZ1	1.81	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:29:LEU:HD11	1:F:179:LEU:HD13	1.52	0.89
2:L:94:ASP:H	2:L:100:LYS:HZ3	1.10	0.89
1:A:105:HIS:CA	1:F:227:LYS:HZ2	1.85	0.89
1:A:338:ASP:OD2	2:B:326:GLN:OE1	1.91	0.89
2:I:357:LEU:O	2:I:363:MET:SD	2.31	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
1:F:30:LEU:HD21	1:F:178:LEU:HD12	0.92	0.88
2:G:94:ASP:C	2:G:100:LYS:HZ1	1.81	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:L:94:ASP:N	2:L:100:LYS:NZ	2.21	0.87
2:L:94:ASP:H	2:L:100:LYS:HZ1	1.21	0.87
2:L:362:ARG:HE	2:L:363:MET:HE2	1.39	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
2:G:362:ARG:HE	2:G:363:MET:HE2	1.39	0.87
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:B:94:ASP:C	2:B:100:LYS:HZ1	1.84	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: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: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
1:F:29:LEU:HD22	1:F:178:LEU:C	2.02	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N:356:ALA:O	2:N:363:MET:HE3	1.77	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
2:I:356:ALA:O	2:I:363:MET:HE3	1.77	0.84
1:K:55:ILE:HD13	1:K:97:LEU:HD11	1.59	0.84
2:B:362:ARG:HE	2:B:363:MET:HE2	1.39	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:G:20:GLY:CA	2:G:178:LEU:CD2	2.46	0.84
2:H:86:ARG:HH12	2:I:141:LYS:HZ1	1.21	0.84
1:A:193:PRO:HB3	2:M:311:LEU:HD21	1.30	0.84
2:H:86:ARG:NH1	2:I:141:LYS:HZ1	1.67	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:D:356:ALA:O	2:D:363:MET:HE3	1.77	0.83
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: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:I:345:ARG:HE	3:J:150:ARG:HH21	0.83	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:M:351:MET:HE1	2:N:326:GLN:HE22	1.42	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
1:F:270:ARG:HH11	2:N:316:LEU:HD23	1.02	0.82
2:L:3:TYR:O	2:L:4:GLN:HG3	1.79	0.82
2: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
1:F:283:ARG:NE	2:N:315:GLU:OE2	2.11	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:32:GLN:HE22	2:L:165:THR:HG23	1.43	0.81
1:K:172:TYR:OH	1:K:281:ASN:ND2	2.12	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:B:3:TYR:O	2:B:4:GLN:HG3	1.79	0.81
2:I:360:HIS:ND1	2:I:363:MET:CE	2.43	0.81
2:N:354:LEU:HD12	3:O:253:MET:HE2	1.61	0.81
2:N:360:HIS:ND1	2:N:363:MET:CE	2.44	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:HB3	2:D:363:MET:CG	2.10	0.81
2:D:360:HIS:ND1	2:D:363:MET:CE	2.44	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:M:351:MET:CE	2:N:326:GLN:NE2	2.35	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
2:I:277:GLU:HA	3:J:149:GLU:HG2	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	2:D:99:THR:HG22	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
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
2:C:359:PHE:CE2	2:D:323:THR:HG23	2.15	0.80
2:H:99:THR:O	2:H:99:THR:HG22	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
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: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
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: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
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:94:ASP:N	2:L:100:LYS:HZ1	1.79	0.79
2:L:99:THR:HG22	2:L:99:THR:O	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:99:THR:HG22	2:N:99:THR:O	1.81	0.79
2:N:360:HIS:CB	2:N:363:MET:CG	2.61	0.79
1:A:104:LEU:O	1:F:227:LYS:NZ	2.10	0.78
1:A:222:LEU:O	1:A:223:MET:HB2	1.83	0.78
2:H:271:ALA:CB	2:H:276:ILE:HD11	2.13	0.78
2:I:99:THR:HG22	2:I:99:THR:O	1.81	0.78
2:I:259:ALA:HB2	2:I:363:MET:CG	2.12	0.78
2:L:6:LEU:CD2	2:L:194:GLU:CG	2.44	0.78
1:F:244:VAL:HG22	1:F:312:LEU:HD21	1.64	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
2:C:271:ALA:CB	2:C:276:ILE:HD11	2.13	0.78
2:D:345:ARG:NE	3:E:150:ARG:NH2	1.90	0.78
2:D:363:MET:HB3	2:D:364:PRO:CD	2.14	0.78
2:B:6:LEU:HD21	2:B:194:GLU:CD	2.08	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:80:ARG:O	2:H:84:GLN:HG3	1.82	0.78
2:H:359:PHE:CE2	2:I:323:THR:HG23	2.18	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
1:A:75:ALA:CB	1:F:207:ASN:CG	2.56	0.78
2:B:99:THR:O	2:B:99:THR:HG22	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:94:ASP:C	2:H:100:LYS:HZ1	1.91	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:4:GLN:OE1	2:L:9:LYS:HD2	1.84	0.78
2:L:180:VAL:CG1	2:L:305:ASP:OD2	2.31	0.78
2:M:341:TYR:CB	2:N:333:LEU:HD13	2.14	0.78
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
1:F:270:ARG:NH2	2:N:316:LEU:HA	1.99	0.77
2:M:86:ARG:HH22	2:N:141:LYS:HE2	1.49	0.77
2:M:111:VAL:HG11	2:M:142:THR:HG21	1.66	0.77
1:A:75:ALA:HB2	1:F:207:ASN:ND2	1.95	0.77
2:B:365:LEU:HD22	2:C:297:LEU:CD1	2.14	0.77
2:C:111:VAL:HG11	2:C:142:THR:HG21	1.66	0.77
2:I:363:MET:HB3	2:I:364:PRO:CD	2.14	0.77
2:L:265:MET:HE1	2:M:294:MET:HE1	1.65	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: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:67:GLY:HA2	2:C:119:ARG:HH12	1.47	0.77
2:C:128:VAL:HG11	2:C:154:LEU:HD22	1.67	0.77
2: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
1:F:262:ARG:NH1	3:J:230:TYR:HB3	1.99	0.77
2:H:351:MET:HE2	2:I:326:GLN:HE22	1.49	0.77
1:A:336:LEU:HD12	2:B:326:GLN:NE2	2.00	0.77
2:C:3:TYR:CD2	2:C:3:TYR:O	2.38	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:97:SER:OG	2:C:100:LYS:HE3	1.83	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:M:201:ARG:HB2	2:M:305:ASP:CG	2.11	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:C:281:LEU:HD23	2:C:285:MET:HE2	1.68	0.76
2:N:6:LEU:O	2:N:218:LEU:HB3	1.85	0.76
2:I:345:ARG:CD	3:J:150:ARG:HH21	1.98	0.76
2:I:360:HIS:HB2	2:I:363:MET:SD	2.26	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
2:G:99:THR:O	2:G:99:THR:HG22	1.83	0.76
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:CD2	2:M:3:TYR:O	2.38	0.76
2:N:42:LEU:HB3	2:N:172:GLN:HB3	1.67	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:4:GLN:OE1	2:G:9:LYS:HD2	1.84	0.76
2:G:19:VAL:CG2	2:G:186:GLN:CG	2.50	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: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:H:281:LEU:HD23	2:H:285:MET:HE2	1.68	0.75
2:N:257:VAL:O	2:N:360:HIS:HE1	1.69	0.75
2:N:360:HIS:HB2	2:N:363:MET:SD	2.26	0.75
2: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:94:ASP:C	2:C:100:LYS:HZ1	1.95	0.75
2:D:5:VAL:HG13	2:D:222:ASP:CG	2.12	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:257:VAL:O	2:I:360:HIS:HE1	1.69	0.75
2:I:259:ALA:CB	2:I:363:MET:HG2	2.17	0.75
2: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
1:A:315:ASP:CG	1:A:315:ASP:CA	2.61	0.74
3:J:5:PRO:O	3:J:8:ARG:HG2	1.87	0.74
2:L:343:PRO:CA	2:M:283:VAL:HG13	2.17	0.74
2:M:128:VAL:HG11	2:M:154:LEU:HD22	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:82:LEU:HD21	1:K:100:LEU:HD12	1.70	0.74
2:N:357:LEU:CA	2:N:363:MET:SD	2.75	0.74
2:N:360:HIS:CG	2:N:363:MET:HG3	2.23	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:M:281:LEU:HD23	2:M:285:MET:HE2	1.68	0.73
2:C:3:TYR:O	2:C:4:GLN:HG3	1.88	0.73
2:C:156:THR:HG22	2:C:158:ASP:H	1.53	0.73
2: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: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
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:K:315:ASP:CG	1:K:315:ASP:CA	2.61	0.73
2:D:360:HIS:CG	2:D:363:MET:HG3	2.23	0.73
1:F:315:ASP:CG	1:F:315:ASP:CA	2.61	0.73
2:I:358:ALA:HA	2:I:364:PRO:HG2	1.71	0.73
2:L:6:LEU:HD21	2:L:194:GLU:CD	2.12	0.73
3:O:4:TYR:HD1	3:O:175:TRP:HH2	1.34	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
1:A:338:ASP:OD2	2:B:326:GLN:CD	2.32	0.73
2:H:10:TRP:CZ2	2:H:194:GLU:OE2	2.42	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
1:A:194:ASP:HA	2:M:311:LEU:CD1	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:360:HIS:CG	2:I:363:MET:HG3	2.23	0.72
2:L:180:VAL:HB	2:L:304:ASN:C	2.14	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
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:82:LEU:HD21	1:F:100:LEU:HD12	1.70	0.72
1:F:147:LEU:HB3	1:F:148:PRO:HD3	1.70	0.72
2:H:156:THR:HG22	2:H:158:ASP:H	1.54	0.72
2:G:94:ASP:H	2:G:100:LYS:HZ1	1.31	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
2:I:259:ALA:HB1	2:I:363:MET:HG2	1.72	0.72
2:I:277:GLU:HB3	3:J:149:GLU:HG2	0.74	0.71
2:C:215:ARG:NH2	2:D:164:VAL:HG22	2.05	0.71
2:I:5:VAL:HG13	2:I:222:ASP:CG	2.15	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
3:O:117:ALA:O	3:O:120:LEU:HD22	1.89	0.71
2:D:241:LEU:O	3:E:156:ARG:NH1	2.22	0.71
2:D:345:ARG:CD	3:E:150:ARG:HH21	2.02	0.71
2:M:351:MET:HE2	2:N:326:GLN:CD	2.14	0.71
2:N:345:ARG:HH21	3:O:150:ARG:NH2	1.87	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
2:H:351:MET:HE2	2:I:326:GLN:NE2	2.05	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:29:LEU:HD21	1:A:154:ARG:HH12	1.56	0.71
1:A:213:THR:H	1:A:216:HIS:CD2	2.04	0.71
2:B:98:ARG:NH1	2:C:137:ASN:OD1	2.24	0.71
2:C:351:MET:HE2	2:D:326:GLN:HE22	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:283:ARG:CZ	2:N:315:GLU:OE2	2.14	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:94:ASP:N	2:G:100:LYS:HZ3	1.81	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
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
2:C:360:HIS:HB3	2:C:363:MET:O	1.91	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
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:73:CYS:O	2:H:79:CYS:SG	2.50	0.70
2:H:360:HIS:HB3	2:H:363:MET:O	1.91	0.70
1:K:313:LYS:O	1:K:316:TYR:CZ	2.44	0.70
2:B:6:LEU:CD1	2:B:190:ILE:HG21	1.92	0.69
2:C:67:GLY:HA2	2:C:119:ARG:NH1	2.07	0.69
2:C:341:TYR:CE2	2:D:337:LYS:HB2	2.26	0.69
1:F:306:THR:OG1	3:J:310:LEU:HD22	1.92	0.69
1:F:313:LYS:O	1:F:316:TYR:CZ	2.44	0.69
2:M:306:MET:HE1	2:M:313:MET:HE2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:194:ASP:HA	2:M:311:LEU:HD11	1.72	0.69
1:A:222:LEU:HD12	1:A:285:MET:HG2	1.74	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:H:306:MET:HE1	2:H:313:MET:HE2	1.75	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
3:E:32:LEU:HD11	3:E:195:ALA:O	1.91	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:C:94:ASP:O	2:C:100:LYS:NZ	2.25	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:222:LEU:HD12	1:F:285:MET:HG2	1.74	0.69
1:F:308:THR:HG23	1:F:320:VAL:HG13	1.75	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:M:94:ASP:O	2:M:100:LYS:NZ	2.25	0.69
2:N:271:ALA:HB1	2:N:276:ILE:HD12	1.75	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: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:222:LEU:HD11	1:A:285:MET:HE3	1.74	0.68
1:A:308:THR:HG23	1:A:320:VAL:HG13	1.75	0.68
2:I:220:LEU:HD21	3:J:154:THR:HA	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:111:VAL:HG12	3:J:140:TRP:HB2	1.75	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
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
2:N:259:ALA:CB	2:N:363:MET:CG	2.72	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
1:A:133:ARG:HG3	2:G:299:PRO:HG2	1.75	0.68
2:B:6:LEU:CD2	2:B:194:GLU:CD	2.66	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
2:C:93:ILE:HG23	2:D:133:ARG:NH2	2.08	0.68
2:C:306:MET:HE1	2:C:313:MET:HE2	1.75	0.68
3:E:111:VAL:HG12	3:E:140:TRP:HB2	1.75	0.68
2:G:110:ASN:HB3	2:G:113:TYR:HD1	1.58	0.68
2: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
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
1:F:222:LEU:HD11	1:F:285:MET:HE3	1.74	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
1:F:281:ASN:C	1:F:283:ARG:H	2.02	0.68
2:G:93:ILE:HG23	2:G:100:LYS:NZ	2.09	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
2:D:93:ILE:HG22	2:D:100:LYS:HZ3	1.58	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
1:K:281:ASN:C	1:K:283:ARG:H	2.02	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:I:345:ARG:HH12	3:J:150:ARG:CG	2.07	0.68
3:J:74:PRO:HB3	3:J:105:ARG:HD2	1.76	0.68
1:K:333:HIS:CG	2:L:297:LEU:CG	2.76	0.68
2:L:93:ILE:HG23	2:L:100:LYS:NZ	2.09	0.68
2: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
2:G:265:MET:CE	2:H:294:MET:HE1	2.22	0.67
3:O:31:ALA:HB2	3:O:164:LEU:HB3	1.76	0.67
1:F:283:ARG:NH2	2:N:315:GLU:OE1	2.26	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
2:N:260:ASN:O	2:N:262:GLU:N	2.27	0.67
2:N:345:ARG:HH21	3:O:150:ARG:CZ	2.05	0.67
1:A:281:ASN:C	1:A:283:ARG:H	2.02	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:32:GLN:NE2	2:L:165:THR:HA	2.08	0.67
1:K:213:THR:H	1:K:216:HIS:CD2	2.04	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:B:98:ARG:NH1	2:C:137:ASN:CB	2.51	0.67
2:N:73:CYS:O	2:N:79:CYS:SG	2.48	0.67
2: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:O	2:G:73:CYS:SG	2.53	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:222:LEU:HD11	1:K:285:MET:HE3	1.74	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:M:97:SER:HG	2:M:100:LYS:HE3	1.59	0.66
2:B:97:SER:HB2	2:C:144:GLU:CD	2.21	0.66
2:C:256:MET:HE2	2:C:353:LEU:HD21	1.77	0.66
2:D:277:GLU:CD	3:E:149:GLU:HG3	2.20	0.66
2:L:73:CYS:O	2:L:73:CYS:SG	2.53	0.66
2:L:351:MET:HG2	2:M:290:HIS:ND1	2.10	0.66
2:M:181:GLU:HG2	2:M:184:ARG:HD2	1.77	0.66
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:G:93:ILE:HG23	2:G:100:LYS:HZ2	1.61	0.66
2:I:73:CYS:O	2:I:79:CYS:SG	2.48	0.66
2:I:259:ALA:CB	2:I:363:MET:CG	2.72	0.66
2:D:73:CYS:O	2:D:79:CYS:SG	2.48	0.66
2:D:93:ILE:HG22	2:D:100:LYS:NZ	2.10	0.66
2:D:347:MET:O	2:D:351:MET:HG2	1.96	0.66
2:B:94:ASP:H	2:B:100:LYS:HZ1	1.43	0.66
2:H:351:MET:HE1	2:I:326:GLN:HE22	1.61	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:C:344:ASP:HB3	2:C:347:MET:HE3	1.79	0.65
1:A:105:HIS:CA	1:F:227:LYS:HD2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:L:94:ASP:N	2:L:100:LYS:HZ3	1.90	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:H:344:ASP:HB3	2:H:347:MET:HE3	1.78	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
1:A:161:GLU:CD	2:M:318:ARG:CD	2.67	0.65
2:I:345:ARG:NH1	3:J:150:ARG:HG3	2.11	0.65
2:I:355:ARG:NH1	3:J:287:GLN:HB3	2.11	0.65
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:H:256:MET:HE2	2:H:353:LEU:HD21	1.77	0.65
2:M:256:MET:HE2	2:M:353:LEU:HD21	1.77	0.65
2:N:345:ARG:CZ	3:O:150:ARG:NH2	2.60	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
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:48:GLU:HG3	1:F:49:GLU:N	2.12	0.65
1:F:274:ASP:HA	1:F:279:TRP:CE3	2.32	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:93:ILE:HG22	2:N:100:LYS:HZ3	1.62	0.65
3:O:149:GLU:C	3:O:151:LEU:H	2.05	0.65
3:J:149:GLU:C	3:J:151:LEU:H	2.05	0.64
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
3:E:149:GLU:C	3:E:151:LEU:H	2.05	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:H:256:MET:HE1	2:H:332:LEU:HD11	1.80	0.64
2:N:360:HIS:CG	2:N:363:MET:CG	2.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:M:256:MET:HE1	2:M:332:LEU:HD11	1.79	0.64
1:A:274:ASP:HA	1:A:279:TRP:CE3	2.32	0.64
2:I:238:SER:CB	2:I:243:THR:HB	2.25	0.64
2:I:356:ALA:O	2:I:363:MET:CE	2.45	0.64
1:F:270:ARG:HE	2:N:319:THR:CG2	1.95	0.64
1:F:273:PHE:HB3	1:F:279:TRP:CG	2.33	0.64
2:G:354:LEU:HD21	2:H:297:LEU:HD22	1.76	0.64
2:M:73:CYS:O	2:M:73:CYS:SG	2.56	0.64
2:M:343:PRO:HG2	2:M:347:MET:SD	2.37	0.64
2:C:97:SER:HG	2:C:100:LYS:HE3	1.63	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:6:LEU:HG	2:M:222:ASP:OD1	1.97	0.64
2:M:10:TRP:CE2	2:M:190:ILE:CG2	2.78	0.64
2:N:337:LYS:HG3	2:N:338:GLU:N	2.12	0.64
3:O:4:TYR:CD1	3:O:175:TRP:HH2	2.11	0.64
2:C:73:CYS:O	2:C:73:CYS:SG	2.55	0.64
3:E:147:GLU:HG2	3:E:147:GLU:O	1.98	0.64
3:J:147:GLU:HG2	3:J:147:GLU:O	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
2:B:354:LEU:HD21	2:C:297:LEU:HD22	1.80	0.64
2:C:256:MET:HE1	2:C:332:LEU:HD11	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
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:94:ASP:C	2:M:100:LYS:HZ1	2.06	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:215:ARG:NE	2:N:164:VAL:CG1	2.61	0.63
1:A:119:LYS:H	1:A:119:LYS:CD	2.04	0.63
2:H:73:CYS:O	2:H:73:CYS:SG	2.56	0.63
2:M:344:ASP:HB3	2:M:347:MET:HE3	1.78	0.63
2:N:309:ILE:HG21	2:N:313:MET:HG2	1.77	0.63
3:O:329:LEU:HD23	3:O:329:LEU:H	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
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:HD12	3:J:161:LEU:H	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
2:N:366:PRO:HB2	3:O:282:SER:CB	2.29	0.63
3:O:161:LEU:H	3:O:161:LEU:HD12	1.64	0.63
2:D:337:LYS:HG3	2:D:338:GLU:N	2.12	0.63
1:F:29:LEU:CD2	1:F:178:LEU:C	2.71	0.63
2:I:345:ARG:HH12	3:J:150:ARG:HG3	1.62	0.63
3:O:147:GLU:HG2	3:O:147:GLU:O	1.98	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
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: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:73:HIS:HD2	3:O:75:ASP:H	1.45	0.63
3:O:129:LEU:HD11	3:O:158:ARG:HH11	1.64	0.63
1:A:193:PRO:C	2:M:311:LEU:HD21	2.23	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:329:LEU:HD13	2:B:294:MET:HE1	1.82	0.62
2:G:94:ASP:N	2:G:100:LYS:HZ1	1.89	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:HD23	3:J:329:LEU:H	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: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:C:256:MET:HE2	2:C:353:LEU:CD2	2.29	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:281:ASN:C	1:K:283:ARG:N	2.57	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:L:180:VAL:HG23	2:L:304:ASN:ND2	2.14	0.61
3:E:73:HIS:CD2	3:E:75:ASP:H	2.18	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:B:281:LEU:HG	2:B:285:MET:HE2	1.81	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
1:F:281:ASN:C	1:F:283:ARG:N	2.57	0.61
2:H:256:MET:HE2	2:H:353:LEU:CD2	2.29	0.61
2:I:98:ARG:NH2	3:J:91:ASP:OD1	2.33	0.61
2:L:281:LEU:HG	2:L:285:MET:HE2	1.81	0.61
2:M:256:MET:HE2	2:M:353:LEU:CD2	2.29	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
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:G:281:LEU:HG	2:G:285:MET:HE2	1.81	0.61
2:H:250:LEU:HD22	2:H:309:ILE:HD12	1.82	0.61
2:L:223:GLN:OE1	2:M:171:LEU:HD12	2.01	0.61
2: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:10:TRP:CH2	2:L:193:GLU:CD	2.79	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
3:O:6:TRP:HZ3	3:O:175:TRP:CE2	2.17	0.60
3:O:117:ALA:HB2	3:O:143:LEU:HD12	1.83	0.60
1:A:281:ASN:C	1:A:283:ARG:N	2.57	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
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
2:L:6:LEU:CD2	2:L:194:GLU:CD	2.74	0.60
2:M:292:ILE:O	2:M:296:GLN:HG3	2.02	0.60
2:M:341:TYR:CE2	2:N:337:LYS:CB	2.84	0.60
2:M:362:ARG:O	2:M:363:MET:HG3	2.02	0.60
2:B:343:PRO:HG2	2:B:347:MET:SD	2.42	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:354:LEU:CD1	3:O:253:MET:HE2	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:363:MET:CG	2:N:364:PRO:HD2	2.31	0.60
1:A:262:ARG:NH2	3:E:320:GLU:OE1	2.35	0.59
2:C:354:LEU:HD11	2:D:294:MET:SD	2.42	0.59
2:H:84:GLN:CB	2:I:144:GLU:OE1	2.50	0.59
2:H:88:VAL:HG11	2:H:116:ALA:HB3	1.83	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
1:A:255:LEU:HD22	3:E:313:THR:HG21	1.84	0.59
3:E:303:VAL:HB	3:E:306:ILE:HD11	1.83	0.59
3:J:303:VAL:HB	3:J:306:ILE:HD11	1.83	0.59
1:K:10:ARG:HH12	1:K:40:GLN:NE2	2.00	0.59
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
2:D:265:MET:HE1	2:D:350:GLU:HB3	1.85	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:47:ARG:HG3	2:B:47:ARG:O	2.03	0.59
2:B:284:GLU:O	2:B:288:LEU:HG	2.02	0.59
2:C:292:ILE:O	2:C:296:GLN:HG3	2.02	0.59
2:D:140:LEU:HD21	2:D:166:ILE:HG12	1.83	0.59
2:I:47:ARG:CZ	3:J:126:ASN:OD1	2.51	0.59
2:I:265:MET:HE1	2:I:350:GLU:HB3	1.85	0.59
2:N:265:MET:HE1	2:N:350:GLU:HB3	1.85	0.59
2:G:20:GLY:O	2:G:178:LEU:HD22	1.86	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:259:ALA:HB3	2:G:363:MET:CE	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:93:ILE:HG23	2:L:100:LYS:HZ2	1.68	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: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:61:GLY:HA2	2:B:72:PRO:HG3	1.86	0.58
2:B:282:LEU:CD2	2:B:332:LEU:HD12	2.34	0.58
2:C:56:ARG:NH2	2:D:165:THR:HG21	2.18	0.58
2:C:152:PHE:O	2:C:153:LEU:HD23	2.03	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:259:ALA:HB3	2:L:363:MET:CE	2.33	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:H:97:SER:HG	2:H:100:LYS:HE3	1.66	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
3:J:308:ARG:O	3:J:312:ILE:HG13	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:222:LEU:HD12	1:F:285:MET:SD	2.44	0.58
1:F:273:PHE:CE1	1:F:283:ARG:HG3	2.39	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:94:ASP:O	2:I:100:LYS:HE2	2.03	0.58
2:I:184:ARG:HH22	2:I:304:ASN:ND2	2.02	0.58
3:J:46:ARG:CZ	3:J:68:MET:HG3	2.33	0.58
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
2:M:257:VAL:HG11	2:M:320:ILE:CD1	2.34	0.58
1:A:75:ALA:HB2	1:F:207:ASN:CB	2.34	0.58
1:A:273:PHE:CE1	1:A:283:ARG:HG3	2.39	0.58
2:C:94:ASP:C	2:C:100:LYS:NZ	2.62	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:58:LEU:HD23	2:N:153:LEU:HD22	1.86	0.58
2:N:229:ASP:O	2:N:231:GLN:N	2.33	0.58
3:O:308:ARG:O	3:O:312:ILE:HG13	2.04	0.58
1:A:161:GLU:CD	2:M:318:ARG:HD3	2.22	0.58
1:A:279:TRP:CG	1:A:279:TRP:O	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
2:B:306:MET:HE1	2:B:313:MET:HE2	1.86	0.57
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
1:A:105:HIS:HA	1:F:227:LYS:CD	2.33	0.57
2:D:47:ARG:NE	3:E:126:ASN:OD1	2.37	0.57
1:F:279:TRP:CG	1:F:279:TRP:O	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
2:B:246:ASP:HB3	2:B:274:ARG:CD	2.24	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:ALA:HB3	2:B:363:MET:HE3	1.87	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:47:ARG:HG3	2:G:47:ARG:O	2.03	0.57
2:G:61:GLY:HA2	2:G:72:PRO:HG3	1.85	0.57
2:G:246:ASP:CB	2:G:274:ARG:HD3	2.24	0.57
2:H:341:TYR:CB	2:I:333:LEU:HD13	2.35	0.57
1:K:279:TRP:CG	1:K:279:TRP:O	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:M:94:ASP:C	2:M:100:LYS:NZ	2.62	0.57
2:D:58:LEU:HD23	2:D:153:LEU:HD22	1.86	0.57
1:F:270:ARG:HH22	2:N:316:LEU:CA	2.17	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
2:L:306:MET:HE1	2:L:313:MET:HE2	1.86	0.57
1:A:222:LEU:HD12	1:A:285:MET:SD	2.44	0.57
1:A:222:LEU:HD12	1:A:285:MET:CG	2.33	0.57
3:J:8:ARG:HG3	3:J:9:PRO:CD	2.33	0.57
2: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
2:D:186:GLN:HG2	2:D:214:LEU:HD21	1.86	0.57
1:F:270:ARG:NE	2:N:319:THR:HG21	2.20	0.57
2:M:3:TYR:O	2:M:3:TYR:HD2	1.86	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:259:ALA:HB3	2:L:363:MET:HE3	1.87	0.56
2:M:84:GLN:CA	2:N:144:GLU:OE1	2.53	0.56
2:N:128:VAL:HG11	2:N:154:LEU:HD22	1.87	0.56
2:C:291:ARG:HH11	2:C:306:MET:HG3	1.69	0.56
2:D:95:ALA:HA	2:D:100:LYS:HZ1	1.71	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
2:G:306:MET:HE1	2:G:313:MET:HE2	1.86	0.56
1:A:191:LEU:CD2	2:B:23:HIS:ND1	2.67	0.56
2:D:357:LEU:C	2:D:363:MET:SD	2.88	0.56
3:E:280:HIS:O	3:E:281:LEU:HD23	2.05	0.56
1:F:170:LEU:O	1:F:173:CYS:O	2.23	0.56
1:F:270:ARG:NE	2:N:319:THR:CG2	2.68	0.56
2:I:363:MET:CB	2:I:364:PRO:CD	2.78	0.56
1:K:170:LEU:O	1:K:173:CYS:O	2.23	0.56
2:L:328:TYR:OH	2:L:361:PRO:HD2	2.05	0.56
2:M:3:TYR:O	2:M:4:GLN:CG	2.53	0.56
2:N:186:GLN:HG2	2:N:214:LEU:HD21	1.86	0.56
2:N:367:GLU:HB3	2:N:368:PRO:HD2	1.86	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
2:I:357:LEU:C	2:I:363:MET:SD	2.88	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:8:ARG:HG3	3:O:9:PRO:CD	2.33	0.56
3:O:201:ALA:O	3:O:204:LEU:HB2	2.06	0.56
2:B:328:TYR:OH	2:B:361:PRO:HD2	2.05	0.56
2:G:259:ALA:HB3	2:G:363:MET:HE3	1.87	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
2:N:357:LEU:C	2:N:363:MET:SD	2.88	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:8:ARG:HG3	3:E:9:PRO:CD	2.33	0.56
3:E:201:ALA:O	3:E:204:LEU:HB2	2.06	0.56
2:G:341:TYR:O	2:H:336:ARG:NH1	2.35	0.56
2:H:40:ALA:HB1	2:H:170:CYS:SG	2.46	0.56
1:K:262:ARG:NH1	3:O:230:TYR:HB3	2.21	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:L:180:VAL:HG21	2:L:304:ASN:OD1	2.03	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
1:K:255:LEU:CD1	3:O:309:GLU:HG2	2.36	0.56
2:N:259:ALA:HB2	2:N:363:MET:SD	2.46	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:93:ILE:CG2	2:G:100:LYS:HZ2	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:L:94:ASP:CA	2:L:100:LYS:HZ1	2.19	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
2:G:351:MET:HE2	2:H:290:HIS:HA	1.88	0.55
2:H:281:LEU:CD2	2:H:285:MET:HE2	2.36	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:C:351:MET:HA	2:C:351:MET:CE	2.30	0.55
2:H:156:THR:HG22	2:H:158:ASP:N	2.21	0.55
2:I:360:HIS:CG	2:I:363:MET:CE	2.90	0.55
2:L:3:TYR:O	2:L:3:TYR:CD2	2.60	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:5:VAL:CG1	2:D:222:ASP:CG	2.80	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:11:ARG:HD3	2:B:83:GLU:OE2	2.06	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: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
2:C:351:MET:HE2	2:D:326:GLN:NE2	2.21	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:194:GLU:OE1	2:D:194:GLU:HA	2.05	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
2:I:5:VAL:CG1	2:I:222:ASP:CG	2.80	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:L:366:PRO:C	2:L:367:GLU:HG3	2.32	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:3:TYR:O	2:B:3:TYR:CD2	2.60	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:VAL:HG22	2:B:301:ALA:HB3	1.88	0.54
2:B:366:PRO:C	2:B:367:GLU:HG3	2.32	0.54
2:C:97:SER:OG	2:C:100:LYS:CE	2.55	0.54
1:K:262:ARG:NH2	3:O:230:TYR:CB	2.70	0.54
1:K:313:LYS:O	1:K:316:TYR:CE2	2.60	0.54
2:H:94:ASP:C	2:H:100:LYS:NZ	2.62	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:B:265:MET:CE	2:C:294:MET:HE1	2.30	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:11:ARG:HD3	2:L:83:GLU:OE2	2.07	0.54
2:L:309:ILE:HG22	2:L:313:MET:HG2	1.88	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
3:O:34:GLY:C	3:O:199:GLY:HA3	2.30	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:48:GLU:HG3	1:A:49:GLU:H	1.72	0.54
1:A:271:ALA:O	1:A:275:LYS:HG2	2.07	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
2:G:366:PRO:C	2:G:367:GLU:HG3	2.32	0.54
1:K:218:VAL:HA	1:K:221:LEU:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:334:LYS:C	2:G:297:LEU:CD2	2.81	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
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
1:F:270:ARG:HH22	2:N:316:LEU:C	2.17	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:259:ALA:HB2	2:I:363:MET:HG3	1.89	0.53
2:I:302:LEU:HD22	2:I:306:MET:HG2	1.91	0.53
1:K:271:ALA:O	1:K:275:LYS:HG2	2.07	0.53
3:O:4:TYR:HB3	3:O:5:PRO:HD2	1.89	0.53
3:O:5:PRO:HD2	3:O:175:TRP:CZ3	2.43	0.53
1:F:262:ARG:HH12	3:J:230:TYR:HB3	1.70	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
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
1:F:270:ARG:NH2	2:N:315:GLU:O	2.41	0.53
2:I:334:ILE:HG12	3:J:334:LEU:OXT	2.09	0.53
3:J:4:TYR:HB3	3:J:5:PRO:HD2	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:N:357:LEU:HA	2:N:363:MET:HE1	1.91	0.53
3:O:238:HIS:ND1	3:O:239:GLU:N	2.56	0.53
1:A:311:THR:HG23	1:A:318:GLN:CD	2.34	0.53
2:B:259:ALA:CB	2:B:363:MET:HE3	2.39	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
2:N:241:LEU:HD22	3:O:153:ALA:HB1	1.89	0.53
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
1:K:311:THR:HG23	1:K:318:GLN:CD	2.34	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
2:M:281:LEU:CD2	2:M:285:MET:HE2	2.36	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
1:F:311:THR:HG23	1:F:318:GLN:CD	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:B:98:ARG:NH1	2:C:137:ASN:CG	2.51	0.52
2:C:93:ILE:HG23	2:D:133:ARG:HH12	1.73	0.52
2:C:281:LEU:HD23	2:C:285:MET:CE	2.36	0.52
2:D:360:HIS:HB2	2:D:363:MET:CE	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:360:HIS:CG	2:D:363:MET:SD	3.03	0.52
2:M:10:TRP:CH2	2:M:190:ILE:HG23	2.37	0.52
2:M:100:LYS:CB	2:N:133:ARG:NE	2.43	0.52
2:M:156:THR:HG22	2:M:158:ASP:N	2.21	0.52
2:M:360:HIS:HD2	2:M:363:MET:H	1.57	0.52
2:N: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:L:259:ALA:CB	2:L:363:MET:HE3	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
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:95:ALA:HA	2:N:100:LYS:HZ1	1.74	0.52
2:N:240:MET:SD	3:O:157:SER:HB2	2.50	0.52
2:N:250:LEU:HD23	2:N:312:ARG:HH11	1.75	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:10:ARG:HH22	1:K:40:GLN:NE2	2.08	0.52
1:K:25:GLY:O	1:K:115:ASN:HA	2.08	0.52
2:L:93:ILE:HG22	2:L:100:LYS:NZ	2.25	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
2:C:281:LEU:CD2	2:C:285:MET:HE2	2.37	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
2:G:259:ALA:CB	2:G:363:MET:HE3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:268:VAL:O	3:J:271:PRO:HD3	2.09	0.52
2:M:341:TYR:CB	2:N:333:LEU:HD11	2.11	0.52
2:M:351:MET:HE2	2:N:326:GLN:OE1	2.09	0.52
2:N:302:LEU:HD22	2:N:306:MET:HG2	1.90	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
1:F:10:ARG:HH22	1:F:40:GLN:NE2	2.08	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: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:G:20:GLY:HA3	2:G:182:GLN:CD	2.36	0.51
2:H:89:ASP:HB3	2:H:121:LYS:HA	1.92	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
2:M:241:LEU:C	2:M:243:THR:N	2.68	0.51
3:O:27:LEU:O	3:O:143:LEU:N	2.39	0.51
3:O:68:MET:HA	3:O:68:MET:HE3	1.91	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:27:ASP:HB3	1:F:30:LEU:HB2	1.93	0.51
1:F:218:VAL:HG11	1:F:253:GLU:HG3	1.91	0.51
2:N:352:THR:O	2:N:355:ARG:HB3	2.10	0.51
3:O:151:LEU:HD21	3:O:155:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:357:LEU:HA	2:I:363:MET:HE1	1.91	0.51
3:J:68:MET:HA	3:J:68:MET:HE3	1.92	0.51
1:K:315:ASP:HB2	1:K:318:GLN:CD	2.36	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:315:ASP:HB2	1:A:318:GLN:CD	2.36	0.51
1:A:333:HIS:CE1	2:B:298:SER:OG	2.64	0.51
2:G:343:PRO:CG	2:G:347:MET:SD	2.99	0.51
2:H:11:ARG:HH22	2:I:165:THR:HG22	1.74	0.51
2:H:86:ARG:NE	2:I:141:LYS:HB2	2.26	0.51
2:L:347:MET:SD	2:M:290:HIS:CD2	3.03	0.51
2: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: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
1:F:262:ARG:CZ	3:J:230:TYR:HB3	2.40	0.51
3:J:151:LEU:HD21	3:J:155:LEU:HD12	1.92	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:89:ASP:HB3	2:M:121:LYS:HA	1.92	0.51
2:M:278:TRP:HB3	2:M:349:VAL:HG21	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:357:LEU:HA	2:D:363:MET:HE1	1.91	0.51
3:E:68:MET:HA	3:E:68:MET:HE3	1.92	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: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
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
3:O:139:THR:HG22	3:O:140:TRP:N	2.26	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:204:GLN:HE21	2:L:305:ASP:CG	2.18	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
3:E:151:LEU:HD21	3:E:155:LEU:HD12	1.93	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:L:93:ILE:CG2	2:L:100:LYS:HZ2	2.22	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:6:LEU:CD2	2:B:194:GLU:OE2	2.59	0.50
2:B:347:MET:HG3	2:C:290:HIS:CD2	2.46	0.50
2:C:213:SER:OG	2:C:216:ASP:HB2	2.11	0.50
2:G:69:THR:HG22	2:G:71:THR:N	2.01	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:92:GLU:HG2	2:H:124:LEU:HD23	1.94	0.50
2:H:360:HIS:CD2	2:H:362:ARG:H	2.30	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:93:ILE:CG2	2:C:100:LYS:HZ2	2.21	0.50
2:C:102:GLU:HB3	2:C:106:ASP:CB	2.41	0.50
2:D:60:LYS:HE3	2:D:79:CYS:HB3	1.93	0.50
2:D:302:LEU:HD11	2:D:313:MET:HB2	1.94	0.50
1:F:20:ALA:O	1:F:134:SER:HB2	2.12	0.50
1:F:315:ASP:HB2	1:F:318:GLN:CD	2.36	0.50
2:I:184:ARG:HH22	2:I:304:ASN:HD22	1.59	0.50
2:L:19:VAL:HG21	2:L:186:GLN:CD	2.37	0.50
2:M:351:MET:CE	2:M:351:MET:HA	2.30	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:49:VAL:HG12	2:G:50:GLY:N	2.27	0.50
2:G:303:GLY:HA3	2:G:306:MET:HG2	1.93	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
2:B:243:THR:HG22	2:B:244:LEU:N	2.26	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:THR:OG1	3:E:310:LEU:HD22	2.12	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
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:D:200:PRO:HD2	2:D:305:ASP:CG	2.37	0.49
1:F:222:LEU:CD1	1:F:285:MET:HE3	2.42	0.49
2:G:82:ILE:HG23	2:G:90:LEU:CD2	2.42	0.49
2:I:47:ARG:NE	3:J:126:ASN:OD1	2.45	0.49
3:J:46:ARG:NH1	3:J:68:MET:HG3	2.27	0.49
3:J:145:THR:HG22	3:J:147:GLU:N	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
3:O:41:ILE:HG21	3:O:113:TRP:CG	2.47	0.49
2:C:44:SER:HB2	2:C:159:PRO:HG3	1.94	0.49
2:C:92:GLU:HG2	2:C:124:LEU:HD23	1.94	0.49
2:G:94:ASP:CA	2:G:100:LYS:HZ1	2.25	0.49
2:H:271:ALA:HB1	2:H:276:ILE:CD1	2.36	0.49
2:H:351:MET:HA	2:H:351:MET:CE	2.30	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:G:69:THR:HG22	2:G:70:ALA:N	2.28	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
3:O:100:LEU:HD13	3:O:139:THR:HG21	1.93	0.49
2:C:341:TYR:CB	2:D:333:LEU:HD13	2.41	0.49
2:D:140:LEU:HD22	2:D:169:ARG:CZ	2.43	0.49
2:D:355:ARG:HH12	3:E:287:GLN:HB3	1.74	0.49
2:G:99:THR:O	2:G:99:THR:CG2	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:F:234:GLN:CD	2:G:304:ASN:ND2	2.70	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:119:LYS:H	1:K:119:LYS:CD	2.05	0.49
1:K:222:LEU:CD1	1:K:285:MET:HE3	2.42	0.49
2:L:49:VAL:HG12	2:L:50:GLY:N	2.27	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:257:VAL:HG11	2:N:320:ILE:HD13	1.95	0.49
2:N:276:ILE:HG22	2:N:277:GLU:N	2.28	0.49
1:A:172:TYR:O	1:A:216:HIS:HE1	1.96	0.49
2:D:200:PRO:HB2	2:D:305:ASP:N	2.28	0.49
2:D:277:GLU:HA	3:E:149:GLU:CG	2.42	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
3:J:312:ILE:O	3:J:316:LEU:HG	2.13	0.49
2:N:52:THR:O	2:N:55:ALA:HB3	2.13	0.49
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
3:E:149:GLU:C	3:E:151:LEU:N	2.71	0.49
1:F:48:GLU:CG	1:F:49:GLU:N	2.76	0.49
2:G:362:ARG:NE	2:G:363:MET:HE2	2.19	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
1:F:234:GLN:CD	2:G:304:ASN:HD22	2.14	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:B:307:ALA:HA	2:B:310:GLU:CD	2.38	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:274:ASP:HA	1:F:279:TRP:CZ3	2.47	0.49
2:G:307:ALA:HA	2:G:310:GLU:CD	2.38	0.49
2:I:140:LEU:HD22	2:I:169:ARG:CZ	2.43	0.49
3:J:149:GLU:C	3:J:151:LEU:N	2.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:THR:HG22	2:B:70:ALA:N	2.28	0.48
2:B:362:ARG:NE	2:B:363:MET:HE2	2.19	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:10:TRP:HZ2	2:G:194:GLU:CD	2.21	0.48
2:G:12:PRO:CD	2:G:215:ARG:NH1	2.70	0.48
3:J:85:LYS:NZ	3:J:85:LYS:HB3	2.28	0.48
2:L:82:ILE:HG23	2:L:90:LEU:CD2	2.42	0.48
2:L:201:ARG:O	2:L:205:LEU:HG	2.11	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:HA	1:F:183:GLN:HE21	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:L:362:ARG:NE	2:L:363:MET:HE2	2.19	0.48
2:M:56:ARG:NH2	2:N:165:THR:HG21	2.27	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
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:52:THR:O	2:D:55:ALA:HB3	2.13	0.48
2:D:302:LEU:HD11	2:D:313:MET:CB	2.44	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
2:I:337:LYS:HD3	3:J:334:LEU:HB2	1.96	0.48
3:J:27:LEU:O	3:J:143:LEU:N	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:307:ALA:HA	2:L:310:GLU:CD	2.38	0.48
3:O:85:LYS:HB3	3:O:85:LYS:NZ	2.28	0.48
2:D:260:ASN:O	2:D:260:ASN:OD1	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:L:204:GLN:NE2	2:L:305:ASP:CG	2.67	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:66:THR:O	2:C:66:THR:HG22	2.14	0.48
2:C:341:TYR:CE2	2:D:337:LYS:CB	2.96	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
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:I:229:ASP:C	2:I:231:GLN:N	2.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:286:LEU:HD11	2:B:333:LEU:HA	1.96	0.47
2:H:351:MET:HE2	2:I:326:GLN:CD	2.38	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:M:362:ARG:C	2:M:363:MET:HG3	2.39	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:HB2	2:D:51:LYS:HE3	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
2:L:244:LEU:HD23	2:L:244:LEU:HA	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:74:PHE:CZ	1:F:203:GLU:OE1	2.62	0.47
1:A:221:LEU:HD23	1:A:221:LEU:HA	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
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:66:THR:O	2:H:66:THR:HG22	2.14	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:I:10:TRP:CE2	2:I:190:ILE:HG23	2.49	0.47
2:N:260:ASN:O	2:N:260:ASN:OD1	2.32	0.47
1:A:105:HIS:CB	1:F:227:LYS:CD	2.66	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:98:LEU:O	1:F:101:THR:HG22	2.14	0.47
1:F:262:ARG:CZ	3:J:230:TYR:CD2	2.97	0.47
2:G:10:TRP:CE3	2:G:190:ILE:CG2	2.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:262:ARG:HH12	3:O:228:ASP:CG	2.23	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:60:ASP:O	1:A:64:ILE:HD12	2.15	0.47
1:A:194:ASP:CA	2:M:311:LEU:CD1	2.80	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:50:GLY:O	2:B:54:ILE:HG13	2.15	0.47
2:B:333:LEU:CD1	2:B:337:LYS:HE3	2.45	0.47
2:D:229:ASP:C	2:D:231:GLN:N	2.71	0.47
3:E:241:ALA:N	3:E:242:PRO:HD2	2.29	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:L:292:ILE:O	2:L:296:GLN:HG3	2.14	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:M:316:LEU:HB3	2:M:320:ILE:HD12	1.96	0.47
2:N:220:LEU:HD21	3:O:154:THR:HB	1.96	0.47
2:N:246:ASP:HB2	2:N:248:GLN:CG	2.45	0.47
1:A:119:LYS:HD3	1:A:119:LYS:N	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:292:ILE:O	2:G:296:GLN:HG3	2.14	0.47
2:H:6:LEU:CB	2:H:222:ASP:OD1	2.63	0.47
1:K:262:ARG:CZ	3:O:230:TYR:CD2	2.98	0.47
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:N:244:LEU:HD11	2:N:276:ILE:CG2	2.45	0.47
2:N:334:ILE:HG12	3:O:334:LEU:OXT	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:362:ARG:C	2:H:363:MET:HG3	2.39	0.47
2:I:256:MET:HA	2:I:357:LEU:HD11	1.97	0.47
2:I:358:ALA:C	2:I:360:HIS:H	2.23	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:C:362:ARG:C	2:C:363:MET:HG3	2.40	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
2:D:358:ALA:C	2:D:360:HIS:H	2.23	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
2:I:316:LEU:HD22	2:I:320:ILE:CD1	2.45	0.46
1:K:60:ASP:O	1:K:64:ILE:HD12	2.15	0.46
1:K:263:GLN:OE1	1:K:272:LEU:HD11	2.16	0.46
2:M:201:ARG:NH2	2:M:308:ALA:CB	2.78	0.46
2:N:265:MET:HE2	3:O:257:LYS:HE2	1.97	0.46
1:A:183:GLN:HE21	1:A:183:GLN:HA	1.78	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:66:THR:O	2:M:66:THR:HG22	2.14	0.46
2:M:126:ASP:HA	2:M:155:ALA:HB3	1.96	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:A:223:MET:HE3	1:A:223:MET:HB3	1.59	0.46
1:F:10:ARG:NH2	1:F:40:GLN:HE22	2.11	0.46
1:F:19:ALA:CB	1:F:133:ARG:HD3	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:222:LEU:CD1	1:A:285:MET:HE3	2.42	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: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:229:ASP:C	2:N:231:GLN:N	2.71	0.46
2:N:291:ARG:O	2:N:295:VAL:HG23	2.16	0.46
2:N:358:ALA:C	2:N:360:HIS:H	2.23	0.46
1:A:333:HIS:CE1	2:B:298:SER:HG	2.33	0.46
2:C:149:HIS:H	2:C:149:HIS:CD2	2.34	0.46
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:60:ASP:O	1:F:64:ILE:HD12	2.15	0.46
1:F:298:LEU:O	1:F:302:VAL:HG23	2.16	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:M:56:ARG:HH21	2:N:165:THR:HG23	1.79	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:93:ILE:HG22	2:I:100:LYS:HZ2	1.80	0.46
2:I:291:ARG:O	2:I:295:VAL:HG23	2.16	0.46
1:K:315:ASP:HB2	1:K:318:GLN:NE2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:73:CYS:SG	2:M:76:CYS:HB3	2.56	0.46
2:M:359:PHE:CZ	2:N:323:THR:HG22	2.50	0.46
2:C:7:ALA:O	2:D:168:SER:HB2	2.16	0.46
2:C:216:ASP:O	2:C:220:LEU:HG	2.15	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:HB2	2:C:51:LYS:HE3	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
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:56:ARG:NH1	2:L:82:ILE:O	2.49	0.46
2:L:316:LEU:HD22	2:L:320:ILE:HD11	1.98	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:OD1	2:C:260:ASN:O	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:73:CYS:SG	2:H:76:CYS:HB3	2.56	0.45
2:H:260:ASN:OD1	2:H:260:ASN:O	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:282:SER:OG	3:J:285:ARG:HB2	2.16	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:56:ARG:NH1	2:B:82:ILE:O	2.49	0.45
2:B:186:GLN:HG2	2:B:214:LEU:HD21	1.98	0.45
2:C:3:TYR:CD2	2:C:3:TYR:C	2.94	0.45
2:C:73:CYS:SG	2:C:76:CYS:HB3	2.56	0.45
2:C:252:LEU:CD1	2:C:281:LEU:HD21	2.47	0.45
2:C:271:ALA:HB1	2:C:276:ILE:CD1	2.36	0.45
2:D:338:GLU:HA	2:D:341:TYR:HD1	1.81	0.45
2:I:191:LEU:HD12	2:I:203:LEU:HD21	1.99	0.45
3:J:14:LEU:HD13	3:J:44:LEU:HD11	1.98	0.45
3:J:253:MET:O	3:J:256:LEU:N	2.50	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
3:O:57:LYS:HA	3:O:57:LYS:HD2	1.67	0.45
2:B:4:GLN:CD	2:B:9:LYS:HD2	2.42	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:O	1:K:312:LEU:HG	2.15	0.45
2:L:22:GLU:H	2:L:22:GLU:HG3	1.09	0.45
2:L:363:MET:HE3	2:L:363:MET:HB2	1.67	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:19:ALA:CB	1:A:133:ARG:HD3	2.46	0.45
1:A:133:ARG:HG3	2:G:299:PRO:CG	2.45	0.45
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:O	1:F:279:TRP:CD2	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:94:ASP:N	2:M:100:LYS:HZ3	2.14	0.45
2:M:238:SER:CB	2:M:245:ASP:OD1	2.65	0.45
2:N:142:THR:O	2:N:146:PRO:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:A:279:TRP:CD2	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
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
2:B:219:SER:O	2:B:223:GLN:HG3	2.17	0.45
2:B:270:GLU:HG2	2:B:274:ARG:CZ	2.46	0.45
3:E:27:LEU:HG	3:E:29:ILE:CD1	2.47	0.45
3:E:257:LYS:HB3	3:E:262:ALA:HB3	1.98	0.45
2:G:11:ARG:HA	2:G:215:ARG:NH1	2.31	0.45
2:H:37:ILE:HD12	2:H:62:LEU:HD21	1.99	0.45
2:H:102:GLU:HB3	2:H:106:ASP:HB2	1.99	0.45
2:I:42:LEU:HD12	2:I:172:GLN:OE1	2.16	0.45
2:I:201:ARG:N	2:I:305:ASP:HB2	2.28	0.45
3:J:257:LYS:HB3	3:J:262:ALA:HB3	1.98	0.45
1:K:32:GLN:HE22	2:L:165:THR:HA	1.79	0.45
2:L:93:ILE:CG2	2:L:100:LYS:HZ3	2.29	0.45
3:O:14:LEU:HD13	3:O:44:LEU:HD11	1.98	0.45
2:B:304:ASN:OD1	2:B:304:ASN:C	2.60	0.45
2:D:140:LEU:HD11	2:D:165:THR:HB	1.99	0.45
1:F:48:GLU:CG	1:F:49:GLU:H	2.30	0.45
1:F:315:ASP:H	1:F:318:GLN:HE21	1.65	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:MET:HE3	2:B:363:MET:HB2	1.67	0.45
2:C:21:GLN:HE22	2:C:49:VAL:HG13	1.82	0.45
2:C:99:THR:O	2:C:99:THR:CG2	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:94:ASP:O	2:I:100:LYS:CE	2.65	0.45
2:I:131:LEU:HB2	2:I:136:PHE:CD1	2.52	0.45
2:L:223:GLN:OE1	2:M:171:LEU:HD11	2.17	0.45
2:L:248:GLN:HA	2:L:251:SER:OG	2.17	0.45
2:M:5:VAL:HG11	2:N:171:LEU:HB2	1.99	0.45
2:M:149:HIS:CD2	2:M:149:HIS:H	2.34	0.45
3:O:253:MET:O	3:O:256:LEU:N	2.49	0.45
2:B:351:MET:HG2	2:C:290:HIS:ND1	2.32	0.45
2:C:147:PRO:HB2	2:C:149:HIS:CD2	2.53	0.45
1:F:25:GLY:N	1:F:114:GLY:O	2.41	0.45
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: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:HA	2:N:302:LEU:HD23	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:176:LYS:C	2:G:178:LEU:N	2.75	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
2:G:360:HIS:CD2	2:G:361:PRO:HD2	2.52	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:HA	3:J:57:LYS:HD2	1.67	0.44
1:K:57:PRO:HB3	1:K:90:ASN:ND2	2.33	0.44
1:K:191:LEU:HA	1:K:191:LEU:HD23	1.80	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:HD2	3:E:57:LYS:HA	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:G:256:MET:HE2	2:G:332:LEU:HD21	1.99	0.44
2:I:200:PRO:CB	2:I:304:ASN:CB	2.92	0.44
2:L:341:TYR:C	2:M:336:ARG:NH1	2.75	0.44
2:M:5:VAL:HB	2:M:222:ASP:OD2	2.17	0.44
2:M:260:ASN:O	2:M:260:ASN:OD1	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:GLN:HA	2:B:251:SER:OG	2.17	0.44
2:B:256:MET:HE2	2:B:332:LEU:HD21	2.00	0.44
2:D:135:SER:O	2:D:138:ALA:HB3	2.17	0.44
1:F:56:ASP:HB3	1:F:58:ASN:H	1.83	0.44
1:F:191:LEU:O	1:F:193:PRO:HD3	2.18	0.44
2:H:167:LEU:HB3	2:H:172:GLN:NE2	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
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: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:HD3	1:K:119:LYS:N	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:21:GLN:HE22	2:M:49:VAL:HG13	1.82	0.44
2:M:147:PRO:HB2	2:M:149:HIS:CD2	2.52	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
1:A:329:LEU:CD1	2:B:294:MET:HE1	2.47	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:304:ASN:OD1	2:G:304:ASN:C	2.60	0.44
2:L:256:MET:HE2	2:L:332:LEU:HD21	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:304:ASN:C	2:L:304:ASN:OD1	2.60	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
1:A:213:THR:C	1:A:215:PHE:N	2.75	0.43
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
2:G:63:ASN:O	2:G:64:CYS:C	2.61	0.43
3:J:30:GLN:HA	3:J:145:THR:O	2.17	0.43
2:M:3:TYR:CD2	2:M:3:TYR:N	2.83	0.43
2:M:245:ASP:HB2	2:M:248:GLN:HG3	1.99	0.43
2:N:66:THR:HG22	2:N:66:THR:O	2.18	0.43
2:N:244:LEU:CD1	2:N:276:ILE:HD13	2.48	0.43
2:N:258:GLU:O	2:N:259:ALA:HB3	2.17	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
1:A:183:GLN:OE1	2:B:172:GLN:HG3	2.17	0.43
2:B:214:LEU:O	2:B:215:ARG:C	2.61	0.43
1:F:213:THR:C	1:F:215:PHE:N	2.75	0.43
2:H:264:VAL:O	2:H:268:ILE:HG13	2.18	0.43
2:I:6:LEU:C	2:I:222:ASP:OD2	2.61	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:42:LEU:HD23	2:L:172:GLN:HG2	1.99	0.43
2:L:250:LEU:HD22	2:L:309:ILE:CG2	2.48	0.43
2:M:201:ARG:HH21	2:M:308:ALA:CB	2.30	0.43
2:M:237:VAL:C	2:M:239:ALA:N	2.76	0.43
2:N:140:LEU:HD11	2:N:165:THR:HB	1.99	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:84:LEU:HD12	1:F:84:LEU:HA	1.84	0.43
1:F:191:LEU:HD23	1:F:191:LEU:HA	1.80	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:360:HIS:CD2	2:L:361:PRO:HD2	2.52	0.43
2:M:10:TRP:CH2	2:M:190:ILE:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:86:ARG:CZ	2:N:141:LYS:CB	2.83	0.43
2:M:102:GLU:HB3	2:M:106:ASP:HB2	1.99	0.43
2:N:62:LEU:O	2:N:119:ARG:HD2	2.18	0.43
2:N:257:VAL:O	2:N:257:VAL:HG12	2.17	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
2:I:309:ILE:O	2:I:310:GLU:C	2.61	0.43
3:J:117:ALA:HB2	3:J:143:LEU:CD1	2.47	0.43
1:K:213:THR:C	1:K:215:PHE:N	2.75	0.43
2:L:4:GLN:CD	2:L:9:LYS:HD2	2.42	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:6:LEU:HD23	2:B:194:GLU:CD	2.42	0.43
2:B:140:LEU:HD23	2:B:140:LEU:HA	1.84	0.43
2:B:250:LEU:HD22	2:B:309:ILE:CG2	2.48	0.43
2:D:246:ASP:C	2:D:248:GLN:H	2.26	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
1:K:100:LEU:O	1:K:103:LEU:HB3	2.18	0.43
1:K:183:GLN:OE1	2:L:172:GLN:HG3	2.18	0.43
2:L:42:LEU:HD11	2:L:156:THR:HG22	2.01	0.43
2: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:84:GLN:HG2	2:D:144:GLU:OE1	2.17	0.43
2:C:102:GLU:HB3	2:C:106:ASP:HB2	1.99	0.43
1:F:50:HIS:O	1:F:51:HIS:CD2	2.72	0.43
1:F:270:ARG:NH2	2:N:319:THR:H	2.16	0.43
2:I:246:ASP:C	2:I:248:GLN:H	2.26	0.43
3:J:30:GLN:O	3:J:30:GLN:HG3	2.18	0.43
1:K:48:GLU:CG	1:K:49:GLU:H	2.30	0.43
2:L:63:ASN:O	2:L:64:CYS:C	2.61	0.43
2:L:278:TRP:CE3	2:L:349:VAL:HG21	2.53	0.43
2:M:276:ILE:H	2:M:276:ILE:HG13	1.66	0.43
2:N:246:ASP:C	2:N:248:GLN:H	2.26	0.43
2:N:282:LEU:HD23	2:N:285:MET:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:ASN:O	2:B:64:CYS:C	2.61	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
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:21:GLN:O	2:N:22:GLU:C	2.62	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
1:A:253:GLU:OE1	1:A:286:MET:HE1	2.19	0.43
2:D:143:LEU:HD23	2:D:143:LEU:HA	1.89	0.43
2:D:309:ILE:O	2:D:310:GLU:C	2.61	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:H:351:MET:HE3	2:H:354:LEU:HB2	2.01	0.43
2:I:338:GLU:OE2	3:J:295:HIS:NE2	2.52	0.43
2:L:214:LEU:O	2:L:215:ARG:C	2.61	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
2:G:4:GLN:CD	2:G:9:LYS:HD2	2.42	0.43
2:G:363:MET:HE3	2:G:363:MET:HB2	1.67	0.43
1:K:50:HIS:O	1:K:51:HIS:CD2	2.72	0.43
1:K:325:GLU:O	1:K:329:LEU:HG	2.18	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:G:214:LEU:O	2:G:215:ARG:C	2.61	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
1:K:253:GLU:OE1	1:K:286:MET:HE1	2.19	0.43
2:L:10:TRP:CZ2	2:L:193:GLU:CG	3.02	0.43
2:L:93:ILE:HG23	2:L:100:LYS:HZ3	1.80	0.43
2:M:42:LEU:HD12	2:M:154:LEU:HB2	2.00	0.43
2:M:345:ARG:O	2:M:349:VAL:HG23	2.19	0.43
3:E:149:GLU:O	3:E:151:LEU:N	2.52	0.42
1:F:228:ARG:H	1:F:228:ARG:HG2	1.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:253:GLU:OE1	1:F:286:MET:HE1	2.19	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:76:CYS:SG	2:N:78:ASN:HB2	2.59	0.42
2:N:347:MET:O	2:N:351:MET:CG	2.65	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:42:LEU:HD12	2:C:154:LEU:HB2	2.00	0.42
2:C:156:THR:HG22	2:C:157:THR:N	2.34	0.42
2:D:21:GLN:O	2:D:22:GLU:C	2.62	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:H:351:MET:HE2	2:I:326:GLN:OE1	2.19	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:C:351:MET:HE3	2:C:354:LEU:HB2	2.00	0.42
2:G:20:GLY:CA	2:G:182:GLN:NE2	2.83	0.42
2:I:21:GLN:O	2:I:22:GLU:C	2.62	0.42
3:J:245:LEU:HB2	3:J:297:ARG:HG3	2.01	0.42
1:K:3:ARG:HG2	1:K:136:GLN:NE2	2.33	0.42
1:K:29:LEU:O	1:K:33:GLU:HG3	2.19	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
2:N:309:ILE:O	2:N:310:GLU:C	2.61	0.42
3:O:30:GLN:O	3:O:30:GLN:HG3	2.18	0.42
2:D:76:CYS:SG	2:D:78:ASN:HB2	2.59	0.42
3:E:35:MET:HE2	3:E:166:PRO:HA	2.00	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:277:GLU:OE1	3:O:149:GLU:HG3	2.19	0.42
2:N:289:LEU:HD23	2:N:289:LEU:HA	1.81	0.42
3:O:170:GLN:H	3:O:170:GLN:HG2	1.65	0.42
2:C:18:VAL:HG12	2:C:19:VAL:N	2.35	0.42
3:E:117:ALA:HB2	3:E:143:LEU:CD1	2.47	0.42
1:F:223:MET:HE2	1:F:288:GLU:O	2.20	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
2:G:259:ALA:HB3	2:G:363:MET:HE1	2.02	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
2:N:360:HIS:HB2	2:N:363:MET:HE3	2.02	0.42
2:B:259:ALA:HB3	2:B:363:MET:HE1	2.02	0.42
2:D:257:VAL:O	2:D:360:HIS:CE1	2.61	0.42
3:E:35:MET:CE	3:E:166:PRO:HA	2.50	0.42
1:F:124:ALA:O	1:F:125:ALA:C	2.63	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:79:THR:HG22	1:K:80:LEU:N	2.34	0.42
1:K:246:LEU:HD23	1:K:246:LEU:HA	1.87	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
1:A:28:PRO:CB	2:B:164:VAL:HG21	2.25	0.42
2:C:342:ALA:HA	2:D:333:LEU:HD21	2.01	0.42
2:D:50:GLY:O	2:D:51:LYS:C	2.63	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
2:M:306:MET:CE	2:M:313:MET:HE2	2.47	0.42
2:M:351:MET:HE3	2:M:354:LEU:HB2	2.00	0.42
3:O:225:PRO:HB3	3:O:276:GLU:OE2	2.20	0.42
2:B:4:GLN:OE1	2:B:9:LYS:CD	2.64	0.42
2:B:42:LEU:HD11	2:B:156:THR:HG22	2.00	0.42
3:E:225:PRO:HB3	3:E:276:GLU:OE2	2.20	0.42
3:E:237:ASN:C	3:E:237:ASN:HD22	2.28	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:I:351:MET:SD	3:J:290:LEU:HD13	2.59	0.42
3:J:311:LEU:HD12	3:J:311:LEU:HA	1.86	0.42
1:K:311:THR:O	1:K:318:GLN:NE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:333:HIS:HB2	2:L:297:LEU:CD2	2.32	0.42
2:L:341:TYR:C	2:M:336:ARG:HH11	2.22	0.42
2:M:291:ARG:HD2	2:M:306:MET:HE2	2.02	0.42
2:N:50:GLY:O	2:N:51:LYS:C	2.63	0.42
3:O:18:TYR:HB3	3:O:48:LEU:HD21	2.01	0.42
2:B:94:ASP:C	2:B:100:LYS:NZ	2.67	0.42
2:B:97:SER:CB	2:C:144:GLU:CD	2.86	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:C:291:ARG:HD2	2:C:306:MET:HE2	2.02	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:5:PRO:HD3	3:O:175:TRP:CZ3	2.54	0.42
3:O:149:GLU:O	3:O:151:LEU:N	2.53	0.42
2:B:10:TRP:CZ2	2:B:193:GLU:CD	2.97	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
2:D:333:LEU:O	2:D:334:ILE:C	2.63	0.42
1:F:4:LEU:CD1	1:F:137:VAL:HG22	2.50	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
2:G:10:TRP:CE3	2:G:190:ILE:CG1	3.01	0.42
2:G:21:GLN:HE22	2:G:49:VAL:CG1	2.32	0.42
2:G:37:ILE:HG12	2:G:62:LEU:HD21	2.02	0.42
2:H:6:LEU:HB2	2:H:222:ASP:OD1	2.19	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:N:333:LEU:O	2:N:334:ILE:C	2.63	0.42
2:C:137:ASN:HA	2:C:140:LEU:HD12	2.02	0.41
2:G:104:THR:HG22	2:G:108:LEU:CD1	2.50	0.41
2:I:50:GLY:O	2:I:51:LYS:C	2.63	0.41
2:I:351:MET:HE3	2:I:351:MET:HB3	1.92	0.41
1:K:264:SER:O	1:K:265:ALA:CB	2.68	0.41
1:K:295:GLN:H	1:K:295:GLN:CD	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:124:ALA:O	1:A:125:ALA:C	2.63	0.41
2:B:37:ILE:HG12	2:B:62:LEU:HD21	2.02	0.41
2:B:276:ILE:CG2	2:B:277:GLU:N	2.82	0.41
2:C:3:TYR:CD2	2:C:3:TYR:N	2.86	0.41
2:C:147:PRO:HB2	2:C:149:HIS:NE2	2.35	0.41
2:D:244:LEU:HD11	2:D:276:ILE:HG21	2.01	0.41
2:D:282:LEU:HD23	2:D:285:MET:HE3	2.01	0.41
2:D:360:HIS:HB2	2:D:363:MET:HE3	2.02	0.41
1:F:79:THR:HG22	1:F:80:LEU:N	2.34	0.41
1:F:295:GLN:CD	1:F:295:GLN:H	2.28	0.41
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:I:333:LEU:O	2:I:334:ILE:C	2.63	0.41
2:L:180:VAL:HG23	2:L:304:ASN:CG	2.25	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:L:343:PRO:HD3	2:M:286:LEU:HB3	2.01	0.41
2:M:156:THR:HG22	2:M:157:THR:N	2.34	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:G:93:ILE:CG2	2:G:100:LYS:HZ3	2.33	0.41
2:H:78:ASN:O	2:H:82:ILE:HG13	2.20	0.41
2:H:156:THR:HG22	2:H:157:THR:N	2.34	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:320:ILE:HA	2:N:321:PRO:HD3	1.90	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:171:TYR:CD2	3:E:171:TYR:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:64:ILE:HG12	1:F:96:GLN:HB3	2.02	0.41
1:F:262:ARG:HD2	3:J:230:TYR:CD2	2.55	0.41
2:H:56:ARG:HH22	2:I:165:THR:HG21	1.84	0.41
2:H:237:VAL:C	2:H:239:ALA:N	2.76	0.41
2:I:282:LEU:HD23	2:I:285:MET:HE3	2.01	0.41
1:K:124:ALA:O	1:K:125:ALA:C	2.63	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:34:GLY:O	3:O:199:GLY:N	2.51	0.41
3:O:171:TYR:CD2	3:O:171:TYR:N	2.88	0.41
1:A:295:GLN:H	1:A:295:GLN:CD	2.28	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
1:A:159:ASN:OD1	2:M:319:THR:HG21	2.20	0.41
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:28:LEU:HD23	2:I:28:LEU:HA	1.90	0.41
2:I:271:ALA:O	2:I:276:ILE:HG13	2.20	0.41
2:I:360:HIS:HB2	2:I:363:MET:HE3	2.02	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:4:LEU:CD1	1:A:137:VAL:HG22	2.50	0.41
2:D:5:VAL:HG12	2:D:222:ASP:OD2	2.21	0.41
2:D:271:ALA:O	2:D:276:ILE:HG13	2.20	0.41
1:F:29:LEU:HB2	1:F:179:LEU:CB	2.43	0.41
1:F:193:PRO:HA	2:G:36:ARG:HH22	1.86	0.41
1:F:223:MET:HE3	1:F:223:MET:HB3	1.59	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
1:K:222:LEU:HD11	1:K:285:MET:CE	2.47	0.41
2:L:43:PHE:O	2:L:155:ALA:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	3:E:252:LEU:HA	1.83	0.41
1:F:270:ARG:HG2	1:F:283:ARG:NH2	2.36	0.41
2:G:22:GLU:H	2:G:22:GLU:HG3	1.09	0.41
2:N:119:ARG:H	2:N:119:ARG:HG3	1.65	0.41
3:O:244:ARG:O	3:O:247:TRP:HB2	2.21	0.41
1:A:64:ILE:HG12	1:A:96:GLN:HB3	2.02	0.41
1:A:264:SER:O	1:A:265:ALA:CB	2.68	0.41
1:A:281:ASN:O	1:A:281:ASN:OD1	2.39	0.41
2:B:98:ARG:HD3	2:C:141:LYS:HE2	2.03	0.41
2:B:104:THR:HG22	2:B:108:LEU:CD1	2.50	0.41
2:B:248:GLN:CD	2:B:267:LEU:HD22	2.46	0.41
2:C:210:ALA:HB1	2:C:213:SER:OG	2.20	0.41
2:D:42:LEU:HB3	2:D:172:GLN:CB	2.43	0.41
2:D:69:THR:HG22	2:D:71:THR:H	1.86	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
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:G:248:GLN:CD	2:G:267:LEU:HD22	2.46	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
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:142:PRO:CD	1:K:178:LEU:HD11	2.50	0.41
1:K:333:HIS:CB	2:L:297:LEU:CD2	2.61	0.41
1:K:333:HIS:CE1	2:L:297:LEU:HG	2.56	0.41
2:L:10:TRP:CD2	2:L:190:ILE:HG12	2.55	0.41
2:N:51:LYS:HB2	2:N:51:LYS:HE3	1.76	0.41
2:N:105:ARG:HD2	2:N:134:HIS:NE2	2.36	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:71:MET:HE2	1:A:80:LEU:HD22	2.03	0.41
1:A:105:HIS:HB2	1:F:225:LYS:HE3	0.88	0.41
1:A:223:MET:HE2	1:A:288:GLU:O	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:283:VAL:HA	2:H:286:LEU:HD12	2.03	0.41
2:H:291:ARG:HD2	2:H:306:MET:HE2	2.02	0.41
2:I:250:LEU:CD2	2:I:309:ILE:HG23	2.51	0.41
2:I:302:LEU:HD13	2:I:310:GLU:HA	2.03	0.41
3:J:27:LEU:HG	3:J:29:ILE:HD11	2.03	0.41
3:J:329:LEU:HD23	3:J:329:LEU:N	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:D:244:LEU:HD21	2:D:276:ILE:HG23	2.03	0.40
3:E:73:HIS:HE1	3:E:106:LEU:HD22	1.86	0.40
3:E:311:LEU:HD12	3:E:311:LEU:HA	1.86	0.40
1:F:29:LEU:HD13	1:F:179:LEU:CA	2.37	0.40
2:I:220:LEU:CD2	3:J:154:THR:HA	2.47	0.40
2:I:343:PRO:CG	2:I:347:MET:SD	3.09	0.40
3:J:73:HIS:CE1	3:J:106:LEU:HD22	2.56	0.40
1:K:64:ILE:HG12	1:K:96:GLN:HB3	2.02	0.40
1:K:310:LEU:HA	1:K:310:LEU:HD23	1.61	0.40
2:N:250:LEU:CD2	2:N:309:ILE:HG23	2.51	0.40
2:N:302:LEU:HD13	2:N:310:GLU:HA	2.03	0.40
3:O:6:TRP:HH2	3:O:175:TRP:CZ2	2.39	0.40
3:O:25:HIS:O	3:O:141:PHE:HB2	2.22	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:H:210:ALA:HB1	2:H:213:SER:OG	2.20	0.40
3:J:73:HIS:HE1	3:J:106:LEU:HD22	1.86	0.40
3:J:121:THR:O	3:J:124:ALA:HB3	2.21	0.40
1:K:84:LEU:HD12	1:K:84:LEU:HA	1.84	0.40
1:K:223:MET:HE2	1:K:288:GLU:O	2.20	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:75:ALA:CB	1:F:207:ASN:CB	2.97	0.40
1:A:270:ARG:HG2	1:A:283:ARG:NH2	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:51:LYS:HB2	2:H:51:LYS:HE3	1.77	0.40
2:I:42:LEU:HD23	2:I:154:LEU:HB2	2.02	0.40
2:I:105:ARG:HD2	2:I:134:HIS:NE2	2.36	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:32:LEU:HD23	2:L:32:LEU:HA	1.94	0.40
2:M:215:ARG:CD	2:N:164:VAL:HG11	2.51	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: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: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:D:289:LEU:HA	2:D:289:LEU:HD23	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:40:GLN:HE21	1:F:40:GLN:HB3	1.69	0.40
1:F:71:MET:HE2	1:F:80:LEU:HD22	2.03	0.40
1:F:190:LEU:HA	1:F:190:LEU:HD23	1.85	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
1:K:223:MET:HB3	1:K:223:MET:HE3	1.59	0.40
2:L:248:GLN:CD	2:L:267:LEU:HD22	2.46	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
3:O:192:ARG:C	3:O:194:SER:H	2.30	0.40
1:A:105:HIS:HA	1:F:227:LYS:HD2	1.94	0.40
2:B:22:GLU:H	2:B:22:GLU:HG3	1.09	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
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:L:259:ALA:HB3	2:L:363:MET:HE1	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:126:ASP:OD1	2:M:127:GLU:HG3	2.22	0.40
2:N:297:LEU:HD12	2:N:297:LEU:HA	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:B:4:GLN:NE2	3:J:59:CYS:O[2_646]	1.33	0.87
2:C:192:ASN:ND2	1:F:77:ARG:NE[2_546]	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
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
3:E:63:ARG:CZ	2:H:361:PRO:CA[1_455]	1.48	0.72
1:K:277:ARG:CZ	2:N:66:THR:CG2[1_655]	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:192:ASN:O	1:F:76:SER:CA[2_546]	1.80	0.40
2:G:75:VAL:C	2:I:270:GLU:OE2[1_455]	1.80	0.40
2:C:188:GLU:CD	1:F:77:ARG:NH2[2_546]	1.81	0.39
2:C:192:ASN:OD1	1:F:107:ASP:OD1[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:192:ASN:ND2	1:F:77:ARG:CD[2_546]	1.85	0.35
2:C:193:GLU:N	1:F:75:ALA:O[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
2:B:3:TYR:CZ	3:J:54:GLN:CG[2_646]	1.96	0.24
3:J:19:GLN:OE1	2:L:299:PRO:CG[2_756]	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:B:4:GLN:NE2	3:J:59:CYS:C[2_646]	2.02	0.18
2:C:192:ASN:C	1:F:76:SER:CA[2_546]	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:B:193:GLU:OE1	3:J:69:GLN:NE2[2_646]	2.06	0.14
2:C:193:GLU:O	1:F:75:ALA:N[2_546]	2.06	0.14
2:C:195:HIS:CG	1:F:74:PHE:O[2_546]	2.06	0.14
1:A:277:ARG:CZ	2:D:66:THR:C[1_655]	2.07	0.13
2:B:361:PRO:O	3:O:184:GLN:CG[2_646]	2.07	0.13
2:C:192:ASN:O	1:F:76:SER:C[2_546]	2.07	0.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:3:TYR:CD2	3:J:54:GLN:OE1[2_646]	2.17	0.03
2:C:198:HIS:O	1:F:106:ASP:OD2[2_546]	2.17	0.03
3:E:63:ARG:NH2	2:H:360:HIS:O[1_455]	2.17	0.03
2:C:192:ASN:C	1:F:75:ALA:O[2_546]	2.18	0.02
3:E:63:ARG:CZ	2:H:361:PRO:N[1_455]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	330/343 (96%)	301 (91%)	22 (7%)	7 (2%)	5	31
1	F	330/343 (96%)	301 (91%)	22 (7%)	7 (2%)	5	31
1	K	330/343 (96%)	301 (91%)	22 (7%)	7 (2%)	5	31
2	B	358/376 (95%)	327 (91%)	23 (6%)	8 (2%)	5	31
2	C	358/376 (95%)	329 (92%)	23 (6%)	6 (2%)	7	35
2	D	357/376 (95%)	320 (90%)	27 (8%)	10 (3%)	4	27
2	G	358/376 (95%)	328 (92%)	22 (6%)	8 (2%)	5	31
2	H	358/376 (95%)	329 (92%)	22 (6%)	7 (2%)	6	32
2	I	357/376 (95%)	320 (90%)	27 (8%)	10 (3%)	4	27
2	L	358/376 (95%)	327 (91%)	23 (6%)	8 (2%)	5	31
2	M	358/376 (95%)	329 (92%)	22 (6%)	7 (2%)	6	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	357/376 (95%)	320 (90%)	27 (8%)	10 (3%)	4	27
3	E	326/334 (98%)	296 (91%)	28 (9%)	2 (1%)	21	55
3	J	326/334 (98%)	296 (91%)	28 (9%)	2 (1%)	21	55
3	O	326/334 (98%)	296 (91%)	28 (9%)	2 (1%)	21	55
All	All	5187/5415 (96%)	4720 (91%)	366 (7%)	101 (2%)	6	33

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	256 (90%)	29 (10%)	7	26
1	F	285/291 (98%)	256 (90%)	29 (10%)	7	26
1	K	285/291 (98%)	256 (90%)	29 (10%)	7	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	303/312 (97%)	279 (92%)	24 (8%)	11	36
2	C	303/312 (97%)	287 (95%)	16 (5%)	20	46
2	D	302/312 (97%)	281 (93%)	21 (7%)	14	40
2	G	303/312 (97%)	279 (92%)	24 (8%)	11	36
2	H	303/312 (97%)	287 (95%)	16 (5%)	20	46
2	I	302/312 (97%)	281 (93%)	21 (7%)	14	40
2	L	303/312 (97%)	279 (92%)	24 (8%)	11	36
2	M	303/312 (97%)	287 (95%)	16 (5%)	20	46
2	N	302/312 (97%)	281 (93%)	21 (7%)	14	40
3	E	270/270 (100%)	240 (89%)	30 (11%)	6	23
3	J	270/270 (100%)	240 (89%)	30 (11%)	6	23
3	O	270/270 (100%)	240 (89%)	30 (11%)	6	23
All	All	4389/4491 (98%)	4029 (92%)	360 (8%)	10	34

All (360) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	54	SER
1	A	64	ILE
1	A	84	LEU
1	A	98	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
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	221	LEU
1	A	223	MET

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Mol	Chain	Res	Type
1	A	228	ARG
1	A	230	LEU
1	A	266	HIS
1	A	279	TRP
1	A	292	ARG
1	A	296	THR
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	51	LYS
2	B	52	THR
2	B	71	THR
2	B	88	VAL
2	B	97	SER
2	B	128	VAL
2	B	157	THR
2	B	160	GLN
2	B	165	THR
2	B	176	LYS
2	B	219	SER
2	B	240	MET
2	B	251	SER
2	B	252	LEU
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
2	C	69	THR
2	C	76	CYS
2	C	117	ARG
2	C	130	MET
2	C	166	ILE
2	C	251	SER
2	C	309	ILE

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Mol	Chain	Res	Type
2	C	318	ARG
2	C	323	THR
2	C	327	LEU
2	C	344	ASP
2	C	357	LEU
2	C	367	GLU
2	D	6	LEU
2	D	17	ASP
2	D	42	LEU
2	D	46	THR
2	D	47	ARG
2	D	71	THR
2	D	76	CYS
2	D	137	ASN
2	D	160	GLN
2	D	164	VAL
2	D	167	LEU
2	D	194	GLU
2	D	248	GLN
2	D	251	SER
2	D	253	VAL
2	D	298	SER
2	D	318	ARG
2	D	333	LEU
2	D	351	MET
2	D	357	LEU
2	D	363	MET
3	E	13	LYS
3	E	15	VAL
3	E	35	MET
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	156	ARG
3	E	159	CYS
3	E	170	GLN
3	E	175	TRP
3	E	202	LEU

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Mol	Chain	Res	Type
3	E	206	GLN
3	E	216	LEU
3	E	220	LEU
3	E	245	LEU
3	E	252	LEU
3	E	256	LEU
3	E	274	VAL
3	E	277	LEU
3	E	285	ARG
3	E	290	LEU
3	E	296	ILE
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	64	ILE
1	F	84	LEU
1	F	98	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	221	LEU
1	F	223	MET
1	F	228	ARG
1	F	230	LEU
1	F	266	HIS
1	F	279	TRP
1	F	292	ARG
1	F	296	THR

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Mol	Chain	Res	Type
1	F	305	LEU
1	F	330	LEU
2	G	3	TYR
2	G	14	THR
2	G	17	ASP
2	G	18	VAL
2	G	22	GLU
2	G	47	ARG
2	G	51	LYS
2	G	52	THR
2	G	71	THR
2	G	88	VAL
2	G	97	SER
2	G	128	VAL
2	G	157	THR
2	G	160	GLN
2	G	165	THR
2	G	176	LYS
2	G	219	SER
2	G	240	MET
2	G	251	SER
2	G	252	LEU
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	166	ILE
2	H	251	SER
2	H	309	ILE
2	H	318	ARG
2	H	323	THR
2	H	327	LEU
2	H	344	ASP
2	H	357	LEU
2	H	367	GLU

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Mol	Chain	Res	Type
2	I	6	LEU
2	I	17	ASP
2	I	42	LEU
2	I	46	THR
2	I	47	ARG
2	I	71	THR
2	I	76	CYS
2	I	137	ASN
2	I	160	GLN
2	I	164	VAL
2	I	167	LEU
2	I	194	GLU
2	I	248	GLN
2	I	251	SER
2	I	253	VAL
2	I	298	SER
2	I	318	ARG
2	I	333	LEU
2	I	351	MET
2	I	357	LEU
2	I	363	MET
3	J	13	LYS
3	J	15	VAL
3	J	35	MET
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	156	ARG
3	J	159	CYS
3	J	170	GLN
3	J	175	TRP
3	J	202	LEU
3	J	206	GLN
3	J	216	LEU
3	J	220	LEU
3	J	245	LEU
3	J	252	LEU
3	J	256	LEU

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Mol	Chain	Res	Type
3	J	274	VAL
3	J	277	LEU
3	J	285	ARG
3	J	290	LEU
3	J	296	ILE
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	64	ILE
1	K	84	LEU
1	K	98	LEU
1	K	101	THR
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	221	LEU
1	K	223	MET
1	K	228	ARG
1	K	230	LEU
1	K	266	HIS
1	K	279	TRP
1	K	292	ARG
1	K	296	THR
1	K	305	LEU
1	K	330	LEU
2	L	3	TYR
2	L	14	THR
2	L	17	ASP
2	L	18	VAL

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Mol	Chain	Res	Type
2	L	22	GLU
2	L	47	ARG
2	L	51	LYS
2	L	52	THR
2	L	71	THR
2	L	88	VAL
2	L	97	SER
2	L	128	VAL
2	L	157	THR
2	L	160	GLN
2	L	165	THR
2	L	176	LYS
2	L	219	SER
2	L	240	MET
2	L	251	SER
2	L	252	LEU
2	L	333	LEU
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	166	ILE
2	M	251	SER
2	M	309	ILE
2	M	318	ARG
2	M	323	THR
2	M	327	LEU
2	M	344	ASP
2	M	357	LEU
2	M	367	GLU
2	N	6	LEU
2	N	17	ASP
2	N	42	LEU
2	N	46	THR
2	N	47	ARG
2	N	71	THR

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Mol	Chain	Res	Type
2	N	76	CYS
2	N	137	ASN
2	N	160	GLN
2	N	164	VAL
2	N	167	LEU
2	N	194	GLU
2	N	248	GLN
2	N	251	SER
2	N	253	VAL
2	N	298	SER
2	N	318	ARG
2	N	333	LEU
2	N	351	MET
2	N	357	LEU
2	N	363	MET
3	O	13	LYS
3	O	15	VAL
3	O	35	MET
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	156	ARG
3	O	159	CYS
3	O	170	GLN
3	O	175	TRP
3	O	202	LEU
3	O	206	GLN
3	O	216	LEU
3	O	220	LEU
3	O	245	LEU
3	O	252	LEU
3	O	256	LEU
3	O	274	VAL
3	O	277	LEU
3	O	285	ARG
3	O	290	LEU
3	O	296	ILE
3	O	299	GLN

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Mol	Chain	Res	Type
3	O	310	LEU
3	O	315	LEU
3	O	329	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) 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	168	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	303	GLN
1	A	314	GLN
1	A	318	GLN
2	B	21	GLN
2	B	137	ASN
2	B	189	HIS
2	B	198	HIS
2	B	360	HIS
2	C	78	ASN
2	C	198	HIS
2	C	223	GLN
2	C	360	HIS
2	D	38	HIS
2	D	110	ASN
2	D	129	HIS
2	D	185	HIS
2	D	198	HIS
2	D	248	GLN
2	D	290	HIS
2	D	304	ASN
2	D	326	GLN
2	D	360	HIS
3	E	73	HIS

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Mol	Chain	Res	Type
3	E	162	HIS
3	E	237	ASN
3	E	240	GLN
3	E	246	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	168	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	23	HIS
2	G	137	ASN
2	G	174	HIS
2	G	198	HIS
2	G	360	HIS
2	H	78	ASN
2	H	198	HIS
2	H	360	HIS
2	I	110	ASN
2	I	129	HIS
2	I	185	HIS
2	I	198	HIS
2	I	248	GLN
2	I	290	HIS
2	I	304	ASN
2	I	326	GLN
2	I	360	HIS
3	J	73	HIS
3	J	162	HIS
3	J	209	ASN

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Mol	Chain	Res	Type
3	J	237	ASN
3	J	240	GLN
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	168	GLN
1	K	183	GLN
1	K	216	HIS
1	K	259	ASN
1	K	266	HIS
1	K	276	HIS
1	K	281	ASN
1	K	295	GLN
1	K	297	GLN
1	K	303	GLN
1	K	314	GLN
1	K	318	GLN
1	K	333	HIS
2	L	137	ASN
2	L	198	HIS
2	L	204	GLN
2	L	360	HIS
2	M	78	ASN
2	M	198	HIS
2	M	223	GLN
2	M	360	HIS
2	N	110	ASN
2	N	129	HIS
2	N	185	HIS
2	N	198	HIS
2	N	223	GLN
2	N	248	GLN
2	N	290	HIS
2	N	326	GLN
2	N	360	HIS
3	O	73	HIS
3	O	162	HIS

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Mol	Chain	Res	Type
3	O	209	ASN
3	O	237	ASN
3	O	240	GLN
3	O	246	HIS
3	O	260	HIS
3	O	299	GLN
3	O	307	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	336/343 (97%)	0.16	11 (3%)	49	34	69, 78, 90, 90	0
1	F	336/343 (97%)	0.50	16 (4%)	35	27	127, 241, 267, 267	0
1	K	336/343 (97%)	0.09	5 (1%)	72	50	56, 67, 79, 79	0
2	B	364/376 (96%)	0.11	14 (3%)	44	32	85, 90, 111, 111	0
2	C	364/376 (96%)	0.09	3 (0%)	82	64	61, 66, 76, 85	0
2	D	363/376 (96%)	0.06	9 (2%)	58	41	57, 67, 70, 70	0
2	G	364/376 (96%)	0.32	17 (4%)	36	28	84, 208, 291, 291	0
2	H	364/376 (96%)	0.05	5 (1%)	73	52	59, 171, 228, 228	0
2	I	363/376 (96%)	-0.02	7 (1%)	66	46	66, 67, 151, 151	0
2	L	364/376 (96%)	0.06	7 (1%)	66	46	66, 94, 101, 101	0
2	M	364/376 (96%)	0.08	7 (1%)	66	46	79, 127, 140, 140	0
2	N	363/376 (96%)	0.01	5 (1%)	73	52	102, 107, 133, 133	0
3	E	332/334 (99%)	-0.08	2 (0%)	85	69	30, 46, 62, 62	0
3	J	332/334 (99%)	-0.10	3 (0%)	81	62	52, 66, 71, 71	0
3	O	332/334 (99%)	0.03	6 (1%)	67	47	75, 182, 266, 266	0
All	All	5277/5415 (97%)	0.09	117 (2%)	62	44	30, 79, 267, 291	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	365	LEU	5.0
1	F	181	LEU	4.3
1	A	60	ASP	4.0
2	G	42	LEU	3.9
1	K	130	LEU	3.9
3	E	159	CYS	3.8
2	M	299	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	185	LEU	3.7
2	G	139	LEU	3.5
1	A	103	LEU	3.4
2	D	171	LEU	3.3
1	F	100	LEU	3.3
2	B	340	PRO	3.3
3	J	51	GLN	3.3
2	D	305	ASP	3.3
2	G	221	THR	3.2
1	F	188	LEU	3.2
2	D	359	PHE	3.2
3	O	125	ALA	3.1
2	B	3	TYR	3.1
2	G	128	VAL	3.0
2	B	354	LEU	3.0
1	F	197	LEU	3.0
1	K	100	LEU	3.0
1	A	338	ASP	2.9
2	G	357	LEU	2.9
2	N	104	THR	2.9
2	B	6	LEU	2.9
3	J	54	GLN	2.9
2	H	218	LEU	2.9
1	F	338	ASP	2.8
2	B	249	ALA	2.8
2	M	305	ASP	2.8
1	F	112	VAL	2.8
2	C	104	THR	2.8
2	D	358	ALA	2.8
2	L	6	LEU	2.8
2	B	362	ARG	2.7
1	F	110	LEU	2.7
2	I	327	LEU	2.7
2	N	354	LEU	2.7
2	H	94	ASP	2.6
2	G	277	GLU	2.6
2	B	5	VAL	2.6
1	F	91	ALA	2.6
1	F	82	LEU	2.5
3	E	334	LEU	2.5
1	F	80	LEU	2.5
2	I	19	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
3	O	256	LEU	2.5
2	D	55	ALA	2.5
3	J	159	CYS	2.5
2	G	136	PHE	2.4
1	A	112	VAL	2.4
2	L	152	PHE	2.4
1	K	188	LEU	2.4
1	A	59	THR	2.4
2	D	173	PHE	2.4
1	K	59	THR	2.4
1	A	219	ASP	2.4
2	B	268	ILE	2.4
2	B	7	ALA	2.4
2	G	170	CYS	2.4
1	A	53	PHE	2.3
2	B	282	LEU	2.3
2	B	357	LEU	2.3
1	A	267	THR	2.3
2	M	256	MET	2.3
2	M	224	ALA	2.3
2	G	166	ILE	2.3
2	B	101	VAL	2.3
2	G	290	HIS	2.3
2	M	295	VAL	2.3
2	M	354	LEU	2.3
2	G	27	ALA	2.3
1	F	170	LEU	2.3
1	K	82	LEU	2.3
2	D	271	ALA	2.3
2	I	6	LEU	2.2
1	F	92	ALA	2.2
2	B	229	ASP	2.2
1	A	55	ILE	2.2
1	F	182	ALA	2.2
3	O	185	ASP	2.2
2	H	162	LEU	2.2
2	N	364	PRO	2.2
2	L	363	MET	2.2
2	N	353	LEU	2.2
2	I	133	ARG	2.2
2	G	232	VAL	2.2
2	G	173	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	64	CYS	2.1
1	A	278	VAL	2.1
2	D	241	LEU	2.1
2	M	245	ASP	2.1
2	L	359	PHE	2.1
2	I	364	PRO	2.1
2	I	104	THR	2.1
2	G	91	ILE	2.1
2	C	49	VAL	2.1
2	I	366	PRO	2.1
2	H	214	LEU	2.1
2	L	123	TYR	2.1
3	O	248	LEU	2.1
2	G	356	ALA	2.1
1	F	79	THR	2.1
2	G	155	ALA	2.1
2	N	325	ILE	2.0
2	H	209	ALA	2.0
2	L	351	MET	2.0
1	A	328	SER	2.0
2	L	32	LEU	2.0
3	O	176	LEU	2.0
1	F	202	VAL	2.0
2	G	156	THR	2.0
2	C	108	LEU	2.0
3	O	252	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.