Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2026 – 11:09 AM UTC

PDB ID	:	4K95 / pdb_00004k95
Title	:	Crystal Structure of Parkin
Authors	:	Seirafi, M.; Menade, M.; Sauve, V.; Kozlov, G.; Trempe, J.-F.; Nagar, B.; Gehring, K.
Deposited on	:	2013-04-19
Resolution	:	6.50 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:

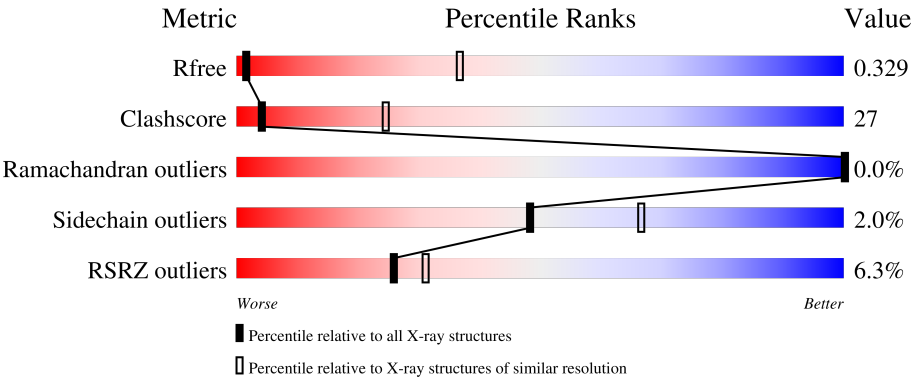
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 6.50 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	1162 (9.00-4.00)
Clashscore	190562	1020 (8.98-4.02)
Ramachandran outliers	187476	1050 (9.00-4.00)
Sidechain outliers	187428	1014 (9.00-4.00)
RSRZ outliers	180081	1155 (9.00-4.00)

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

Mol	Chain	Length	Quality of chain
1	A	470	5% 54% 23% • 20%
1	B	470	5% 51% 26% • 20%
1	C	470	4% 54% 23% • 20%
1	D	470	4% 55% 22% • 20%
1	E	470	5% 54% 23% • 20%

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Mol	Chain	Length	Quality of chain
1	F	470	5% 53% 24% 20%
1	G	470	6% 54% 23% 20%
1	H	470	6% 55% 22% 20%
1	I	470	4% 55% 22% 20%
1	J	470	5% 54% 24% 20%
1	K	470	5% 53% 24% 20%
1	L	470	6% 54% 24% 20%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 35796 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 E3 ubiquitin-protein ligase parkin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	4	0
			2975	1850	542	543	40			
1	B	375	Total	C	N	O	S	0	4	0
			2975	1850	542	543	40			
1	C	375	Total	C	N	O	S	0	4	0
			2975	1850	542	543	40			
1	D	375	Total	C	N	O	S	0	4	0
			2975	1850	542	543	40			
1	E	375	Total	C	N	O	S	0	4	0
			2975	1850	542	543	40			
1	F	375	Total	C	N	O	S	0	4	0
			2975	1850	542	543	40			
1	G	375	Total	C	N	O	S	0	4	0
			2975	1850	542	543	40			
1	H	375	Total	C	N	O	S	0	4	0
			2975	1850	542	543	40			
1	I	375	Total	C	N	O	S	0	4	0
			2975	1850	542	543	40			
1	J	375	Total	C	N	O	S	0	4	0
			2975	1850	542	543	40			
1	K	375	Total	C	N	O	S	0	4	0
			2975	1850	542	543	40			
1	L	375	Total	C	N	O	S	0	4	0
			2975	1850	542	543	40			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q9JK66
A	-3	PRO	-	expression tag	UNP Q9JK66
A	-2	LEU	-	expression tag	UNP Q9JK66
A	-1	GLY	-	expression tag	UNP Q9JK66
A	0	SER	-	expression tag	UNP Q9JK66

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Chain	Residue	Modelled	Actual	Comment	Reference
A	138	ALA	GLU	conflict	UNP Q9JK66
A	348	ARG	LYS	conflict	UNP Q9JK66
B	-4	GLY	-	expression tag	UNP Q9JK66
B	-3	PRO	-	expression tag	UNP Q9JK66
B	-2	LEU	-	expression tag	UNP Q9JK66
B	-1	GLY	-	expression tag	UNP Q9JK66
B	0	SER	-	expression tag	UNP Q9JK66
B	138	ALA	GLU	conflict	UNP Q9JK66
B	348	ARG	LYS	conflict	UNP Q9JK66
C	-4	GLY	-	expression tag	UNP Q9JK66
C	-3	PRO	-	expression tag	UNP Q9JK66
C	-2	LEU	-	expression tag	UNP Q9JK66
C	-1	GLY	-	expression tag	UNP Q9JK66
C	0	SER	-	expression tag	UNP Q9JK66
C	138	ALA	GLU	conflict	UNP Q9JK66
C	348	ARG	LYS	conflict	UNP Q9JK66
D	-4	GLY	-	expression tag	UNP Q9JK66
D	-3	PRO	-	expression tag	UNP Q9JK66
D	-2	LEU	-	expression tag	UNP Q9JK66
D	-1	GLY	-	expression tag	UNP Q9JK66
D	0	SER	-	expression tag	UNP Q9JK66
D	138	ALA	GLU	conflict	UNP Q9JK66
D	348	ARG	LYS	conflict	UNP Q9JK66
E	-4	GLY	-	expression tag	UNP Q9JK66
E	-3	PRO	-	expression tag	UNP Q9JK66
E	-2	LEU	-	expression tag	UNP Q9JK66
E	-1	GLY	-	expression tag	UNP Q9JK66
E	0	SER	-	expression tag	UNP Q9JK66
E	138	ALA	GLU	conflict	UNP Q9JK66
E	348	ARG	LYS	conflict	UNP Q9JK66
F	-4	GLY	-	expression tag	UNP Q9JK66
F	-3	PRO	-	expression tag	UNP Q9JK66
F	-2	LEU	-	expression tag	UNP Q9JK66
F	-1	GLY	-	expression tag	UNP Q9JK66
F	0	SER	-	expression tag	UNP Q9JK66
F	138	ALA	GLU	conflict	UNP Q9JK66
F	348	ARG	LYS	conflict	UNP Q9JK66
G	-4	GLY	-	expression tag	UNP Q9JK66
G	-3	PRO	-	expression tag	UNP Q9JK66
G	-2	LEU	-	expression tag	UNP Q9JK66
G	-1	GLY	-	expression tag	UNP Q9JK66
G	0	SER	-	expression tag	UNP Q9JK66

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Chain	Residue	Modelled	Actual	Comment	Reference
G	138	ALA	GLU	conflict	UNP Q9JK66
G	348	ARG	LYS	conflict	UNP Q9JK66
H	-4	GLY	-	expression tag	UNP Q9JK66
H	-3	PRO	-	expression tag	UNP Q9JK66
H	-2	LEU	-	expression tag	UNP Q9JK66
H	-1	GLY	-	expression tag	UNP Q9JK66
H	0	SER	-	expression tag	UNP Q9JK66
H	138	ALA	GLU	conflict	UNP Q9JK66
H	348	ARG	LYS	conflict	UNP Q9JK66
I	-4	GLY	-	expression tag	UNP Q9JK66
I	-3	PRO	-	expression tag	UNP Q9JK66
I	-2	LEU	-	expression tag	UNP Q9JK66
I	-1	GLY	-	expression tag	UNP Q9JK66
I	0	SER	-	expression tag	UNP Q9JK66
I	138	ALA	GLU	conflict	UNP Q9JK66
I	348	ARG	LYS	conflict	UNP Q9JK66
J	-4	GLY	-	expression tag	UNP Q9JK66
J	-3	PRO	-	expression tag	UNP Q9JK66
J	-2	LEU	-	expression tag	UNP Q9JK66
J	-1	GLY	-	expression tag	UNP Q9JK66
J	0	SER	-	expression tag	UNP Q9JK66
J	138	ALA	GLU	conflict	UNP Q9JK66
J	348	ARG	LYS	conflict	UNP Q9JK66
K	-4	GLY	-	expression tag	UNP Q9JK66
K	-3	PRO	-	expression tag	UNP Q9JK66
K	-2	LEU	-	expression tag	UNP Q9JK66
K	-1	GLY	-	expression tag	UNP Q9JK66
K	0	SER	-	expression tag	UNP Q9JK66
K	138	ALA	GLU	conflict	UNP Q9JK66
K	348	ARG	LYS	conflict	UNP Q9JK66
L	-4	GLY	-	expression tag	UNP Q9JK66
L	-3	PRO	-	expression tag	UNP Q9JK66
L	-2	LEU	-	expression tag	UNP Q9JK66
L	-1	GLY	-	expression tag	UNP Q9JK66
L	0	SER	-	expression tag	UNP Q9JK66
L	138	ALA	GLU	conflict	UNP Q9JK66
L	348	ARG	LYS	conflict	UNP Q9JK66

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf

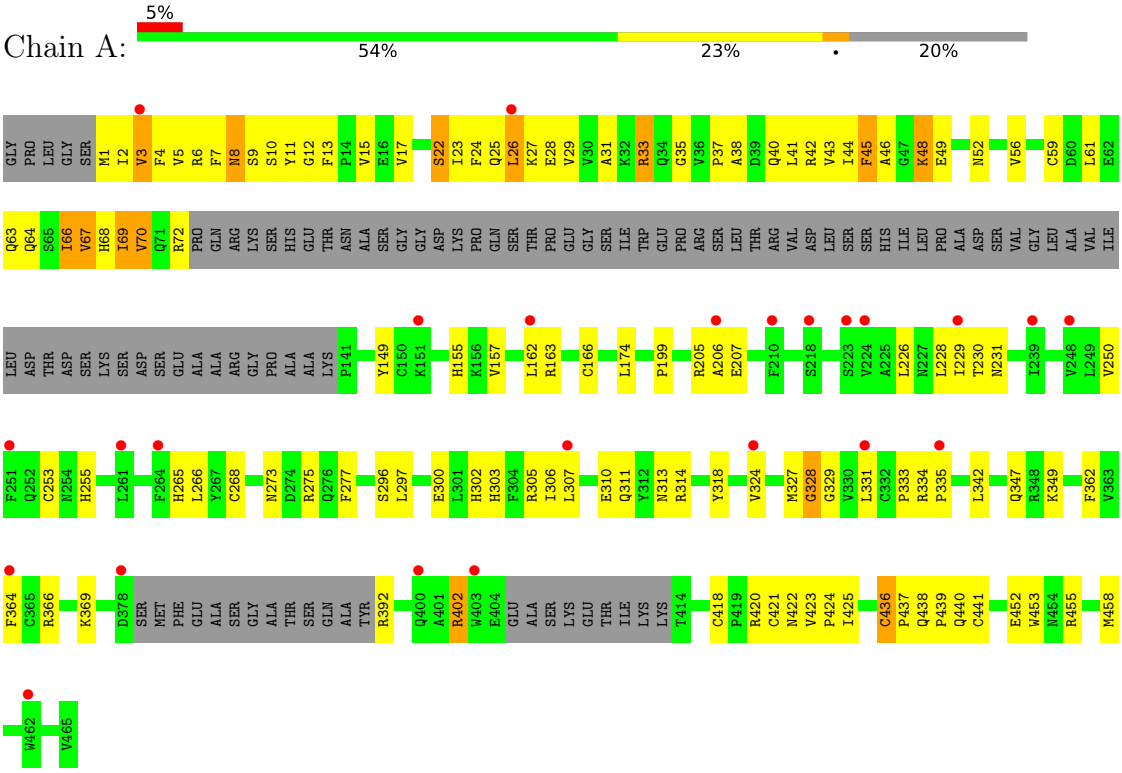
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	8	Total Zn 8 8	0	0
2	B	8	Total Zn 8 8	0	0
2	C	8	Total Zn 8 8	0	0
2	D	8	Total Zn 8 8	0	0
2	E	8	Total Zn 8 8	0	0
2	F	8	Total Zn 8 8	0	0
2	G	8	Total Zn 8 8	0	0
2	H	8	Total Zn 8 8	0	0
2	I	8	Total Zn 8 8	0	0
2	J	8	Total Zn 8 8	0	0
2	K	8	Total Zn 8 8	0	0
2	L	8	Total Zn 8 8	0	0

3 Residue-property plots (i)

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

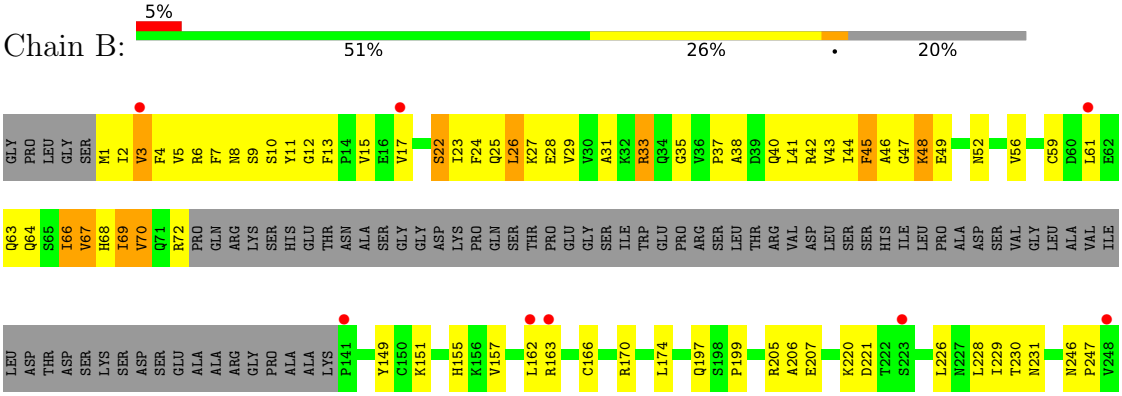
• Molecule 1: E3 ubiquitin-protein ligase parkin

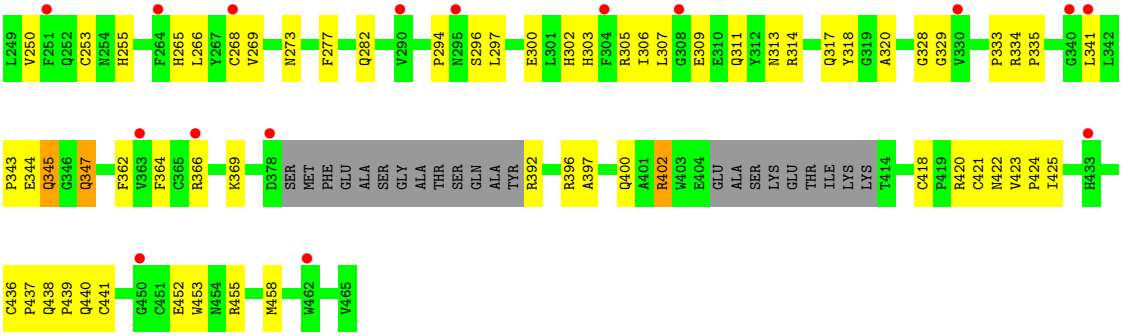
Chain A:



• Molecule 1: E3 ubiquitin-protein ligase parkin

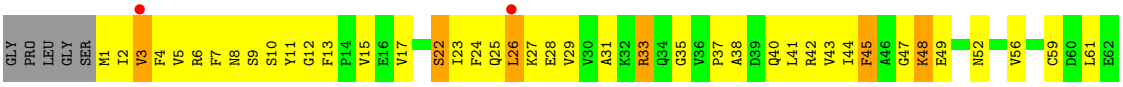
Chain B:



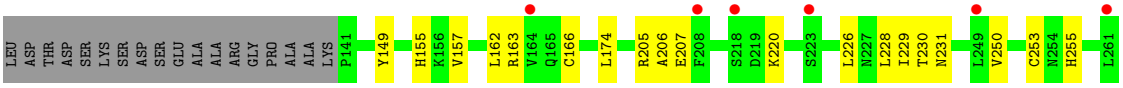


• Molecule 1: E3 ubiquitin-protein ligase parkin

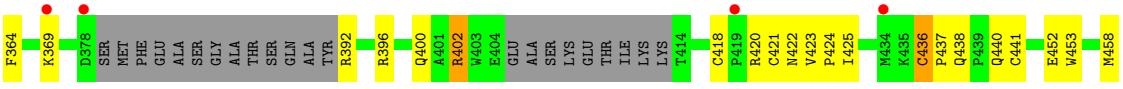








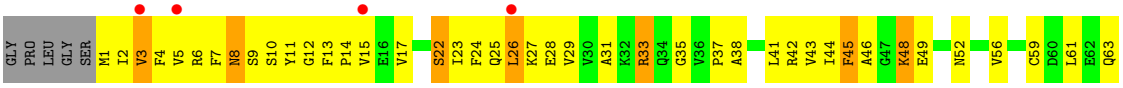


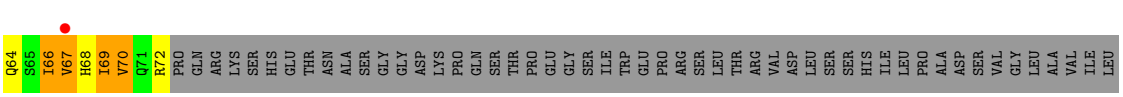




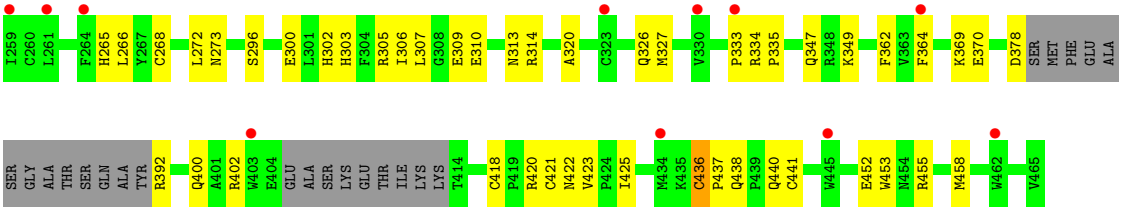
• Molecule 1: E3 ubiquitin-protein ligase parkin







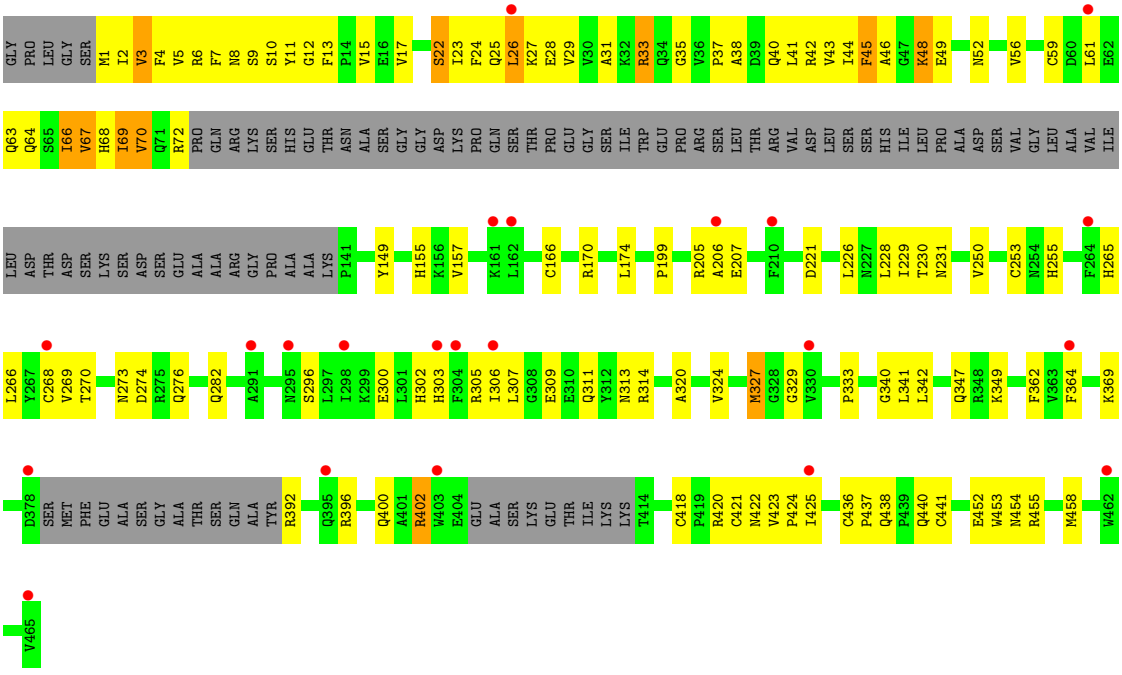




• Molecule 1: E3 ubiquitin-protein ligase parkin

Chain E:

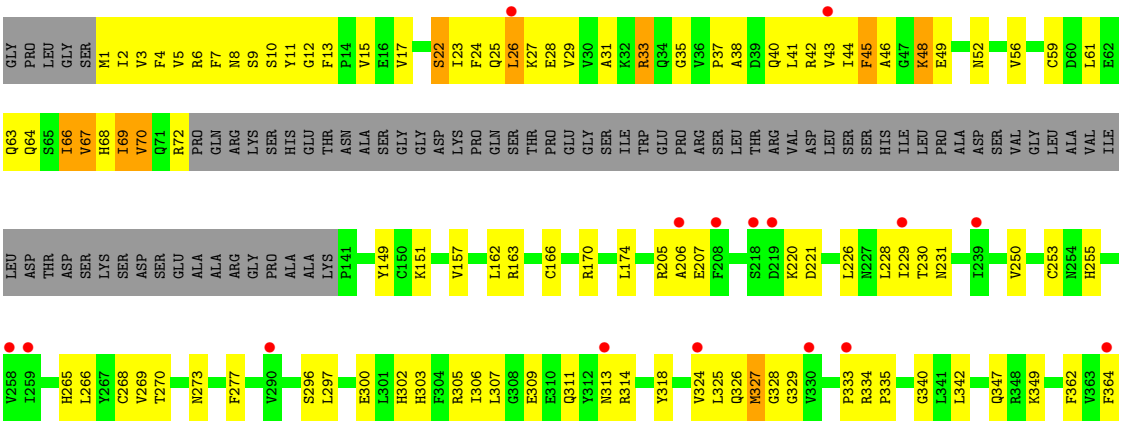


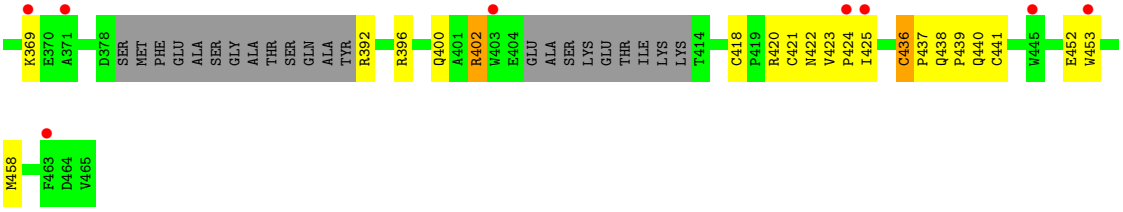


• Molecule 1: E3 ubiquitin-protein ligase parkin

Chain F:



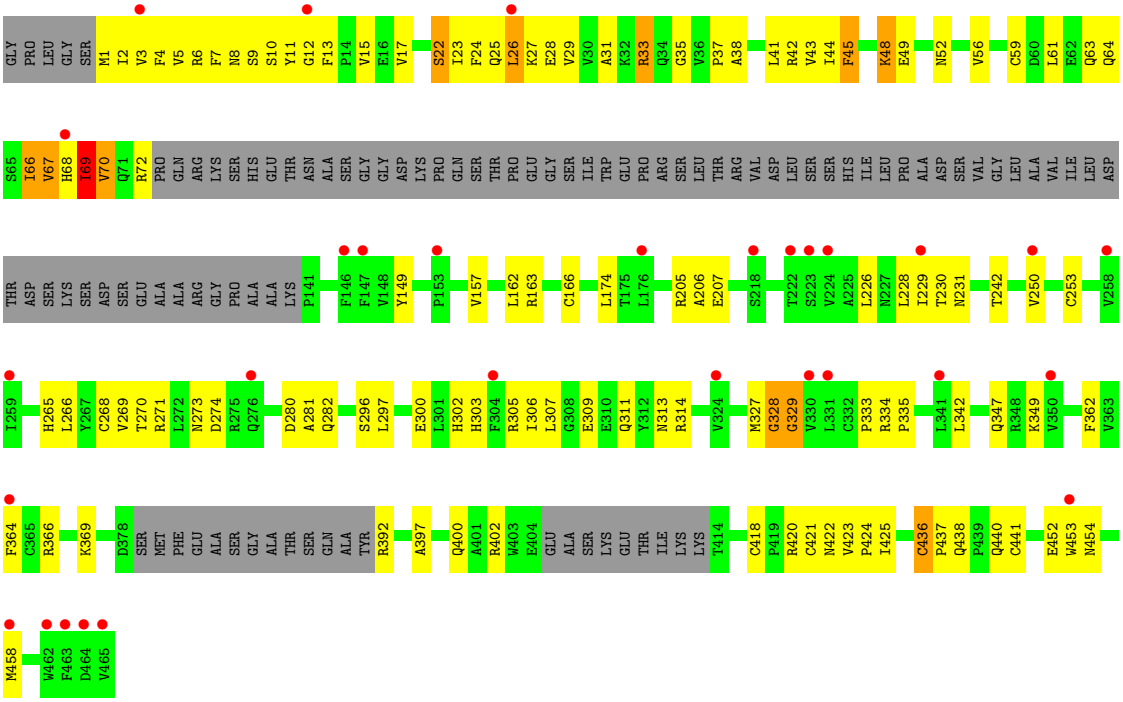




• Molecule 1: E3 ubiquitin-protein ligase parkin

Chain G:

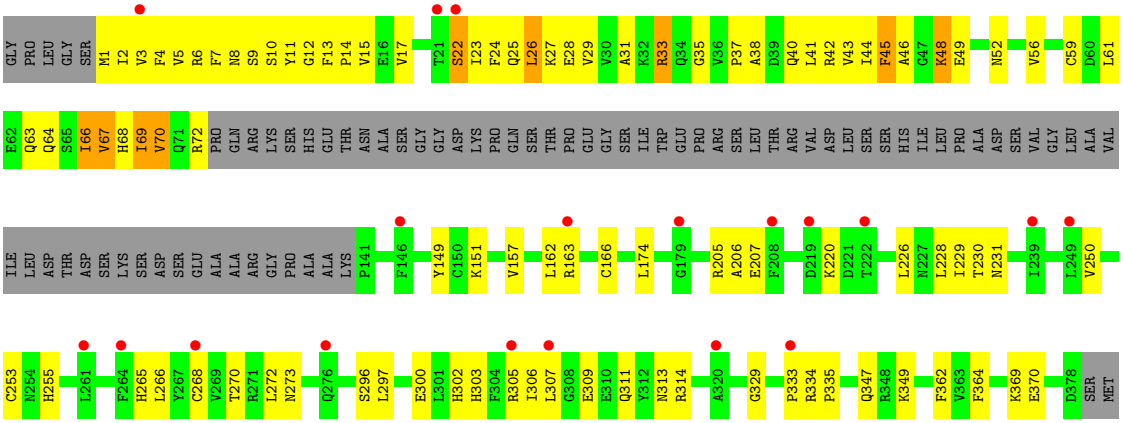


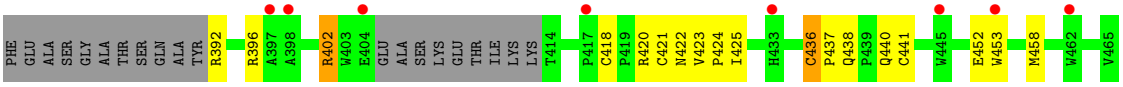


• Molecule 1: E3 ubiquitin-protein ligase parkin

Chain H:



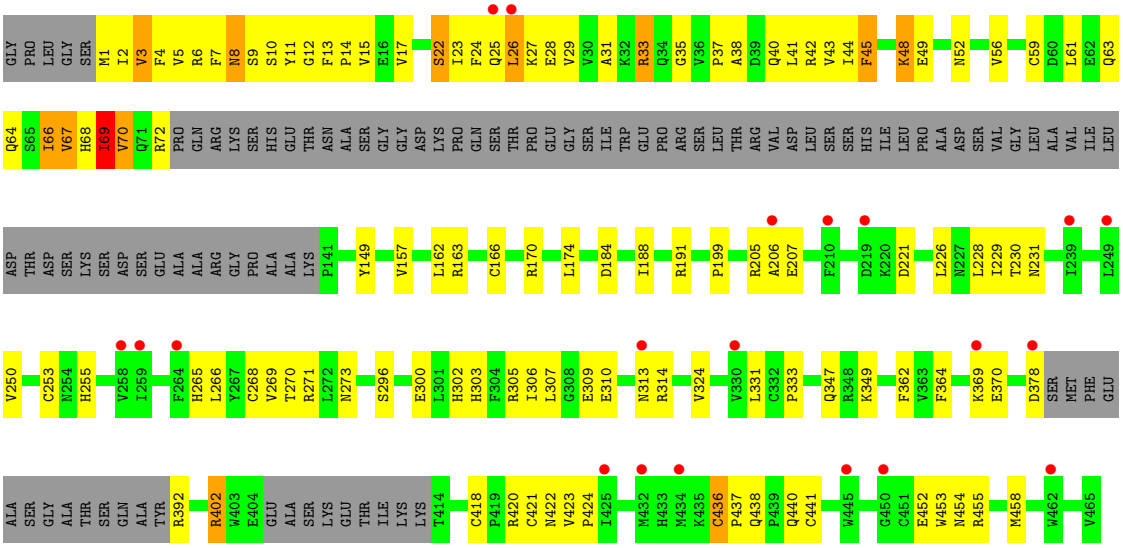




• Molecule 1: E3 ubiquitin-protein ligase parkin

Chain I:

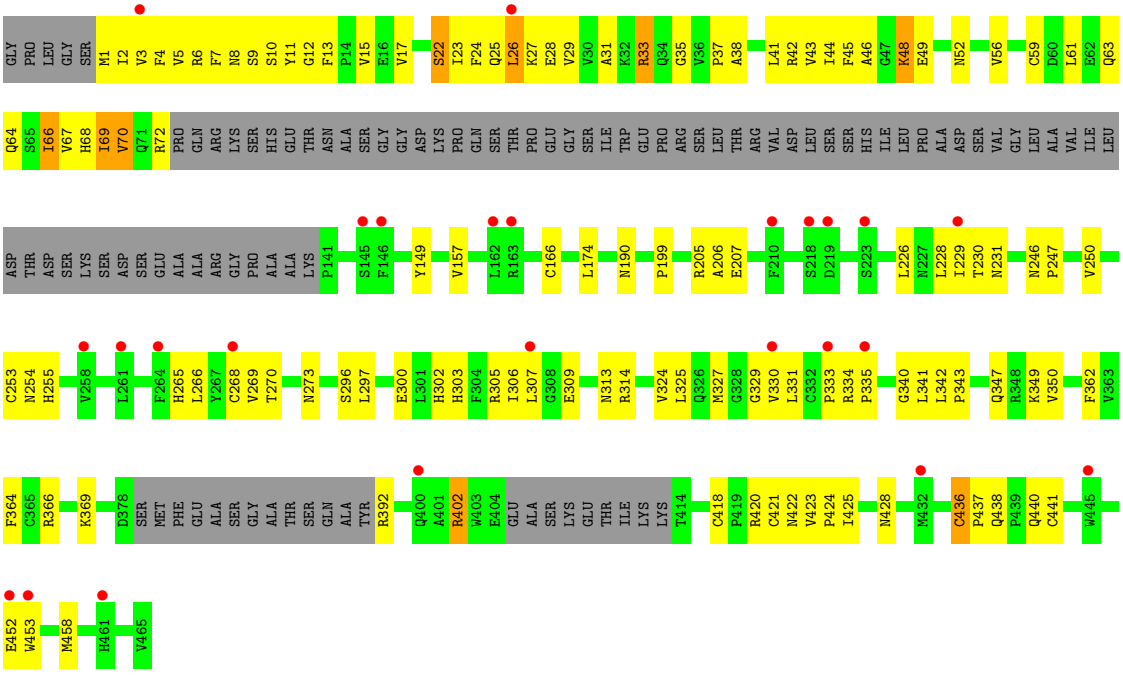




• Molecule 1: E3 ubiquitin-protein ligase parkin

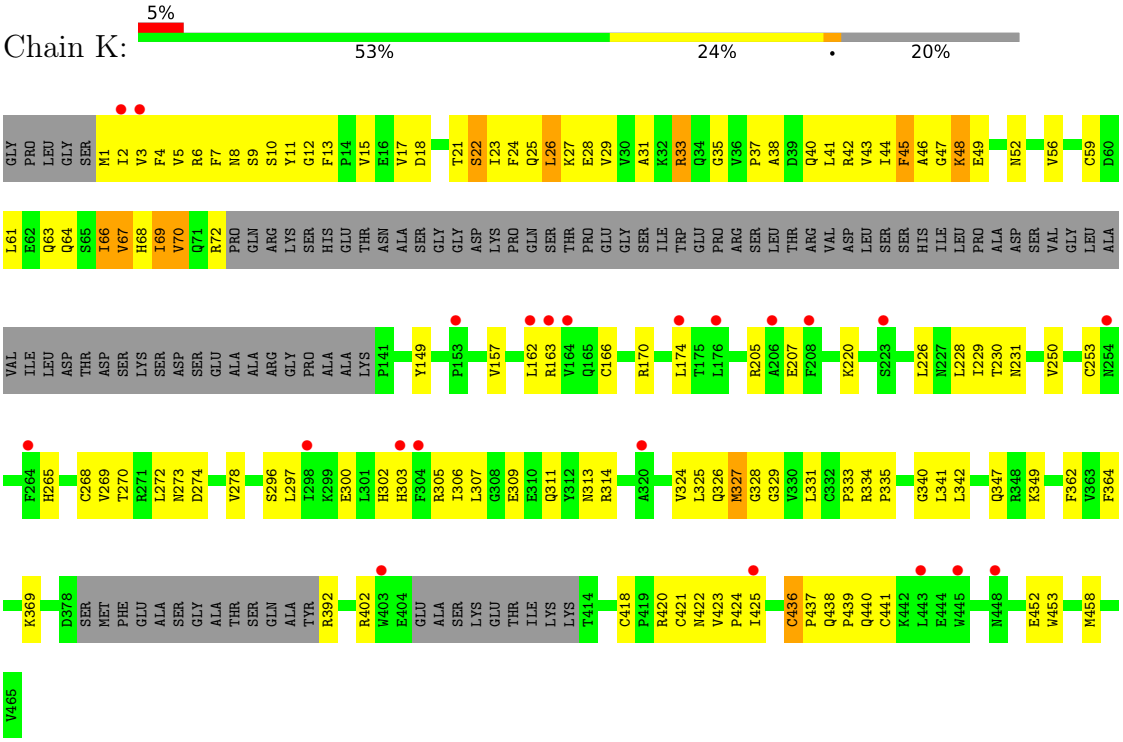
Chain J:





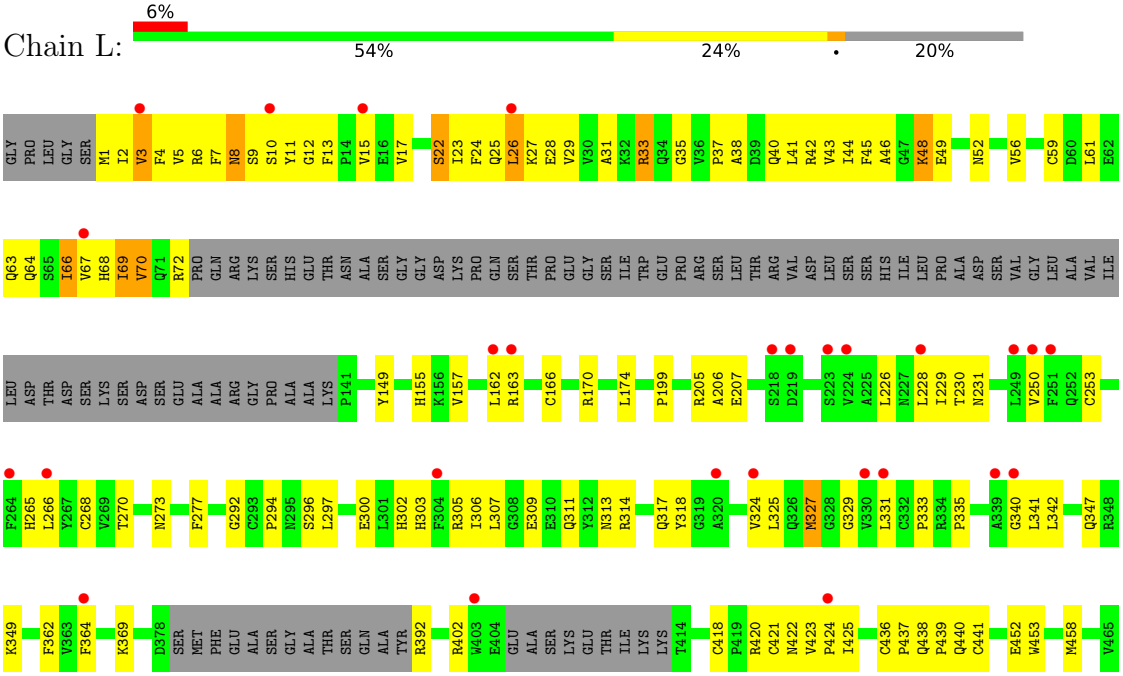
• Molecule 1: E3 ubiquitin-protein ligase parkin

Chain K:



• Molecule 1: E3 ubiquitin-protein ligase parkin

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	208.60Å 277.44Å 125.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.33 – 6.50 49.33 – 6.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.33-6.50) 99.5 (49.33-6.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.29 (at 6.68Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.307 , 0.327 0.304 , 0.329	Depositor DCC
R_{free} test set	752 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	237.2	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 346.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.77	EDS
Total number of atoms	35796	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.56	2/3051 (0.1%)	0.92	16/4125 (0.4%)
1	B	0.56	2/3051 (0.1%)	0.92	16/4125 (0.4%)
1	C	0.56	2/3051 (0.1%)	0.92	16/4125 (0.4%)
1	D	0.56	1/3051 (0.0%)	0.91	15/4125 (0.4%)
1	E	0.56	2/3051 (0.1%)	0.91	15/4125 (0.4%)
1	F	0.57	2/3051 (0.1%)	0.93	15/4125 (0.4%)
1	G	0.57	2/3051 (0.1%)	0.93	16/4125 (0.4%)
1	H	0.56	2/3051 (0.1%)	0.91	15/4125 (0.4%)
1	I	0.56	2/3051 (0.1%)	0.91	15/4125 (0.4%)
1	J	0.56	2/3051 (0.1%)	0.91	14/4125 (0.3%)
1	K	0.58	2/3051 (0.1%)	0.94	16/4125 (0.4%)
1	L	0.56	2/3051 (0.1%)	0.91	15/4125 (0.4%)
All	All	0.56	23/36612 (0.1%)	0.92	184/49500 (0.4%)

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	F	0	1
1	K	0	1
All	All	0	2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	423	VAL	C-N	5.73	1.41	1.33
1	B	423	VAL	C-N	5.71	1.41	1.33
1	E	423	VAL	C-N	5.67	1.41	1.33
1	G	423	VAL	C-N	5.67	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	423	VAL	C-N	5.66	1.41	1.33
1	A	423	VAL	C-N	5.65	1.41	1.33
1	F	423	VAL	C-N	5.64	1.41	1.33
1	I	423	VAL	C-N	5.64	1.41	1.33
1	D	423	VAL	C-N	5.64	1.41	1.33
1	C	423	VAL	C-N	5.62	1.41	1.33
1	H	423	VAL	C-N	5.62	1.41	1.33
1	L	423	VAL	C-N	5.60	1.40	1.33
1	H	424	PRO	N-CD	5.14	1.54	1.47
1	J	424	PRO	N-CD	5.10	1.54	1.47
1	A	424	PRO	N-CD	5.09	1.54	1.47
1	F	424	PRO	N-CD	5.08	1.54	1.47
1	I	424	PRO	N-CD	5.08	1.54	1.47
1	B	424	PRO	N-CD	5.08	1.54	1.47
1	E	424	PRO	N-CD	5.07	1.54	1.47
1	L	424	PRO	N-CD	5.06	1.54	1.47
1	G	424	PRO	N-CD	5.04	1.54	1.47
1	K	424	PRO	N-CD	5.04	1.54	1.47
1	C	424	PRO	N-CD	5.03	1.54	1.47

All (184) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	328	GLY	N-CA-C	-10.74	100.50	115.32
1	F	328	GLY	N-CA-C	-9.88	102.22	115.36
1	C	329	GLY	N-CA-C	9.28	126.70	112.51
1	B	329	GLY	N-CA-C	9.06	124.14	112.54
1	G	328	GLY	N-CA-C	-8.91	103.79	115.47
1	K	328	GLY	CA-C-O	7.11	127.03	119.06
1	F	69	ILE	CB-CA-C	-6.88	100.59	110.83
1	E	69	ILE	CB-CA-C	-6.87	100.60	110.83
1	L	69	ILE	CB-CA-C	-6.87	100.60	110.83
1	B	69	ILE	CB-CA-C	-6.84	100.63	110.83
1	K	69	ILE	CB-CA-C	-6.84	100.63	110.83
1	G	69	ILE	CB-CA-C	-6.84	100.64	110.83
1	D	69	ILE	CB-CA-C	-6.84	100.64	110.83
1	A	69	ILE	CB-CA-C	-6.83	100.65	110.83
1	H	69	ILE	CB-CA-C	-6.83	100.65	110.83
1	I	69	ILE	CB-CA-C	-6.83	100.66	110.83
1	J	69	ILE	CB-CA-C	-6.81	100.69	110.83
1	C	69	ILE	CB-CA-C	-6.80	100.57	110.63
1	D	423	VAL	CA-C-N	-6.61	112.96	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	423	VAL	C-N-CA	-6.61	112.96	119.76
1	I	423	VAL	CA-C-N	-6.61	112.96	119.76
1	I	423	VAL	C-N-CA	-6.61	112.96	119.76
1	J	423	VAL	CA-C-N	-6.60	112.96	119.76
1	J	423	VAL	C-N-CA	-6.60	112.96	119.76
1	K	423	VAL	CA-C-N	-6.58	112.98	119.76
1	K	423	VAL	C-N-CA	-6.58	112.98	119.76
1	L	423	VAL	CA-C-N	-6.58	112.98	119.76
1	L	423	VAL	C-N-CA	-6.58	112.98	119.76
1	F	423	VAL	CA-C-N	-6.57	112.99	119.76
1	F	423	VAL	C-N-CA	-6.57	112.99	119.76
1	G	423	VAL	CA-C-N	-6.56	113.00	119.76
1	G	423	VAL	C-N-CA	-6.56	113.00	119.76
1	A	328	GLY	N-CA-C	-6.55	106.65	115.36
1	A	423	VAL	CA-C-N	-6.55	113.01	119.76
1	A	423	VAL	C-N-CA	-6.55	113.01	119.76
1	C	423	VAL	CA-C-N	-6.55	113.02	119.76
1	C	423	VAL	C-N-CA	-6.55	113.02	119.76
1	B	423	VAL	CA-C-N	-6.55	113.02	119.76
1	B	423	VAL	C-N-CA	-6.55	113.02	119.76
1	E	423	VAL	CA-C-N	-6.54	113.03	119.76
1	E	423	VAL	C-N-CA	-6.54	113.03	119.76
1	H	423	VAL	CA-C-N	-6.54	113.03	119.76
1	H	423	VAL	C-N-CA	-6.54	113.03	119.76
1	K	67	VAL	N-CA-C	6.34	118.89	108.99
1	A	67	VAL	N-CA-C	6.34	118.88	108.99
1	G	67	VAL	N-CA-C	6.33	118.86	108.99
1	D	67	VAL	N-CA-C	6.33	118.86	108.99
1	B	67	VAL	N-CA-C	6.32	118.85	108.99
1	I	67	VAL	N-CA-C	6.32	118.85	108.99
1	J	67	VAL	N-CA-C	6.32	118.84	108.99
1	E	67	VAL	N-CA-C	6.31	118.83	108.99
1	L	67	VAL	N-CA-C	6.31	118.83	108.99
1	H	67	VAL	N-CA-C	6.28	118.78	108.99
1	C	67	VAL	N-CA-C	6.28	118.78	108.99
1	F	67	VAL	N-CA-C	6.27	118.78	108.99
1	B	23	ILE	CB-CA-C	-5.76	104.53	112.24
1	G	329	GLY	N-CA-C	-5.75	105.17	112.54
1	C	23	ILE	CB-CA-C	-5.74	104.52	112.04
1	D	23	ILE	CB-CA-C	-5.72	104.54	112.04
1	G	23	ILE	CB-CA-C	-5.72	104.58	112.24
1	F	23	ILE	CB-CA-C	-5.70	104.58	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	23	ILE	CB-CA-C	-5.69	104.58	112.04
1	K	23	ILE	CB-CA-C	-5.69	104.59	112.04
1	L	23	ILE	CB-CA-C	-5.69	104.59	112.04
1	H	23	ILE	CB-CA-C	-5.67	104.61	112.04
1	A	23	ILE	CB-CA-C	-5.67	104.62	112.04
1	I	23	ILE	CB-CA-C	-5.65	104.64	112.04
1	J	23	ILE	CB-CA-C	-5.63	104.67	112.04
1	A	48	LYS	N-CA-C	5.58	117.53	108.26
1	K	48	LYS	N-CA-C	5.58	117.51	108.26
1	C	48	LYS	N-CA-C	5.57	117.51	108.26
1	E	48	LYS	N-CA-C	5.57	117.51	108.26
1	D	48	LYS	N-CA-C	5.57	117.50	108.26
1	J	48	LYS	N-CA-C	5.57	117.50	108.26
1	B	48	LYS	N-CA-C	5.57	117.50	108.26
1	H	329	GLY	N-CA-C	5.57	121.02	112.51
1	I	48	LYS	N-CA-C	5.57	117.50	108.26
1	F	48	LYS	N-CA-C	5.56	117.49	108.26
1	L	48	LYS	N-CA-C	5.54	117.46	108.26
1	H	48	LYS	N-CA-C	5.54	117.45	108.26
1	B	33	ARG	N-CA-C	-5.52	105.27	112.23
1	A	33	ARG	N-CA-C	-5.51	105.28	112.23
1	F	33	ARG	N-CA-C	-5.51	105.28	112.23
1	L	33	ARG	N-CA-C	-5.51	105.29	112.23
1	H	33	ARG	N-CA-C	-5.50	105.30	112.23
1	E	33	ARG	N-CA-C	-5.50	105.31	112.23
1	G	48	LYS	N-CA-C	5.50	117.38	108.26
1	C	33	ARG	N-CA-C	-5.49	105.31	112.23
1	D	33	ARG	N-CA-C	-5.49	105.32	112.23
1	G	33	ARG	N-CA-C	-5.49	105.32	112.23
1	I	33	ARG	N-CA-C	-5.49	105.32	112.23
1	K	33	ARG	N-CA-C	-5.47	105.34	112.23
1	J	33	ARG	N-CA-C	-5.46	105.35	112.23
1	F	35	GLY	CA-C-N	-5.46	118.58	123.33
1	F	35	GLY	C-N-CA	-5.46	118.58	123.33
1	D	35	GLY	CA-C-N	-5.45	118.58	123.33
1	D	35	GLY	C-N-CA	-5.45	118.58	123.33
1	C	35	GLY	CA-C-N	-5.44	118.60	123.33
1	C	35	GLY	C-N-CA	-5.44	118.60	123.33
1	F	70	VAL	CB-CA-C	-5.42	103.44	111.19
1	E	70	VAL	CB-CA-C	-5.41	103.46	111.19
1	J	35	GLY	CA-C-N	-5.39	118.64	123.33
1	J	35	GLY	C-N-CA	-5.39	118.64	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	35	GLY	CA-C-N	-5.39	118.64	123.33
1	H	35	GLY	C-N-CA	-5.39	118.64	123.33
1	I	35	GLY	CA-C-N	-5.39	118.64	123.33
1	I	35	GLY	C-N-CA	-5.39	118.64	123.33
1	K	70	VAL	CB-CA-C	-5.39	103.48	111.19
1	L	70	VAL	CB-CA-C	-5.38	103.49	111.19
1	L	35	GLY	CA-C-N	-5.38	118.65	123.33
1	L	35	GLY	C-N-CA	-5.38	118.65	123.33
1	K	35	GLY	CA-C-N	-5.38	118.65	123.33
1	K	35	GLY	C-N-CA	-5.38	118.65	123.33
1	G	35	GLY	CA-C-N	-5.38	118.65	123.33
1	G	35	GLY	C-N-CA	-5.38	118.65	123.33
1	A	35	GLY	CA-C-N	-5.37	118.66	123.33
1	A	35	GLY	C-N-CA	-5.37	118.66	123.33
1	E	35	GLY	CA-C-N	-5.36	118.67	123.33
1	E	35	GLY	C-N-CA	-5.36	118.67	123.33
1	B	35	GLY	CA-C-N	-5.30	118.72	123.33
1	B	35	GLY	C-N-CA	-5.30	118.72	123.33
1	K	45	PHE	N-CA-C	5.25	117.93	108.48
1	F	26	LEU	N-CA-C	5.25	117.08	111.36
1	E	26	LEU	N-CA-C	5.24	117.07	111.36
1	C	45	PHE	N-CA-C	5.23	117.90	108.48
1	I	45	PHE	N-CA-C	5.23	117.89	108.48
1	F	45	PHE	N-CA-C	5.22	117.89	108.48
1	G	45	PHE	N-CA-C	5.22	117.88	108.48
1	E	45	PHE	N-CA-C	5.22	117.87	108.48
1	J	45	PHE	N-CA-C	5.22	117.87	108.48
1	A	26	LEU	N-CA-C	5.21	117.04	111.36
1	L	26	LEU	N-CA-C	5.21	117.04	111.36
1	L	45	PHE	N-CA-C	5.21	117.86	108.48
1	D	45	PHE	N-CA-C	5.21	117.86	108.48
1	B	26	LEU	N-CA-C	5.21	117.04	111.36
1	D	26	LEU	N-CA-C	5.21	117.04	111.36
1	H	45	PHE	N-CA-C	5.21	117.85	108.48
1	C	26	LEU	N-CA-C	5.21	117.03	111.36
1	B	45	PHE	N-CA-C	5.20	117.84	108.48
1	B	70	VAL	CB-CA-C	-5.20	103.41	110.90
1	A	45	PHE	N-CA-C	5.20	117.84	108.48
1	D	70	VAL	CB-CA-C	-5.20	103.41	110.90
1	G	70	VAL	CB-CA-C	-5.20	103.42	110.90
1	C	70	VAL	CB-CA-C	-5.19	103.42	110.90
1	J	26	LEU	N-CA-C	5.19	117.02	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	70	VAL	CB-CA-C	-5.19	103.43	110.90
1	K	26	LEU	N-CA-C	5.19	117.02	111.36
1	H	70	VAL	CB-CA-C	-5.19	103.43	110.90
1	I	70	VAL	CB-CA-C	-5.18	103.44	110.90
1	B	436	CYS	CA-C-N	5.17	124.87	119.64
1	B	436	CYS	C-N-CA	5.17	124.87	119.64
1	G	26	LEU	N-CA-C	5.17	117.00	111.36
1	I	26	LEU	N-CA-C	5.17	116.99	111.36
1	H	26	LEU	N-CA-C	5.16	116.98	111.36
1	A	70	VAL	CB-CA-C	-5.15	103.48	110.90
1	H	436	CYS	CA-C-N	5.15	124.84	119.64
1	H	436	CYS	C-N-CA	5.15	124.84	119.64
1	J	436	CYS	CA-C-N	5.12	124.82	119.64
1	J	436	CYS	C-N-CA	5.12	124.82	119.64
1	C	436	CYS	CA-C-N	5.12	124.81	119.64
1	C	436	CYS	C-N-CA	5.12	124.81	119.64
1	F	436	CYS	CA-C-N	5.11	124.80	119.64
1	F	436	CYS	C-N-CA	5.11	124.80	119.64
1	I	436	CYS	CA-C-N	5.11	124.80	119.64
1	I	436	CYS	C-N-CA	5.11	124.80	119.64
1	L	436	CYS	CA-C-N	5.11	124.80	119.64
1	L	436	CYS	C-N-CA	5.11	124.80	119.64
1	A	436	CYS	CA-C-N	5.10	124.79	119.64
1	A	436	CYS	C-N-CA	5.10	124.79	119.64
1	E	436	CYS	CA-C-N	5.07	124.76	119.64
1	E	436	CYS	C-N-CA	5.07	124.76	119.64
1	D	436	CYS	CA-C-N	5.07	124.76	119.64
1	D	436	CYS	C-N-CA	5.07	124.76	119.64
1	K	436	CYS	CA-C-N	5.06	124.75	119.64
1	K	436	CYS	C-N-CA	5.06	124.75	119.64
1	A	3	VAL	N-CA-C	5.04	115.16	108.11
1	G	436	CYS	CA-C-N	5.03	124.72	119.64
1	G	436	CYS	C-N-CA	5.03	124.72	119.64
1	D	3	VAL	N-CA-C	5.03	115.15	108.11
1	E	3	VAL	N-CA-C	5.02	115.14	108.11
1	I	3	VAL	N-CA-C	5.02	115.13	108.11
1	B	3	VAL	N-CA-C	5.01	115.13	108.11
1	L	3	VAL	N-CA-C	5.01	115.13	108.11
1	C	3	VAL	N-CA-C	5.01	115.12	108.11

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	327	MET	Mainchain
1	K	327	MET	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2975	0	2830	147	0
1	B	2975	0	2830	209	12
1	C	2975	0	2826	164	4
1	D	2975	0	2831	161	6
1	E	2975	0	2831	194	3
1	F	2975	0	2829	196	8
1	G	2975	0	2832	142	8
1	H	2975	0	2828	153	0
1	I	2975	0	2831	189	1
1	J	2975	0	2831	186	1
1	K	2975	0	2829	168	12
1	L	2975	0	2832	193	6
2	A	8	0	0	0	0
2	B	8	0	0	0	0
2	C	8	0	0	0	0
2	D	8	0	0	0	0
2	E	8	0	0	0	0
2	F	8	0	0	0	0
2	G	8	0	0	0	0
2	H	8	0	0	0	0
2	I	8	0	0	0	0
2	J	8	0	0	0	0
2	K	8	0	0	0	0
2	L	8	0	0	0	0
All	All	35796	0	33960	1910	31

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 27.

All (1910) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:ALA:CA	1:E:392:ARG:HH11	1.05	1.64
1:D:46:ALA:CA	1:D:392:ARG:HH11	1.09	1.58
1:C:44:ILE:CD1	1:C:266:LEU:CD2	1.77	1.58
1:L:11:TYR:CZ	1:L:333:PRO:HB2	1.34	1.58
1:B:44:ILE:HD13	1:B:266:LEU:CD2	1.06	1.54
1:J:44:ILE:HD13	1:J:266:LEU:CD2	1.12	1.54
1:C:44:ILE:HD13	1:C:266:LEU:CD2	1.10	1.52
1:H:46:ALA:CA	1:H:392:ARG:HH11	1.20	1.51
1:F:46:ALA:CA	1:F:392:ARG:HH11	0.87	1.51
1:J:44:ILE:CD1	1:J:266:LEU:HD22	1.40	1.49
1:F:44:ILE:HD13	1:F:266:LEU:CD2	1.37	1.48
1:C:44:ILE:CG1	1:C:266:LEU:HD21	1.44	1.47
1:B:396:ARG:NH1	1:F:396:ARG:C	1.67	1.46
1:J:46:ALA:HA	1:J:392:ARG:CD	1.45	1.46
1:F:46:ALA:CA	1:F:392:ARG:NH1	1.72	1.46
1:D:46:ALA:CB	1:D:392:ARG:NH1	1.79	1.45
1:D:11:TYR:CD1	1:D:369:LYS:CE	1.98	1.44
1:J:46:ALA:CA	1:J:392:ARG:HH11	1.28	1.43
1:E:46:ALA:HB2	1:E:392:ARG:NH1	1.27	1.43
1:E:44:ILE:HD13	1:E:266:LEU:CD2	1.49	1.42
1:B:44:ILE:CD1	1:B:266:LEU:CD2	1.94	1.42
1:H:11:TYR:CD1	1:H:369:LYS:CE	2.03	1.41
1:C:11:TYR:CD1	1:C:369:LYS:CE	2.03	1.41
1:E:46:ALA:CB	1:E:392:ARG:NH1	1.81	1.40
1:F:46:ALA:CB	1:F:392:ARG:NH1	1.83	1.38
1:B:46:ALA:C	1:B:392:ARG:CD	1.98	1.37
1:C:11:TYR:CD1	1:C:369:LYS:HE2	1.59	1.37
1:J:44:ILE:CD1	1:J:266:LEU:CD2	1.96	1.36
1:C:44:ILE:CD1	1:C:266:LEU:HD21	1.45	1.35
1:B:46:ALA:CA	1:B:392:ARG:CD	2.02	1.35
1:I:11:TYR:CZ	1:I:333:PRO:HB2	1.59	1.35
1:C:11:TYR:CZ	1:C:333:PRO:HB2	1.61	1.35
1:E:327:MET:CB	1:E:342:LEU:HD21	1.55	1.35
1:E:327:MET:HB3	1:E:342:LEU:CD2	1.57	1.34
1:D:46:ALA:HA	1:D:392:ARG:NH1	1.29	1.34
1:L:46:ALA:CA	1:L:392:ARG:HH11	1.39	1.34
1:I:11:TYR:CZ	1:I:333:PRO:CB	2.12	1.33
1:L:11:TYR:CE1	1:L:333:PRO:CB	2.12	1.33
1:H:44:ILE:HD13	1:H:266:LEU:CD2	1.59	1.32
1:E:46:ALA:CB	1:E:392:ARG:HH11	1.35	1.32
1:C:44:ILE:HD13	1:C:266:LEU:CG	1.60	1.32
1:D:11:TYR:CD1	1:D:369:LYS:HE2	1.58	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:ALA:HB2	1:F:392:ARG:NH1	1.44	1.31
1:A:44:ILE:HD13	1:A:266:LEU:CD2	1.60	1.30
1:H:46:ALA:HA	1:H:392:ARG:NH1	1.47	1.30
1:D:11:TYR:CE1	1:D:369:LYS:HE3	1.65	1.29
1:K:327:MET:O	1:K:342:LEU:HD22	1.20	1.29
1:D:6:ARG:NE	1:D:66:ILE:HD11	1.47	1.29
1:J:6:ARG:NE	1:J:66:ILE:HD11	1.47	1.29
1:B:11:TYR:CZ	1:B:333:PRO:HB2	1.67	1.29
1:L:6:ARG:NE	1:L:66:ILE:HD11	1.47	1.28
1:H:6:ARG:NH1	1:H:273:ASN:CB	1.95	1.28
1:K:6:ARG:NE	1:K:66:ILE:HD11	1.47	1.28
1:C:72:ARG:NH2	1:C:265:HIS:HD2	1.29	1.27
1:B:46:ALA:C	1:B:392:ARG:HD2	1.58	1.27
1:F:6:ARG:NE	1:F:66:ILE:HD11	1.47	1.27
1:D:46:ALA:CA	1:D:392:ARG:NH1	1.79	1.27
1:E:6:ARG:NE	1:E:66:ILE:HD11	1.47	1.27
1:B:6:ARG:NE	1:B:66:ILE:HD11	1.47	1.26
1:G:6:ARG:NE	1:G:66:ILE:HD11	1.47	1.26
1:I:11:TYR:OH	1:I:333:PRO:HB2	1.15	1.26
1:B:11:TYR:OH	1:B:333:PRO:HB2	1.34	1.26
1:I:184:ASP:O	1:I:188:ILE:HG22	1.33	1.26
1:A:6:ARG:NE	1:A:66:ILE:HD11	1.47	1.26
1:I:6:ARG:NE	1:I:66:ILE:HD11	1.47	1.26
1:C:11:TYR:CZ	1:C:333:PRO:CB	2.16	1.25
1:J:327:MET:O	1:J:342:LEU:HD21	1.16	1.25
1:F:11:TYR:OH	1:F:333:PRO:HB2	1.23	1.25
1:L:11:TYR:CE1	1:L:333:PRO:HB2	1.69	1.25
1:C:11:TYR:OH	1:C:333:PRO:CB	1.85	1.25
1:H:6:ARG:NH1	1:H:273:ASN:HB3	1.50	1.25
1:B:44:ILE:CD1	1:B:266:LEU:HD21	1.55	1.25
1:E:46:ALA:CA	1:E:392:ARG:NH1	1.91	1.24
1:J:190:ASN:OD1	1:J:205:ARG:HD2	1.20	1.24
1:J:327:MET:O	1:J:342:LEU:CD2	1.84	1.24
1:K:327:MET:O	1:K:342:LEU:CD2	1.82	1.24
1:H:11:TYR:CD1	1:H:369:LYS:HE2	1.66	1.24
1:D:11:TYR:CD1	1:D:369:LYS:HE3	1.64	1.23
1:I:188:ILE:HD13	1:I:191:ARG:NH2	1.51	1.22
1:B:396:ARG:NH1	1:F:396:ARG:O	1.72	1.22
1:E:327:MET:CG	1:E:342:LEU:HD11	1.68	1.22
1:C:11:TYR:CE1	1:C:333:PRO:CB	2.22	1.22
1:H:46:ALA:CA	1:H:392:ARG:NH1	1.98	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:ARG:NE	1:D:313:ASN:OD1	1.71	1.22
1:H:11:TYR:CD1	1:H:369:LYS:HE3	1.70	1.22
1:I:11:TYR:OH	1:I:333:PRO:CB	1.85	1.21
1:D:44:ILE:HD13	1:D:266:LEU:CD2	1.70	1.21
1:G:44:ILE:HD13	1:G:266:LEU:CD1	1.71	1.21
1:L:11:TYR:CE1	1:L:333:PRO:O	1.95	1.20
1:H:14:PRO:CD	1:H:370:GLU:OE1	1.89	1.20
1:F:44:ILE:CD1	1:F:266:LEU:HD22	1.71	1.19
1:F:46:ALA:CB	1:F:392:ARG:HH11	1.48	1.19
1:E:327:MET:HG2	1:E:342:LEU:CD1	1.73	1.19
1:B:44:ILE:CD1	1:B:266:LEU:HD22	1.66	1.18
1:E:46:ALA:HA	1:E:392:ARG:CD	1.73	1.18
1:C:11:TYR:CE1	1:C:333:PRO:HB3	1.78	1.18
1:J:46:ALA:HB2	1:J:392:ARG:NH1	1.56	1.18
1:L:324:VAL:HG11	1:L:340:GLY:CA	1.71	1.18
1:J:452:GLU:CD	1:L:309:GLU:OE2	1.85	1.17
1:H:44:ILE:HD13	1:H:266:LEU:HD22	1.21	1.17
1:K:11:TYR:CZ	1:K:333:PRO:HB2	1.78	1.17
1:A:313:ASN:OD1	1:F:420:ARG:NE	1.76	1.17
1:L:324:VAL:HG11	1:L:340:GLY:HA3	1.22	1.17
1:F:44:ILE:CD1	1:F:266:LEU:CD2	2.21	1.17
1:G:6:ARG:NE	1:G:66:ILE:CD1	2.08	1.17
1:L:11:TYR:CE1	1:L:333:PRO:CA	2.27	1.17
1:B:199:PRO:HD3	1:D:170:ARG:NE	1.59	1.17
1:B:11:TYR:CZ	1:B:333:PRO:CB	2.27	1.16
1:C:44:ILE:CD1	1:C:266:LEU:HD22	1.56	1.16
1:J:6:ARG:NE	1:J:66:ILE:CD1	2.08	1.16
1:L:6:ARG:NE	1:L:66:ILE:CD1	2.09	1.16
1:K:11:TYR:OH	1:K:333:PRO:O	1.62	1.16
1:L:44:ILE:HD13	1:L:266:LEU:CD2	1.75	1.16
1:E:327:MET:HG2	1:E:342:LEU:HD11	1.20	1.16
1:F:6:ARG:NE	1:F:66:ILE:CD1	2.08	1.16
1:L:11:TYR:CZ	1:L:333:PRO:CB	2.26	1.16
1:L:11:TYR:HE1	1:L:333:PRO:CA	1.59	1.16
1:I:44:ILE:HD13	1:I:266:LEU:CD2	1.76	1.15
1:F:46:ALA:HA	1:F:392:ARG:NH1	1.41	1.15
1:B:46:ALA:C	1:B:392:ARG:HD3	1.62	1.15
1:E:44:ILE:CD1	1:E:266:LEU:HD22	1.76	1.15
1:D:6:ARG:NE	1:D:66:ILE:CD1	2.09	1.15
1:E:329:GLY:HA3	1:E:341:LEU:O	1.44	1.15
1:E:6:ARG:NE	1:E:66:ILE:CD1	2.08	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:11:TYR:CE1	1:G:333:PRO:HB2	1.81	1.14
1:K:6:ARG:NE	1:K:66:ILE:CD1	2.08	1.14
1:B:6:ARG:NE	1:B:66:ILE:CD1	2.09	1.14
1:A:6:ARG:NE	1:A:66:ILE:CD1	2.09	1.14
1:K:324:VAL:HG11	1:K:340:GLY:HA3	1.28	1.14
1:J:452:GLU:CG	1:L:309:GLU:OE2	1.95	1.14
1:B:44:ILE:CG1	1:B:266:LEU:HD21	1.78	1.13
1:I:6:ARG:NE	1:I:66:ILE:CD1	2.08	1.13
1:J:325:LEU:HD21	1:J:331:LEU:CD1	1.76	1.13
1:J:325:LEU:CD2	1:J:331:LEU:HD11	1.78	1.13
1:K:327:MET:HB3	1:K:342:LEU:HD21	1.31	1.12
1:D:72:ARG:HH22	1:D:265:HIS:CD2	1.68	1.12
1:J:46:ALA:CA	1:J:392:ARG:NH1	2.12	1.12
1:K:309:GLU:OE2	1:L:452:GLU:HG2	1.48	1.12
1:J:44:ILE:CG1	1:J:266:LEU:HD21	1.79	1.12
1:K:47:GLY:HA3	1:K:392:ARG:HB3	1.25	1.12
1:B:420:ARG:HE	1:D:313:ASN:CG	1.58	1.12
1:E:46:ALA:HA	1:E:392:ARG:HD2	1.20	1.12
1:G:11:TYR:CE1	1:G:333:PRO:CB	2.31	1.12
1:K:327:MET:HB3	1:K:342:LEU:CD2	1.78	1.12
1:C:11:TYR:CD1	1:C:369:LYS:HE3	1.75	1.11
1:C:44:ILE:HD13	1:C:266:LEU:CD1	1.78	1.11
1:C:72:ARG:NH2	1:C:265:HIS:CD2	2.17	1.11
1:J:44:ILE:CB	1:J:266:LEU:HD21	1.80	1.11
1:J:46:ALA:CA	1:J:392:ARG:CD	2.26	1.11
1:F:327:MET:HB3	1:F:342:LEU:HD21	1.32	1.11
1:I:11:TYR:OH	1:I:333:PRO:O	1.68	1.11
1:I:14:PRO:HD2	1:I:370:GLU:OE1	1.48	1.11
1:K:327:MET:C	1:K:342:LEU:CD2	2.23	1.11
1:I:11:TYR:OH	1:I:333:PRO:C	1.95	1.10
1:D:2:ILE:HD12	1:D:378:ASP:OD2	1.52	1.10
1:G:44:ILE:HD13	1:G:266:LEU:CD2	1.82	1.10
1:D:46:ALA:HB2	1:D:392:ARG:NH1	1.60	1.09
1:J:325:LEU:HD21	1:J:331:LEU:HD11	1.31	1.09
1:J:46:ALA:CB	1:J:392:ARG:NH1	2.15	1.09
1:D:46:ALA:HB2	1:D:392:ARG:HH12	1.14	1.09
1:D:46:ALA:CB	1:D:392:ARG:HH11	1.51	1.08
1:J:46:ALA:CB	1:J:392:ARG:HH11	1.66	1.08
1:H:6:ARG:HH11	1:H:273:ASN:HB3	1.01	1.08
1:I:72:ARG:NH2	1:I:265:HIS:HD2	1.51	1.08
1:L:10:SER:HA	1:L:273:ASN:O	1.52	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:324:VAL:CG1	1:L:340:GLY:HA3	1.82	1.08
1:B:420:ARG:NH2	1:D:313:ASN:OD1	1.87	1.08
1:C:11:TYR:OH	1:C:333:PRO:HB2	0.90	1.08
1:C:313:ASN:OD1	1:H:420:ARG:NE	1.87	1.08
1:H:6:ARG:HH12	1:H:273:ASN:HB2	1.12	1.08
1:E:10:SER:HA	1:E:273:ASN:O	1.51	1.07
1:H:6:ARG:NH1	1:H:273:ASN:HB2	1.66	1.06
1:B:46:ALA:O	1:B:392:ARG:HD3	1.53	1.06
1:B:420:ARG:CZ	1:D:313:ASN:OD1	2.03	1.06
1:I:44:ILE:HD13	1:I:266:LEU:CD1	1.85	1.06
1:J:452:GLU:HG2	1:L:309:GLU:OE2	1.54	1.06
1:L:46:ALA:HA	1:L:392:ARG:HH11	0.93	1.06
1:D:44:ILE:CD1	1:D:266:LEU:HD22	1.86	1.05
1:D:72:ARG:NH2	1:D:265:HIS:CD2	2.24	1.05
1:F:46:ALA:HA	1:F:392:ARG:CD	1.87	1.05
1:I:188:ILE:HG23	1:I:191:ARG:HB2	1.36	1.05
1:I:72:ARG:NH2	1:I:265:HIS:CD2	2.25	1.05
1:D:44:ILE:HD13	1:D:266:LEU:HD22	1.06	1.04
1:L:11:TYR:HE1	1:L:333:PRO:C	1.65	1.04
1:G:11:TYR:HE1	1:G:333:PRO:CB	1.67	1.04
1:J:46:ALA:CA	1:J:392:ARG:HD2	1.84	1.04
1:L:327:MET:CB	1:L:342:LEU:HD21	1.87	1.04
1:E:46:ALA:HA	1:E:392:ARG:HH11	1.06	1.04
1:K:327:MET:CB	1:K:342:LEU:HD21	1.87	1.04
1:B:11:TYR:HE1	1:B:333:PRO:HA	1.24	1.03
1:B:396:ARG:NH1	1:F:396:ARG:CA	2.13	1.03
1:K:324:VAL:HG11	1:K:340:GLY:CA	1.88	1.03
1:L:46:ALA:CA	1:L:392:ARG:NH1	2.21	1.03
1:B:309:GLU:OE2	1:I:452:GLU:HG2	1.58	1.03
1:H:14:PRO:HD3	1:H:370:GLU:OE1	1.56	1.03
1:L:46:ALA:HB2	1:L:392:ARG:NH1	1.72	1.03
1:C:44:ILE:HD11	1:C:266:LEU:HD22	1.41	1.03
1:H:44:ILE:HD13	1:H:266:LEU:HD21	1.41	1.03
1:L:46:ALA:HA	1:L:392:ARG:NH1	1.74	1.03
1:B:396:ARG:C	1:F:396:ARG:NH2	2.12	1.02
1:F:72:ARG:NH2	1:F:265:HIS:HD2	1.56	1.02
1:A:44:ILE:CD1	1:A:266:LEU:HD22	1.88	1.02
1:D:72:ARG:NH2	1:D:265:HIS:HD2	1.58	1.02
1:F:11:TYR:OH	1:F:333:PRO:CB	2.07	1.02
1:L:44:ILE:HD13	1:L:266:LEU:HD22	1.06	1.02
1:E:327:MET:SD	1:E:342:LEU:HD11	1.98	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:TYR:CE1	1:B:333:PRO:CB	2.43	1.01
1:I:11:TYR:HH	1:I:333:PRO:C	1.65	1.01
1:L:46:ALA:CB	1:L:392:ARG:NH1	2.23	1.01
1:E:44:ILE:CD1	1:E:266:LEU:CD2	2.32	1.01
1:J:324:VAL:HG12	1:J:331:LEU:HD21	1.41	1.01
1:L:329:GLY:HA3	1:L:341:LEU:O	1.61	1.01
1:B:46:ALA:HA	1:B:392:ARG:CD	1.53	1.01
1:I:72:ARG:HH22	1:I:265:HIS:HD2	1.04	1.01
1:H:14:PRO:HD2	1:H:370:GLU:OE1	1.55	1.01
1:H:68:HIS:CE1	1:H:270:THR:HA	1.95	1.01
1:B:46:ALA:CA	1:B:392:ARG:HD2	1.74	1.00
1:K:11:TYR:CE1	1:K:333:PRO:CA	2.43	1.00
1:G:420:ARG:NE	1:H:313:ASN:OD1	1.93	1.00
1:J:44:ILE:CD1	1:J:266:LEU:HD21	1.83	1.00
1:L:325:LEU:HD21	1:L:331:LEU:HG	1.39	1.00
1:J:46:ALA:HA	1:J:392:ARG:HD2	1.02	1.00
1:A:44:ILE:HD13	1:A:266:LEU:HD22	1.02	1.00
1:L:46:ALA:CB	1:L:392:ARG:HH11	1.75	1.00
1:C:44:ILE:HG12	1:C:266:LEU:HD21	1.40	1.00
1:F:6:ARG:HE	1:F:66:ILE:HD11	1.10	1.00
1:J:199:PRO:HD3	1:L:170:ARG:CZ	1.92	0.99
1:A:6:ARG:HE	1:A:66:ILE:HD11	1.10	0.99
1:F:44:ILE:CG1	1:F:266:LEU:HD21	1.93	0.99
1:I:188:ILE:CD1	1:I:191:ARG:NH2	2.25	0.99
1:B:44:ILE:HD13	1:B:266:LEU:HD22	0.99	0.99
1:E:11:TYR:OH	1:E:333:PRO:HB2	1.63	0.99
1:F:327:MET:O	1:F:342:LEU:HD22	1.62	0.99
1:J:46:ALA:N	1:J:392:ARG:HH11	1.59	0.99
1:C:400:GLN:HG2	1:E:396:ARG:NH1	1.76	0.99
1:D:24:PHE:CE2	1:D:25:GLN:HG3	1.98	0.99
1:I:24:PHE:CE2	1:I:25:GLN:HG3	1.98	0.98
1:L:24:PHE:CE2	1:L:25:GLN:HG3	1.98	0.98
1:E:329:GLY:CA	1:E:341:LEU:O	2.11	0.98
1:G:24:PHE:CE2	1:G:25:GLN:HG3	1.98	0.98
1:I:14:PRO:CD	1:I:370:GLU:OE1	2.12	0.98
1:J:420:ARG:HE	1:L:313:ASN:CG	1.64	0.98
1:B:11:TYR:OH	1:B:333:PRO:O	1.79	0.98
1:J:24:PHE:CE2	1:J:25:GLN:HG3	1.98	0.98
1:A:24:PHE:CE2	1:A:25:GLN:HG3	1.98	0.98
1:F:24:PHE:CE2	1:F:25:GLN:HG3	1.98	0.98
1:A:313:ASN:CG	1:F:420:ARG:HE	1.71	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:11:TYR:CG	1:H:369:LYS:CE	2.47	0.97
1:H:24:PHE:CE2	1:H:25:GLN:HG3	1.98	0.97
1:K:24:PHE:CE2	1:K:25:GLN:HG3	1.98	0.97
1:B:24:PHE:CE2	1:B:25:GLN:HG3	1.98	0.97
1:L:327:MET:HB3	1:L:342:LEU:CD2	1.95	0.97
1:C:24:PHE:CE2	1:C:25:GLN:HG3	1.98	0.97
1:B:44:ILE:HD13	1:B:266:LEU:HD21	1.00	0.97
1:F:46:ALA:HA	1:F:392:ARG:HD2	1.45	0.97
1:E:324:VAL:HG11	1:E:340:GLY:HA3	1.45	0.96
1:J:452:GLU:OE2	1:L:309:GLU:CD	2.07	0.96
1:L:327:MET:HB3	1:L:342:LEU:HD21	0.99	0.96
1:L:327:MET:HG2	1:L:342:LEU:HD11	1.47	0.96
1:E:24:PHE:CE2	1:E:25:GLN:HG3	1.98	0.96
1:C:11:TYR:CG	1:C:369:LYS:HE2	1.99	0.96
1:F:327:MET:O	1:F:342:LEU:CD2	2.14	0.96
1:I:72:ARG:HH22	1:I:265:HIS:CD2	1.81	0.96
1:B:11:TYR:CD1	1:B:369:LYS:CE	2.49	0.96
1:K:6:ARG:HE	1:K:66:ILE:HD11	1.09	0.96
1:L:11:TYR:CE1	1:L:333:PRO:C	2.39	0.96
1:E:72:ARG:HH22	1:E:265:HIS:HD2	1.14	0.96
1:C:313:ASN:CG	1:H:420:ARG:HE	1.72	0.95
1:G:11:TYR:CZ	1:G:333:PRO:HB2	1.99	0.95
1:G:44:ILE:HD13	1:G:266:LEU:HD11	1.49	0.95
1:B:11:TYR:CD1	1:B:369:LYS:HE2	2.02	0.95
1:J:72:ARG:HH22	1:J:265:HIS:HD2	1.04	0.95
1:F:72:ARG:NH2	1:F:265:HIS:CD2	2.34	0.95
1:C:11:TYR:CE1	1:C:369:LYS:HE3	2.02	0.95
1:C:313:ASN:OD1	1:H:420:ARG:NH2	2.00	0.95
1:C:72:ARG:HH22	1:C:265:HIS:HD2	1.06	0.94
1:A:44:ILE:CD1	1:A:266:LEU:CD2	2.45	0.94
1:F:327:MET:HB3	1:F:342:LEU:CD2	1.97	0.94
1:I:6:ARG:HE	1:I:66:ILE:HD11	1.10	0.94
1:A:11:TYR:OH	1:A:333:PRO:HB2	1.66	0.94
1:L:325:LEU:CD2	1:L:331:LEU:HG	1.98	0.94
1:E:46:ALA:CA	1:E:392:ARG:HD2	1.97	0.94
1:K:68:HIS:CE1	1:K:274:ASP:OD1	2.21	0.94
1:I:11:TYR:CE1	1:I:333:PRO:HA	2.02	0.94
1:I:44:ILE:HD13	1:I:266:LEU:HD22	1.49	0.94
1:C:70:VAL:CG1	1:C:269:VAL:HG11	1.97	0.94
1:L:44:ILE:CD1	1:L:266:LEU:HD22	1.96	0.94
1:K:11:TYR:CZ	1:K:333:PRO:CB	2.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:72:ARG:NH2	1:G:265:HIS:HD2	1.65	0.93
1:K:11:TYR:CZ	1:K:333:PRO:O	2.21	0.93
1:C:11:TYR:HE1	1:C:333:PRO:CA	1.81	0.93
1:E:44:ILE:CB	1:E:266:LEU:HD21	1.98	0.93
1:B:313:ASN:HB3	1:I:420:ARG:HG3	1.47	0.93
1:F:44:ILE:CD1	1:F:266:LEU:HD21	1.99	0.93
1:I:188:ILE:HD13	1:I:191:ARG:HH21	1.32	0.93
1:F:44:ILE:HD13	1:F:266:LEU:HD21	1.47	0.93
1:L:325:LEU:HD21	1:L:331:LEU:CG	1.97	0.93
1:C:44:ILE:CD1	1:C:266:LEU:CD1	2.44	0.93
1:D:44:ILE:HG21	1:D:266:LEU:HD21	1.48	0.93
1:C:11:TYR:HE1	1:C:333:PRO:HA	1.30	0.93
1:F:72:ARG:HH22	1:F:265:HIS:HD2	0.99	0.92
1:K:11:TYR:CE1	1:K:333:PRO:CB	2.53	0.92
1:F:72:ARG:HH22	1:F:265:HIS:CD2	1.87	0.92
1:J:6:ARG:HE	1:J:66:ILE:HD11	1.10	0.92
1:B:11:TYR:CE1	1:B:333:PRO:CA	2.52	0.92
1:C:11:TYR:CG	1:C:369:LYS:CE	2.52	0.92
1:F:46:ALA:HA	1:F:392:ARG:CZ	2.00	0.92
1:I:11:TYR:OH	1:I:333:PRO:CA	2.18	0.92
1:D:6:ARG:HE	1:D:66:ILE:CD1	1.78	0.92
1:K:70:VAL:CG1	1:K:269:VAL:HG11	1.99	0.92
1:F:10:SER:HA	1:F:273:ASN:O	1.68	0.92
1:L:324:VAL:CG1	1:L:340:GLY:CA	2.45	0.92
1:G:328:GLY:O	1:G:366:ARG:NH2	2.03	0.92
1:L:6:ARG:HE	1:L:66:ILE:HD11	1.10	0.92
1:J:46:ALA:CA	1:J:392:ARG:HD3	1.98	0.91
1:K:313:ASN:OD1	1:L:420:ARG:NH2	2.03	0.91
1:B:199:PRO:HD3	1:D:170:ARG:HE	1.28	0.91
1:D:11:TYR:HD1	1:D:369:LYS:HE2	1.16	0.91
1:F:44:ILE:HD13	1:F:266:LEU:HD22	0.92	0.91
1:H:11:TYR:CE1	1:H:369:LYS:HE3	2.04	0.91
1:A:6:ARG:HE	1:A:66:ILE:CD1	1.78	0.91
1:B:309:GLU:OE2	1:I:452:GLU:CG	2.19	0.91
1:E:46:ALA:CA	1:E:392:ARG:CD	2.47	0.91
1:F:46:ALA:HA	1:F:392:ARG:HH11	0.77	0.91
1:K:11:TYR:CE1	1:K:333:PRO:HA	2.04	0.91
1:I:11:TYR:HE1	1:I:333:PRO:HA	1.34	0.91
1:K:47:GLY:CA	1:K:392:ARG:HB3	2.01	0.91
1:C:72:ARG:CZ	1:C:265:HIS:CD2	2.54	0.90
1:E:44:ILE:CG1	1:E:266:LEU:HD21	2.00	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:44:ILE:CD1	1:G:266:LEU:CD2	2.49	0.90
1:L:11:TYR:OH	1:L:333:PRO:HB2	1.70	0.90
1:B:11:TYR:OH	1:B:333:PRO:CB	2.14	0.90
1:I:44:ILE:CD1	1:I:266:LEU:CD2	2.49	0.90
1:J:72:ARG:NH2	1:J:265:HIS:HD2	1.68	0.90
1:B:6:ARG:HE	1:B:66:ILE:CD1	1.77	0.90
1:B:44:ILE:HD13	1:B:266:LEU:CG	2.02	0.90
1:E:6:ARG:HE	1:E:66:ILE:HD11	1.10	0.90
1:J:199:PRO:CG	1:L:170:ARG:HE	1.85	0.90
1:G:6:ARG:HE	1:G:66:ILE:CD1	1.77	0.89
1:I:6:ARG:HE	1:I:66:ILE:CD1	1.77	0.89
1:E:44:ILE:HD13	1:E:266:LEU:HD22	0.91	0.89
1:H:46:ALA:HA	1:H:392:ARG:CD	2.01	0.89
1:B:11:TYR:CE1	1:B:333:PRO:HA	2.07	0.89
1:D:6:ARG:HE	1:D:66:ILE:HD11	1.10	0.89
1:D:400:GLN:HG2	1:H:396:ARG:CZ	2.02	0.89
1:J:44:ILE:CG1	1:J:266:LEU:CD2	2.44	0.89
1:K:327:MET:C	1:K:342:LEU:HD21	1.96	0.89
1:I:11:TYR:CE1	1:I:333:PRO:CA	2.56	0.89
1:C:440:GLN:OE1	1:C:440:GLN:N	2.06	0.89
1:E:440:GLN:OE1	1:E:440:GLN:N	2.06	0.89
1:G:440:GLN:OE1	1:G:440:GLN:N	2.06	0.89
1:D:440:GLN:N	1:D:440:GLN:OE1	2.06	0.88
1:H:11:TYR:CG	1:H:369:LYS:HE3	2.07	0.88
1:I:44:ILE:CG1	1:I:266:LEU:HD21	2.03	0.88
1:L:440:GLN:N	1:L:440:GLN:OE1	2.06	0.88
1:C:400:GLN:HG2	1:E:396:ARG:HH11	1.35	0.88
1:G:11:TYR:CE1	1:G:333:PRO:HB3	2.07	0.88
1:B:155:HIS:CE1	1:I:452:GLU:HG3	2.09	0.88
1:C:313:ASN:OD1	1:H:420:ARG:CZ	2.22	0.88
1:K:11:TYR:HE1	1:K:333:PRO:HA	1.37	0.88
1:F:46:ALA:N	1:F:392:ARG:NH1	2.21	0.88
1:J:440:GLN:OE1	1:J:440:GLN:N	2.06	0.88
1:L:324:VAL:HG11	1:L:340:GLY:HA2	1.55	0.88
1:B:47:GLY:N	1:B:392:ARG:HD2	1.89	0.88
1:F:440:GLN:OE1	1:F:440:GLN:N	2.06	0.88
1:H:46:ALA:CB	1:H:392:ARG:NH1	2.36	0.88
1:J:325:LEU:CD2	1:J:331:LEU:CD1	2.46	0.88
1:K:11:TYR:CE1	1:K:333:PRO:O	2.27	0.88
1:L:325:LEU:HD21	1:L:331:LEU:CD1	2.03	0.87
1:B:440:GLN:OE1	1:B:440:GLN:N	2.06	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6:ARG:HE	1:G:66:ILE:HD11	1.09	0.87
1:H:440:GLN:OE1	1:H:440:GLN:N	2.06	0.87
1:L:8:ASN:O	1:L:335:PRO:HB3	1.75	0.87
1:B:6:ARG:HE	1:B:66:ILE:HD11	1.10	0.87
1:F:46:ALA:N	1:F:392:ARG:HH11	1.71	0.87
1:A:440:GLN:N	1:A:440:GLN:OE1	2.06	0.87
1:F:44:ILE:CB	1:F:266:LEU:HD21	2.05	0.87
1:K:440:GLN:OE1	1:K:440:GLN:N	2.06	0.87
1:F:11:TYR:CD1	1:F:369:LYS:HE2	2.09	0.87
1:L:6:ARG:HE	1:L:66:ILE:CD1	1.77	0.87
1:H:6:ARG:HH11	1:H:273:ASN:CB	1.75	0.86
1:J:10:SER:HA	1:J:273:ASN:O	1.75	0.86
1:H:46:ALA:HA	1:H:392:ARG:HH11	0.71	0.86
1:I:440:GLN:N	1:I:440:GLN:OE1	2.06	0.86
1:D:400:GLN:HE21	1:H:396:ARG:HD3	1.40	0.86
1:J:72:ARG:HH22	1:J:265:HIS:CD2	1.93	0.86
1:D:72:ARG:HH22	1:D:265:HIS:HD2	0.88	0.86
1:D:400:GLN:HG2	1:H:396:ARG:NH1	1.90	0.86
1:F:327:MET:CB	1:F:342:LEU:HD21	2.06	0.86
1:J:6:ARG:HE	1:J:66:ILE:CD1	1.78	0.86
1:C:11:TYR:CZ	1:C:333:PRO:HB3	1.99	0.86
1:H:46:ALA:N	1:H:392:ARG:HH11	1.73	0.86
1:J:313:ASN:OD1	1:K:420:ARG:NE	2.08	0.86
1:J:72:ARG:NH2	1:J:265:HIS:CD2	2.44	0.86
1:C:396:ARG:NE	1:E:400:GLN:HE21	1.74	0.86
1:F:6:ARG:HE	1:F:66:ILE:CD1	1.77	0.86
1:G:44:ILE:CG1	1:G:266:LEU:HD21	2.06	0.86
1:H:11:TYR:CG	1:H:369:LYS:HE2	2.09	0.86
1:D:46:ALA:HA	1:D:392:ARG:HH11	0.70	0.85
1:K:6:ARG:HE	1:K:66:ILE:CD1	1.77	0.85
1:D:44:ILE:CG2	1:D:266:LEU:HD21	2.06	0.85
1:D:44:ILE:CB	1:D:266:LEU:HD21	2.06	0.85
1:B:317:GLN:HE22	1:I:440:GLN:C	1.84	0.85
1:C:44:ILE:HD13	1:C:266:LEU:HD22	1.19	0.85
1:I:188:ILE:CD1	1:I:191:ARG:HH21	1.87	0.85
1:J:440:GLN:O	1:L:317:GLN:NE2	2.08	0.85
1:J:330:VAL:HG11	1:J:350:VAL:HG11	1.57	0.84
1:F:11:TYR:CZ	1:F:333:PRO:HB2	2.12	0.84
1:I:11:TYR:CE1	1:I:333:PRO:CB	2.60	0.84
1:B:345:GLN:OE1	1:B:347:GLN:HB2	1.77	0.84
1:F:46:ALA:HB2	1:F:392:ARG:HH12	1.39	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:GLN:NE2	1:I:440:GLN:O	2.10	0.84
1:H:68:HIS:HE1	1:H:270:THR:HA	1.42	0.84
1:J:199:PRO:CG	1:L:170:ARG:NE	2.40	0.84
1:A:199:PRO:HG2	1:E:170:ARG:HG3	1.60	0.84
1:J:46:ALA:HA	1:J:392:ARG:HH11	1.26	0.84
1:C:11:TYR:HD1	1:C:369:LYS:HE2	1.34	0.84
1:G:44:ILE:CD1	1:G:266:LEU:HD21	2.07	0.84
1:L:72:ARG:HH22	1:L:265:HIS:HD2	1.24	0.84
1:A:72:ARG:HH22	1:A:265:HIS:HD2	1.25	0.84
1:A:327:MET:HB3	1:A:342:LEU:HD21	1.59	0.84
1:G:44:ILE:HD13	1:G:266:LEU:HD21	1.60	0.84
1:J:190:ASN:OD1	1:J:205:ARG:CD	2.16	0.84
1:C:44:ILE:CG1	1:C:266:LEU:CD2	2.32	0.84
1:B:24:PHE:HB3	1:B:52:ASN:HD21	1.43	0.83
1:A:24:PHE:HB3	1:A:52:ASN:HD21	1.43	0.83
1:I:24:PHE:HB3	1:I:52:ASN:HD21	1.43	0.83
1:G:72:ARG:NH2	1:G:265:HIS:CD2	2.46	0.83
1:J:24:PHE:HB3	1:J:52:ASN:HD21	1.43	0.83
1:L:329:GLY:CA	1:L:341:LEU:O	2.26	0.83
1:H:24:PHE:HB3	1:H:52:ASN:HD21	1.43	0.83
1:J:325:LEU:HD21	1:J:331:LEU:HD12	1.57	0.83
1:C:11:TYR:CE1	1:C:333:PRO:CA	2.58	0.83
1:E:46:ALA:N	1:E:392:ARG:HH11	1.75	0.83
1:G:24:PHE:HB3	1:G:52:ASN:HD21	1.43	0.83
1:C:24:PHE:HB3	1:C:52:ASN:HD21	1.43	0.83
1:L:11:TYR:CZ	1:L:333:PRO:O	2.31	0.83
1:E:72:ARG:HH22	1:E:265:HIS:CD2	1.96	0.82
1:G:44:ILE:CD1	1:G:266:LEU:CD1	2.57	0.82
1:I:44:ILE:HD13	1:I:266:LEU:HD13	1.59	0.82
1:K:324:VAL:CG1	1:K:340:GLY:HA3	2.07	0.82
1:E:46:ALA:HA	1:E:392:ARG:NH1	1.69	0.82
1:G:327:MET:HB3	1:G:342:LEU:HD21	1.62	0.82
1:B:11:TYR:HE1	1:B:333:PRO:CA	1.90	0.82
1:K:11:TYR:OH	1:K:333:PRO:C	2.22	0.82
1:C:47:GLY:HA3	1:C:392:ARG:HB3	1.62	0.82
1:L:24:PHE:HB3	1:L:52:ASN:HD21	1.43	0.82
1:E:6:ARG:HE	1:E:66:ILE:CD1	1.77	0.82
1:K:72:ARG:NH2	1:K:265:HIS:HD2	1.77	0.82
1:L:44:ILE:CB	1:L:266:LEU:HD21	2.10	0.82
1:D:24:PHE:HB3	1:D:52:ASN:HD21	1.43	0.82
1:F:6:ARG:CD	1:F:66:ILE:HD11	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:327:MET:CG	1:L:342:LEU:HD11	2.10	0.82
1:D:2:ILE:CD1	1:D:378:ASP:OD2	2.28	0.82
1:D:199:PRO:HG2	1:I:170:ARG:HG3	1.61	0.81
1:E:44:ILE:HD13	1:E:266:LEU:HD21	1.62	0.81
1:B:400:GLN:CD	1:F:396:ARG:HG2	2.05	0.81
1:H:46:ALA:N	1:H:392:ARG:NH1	2.28	0.81
1:I:324:VAL:HG11	1:I:331:LEU:HD21	1.60	0.81
1:J:327:MET:C	1:J:342:LEU:HD21	2.04	0.81
1:K:24:PHE:HB3	1:K:52:ASN:HD21	1.43	0.81
1:E:6:ARG:CD	1:E:66:ILE:HD11	2.10	0.81
1:E:38:ALA:HA	1:E:41:LEU:HD12	1.63	0.81
1:I:11:TYR:CZ	1:I:333:PRO:CA	2.64	0.81
1:A:6:ARG:CD	1:A:66:ILE:HD11	2.11	0.81
1:B:11:TYR:OH	1:B:333:PRO:C	2.23	0.81
1:F:24:PHE:HB3	1:F:52:ASN:HD21	1.43	0.81
1:J:38:ALA:HA	1:J:41:LEU:HD12	1.63	0.81
1:D:38:ALA:HA	1:D:41:LEU:HD12	1.63	0.81
1:F:38:ALA:HA	1:F:41:LEU:HD12	1.63	0.81
1:L:6:ARG:CD	1:L:66:ILE:HD11	2.11	0.81
1:B:46:ALA:HA	1:B:392:ARG:HD2	1.36	0.81
1:C:452:GLU:HG2	1:G:309:GLU:OE2	1.79	0.81
1:E:420:ARG:NE	1:F:313:ASN:OD1	2.13	0.81
1:G:6:ARG:CD	1:G:66:ILE:HD11	2.10	0.81
1:G:44:ILE:HD13	1:G:266:LEU:CG	2.11	0.81
1:I:6:ARG:CD	1:I:66:ILE:HD11	2.10	0.81
1:A:38:ALA:HA	1:A:41:LEU:HD12	1.63	0.80
1:C:396:ARG:HE	1:E:400:GLN:HE21	1.27	0.80
1:J:199:PRO:HG3	1:L:170:ARG:HE	1.45	0.80
1:D:6:ARG:CD	1:D:66:ILE:HD11	2.11	0.80
1:K:309:GLU:OE2	1:L:452:GLU:CG	2.28	0.80
1:G:11:TYR:OH	1:G:333:PRO:HB2	1.80	0.80
1:J:324:VAL:CG1	1:J:331:LEU:HD21	2.10	0.80
1:E:24:PHE:HB3	1:E:52:ASN:HD21	1.43	0.80
1:L:38:ALA:HA	1:L:41:LEU:HD12	1.63	0.80
1:B:6:ARG:CD	1:B:66:ILE:HD11	2.11	0.80
1:K:6:ARG:CD	1:K:66:ILE:HD11	2.11	0.80
1:K:68:HIS:HE1	1:K:274:ASP:OD1	1.64	0.80
1:L:11:TYR:HE1	1:L:333:PRO:HA	1.46	0.80
1:C:38:ALA:HA	1:C:41:LEU:HD12	1.63	0.80
1:D:44:ILE:CD1	1:D:266:LEU:CD2	2.49	0.80
1:E:324:VAL:HG11	1:E:340:GLY:CA	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ALA:HA	1:B:41:LEU:HD12	1.63	0.80
1:L:11:TYR:HE1	1:L:333:PRO:O	1.46	0.80
1:D:420:ARG:NE	1:I:313:ASN:OD1	2.15	0.80
1:G:452:GLU:HG2	1:H:309:GLU:OE2	1.81	0.80
1:A:44:ILE:CB	1:A:266:LEU:HD21	2.12	0.80
1:J:44:ILE:HB	1:J:266:LEU:HD21	1.62	0.80
1:I:38:ALA:HA	1:I:41:LEU:HD12	1.63	0.80
1:K:38:ALA:HA	1:K:41:LEU:HD12	1.63	0.79
1:K:329:GLY:HA2	1:K:341:LEU:O	1.82	0.79
1:F:11:TYR:CZ	1:F:333:PRO:CB	2.65	0.79
1:J:6:ARG:CD	1:J:66:ILE:HD11	2.10	0.79
1:H:11:TYR:HD1	1:H:369:LYS:HE2	1.40	0.79
1:I:11:TYR:CZ	1:I:333:PRO:HB3	2.14	0.79
1:I:44:ILE:CD1	1:I:266:LEU:HD22	2.10	0.79
1:A:11:TYR:CZ	1:A:333:PRO:HB2	2.16	0.79
1:A:44:ILE:CG1	1:A:266:LEU:HD21	2.13	0.79
1:C:309:GLU:OE2	1:H:452:GLU:HG2	1.82	0.79
1:G:11:TYR:CD1	1:G:369:LYS:HE3	2.18	0.79
1:H:38:ALA:HA	1:H:41:LEU:HD12	1.63	0.79
1:E:324:VAL:CG1	1:E:340:GLY:HA3	2.12	0.79
1:G:38:ALA:HA	1:G:41:LEU:HD12	1.63	0.79
1:E:46:ALA:HB2	1:E:392:ARG:HH12	1.39	0.78
1:H:10:SER:HA	1:H:273:ASN:O	1.82	0.78
1:B:72:ARG:NH2	1:B:265:HIS:HD2	1.81	0.78
1:A:452:GLU:HG2	1:E:309:GLU:OE2	1.82	0.78
1:C:72:ARG:HH22	1:C:265:HIS:CD2	1.91	0.78
1:H:44:ILE:CD1	1:H:266:LEU:CD2	2.52	0.78
1:L:46:ALA:HA	1:L:392:ARG:HD2	1.64	0.78
1:B:11:TYR:CD1	1:B:369:LYS:HE3	2.18	0.78
1:E:72:ARG:NH2	1:E:265:HIS:HD2	1.81	0.78
1:G:397:ALA:O	1:G:400:GLN:HG2	1.83	0.78
1:H:46:ALA:HB2	1:H:392:ARG:NH1	1.98	0.78
1:E:11:TYR:CZ	1:E:333:PRO:HB2	2.17	0.78
1:H:44:ILE:CD1	1:H:266:LEU:HD22	2.10	0.78
1:K:11:TYR:OH	1:K:333:PRO:HB2	1.83	0.78
1:I:188:ILE:HG23	1:I:191:ARG:CB	2.12	0.77
1:D:44:ILE:CG1	1:D:266:LEU:HD21	2.14	0.77
1:E:452:GLU:HG2	1:F:309:GLU:OE2	1.84	0.77
1:G:70:VAL:CG1	1:G:269:VAL:HG11	2.13	0.77
1:F:6:ARG:CZ	1:F:66:ILE:HD13	2.14	0.77
1:J:199:PRO:CD	1:L:170:ARG:NE	2.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:TYR:CE1	1:B:333:PRO:HB3	2.17	0.77
1:B:72:ARG:HH22	1:B:265:HIS:HD2	1.32	0.77
1:D:452:GLU:HG2	1:I:309:GLU:OE2	1.84	0.77
1:J:199:PRO:HD3	1:L:170:ARG:NE	1.99	0.77
1:E:44:ILE:CD1	1:E:266:LEU:HD21	2.13	0.77
1:G:6:ARG:CZ	1:G:66:ILE:HD13	2.14	0.77
1:L:11:TYR:CE1	1:L:333:PRO:HA	2.19	0.77
1:E:72:ARG:NH2	1:E:265:HIS:CD2	2.52	0.77
1:J:6:ARG:CZ	1:J:66:ILE:HD13	2.15	0.77
1:D:6:ARG:CZ	1:D:66:ILE:HD13	2.15	0.77
1:E:6:ARG:CZ	1:E:66:ILE:HD13	2.15	0.77
1:K:6:ARG:CZ	1:K:66:ILE:HD13	2.15	0.77
1:B:11:TYR:HH	1:B:333:PRO:C	1.92	0.77
1:A:46:ALA:HA	1:A:392:ARG:HD2	1.66	0.76
1:B:27:LYS:NZ	1:B:41:LEU:O	2.18	0.76
1:E:46:ALA:N	1:E:392:ARG:NH1	2.31	0.76
1:F:27:LYS:NZ	1:F:41:LEU:O	2.19	0.76
1:F:324:VAL:HG11	1:F:340:GLY:CA	2.16	0.76
1:H:27:LYS:NZ	1:H:41:LEU:O	2.18	0.76
1:J:46:ALA:N	1:J:392:ARG:NH1	2.28	0.76
1:E:11:TYR:CZ	1:E:333:PRO:CB	2.69	0.76
1:J:329:GLY:HA2	1:J:366:ARG:HH22	1.49	0.76
1:A:22:SER:HB2	1:A:24:PHE:CE1	2.21	0.76
1:G:27:LYS:NZ	1:G:41:LEU:O	2.19	0.76
1:I:6:ARG:CZ	1:I:66:ILE:HD13	2.15	0.76
1:I:188:ILE:HD13	1:I:191:ARG:CZ	2.16	0.76
1:K:22:SER:HB2	1:K:24:PHE:CE1	2.21	0.76
1:A:72:ARG:HH22	1:A:265:HIS:CD2	2.04	0.76
1:B:6:ARG:CZ	1:B:66:ILE:HD13	2.15	0.76
1:G:22:SER:HB2	1:G:24:PHE:CE1	2.21	0.76
1:F:46:ALA:CA	1:F:392:ARG:CD	2.60	0.76
1:G:44:ILE:HG12	1:G:266:LEU:HD21	1.67	0.76
1:K:27:LYS:NZ	1:K:41:LEU:O	2.19	0.76
1:I:22:SER:HB2	1:I:24:PHE:CE1	2.21	0.76
1:I:44:ILE:HD13	1:I:266:LEU:CG	2.15	0.76
1:I:188:ILE:CG2	1:I:191:ARG:HB2	2.13	0.76
1:A:27:LYS:NZ	1:A:41:LEU:O	2.19	0.75
1:I:44:ILE:HG21	1:I:266:LEU:HD21	1.67	0.75
1:B:155:HIS:HD1	1:I:452:GLU:CD	1.94	0.75
1:C:22:SER:HB2	1:C:24:PHE:CE1	2.21	0.75
1:L:22:SER:HB2	1:L:24:PHE:CE1	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:SER:HB2	1:E:24:PHE:CE1	2.21	0.75
1:J:22:SER:HB2	1:J:24:PHE:CE1	2.21	0.75
1:L:72:ARG:HH22	1:L:265:HIS:CD2	2.03	0.75
1:A:313:ASN:OD1	1:F:420:ARG:CZ	2.35	0.75
1:J:452:GLU:OE2	1:L:309:GLU:OE2	2.00	0.75
1:A:6:ARG:CZ	1:A:66:ILE:HD13	2.15	0.75
1:D:27:LYS:NZ	1:D:41:LEU:O	2.18	0.75
1:F:22:SER:HB2	1:F:24:PHE:CE1	2.21	0.75
1:L:6:ARG:CZ	1:L:66:ILE:HD13	2.15	0.75
1:K:11:TYR:HE1	1:K:333:PRO:CA	1.89	0.75
1:H:22:SER:HB2	1:H:24:PHE:CE1	2.21	0.75
1:I:27:LYS:NZ	1:I:41:LEU:O	2.18	0.75
1:A:46:ALA:HA	1:A:392:ARG:CD	2.17	0.74
1:C:44:ILE:CB	1:C:266:LEU:HD21	2.16	0.74
1:E:27:LYS:NZ	1:E:41:LEU:O	2.18	0.74
1:A:44:ILE:HG21	1:A:266:LEU:HD21	1.69	0.74
1:B:22:SER:HB2	1:B:24:PHE:CE1	2.21	0.74
1:D:22:SER:HB2	1:D:24:PHE:CE1	2.21	0.74
1:H:11:TYR:CE1	1:H:369:LYS:CE	2.67	0.74
1:F:46:ALA:CA	1:F:392:ARG:HD2	2.16	0.74
1:K:70:VAL:HG12	1:K:269:VAL:HG11	1.69	0.74
1:L:27:LYS:NZ	1:L:41:LEU:O	2.19	0.74
1:B:46:ALA:CA	1:B:392:ARG:HD3	1.94	0.74
1:K:170:ARG:NE	1:L:199:PRO:HD3	2.01	0.74
1:J:6:ARG:NE	1:J:66:ILE:HD13	2.03	0.74
1:J:27:LYS:NZ	1:J:41:LEU:O	2.19	0.74
1:L:6:ARG:NE	1:L:66:ILE:HD13	2.03	0.74
1:D:199:PRO:CG	1:I:170:ARG:HG3	2.17	0.74
1:I:44:ILE:CD1	1:I:266:LEU:CD1	2.64	0.74
1:A:452:GLU:HG3	1:E:155:HIS:CE1	2.23	0.73
1:G:420:ARG:HE	1:H:313:ASN:CG	1.96	0.73
1:L:46:ALA:HA	1:L:392:ARG:CD	2.18	0.73
1:A:199:PRO:HD3	1:E:170:ARG:NE	2.02	0.73
1:A:420:ARG:HG3	1:E:313:ASN:HB3	1.69	0.73
1:G:6:ARG:NE	1:G:66:ILE:HD13	2.03	0.73
1:K:327:MET:HB3	1:K:342:LEU:CD1	2.18	0.73
1:A:6:ARG:NE	1:A:66:ILE:HD13	2.03	0.73
1:G:44:ILE:CD1	1:G:266:LEU:HD11	2.17	0.73
1:C:27:LYS:NZ	1:C:41:LEU:O	2.19	0.73
1:I:11:TYR:CD1	1:I:369:LYS:HE2	2.23	0.73
1:G:44:ILE:HD13	1:G:266:LEU:HD13	1.67	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:44:ILE:CD1	1:H:266:LEU:HD21	2.14	0.73
1:B:199:PRO:CD	1:D:170:ARG:HE	2.00	0.73
1:C:324:VAL:O	1:C:342:LEU:HD21	1.89	0.73
1:D:46:ALA:HB1	1:D:392:ARG:NH1	1.96	0.73
1:I:44:ILE:HG12	1:I:266:LEU:HD21	1.70	0.73
1:H:46:ALA:HA	1:H:392:ARG:CZ	2.19	0.72
1:F:44:ILE:HD13	1:F:266:LEU:CG	2.19	0.72
1:L:44:ILE:CD1	1:L:266:LEU:CD2	2.59	0.72
1:B:197:GLN:O	1:D:170:ARG:NH2	2.21	0.72
1:A:155:HIS:HE1	1:F:452:GLU:HG3	1.55	0.72
1:E:46:ALA:HA	1:E:392:ARG:CZ	2.19	0.72
1:B:400:GLN:OE1	1:F:396:ARG:HG2	1.89	0.72
1:D:11:TYR:CE1	1:D:369:LYS:CE	2.44	0.72
1:J:46:ALA:HA	1:J:392:ARG:NH1	1.89	0.72
1:A:46:ALA:C	1:A:392:ARG:HD2	2.14	0.72
1:D:14:PRO:HD2	1:D:370:GLU:OE1	1.89	0.72
1:F:70:VAL:CG1	1:F:269:VAL:HG11	2.20	0.72
1:B:199:PRO:CD	1:D:170:ARG:NE	2.46	0.72
1:G:70:VAL:HG11	1:G:269:VAL:HG11	1.72	0.71
1:L:44:ILE:HG21	1:L:266:LEU:HD21	1.72	0.71
1:E:327:MET:HG2	1:E:342:LEU:HD13	1.70	0.71
1:E:44:ILE:HG21	1:E:266:LEU:HD21	1.72	0.71
1:G:327:MET:C	1:G:329:GLY:H	1.97	0.71
1:E:44:ILE:CG2	1:E:266:LEU:HD21	2.20	0.71
1:L:327:MET:HG2	1:L:342:LEU:CD1	2.18	0.71
1:D:11:TYR:CG	1:D:369:LYS:CE	2.73	0.71
1:F:324:VAL:HG11	1:F:340:GLY:HA3	1.71	0.71
1:E:6:ARG:NE	1:E:66:ILE:HD13	2.03	0.71
1:B:452:GLU:HG2	1:D:309:GLU:OE2	1.90	0.71
1:A:155:HIS:CE1	1:F:452:GLU:HG3	2.26	0.70
1:C:396:ARG:CD	1:E:400:GLN:CG	2.69	0.70
1:K:327:MET:SD	1:K:342:LEU:HD11	2.31	0.70
1:C:1:MET:N	1:C:17:VAL:O	2.25	0.70
1:G:327:MET:HB3	1:G:342:LEU:CD2	2.22	0.70
1:I:8:ASN:OD1	1:I:310:GLU:OE2	2.09	0.70
1:F:6:ARG:CZ	1:F:66:ILE:CD1	2.70	0.70
1:J:1:MET:N	1:J:17:VAL:O	2.25	0.70
1:J:327:MET:O	1:J:342:LEU:HD22	1.91	0.70
1:C:396:ARG:CD	1:E:400:GLN:HE21	2.05	0.70
1:H:46:ALA:HA	1:H:392:ARG:HD2	1.74	0.70
1:J:6:ARG:CZ	1:J:66:ILE:CD1	2.70	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:ARG:CZ	1:D:66:ILE:CD1	2.70	0.69
1:E:6:ARG:CZ	1:E:66:ILE:CD1	2.70	0.69
1:F:1:MET:N	1:F:17:VAL:O	2.25	0.69
1:E:68:HIS:CD2	1:E:270:THR:HG23	2.27	0.69
1:I:184:ASP:O	1:I:188:ILE:CG2	2.26	0.69
1:H:1:MET:N	1:H:17:VAL:O	2.25	0.69
1:I:44:ILE:CD1	1:I:266:LEU:HD21	2.21	0.69
1:G:6:ARG:CZ	1:G:66:ILE:CD1	2.69	0.69
1:I:6:ARG:CZ	1:I:66:ILE:CD1	2.70	0.69
1:J:46:ALA:HA	1:J:392:ARG:NE	2.07	0.69
1:H:14:PRO:CD	1:H:370:GLU:CD	2.65	0.69
1:B:44:ILE:CB	1:B:266:LEU:HD21	2.22	0.69
1:D:1:MET:N	1:D:17:VAL:O	2.25	0.69
1:I:1:MET:N	1:I:17:VAL:O	2.25	0.69
1:K:6:ARG:CZ	1:K:66:ILE:CD1	2.70	0.69
1:L:6:ARG:CZ	1:L:66:ILE:CD1	2.70	0.69
1:K:72:ARG:HH22	1:K:265:HIS:HD2	1.40	0.69
1:A:452:GLU:OE2	1:E:155:HIS:ND1	2.21	0.69
1:F:11:TYR:CD1	1:F:369:LYS:CE	2.75	0.69
1:A:6:ARG:CZ	1:A:66:ILE:CD1	2.70	0.68
1:I:324:VAL:HG11	1:I:331:LEU:CD2	2.23	0.68
1:C:44:ILE:CD1	1:C:266:LEU:HD11	2.21	0.68
1:I:11:TYR:CD1	1:I:369:LYS:CE	2.76	0.68
1:A:155:HIS:CE1	1:F:452:GLU:CG	2.76	0.68
1:D:8:ASN:OD1	1:D:310:GLU:OE2	2.12	0.68
1:K:327:MET:CB	1:K:342:LEU:CD2	2.59	0.68
1:A:8:ASN:OD1	1:A:310:GLU:OE2	2.11	0.68
1:A:44:ILE:CG2	1:A:266:LEU:HD21	2.24	0.68
1:B:1:MET:N	1:B:17:VAL:O	2.25	0.68
1:D:46:ALA:HA	1:D:392:ARG:CZ	2.20	0.68
1:H:14:PRO:HD2	1:H:370:GLU:CD	2.18	0.68
1:K:324:VAL:CG1	1:K:340:GLY:CA	2.68	0.68
1:B:317:GLN:NE2	1:I:440:GLN:C	2.52	0.68
1:J:44:ILE:HD13	1:J:266:LEU:CG	2.16	0.68
1:L:44:ILE:CG2	1:L:266:LEU:HD21	2.24	0.67
1:F:44:ILE:CG1	1:F:266:LEU:CD2	2.64	0.67
1:L:1:MET:N	1:L:17:VAL:O	2.25	0.67
1:D:44:ILE:HG21	1:D:266:LEU:CD2	2.24	0.67
1:E:11:TYR:OH	1:E:333:PRO:CB	2.31	0.67
1:A:46:ALA:CA	1:A:392:ARG:HD2	2.24	0.67
1:B:440:GLN:HB2	1:D:320:ALA:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:ARG:NE	1:G:313:ASN:OD1	2.25	0.67
1:E:1:MET:N	1:E:17:VAL:O	2.25	0.67
1:G:420:ARG:CZ	1:H:313:ASN:OD1	2.42	0.67
1:K:1:MET:N	1:K:17:VAL:O	2.25	0.67
1:C:400:GLN:CG	1:E:396:ARG:NH1	2.57	0.67
1:F:7:PHE:HD1	1:F:69:ILE:HB	1.60	0.67
1:J:325:LEU:HD23	1:J:331:LEU:HD11	1.77	0.67
1:L:72:ARG:NH2	1:L:265:HIS:CD2	2.62	0.67
1:G:1:MET:N	1:G:17:VAL:O	2.25	0.67
1:K:11:TYR:CE1	1:K:333:PRO:C	2.72	0.67
1:B:44:ILE:HD11	1:B:266:LEU:HD22	1.72	0.67
1:C:7:PHE:HD1	1:C:69:ILE:HB	1.60	0.67
1:E:7:PHE:HD1	1:E:69:ILE:HB	1.60	0.67
1:E:455:ARG:HD2	1:F:221:ASP:OD1	1.95	0.66
1:C:44:ILE:HD13	1:C:266:LEU:HD21	1.16	0.66
1:E:11:TYR:CE1	1:E:333:PRO:HA	2.29	0.66
1:K:7:PHE:HD1	1:K:69:ILE:HB	1.60	0.66
1:L:7:PHE:HD1	1:L:69:ILE:HB	1.60	0.66
1:J:46:ALA:CB	1:J:392:ARG:HD3	2.26	0.66
1:F:327:MET:C	1:F:342:LEU:CD2	2.68	0.66
1:I:6:ARG:NE	1:I:66:ILE:HD13	2.03	0.66
1:A:7:PHE:HD1	1:A:69:ILE:HB	1.60	0.66
1:B:11:TYR:CG	1:B:369:LYS:HE2	2.31	0.66
1:A:155:HIS:ND1	1:F:452:GLU:OE2	2.18	0.66
1:E:44:ILE:CG1	1:E:266:LEU:CD2	2.68	0.66
1:A:63:GLN:NE2	1:A:64:GLN:HG3	2.11	0.66
1:D:7:PHE:HD1	1:D:69:ILE:HB	1.60	0.66
1:D:400:GLN:NE2	1:H:396:ARG:HD3	2.11	0.66
1:G:7:PHE:HD1	1:G:69:ILE:HB	1.60	0.66
1:J:313:ASN:OD1	1:K:420:ARG:NH2	2.28	0.66
1:L:11:TYR:OH	1:L:333:PRO:C	2.39	0.66
1:A:199:PRO:CG	1:E:170:ARG:HG3	2.26	0.66
1:C:63:GLN:NE2	1:C:64:GLN:HG3	2.11	0.66
1:A:1:MET:N	1:A:17:VAL:O	2.25	0.66
1:I:7:PHE:HD1	1:I:69:ILE:HB	1.60	0.66
1:D:63:GLN:NE2	1:D:64:GLN:HG3	2.11	0.65
1:H:63:GLN:NE2	1:H:64:GLN:HG3	2.11	0.65
1:K:170:ARG:HG3	1:L:199:PRO:HG2	1.78	0.65
1:G:63:GLN:NE2	1:G:64:GLN:HG3	2.11	0.65
1:K:63:GLN:NE2	1:K:64:GLN:HG3	2.11	0.65
1:L:27:LYS:HE3	1:L:41:LEU:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:GLN:NE2	1:B:64:GLN:HG3	2.11	0.65
1:E:27:LYS:HE3	1:E:41:LEU:HB2	1.79	0.65
1:H:27:LYS:HE3	1:H:41:LEU:HB2	1.78	0.65
1:J:7:PHE:HD1	1:J:69:ILE:HB	1.60	0.65
1:J:324:VAL:CG1	1:J:331:LEU:CD2	2.74	0.65
1:B:6:ARG:CZ	1:B:66:ILE:CD1	2.70	0.65
1:B:7:PHE:HD1	1:B:69:ILE:HB	1.60	0.65
1:D:27:LYS:HE3	1:D:41:LEU:HB2	1.78	0.65
1:F:27:LYS:HE3	1:F:41:LEU:HB2	1.79	0.65
1:F:63:GLN:NE2	1:F:64:GLN:HG3	2.11	0.65
1:D:44:ILE:CG1	1:D:266:LEU:CD2	2.74	0.65
1:D:229:ILE:HD11	1:D:306:ILE:HD11	1.79	0.65
1:H:7:PHE:HD1	1:H:69:ILE:HB	1.60	0.65
1:J:331:LEU:HD23	1:J:340:GLY:HA2	1.79	0.65
1:K:229:ILE:HD11	1:K:306:ILE:HD11	1.79	0.65
1:L:63:GLN:NE2	1:L:64:GLN:HG3	2.11	0.65
1:L:327:MET:SD	1:L:342:LEU:HD11	2.36	0.65
1:K:327:MET:CA	1:K:342:LEU:HD21	2.26	0.65
1:B:11:TYR:CZ	1:B:333:PRO:HB3	2.30	0.65
1:C:27:LYS:HE3	1:C:41:LEU:HB2	1.78	0.65
1:C:44:ILE:HG12	1:C:266:LEU:CD2	2.14	0.65
1:J:63:GLN:NE2	1:J:64:GLN:HG3	2.11	0.65
1:K:27:LYS:HE3	1:K:41:LEU:HB2	1.79	0.65
1:A:27:LYS:HE3	1:A:41:LEU:HB2	1.79	0.65
1:H:70:VAL:HG21	1:H:72:ARG:CZ	2.27	0.65
1:C:70:VAL:HG21	1:C:72:ARG:CZ	2.27	0.64
1:G:27:LYS:HE3	1:G:41:LEU:HB2	1.78	0.64
1:I:63:GLN:NE2	1:I:64:GLN:HG3	2.11	0.64
1:J:68:HIS:CD2	1:J:270:THR:HG23	2.33	0.64
1:B:155:HIS:ND1	1:I:452:GLU:OE2	2.25	0.64
1:C:229:ILE:HD11	1:C:306:ILE:HD11	1.79	0.64
1:C:396:ARG:CD	1:E:400:GLN:HG2	2.26	0.64
1:F:229:ILE:HD11	1:F:306:ILE:HD11	1.79	0.64
1:G:229:ILE:HD11	1:G:306:ILE:HD11	1.79	0.64
1:E:6:ARG:HG2	1:E:11:TYR:O	1.98	0.64
1:I:27:LYS:HE3	1:I:41:LEU:HB2	1.78	0.64
1:J:229:ILE:HD11	1:J:306:ILE:HD11	1.79	0.64
1:J:420:ARG:NE	1:L:313:ASN:CG	2.34	0.64
1:A:6:ARG:HG2	1:A:11:TYR:O	1.98	0.64
1:A:70:VAL:HG21	1:A:72:ARG:CZ	2.28	0.64
1:A:72:ARG:NH2	1:A:265:HIS:CD2	2.66	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:SER:O	1:E:273:ASN:HA	1.96	0.64
1:J:313:ASN:CG	1:K:420:ARG:HE	2.04	0.64
1:J:440:GLN:C	1:L:317:GLN:HE22	2.06	0.64
1:K:6:ARG:HG2	1:K:11:TYR:O	1.98	0.64
1:A:46:ALA:CA	1:A:392:ARG:CD	2.76	0.64
1:A:452:GLU:CD	1:E:155:HIS:HD1	2.04	0.64
1:B:6:ARG:HG2	1:B:11:TYR:O	1.98	0.64
1:B:229:ILE:HD11	1:B:306:ILE:HD11	1.79	0.64
1:B:273:ASN:OD1	1:B:314:ARG:NH2	2.31	0.64
1:C:6:ARG:HD2	1:C:9:SER:O	1.97	0.64
1:C:327:MET:O	1:C:342:LEU:HD22	1.96	0.64
1:D:70:VAL:HG21	1:D:72:ARG:CZ	2.28	0.64
1:F:273:ASN:OD1	1:F:314:ARG:NH2	2.31	0.64
1:B:27:LYS:HE3	1:B:41:LEU:HB2	1.78	0.64
1:E:63:GLN:NE2	1:E:64:GLN:HG3	2.11	0.64
1:H:6:ARG:HD2	1:H:9:SER:O	1.97	0.64
1:I:229:ILE:HD11	1:I:306:ILE:HD11	1.79	0.64
1:J:309:GLU:OE2	1:K:452:GLU:HG2	1.98	0.64
1:L:72:ARG:NH2	1:L:265:HIS:HD2	1.94	0.64
1:L:273:ASN:OD1	1:L:314:ARG:NH2	2.31	0.64
1:E:46:ALA:CB	1:E:392:ARG:CZ	2.73	0.64
1:G:6:ARG:HG2	1:G:11:TYR:O	1.98	0.64
1:H:229:ILE:HD11	1:H:306:ILE:HD11	1.79	0.64
1:J:46:ALA:HA	1:J:392:ARG:CZ	2.27	0.64
1:D:6:ARG:HG2	1:D:11:TYR:O	1.98	0.64
1:I:273:ASN:OD1	1:I:314:ARG:NH2	2.31	0.64
1:J:6:ARG:HG2	1:J:11:TYR:O	1.98	0.64
1:E:70:VAL:HG21	1:E:72:ARG:CZ	2.28	0.63
1:E:229:ILE:HD11	1:E:306:ILE:HD11	1.79	0.63
1:G:44:ILE:CD1	1:G:266:LEU:HD22	2.27	0.63
1:G:70:VAL:HG21	1:G:72:ARG:CZ	2.28	0.63
1:G:420:ARG:NH2	1:H:313:ASN:OD1	2.30	0.63
1:H:273:ASN:OD1	1:H:314:ARG:NH2	2.31	0.63
1:A:273:ASN:OD1	1:A:314:ARG:NH2	2.31	0.63
1:I:6:ARG:HG2	1:I:11:TYR:O	1.98	0.63
1:I:70:VAL:HG21	1:I:72:ARG:CZ	2.28	0.63
1:K:273:ASN:OD1	1:K:314:ARG:NH2	2.31	0.63
1:L:70:VAL:HG21	1:L:72:ARG:CZ	2.27	0.63
1:F:70:VAL:HG21	1:F:72:ARG:CZ	2.27	0.63
1:B:70:VAL:HG21	1:B:72:ARG:CZ	2.28	0.63
1:I:44:ILE:CD1	1:I:266:LEU:HD13	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:27:LYS:HE3	1:J:41:LEU:HB2	1.78	0.63
1:J:70:VAL:HG21	1:J:72:ARG:CZ	2.28	0.63
1:K:70:VAL:HG21	1:K:72:ARG:CZ	2.28	0.63
1:L:325:LEU:HD21	1:L:331:LEU:HD11	1.80	0.63
1:L:325:LEU:CD2	1:L:331:LEU:CG	2.69	0.63
1:D:455:ARG:HD2	1:I:221:ASP:OD1	1.99	0.63
1:F:46:ALA:HA	1:F:392:ARG:NE	2.13	0.63
1:A:229:ILE:HD11	1:A:306:ILE:HD11	1.79	0.63
1:F:72:ARG:CZ	1:F:265:HIS:CD2	2.81	0.63
1:J:273:ASN:OD1	1:J:314:ARG:NH2	2.31	0.63
1:L:63:GLN:HE21	1:L:64:GLN:HE21	1.47	0.63
1:C:396:ARG:HD2	1:E:400:GLN:NE2	2.13	0.63
1:H:63:GLN:HE21	1:H:64:GLN:HE21	1.47	0.63
1:L:6:ARG:HG2	1:L:11:TYR:O	1.98	0.63
1:G:273:ASN:OD1	1:G:314:ARG:NH2	2.31	0.62
1:J:199:PRO:HG2	1:L:170:ARG:HG3	1.81	0.62
1:B:72:ARG:NH2	1:B:265:HIS:CD2	2.65	0.62
1:C:273:ASN:OD1	1:C:314:ARG:NH2	2.31	0.62
1:E:63:GLN:HE21	1:E:64:GLN:HE21	1.47	0.62
1:F:6:ARG:HG2	1:F:11:TYR:O	1.98	0.62
1:F:63:GLN:HE21	1:F:64:GLN:HE21	1.47	0.62
1:I:63:GLN:HE21	1:I:64:GLN:HE21	1.47	0.62
1:L:229:ILE:HD11	1:L:306:ILE:HD11	1.79	0.62
1:B:155:HIS:CE1	1:I:452:GLU:CG	2.82	0.62
1:E:273:ASN:OD1	1:E:314:ARG:NH2	2.31	0.62
1:D:273:ASN:OD1	1:D:314:ARG:NH2	2.31	0.62
1:F:327:MET:SD	1:F:342:LEU:HD11	2.40	0.62
1:B:6:ARG:NE	1:B:66:ILE:HD13	2.03	0.62
1:D:63:GLN:HE21	1:D:64:GLN:HE21	1.47	0.62
1:K:63:GLN:HE21	1:K:64:GLN:HE21	1.47	0.62
1:G:11:TYR:CD1	1:G:369:LYS:CE	2.83	0.62
1:I:11:TYR:CZ	1:I:333:PRO:O	2.53	0.62
1:A:313:ASN:OD1	1:F:420:ARG:NH2	2.32	0.62
1:K:170:ARG:CZ	1:L:199:PRO:HD3	2.30	0.62
1:C:327:MET:HB3	1:C:342:LEU:HD22	1.82	0.62
1:G:63:GLN:HE21	1:G:64:GLN:HE21	1.47	0.62
1:G:327:MET:C	1:G:329:GLY:N	2.58	0.62
1:I:324:VAL:CG1	1:I:331:LEU:HD21	2.29	0.62
1:J:420:ARG:HE	1:L:313:ASN:CB	2.12	0.62
1:A:44:ILE:HD13	1:A:266:LEU:HD21	1.68	0.61
1:C:63:GLN:HE21	1:C:64:GLN:HE21	1.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2:ILE:HB	1:H:63:GLN:HE22	1.65	0.61
1:J:46:ALA:C	1:J:392:ARG:CD	2.72	0.61
1:A:11:TYR:OH	1:A:333:PRO:O	2.15	0.61
1:B:2:ILE:HB	1:B:63:GLN:HE22	1.65	0.61
1:F:44:ILE:HG21	1:F:266:LEU:HD21	1.81	0.61
1:A:11:TYR:CZ	1:A:333:PRO:CB	2.83	0.61
1:C:2:ILE:HB	1:C:63:GLN:HE22	1.65	0.61
1:C:327:MET:HB3	1:C:342:LEU:CD2	2.31	0.61
1:C:418:CYS:O	1:C:422:ASN:N	2.30	0.61
1:E:2:ILE:HB	1:E:63:GLN:HE22	1.65	0.61
1:K:2:ILE:HB	1:K:63:GLN:HE22	1.65	0.61
1:K:325:LEU:HD21	1:K:331:LEU:HG	1.83	0.61
1:A:46:ALA:C	1:A:392:ARG:CD	2.73	0.61
1:A:72:ARG:NH2	1:A:265:HIS:HD2	1.98	0.61
1:L:2:ILE:HB	1:L:63:GLN:HE22	1.65	0.61
1:A:2:ILE:HB	1:A:63:GLN:HE22	1.65	0.61
1:B:44:ILE:HD13	1:B:266:LEU:CD1	2.29	0.61
1:F:2:ILE:HB	1:F:63:GLN:HE22	1.65	0.61
1:F:44:ILE:CG2	1:F:266:LEU:HD21	2.30	0.61
1:B:63:GLN:HE21	1:B:64:GLN:HE21	1.47	0.61
1:C:44:ILE:CD1	1:C:266:LEU:HD13	2.30	0.61
1:E:46:ALA:HB2	1:E:392:ARG:CZ	2.21	0.61
1:G:271:ARG:HH12	1:G:392:ARG:NH1	1.99	0.61
1:H:418:CYS:O	1:H:422:ASN:N	2.30	0.61
1:I:2:ILE:HB	1:I:63:GLN:HE22	1.65	0.61
1:J:2:ILE:HB	1:J:63:GLN:HE22	1.65	0.61
1:B:11:TYR:CG	1:B:369:LYS:CE	2.84	0.61
1:C:72:ARG:NH1	1:C:265:HIS:CD2	2.68	0.61
1:E:46:ALA:HA	1:E:392:ARG:NE	2.16	0.61
1:B:170:ARG:CZ	1:I:199:PRO:HD3	2.31	0.60
1:B:199:PRO:HD3	1:D:170:ARG:CZ	2.30	0.60
1:B:396:ARG:HG2	1:F:400:GLN:CD	2.25	0.60
1:C:11:TYR:CB	1:C:369:LYS:HE2	2.31	0.60
1:G:397:ALA:O	1:G:400:GLN:CG	2.49	0.60
1:J:6:ARG:HG2	1:J:11:TYR:C	2.26	0.60
1:J:24:PHE:CD2	1:J:25:GLN:HG3	2.36	0.60
1:J:63:GLN:HE21	1:J:64:GLN:HE21	1.47	0.60
1:L:24:PHE:CD2	1:L:25:GLN:HG3	2.36	0.60
1:B:396:ARG:HG2	1:F:400:GLN:NE2	2.16	0.60
1:E:6:ARG:HG2	1:E:11:TYR:C	2.26	0.60
1:E:29:VAL:O	1:E:33:ARG:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6:ARG:HG2	1:G:11:TYR:C	2.26	0.60
1:I:24:PHE:CD2	1:I:25:GLN:HG3	2.36	0.60
1:K:11:TYR:HH	1:K:333:PRO:C	1.92	0.60
1:A:63:GLN:HE21	1:A:64:GLN:HE21	1.47	0.60
1:E:199:PRO:HG2	1:F:170:ARG:HG3	1.83	0.60
1:F:44:ILE:HD13	1:F:266:LEU:CD1	2.31	0.60
1:D:2:ILE:HB	1:D:63:GLN:HE22	1.65	0.60
1:K:327:MET:HB3	1:K:342:LEU:HD11	1.81	0.60
1:C:24:PHE:CD2	1:C:25:GLN:HG3	2.36	0.60
1:F:29:VAL:O	1:F:33:ARG:HB2	2.02	0.60
1:A:452:GLU:HG3	1:E:155:HIS:HE1	1.65	0.60
1:G:2:ILE:HB	1:G:63:GLN:HE22	1.65	0.60
1:K:6:ARG:HG2	1:K:11:TYR:C	2.26	0.60
1:K:29:VAL:O	1:K:33:ARG:HB2	2.02	0.60
1:B:6:ARG:HG2	1:B:11:TYR:C	2.27	0.60
1:C:396:ARG:HD2	1:E:400:GLN:HE21	1.66	0.60
1:E:24:PHE:CD2	1:E:25:GLN:HG3	2.36	0.60
1:H:24:PHE:CD2	1:H:25:GLN:HG3	2.36	0.60
1:J:44:ILE:CG2	1:J:266:LEU:HD21	2.32	0.60
1:G:9:SER:OG	1:G:10:SER:N	2.35	0.60
1:J:313:ASN:OD1	1:K:420:ARG:CZ	2.50	0.60
1:L:44:ILE:CG1	1:L:266:LEU:HD21	2.31	0.60
1:A:6:ARG:HG2	1:A:11:TYR:C	2.26	0.60
1:A:327:MET:HB3	1:A:342:LEU:CD2	2.30	0.60
1:I:70:VAL:CG1	1:I:269:VAL:HG11	2.30	0.60
1:K:324:VAL:HG11	1:K:340:GLY:HA2	1.81	0.60
1:A:452:GLU:CG	1:E:309:GLU:OE2	2.50	0.60
1:L:29:VAL:O	1:L:33:ARG:HB2	2.02	0.60
1:C:9:SER:OG	1:C:10:SER:N	2.35	0.59
1:D:24:PHE:CD2	1:D:25:GLN:HG3	2.36	0.59
1:D:29:VAL:O	1:D:33:ARG:HB2	2.01	0.59
1:I:6:ARG:HG2	1:I:11:TYR:C	2.26	0.59
1:I:188:ILE:HG23	1:I:188:ILE:O	2.01	0.59
1:A:455:ARG:HD2	1:E:221:ASP:OD1	2.01	0.59
1:B:24:PHE:CD2	1:B:25:GLN:HG3	2.36	0.59
1:D:6:ARG:HG2	1:D:11:TYR:C	2.26	0.59
1:G:24:PHE:CD2	1:G:25:GLN:HG3	2.36	0.59
1:I:29:VAL:O	1:I:33:ARG:HB2	2.02	0.59
1:I:72:ARG:CZ	1:I:265:HIS:CD2	2.85	0.59
1:J:29:VAL:O	1:J:33:ARG:HB2	2.01	0.59
1:C:22:SER:CB	1:C:24:PHE:CE1	2.86	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:ARG:CZ	1:D:265:HIS:CD2	2.85	0.59
1:F:24:PHE:HB3	1:F:52:ASN:ND2	2.17	0.59
1:I:271:ARG:HH12	1:I:392:ARG:NH1	2.00	0.59
1:K:24:PHE:CD2	1:K:25:GLN:HG3	2.36	0.59
1:L:324:VAL:HG13	1:L:340:GLY:HA3	1.82	0.59
1:A:24:PHE:CD2	1:A:25:GLN:HG3	2.36	0.59
1:C:29:VAL:O	1:C:33:ARG:HB2	2.02	0.59
1:J:324:VAL:CG1	1:J:340:GLY:HA3	2.32	0.59
1:L:6:ARG:HG2	1:L:11:TYR:C	2.26	0.59
1:D:22:SER:CB	1:D:24:PHE:CE1	2.86	0.59
1:F:6:ARG:HG2	1:F:11:TYR:C	2.26	0.59
1:I:44:ILE:CG2	1:I:266:LEU:HD21	2.33	0.59
1:I:68:HIS:CE1	1:I:273:ASN:CB	2.86	0.59
1:E:22:SER:CB	1:E:24:PHE:CE1	2.86	0.59
1:E:46:ALA:CA	1:E:392:ARG:HD3	2.30	0.59
1:E:46:ALA:C	1:E:392:ARG:HD2	2.28	0.59
1:F:24:PHE:CD2	1:F:25:GLN:HG3	2.36	0.59
1:B:6:ARG:NH2	1:B:66:ILE:HD13	2.18	0.59
1:B:29:VAL:O	1:B:33:ARG:HB2	2.01	0.59
1:C:396:ARG:NE	1:E:400:GLN:HG2	2.17	0.59
1:D:9:SER:OG	1:D:10:SER:N	2.35	0.59
1:H:29:VAL:O	1:H:33:ARG:HB2	2.01	0.59
1:H:46:ALA:H	1:H:392:ARG:NH1	1.99	0.59
1:J:324:VAL:HG12	1:J:331:LEU:CD2	2.25	0.59
1:A:29:VAL:O	1:A:33:ARG:HB2	2.02	0.59
1:D:6:ARG:NH2	1:D:66:ILE:HD13	2.18	0.59
1:E:11:TYR:HE1	1:E:333:PRO:HA	1.68	0.59
1:F:9:SER:OG	1:F:10:SER:N	2.35	0.59
1:G:29:VAL:O	1:G:33:ARG:HB2	2.02	0.59
1:I:9:SER:OG	1:I:10:SER:N	2.35	0.59
1:K:6:ARG:NH2	1:K:66:ILE:HD13	2.18	0.59
1:A:44:ILE:CD1	1:A:266:LEU:HD21	2.24	0.59
1:C:3:VAL:HG22	1:C:15:VAL:O	2.03	0.59
1:C:70:VAL:HG13	1:C:269:VAL:HG11	1.85	0.59
1:F:22:SER:CB	1:F:24:PHE:CE1	2.86	0.59
1:G:6:ARG:NH2	1:G:66:ILE:HD13	2.17	0.59
1:J:9:SER:OG	1:J:10:SER:N	2.35	0.59
1:L:22:SER:CB	1:L:24:PHE:CE1	2.86	0.59
1:B:455:ARG:HD2	1:D:221:ASP:OD1	2.03	0.58
1:C:24:PHE:HB3	1:C:52:ASN:ND2	2.17	0.58
1:G:24:PHE:HB3	1:G:52:ASN:ND2	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:72:ARG:NH1	1:K:265:HIS:CD2	2.71	0.58
1:A:22:SER:CB	1:A:24:PHE:CE1	2.86	0.58
1:B:47:GLY:HA3	1:B:392:ARG:HB3	1.85	0.58
1:E:9:SER:OG	1:E:10:SER:N	2.35	0.58
1:E:24:PHE:HB3	1:E:52:ASN:ND2	2.17	0.58
1:G:44:ILE:HD13	1:G:266:LEU:HD22	1.78	0.58
1:I:3:VAL:HG22	1:I:15:VAL:O	2.03	0.58
1:L:6:ARG:NH2	1:L:66:ILE:HD13	2.18	0.58
1:A:9:SER:OG	1:A:10:SER:N	2.35	0.58
1:B:155:HIS:ND1	1:I:452:GLU:CG	2.67	0.58
1:C:11:TYR:HB3	1:C:369:LYS:HE2	1.84	0.58
1:I:22:SER:CB	1:I:24:PHE:CE1	2.86	0.58
1:K:22:SER:CB	1:K:24:PHE:CE1	2.86	0.58
1:L:3:VAL:HG22	1:L:15:VAL:O	2.03	0.58
1:F:3:VAL:HG22	1:F:15:VAL:O	2.03	0.58
1:G:3:VAL:HG22	1:G:15:VAL:O	2.03	0.58
1:H:22:SER:CB	1:H:24:PHE:CE1	2.86	0.58
1:J:3:VAL:HG22	1:J:15:VAL:O	2.03	0.58
1:B:22:SER:CB	1:B:24:PHE:CE1	2.86	0.58
1:B:396:ARG:O	1:F:396:ARG:CZ	2.27	0.58
1:E:6:ARG:NH2	1:E:66:ILE:HD13	2.18	0.58
1:E:327:MET:CG	1:E:342:LEU:CD1	2.49	0.58
1:I:6:ARG:NH2	1:I:66:ILE:HD13	2.18	0.58
1:J:6:ARG:NH2	1:J:66:ILE:HD13	2.18	0.58
1:A:418:CYS:O	1:A:422:ASN:N	2.31	0.58
1:E:3:VAL:HG22	1:E:15:VAL:O	2.03	0.58
1:G:72:ARG:CZ	1:G:265:HIS:CD2	2.86	0.58
1:J:22:SER:CB	1:J:24:PHE:CE1	2.86	0.58
1:F:6:ARG:NH2	1:F:66:ILE:HD13	2.17	0.58
1:G:22:SER:CB	1:G:24:PHE:CE1	2.86	0.58
1:J:46:ALA:C	1:J:392:ARG:HD2	2.28	0.58
1:K:72:ARG:NH2	1:K:265:HIS:CD2	2.67	0.58
1:C:24:PHE:CB	1:C:52:ASN:HD21	2.17	0.58
1:B:345:GLN:CD	1:B:345:GLN:H	2.11	0.58
1:C:44:ILE:HD12	1:C:266:LEU:CD1	2.33	0.58
1:E:44:ILE:HB	1:E:266:LEU:HD21	1.86	0.58
1:H:24:PHE:HB3	1:H:52:ASN:ND2	2.17	0.58
1:J:330:VAL:CG1	1:J:350:VAL:HG11	2.30	0.58
1:K:72:ARG:CZ	1:K:265:HIS:CD2	2.87	0.58
1:B:3:VAL:HG22	1:B:15:VAL:O	2.03	0.58
1:E:418:CYS:O	1:E:422:ASN:N	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:418:CYS:O	1:G:422:ASN:N	2.30	0.58
1:H:9:SER:OG	1:H:10:SER:N	2.35	0.58
1:I:11:TYR:CE2	1:I:333:PRO:HB2	2.34	0.58
1:I:44:ILE:HD13	1:I:266:LEU:HD21	1.74	0.58
1:I:68:HIS:CE1	1:I:273:ASN:HB3	2.39	0.58
1:B:420:ARG:HG3	1:D:313:ASN:HB3	1.86	0.57
1:H:3:VAL:HG22	1:H:15:VAL:O	2.03	0.57
1:K:9:SER:OG	1:K:10:SER:N	2.35	0.57
1:K:11:TYR:HE1	1:K:333:PRO:C	2.10	0.57
1:D:3:VAL:HG22	1:D:15:VAL:O	2.03	0.57
1:K:418:CYS:O	1:K:422:ASN:N	2.31	0.57
1:L:46:ALA:HB2	1:L:392:ARG:HH12	1.65	0.57
1:A:6:ARG:NH2	1:A:66:ILE:HD13	2.18	0.57
1:B:9:SER:OG	1:B:10:SER:N	2.35	0.57
1:B:24:PHE:HB3	1:B:52:ASN:ND2	2.17	0.57
1:F:46:ALA:C	1:F:392:ARG:HD2	2.30	0.57
1:A:3:VAL:HG22	1:A:15:VAL:O	2.03	0.57
1:B:199:PRO:HG2	1:D:170:ARG:HG3	1.87	0.57
1:D:24:PHE:HB3	1:D:52:ASN:ND2	2.17	0.57
1:K:3:VAL:HG22	1:K:15:VAL:O	2.03	0.57
1:B:24:PHE:CB	1:B:52:ASN:HD21	2.17	0.57
1:J:418:CYS:O	1:J:422:ASN:N	2.30	0.57
1:I:2:ILE:HG13	1:I:378:ASP:OD2	2.04	0.57
1:L:9:SER:OG	1:L:10:SER:N	2.35	0.57
1:L:24:PHE:HB3	1:L:52:ASN:ND2	2.17	0.57
1:D:400:GLN:HE21	1:H:396:ARG:CD	2.14	0.57
1:D:418:CYS:O	1:D:422:ASN:N	2.30	0.57
1:I:44:ILE:CG1	1:I:266:LEU:CD2	2.79	0.57
1:B:155:HIS:HE1	1:I:452:GLU:HG3	1.63	0.57
1:I:11:TYR:CE1	1:I:333:PRO:HB3	2.37	0.57
1:J:452:GLU:OE2	1:L:155:HIS:ND1	2.36	0.57
1:A:11:TYR:CD1	1:A:369:LYS:HE2	2.40	0.57
1:B:420:ARG:NE	1:D:313:ASN:CG	2.40	0.57
1:F:324:VAL:HG11	1:F:340:GLY:HA2	1.87	0.57
1:G:397:ALA:C	1:G:400:GLN:HG2	2.30	0.56
1:J:46:ALA:HB1	1:J:392:ARG:HD3	1.85	0.56
1:A:44:ILE:CG1	1:A:266:LEU:CD2	2.81	0.56
1:A:24:PHE:HB3	1:A:52:ASN:ND2	2.17	0.56
1:B:418:CYS:O	1:B:422:ASN:N	2.31	0.56
1:C:72:ARG:NH1	1:C:265:HIS:NE2	2.54	0.56
1:F:327:MET:C	1:F:342:LEU:HD21	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:255:HIS:CE1	1:H:402:ARG:NH2	2.73	0.56
1:I:11:TYR:CG	1:I:369:LYS:HE2	2.40	0.56
1:J:24:PHE:HB3	1:J:52:ASN:ND2	2.17	0.56
1:D:420:ARG:NH2	1:I:313:ASN:OD1	2.38	0.56
1:E:27:LYS:HE2	1:E:38:ALA:HB1	1.88	0.56
1:H:27:LYS:HE2	1:H:38:ALA:HB1	1.88	0.56
1:L:11:TYR:CZ	1:L:333:PRO:C	2.77	0.56
1:L:44:ILE:HB	1:L:266:LEU:HD21	1.86	0.56
1:C:396:ARG:HD2	1:E:400:GLN:CG	2.34	0.56
1:F:27:LYS:HE2	1:F:38:ALA:HB1	1.88	0.56
1:L:418:CYS:O	1:L:422:ASN:N	2.31	0.56
1:D:27:LYS:HE2	1:D:38:ALA:HB1	1.88	0.56
1:F:6:ARG:NE	1:F:66:ILE:HD13	2.02	0.56
1:F:68:HIS:CD2	1:F:270:THR:HG23	2.41	0.56
1:I:27:LYS:HE2	1:I:38:ALA:HB1	1.88	0.56
1:I:418:CYS:O	1:I:422:ASN:N	2.31	0.56
1:J:46:ALA:C	1:J:392:ARG:HD3	2.29	0.56
1:K:27:LYS:HE2	1:K:38:ALA:HB1	1.88	0.56
1:B:27:LYS:HE2	1:B:38:ALA:HB1	1.88	0.56
1:B:341:LEU:C	1:B:343:PRO:HD3	2.31	0.56
1:D:24:PHE:CB	1:D:52:ASN:HD21	2.17	0.56
1:F:24:PHE:CB	1:F:52:ASN:HD21	2.17	0.56
1:G:242:THR:HG22	1:G:400:GLN:NE2	2.21	0.56
1:F:418:CYS:O	1:F:422:ASN:N	2.30	0.56
1:B:44:ILE:CG1	1:B:266:LEU:CD2	2.61	0.55
1:J:24:PHE:CB	1:J:52:ASN:HD21	2.17	0.55
1:A:452:GLU:CG	1:E:155:HIS:CE1	2.89	0.55
1:B:46:ALA:CB	1:B:392:ARG:CD	2.80	0.55
1:C:327:MET:C	1:C:342:LEU:HD22	2.32	0.55
1:C:420:ARG:NH2	1:G:313:ASN:OD1	2.38	0.55
1:K:24:PHE:HB3	1:K:52:ASN:ND2	2.17	0.55
1:L:27:LYS:HE2	1:L:38:ALA:HB1	1.88	0.55
1:A:328:GLY:O	1:A:366:ARG:NH2	2.40	0.55
1:B:11:TYR:OH	1:B:333:PRO:CA	2.55	0.55
1:E:455:ARG:CD	1:F:221:ASP:OD1	2.54	0.55
1:F:46:ALA:C	1:F:392:ARG:CD	2.79	0.55
1:H:46:ALA:HA	1:H:392:ARG:HD3	1.86	0.55
1:L:11:TYR:OH	1:L:333:PRO:O	2.25	0.55
1:B:46:ALA:CB	1:B:392:ARG:HD3	2.35	0.55
1:B:221:ASP:OD1	1:I:455:ARG:HD2	2.06	0.55
1:J:27:LYS:HE2	1:J:38:ALA:HB1	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:LYS:HE2	1:A:38:ALA:HB1	1.88	0.55
1:K:313:ASN:OD1	1:L:420:ARG:CZ	2.55	0.55
1:K:24:PHE:CB	1:K:52:ASN:HD21	2.17	0.55
1:C:27:LYS:HE2	1:C:38:ALA:HB1	1.88	0.55
1:C:155:HIS:CE1	1:H:452:GLU:HG3	2.42	0.54
1:A:24:PHE:CB	1:A:52:ASN:HD21	2.17	0.54
1:G:24:PHE:CB	1:G:52:ASN:HD21	2.17	0.54
1:B:11:TYR:HB3	1:B:369:LYS:HE2	1.88	0.54
1:C:11:TYR:CG	1:C:369:LYS:HE3	2.28	0.54
1:E:11:TYR:CE1	1:E:333:PRO:CA	2.90	0.54
1:L:4:PHE:HB2	1:L:66:ILE:HA	1.90	0.54
1:E:46:ALA:C	1:E:392:ARG:CD	2.80	0.54
1:J:4:PHE:HB2	1:J:66:ILE:HA	1.90	0.54
1:J:324:VAL:HG13	1:J:340:GLY:HA3	1.88	0.54
1:K:4:PHE:HB2	1:K:66:ILE:HA	1.90	0.54
1:K:72:ARG:CZ	1:K:265:HIS:HD2	2.19	0.54
1:B:4:PHE:HB2	1:B:66:ILE:HA	1.90	0.54
1:G:4:PHE:HB2	1:G:66:ILE:HA	1.90	0.54
1:G:27:LYS:HE2	1:G:38:ALA:HB1	1.88	0.54
1:D:4:PHE:HB2	1:D:66:ILE:HA	1.90	0.54
1:I:24:PHE:CB	1:I:52:ASN:HD21	2.17	0.54
1:L:24:PHE:CB	1:L:52:ASN:HD21	2.17	0.54
1:B:170:ARG:NE	1:I:199:PRO:HD3	2.23	0.54
1:B:397:ALA:N	1:F:396:ARG:NH2	2.55	0.54
1:C:309:GLU:OE2	1:H:452:GLU:CG	2.55	0.54
1:L:11:TYR:CE1	1:L:333:PRO:HB3	2.32	0.54
1:F:327:MET:C	1:F:329:GLY:H	2.07	0.53
1:E:44:ILE:HG21	1:E:266:LEU:CD2	2.38	0.53
1:F:157:VAL:HG21	1:F:306:ILE:HG12	1.91	0.53
1:G:157:VAL:HG21	1:G:306:ILE:HG12	1.91	0.53
1:H:68:HIS:CE1	1:H:273:ASN:HB2	2.43	0.53
1:K:327:MET:HB3	1:K:342:LEU:HD22	1.83	0.53
1:K:327:MET:CB	1:K:342:LEU:HD11	2.38	0.53
1:L:157:VAL:HG21	1:L:306:ILE:HG12	1.91	0.53
1:C:44:ILE:HD13	1:C:266:LEU:HD13	1.84	0.53
1:A:56:VAL:HA	1:A:59:CYS:SG	2.49	0.53
1:E:4:PHE:HB2	1:E:66:ILE:HA	1.90	0.53
1:E:24:PHE:CB	1:E:52:ASN:HD21	2.17	0.53
1:K:327:MET:HB3	1:K:342:LEU:CG	2.37	0.53
1:C:4:PHE:HB2	1:C:66:ILE:HA	1.90	0.53
1:E:268:CYS:HB2	1:E:307:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:4:PHE:HB2	1:I:66:ILE:HA	1.90	0.53
1:K:170:ARG:NE	1:L:199:PRO:CD	2.69	0.53
1:L:56:VAL:HA	1:L:59:CYS:SG	2.49	0.53
1:L:325:LEU:HD23	1:L:331:LEU:HG	1.87	0.53
1:B:56:VAL:HA	1:B:59:CYS:SG	2.49	0.53
1:D:6:ARG:NE	1:D:66:ILE:HD13	2.03	0.53
1:D:199:PRO:HD3	1:I:170:ARG:NE	2.23	0.53
1:E:329:GLY:N	1:E:342:LEU:HD23	2.24	0.53
1:E:453:TRP:HE1	1:E:458:MET:HE3	1.74	0.53
1:G:56:VAL:HA	1:G:59:CYS:SG	2.49	0.53
1:G:268:CYS:HB2	1:G:307:LEU:HD21	1.91	0.53
1:I:56:VAL:HA	1:I:59:CYS:SG	2.49	0.53
1:K:56:VAL:HA	1:K:59:CYS:SG	2.49	0.53
1:K:453:TRP:HE1	1:K:458:MET:HE3	1.74	0.53
1:A:268:CYS:HB2	1:A:307:LEU:HD21	1.91	0.53
1:B:320:ALA:HB2	1:I:440:GLN:HB2	1.91	0.53
1:C:56:VAL:HA	1:C:59:CYS:SG	2.49	0.53
1:C:268:CYS:HB2	1:C:307:LEU:HD21	1.91	0.53
1:C:453:TRP:HE1	1:C:458:MET:HE3	1.74	0.53
1:F:453:TRP:HE1	1:F:458:MET:HE3	1.74	0.53
1:J:46:ALA:HB2	1:J:392:ARG:CZ	2.35	0.53
1:J:453:TRP:HE1	1:J:458:MET:HE3	1.74	0.53
1:L:453:TRP:HE1	1:L:458:MET:HE3	1.74	0.53
1:D:56:VAL:HA	1:D:59:CYS:SG	2.49	0.53
1:D:157:VAL:HG21	1:D:306:ILE:HG12	1.91	0.53
1:E:157:VAL:HG21	1:E:306:ILE:HG12	1.91	0.53
1:H:56:VAL:HA	1:H:59:CYS:SG	2.49	0.53
1:H:268:CYS:HB2	1:H:307:LEU:HD21	1.91	0.53
1:B:453:TRP:HE1	1:B:458:MET:HE3	1.73	0.53
1:D:420:ARG:HE	1:I:313:ASN:CG	2.15	0.53
1:H:453:TRP:HE1	1:H:458:MET:HE3	1.74	0.53
1:I:453:TRP:HE1	1:I:458:MET:HE3	1.74	0.53
1:L:268:CYS:HB2	1:L:307:LEU:HD21	1.91	0.53
1:F:11:TYR:CE1	1:F:369:LYS:HE3	2.44	0.53
1:H:44:ILE:CG1	1:H:266:LEU:HD21	2.39	0.53
1:J:44:ILE:HD13	1:J:266:LEU:HD22	0.53	0.53
1:J:46:ALA:H	1:J:392:ARG:NH1	2.06	0.53
1:J:157:VAL:HG21	1:J:306:ILE:HG12	1.91	0.53
1:B:268:CYS:HB2	1:B:307:LEU:HD21	1.91	0.52
1:F:56:VAL:HA	1:F:59:CYS:SG	2.49	0.52
1:H:24:PHE:CB	1:H:52:ASN:HD21	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:68:HIS:ND1	1:H:270:THR:HA	2.20	0.52
1:B:157:VAL:HG21	1:B:306:ILE:HG12	1.91	0.52
1:D:453:TRP:HE1	1:D:458:MET:HE3	1.74	0.52
1:F:4:PHE:HB2	1:F:66:ILE:HA	1.90	0.52
1:F:11:TYR:CE1	1:F:333:PRO:CB	2.92	0.52
1:I:157:VAL:HG21	1:I:306:ILE:HG12	1.91	0.52
1:K:313:ASN:OD1	1:L:420:ARG:NE	2.42	0.52
1:G:44:ILE:CD1	1:G:266:LEU:HD13	2.35	0.52
1:H:4:PHE:HB2	1:H:66:ILE:HA	1.90	0.52
1:K:157:VAL:HG21	1:K:306:ILE:HG12	1.91	0.52
1:A:453:TRP:HE1	1:A:458:MET:HE3	1.74	0.52
1:C:70:VAL:HG11	1:C:269:VAL:HG11	1.89	0.52
1:F:9:SER:O	1:F:273:ASN:HA	2.10	0.52
1:I:24:PHE:HB3	1:I:52:ASN:ND2	2.17	0.52
1:K:327:MET:C	1:K:329:GLY:N	2.64	0.52
1:L:9:SER:O	1:L:273:ASN:HA	2.09	0.52
1:A:4:PHE:HB2	1:A:66:ILE:HA	1.90	0.52
1:E:56:VAL:HA	1:E:59:CYS:SG	2.49	0.52
1:J:72:ARG:CZ	1:J:265:HIS:CD2	2.93	0.52
1:K:68:HIS:CD2	1:K:270:THR:HG23	2.44	0.52
1:A:157:VAL:HG21	1:A:306:ILE:HG12	1.91	0.52
1:F:327:MET:C	1:F:329:GLY:N	2.67	0.52
1:G:397:ALA:HA	1:G:400:GLN:HG2	1.91	0.52
1:H:11:TYR:HB3	1:H:369:LYS:HE2	1.91	0.52
1:I:268:CYS:HB2	1:I:307:LEU:HD21	1.91	0.52
1:J:56:VAL:HA	1:J:59:CYS:SG	2.49	0.52
1:K:68:HIS:CE1	1:K:274:ASP:CG	2.88	0.52
1:F:268:CYS:HB2	1:F:307:LEU:HD21	1.91	0.52
1:I:68:HIS:CE1	1:I:273:ASN:HB2	2.45	0.52
1:C:157:VAL:HG21	1:C:306:ILE:HG12	1.91	0.52
1:D:44:ILE:HD13	1:D:266:LEU:CD1	2.39	0.52
1:G:453:TRP:HE1	1:G:458:MET:HE3	1.74	0.52
1:J:268:CYS:HB2	1:J:307:LEU:HD21	1.91	0.52
1:E:421:CYS:HB3	1:E:441:CYS:SG	2.50	0.51
1:H:157:VAL:HG21	1:H:306:ILE:HG12	1.91	0.51
1:K:11:TYR:HB3	1:K:369:LYS:HE2	1.92	0.51
1:C:15:VAL:HG11	1:C:26:LEU:HD13	1.92	0.51
1:D:268:CYS:HB2	1:D:307:LEU:HD21	1.91	0.51
1:K:11:TYR:CZ	1:K:333:PRO:CA	2.92	0.51
1:A:421:CYS:HB3	1:A:441:CYS:SG	2.50	0.51
1:E:9:SER:O	1:E:273:ASN:CA	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:454:ASN:HB3	1:F:151:LYS:O	2.10	0.51
1:F:15:VAL:HG11	1:F:26:LEU:HD13	1.92	0.51
1:G:421:CYS:HB3	1:G:441:CYS:SG	2.50	0.51
1:I:421:CYS:HB3	1:I:441:CYS:SG	2.50	0.51
1:J:421:CYS:HB3	1:J:441:CYS:SG	2.50	0.51
1:B:11:TYR:CZ	1:B:333:PRO:O	2.63	0.51
1:B:421:CYS:HB3	1:B:441:CYS:SG	2.50	0.51
1:E:324:VAL:O	1:E:327:MET:HB2	2.10	0.51
1:G:15:VAL:HG11	1:G:26:LEU:HD13	1.92	0.51
1:H:421:CYS:HB3	1:H:441:CYS:SG	2.50	0.51
1:I:6:ARG:CG	1:I:66:ILE:HD11	2.41	0.51
1:J:15:VAL:HG11	1:J:26:LEU:HD13	1.92	0.51
1:K:15:VAL:HG11	1:K:26:LEU:HD13	1.92	0.51
1:L:6:ARG:CG	1:L:66:ILE:HD11	2.41	0.51
1:G:242:THR:HG22	1:G:400:GLN:HE22	1.76	0.51
1:K:268:CYS:HB2	1:K:307:LEU:HD21	1.91	0.51
1:B:70:VAL:CG1	1:B:269:VAL:HG11	2.41	0.51
1:E:43:VAL:HG13	1:E:68:HIS:O	2.11	0.51
1:J:6:ARG:CG	1:J:66:ILE:HD11	2.41	0.51
1:K:43:VAL:HG13	1:K:68:HIS:O	2.11	0.51
1:K:421:CYS:HB3	1:K:441:CYS:SG	2.50	0.51
1:F:421:CYS:HB3	1:F:441:CYS:SG	2.50	0.51
1:H:6:ARG:HH12	1:H:68:HIS:CE1	2.28	0.51
1:L:421:CYS:HB3	1:L:441:CYS:SG	2.50	0.51
1:A:327:MET:C	1:A:329:GLY:H	2.18	0.51
1:B:6:ARG:CG	1:B:66:ILE:HD11	2.41	0.51
1:C:11:TYR:CE1	1:C:369:LYS:CE	2.71	0.51
1:C:400:GLN:HA	1:E:396:ARG:NH1	2.26	0.51
1:F:6:ARG:CG	1:F:66:ILE:HD11	2.41	0.51
1:I:43:VAL:HG13	1:I:68:HIS:O	2.11	0.51
1:C:396:ARG:NE	1:E:400:GLN:NE2	2.54	0.51
1:D:421:CYS:HB3	1:D:441:CYS:SG	2.50	0.51
1:F:43:VAL:HG13	1:F:68:HIS:O	2.11	0.51
1:L:11:TYR:OH	1:L:333:PRO:CB	2.46	0.51
1:C:421:CYS:HB3	1:C:441:CYS:SG	2.50	0.50
1:A:6:ARG:CG	1:A:66:ILE:HD11	2.41	0.50
1:C:43:VAL:HG13	1:C:68:HIS:O	2.11	0.50
1:D:6:ARG:CG	1:D:66:ILE:HD11	2.41	0.50
1:D:11:TYR:HE1	1:D:333:PRO:HA	1.76	0.50
1:L:15:VAL:HG11	1:L:26:LEU:HD13	1.92	0.50
1:B:15:VAL:HG11	1:B:26:LEU:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:VAL:HG11	1:E:26:LEU:HD13	1.92	0.50
1:F:46:ALA:CA	1:F:392:ARG:HD3	2.40	0.50
1:H:11:TYR:CB	1:H:369:LYS:HE2	2.41	0.50
1:I:44:ILE:HD13	1:I:266:LEU:HD11	1.83	0.50
1:J:329:GLY:CA	1:J:366:ARG:HH22	2.23	0.50
1:L:43:VAL:HG13	1:L:68:HIS:O	2.11	0.50
1:A:43:VAL:HG13	1:A:68:HIS:O	2.11	0.50
1:B:43:VAL:HG13	1:B:68:HIS:O	2.11	0.50
1:C:44:ILE:HD12	1:C:266:LEU:HD11	1.94	0.50
1:J:43:VAL:HG13	1:J:68:HIS:O	2.11	0.50
1:K:6:ARG:CG	1:K:66:ILE:HD11	2.41	0.50
1:K:11:TYR:HE1	1:K:333:PRO:O	1.86	0.50
1:A:15:VAL:HG11	1:A:26:LEU:HD13	1.92	0.50
1:D:15:VAL:HG11	1:D:26:LEU:HD13	1.92	0.50
1:G:11:TYR:HH	1:G:333:PRO:HB2	1.72	0.50
1:I:15:VAL:HG11	1:I:26:LEU:HD13	1.92	0.50
1:J:324:VAL:HG11	1:J:331:LEU:CD2	2.41	0.50
1:L:44:ILE:HG21	1:L:266:LEU:CD2	2.39	0.50
1:B:455:ARG:CD	1:D:221:ASP:OD1	2.60	0.50
1:G:6:ARG:CG	1:G:66:ILE:HD11	2.41	0.50
1:H:15:VAL:HG11	1:H:26:LEU:HD13	1.92	0.50
1:H:43:VAL:HG13	1:H:68:HIS:O	2.11	0.50
1:A:155:HIS:HD1	1:F:452:GLU:CD	2.12	0.50
1:H:347:GLN:HG3	1:H:349:LYS:H	1.77	0.50
1:D:43:VAL:HG13	1:D:68:HIS:O	2.11	0.50
1:E:199:PRO:CG	1:F:170:ARG:HG3	2.41	0.50
1:G:43:VAL:HG13	1:G:68:HIS:O	2.11	0.50
1:J:347:GLN:HG3	1:J:349:LYS:H	1.77	0.49
1:K:68:HIS:NE2	1:K:274:ASP:OD2	2.45	0.49
1:B:44:ILE:HG12	1:B:266:LEU:HD21	1.87	0.49
1:B:155:HIS:HD1	1:I:452:GLU:CG	2.24	0.49
1:E:6:ARG:CG	1:E:66:ILE:HD11	2.41	0.49
1:E:324:VAL:CG1	1:E:340:GLY:CA	2.82	0.49
1:H:44:ILE:HG23	1:H:48:LYS:C	2.38	0.49
1:I:14:PRO:HD3	1:I:370:GLU:OE1	2.09	0.49
1:B:44:ILE:HG23	1:B:48:LYS:C	2.38	0.49
1:G:420:ARG:HG3	1:H:313:ASN:HB3	1.95	0.49
1:I:44:ILE:CD1	1:I:266:LEU:HD11	2.38	0.49
1:K:347:GLN:HG3	1:K:349:LYS:H	1.77	0.49
1:D:44:ILE:HG23	1:D:48:LYS:C	2.38	0.49
1:D:347:GLN:HG3	1:D:349:LYS:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:420:ARG:CZ	1:I:313:ASN:OD1	2.60	0.49
1:E:44:ILE:HG23	1:E:48:LYS:C	2.37	0.49
1:E:347:GLN:HG3	1:E:349:LYS:H	1.77	0.49
1:F:347:GLN:HG3	1:F:349:LYS:H	1.77	0.49
1:K:24:PHE:CE2	1:K:25:GLN:CG	2.87	0.49
1:K:327:MET:C	1:K:329:GLY:H	2.05	0.49
1:A:44:ILE:HG23	1:A:48:LYS:C	2.38	0.49
1:C:44:ILE:HG23	1:C:48:LYS:C	2.38	0.49
1:I:44:ILE:CB	1:I:266:LEU:HD21	2.42	0.49
1:K:170:ARG:HE	1:L:199:PRO:CG	2.25	0.49
1:F:44:ILE:HG23	1:F:48:LYS:C	2.38	0.49
1:I:11:TYR:CG	1:I:369:LYS:CE	2.95	0.49
1:H:72:ARG:HH22	1:H:265:HIS:HD2	1.59	0.49
1:K:68:HIS:NE2	1:K:274:ASP:OD1	2.46	0.49
1:A:11:TYR:CE1	1:A:333:PRO:CB	2.95	0.49
1:B:438:GLN:HB3	1:B:440:GLN:CD	2.38	0.49
1:D:70:VAL:HG21	1:D:72:ARG:NH2	2.28	0.49
1:G:24:PHE:O	1:G:28:GLU:HG3	2.13	0.49
1:G:347:GLN:HG3	1:G:349:LYS:H	1.77	0.49
1:K:24:PHE:O	1:K:28:GLU:HG3	2.13	0.49
1:K:327:MET:O	1:K:342:LEU:HD23	2.00	0.49
1:L:438:GLN:HB3	1:L:440:GLN:CD	2.38	0.49
1:A:438:GLN:HB3	1:A:440:GLN:CD	2.38	0.49
1:K:44:ILE:HG23	1:K:48:LYS:C	2.38	0.49
1:A:24:PHE:O	1:A:28:GLU:HG3	2.13	0.49
1:A:70:VAL:HG21	1:A:72:ARG:NH2	2.28	0.49
1:A:347:GLN:HG3	1:A:349:LYS:H	1.77	0.49
1:B:24:PHE:O	1:B:28:GLU:HG3	2.13	0.49
1:G:44:ILE:HG23	1:G:48:LYS:C	2.37	0.49
1:I:44:ILE:HG23	1:I:48:LYS:C	2.37	0.49
1:I:44:ILE:HB	1:I:266:LEU:HD11	1.95	0.49
1:J:24:PHE:O	1:J:28:GLU:HG3	2.13	0.49
1:J:44:ILE:HG23	1:J:48:LYS:C	2.38	0.49
1:K:327:MET:C	1:K:342:LEU:HD22	2.03	0.49
1:A:10:SER:HA	1:A:273:ASN:O	2.12	0.48
1:I:24:PHE:O	1:I:28:GLU:HG3	2.13	0.48
1:K:438:GLN:HB3	1:K:440:GLN:CD	2.38	0.48
1:A:324:VAL:HG11	1:A:331:LEU:CD2	2.43	0.48
1:D:14:PRO:HD2	1:D:370:GLU:CD	2.38	0.48
1:G:70:VAL:HG21	1:G:72:ARG:NH2	2.28	0.48
1:I:438:GLN:HB3	1:I:440:GLN:CD	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:24:PHE:O	1:L:28:GLU:HG3	2.13	0.48
1:L:44:ILE:CD1	1:L:266:LEU:HD21	2.43	0.48
1:L:44:ILE:HG23	1:L:48:LYS:C	2.38	0.48
1:L:70:VAL:HG21	1:L:72:ARG:NH2	2.28	0.48
1:B:46:ALA:HB1	1:B:392:ARG:HD3	1.95	0.48
1:B:452:GLU:CG	1:D:309:GLU:OE2	2.60	0.48
1:C:438:GLN:HB3	1:C:440:GLN:CD	2.38	0.48
1:H:70:VAL:HG21	1:H:72:ARG:NH2	2.28	0.48
1:I:11:TYR:CD1	1:I:369:LYS:HE3	2.49	0.48
1:I:70:VAL:HG13	1:I:269:VAL:HG11	1.94	0.48
1:J:46:ALA:CB	1:J:392:ARG:CD	2.89	0.48
1:E:24:PHE:O	1:E:28:GLU:HG3	2.13	0.48
1:E:327:MET:CG	1:E:342:LEU:HD21	2.36	0.48
1:I:347:GLN:HG3	1:I:349:LYS:H	1.77	0.48
1:K:11:TYR:CZ	1:K:333:PRO:C	2.85	0.48
1:L:347:GLN:HG3	1:L:349:LYS:H	1.77	0.48
1:C:347:GLN:HG3	1:C:349:LYS:H	1.77	0.48
1:B:396:ARG:HH11	1:F:396:ARG:HD2	1.25	0.48
1:E:68:HIS:NE2	1:E:270:THR:HG23	2.29	0.48
1:H:9:SER:O	1:H:273:ASN:HB3	2.14	0.48
1:H:149:TYR:CD2	1:H:305[A]:ARG:HD3	2.49	0.48
1:J:333:PRO:HB3	1:J:369:LYS:HE3	1.96	0.48
1:C:70:VAL:HG21	1:C:72:ARG:NH2	2.28	0.48
1:E:70:VAL:HG21	1:E:72:ARG:NH2	2.28	0.48
1:E:438:GLN:HB3	1:E:440:GLN:CD	2.38	0.48
1:F:24:PHE:O	1:F:28:GLU:HG3	2.13	0.48
1:G:438:GLN:HB3	1:G:440:GLN:CD	2.38	0.48
1:H:24:PHE:CE2	1:H:25:GLN:CG	2.87	0.48
1:J:70:VAL:CG1	1:J:269:VAL:HG11	2.43	0.48
1:K:170:ARG:HE	1:L:199:PRO:HG3	1.78	0.48
1:B:334:ARG:HA	1:B:335:PRO:HD3	1.77	0.48
1:D:438:GLN:HB3	1:D:440:GLN:CD	2.38	0.48
1:E:24:PHE:CE2	1:E:25:GLN:CG	2.87	0.48
1:E:149:TYR:CD2	1:E:305[A]:ARG:HD3	2.49	0.48
1:F:70:VAL:HG21	1:F:72:ARG:NH2	2.28	0.48
1:F:149:TYR:CD2	1:F:305[A]:ARG:HD3	2.49	0.48
1:H:333:PRO:HB3	1:H:369:LYS:HE3	1.96	0.48
1:I:70:VAL:HG21	1:I:72:ARG:NH2	2.28	0.48
1:I:149:TYR:CD2	1:I:305[A]:ARG:HD3	2.49	0.48
1:J:438:GLN:HB3	1:J:440:GLN:CD	2.38	0.48
1:A:149:TYR:CD2	1:A:305[A]:ARG:HD3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:VAL:HG21	1:B:72:ARG:NH2	2.28	0.48
1:C:149:TYR:CD2	1:C:305[A]:ARG:HD3	2.49	0.48
1:D:149:TYR:CD2	1:D:305[A]:ARG:HD3	2.49	0.48
1:F:72:ARG:NH1	1:F:265:HIS:CD2	2.82	0.48
1:F:324:VAL:CG1	1:F:340:GLY:HA3	2.40	0.48
1:H:24:PHE:O	1:H:28:GLU:HG3	2.13	0.48
1:H:438:GLN:HB3	1:H:440:GLN:CD	2.38	0.48
1:J:149:TYR:CD2	1:J:305[A]:ARG:HD3	2.49	0.48
1:K:70:VAL:HG21	1:K:72:ARG:NH2	2.28	0.48
1:L:9:SER:O	1:L:273:ASN:CA	2.62	0.48
1:L:327:MET:CG	1:L:342:LEU:HD21	2.43	0.48
1:B:151:LYS:O	1:I:454:ASN:HB3	2.14	0.47
1:D:24:PHE:O	1:D:28:GLU:HG3	2.13	0.47
1:F:438:GLN:HB3	1:F:440:GLN:CD	2.38	0.47
1:J:70:VAL:HG21	1:J:72:ARG:NH2	2.28	0.47
1:C:40:GLN:O	1:C:72:ARG:N	2.34	0.47
1:F:333:PRO:HB3	1:F:369:LYS:HE3	1.96	0.47
1:L:11:TYR:HH	1:L:333:PRO:C	2.21	0.47
1:D:11:TYR:HE1	1:D:333:PRO:CA	2.15	0.47
1:H:228:LEU:HG	1:H:303:HIS:CE1	2.50	0.47
1:J:302:HIS:HB3	1:J:305[B]:ARG:HH11	1.80	0.47
1:K:333:PRO:HB3	1:K:369:LYS:HE3	1.96	0.47
1:A:11:TYR:CD1	1:A:369:LYS:CE	2.98	0.47
1:B:302:HIS:HB3	1:B:305[B]:ARG:HH11	1.80	0.47
1:B:333:PRO:HB3	1:B:369:LYS:HE3	1.96	0.47
1:F:228:LEU:HG	1:F:303:HIS:CE1	2.50	0.47
1:G:42:ARG:HD2	1:G:49:GLU:OE1	2.15	0.47
1:G:270:THR:HG21	1:G:392:ARG:HH12	1.79	0.47
1:H:302:HIS:HB3	1:H:305[B]:ARG:HH11	1.80	0.47
1:I:436:CYS:HA	1:I:437:PRO:HD3	1.71	0.47
1:J:46:ALA:CB	1:J:392:ARG:CZ	2.91	0.47
1:K:40:GLN:O	1:K:72:ARG:N	2.34	0.47
1:K:327:MET:SD	1:K:342:LEU:CD1	3.00	0.47
1:E:333:PRO:HB3	1:E:369:LYS:HE3	1.96	0.47
1:F:46:ALA:CB	1:F:392:ARG:CZ	2.78	0.47
1:G:149:TYR:CD2	1:G:305[A]:ARG:HD3	2.49	0.47
1:G:302:HIS:HB3	1:G:305[B]:ARG:HH11	1.80	0.47
1:I:270:THR:HG21	1:I:392:ARG:HH12	1.79	0.47
1:I:333:PRO:HB3	1:I:369:LYS:HE3	1.96	0.47
1:L:44:ILE:CG1	1:L:266:LEU:CD2	2.91	0.47
1:L:228:LEU:HG	1:L:303:HIS:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:LEU:HG	1:B:303:HIS:CE1	2.50	0.47
1:B:452:GLU:HG3	1:D:155:HIS:CE1	2.49	0.47
1:C:24:PHE:O	1:C:28:GLU:HG3	2.13	0.47
1:C:333:PRO:HB3	1:C:369:LYS:HE3	1.96	0.47
1:D:228:LEU:HG	1:D:303:HIS:CE1	2.50	0.47
1:F:302:HIS:HB3	1:F:305[B]:ARG:HH11	1.80	0.47
1:L:42:ARG:HD2	1:L:49:GLU:OE1	2.15	0.47
1:A:228:LEU:HG	1:A:303:HIS:CE1	2.50	0.47
1:B:42:ARG:HD2	1:B:49:GLU:OE1	2.15	0.47
1:B:149:TYR:CD2	1:B:305[A]:ARG:HD3	2.49	0.47
1:D:42:ARG:HD2	1:D:49:GLU:OE1	2.15	0.47
1:G:228:LEU:HG	1:G:303:HIS:CE1	2.50	0.47
1:L:325:LEU:HD11	1:L:331:LEU:HD11	1.96	0.47
1:A:333:PRO:HB3	1:A:369:LYS:HE3	1.96	0.47
1:D:302:HIS:HB3	1:D:305[B]:ARG:HH11	1.80	0.47
1:E:40:GLN:O	1:E:72:ARG:N	2.34	0.47
1:E:46:ALA:HB1	1:E:392:ARG:HD3	1.97	0.47
1:L:333:PRO:HB3	1:L:369:LYS:HE3	1.96	0.47
1:B:155:HIS:ND1	1:I:452:GLU:HG3	2.29	0.47
1:C:42:ARG:HD2	1:C:49:GLU:OE1	2.15	0.47
1:D:10:SER:HA	1:D:273:ASN:O	2.15	0.47
1:E:228:LEU:HG	1:E:303:HIS:CE1	2.50	0.47
1:G:297:LEU:HD23	1:G:297:LEU:HA	1.78	0.47
1:H:72:ARG:NH2	1:H:265:HIS:HD2	2.13	0.47
1:K:228:LEU:HG	1:K:303:HIS:CE1	2.50	0.47
1:C:228:LEU:HG	1:C:303:HIS:CE1	2.50	0.47
1:E:11:TYR:CZ	1:E:333:PRO:CA	2.97	0.47
1:E:42:ARG:HD2	1:E:49:GLU:OE1	2.15	0.47
1:E:302:HIS:HB3	1:E:305[B]:ARG:HH11	1.80	0.47
1:H:42:ARG:HD2	1:H:49:GLU:OE1	2.15	0.47
1:K:149:TYR:CD2	1:K:305[A]:ARG:HD3	2.49	0.47
1:C:24:PHE:CE2	1:C:25:GLN:CG	2.87	0.46
1:C:396:ARG:CD	1:E:400:GLN:HG3	2.44	0.46
1:C:400:GLN:HA	1:E:396:ARG:HH12	1.78	0.46
1:F:11:TYR:CZ	1:F:333:PRO:HB3	2.46	0.46
1:G:271:ARG:NH1	1:G:392:ARG:NH1	2.62	0.46
1:J:334:ARG:HA	1:J:335:PRO:HD3	1.77	0.46
1:B:396:ARG:HD3	1:F:400:GLN:HG2	1.96	0.46
1:C:420:ARG:HE	1:G:313:ASN:CG	2.23	0.46
1:F:42:ARG:HD2	1:F:49:GLU:OE1	2.15	0.46
1:K:18:ASP:H	1:K:21:THR:HG1	1.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:149:TYR:CD2	1:L:305[A]:ARG:HD3	2.49	0.46
1:L:302:HIS:HB3	1:L:305[B]:ARG:HH11	1.80	0.46
1:A:40:GLN:O	1:A:72:ARG:N	2.34	0.46
1:B:309:GLU:CD	1:I:452:GLU:HG2	2.37	0.46
1:B:40:GLN:O	1:B:72:ARG:N	2.34	0.46
1:A:302:HIS:HB3	1:A:305[B]:ARG:HH11	1.80	0.46
1:B:309:GLU:OE2	1:I:452:GLU:CD	2.58	0.46
1:B:345:GLN:CD	1:B:345:GLN:N	2.73	0.46
1:G:24:PHE:CE2	1:G:25:GLN:CG	2.87	0.46
1:G:333:PRO:HB3	1:G:369:LYS:HE3	1.96	0.46
1:K:302:HIS:HB3	1:K:305[B]:ARG:HH11	1.80	0.46
1:L:9:SER:O	1:L:273:ASN:CB	2.64	0.46
1:C:302:HIS:HB3	1:C:305[B]:ARG:HH11	1.80	0.46
1:D:24:PHE:CE2	1:D:25:GLN:CG	2.86	0.46
1:G:454:ASN:HB3	1:H:151:LYS:O	2.16	0.46
1:J:228:LEU:HG	1:J:303:HIS:CE1	2.50	0.46
1:A:42:ARG:HD2	1:A:49:GLU:OE1	2.15	0.46
1:C:5:VAL:O	1:C:12:GLY:HA2	2.16	0.46
1:E:27:LYS:O	1:E:31:ALA:N	2.49	0.46
1:E:199:PRO:HD3	1:F:170:ARG:NE	2.31	0.46
1:I:228:LEU:HG	1:I:303:HIS:CE1	2.50	0.46
1:J:329:GLY:HA3	1:J:343:PRO:HD2	1.98	0.46
1:K:42:ARG:HD2	1:K:49:GLU:OE1	2.15	0.46
1:C:436:CYS:HA	1:C:437:PRO:HD3	1.71	0.46
1:I:42:ARG:HD2	1:I:49:GLU:OE1	2.15	0.46
1:B:396:ARG:HD3	1:F:400:GLN:CG	2.46	0.46
1:F:5:VAL:O	1:F:12:GLY:HA2	2.16	0.46
1:H:334:ARG:HA	1:H:335:PRO:HD3	1.77	0.46
1:I:271:ARG:NH1	1:I:392:ARG:NH1	2.63	0.46
1:J:42:ARG:HD2	1:J:49:GLU:OE1	2.15	0.46
1:B:199:PRO:CD	1:D:170:ARG:HG3	2.46	0.46
1:D:333:PRO:HB3	1:D:369:LYS:HE3	1.96	0.46
1:J:5:VAL:O	1:J:12:GLY:HA2	2.16	0.46
1:J:329:GLY:C	1:J:366:ARG:NH2	2.73	0.46
1:K:436:CYS:HA	1:K:437:PRO:HD3	1.71	0.46
1:L:324:VAL:O	1:L:327:MET:HB2	2.16	0.46
1:A:27:LYS:O	1:A:31:ALA:N	2.49	0.45
1:A:440:GLN:HB2	1:E:320:ALA:HB2	1.98	0.45
1:C:11:TYR:CE1	1:C:333:PRO:HA	2.22	0.45
1:C:27:LYS:O	1:C:31:ALA:N	2.49	0.45
1:E:420:ARG:CZ	1:F:313:ASN:OD1	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:420:ARG:NH2	1:F:313:ASN:OD1	2.49	0.45
1:H:5:VAL:O	1:H:12:GLY:HA2	2.16	0.45
1:A:46:ALA:O	1:A:392:ARG:HD3	2.16	0.45
1:B:396:ARG:CG	1:F:400:GLN:CD	2.89	0.45
1:I:302:HIS:HB3	1:I:305[B]:ARG:HH11	1.80	0.45
1:J:27:LYS:O	1:J:31:ALA:N	2.49	0.45
1:B:11:TYR:CG	1:B:369:LYS:HE3	2.51	0.45
1:C:396:ARG:HE	1:E:400:GLN:NE2	2.04	0.45
1:J:9:SER:O	1:J:273:ASN:HB3	2.17	0.45
1:K:3:VAL:HG23	1:K:15:VAL:HB	1.99	0.45
1:L:324:VAL:CG1	1:L:340:GLY:HA2	2.29	0.45
1:B:3:VAL:HG23	1:B:15:VAL:HB	1.99	0.45
1:B:5:VAL:O	1:B:12:GLY:HA2	2.16	0.45
1:B:320:ALA:CB	1:I:440:GLN:HB2	2.46	0.45
1:C:313:ASN:HB3	1:H:420:ARG:HG3	1.99	0.45
1:E:5:VAL:O	1:E:12:GLY:HA2	2.16	0.45
1:F:46:ALA:C	1:F:392:ARG:HD3	2.40	0.45
1:F:436:CYS:HA	1:F:437:PRO:HD3	1.71	0.45
1:H:46:ALA:CA	1:H:392:ARG:CD	2.85	0.45
1:L:5:VAL:O	1:L:12:GLY:HA2	2.16	0.45
1:A:3:VAL:HG23	1:A:15:VAL:HB	1.99	0.45
1:A:155:HIS:CE1	1:F:452:GLU:HG2	2.51	0.45
1:F:324:VAL:CG1	1:F:340:GLY:CA	2.93	0.45
1:I:40:GLN:O	1:I:72:ARG:N	2.34	0.45
1:J:44:ILE:HG21	1:J:266:LEU:HD21	1.99	0.45
1:G:3:VAL:HG23	1:G:15:VAL:HB	1.99	0.45
1:H:68:HIS:CE1	1:H:273:ASN:CB	2.98	0.45
1:B:11:TYR:CB	1:B:369:LYS:HE2	2.47	0.45
1:D:436:CYS:HA	1:D:437:PRO:HD3	1.71	0.45
1:G:5:VAL:O	1:G:12:GLY:HA2	2.16	0.45
1:G:11:TYR:HE1	1:G:333:PRO:CA	2.26	0.45
1:I:3:VAL:HG23	1:I:15:VAL:HB	1.99	0.45
1:J:325:LEU:HD23	1:J:331:LEU:CD1	2.40	0.45
1:A:5:VAL:O	1:A:12:GLY:HA2	2.16	0.45
1:B:199:PRO:CG	1:D:170:ARG:HG3	2.46	0.45
1:D:3:VAL:HG23	1:D:15:VAL:HB	1.99	0.45
1:J:324:VAL:HG11	1:J:340:GLY:HA3	1.99	0.45
1:K:297:LEU:HD23	1:K:297:LEU:HA	1.78	0.45
1:K:313:ASN:CG	1:L:420:ARG:HE	2.25	0.45
1:F:40:GLN:O	1:F:72:ARG:N	2.34	0.45
1:F:300:GLU:HB3	1:F:302:HIS:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:27:LYS:O	1:H:31:ALA:N	2.49	0.45
1:B:300:GLU:HB3	1:B:302:HIS:NE2	2.32	0.45
1:H:436:CYS:HA	1:H:437:PRO:HD3	1.71	0.45
1:I:5:VAL:O	1:I:12:GLY:HA2	2.16	0.45
1:E:6:ARG:NH1	1:E:274:ASP:OD1	2.51	0.44
1:E:300:GLU:HB3	1:E:302:HIS:NE2	2.32	0.44
1:J:3:VAL:HG23	1:J:15:VAL:HB	1.99	0.44
1:C:313:ASN:CG	1:H:420:ARG:NE	2.54	0.44
1:F:27:LYS:O	1:F:31:ALA:N	2.49	0.44
1:K:300:GLU:HB3	1:K:302:HIS:NE2	2.32	0.44
1:K:309:GLU:OE2	1:L:452:GLU:CD	2.59	0.44
1:B:313:ASN:HB3	1:I:420:ARG:CG	2.33	0.44
1:D:5:VAL:O	1:D:12:GLY:HA2	2.16	0.44
1:E:44:ILE:HD13	1:E:266:LEU:CD1	2.46	0.44
1:H:300:GLU:HB3	1:H:302:HIS:NE2	2.32	0.44
1:L:3:VAL:HG23	1:L:15:VAL:HB	1.99	0.44
1:A:300:GLU:HB3	1:A:302:HIS:NE2	2.32	0.44
1:B:46:ALA:O	1:B:392:ARG:CD	2.32	0.44
1:H:37:PRO:O	1:H:41:LEU:HG	2.18	0.44
1:J:199:PRO:HG2	1:L:170:ARG:HE	1.78	0.44
1:K:5:VAL:O	1:K:12:GLY:HA2	2.16	0.44
1:A:24:PHE:CE2	1:A:25:GLN:CG	2.87	0.44
1:D:37:PRO:O	1:D:41:LEU:HG	2.18	0.44
1:F:24:PHE:CE2	1:F:25:GLN:CG	2.87	0.44
1:G:11:TYR:HD1	1:G:369:LYS:CE	2.29	0.44
1:L:300:GLU:HB3	1:L:302:HIS:NE2	2.32	0.44
1:C:3:VAL:HG23	1:C:15:VAL:HB	1.99	0.44
1:C:300:GLU:HB3	1:C:302:HIS:NE2	2.32	0.44
1:C:327:MET:C	1:C:342:LEU:CD2	2.90	0.44
1:D:27:LYS:O	1:D:31:ALA:N	2.49	0.44
1:E:37:PRO:O	1:E:41:LEU:HG	2.18	0.44
1:F:11:TYR:HE1	1:F:333:PRO:HA	1.80	0.44
1:H:44:ILE:CB	1:H:266:LEU:HD21	2.47	0.44
1:J:24:PHE:CE2	1:J:25:GLN:CG	2.87	0.44
1:J:37:PRO:O	1:J:41:LEU:HG	2.18	0.44
1:K:37:PRO:O	1:K:41:LEU:HG	2.18	0.44
1:L:37:PRO:O	1:L:41:LEU:HG	2.18	0.44
1:D:300:GLU:HB3	1:D:302:HIS:NE2	2.32	0.44
1:E:3:VAL:HG23	1:E:15:VAL:HB	1.99	0.44
1:H:40:GLN:O	1:H:72:ARG:N	2.34	0.44
1:J:329:GLY:O	1:J:366:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:330:VAL:O	1:J:341:LEU:HB2	2.18	0.44
1:K:27:LYS:O	1:K:31:ALA:N	2.49	0.44
1:G:27:LYS:NZ	1:G:38:ALA:O	2.49	0.44
1:C:37:PRO:O	1:C:41:LEU:HG	2.18	0.44
1:C:297:LEU:HD23	1:C:297:LEU:HA	1.78	0.44
1:D:46:ALA:HA	1:D:392:ARG:HD2	1.99	0.44
1:E:253:CYS:HB3	1:E:296:SER:HB3	2.00	0.44
1:F:3:VAL:HG23	1:F:15:VAL:HB	1.99	0.44
1:G:205:ARG:HH21	1:G:207:GLU:CG	2.31	0.44
1:A:44:ILE:HG21	1:A:266:LEU:CD2	2.43	0.43
1:B:4:PHE:HB3	1:B:66:ILE:HD12	2.00	0.43
1:F:11:TYR:OH	1:F:333:PRO:O	2.29	0.43
1:F:46:ALA:H	1:F:392:ARG:NH1	2.12	0.43
1:H:205:ARG:HH21	1:H:207:GLU:CG	2.31	0.43
1:I:300:GLU:HB3	1:I:302:HIS:NE2	2.33	0.43
1:B:205:ARG:HH21	1:B:207:GLU:CG	2.31	0.43
1:E:44:ILE:HD13	1:E:266:LEU:CG	2.35	0.43
1:E:70:VAL:CG1	1:E:269:VAL:HG11	2.48	0.43
1:F:37:PRO:O	1:F:41:LEU:HG	2.17	0.43
1:J:205:ARG:HH21	1:J:207:GLU:CG	2.31	0.43
1:K:205:ARG:HH21	1:K:207:GLU:CG	2.31	0.43
1:B:37:PRO:O	1:B:41:LEU:HG	2.18	0.43
1:C:205:ARG:HH21	1:C:207:GLU:CG	2.31	0.43
1:E:4:PHE:HB3	1:E:66:ILE:HD12	2.00	0.43
1:F:11:TYR:CE1	1:F:369:LYS:CE	3.00	0.43
1:H:253:CYS:HB3	1:H:296:SER:HB3	2.00	0.43
1:J:300:GLU:HB3	1:J:302:HIS:NE2	2.32	0.43
1:C:253:CYS:HB3	1:C:296:SER:HB3	2.00	0.43
1:C:334:ARG:HA	1:C:335:PRO:HD3	1.77	0.43
1:D:334:ARG:HA	1:D:335:PRO:HD3	1.77	0.43
1:D:455:ARG:CD	1:I:221:ASP:OD1	2.64	0.43
1:G:397:ALA:HA	1:G:400:GLN:CD	2.43	0.43
1:J:436:CYS:HA	1:J:437:PRO:HD3	1.71	0.43
1:B:43:VAL:HG22	1:B:69:ILE:HG12	2.01	0.43
1:C:43:VAL:HG22	1:C:69:ILE:HG12	2.01	0.43
1:H:3:VAL:HG23	1:H:15:VAL:HB	1.99	0.43
1:K:329:GLY:N	1:K:342:LEU:HD23	2.33	0.43
1:A:297:LEU:HD23	1:A:297:LEU:HA	1.78	0.43
1:F:11:TYR:CE1	1:F:333:PRO:HB3	2.53	0.43
1:F:220:LYS:HA	1:F:220:LYS:HD3	1.90	0.43
1:G:300:GLU:HB3	1:G:302:HIS:NE2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2:ILE:CD1	1:I:378:ASP:OD2	2.67	0.43
1:L:4:PHE:HB3	1:L:66:ILE:HD12	2.00	0.43
1:A:199:PRO:HG3	1:E:170:ARG:HE	1.83	0.43
1:A:362:PHE:CE2	1:A:364:PHE:HB3	2.54	0.43
1:D:44:ILE:HD13	1:D:266:LEU:CG	2.41	0.43
1:D:44:ILE:HD13	1:D:266:LEU:HD13	2.00	0.43
1:G:4:PHE:HB3	1:G:66:ILE:HD12	2.01	0.43
1:G:27:LYS:O	1:G:31:ALA:N	2.49	0.43
1:G:436:CYS:HA	1:G:437:PRO:HD3	1.71	0.43
1:J:68:HIS:NE2	1:J:270:THR:HG23	2.33	0.43
1:L:205:ARG:HH21	1:L:207:GLU:CG	2.31	0.43
1:A:37:PRO:O	1:A:41:LEU:HG	2.18	0.43
1:B:220:LYS:HA	1:B:220:LYS:HD3	1.90	0.43
1:E:230:THR:HG22	1:E:231:ASN:O	2.19	0.43
1:F:205:ARG:HH21	1:F:207:GLU:CG	2.31	0.43
1:G:37:PRO:O	1:G:41:LEU:HG	2.18	0.43
1:G:43:VAL:HG22	1:G:69:ILE:HG12	2.01	0.43
1:G:397:ALA:CA	1:G:400:GLN:HG2	2.49	0.43
1:H:255:HIS:ND1	1:H:402:ARG:NH2	2.67	0.43
1:H:362:PHE:CE2	1:H:364:PHE:HB3	2.54	0.43
1:I:37:PRO:O	1:I:41:LEU:HG	2.18	0.43
1:I:362:PHE:CE2	1:I:364:PHE:HB3	2.54	0.43
1:J:362:PHE:CE2	1:J:364:PHE:HB3	2.54	0.43
1:K:43:VAL:HG22	1:K:69:ILE:HG12	2.01	0.43
1:B:24:PHE:CE2	1:B:25:GLN:CG	2.87	0.43
1:D:43:VAL:HG22	1:D:69:ILE:HG12	2.01	0.43
1:D:230:THR:HG22	1:D:231:ASN:O	2.19	0.43
1:E:205:ARG:HH21	1:E:207:GLU:CG	2.31	0.43
1:G:362:PHE:CE2	1:G:364:PHE:HB3	2.54	0.43
1:I:188:ILE:CG2	1:I:191:ARG:CB	2.86	0.43
1:J:253:CYS:HB3	1:J:296:SER:HB3	2.00	0.43
1:A:4:PHE:HB3	1:A:66:ILE:HD12	2.00	0.43
1:A:205:ARG:HH21	1:A:207:GLU:CG	2.31	0.43
1:A:253:CYS:HB3	1:A:296:SER:HB3	2.00	0.43
1:B:253:CYS:HB3	1:B:296:SER:HB3	2.00	0.43
1:B:400:GLN:OE1	1:F:396:ARG:CG	2.64	0.43
1:C:155:HIS:HE1	1:H:452:GLU:HG3	1.81	0.43
1:F:362:PHE:CE2	1:F:364:PHE:HB3	2.54	0.43
1:H:46:ALA:CA	1:H:392:ARG:HD3	2.47	0.43
1:I:43:VAL:HG22	1:I:69:ILE:HG12	2.01	0.43
1:K:230:THR:HG22	1:K:231:ASN:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:362:PHE:CE2	1:K:364:PHE:HB3	2.54	0.43
1:L:438:GLN:HA	1:L:439:PRO:HD3	1.87	0.43
1:A:230:THR:HG22	1:A:231:ASN:O	2.19	0.42
1:B:11:TYR:CE1	1:B:369:LYS:HE3	2.54	0.42
1:D:362:PHE:CE2	1:D:364:PHE:HB3	2.54	0.42
1:E:166:CYS:HA	1:E:174:LEU:HD13	2.01	0.42
1:G:230:THR:HG22	1:G:231:ASN:O	2.19	0.42
1:H:11:TYR:HE1	1:H:333:PRO:HA	1.00	0.42
1:L:362:PHE:CE2	1:L:364:PHE:HB3	2.54	0.42
1:A:166:CYS:HA	1:A:174:LEU:HD13	2.01	0.42
1:B:313:ASN:CB	1:I:420:ARG:HG3	2.34	0.42
1:D:253:CYS:HB3	1:D:296:SER:HB3	2.00	0.42
1:F:230:THR:HG22	1:F:231:ASN:O	2.19	0.42
1:I:230:THR:HG22	1:I:231:ASN:O	2.19	0.42
1:K:13:PHE:CE2	1:K:33:ARG:CZ	3.03	0.42
1:L:24:PHE:CE2	1:L:25:GLN:CG	2.87	0.42
1:L:27:LYS:O	1:L:31:ALA:N	2.49	0.42
1:B:230:THR:HG22	1:B:231:ASN:O	2.19	0.42
1:B:362:PHE:CE2	1:B:364:PHE:HB3	2.54	0.42
1:C:420:ARG:CZ	1:G:313:ASN:OD1	2.66	0.42
1:F:166:CYS:HA	1:F:174:LEU:HD13	2.01	0.42
1:I:27:LYS:O	1:I:31:ALA:N	2.49	0.42
1:K:253:CYS:HB3	1:K:296:SER:HB3	2.00	0.42
1:A:334:ARG:HA	1:A:335:PRO:HD3	1.77	0.42
1:B:328:GLY:O	1:B:366:ARG:NH2	2.50	0.42
1:C:166:CYS:HA	1:C:174:LEU:HD13	2.01	0.42
1:D:438:GLN:HB3	1:D:440:GLN:NE2	2.35	0.42
1:E:43:VAL:HG22	1:E:69:ILE:HG12	2.01	0.42
1:E:59:CYS:SG	1:E:61:LEU:HB2	2.60	0.42
1:F:253:CYS:HB3	1:F:296:SER:HB3	2.00	0.42
1:F:438:GLN:HB3	1:F:440:GLN:NE2	2.35	0.42
1:I:253:CYS:HB3	1:I:296:SER:HB3	2.00	0.42
1:J:230:THR:HG22	1:J:231:ASN:O	2.19	0.42
1:K:68:HIS:NE2	1:K:274:ASP:CG	2.78	0.42
1:K:438:GLN:HB3	1:K:440:GLN:NE2	2.35	0.42
1:C:362:PHE:CE2	1:C:364:PHE:HB3	2.54	0.42
1:C:438:GLN:HB3	1:C:440:GLN:NE2	2.35	0.42
1:E:362:PHE:CE2	1:E:364:PHE:HB3	2.54	0.42
1:G:11:TYR:CE1	1:G:369:LYS:HE3	2.55	0.42
1:G:253:CYS:HB3	1:G:296:SER:HB3	2.00	0.42
1:H:438:GLN:HB3	1:H:440:GLN:NE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:4:PHE:HB3	1:I:66:ILE:HD12	2.01	0.42
1:J:13:PHE:CE2	1:J:33:ARG:CZ	3.03	0.42
1:K:72:ARG:HH12	1:K:265:HIS:CD2	2.37	0.42
1:K:166:CYS:HA	1:K:174:LEU:HD13	2.01	0.42
1:L:43:VAL:HG22	1:L:69:ILE:HG12	2.01	0.42
1:L:166:CYS:HA	1:L:174:LEU:HD13	2.02	0.42
1:B:59:CYS:SG	1:B:61:LEU:HB2	2.60	0.42
1:B:309:GLU:OE2	1:I:452:GLU:CB	2.67	0.42
1:C:220:LYS:HA	1:C:220:LYS:HD3	1.90	0.42
1:F:4:PHE:HB3	1:F:66:ILE:HD12	2.01	0.42
1:F:43:VAL:HG22	1:F:69:ILE:HG12	2.01	0.42
1:F:44:ILE:CD1	1:F:266:LEU:CD1	2.97	0.42
1:G:13:PHE:CE2	1:G:33:ARG:CZ	3.03	0.42
1:G:68:HIS:CE1	1:G:274:ASP:OD1	2.73	0.42
1:G:334:ARG:HA	1:G:335:PRO:HD3	1.77	0.42
1:H:13:PHE:CE2	1:H:33:ARG:CZ	3.03	0.42
1:H:43:VAL:HG22	1:H:69:ILE:HG12	2.01	0.42
1:H:272:LEU:HD23	1:H:272:LEU:HA	1.91	0.42
1:I:205:ARG:HH21	1:I:207:GLU:CG	2.31	0.42
1:J:438:GLN:HB3	1:J:440:GLN:NE2	2.35	0.42
1:L:59:CYS:SG	1:L:61:LEU:HB2	2.60	0.42
1:L:253:CYS:HB3	1:L:296:SER:HB3	2.00	0.42
1:A:43:VAL:HG22	1:A:69:ILE:HG12	2.01	0.42
1:B:297:LEU:HD23	1:B:297:LEU:HA	1.78	0.42
1:B:438:GLN:HA	1:B:439:PRO:HD3	1.87	0.42
1:C:4:PHE:HB3	1:C:66:ILE:HD12	2.00	0.42
1:E:13:PHE:CE2	1:E:33:ARG:CZ	3.03	0.42
1:F:438:GLN:HA	1:F:439:PRO:HD3	1.87	0.42
1:H:4:PHE:HB3	1:H:66:ILE:HD12	2.00	0.42
1:H:59:CYS:SG	1:H:61:LEU:HB2	2.60	0.42
1:H:230:THR:HG22	1:H:231:ASN:O	2.19	0.42
1:H:297:LEU:HD23	1:H:297:LEU:HA	1.78	0.42
1:I:188:ILE:CG2	1:I:188:ILE:O	2.68	0.42
1:J:166:CYS:HA	1:J:174:LEU:HD13	2.01	0.42
1:J:452:GLU:HG3	1:L:155:HIS:CE1	2.54	0.42
1:K:4:PHE:HB3	1:K:66:ILE:HD12	2.00	0.42
1:K:10:SER:HA	1:K:273:ASN:O	2.19	0.42
1:K:334:ARG:HA	1:K:335:PRO:HD3	1.77	0.42
1:C:6:ARG:NH1	1:C:68:HIS:ND1	2.55	0.42
1:D:4:PHE:HB3	1:D:66:ILE:HD12	2.00	0.42
1:D:205:ARG:HH21	1:D:207:GLU:CG	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:425:ILE:HD12	1:E:437:PRO:HD3	2.02	0.42
1:G:166:CYS:HA	1:G:174:LEU:HD13	2.02	0.42
1:J:43:VAL:HG22	1:J:69:ILE:HG12	2.01	0.42
1:L:230:THR:HG22	1:L:231:ASN:O	2.19	0.42
1:L:438:GLN:HB3	1:L:440:GLN:NE2	2.35	0.42
1:A:438:GLN:HB3	1:A:440:GLN:NE2	2.35	0.42
1:B:13:PHE:CE2	1:B:33:ARG:CZ	3.03	0.42
1:C:13:PHE:CE2	1:C:33:ARG:CZ	3.03	0.42
1:E:329:GLY:H	1:E:342:LEU:HD23	1.83	0.42
1:H:166:CYS:HA	1:H:174:LEU:HD13	2.01	0.42
1:K:46:ALA:O	1:K:392:ARG:HA	2.19	0.42
1:D:13:PHE:CE2	1:D:33:ARG:CZ	3.03	0.42
1:E:174:LEU:HD22	1:E:206:ALA:HA	2.02	0.42
1:H:425:ILE:HD12	1:H:437:PRO:HD3	2.02	0.42
1:I:13:PHE:CE2	1:I:33:ARG:CZ	3.03	0.42
1:J:59:CYS:SG	1:J:61:LEU:HB2	2.60	0.42
1:L:13:PHE:CE2	1:L:33:ARG:CZ	3.03	0.42
1:L:68:HIS:CD2	1:L:270:THR:HG23	2.55	0.42
1:B:425:ILE:HD12	1:B:437:PRO:HD3	2.02	0.41
1:I:59:CYS:SG	1:I:61:LEU:HB2	2.60	0.41
1:B:27:LYS:O	1:B:31:ALA:N	2.49	0.41
1:B:307:LEU:HB3	1:B:311:GLN:HB2	2.03	0.41
1:D:59:CYS:SG	1:D:61:LEU:HB2	2.60	0.41
1:F:59:CYS:SG	1:F:61:LEU:HB2	2.60	0.41
1:G:59:CYS:SG	1:G:61:LEU:HB2	2.60	0.41
1:I:438:GLN:HB3	1:I:440:GLN:NE2	2.35	0.41
1:J:246:ASN:HA	1:J:247:PRO:HA	1.91	0.41
1:K:272:LEU:HD23	1:K:272:LEU:HA	1.91	0.41
1:A:438:GLN:HA	1:A:439:PRO:HD3	1.87	0.41
1:B:166:CYS:HA	1:B:174:LEU:HD13	2.01	0.41
1:B:199:PRO:CG	1:D:170:ARG:HE	2.33	0.41
1:E:46:ALA:CB	1:E:392:ARG:HD3	2.49	0.41
1:F:162:LEU:HD12	1:F:163:ARG:H	1.86	0.41
1:G:438:GLN:HB3	1:G:440:GLN:NE2	2.35	0.41
1:H:220:LYS:HD3	1:H:220:LYS:HA	1.90	0.41
1:J:174:LEU:HD22	1:J:206:ALA:HA	2.02	0.41
1:J:329:GLY:HA2	1:J:366:ARG:NH2	2.26	0.41
1:K:438:GLN:HA	1:K:439:PRO:HD3	1.87	0.41
1:A:13:PHE:CE2	1:A:33:ARG:CZ	3.03	0.41
1:A:275:ARG:HE	1:A:275:ARG:HB3	1.71	0.41
1:B:452:GLU:OE2	1:D:155:HIS:ND1	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:CYS:SG	1:C:61:LEU:HB2	2.60	0.41
1:F:13:PHE:CE2	1:F:33:ARG:CZ	3.03	0.41
1:G:162:LEU:HD12	1:G:163:ARG:H	1.86	0.41
1:H:307:LEU:HB3	1:H:311:GLN:HB2	2.03	0.41
1:J:4:PHE:HB3	1:J:66:ILE:HD12	2.01	0.41
1:K:59:CYS:SG	1:K:61:LEU:HB2	2.60	0.41
1:K:162:LEU:HD12	1:K:163:ARG:H	1.86	0.41
1:K:425:ILE:HD12	1:K:437:PRO:HD3	2.02	0.41
1:B:438:GLN:HB3	1:B:440:GLN:NE2	2.35	0.41
1:E:307:LEU:HB3	1:E:311:GLN:HB2	2.03	0.41
1:F:297:LEU:HD23	1:F:297:LEU:HA	1.78	0.41
1:G:174:LEU:HD22	1:G:206:ALA:HA	2.02	0.41
1:I:24:PHE:CE2	1:I:25:GLN:CG	2.87	0.41
1:A:59:CYS:SG	1:A:61:LEU:HB2	2.60	0.41
1:A:436:CYS:HA	1:A:437:PRO:HD3	1.71	0.41
1:B:44:ILE:CD1	1:B:266:LEU:CD1	2.95	0.41
1:C:230:THR:HG22	1:C:231:ASN:O	2.19	0.41
1:D:166:CYS:HA	1:D:174:LEU:HD13	2.01	0.41
1:L:162:LEU:HD12	1:L:163:ARG:H	1.86	0.41
1:A:174:LEU:HD22	1:A:206:ALA:HA	2.02	0.41
1:C:45:PHE:HB2	1:C:67:VAL:HG12	2.03	0.41
1:C:162:LEU:HD12	1:C:163:ARG:H	1.86	0.41
1:C:174:LEU:HD22	1:C:206:ALA:HA	2.02	0.41
1:F:72:ARG:NH1	1:F:265:HIS:NE2	2.69	0.41
1:F:174:LEU:HD22	1:F:206:ALA:HA	2.02	0.41
1:G:45:PHE:HB2	1:G:67:VAL:HG12	2.03	0.41
1:I:174:LEU:HD22	1:I:206:ALA:HA	2.02	0.41
1:F:9:SER:O	1:F:273:ASN:CA	2.68	0.41
1:G:307:LEU:HB3	1:G:311:GLN:HB2	2.03	0.41
1:H:45:PHE:HB2	1:H:67:VAL:HG12	2.03	0.41
1:I:166:CYS:HA	1:I:174:LEU:HD13	2.02	0.41
1:A:255:HIS:HB3	1:A:402:ARG:HG2	2.03	0.41
1:B:162:LEU:HD12	1:B:163:ARG:H	1.86	0.41
1:D:425:ILE:HD12	1:D:437:PRO:HD3	2.02	0.41
1:E:45:PHE:HB2	1:E:67:VAL:HG12	2.03	0.41
1:E:255:HIS:HB3	1:E:402:ARG:HG2	2.03	0.41
1:E:438:GLN:HB3	1:E:440:GLN:NE2	2.35	0.41
1:F:307:LEU:HB3	1:F:311:GLN:HB2	2.03	0.41
1:F:334:ARG:HA	1:F:335:PRO:HD3	1.77	0.41
1:H:11:TYR:OH	1:H:333:PRO:O	2.21	0.41
1:H:255:HIS:HB3	1:H:402:ARG:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:45:PHE:HB2	1:I:67:VAL:HG12	2.03	0.41
1:J:199:PRO:HG3	1:L:170:ARG:NE	2.15	0.41
1:K:45:PHE:HB2	1:K:67:VAL:HG12	2.03	0.41
1:K:329:GLY:CA	1:K:341:LEU:O	2.61	0.41
1:L:8:ASN:HB3	1:L:335:PRO:HB3	2.02	0.41
1:L:40:GLN:O	1:L:72:ARG:N	2.34	0.41
1:L:425:ILE:HD12	1:L:437:PRO:HD3	2.03	0.41
1:A:45:PHE:HB2	1:A:67:VAL:HG12	2.03	0.41
1:A:452:GLU:CG	1:E:155:HIS:ND1	2.84	0.41
1:B:277:PHE:HB2	1:B:318:TYR:CZ	2.56	0.41
1:D:45:PHE:HB2	1:D:67:VAL:HG12	2.03	0.41
1:E:42:ARG:CG	1:E:72:ARG:HG3	2.51	0.41
1:F:42:ARG:CG	1:F:72:ARG:HG3	2.51	0.41
1:I:162:LEU:HD12	1:I:163:ARG:H	1.86	0.41
1:J:44:ILE:HG21	1:J:266:LEU:CD2	2.51	0.41
1:L:9:SER:O	1:L:273:ASN:HB3	2.21	0.41
1:A:162:LEU:HD12	1:A:163:ARG:H	1.86	0.40
1:B:246:ASN:HA	1:B:247:PRO:HA	1.91	0.40
1:B:255:HIS:HB3	1:B:402:ARG:HG2	2.03	0.40
1:C:255:HIS:HB3	1:C:402:ARG:HG2	2.03	0.40
1:C:307:LEU:HB3	1:C:311:GLN:HB2	2.02	0.40
1:D:272:LEU:HD23	1:D:272:LEU:HA	1.91	0.40
1:F:255:HIS:HB3	1:F:402:ARG:HG2	2.03	0.40
1:F:277:PHE:HB2	1:F:318:TYR:CZ	2.56	0.40
1:F:425:ILE:HD12	1:F:437:PRO:HD3	2.02	0.40
1:G:425:ILE:HD12	1:G:437:PRO:HD3	2.02	0.40
1:J:199:PRO:CD	1:L:170:ARG:CZ	2.76	0.40
1:K:42:ARG:CG	1:K:72:ARG:HG3	2.52	0.40
1:L:174:LEU:HD22	1:L:206:ALA:HA	2.02	0.40
1:A:277:PHE:HB2	1:A:318:TYR:CZ	2.56	0.40
1:A:425:ILE:HD12	1:A:437:PRO:HD3	2.02	0.40
1:B:42:ARG:CG	1:B:72:ARG:HG3	2.52	0.40
1:C:42:ARG:CG	1:C:72:ARG:HG3	2.52	0.40
1:D:42:ARG:CG	1:D:72:ARG:HG3	2.51	0.40
1:D:162:LEU:HD12	1:D:163:ARG:H	1.86	0.40
1:D:220:LYS:HA	1:D:220:LYS:HD3	1.90	0.40
1:F:45:PHE:HB2	1:F:67:VAL:HG12	2.03	0.40
1:G:42:ARG:CG	1:G:72:ARG:HG3	2.52	0.40
1:G:72:ARG:HH22	1:G:265:HIS:CD2	2.35	0.40
1:I:255:HIS:HB3	1:I:402:ARG:HG2	2.03	0.40
1:J:72:ARG:NH1	1:J:265:HIS:CD2	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:255:HIS:HB3	1:J:402:ARG:HG2	2.03	0.40
1:K:220:LYS:HD3	1:K:220:LYS:HA	1.90	0.40
1:L:277:PHE:HB2	1:L:318:TYR:CZ	2.56	0.40
1:A:46:ALA:C	1:A:392:ARG:HD3	2.46	0.40
1:A:327:MET:C	1:A:329:GLY:N	2.77	0.40
1:B:45:PHE:HB2	1:B:67:VAL:HG12	2.03	0.40
1:H:174:LEU:HD22	1:H:206:ALA:HA	2.02	0.40
1:I:42:ARG:CG	1:I:72:ARG:HG3	2.51	0.40
1:A:307:LEU:HB3	1:A:311:GLN:HB2	2.03	0.40
1:B:174:LEU:HD22	1:B:206:ALA:HA	2.02	0.40
1:C:277:PHE:HB2	1:C:318:TYR:CZ	2.56	0.40
1:C:425:ILE:HD12	1:C:437:PRO:HD3	2.02	0.40
1:D:174:LEU:HD22	1:D:206:ALA:HA	2.02	0.40
1:H:162:LEU:HD12	1:H:163:ARG:H	1.86	0.40
1:K:307:LEU:HB3	1:K:311:GLN:HB2	2.03	0.40
1:F:11:TYR:CD1	1:F:369:LYS:HE3	2.56	0.40
1:H:42:ARG:CG	1:H:72:ARG:HG3	2.52	0.40
1:J:42:ARG:CG	1:J:72:ARG:HG3	2.51	0.40
1:J:297:LEU:HA	1:J:297:LEU:HD23	1.78	0.40
1:J:330:VAL:HG21	1:J:364:PHE:HE2	1.87	0.40
1:J:425:ILE:HD12	1:J:437:PRO:HD3	2.02	0.40
1:L:297:LEU:HD23	1:L:297:LEU:HA	1.78	0.40
1:L:307:LEU:HB3	1:L:311:GLN:HB2	2.03	0.40

All (31) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:254:ASN:ND2	1:J:428:ASN:OD1[2_655]	1.25	0.95
1:F:326:GLN:O	1:G:282:GLN:CG[1_554]	1.30	0.90
1:D:327:MET:CG	1:L:294:PRO:CB[4_455]	1.35	0.85
1:C:282:GLN:NE2	1:E:276:GLN:NE2[2_555]	1.41	0.79
1:B:282:GLN:NE2	1:K:326:GLN:CA[1_554]	1.42	0.78
1:F:325:LEU:O	1:G:282:GLN:NE2[1_554]	1.55	0.65
1:D:326:GLN:O	1:L:292:GLY:O[4_455]	1.58	0.62
1:B:282:GLN:CB	1:K:326:GLN:OE1[1_554]	1.70	0.50
1:B:282:GLN:CG	1:K:326:GLN:OE1[1_554]	1.72	0.48
1:D:327:MET:O	1:L:294:PRO:CD[4_455]	1.75	0.45
1:F:326:GLN:C	1:G:282:GLN:CG[1_554]	1.82	0.38
1:B:282:GLN:CD	1:K:326:GLN:CG[1_554]	1.84	0.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:GLN:OE1	1:E:282:GLN:N[2_555]	1.87	0.33
1:B:282:GLN:CG	1:K:326:GLN:CB[1_554]	1.91	0.29
1:F:326:GLN:OE1	1:G:281:ALA:N[1_554]	1.92	0.28
1:D:327:MET:CB	1:L:294:PRO:CB[4_455]	1.93	0.27
1:B:282:GLN:CG	1:K:326:GLN:CG[1_554]	1.94	0.26
1:B:282:GLN:N	1:K:326:GLN:OE1[1_554]	1.95	0.25
1:B:282:GLN:NE2	1:K:326:GLN:CB[1_554]	1.96	0.24
1:B:282:GLN:NE2	1:K:326:GLN:CG[1_554]	1.98	0.22
1:D:327:MET:C	1:L:294:PRO:CD[4_455]	2.01	0.19
1:B:294:PRO:CB	1:K:278:VAL:CG2[1_554]	2.03	0.17
1:D:327:MET:O	1:L:294:PRO:CG[4_455]	2.03	0.17
1:B:282:GLN:CG	1:K:326:GLN:CD[1_554]	2.05	0.15
1:F:326:GLN:CA	1:G:282:GLN:CG[1_554]	2.07	0.13
1:C:342:LEU:O	1:I:191:ARG:NH2[4_455]	2.09	0.11
1:F:326:GLN:CD	1:G:280:ASP:OD1[1_554]	2.10	0.10
1:F:326:GLN:OE1	1:G:280:ASP:OD1[1_554]	2.11	0.09
1:B:282:GLN:CA	1:K:326:GLN:OE1[1_554]	2.18	0.02
1:C:326:GLN:O	1:E:282:GLN:CG[2_555]	2.19	0.01
1:F:326:GLN:OE1	1:G:280:ASP:C[1_554]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	371/470 (79%)	361 (97%)	10 (3%)	0	100	100
1	B	371/470 (79%)	358 (96%)	12 (3%)	1 (0%)	36	72
1	C	371/470 (79%)	361 (97%)	10 (3%)	0	100	100
1	D	371/470 (79%)	361 (97%)	10 (3%)	0	100	100
1	E	371/470 (79%)	361 (97%)	10 (3%)	0	100	100
1	F	371/470 (79%)	360 (97%)	11 (3%)	0	100	100
1	G	371/470 (79%)	361 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	371/470 (79%)	361 (97%)	10 (3%)	0	100	100
1	I	371/470 (79%)	361 (97%)	10 (3%)	0	100	100
1	J	371/470 (79%)	361 (97%)	10 (3%)	0	100	100
1	K	371/470 (79%)	360 (97%)	11 (3%)	0	100	100
1	L	371/470 (79%)	361 (97%)	10 (3%)	0	100	100
All	All	4452/5640 (79%)	4327 (97%)	124 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	344	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/403 (82%)	325 (98%)	6 (2%)	51	68
1	B	331/403 (82%)	323 (98%)	8 (2%)	43	64
1	C	331/403 (82%)	325 (98%)	6 (2%)	51	68
1	D	331/403 (82%)	325 (98%)	6 (2%)	51	68
1	E	331/403 (82%)	324 (98%)	7 (2%)	47	65
1	F	331/403 (82%)	325 (98%)	6 (2%)	51	68
1	G	331/403 (82%)	324 (98%)	7 (2%)	47	65
1	H	331/403 (82%)	325 (98%)	6 (2%)	51	68
1	I	331/403 (82%)	324 (98%)	7 (2%)	47	65
1	J	331/403 (82%)	325 (98%)	6 (2%)	51	68
1	K	331/403 (82%)	325 (98%)	6 (2%)	51	68
1	L	331/403 (82%)	324 (98%)	7 (2%)	47	65
All	All	3972/4836 (82%)	3894 (98%)	78 (2%)	48	66

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	22	SER
1	A	66	ILE
1	A	226	LEU
1	A	250	VAL
1	A	402	ARG
1	B	8	ASN
1	B	22	SER
1	B	66	ILE
1	B	226	LEU
1	B	250	VAL
1	B	345	GLN
1	B	347	GLN
1	B	402	ARG
1	C	8	ASN
1	C	22	SER
1	C	66	ILE
1	C	226	LEU
1	C	250	VAL
1	C	402	ARG
1	D	8	ASN
1	D	22	SER
1	D	66	ILE
1	D	226	LEU
1	D	250	VAL
1	D	402	ARG
1	E	8	ASN
1	E	22	SER
1	E	66	ILE
1	E	226	LEU
1	E	250	VAL
1	E	327	MET
1	E	402	ARG
1	F	8	ASN
1	F	22	SER
1	F	66	ILE
1	F	226	LEU
1	F	250	VAL
1	F	402	ARG
1	G	8	ASN
1	G	22	SER
1	G	66	ILE

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Mol	Chain	Res	Type
1	G	69	ILE
1	G	226	LEU
1	G	250	VAL
1	G	402	ARG
1	H	8	ASN
1	H	22	SER
1	H	66	ILE
1	H	226	LEU
1	H	250	VAL
1	H	402	ARG
1	I	8	ASN
1	I	22	SER
1	I	66	ILE
1	I	69	ILE
1	I	226	LEU
1	I	250	VAL
1	I	402	ARG
1	J	8	ASN
1	J	22	SER
1	J	66	ILE
1	J	226	LEU
1	J	250	VAL
1	J	402	ARG
1	K	8	ASN
1	K	22	SER
1	K	66	ILE
1	K	226	LEU
1	K	250	VAL
1	K	402	ARG
1	L	8	ASN
1	L	22	SER
1	L	66	ILE
1	L	226	LEU
1	L	250	VAL
1	L	327	MET
1	L	402	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	34	GLN

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Mol	Chain	Res	Type
1	A	40	GLN
1	A	52	ASN
1	A	64	GLN
1	A	71	GLN
1	A	252	GLN
1	A	265	HIS
1	B	8	ASN
1	B	34	GLN
1	B	40	GLN
1	B	52	ASN
1	B	64	GLN
1	B	68	HIS
1	B	71	GLN
1	B	252	GLN
1	B	265	HIS
1	B	311	GLN
1	B	317	GLN
1	B	347	GLN
1	C	8	ASN
1	C	34	GLN
1	C	40	GLN
1	C	52	ASN
1	C	64	GLN
1	C	68	HIS
1	C	71	GLN
1	C	252	GLN
1	C	265	HIS
1	C	311	GLN
1	D	34	GLN
1	D	40	GLN
1	D	52	ASN
1	D	64	GLN
1	D	71	GLN
1	D	252	GLN
1	D	265	HIS
1	D	400	GLN
1	E	34	GLN
1	E	40	GLN
1	E	52	ASN
1	E	64	GLN
1	E	71	GLN
1	E	252	GLN

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Mol	Chain	Res	Type
1	E	265	HIS
1	E	400	GLN
1	F	8	ASN
1	F	34	GLN
1	F	40	GLN
1	F	52	ASN
1	F	64	GLN
1	F	68	HIS
1	F	71	GLN
1	F	252	GLN
1	F	265	HIS
1	G	34	GLN
1	G	40	GLN
1	G	52	ASN
1	G	64	GLN
1	G	68	HIS
1	G	71	GLN
1	G	252	GLN
1	G	265	HIS
1	G	311	GLN
1	G	400	GLN
1	H	34	GLN
1	H	40	GLN
1	H	52	ASN
1	H	64	GLN
1	H	71	GLN
1	H	252	GLN
1	H	265	HIS
1	H	311	GLN
1	I	8	ASN
1	I	34	GLN
1	I	40	GLN
1	I	52	ASN
1	I	64	GLN
1	I	71	GLN
1	I	252	GLN
1	I	265	HIS
1	I	311	GLN
1	J	34	GLN
1	J	40	GLN
1	J	52	ASN
1	J	64	GLN

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Mol	Chain	Res	Type
1	J	68	HIS
1	J	71	GLN
1	J	252	GLN
1	J	265	HIS
1	J	311	GLN
1	K	34	GLN
1	K	40	GLN
1	K	52	ASN
1	K	64	GLN
1	K	68	HIS
1	K	71	GLN
1	K	252	GLN
1	K	265	HIS
1	K	311	GLN
1	L	34	GLN
1	L	40	GLN
1	L	52	ASN
1	L	64	GLN
1	L	71	GLN
1	L	252	GLN
1	L	265	HIS
1	L	317	GLN

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

Of 96 ligands modelled in this entry, 96 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	375/470 (79%)	0.41	24 (6%)	25	30	20, 41, 105, 105	4 (1%)
1	B	375/470 (79%)	0.38	24 (6%)	25	30	35, 71, 152, 152	4 (1%)
1	C	375/470 (79%)	0.32	19 (5%)	33	35	20, 39, 110, 110	4 (1%)
1	D	375/470 (79%)	0.34	21 (5%)	30	34	27, 55, 154, 154	4 (1%)
1	E	375/470 (79%)	0.31	22 (5%)	28	32	14, 28, 118, 118	4 (1%)
1	F	375/470 (79%)	0.28	24 (6%)	25	30	19, 38, 116, 116	4 (1%)
1	G	375/470 (79%)	0.44	30 (8%)	18	25	25, 50, 131, 131	4 (1%)
1	H	375/470 (79%)	0.43	27 (7%)	21	27	38, 75, 206, 206	4 (1%)
1	I	375/470 (79%)	0.28	20 (5%)	32	34	33, 65, 172, 172	4 (1%)
1	J	375/470 (79%)	0.42	25 (6%)	24	29	51, 102, 172, 172	4 (1%)
1	K	375/470 (79%)	0.26	22 (5%)	28	32	39, 77, 176, 176	4 (1%)
1	L	375/470 (79%)	0.41	27 (7%)	21	27	70, 140, 214, 214	4 (1%)
All	All	4500/5640 (79%)	0.36	285 (6%)	26	31	14, 75, 172, 214	48 (1%)

All (285) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	249	LEU	7.4
1	E	304	PHE	6.5
1	L	340	GLY	6.4
1	K	208	PHE	6.2
1	I	258	VAL	6.1
1	B	330	VAL	6.1
1	L	26	LEU	6.0
1	H	453	TRP	6.0
1	D	26	LEU	5.7
1	L	330	VAL	5.5
1	G	350	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	26	LEU	5.4
1	G	364	PHE	5.4
1	E	26	LEU	5.4
1	K	164	VAL	5.3
1	G	462	TRP	5.3
1	C	264	PHE	5.2
1	J	330	VAL	4.9
1	B	162	LEU	4.8
1	A	3	VAL	4.8
1	H	268	CYS	4.8
1	E	330	VAL	4.8
1	J	3	VAL	4.7
1	L	3	VAL	4.5
1	G	3	VAL	4.5
1	G	453	TRP	4.5
1	G	330	VAL	4.4
1	F	369	LYS	4.4
1	H	462	TRP	4.4
1	I	445	TRP	4.3
1	F	258	VAL	4.3
1	G	147	PHE	4.3
1	D	330	VAL	4.3
1	I	264	PHE	4.3
1	J	146	PHE	4.2
1	J	26	LEU	4.1
1	H	445	TRP	4.1
1	A	462	TRP	4.1
1	D	259	ILE	4.0
1	J	264	PHE	4.0
1	I	462	TRP	4.0
1	H	22	SER	3.9
1	E	303	HIS	3.9
1	A	206	ALA	3.9
1	D	462	TRP	3.9
1	C	330	VAL	3.8
1	I	259	ILE	3.8
1	I	432	MET	3.8
1	L	339	ALA	3.8
1	G	464[A]	ASP	3.7
1	G	26	LEU	3.7
1	B	248	VAL	3.7
1	A	264	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	324	VAL	3.6
1	I	206	ALA	3.6
1	D	5	VAL	3.5
1	G	465	VAL	3.5
1	E	61	LEU	3.4
1	L	162	LEU	3.4
1	F	364	PHE	3.4
1	K	174	LEU	3.4
1	A	400	GLN	3.4
1	K	206	ALA	3.4
1	F	239	ILE	3.4
1	C	249	LEU	3.4
1	G	463	PHE	3.4
1	C	26	LEU	3.4
1	B	462	TRP	3.3
1	L	324	VAL	3.3
1	I	239	ILE	3.3
1	J	218	SER	3.3
1	E	268	CYS	3.3
1	L	67	VAL	3.3
1	A	261	LEU	3.3
1	F	208	PHE	3.2
1	J	445	TRP	3.2
1	G	324	VAL	3.2
1	A	223	SER	3.2
1	B	3	VAL	3.2
1	K	264	PHE	3.2
1	A	324	VAL	3.2
1	C	164	VAL	3.2
1	E	378	ASP	3.2
1	K	162	LEU	3.1
1	I	425	ILE	3.1
1	E	264	PHE	3.1
1	I	249	LEU	3.1
1	A	162	LEU	3.1
1	J	162	LEU	3.1
1	D	3	VAL	3.1
1	J	335	PRO	3.1
1	G	146	PHE	3.1
1	E	298	ILE	3.1
1	L	250	VAL	3.1
1	H	219	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	268	CYS	3.0
1	L	403	TRP	3.0
1	D	264	PHE	3.0
1	K	304	PHE	3.0
1	H	264	PHE	3.0
1	F	259	ILE	3.0
1	A	218	SER	3.0
1	D	249	LEU	2.9
1	D	403	TRP	2.9
1	G	222	THR	2.9
1	B	433	HIS	2.9
1	F	43	VAL	2.9
1	K	3	VAL	2.9
1	G	458	MET	2.9
1	J	452	GLU	2.9
1	A	403	TRP	2.9
1	C	261	LEU	2.9
1	K	403	TRP	2.8
1	L	320	ALA	2.8
1	E	295	ASN	2.8
1	E	210	PHE	2.8
1	L	264	PHE	2.8
1	H	397	ALA	2.8
1	A	331	LEU	2.8
1	G	331	LEU	2.8
1	C	218	SER	2.8
1	E	161	LYS	2.8
1	I	378	ASP	2.8
1	L	224	VAL	2.8
1	C	340	GLY	2.7
1	K	320	ALA	2.7
1	I	25	GLN	2.7
1	J	461	HIS	2.7
1	K	303	HIS	2.7
1	E	462	TRP	2.7
1	J	145	SER	2.7
1	F	425	ILE	2.7
1	C	369	LYS	2.7
1	F	218	SER	2.7
1	G	223	SER	2.7
1	B	340	GLY	2.7
1	G	218	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	417	PRO	2.6
1	D	323	CYS	2.6
1	H	433	HIS	2.6
1	J	163	ARG	2.6
1	B	295	ASN	2.6
1	H	307	LEU	2.5
1	A	224	VAL	2.5
1	B	366	ARG	2.5
1	B	223	SER	2.5
1	L	266	LEU	2.5
1	I	434	MET	2.5
1	L	15	VAL	2.5
1	L	218	SER	2.5
1	B	264	PHE	2.5
1	C	208	PHE	2.5
1	C	3	VAL	2.5
1	E	291	ALA	2.5
1	L	163	ARG	2.5
1	J	307	LEU	2.5
1	G	68	HIS	2.5
1	L	228	LEU	2.5
1	F	290	VAL	2.5
1	F	330	VAL	2.5
1	G	341	LEU	2.4
1	A	307	LEU	2.4
1	B	61	LEU	2.4
1	B	341	LEU	2.4
1	F	324	VAL	2.4
1	F	26	LEU	2.4
1	K	425	ILE	2.4
1	D	162	LEU	2.4
1	K	443	LEU	2.4
1	B	290	VAL	2.4
1	H	276	GLN	2.4
1	K	153	PRO	2.4
1	J	223	SER	2.4
1	G	12	GLY	2.4
1	F	219	ASP	2.4
1	G	229	ILE	2.4
1	F	333	PRO	2.4
1	L	10	SER	2.4
1	L	331	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	206	ALA	2.4
1	E	425	ILE	2.4
1	A	378	ASP	2.4
1	A	248	VAL	2.4
1	B	363	VAL	2.4
1	G	224	VAL	2.4
1	D	261	LEU	2.4
1	H	146	PHE	2.3
1	L	251	PHE	2.3
1	K	223	SER	2.3
1	E	403	TRP	2.3
1	K	445	TRP	2.3
1	D	216	PRO	2.3
1	F	424	PRO	2.3
1	J	210	PHE	2.3
1	F	371	ALA	2.3
1	G	250	VAL	2.3
1	G	258	VAL	2.3
1	H	261	LEU	2.3
1	C	298	ILE	2.3
1	I	450	GLY	2.3
1	C	223	SER	2.3
1	A	364	PHE	2.3
1	D	248	VAL	2.3
1	B	163	ARG	2.3
1	F	463	PHE	2.3
1	J	453	TRP	2.3
1	A	251	PHE	2.3
1	J	229	ILE	2.3
1	J	219	ASP	2.3
1	E	162	LEU	2.3
1	L	424	PRO	2.3
1	G	176	LEU	2.3
1	J	432	MET	2.3
1	L	219	ASP	2.3
1	L	304	PHE	2.2
1	H	333	PRO	2.2
1	I	330	VAL	2.2
1	B	304	PHE	2.2
1	C	378	ASP	2.2
1	G	276	GLN	2.2
1	B	450	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	67	VAL	2.2
1	H	398	ALA	2.2
1	A	335	PRO	2.2
1	H	320	ALA	2.2
1	B	251	PHE	2.2
1	I	210	PHE	2.2
1	K	298	ILE	2.2
1	H	249	LEU	2.2
1	H	404	GLU	2.2
1	A	210	PHE	2.2
1	H	305[A]	ARG	2.2
1	K	163	ARG	2.2
1	F	403	TRP	2.2
1	I	219	ASP	2.1
1	A	229	ILE	2.1
1	B	308	GLY	2.1
1	B	378	ASP	2.1
1	J	333	PRO	2.1
1	A	239	ILE	2.1
1	H	239	ILE	2.1
1	I	369	LYS	2.1
1	J	261	LEU	2.1
1	K	176	LEU	2.1
1	B	17	VAL	2.1
1	A	151	LYS	2.1
1	C	419	PRO	2.1
1	G	153	PRO	2.1
1	I	313	ASN	2.1
1	D	434	MET	2.1
1	H	222	THR	2.1
1	C	341	LEU	2.1
1	F	229	ILE	2.1
1	H	3	VAL	2.1
1	K	254	ASN	2.1
1	E	206	ALA	2.1
1	G	259	ILE	2.1
1	H	208	PHE	2.1
1	K	2	ILE	2.1
1	L	223	SER	2.1
1	B	141	PRO	2.1
1	D	333	PRO	2.1
1	J	258	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	434	MET	2.1
1	J	268	CYS	2.1
1	D	176	LEU	2.1
1	I	26	LEU	2.1
1	E	395	GLN	2.1
1	J	400	GLN	2.1
1	D	364	PHE	2.1
1	H	179	GLY	2.1
1	D	15	VAL	2.1
1	E	306	ILE	2.0
1	F	313	ASN	2.0
1	K	448	ASN	2.0
1	F	453	TRP	2.0
1	C	290	VAL	2.0
1	G	304	PHE	2.0
1	L	364	PHE	2.0
1	E	465	VAL	2.0
1	F	445	TRP	2.0
1	H	163	ARG	2.0
1	E	364	PHE	2.0
1	D	445	TRP	2.0
1	H	21	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	H	506	1/1	0.81	0.19	205,205,205,205	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	H	505	1/1	0.85	0.10	205,205,205,205	0
2	ZN	J	505	1/1	0.85	0.10	171,171,171,171	0
2	ZN	L	508	1/1	0.85	0.09	139,139,139,139	0
2	ZN	I	506	1/1	0.86	0.21	171,171,171,171	0
2	ZN	G	505	1/1	0.90	0.09	131,131,131,131	0
2	ZN	J	508	1/1	0.93	0.08	101,101,101,101	0
2	ZN	G	508	1/1	0.93	0.09	49,49,49,49	0
2	ZN	A	505	1/1	0.94	0.07	105,105,105,105	0
2	ZN	L	503	1/1	0.94	0.06	139,139,139,139	0
2	ZN	B	506	1/1	0.94	0.11	151,151,151,151	0
2	ZN	J	507	1/1	0.95	0.07	101,101,101,101	0
2	ZN	E	505	1/1	0.95	0.09	117,117,117,117	0
2	ZN	K	506	1/1	0.95	0.11	176,176,176,176	0
2	ZN	K	508	1/1	0.95	0.08	77,77,77,77	0
2	ZN	F	505	1/1	0.95	0.07	105,105,105,105	0
2	ZN	L	504	1/1	0.95	0.05	139,139,139,139	0
2	ZN	J	506	1/1	0.95	0.10	171,171,171,171	0
2	ZN	B	505	1/1	0.96	0.05	151,151,151,151	0
2	ZN	H	508	1/1	0.96	0.06	75,75,75,75	0
2	ZN	K	504	1/1	0.96	0.06	77,77,77,77	0
2	ZN	L	507	1/1	0.96	0.06	139,139,139,139	0
2	ZN	I	505	1/1	0.96	0.04	171,171,171,171	0
2	ZN	L	502	1/1	0.97	0.06	139,139,139,139	0
2	ZN	B	508	1/1	0.97	0.05	70,70,70,70	0
2	ZN	K	505	1/1	0.97	0.06	176,176,176,176	0
2	ZN	D	506	1/1	0.97	0.04	153,153,153,153	0
2	ZN	H	503	1/1	0.97	0.11	75,75,75,75	0
2	ZN	J	503	1/1	0.98	0.03	101,101,101,101	0
2	ZN	J	504	1/1	0.98	0.04	101,101,101,101	0
2	ZN	G	506	1/1	0.98	0.09	131,131,131,131	0
2	ZN	G	507	1/1	0.98	0.03	49,49,49,49	0
2	ZN	C	505	1/1	0.98	0.13	104,104,104,104	0
2	ZN	H	501	1/1	0.98	0.06	75,75,75,75	0
2	ZN	D	505	1/1	0.98	0.04	153,153,153,153	0
2	ZN	B	504	1/1	0.98	0.06	70,70,70,70	0
2	ZN	A	501	1/1	0.98	0.06	40,40,40,40	0
2	ZN	H	507	1/1	0.98	0.07	75,75,75,75	0
2	ZN	E	508	1/1	0.98	0.05	28,28,28,28	0
2	ZN	I	503	1/1	0.98	0.05	65,65,65,65	0
2	ZN	A	508	1/1	0.98	0.06	40,40,40,40	0
2	ZN	L	506	1/1	0.98	0.10	213,213,213,213	0
2	ZN	B	502	1/1	0.98	0.04	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	I	508	1/1	0.98	0.05	65,65,65,65	0
2	ZN	I	507	1/1	0.99	0.03	65,65,65,65	0
2	ZN	F	501	1/1	0.99	0.15	38,38,38,38	0
2	ZN	J	502	1/1	0.99	0.03	101,101,101,101	0
2	ZN	C	501	1/1	0.99	0.09	39,39,39,39	0
2	ZN	F	506	1/1	0.99	0.06	105,105,105,105	0
2	ZN	A	507	1/1	0.99	0.04	40,40,40,40	0
2	ZN	C	506	1/1	0.99	0.04	104,104,104,104	0
2	ZN	C	508	1/1	0.99	0.05	39,39,39,39	0
2	ZN	D	502	1/1	0.99	0.06	54,54,54,54	0
2	ZN	K	501	1/1	0.99	0.13	77,77,77,77	0
2	ZN	K	502	1/1	0.99	0.05	77,77,77,77	0
2	ZN	K	503	1/1	0.99	0.04	77,77,77,77	0
2	ZN	D	503	1/1	0.99	0.12	54,54,54,54	0
2	ZN	A	503	1/1	0.99	0.10	40,40,40,40	0
2	ZN	H	504	1/1	0.99	0.03	75,75,75,75	0
2	ZN	K	507	1/1	0.99	0.01	77,77,77,77	0
2	ZN	B	501	1/1	0.99	0.16	70,70,70,70	0
2	ZN	L	501	1/1	0.99	0.07	139,139,139,139	0
2	ZN	D	507	1/1	0.99	0.09	54,54,54,54	0
2	ZN	D	508	1/1	0.99	0.07	54,54,54,54	0
2	ZN	E	503	1/1	0.99	0.10	28,28,28,28	0
2	ZN	L	505	1/1	0.99	0.06	213,213,213,213	0
2	ZN	B	507	1/1	0.99	0.05	70,70,70,70	0
2	ZN	E	506	1/1	0.99	0.12	117,117,117,117	0
2	ZN	A	506	1/1	0.99	0.03	105,105,105,105	0
2	ZN	F	504	1/1	1.00	0.05	38,38,38,38	0
2	ZN	C	504	1/1	1.00	0.04	39,39,39,39	0
2	ZN	A	502	1/1	1.00	0.03	40,40,40,40	0
2	ZN	J	501	1/1	1.00	0.11	101,101,101,101	0
2	ZN	F	507	1/1	1.00	0.06	38,38,38,38	0
2	ZN	F	508	1/1	1.00	0.10	38,38,38,38	0
2	ZN	G	501	1/1	1.00	0.06	49,49,49,49	0
2	ZN	G	502	1/1	1.00	0.01	49,49,49,49	0
2	ZN	G	503	1/1	1.00	0.05	49,49,49,49	0
2	ZN	G	504	1/1	1.00	0.10	49,49,49,49	0
2	ZN	A	504	1/1	1.00	0.04	40,40,40,40	0
2	ZN	C	507	1/1	1.00	0.03	39,39,39,39	0
2	ZN	E	501	1/1	1.00	0.09	28,28,28,28	0
2	ZN	E	502	1/1	1.00	0.02	28,28,28,28	0
2	ZN	B	503	1/1	1.00	0.02	70,70,70,70	0
2	ZN	H	502	1/1	1.00	0.05	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	E	504	1/1	1.00	0.05	28,28,28,28	0
2	ZN	D	501	1/1	1.00	0.13	54,54,54,54	0
2	ZN	C	502	1/1	1.00	0.04	39,39,39,39	0
2	ZN	E	507	1/1	1.00	0.05	28,28,28,28	0
2	ZN	C	503	1/1	1.00	0.07	39,39,39,39	0
2	ZN	D	504	1/1	1.00	0.03	54,54,54,54	0
2	ZN	I	501	1/1	1.00	0.10	65,65,65,65	0
2	ZN	I	502	1/1	1.00	0.04	65,65,65,65	0
2	ZN	F	502	1/1	1.00	0.04	38,38,38,38	0
2	ZN	I	504	1/1	1.00	0.12	65,65,65,65	0
2	ZN	F	503	1/1	1.00	0.02	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.