



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:05 PM GMT

PDB ID : 4K95
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

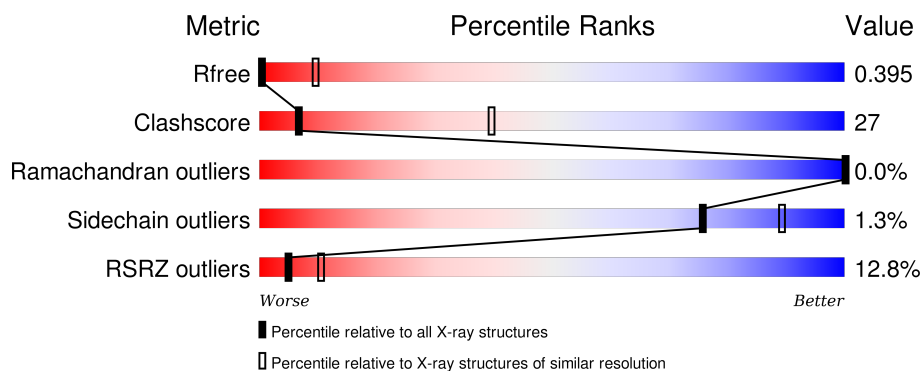
1 Overall quality at a glance

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}	91344	1012 (9.00-3.66)
Clashscore	102246	1060 (9.00-3.70)
Ramachandran outliers	100387	1033 (9.00-3.66)
Sidechain outliers	100360	1004 (9.00-3.66)
RSRZ outliers	91569	1011 (9.00-3.66)

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

Mol	Chain	Length	Quality of chain
1	A	470	<div> <div>7%</div> <div>55%</div> <div>24%</div> <div>•</div> <div>20%</div> </div>
1	B	470	<div> <div>11%</div> <div>53%</div> <div>26%</div> <div>•</div> <div>20%</div> </div>
1	C	470	<div> <div>6%</div> <div>56%</div> <div>24%</div> <div>•</div> <div>20%</div> </div>
1	D	470	<div> <div>9%</div> <div>56%</div> <div>23%</div> <div>•</div> <div>20%</div> </div>
1	E	470	<div> <div>7%</div> <div>55%</div> <div>24%</div> <div>•</div> <div>20%</div> </div>

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Mol	Chain	Length	Quality of chain			
1	F	470	7%	54%	25%	20%
1	G	470	12%	56%	23%	20%
1	H	470	14%	57%	23%	20%
1	I	470	9%	56%	23%	20%
1	J	470	13%	55%	24%	20%
1	K	470	12%	55%	24%	20%
1	L	470	16%	56%	23%	20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	I	506	-	-	-	X

2 Entry composition

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 (three-letter code: ZN) (formula: Zn).

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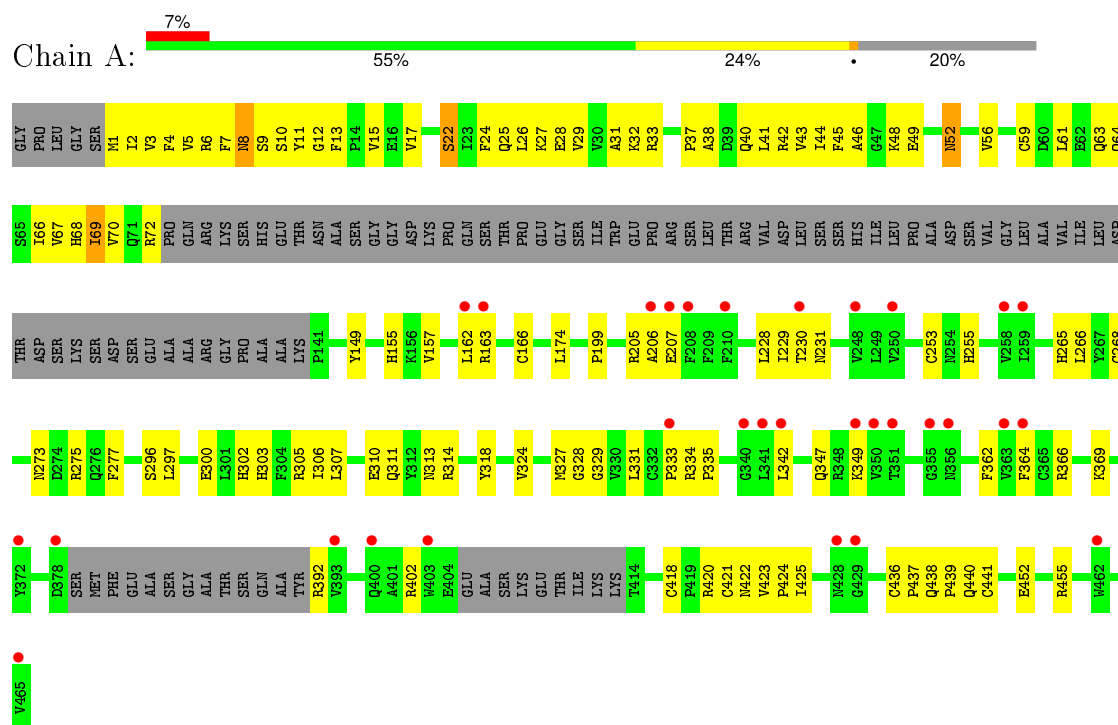
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	8	Total 8 Zn 8	0	0
2	J	8	Total 8 Zn 8	0	0
2	D	8	Total 8 Zn 8	0	0
2	K	8	Total 8 Zn 8	0	0
2	E	8	Total 8 Zn 8	0	0
2	H	8	Total 8 Zn 8	0	0
2	B	8	Total 8 Zn 8	0	0
2	I	8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

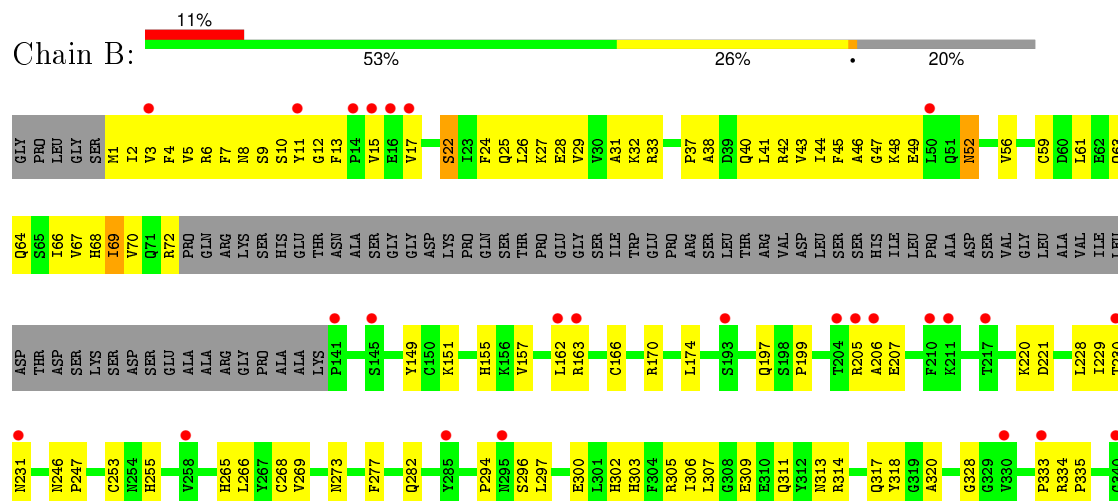
3 Residue-property plots [i](#)

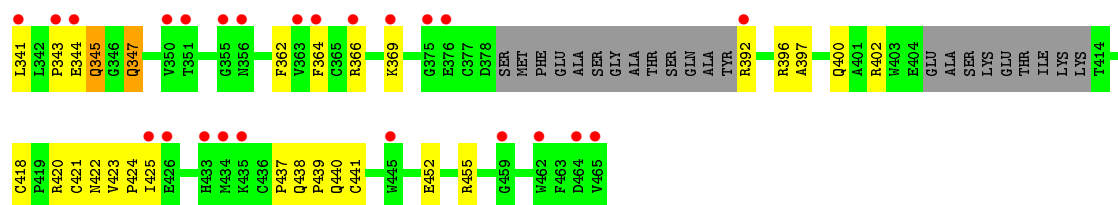
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: E3 ubiquitin-protein ligase parkin

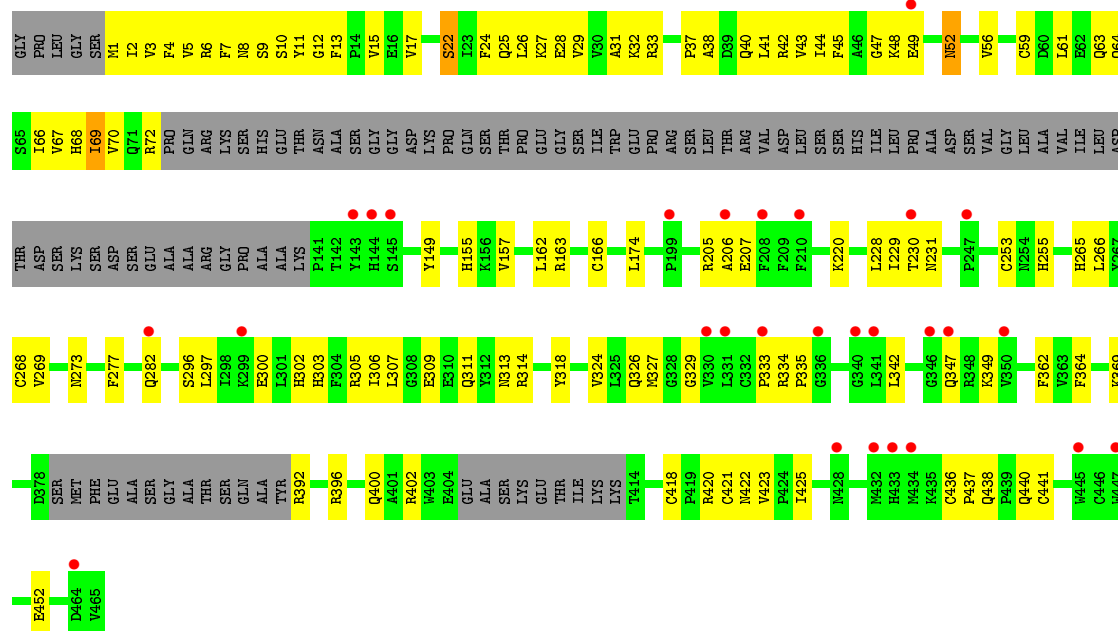


- Molecule 1: E3 ubiquitin-protein ligase parkin

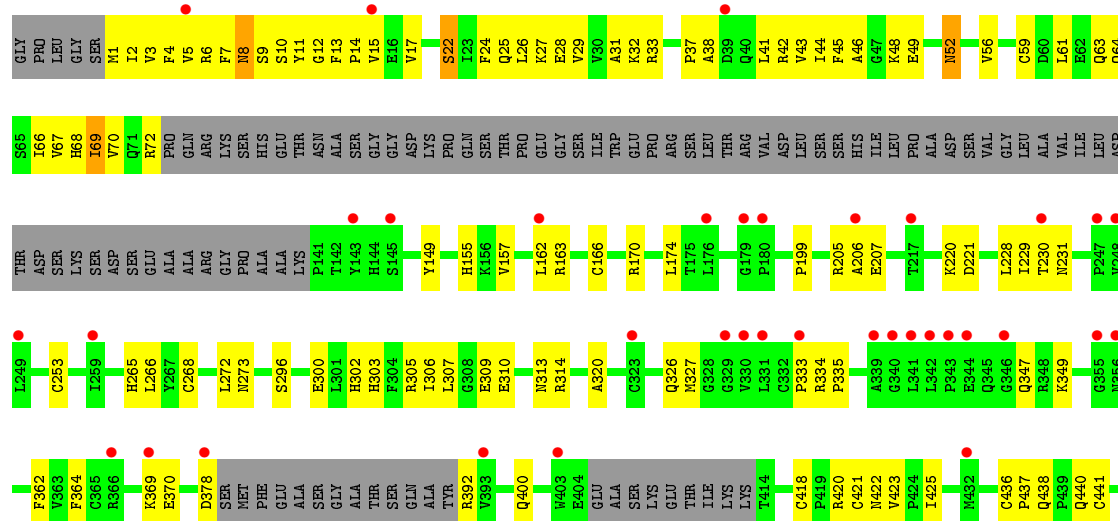


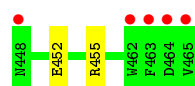


• Molecule 1: E3 ubiquitin-protein ligase parkin

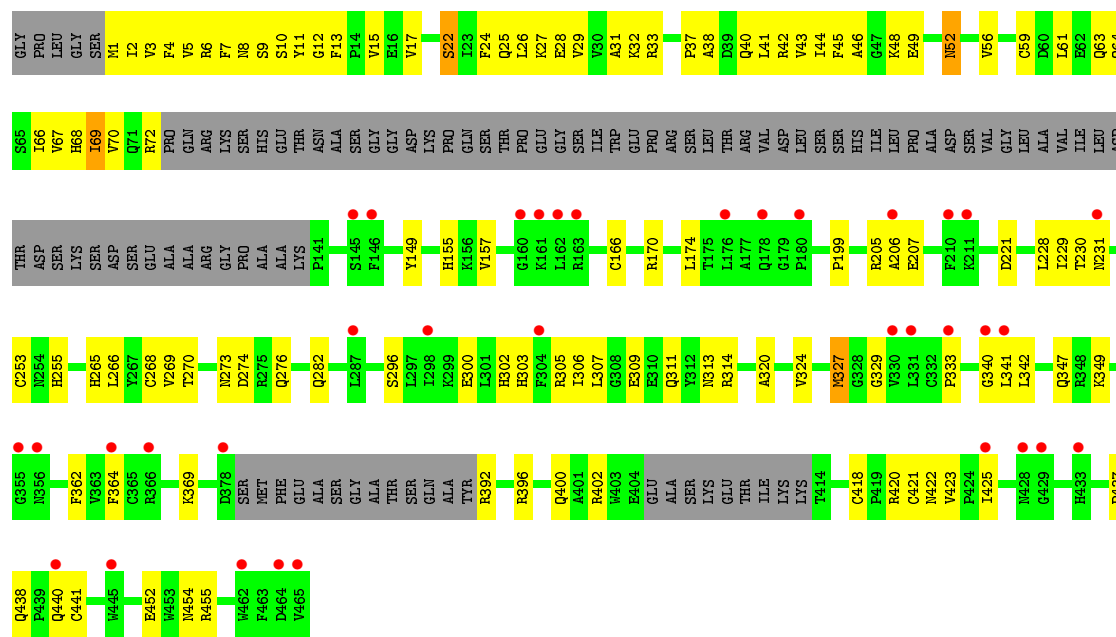


• Molecule 1: E3 ubiquitin-protein ligase parkin

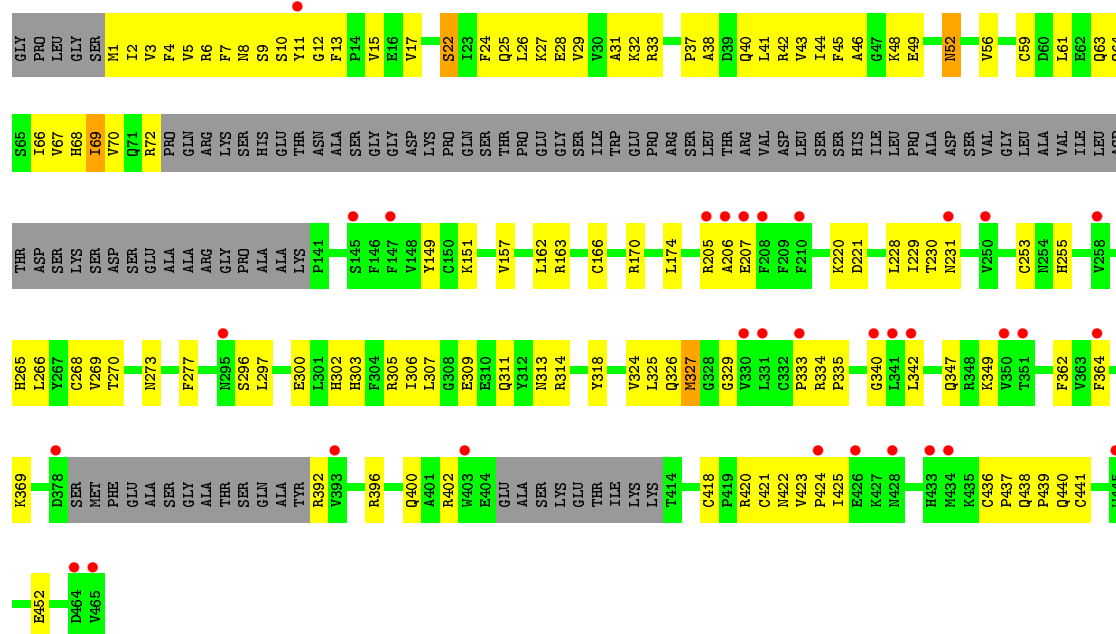




- Molecule 1: E3 ubiquitin-protein ligase parkin

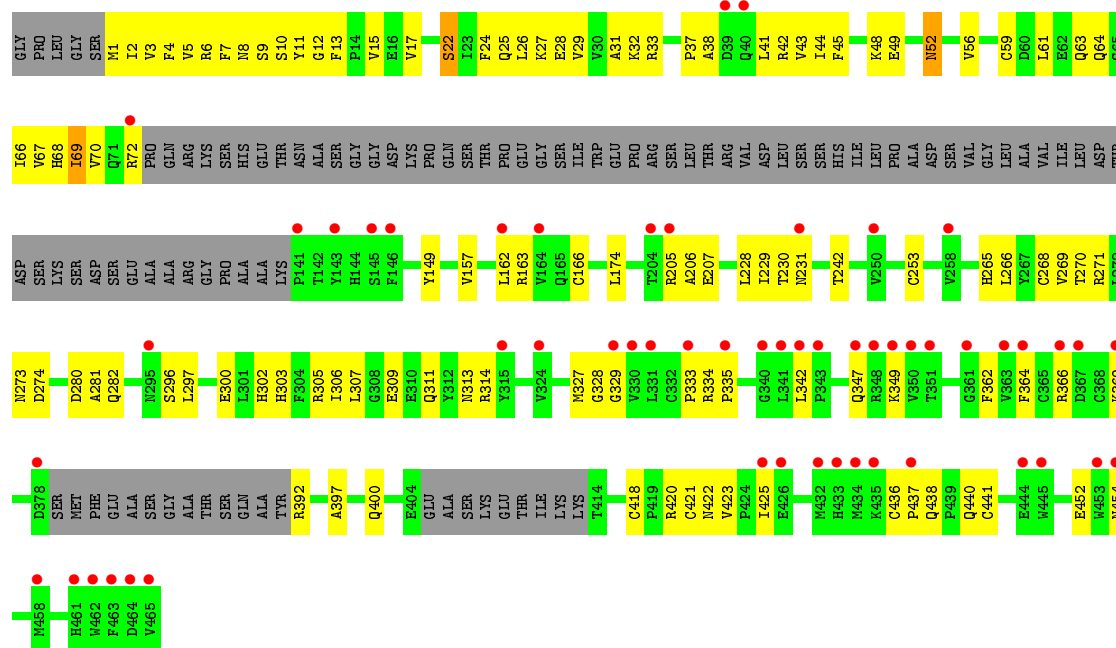


- Molecule 1: E3 ubiquitin-protein ligase parkin



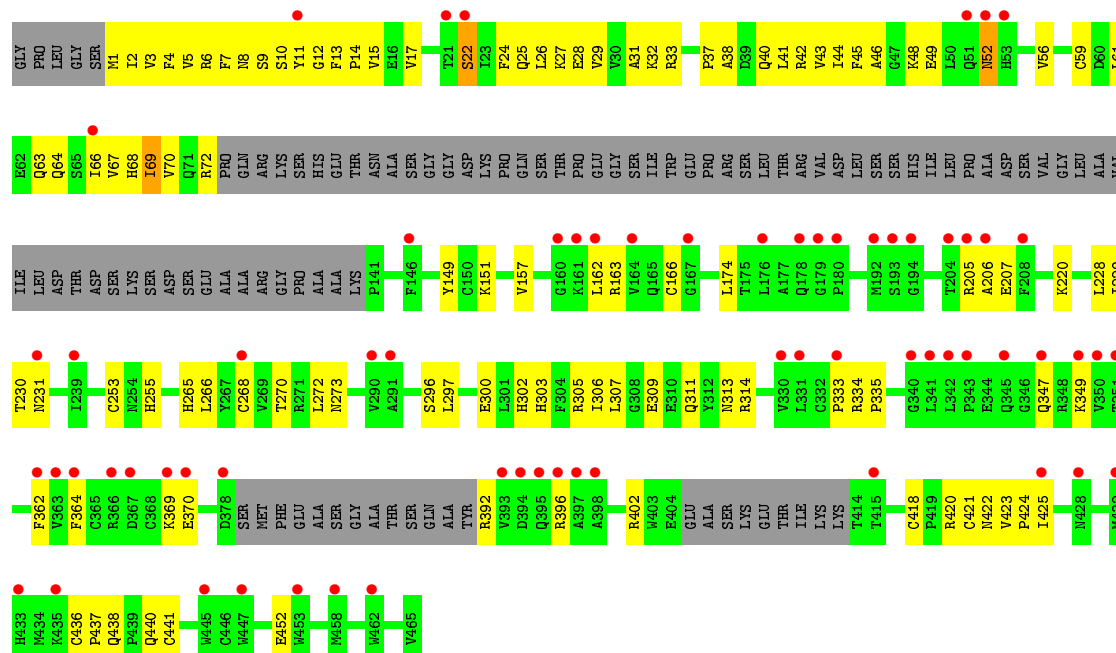
- Molecule 1: E3 ubiquitin-protein ligase parkin

Chain G:



- Molecule 1: E3 ubiquitin-protein ligase parkin

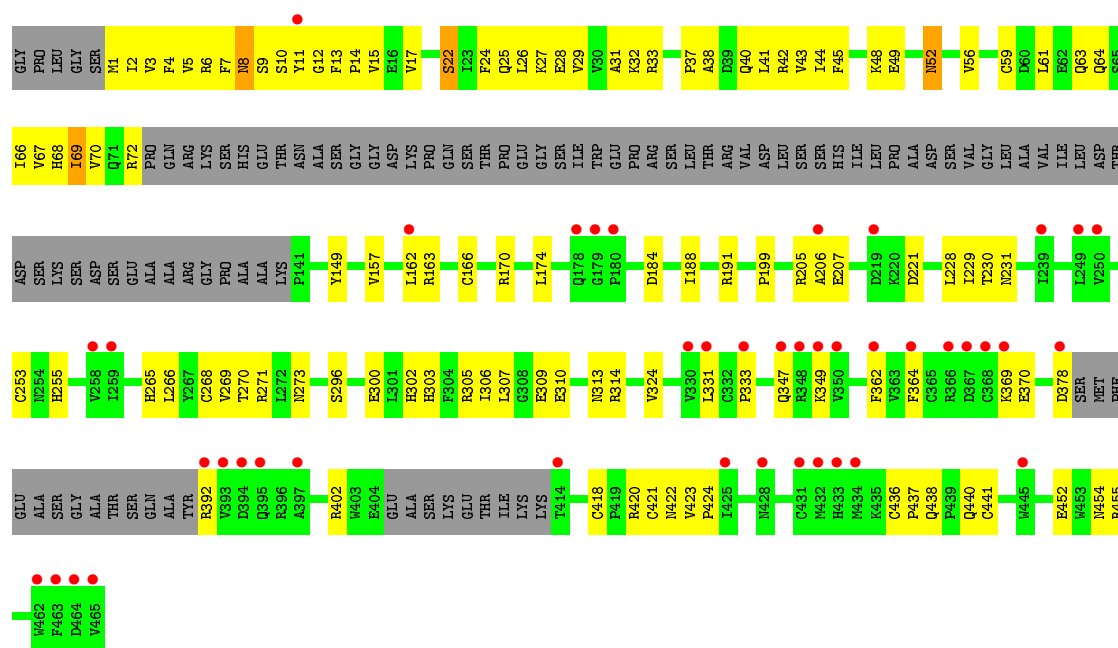
Chain H:



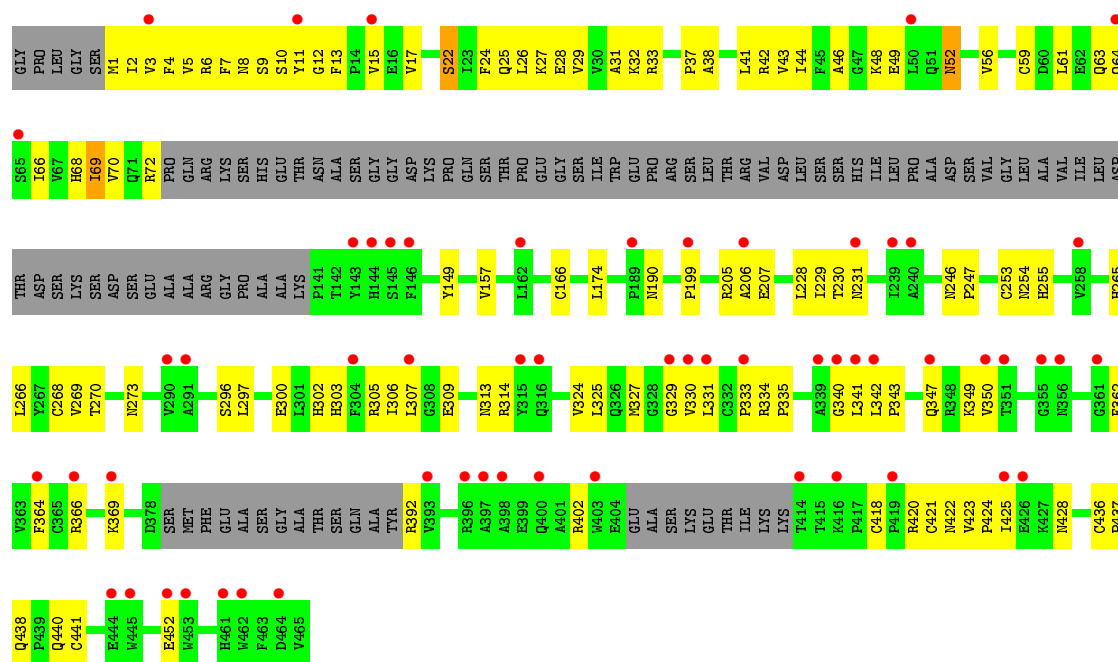
- Molecule 1: E3 ubiquitin-protein ligase parkin

Chain I:

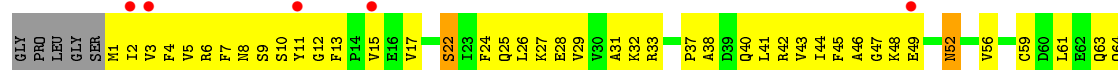


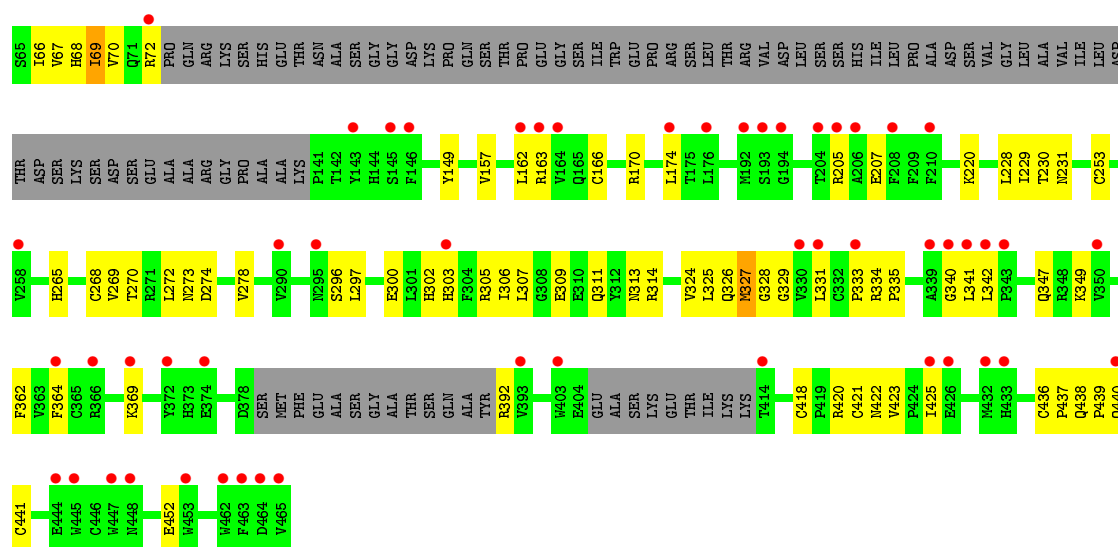


• Molecule 1: E3 ubiquitin-protein ligase parkin

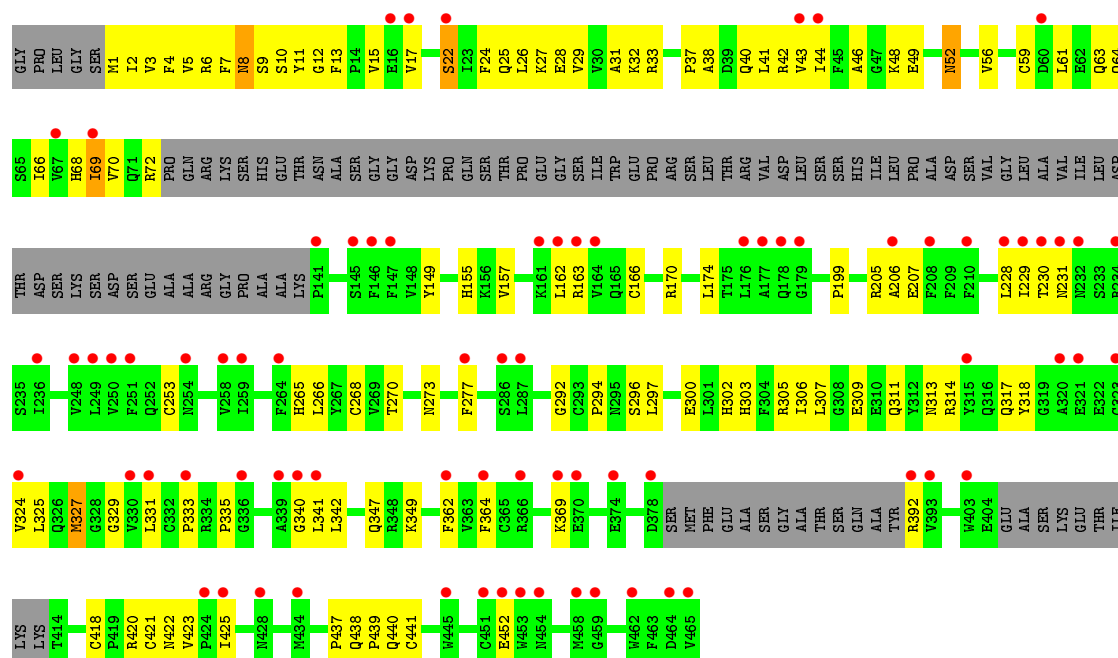


• Molecule 1: E3 ubiquitin-protein ligase parkin





• Molecule 1: E3 ubiquitin-protein ligase parkin



4 Data and refinement statistics

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) 692.9 (49.33-6.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 6.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.307 , 0.327 0.356 , 0.395	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	237.2	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 212.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 14922 reflections	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.43	1/3051 (0.0%)	0.59	2/4125 (0.0%)
1	B	0.43	1/3051 (0.0%)	0.60	2/4125 (0.0%)
1	C	0.43	0/3051	0.60	3/4125 (0.1%)
1	D	0.43	0/3051	0.59	2/4125 (0.0%)
1	E	0.43	0/3051	0.59	2/4125 (0.0%)
1	F	0.44	1/3051 (0.0%)	0.60	2/4125 (0.0%)
1	G	0.43	0/3051	0.60	2/4125 (0.0%)
1	H	0.43	1/3051 (0.0%)	0.59	2/4125 (0.0%)
1	I	0.43	1/3051 (0.0%)	0.59	2/4125 (0.0%)
1	J	0.43	1/3051 (0.0%)	0.59	2/4125 (0.0%)
1	K	0.44	0/3051	0.61	3/4125 (0.1%)
1	L	0.43	0/3051	0.59	2/4125 (0.0%)
All	All	0.43	6/36612 (0.0%)	0.60	26/49500 (0.1%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	424	PRO	N-CD	5.07	1.54	1.47
1	J	424	PRO	N-CD	5.03	1.54	1.47
1	A	424	PRO	N-CD	5.02	1.54	1.47
1	I	424	PRO	N-CD	5.01	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	424	PRO	N-CD	5.01	1.54	1.47
1	B	424	PRO	N-CD	5.01	1.54	1.47

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	423	VAL	C-N-CD	5.82	140.63	128.40
1	J	423	VAL	C-N-CD	5.82	140.62	128.40
1	F	423	VAL	C-N-CD	5.82	140.61	128.40
1	L	423	VAL	C-N-CD	5.82	140.61	128.40
1	G	423	VAL	C-N-CD	5.81	140.61	128.40
1	I	423	VAL	C-N-CD	5.81	140.61	128.40
1	E	423	VAL	C-N-CD	5.81	140.59	128.40
1	A	423	VAL	C-N-CD	5.80	140.59	128.40
1	H	423	VAL	C-N-CD	5.80	140.57	128.40
1	C	423	VAL	C-N-CD	5.79	140.56	128.40
1	K	423	VAL	C-N-CD	5.79	140.55	128.40
1	B	423	VAL	C-N-CD	5.78	140.54	128.40
1	C	69	ILE	CB-CA-C	-5.52	100.57	111.60
1	F	69	ILE	CB-CA-C	-5.51	100.59	111.60
1	E	69	ILE	CB-CA-C	-5.50	100.60	111.60
1	L	69	ILE	CB-CA-C	-5.50	100.60	111.60
1	B	69	ILE	CB-CA-C	-5.48	100.63	111.60
1	K	69	ILE	CB-CA-C	-5.48	100.63	111.60
1	G	69	ILE	CB-CA-C	-5.48	100.64	111.60
1	D	69	ILE	CB-CA-C	-5.48	100.64	111.60
1	A	69	ILE	CB-CA-C	-5.48	100.65	111.60
1	H	69	ILE	CB-CA-C	-5.48	100.65	111.60
1	I	69	ILE	CB-CA-C	-5.47	100.66	111.60
1	J	69	ILE	CB-CA-C	-5.46	100.69	111.60
1	C	329	GLY	N-CA-C	5.44	126.70	113.10
1	K	328	GLY	N-CA-C	-5.04	100.50	113.10

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 ⓘ

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	144	0
1	B	2975	0	2830	208	12
1	C	2975	0	2826	160	4
1	D	2975	0	2831	160	6
1	E	2975	0	2831	193	3
1	F	2975	0	2829	195	8
1	G	2975	0	2832	137	8
1	H	2975	0	2828	151	0
1	I	2975	0	2831	188	1
1	J	2975	0	2831	186	1
1	K	2975	0	2829	162	12
1	L	2975	0	2832	192	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	1886	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 (1886) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:11:TYR:CZ	1:L:333:PRO:HB2	1.34	1.58
1:J:44:ILE:HD13	1:J:266:LEU:CD2	1.12	1.54
1:B:44:ILE:HD13	1:B:266:LEU:CD2	1.06	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: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:B:396:ARG:NH1	1:F:396:ARG:C	1.67	1.43
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: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:I:11:TYR:CZ	1:I:333:PRO:HB2	1.59	1.35
1:B:46:ALA:CA	1:B:392:ARG:CD	2.02	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:B:46:ALA:C	1:B:392:ARG:CD	1.98	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:I:11:TYR:OH	1:I:333:PRO:HB2	1.15	1.26
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: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:I:6:ARG:NE	1:I:66:ILE:HD11	1.47	1.26
1:A:6:ARG:NE	1:A: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:L:11:TYR:CE1	1:L:333:PRO:HB2	1.69	1.25
1:F:11:TYR:OH	1:F:333:PRO:HB2	1.23	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:327:MET:O	1:J:342:LEU:CD2	1.84	1.24
1:J:190:ASN:OD1	1:J:205:ARG:HD2	1.20	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:B:46:ALA:C	1:B:392:ARG:HD2	1.58	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:H:46:ALA:CA	1:H:392:ARG:NH1	1.98	1.22
1:C:11:TYR:CE1	1:C:333:PRO:CB	2.22	1.22
1:H:11:TYR:CD1	1:H:369:LYS:HE3	1.70	1.22
1:B:420:ARG:NE	1:D:313:ASN:OD1	1.71	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:11:TYR:OH	1:I:333:PRO:CB	1.85	1.21
1:G:44:ILE:HD13	1:G:266:LEU:CD1	1.71	1.21
1:D:44:ILE:HD13	1:D:266:LEU:CD2	1.70	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:E:46:ALA:HA	1:E:392:ARG:CD	1.73	1.18
1:B:44:ILE:CD1	1:B:266:LEU:HD22	1.66	1.18
1:J:46:ALA:HB2	1:J:392:ARG:NH1	1.56	1.18
1:C:11:TYR:CE1	1:C:333:PRO:HB3	1.78	1.18
1:L:324:VAL:HG11	1:L:340:GLY:CA	1.71	1.18
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:L:324:VAL:HG11	1:L:340:GLY:HA3	1.22	1.17
1:A:313:ASN:OD1	1:F:420:ARG:NE	1.76	1.17
1:L:11:TYR:CE1	1:L:333:PRO:CA	2.27	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:B:199:PRO:HD3	1:D:170:ARG:NE	1.59	1.17
1:C:44:ILE:CD1	1:C:266:LEU:HD22	1.56	1.16
1:B:11:TYR:CZ	1:B:333:PRO:CB	2.27	1.16
1:L:6:ARG:NE	1:L:66:ILE:CD1	2.09	1.16
1:J:6:ARG:NE	1:J:66:ILE:CD1	2.08	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: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:K:6:ARG:NE	1:K:66:ILE:CD1	2.08	1.14
1:E:6:ARG:NE	1:E:66:ILE:CD1	2.08	1.14
1:G:11:TYR:CE1	1:G:333:PRO:HB2	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:452:GLU:CD	1:L:309:GLU:OE2	1.85	1.13
1:K:327:MET:HB3	1:K:342:LEU:HD21	1.31	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:D:72:ARG:HH22	1:D:265:HIS:CD2	1.68	1.12
1:J:44:ILE:CG1	1:J:266:LEU:HD21	1.79	1.12
1:B:46:ALA:C	1:B:392:ARG:HD3	1.62	1.12
1:K:47:GLY:HA3	1:K:392:ARG:HB3	1.25	1.12
1:E:46:ALA:HA	1:E:392:ARG:HD2	1.20	1.12
1:K:327:MET:HB3	1:K:342:LEU:CD2	1.78	1.12
1:G:11:TYR:CE1	1:G:333:PRO:CB	2.31	1.12
1:C:44:ILE:HD13	1:C:266:LEU:CD1	1.78	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:C:11:TYR:CD1	1:C:369:LYS:HE3	1.75	1.11
1:C:72:ARG:NH2	1:C:265:HIS:CD2	2.17	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:G:44:ILE:HD13	1:G:266:LEU:CD2	1.82	1.10
1:D:2:ILE:HD12	1:D:378:ASP:OD2	1.52	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:L:324:VAL:CG1	1:L:340:GLY:HA3	1.82	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
1:C:11:TYR:OH	1:C:333:PRO:HB2	0.90	1.08
1:H:6:ARG:HH12	1:H:273:ASN:HB2	1.12	1.08
1:B:420:ARG:NH2	1:D:313:ASN:OD1	1.87	1.08
1:C:313:ASN:OD1	1:H:420:ARG:NE	1.87	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:SER:HA	1:E:273:ASN:O	1.51	1.07
1:B:420:ARG:HE	1:D:313:ASN:CG	1.58	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:K:327:MET:C	1:K:342:LEU:CD2	2.23	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:I:11:TYR:OH	1:I:333:PRO:C	1.95	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: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: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:J:46:ALA:CA	1:J:392:ARG:HD2	1.84	1.04
1:G:11:TYR:HE1	1:G:333:PRO:CB	1.67	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:396:ARG:NH1	1:F:396:ARG:CA	2.13	1.03
1:L:46:ALA:CA	1:L:392:ARG:NH1	2.21	1.03
1:B:11:TYR:HE1	1:B:333:PRO:HA	1.24	1.03
1:K:324:VAL:HG11	1:K:340:GLY:CA	1.88	1.03
1:L:46:ALA:HB2	1:L:392:ARG:NH1	1.72	1.03
1:H:14:PRO:HD3	1:H:370:GLU:OE1	1.56	1.03
1:B:309:GLU:OE2	1:I:452:GLU:HG2	1.58	1.03
1:C:44:ILE:HD11	1:C:266:LEU:HD22	1.41	1.03
1:L:46:ALA:HA	1:L:392:ARG:NH1	1.74	1.03
1:H:44:ILE:HD13	1:H:266:LEU:HD21	1.41	1.03
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
1:L:46:ALA:CB	1:L:392:ARG:NH1	2.23	1.01
1:B:11:TYR:CE1	1:B:333:PRO:CB	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:68:HIS:CE1	1:H:270:THR:HA	1.95	1.01
1:H:14:PRO:HD2	1:H:370:GLU:OE1	1.55	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: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:G:420:ARG:NE	1:H:313:ASN:OD1	1.93	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:L:11:TYR:HE1	1:L:333:PRO:C	1.65	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:F:44:ILE:CG1	1:F:266:LEU:HD21	1.93	0.99
1:A:6:ARG:HE	1:A:66:ILE:HD11	1.10	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:J:46:ALA:N	1:J:392:ARG:HH11	1.59	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: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:L:24:PHE:CE2	1:L:25:GLN:HG3	1.98	0.98
1:I:24:PHE:CE2	1:I:25:GLN:HG3	1.98	0.98
1:E:329:GLY:CA	1:E:341:LEU:O	2.11	0.98
1:I:14:PRO:CD	1:I:370:GLU:OE1	2.12	0.98
1:G:24:PHE:CE2	1:G:25:GLN:HG3	1.98	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:F:24:PHE:CE2	1:F:25:GLN:HG3	1.98	0.98
1:A:24:PHE:CE2	1:A:25:GLN:HG3	1.98	0.98
1:B:396:ARG:C	1:F:396:ARG:NH2	2.12	0.98
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:72:ARG:HH22	1:E:265:HIS:HD2	1.14	0.96
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:I:6:ARG:HE	1:I:66:ILE:HD11	1.10	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:A:11:TYR:OH	1:A:333:PRO:HB2	1.66	0.94
1:J:420:ARG:HE	1:L:313:ASN:CG	1.64	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:I:11:TYR:HH	1:I:333:PRO:C	1.69	0.94
1:K:11:TYR:CZ	1:K:333:PRO:CB	2.50	0.93
1:K:11:TYR:CZ	1:K:333:PRO:O	2.21	0.93
1:G:72:ARG:NH2	1:G:265:HIS:HD2	1.65	0.93
1:E:44:ILE:CB	1:E:266:LEU:HD21	1.98	0.93
1:C:11:TYR:HE1	1:C:333:PRO:CA	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:313:ASN:CG	1:F:420:ARG:HE	1.71	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:K:11:TYR:CE1	1:K:333:PRO:CB	2.53	0.92
1:F:72:ARG:HH22	1:F:265:HIS:HD2	0.99	0.92
1:J:6:ARG:HE	1:J:66:ILE:HD11	1.10	0.92
1:F:72:ARG:HH22	1:F:265:HIS:CD2	1.87	0.92
1:F:46:ALA:HA	1:F:392:ARG:CZ	2.00	0.92
1:C:11:TYR:CG	1:C:369:LYS:CE	2.52	0.92
1:B:11:TYR:CE1	1:B:333:PRO:CA	2.52	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:L:324:VAL:CG1	1:L:340:GLY:CA	2.45	0.92
1:F:10:SER:HA	1:F:273:ASN:O	1.68	0.92
1:L:6:ARG:HE	1:L:66:ILE:HD11	1.10	0.92
1:J:452:GLU:OE2	1:L:309:GLU:CD	2.07	0.92
1:G:328:GLY:O	1:G:366:ARG:NH2	2.03	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:F:44:ILE:HD13	1:F:266:LEU:HD22	0.92	0.91
1:D:11:TYR:HD1	1:D:369:LYS:HE2	1.16	0.91
1:B:199:PRO:HD3	1:D:170:ARG:HE	1.28	0.91
1:L:11:TYR:CE1	1:L:333:PRO:C	2.39	0.91
1:H:11:TYR:CE1	1:H:369:LYS:HE3	2.04	0.91
1:C:313:ASN:CG	1:H:420:ARG:HE	1.72	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: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: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:L:11:TYR:OH	1:L:333:PRO:HB2	1.70	0.90
1:E:44:ILE:CG1	1:E:266:LEU:HD21	2.00	0.90
1:C:72:ARG:CZ	1:C:265:HIS:CD2	2.54	0.90
1:G:44:ILE:CD1	1:G:266:LEU:CD2	2.49	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:44:ILE:HD13	1:B:266:LEU:CG	2.02	0.90
1:B:6:ARG:HE	1:B:66:ILE:CD1	1.77	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:I:6:ARG:HE	1:I:66:ILE:CD1	1.77	0.89
1:G:6:ARG:HE	1:G:66:ILE:CD1	1.77	0.89
1:H:46:ALA:HA	1:H:392:ARG:CD	2.01	0.89
1:E:44:ILE:HD13	1:E:266:LEU:HD22	0.91	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:J:44:ILE:CG1	1:J:266:LEU:CD2	2.44	0.89
1:D:400:GLN:HG2	1:H:396:ARG:CZ	2.02	0.89
1:I:11:TYR:CE1	1:I:333:PRO:CA	2.56	0.89
1:G:440:GLN:OE1	1:G:440:GLN:N	2.06	0.89
1:E:440:GLN:N	1:E:440:GLN:OE1	2.06	0.89
1:C:440:GLN:N	1:C:440:GLN:OE1	2.06	0.89
1:D:440:GLN:OE1	1:D:440:GLN:N	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:OE1	1:L:440:GLN:N	2.06	0.88
1:G:11:TYR:CE1	1:G:333:PRO:HB3	2.07	0.88
1:C:400:GLN:HG2	1:E:396:ARG:HH11	1.35	0.88
1:B:155:HIS:CE1	1:I:452:GLU:HG3	2.09	0.88
1:K:11:TYR:HE1	1:K:333:PRO:HA	1.37	0.88
1:C:313:ASN:OD1	1:H:420:ARG:CZ	2.22	0.88
1:F:46:ALA:N	1:F:392:ARG:NH1	2.21	0.88
1:L:324:VAL:HG11	1:L:340:GLY:HA2	1.55	0.88
1:J:440:GLN:N	1:J:440:GLN:OE1	2.06	0.88
1:H:46:ALA:CB	1:H:392:ARG:NH1	2.36	0.88
1:B:47:GLY:N	1:B:392:ARG:HD2	1.89	0.88
1:J:325:LEU:CD2	1:J:331:LEU:CD1	2.46	0.88
1:F:440:GLN:OE1	1:F:440:GLN:N	2.06	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: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:B:440:GLN:N	1:B:440:GLN:OE1	2.06	0.87
1:L:8:ASN:O	1:L:335:PRO:HB3	1.75	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:44:ILE:CB	1:F:266:LEU:HD21	2.05	0.87
1:A:440:GLN:OE1	1:A:440:GLN:N	2.06	0.87
1:K:440:GLN:OE1	1:K:440:GLN:N	2.06	0.87
1:L:6:ARG:HE	1:L:66:ILE:CD1	1.77	0.87
1:F:11:TYR:CD1	1:F:369:LYS:HE2	2.09	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:OE1	1:I:440:GLN:N	2.06	0.86
1:J:72:ARG:HH22	1:J:265:HIS:CD2	1.93	0.86
1:D:400:GLN:HE21	1:H:396:ARG:HD3	1.40	0.86
1:D:72:ARG:HH22	1:D:265:HIS:HD2	0.88	0.86
1:F:327:MET:CB	1:F:342:LEU:HD21	2.06	0.86
1:D:400:GLN:HG2	1:H:396:ARG:NH1	1.90	0.86
1:J:6:ARG:HE	1:J:66:ILE:CD1	1.78	0.86
1:H:46:ALA:N	1:H:392:ARG:HH11	1.73	0.86
1:C:11:TYR:CZ	1:C:333:PRO:HB3	1.99	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:H:11:TYR:CG	1:H:369:LYS:HE2	2.09	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:C:396:ARG:NE	1:E:400:GLN:HE21	1.74	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:C:44:ILE:HD13	1:C:266:LEU:HD22	1.19	0.85
1:K:327:MET:C	1:K:342:LEU:HD21	1.96	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:I:11:TYR:CE1	1:I:333:PRO:CB	2.60	0.84
1:F:11:TYR:CZ	1:F:333:PRO:HB2	2.12	0.84
1:F:46:ALA:HB2	1:F:392:ARG:HH12	1.39	0.84
1:B:345:GLN:OE1	1:B:347:GLN:HB2	1.77	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:B:317:GLN:NE2	1:I:440:GLN:O	2.10	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:46:ALA:HA	1:J:392:ARG:HH11	1.26	0.84
1:A:199:PRO:HG2	1:E:170:ARG:HG3	1.60	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:J:190:ASN:OD1	1:J:205:ARG:CD	2.16	0.84
1:G:44:ILE:HD13	1:G:266:LEU:HD21	1.60	0.84
1:A:327:MET:HB3	1:A:342:LEU:HD21	1.59	0.84
1:A:72:ARG:HH22	1:A:265:HIS:HD2	1.25	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:L:329:GLY:CA	1:L:341:LEU:O	2.26	0.83
1:J:24:PHE:HB3	1:J:52:ASN:HD21	1.43	0.83
1:J:325:LEU:HD21	1:J:331:LEU:HD12	1.57	0.83
1:H:24:PHE:HB3	1:H:52:ASN:HD21	1.43	0.83
1:E:46:ALA:N	1:E:392:ARG:HH11	1.75	0.83
1:C:11:TYR:CE1	1:C:333:PRO:CA	2.58	0.83
1:G:24:PHE:HB3	1:G:52:ASN:HD21	1.43	0.83
1:L:11:TYR:CZ	1:L:333:PRO:O	2.31	0.83
1:C:24:PHE:HB3	1:C:52:ASN:HD21	1.43	0.83
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:E:72:ARG:HH22	1:E:265:HIS:CD2	1.96	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: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:L:44:ILE:CB	1:L:266:LEU:HD21	2.10	0.82
1:K:72:ARG:NH2	1:K:265:HIS:HD2	1.77	0.82
1:F:6:ARG:CD	1:F:66:ILE:HD11	2.10	0.82
1:L:327:MET:CG	1:L:342:LEU:HD11	2.10	0.82
1:D:24:PHE:HB3	1:D:52:ASN:HD21	1.43	0.82
1:D:2:ILE:CD1	1:D:378:ASP:OD2	2.28	0.82
1:E:44:ILE:HD13	1:E:266:LEU:HD21	1.62	0.81
1:D:199:PRO:HG2	1:I:170:ARG:HG3	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:46:ALA:N	1:H:392:ARG:NH1	2.28	0.81
1:K:24:PHE:HB3	1:K:52:ASN:HD21	1.43	0.81
1:I:324:VAL:HG11	1:I:331:LEU:HD21	1.60	0.81
1:E:6:ARG:CD	1:E:66:ILE:HD11	2.10	0.81
1:I:11:TYR:CZ	1:I:333:PRO:CA	2.64	0.81
1:E:38:ALA:HA	1:E:41:LEU:HD12	1.63	0.81
1:A:6:ARG:CD	1:A:66:ILE:HD11	2.11	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:L:6:ARG:CD	1:L:66:ILE:HD11	2.11	0.81
1:F:38:ALA:HA	1:F:41:LEU:HD12	1.63	0.81
1:D:38:ALA:HA	1:D:41:LEU:HD12	1.63	0.81
1:B:46:ALA:HA	1:B:392:ARG:HD2	1.36	0.81
1:I:6:ARG:CD	1:I:66:ILE:HD11	2.10	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: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:J:199:PRO:HG3	1:L:170:ARG:HE	1.45	0.80
1:C:396:ARG:HE	1:E:400:GLN:HE21	1.27	0.80
1:A:38:ALA:HA	1:A:41:LEU:HD12	1.63	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:B:317:GLN:HE22	1:I:440:GLN:C	1.84	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:L:11:TYR:HE1	1:L:333:PRO:HA	1.46	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:E:324:VAL:HG11	1:E:340:GLY:CA	2.11	0.80
1:D:44:ILE:CD1	1:D:266:LEU:CD2	2.49	0.80
1:C:38:ALA:HA	1:C:41:LEU:HD12	1.63	0.80
1:L:11:TYR:HE1	1:L:333:PRO:O	1.46	0.80
1:B:38:ALA:HA	1:B:41:LEU:HD12	1.63	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:J:44:ILE:HB	1:J:266:LEU:HD21	1.62	0.80
1:A:44:ILE:CB	1:A:266:LEU:HD21	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:38:ALA:HA	1:I:41:LEU:HD12	1.63	0.80
1:K:329:GLY:HA2	1:K:341:LEU:O	1.82	0.79
1:K:38:ALA:HA	1:K:41:LEU:HD12	1.63	0.79
1:J:6:ARG:CD	1:J:66:ILE:HD11	2.10	0.79
1:F:11:TYR:CZ	1:F:333:PRO:CB	2.65	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:44:ILE:CG1	1:A:266:LEU:HD21	2.13	0.79
1:G:11:TYR:CD1	1:G:369:LYS:HE3	2.18	0.79
1:A:11:TYR:CZ	1:A:333:PRO:HB2	2.16	0.79
1:C:309:GLU:OE2	1:H:452:GLU:HG2	1.82	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:L:46:ALA:HA	1:L:392:ARG:HD2	1.64	0.78
1:H:44:ILE:CD1	1:H:266:LEU:CD2	2.52	0.78
1:C:72:ARG:HH22	1:C:265:HIS:CD2	1.91	0.78
1:J:452:GLU:OE2	1:L:309:GLU:OE2	2.00	0.78
1:A:452:GLU:HG2	1:E:309:GLU:OE2	1.82	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:H:46:ALA:HB2	1:H:392:ARG:NH1	1.98	0.78
1:G:397:ALA:O	1:G:400:GLN:HG2	1.83	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:E:11:TYR:CZ	1:E:333:PRO:HB2	2.17	0.78
1:K:11:TYR:OH	1:K:333:PRO:C	2.22	0.77
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:G:70:VAL:CG1	1:G:269:VAL:HG11	2.13	0.77
1:E:452:GLU:HG2	1:F:309:GLU:OE2	1.84	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
1:B:11:TYR:CE1	1:B:333:PRO:HB3	2.17	0.77
1:J:199:PRO:HD3	1:L:170:ARG:NE	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:400:GLN:CD	1:F:396:ARG:HG2	2.05	0.77
1:J:6:ARG:CZ	1:J:66:ILE:HD13	2.15	0.77
1:E:72:ARG:NH2	1:E:265:HIS:CD2	2.52	0.77
1:D:6:ARG:CZ	1:D:66:ILE:HD13	2.15	0.77
1:K:6:ARG:CZ	1:K:66:ILE:HD13	2.15	0.77
1:E:6:ARG:CZ	1:E:66:ILE:HD13	2.15	0.77
1:J:327:MET:C	1:J:342:LEU:HD21	2.04	0.77
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:B:27:LYS:NZ	1:B:41:LEU:O	2.18	0.76
1:F:324:VAL:HG11	1:F:340:GLY:CA	2.16	0.76
1:A:46:ALA:HA	1:A:392:ARG:HD2	1.66	0.76
1:J:46:ALA:N	1:J:392:ARG:NH1	2.28	0.76
1:H:27:LYS:NZ	1:H:41:LEU:O	2.18	0.76
1:B:11:TYR:OH	1:B:333:PRO:C	2.23	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:I:6:ARG:CZ	1:I:66:ILE:HD13	2.15	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: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: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:A:72:ARG:HH22	1:A:265:HIS:CD2	2.04	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:I:188:ILE:CG2	1:I:191:ARG:HB2	2.13	0.76
1:I:44:ILE:HD13	1:I:266:LEU:CG	2.15	0.76
1:I:22:SER:HB2	1:I:24:PHE:CE1	2.21	0.76
1:I:44:ILE:HG21	1:I:266:LEU:HD21	1.67	0.75
1:A:27:LYS:NZ	1:A:41:LEU:O	2.19	0.75
1:L:22:SER:HB2	1:L:24:PHE:CE1	2.21	0.75
1:C:22:SER:HB2	1:C:24:PHE:CE1	2.21	0.75
1:J:22:SER:HB2	1:J:24:PHE:CE1	2.21	0.75
1:E:22:SER:HB2	1:E: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ARG:CZ	1:A:66:ILE:HD13	2.15	0.75
1:F:22:SER:HB2	1:F:24:PHE:CE1	2.21	0.75
1:D:27:LYS:NZ	1:D:41:LEU:O	2.18	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: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:46:ALA:HA	1:A:392:ARG:CD	2.17	0.74
1:H:11:TYR:CE1	1:H:369:LYS:CE	2.67	0.74
1:A:44:ILE:HG21	1:A:266:LEU:HD21	1.69	0.74
1:D:22:SER:HB2	1:D:24:PHE:CE1	2.21	0.74
1:B:22:SER:HB2	1:B:24:PHE:CE1	2.21	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:L:6:ARG:NE	1:L:66:ILE:HD13	2.03	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:I:44:ILE:CD1	1:I:266:LEU:CD1	2.64	0.74
1:D:199:PRO:CG	1:I:170:ARG:HG3	2.17	0.74
1:L:46:ALA:HA	1:L:392:ARG:CD	2.18	0.73
1:A:452:GLU:HG3	1:E:155:HIS:CE1	2.23	0.73
1:G:6:ARG:NE	1:G:66:ILE:HD13	2.03	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: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:K:27:LYS:NZ	1:K:41:LEU:O	2.19	0.73
1:B:11:TYR:HH	1:B:333:PRO:C	1.91	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:H:44:ILE:CD1	1:H:266:LEU:HD21	2.14	0.73
1:G:44:ILE:HD13	1:G:266:LEU:HD13	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:46:ALA:HA	1:E:392:ARG:CZ	2.19	0.72
1:A:155:HIS:HE1	1:F:452:GLU:HG3	1.55	0.72
1:J:46:ALA:HA	1:J:392:ARG:NH1	1.89	0.72
1:D:11:TYR:CE1	1:D:369:LYS:CE	2.44	0.72
1:B:400:GLN:OE1	1:F:396:ARG:HG2	1.89	0.72
1:F:70:VAL:CG1	1:F:269:VAL:HG11	2.20	0.72
1:D:14:PRO:HD2	1:D:370:GLU:OE1	1.89	0.72
1:B:199:PRO:CD	1:D:170:ARG:NE	2.46	0.72
1:L:44:ILE:HG21	1:L:266:LEU:HD21	1.72	0.71
1:G:70:VAL:HG11	1:G:269:VAL:HG11	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: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:B:155:HIS:HD1	1:I:452:GLU:CD	1.94	0.71
1:C:396:ARG:CD	1:E:400:GLN:CG	2.69	0.70
1:A:155:HIS:CE1	1:F:452:GLU:HG3	2.26	0.70
1:K:327:MET:SD	1:K:342:LEU:HD11	2.31	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:327:MET:O	1:J:342:LEU:HD22	1.91	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
1:C:396:ARG:CD	1:E:400:GLN:HE21	2.05	0.70
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:I:184:ASP:O	1:I:188:ILE:CG2	2.26	0.69
1:E:68:HIS:CD2	1:E:270:THR:HG23	2.27	0.69
1:I:44:ILE:CD1	1:I:266:LEU:HD21	2.21	0.69
1:J:46:ALA:HA	1:J:392:ARG:NE	2.07	0.69
1:I:6:ARG:CZ	1:I:66:ILE:CD1	2.70	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6:ARG:CZ	1:G:66:ILE:CD1	2.69	0.69
1:L:6:ARG:CZ	1:L:66:ILE:CD1	2.70	0.69
1:B:44:ILE:CB	1:B:266:LEU:HD21	2.22	0.69
1:K:6:ARG:CZ	1:K:66:ILE:CD1	2.70	0.69
1:G:420:ARG:HE	1:H:313:ASN:CG	1.96	0.69
1:I:1:MET:N	1:I:17:VAL:O	2.25	0.69
1:K:72:ARG:HH22	1:K:265:HIS:HD2	1.40	0.69
1:F:11:TYR:CD1	1:F:369:LYS:CE	2.75	0.69
1:A:452:GLU:OE2	1:E:155:HIS:ND1	2.21	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:K:327:MET:CB	1:K:342:LEU:CD2	2.59	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:A:8:ASN:OD1	1:A:310:GLU:OE2	2.11	0.68
1:D:46:ALA:HA	1:D:392:ARG:CZ	2.20	0.68
1:A:44:ILE:CG2	1:A:266:LEU:HD21	2.24	0.68
1:K:324:VAL:CG1	1:K:340:GLY:CA	2.68	0.68
1:B:1:MET:N	1:B:17:VAL:O	2.25	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:A:46:ALA:C	1:A:392:ARG:HD2	2.14	0.67
1:L:1:MET:N	1:L:17:VAL:O	2.25	0.67
1:E:11:TYR:OH	1:E:333:PRO:CB	2.31	0.67
1:D:44:ILE:HG21	1:D:266:LEU:CD2	2.24	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
1:C:420:ARG:NE	1:G:313:ASN:OD1	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:E:1:MET:N	1:E:17:VAL:O	2.25	0.67
1:C:400:GLN:CG	1:E:396:ARG:NH1	2.57	0.67
1:G:327:MET:C	1:G:329:GLY:H	1.97	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:B:44:ILE:HD11	1:B:266:LEU:HD22	1.72	0.67
1:E:7:PHE:HD1	1:E:69:ILE:HB	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:PHE:HD1	1:C: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:I:6:ARG:NE	1:I:66:ILE:HD13	2.03	0.66
1:B:11:TYR:CG	1:B:369:LYS:HE2	2.31	0.66
1:A:7:PHE:HD1	1:A:69:ILE:HB	1.60	0.66
1:E:44:ILE:CG1	1:E:266:LEU:CD2	2.68	0.66
1:A:155:HIS:ND1	1:F:452:GLU:OE2	2.18	0.66
1:D:400:GLN:NE2	1:H:396:ARG:HD3	2.11	0.66
1:J:313:ASN:OD1	1:K:420:ARG:NH2	2.28	0.66
1:G:7:PHE:HD1	1:G:69:ILE:HB	1.60	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: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:K:170:ARG:HG3	1:L:199:PRO:HG2	1.78	0.65
1:H:63:GLN:NE2	1:H:64:GLN:HG3	2.11	0.65
1:L:27:LYS:HE3	1:L:41:LEU:HB2	1.78	0.65
1:K:63:GLN:NE2	1:K:64:GLN:HG3	2.11	0.65
1:G:63:GLN:NE2	1:G:64:GLN:HG3	2.11	0.65
1:J:1:MET:N	1:J:17:VAL:O	2.25	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:B:63:GLN:NE2	1:B:64:GLN:HG3	2.11	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:F:27:LYS:HE3	1:F:41:LEU:HB2	1.79	0.65
1:D:27:LYS:HE3	1:D:41:LEU:HB2	1.78	0.65
1:B:7:PHE:HD1	1:B:69:ILE:HB	1.60	0.65
1:F:63:GLN:NE2	1:F:64:GLN:HG3	2.11	0.65
1:H:7:PHE:HD1	1:H:69:ILE:HB	1.60	0.65
1:D:44:ILE:CG1	1:D:266:LEU:CD2	2.74	0.65
1:L:327:MET:SD	1:L:342:LEU:HD11	2.36	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:331:LEU:HD23	1:J:340:GLY:HA2	1.79	0.65
1:D:229:ILE:HD11	1:D:306:ILE:HD11	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:K:327:MET:CA	1:K:342:LEU:HD21	2.26	0.65
1:C:44:ILE:HG12	1:C:266:LEU:CD2	2.14	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:K:27:LYS:HE3	1:K:41:LEU:HB2	1.79	0.65
1:J:63:GLN:NE2	1:J:64:GLN:HG3	2.11	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:J:68:HIS:CD2	1:J:270:THR:HG23	2.33	0.64
1:C:1:MET:N	1:C:17:VAL:O	2.25	0.64
1:I:63:GLN:NE2	1:I:64:GLN:HG3	2.11	0.64
1:H:14:PRO:CD	1:H:370:GLU:CD	2.65	0.64
1:B:155:HIS:ND1	1:I:452:GLU:OE2	2.25	0.64
1:C:396:ARG:CD	1:E:400:GLN:HG2	2.26	0.64
1:G:229:ILE:HD11	1:G:306:ILE:HD11	1.79	0.64
1:C:229:ILE:HD11	1:C:306:ILE:HD11	1.79	0.64
1:F:229:ILE:HD11	1:F: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:K:6:ARG:HG2	1:K:11:TYR:O	1.98	0.64
1:A:6:ARG:HG2	1:A:11:TYR:O	1.98	0.64
1:E:9:SER:O	1:E:273:ASN:HA	1.96	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
1:B:6:ARG:HG2	1:B:11:TYR:O	1.98	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:A:46:ALA:CA	1:A:392:ARG:CD	2.76	0.64
1:C:327:MET:O	1:C:342:LEU:HD22	1.96	0.64
1:C:6:ARG:HD2	1:C:9:SER:O	1.97	0.64
1:B:273:ASN:OD1	1:B:314:ARG:NH2	2.31	0.64
1:B:229:ILE:HD11	1:B:306:ILE:HD11	1.79	0.64
1:B:27:LYS:HE3	1:B:41:LEU:HB2	1.78	0.64
1:H:6:ARG:HD2	1:H:9:SER:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:273:ASN:OD1	1:L:314:ARG:NH2	2.31	0.64
1:L:72:ARG:NH2	1:L:265:HIS:HD2	1.94	0.64
1:J:309:GLU:OE2	1:K:452:GLU:HG2	1.98	0.64
1:I:229:ILE:HD11	1:I:306:ILE:HD11	1.79	0.64
1:E:63:GLN:NE2	1:E:64:GLN:HG3	2.11	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:F:1:MET:N	1:F:17:VAL:O	2.25	0.64
1:D:6:ARG:HG2	1:D:11:TYR:O	1.98	0.64
1:J:6:ARG:HG2	1:J:11:TYR:O	1.98	0.64
1:I:273:ASN:OD1	1:I:314:ARG:NH2	2.31	0.64
1:G:44:ILE:CD1	1:G:266:LEU:HD22	2.27	0.63
1:G:420:ARG:NH2	1:H:313:ASN:OD1	2.30	0.63
1:E:70:VAL:HG21	1:E:72:ARG:CZ	2.28	0.63
1:G:70:VAL:HG21	1:G:72:ARG:CZ	2.28	0.63
1:E:229:ILE:HD11	1:E:306:ILE:HD11	1.79	0.63
1:H:273:ASN:OD1	1:H: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:L:70:VAL:HG21	1:L:72:ARG:CZ	2.27	0.63
1:A:273:ASN:OD1	1:A:314:ARG:NH2	2.31	0.63
1:K:273:ASN:OD1	1:K:314:ARG:NH2	2.31	0.63
1:F:70:VAL:HG21	1:F:72:ARG:CZ	2.27	0.63
1:I:44:ILE:CD1	1:I:266:LEU:HD13	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: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:J:27:LYS:HE3	1:J:41:LEU:HB2	1.78	0.63
1:B:70:VAL:HG21	1:B:72:ARG:CZ	2.28	0.63
1:F:46:ALA:HA	1:F:392:ARG:NE	2.13	0.63
1:H:14:PRO:HD2	1:H:370:GLU:CD	2.18	0.63
1:D:455:ARG:HD2	1:I:221:ASP:OD1	1.99	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:A:229:ILE:HD11	1:A:306:ILE:HD11	1.79	0.63
1:L:63:GLN:HE21	1:L:64:GLN:HE21	1.47	0.63
1:L:6:ARG:HG2	1:L:11:TYR:O	1.98	0.63
1:C:396:ARG:HD2	1:E:400:GLN:NE2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:63:GLN:HE21	1:H:64:GLN:HE21	1.47	0.63
1:J:199:PRO:HG2	1:L:170:ARG:HG3	1.81	0.62
1:G:273:ASN:OD1	1:G:314:ARG:NH2	2.31	0.62
1:F:6:ARG:HG2	1:F:11:TYR:O	1.98	0.62
1:B:72:ARG:NH2	1:B:265:HIS:CD2	2.65	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:E:63:GLN:HE21	1:E:64:GLN:HE21	1.47	0.62
1:L:229:ILE:HD11	1:L:306:ILE:HD11	1.79	0.62
1:C:273:ASN:OD1	1:C:314:ARG:NH2	2.31	0.62
1:E:273:ASN:OD1	1:E:314:ARG:NH2	2.31	0.62
1:B:155:HIS:CE1	1:I:452:GLU:CG	2.82	0.62
1:F:327:MET:SD	1:F:342:LEU:HD11	2.40	0.62
1:D:273:ASN:OD1	1:D:314:ARG:NH2	2.31	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:I:11:TYR:CZ	1:I:333:PRO:O	2.53	0.62
1:K:11:TYR:CE1	1:K:333:PRO:C	2.72	0.62
1:G:11:TYR:CD1	1:G:369:LYS:CE	2.83	0.62
1:B:396:ARG:O	1:F:396:ARG:CZ	2.27	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:J:420:ARG:HE	1:L:313:ASN:CB	2.12	0.62
1:I:324:VAL:CG1	1:I:331:LEU:HD21	2.29	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: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
1:D:1:MET:N	1:D:17:VAL:O	2.25	0.61
1:F:327:MET:C	1:F:342:LEU:CD2	2.68	0.61
1:H:2:ILE:HB	1:H: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: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:G:1:MET:N	1:G:17:VAL:O	2.25	0.61
1:A:11:TYR:CZ	1:A:333:PRO:CB	2.83	0.61
1:C:327:MET:HB3	1:C:342:LEU:CD2	2.31	0.61
1:C:2:ILE:HB	1:C:63:GLN:HE22	1.65	0.61
1:H:1:MET:N	1:H:17:VAL:O	2.25	0.61
1:K:2:ILE:HB	1:K:63:GLN:HE22	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2:ILE:HB	1:E:63:GLN:HE22	1.65	0.61
1:C:418:CYS:O	1:C:422:ASN:N	2.30	0.61
1:L:11:TYR:OH	1:L:333:PRO:C	2.39	0.61
1:K:325:LEU:HD21	1:K:331:LEU:HG	1.83	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:B:44:ILE:HD13	1:B:266:LEU:CD1	2.29	0.61
1:F:44:ILE:CG2	1:F:266:LEU:HD21	2.30	0.61
1:A:2:ILE:HB	1:A:63:GLN:HE22	1.65	0.61
1:F:2:ILE:HB	1:F:63:GLN:HE22	1.65	0.61
1:E:46:ALA:HB2	1:E:392:ARG:CZ	2.21	0.61
1:C:44:ILE:CD1	1:C:266:LEU:HD13	2.30	0.61
1:B:63:GLN:HE21	1:B:64:GLN:HE21	1.47	0.61
1:J:2:ILE:HB	1:J:63:GLN:HE22	1.65	0.61
1:I:2:ILE:HB	1:I:63:GLN:HE22	1.65	0.61
1:H:418:CYS:O	1:H:422:ASN:N	2.30	0.61
1:G:271:ARG:HH12	1:G:392:ARG:NH1	1.99	0.61
1:E:46:ALA:HA	1:E:392:ARG:NE	2.16	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:C:11:TYR:CB	1:C:369:LYS:HE2	2.31	0.60
1:B:199:PRO:HD3	1:D:170:ARG:CZ	2.30	0.60
1:L:24:PHE:CD2	1:L:25:GLN:HG3	2.36	0.60
1:J:24:PHE:CD2	1:J:25:GLN:HG3	2.36	0.60
1:G:397:ALA:O	1:G:400:GLN:CG	2.49	0.60
1:J:63:GLN:HE21	1:J:64:GLN:HE21	1.47	0.60
1:B:170:ARG:CZ	1:I:199:PRO:HD3	2.31	0.60
1:B:396:ARG:HG2	1:F:400:GLN:NE2	2.16	0.60
1:I:24:PHE:CD2	1:I:25:GLN:HG3	2.36	0.60
1:E:29:VAL:O	1:E:33:ARG:HB2	2.02	0.60
1:F:44:ILE:HD13	1:F:266:LEU:CD1	2.31	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:K:327:MET:HB3	1:K:342:LEU:HD11	1.81	0.60
1:D:2:ILE:HB	1:D:63:GLN:HE22	1.65	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:29:VAL:O	1:K:33:ARG:HB2	2.02	0.60
1:J:44:ILE:CG2	1:J:266:LEU:HD21	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:24:PHE:CD2	1:H:25:GLN:HG3	2.36	0.60
1:E:24:PHE:CD2	1:E:25:GLN:HG3	2.36	0.60
1:C:396:ARG:HD2	1:E:400:GLN:HE21	1.66	0.60
1:L:44:ILE:CG1	1:L:266:LEU:HD21	2.31	0.60
1:J:313:ASN:OD1	1:K:420:ARG:CZ	2.50	0.60
1:G:9:SER:OG	1:G:10:SER:N	2.35	0.60
1:K:324:VAL:HG11	1:K:340:GLY:HA2	1.81	0.60
1:I:70:VAL:CG1	1:I:269:VAL:HG11	2.30	0.60
1:A:327:MET:HB3	1:A:342:LEU:CD2	2.30	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:I:9:SER:OG	1:I:10:SER:N	2.35	0.60
1:D:24:PHE:CD2	1:D:25:GLN:HG3	2.36	0.59
1:C:9:SER:OG	1:C:10:SER:N	2.35	0.59
1:D:29:VAL:O	1:D:33:ARG:HB2	2.01	0.59
1:I:188:ILE:O	1:I:188:ILE:HG23	2.01	0.59
1:J:313:ASN:CG	1:K:420:ARG:HE	2.04	0.59
1:I:72:ARG:CZ	1:I:265:HIS:CD2	2.85	0.59
1:G:24:PHE:CD2	1:G:25:GLN:HG3	2.36	0.59
1:B:24:PHE:CD2	1:B:25:GLN:HG3	2.36	0.59
1:J:440:GLN:C	1:L:317:GLN:HE22	2.06	0.59
1:A:452:GLU:CD	1:E:155:HIS:HD1	2.04	0.59
1:A:455:ARG:HD2	1:E:221:ASP:OD1	2.01	0.59
1:I:29:VAL:O	1:I:33:ARG:HB2	2.02	0.59
1:J:29:VAL:O	1:J:33:ARG:HB2	2.01	0.59
1:L:324:VAL:HG13	1:L:340:GLY:HA3	1.82	0.59
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:K:24:PHE:CD2	1:K:25:GLN:HG3	2.36	0.59
1:C:22:SER:CB	1:C:24:PHE:CE1	2.86	0.59
1:F:9:SER:OG	1:F:10:SER:N	2.35	0.59
1:B:317:GLN:NE2	1:I:440:GLN:C	2.52	0.59
1:I:271:ARG:HH12	1:I:392:ARG:NH1	2.00	0.59
1:J:324:VAL:CG1	1:J:340:GLY:HA3	2.32	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:I:44:ILE:CG2	1:I:266:LEU:HD21	2.33	0.59
1:D:22:SER:CB	1:D:24:PHE:CE1	2.86	0.59
1:I:68:HIS:CE1	1:I:273:ASN:CB	2.86	0.59
1:E:46:ALA:CA	1:E:392:ARG:HD3	2.30	0.59
1:F:24:PHE:CD2	1:F:25:GLN:HG3	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:SER:CB	1:E:24:PHE:CE1	2.86	0.59
1:H:46:ALA:H	1:H:392:ARG:NH1	1.99	0.59
1:B:6:ARG:NH2	1:B:66:ILE:HD13	2.18	0.59
1:J:324:VAL:HG12	1:J:331:LEU:CD2	2.25	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:B:29:VAL:O	1:B:33:ARG:HB2	2.01	0.59
1:D:6:ARG:NH2	1:D:66:ILE:HD13	2.18	0.59
1:K:6:ARG:NH2	1:K:66:ILE:HD13	2.18	0.59
1:E:11:TYR:HE1	1:E:333:PRO:HA	1.68	0.59
1:E:9:SER:OG	1:E:10:SER:N	2.35	0.59
1:J:420:ARG:NE	1:L:313:ASN:CG	2.34	0.59
1:G:29:VAL:O	1:G:33:ARG:HB2	2.02	0.59
1:A:29:VAL:O	1:A:33:ARG:HB2	2.02	0.59
1:A:44:ILE:CD1	1:A:266:LEU:HD21	2.24	0.59
1:C:70:VAL:HG13	1:C:269:VAL:HG11	1.85	0.59
1:G:6:ARG:NH2	1:G:66:ILE:HD13	2.17	0.59
1:L:22:SER:CB	1:L:24:PHE:CE1	2.86	0.59
1:F:22:SER:CB	1:F:24:PHE:CE1	2.86	0.59
1:J:9:SER:OG	1:J:10:SER:N	2.35	0.59
1:C:3:VAL:HG22	1:C:15:VAL:O	2.03	0.59
1:G:24:PHE:HB3	1:G:52:ASN:ND2	2.17	0.58
1:C:24:PHE:HB3	1:C:52:ASN:ND2	2.17	0.58
1:K:72:ARG:NH1	1:K:265:HIS:CD2	2.71	0.58
1:B:455:ARG:HD2	1:D:221:ASP:OD1	2.03	0.58
1:L:6:ARG:NH2	1:L:66:ILE:HD13	2.18	0.58
1:B:47:GLY:HA3	1:B:392:ARG:HB3	1.85	0.58
1:G:44:ILE:HD13	1:G:266:LEU:HD22	1.78	0.58
1:A:22:SER:CB	1:A:24:PHE:CE1	2.86	0.58
1:E:24:PHE:HB3	1:E:52:ASN:ND2	2.17	0.58
1:I:3:VAL:HG22	1:I:15:VAL:O	2.03	0.58
1:C:11:TYR:HB3	1:C:369:LYS:HE2	1.84	0.58
1:B:155:HIS:ND1	1:I:452:GLU:CG	2.67	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:A:9:SER:OG	1:A:10:SER:N	2.35	0.58
1:L:3:VAL:HG22	1:L:15:VAL:O	2.03	0.58
1:H:22:SER:CB	1:H:24:PHE:CE1	2.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3:VAL:HG22	1:J:15:VAL:O	2.03	0.58
1:I:6:ARG:NH2	1:I:66:ILE:HD13	2.18	0.58
1:E:327:MET:CG	1:E:342:LEU:CD1	2.49	0.58
1:J:6:ARG:NH2	1:J:66:ILE:HD13	2.18	0.58
1:E:6:ARG:NH2	1:E:66:ILE:HD13	2.18	0.58
1:B:22:SER:CB	1:B:24:PHE:CE1	2.86	0.58
1:J:22:SER:CB	1:J:24:PHE:CE1	2.86	0.58
1:G:72:ARG:CZ	1:G:265:HIS:CD2	2.86	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: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: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: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:K:72:ARG:CZ	1:K:265:HIS:CD2	2.87	0.58
1:J:330:VAL:CG1	1:J:350:VAL:HG11	2.30	0.58
1:I:11:TYR:CE2	1:I:333:PRO:HB2	2.34	0.58
1:H:9:SER:OG	1:H:10:SER:N	2.35	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: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
1:G:418:CYS:O	1:G:422:ASN:N	2.30	0.58
1:B:420:ARG:HG3	1:D:313:ASN:HB3	1.86	0.57
1:K:9:SER:OG	1:K:10:SER:N	2.35	0.57
1:H:3:VAL:HG22	1:H:15:VAL:O	2.03	0.57
1:L:46:ALA:HB2	1:L:392:ARG:HH12	1.65	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:A:6:ARG:NH2	1:A:66:ILE:HD13	2.18	0.57
1:B:24:PHE:HB3	1:B:52:ASN:ND2	2.17	0.57
1:B:9:SER:OG	1:B:10:SER:N	2.35	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:A:3:VAL:HG22	1:A: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:2:ILE:HG13	1:I:378:ASP:OD2	2.04	0.57
1:I:44:ILE:CG1	1:I:266:LEU:CD2	2.79	0.57
1:D:400:GLN:HE21	1:H:396:ARG:CD	2.14	0.57
1:G:327:MET:C	1:G:329:GLY:N	2.58	0.57
1:D:418:CYS:O	1:D:422:ASN:N	2.30	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:B:155:HIS:HE1	1:I:452:GLU:HG3	1.63	0.57
1:J:46:ALA:C	1:J:392:ARG:CD	2.72	0.57
1:A:11:TYR:CD1	1:A:369:LYS:HE2	2.40	0.57
1:F:324:VAL:HG11	1:F:340:GLY:HA2	1.87	0.57
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:I:11:TYR:CG	1:I:369:LYS:HE2	2.40	0.56
1:C:72:ARG:NH1	1:C:265:HIS:NE2	2.54	0.56
1:J:24:PHE:HB3	1:J:52:ASN:ND2	2.17	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:H:255:HIS:CE1	1:H:402:ARG:NH2	2.73	0.56
1:E:27:LYS:HE2	1:E:38:ALA:HB1	1.88	0.56
1:D:420:ARG:NH2	1:I:313:ASN:OD1	2.38	0.56
1:H:27:LYS:HE2	1:H:38:ALA:HB1	1.88	0.56
1:A:46:ALA:C	1:A:392:ARG:CD	2.73	0.56
1:L:44:ILE:HB	1:L:266:LEU:HD21	1.86	0.56
1:J:6:ARG:HG2	1:J:11:TYR:C	2.26	0.56
1:K:6:ARG:HG2	1:K:11:TYR:C	2.26	0.56
1:G:6:ARG:HG2	1:G:11:TYR:C	2.26	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:L:6:ARG:HG2	1:L:11:TYR:C	2.26	0.56
1:B:396:ARG:HG2	1:F:400:GLN:CD	2.25	0.56
1:F:6:ARG:NE	1:F:66:ILE:HD13	2.02	0.56
1:E:6:ARG:HG2	1:E:11:TYR:C	2.26	0.56
1:D:27:LYS:HE2	1:D:38:ALA:HB1	1.88	0.56
1:I:27:LYS:HE2	1:I:38:ALA:HB1	1.88	0.56
1:K:27:LYS:HE2	1:K:38:ALA:HB1	1.88	0.56
1:F:68:HIS:CD2	1:F:270:THR:HG23	2.41	0.56
1:I:418:CYS:O	1:I:422:ASN:N	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:11:TYR:CZ	1:L:333:PRO:C	2.77	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:B:27:LYS:HE2	1:B:38:ALA:HB1	1.88	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:B:6:ARG:HG2	1:B:11:TYR:C	2.27	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:C:420:ARG:NH2	1:G:313:ASN:OD1	2.38	0.55
1:L:11:TYR:OH	1:L:333:PRO:O	2.25	0.55
1:H:46:ALA:HA	1:H:392:ARG:HD3	1.86	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:A:328:GLY:O	1:A:366:ARG:NH2	2.40	0.55
1:B:46:ALA:CB	1:B:392:ARG:HD3	2.35	0.55
1:J:27:LYS:HE2	1:J:38:ALA:HB1	1.88	0.55
1:B:221:ASP:OD1	1:I:455:ARG:HD2	2.06	0.55
1:A:27:LYS:HE2	1:A:38:ALA:HB1	1.88	0.55
1:A:6:ARG:HG2	1:A:11:TYR:C	2.26	0.55
1:K:313:ASN:OD1	1:L:420:ARG:CZ	2.55	0.55
1:D:6:ARG:HG2	1:D:11:TYR:C	2.26	0.55
1:I:6:ARG:HG2	1:I:11:TYR:C	2.26	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:F:6:ARG:HG2	1:F:11:TYR:C	2.26	0.55
1:C:155:HIS:CE1	1:H:452:GLU:HG3	2.42	0.54
1:K:11:TYR:HH	1:K:333:PRO:C	1.93	0.54
1:E:46:ALA:C	1:E:392:ARG:HD2	2.28	0.54
1:G:24:PHE:CB	1:G:52:ASN:HD21	2.17	0.54
1:A:24:PHE:CB	1:A:52:ASN:HD21	2.17	0.54
1:L:4:PHE:HB2	1:L:66:ILE:HA	1.90	0.54
1:C:11:TYR:CG	1:C:369:LYS:HE3	2.28	0.54
1:B:11:TYR:HB3	1:B:369:LYS:HE2	1.88	0.54
1:E:11:TYR:CE1	1:E:333:PRO:CA	2.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:11:TYR:CE1	1:L:333:PRO:HB3	2.32	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:B:170:ARG:NE	1:I:199:PRO:HD3	2.23	0.54
1:E:44:ILE:HG21	1:E:266:LEU:CD2	2.38	0.53
1:K:327:MET:CB	1:K:342:LEU:HD11	2.38	0.53
1:K:327:MET:HB3	1:K:342:LEU:HD22	1.83	0.53
1:H:68:HIS:CE1	1:H:273:ASN:HB2	2.43	0.53
1:G:157:VAL:HG21	1:G:306:ILE:HG12	1.91	0.53
1:F:157:VAL:HG21	1:F:306:ILE:HG12	1.91	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:J:46:ALA:C	1:J:392:ARG:HD2	2.28	0.53
1:K:327:MET:HB3	1:K:342:LEU:CG	2.37	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:B:345:GLN:CD	1:B:345:GLN:H	2.11	0.53
1:A:56:VAL:HA	1:A:59:CYS:SG	2.49	0.53
1:I:4:PHE:HB2	1:I:66:ILE:HA	1.90	0.53
1:L:325:LEU:HD23	1:L:331:LEU:HG	1.87	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:E:268:CYS:HB2	1:E:307:LEU:HD21	1.91	0.53
1:C:4:PHE:HB2	1:C:66:ILE:HA	1.90	0.53
1:D:6:ARG:NE	1:D:66:ILE:HD13	2.03	0.53
1:E:329:GLY:N	1:E:342:LEU:HD23	2.24	0.53
1:D:199:PRO:HD3	1:I:170:ARG:NE	2.23	0.53
1:B:56:VAL:HA	1:B:59:CYS:SG	2.49	0.53
1:K:56:VAL:HA	1:K:59:CYS:SG	2.49	0.53
1:G:268:CYS:HB2	1:G:307:LEU:HD21	1.91	0.53
1:G:56:VAL:HA	1:G:59:CYS:SG	2.49	0.53
1:I:56:VAL:HA	1:I:59:CYS:SG	2.49	0.53
1:J:46:ALA:HB2	1:J:392:ARG:CZ	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ALA:HB2	1:I:440:GLN:HB2	1.91	0.53
1:A:268:CYS:HB2	1:A:307:LEU:HD21	1.91	0.53
1:C:268:CYS:HB2	1:C:307:LEU:HD21	1.91	0.53
1:C:56:VAL:HA	1:C: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:D:56:VAL:HA	1:D:59:CYS:SG	2.49	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:F:46:ALA:C	1:F:392:ARG:HD2	2.30	0.53
1:L:268:CYS:HB2	1:L:307:LEU:HD21	1.91	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:H:44:ILE:CG1	1:H:266:LEU:HD21	2.39	0.53
1:F:11:TYR:CE1	1:F:369:LYS:HE3	2.44	0.53
1:J:157:VAL:HG21	1:J:306:ILE:HG12	1.91	0.53
1:H:68:HIS:ND1	1:H:270:THR:HA	2.20	0.52
1:H:24:PHE:CB	1:H:52:ASN:HD21	2.17	0.52
1:F:56:VAL:HA	1:F:59:CYS:SG	2.49	0.52
1:B:268:CYS:HB2	1:B:307:LEU:HD21	1.91	0.52
1:K:11:TYR:HE1	1:K:333:PRO:C	2.10	0.52
1:F:11:TYR:CE1	1:F:333:PRO:CB	2.92	0.52
1:F:4:PHE:HB2	1:F:66:ILE:HA	1.90	0.52
1:K:313:ASN:OD1	1:L:420:ARG:NE	2.42	0.52
1:B:157:VAL:HG21	1:B:306:ILE:HG12	1.91	0.52
1:I:157:VAL:HG21	1:I:306:ILE:HG12	1.91	0.52
1:G:44:ILE:CD1	1:G:266:LEU:HD13	2.35	0.52
1:K:157:VAL:HG21	1:K:306:ILE:HG12	1.91	0.52
1:H:4:PHE:HB2	1:H:66:ILE:HA	1.90	0.52
1:C:70:VAL:HG11	1:C:269:VAL:HG11	1.89	0.52
1:L:9:SER:O	1:L:273:ASN:HA	2.09	0.52
1:I:24:PHE:HB3	1:I:52:ASN:ND2	2.17	0.52
1:F:9:SER:O	1:F:273:ASN:HA	2.10	0.52
1:A:4:PHE:HB2	1:A:66:ILE:HA	1.90	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:E:56:VAL:HA	1:E:59:CYS:SG	2.49	0.52
1:H:11:TYR:HB3	1:H:369:LYS:HE2	1.91	0.52
1:G:397:ALA:HA	1:G:400:GLN:HG2	1.91	0.52
1:A:157:VAL:HG21	1:A:306:ILE:HG12	1.91	0.52
1:F:327:MET:C	1:F:342:LEU:HD21	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:397:ALA:C	1:G:400:GLN:HG2	2.30	0.52
1:J:56:VAL:HA	1:J:59:CYS:SG	2.49	0.52
1:I:268:CYS:HB2	1:I:307:LEU:HD21	1.91	0.52
1:I:68:HIS:CE1	1:I:273:ASN:HB2	2.45	0.52
1:F:268:CYS:HB2	1:F:307:LEU:HD21	1.91	0.52
1:D:44:ILE:HD13	1:D:266:LEU:CD1	2.39	0.52
1:C:157:VAL:HG21	1:C:306:ILE:HG12	1.91	0.52
1:J:268:CYS:HB2	1:J:307:LEU:HD21	1.91	0.52
1:K:11:TYR:HB3	1:K:369:LYS:HE2	1.92	0.51
1:H:157:VAL:HG21	1:H:306:ILE:HG12	1.91	0.51
1:E:421:CYS:HB3	1:E:441:CYS:SG	2.50	0.51
1:K:11:TYR:CZ	1:K:333:PRO:CA	2.92	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:B:420:ARG:NE	1:D:313:ASN:CG	2.40	0.51
1:E:9:SER:O	1:E:273:ASN:CA	2.59	0.51
1:F:15:VAL:HG11	1:F:26:LEU:HD13	1.92	0.51
1:E:454:ASN:HB3	1:F:151:LYS:O	2.10	0.51
1:G:421:CYS:HB3	1:G:441:CYS:SG	2.50	0.51
1:A:421:CYS:HB3	1:A: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:L:6:ARG:CG	1:L:66:ILE:HD11	2.41	0.51
1:I:6:ARG:CG	1:I:66:ILE:HD11	2.41	0.51
1:E:324:VAL:O	1:E:327:MET:HB2	2.10	0.51
1:B:11:TYR:CZ	1:B:333:PRO:O	2.63	0.51
1:G:15:VAL:HG11	1:G:26:LEU:HD13	1.92	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:H:421:CYS:HB3	1:H:441:CYS:SG	2.50	0.51
1:B:421:CYS:HB3	1:B:441:CYS:SG	2.50	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: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: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:K:421:CYS:HB3	1:K:441:CYS:SG	2.50	0.51
1:H:6:ARG:HH12	1:H:68:HIS:CE1	2.28	0.51
1:B:341:LEU:C	1:B:343:PRO:HD3	2.31	0.51
1:L:421:CYS:HB3	1:L:441:CYS:SG	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:421:CYS:HB3	1:F:441:CYS:SG	2.50	0.51
1:C:11:TYR:CE1	1:C:369:LYS:CE	2.71	0.51
1:B:6:ARG:CG	1:B:66:ILE:HD11	2.41	0.51
1:F:6:ARG:CG	1:F:66:ILE:HD11	2.41	0.51
1:C:400:GLN:HA	1:E:396:ARG:NH1	2.26	0.51
1:I:43:VAL:HG13	1:I:68:HIS:O	2.11	0.51
1:L:11:TYR:OH	1:L:333:PRO:CB	2.46	0.51
1:C:396:ARG:NE	1:E:400:GLN:NE2	2.54	0.51
1:C:327:MET:C	1:C:342:LEU:HD22	2.32	0.51
1:F:43:VAL:HG13	1:F:68:HIS:O	2.11	0.51
1:D:421:CYS:HB3	1:D:441:CYS:SG	2.50	0.51
1:F:46:ALA:C	1:F:392:ARG:CD	2.79	0.50
1:C:421:CYS:HB3	1:C:441:CYS:SG	2.50	0.50
1:D:11:TYR:HE1	1:D:333:PRO:HA	1.76	0.50
1:D:6:ARG:CG	1:D:66:ILE:HD11	2.41	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:L:15:VAL:HG11	1:L: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:E:15:VAL:HG11	1:E:26:LEU:HD13	1.92	0.50
1:B:15:VAL:HG11	1:B:26:LEU:HD13	1.92	0.50
1:C:44:ILE:HD12	1:C:266:LEU:HD11	1.94	0.50
1:J:46:ALA:C	1:J:392:ARG:HD3	2.29	0.50
1:F:327:MET:C	1:F:329:GLY:H	2.07	0.50
1:A:43:VAL:HG13	1:A:68:HIS:O	2.11	0.50
1:J:43:VAL:HG13	1:J:68:HIS:O	2.11	0.50
1:B:43:VAL:HG13	1:B:68:HIS:O	2.11	0.50
1:K:11:TYR:HE1	1:K:333:PRO:O	1.86	0.50
1:K:6:ARG:CG	1:K:66:ILE:HD11	2.41	0.50
1:L:44:ILE:HG21	1:L:266:LEU:CD2	2.39	0.50
1:J:324:VAL:HG11	1:J:331:LEU:CD2	2.41	0.50
1:I:15:VAL:HG11	1:I:26:LEU:HD13	1.92	0.50
1:D:15:VAL:HG11	1:D:26:LEU:HD13	1.92	0.50
1:A:15:VAL:HG11	1:A:26:LEU:HD13	1.92	0.50
1:H:43:VAL:HG13	1:H:68:HIS:O	2.11	0.50
1:G:6:ARG:CG	1:G:66:ILE:HD11	2.41	0.50
1:B:455:ARG:CD	1:D:221:ASP:OD1	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:15:VAL:HG11	1:H:26:LEU:HD13	1.92	0.50
1:H:347:GLN:HG3	1:H:349:LYS:H	1.77	0.50
1:G:43:VAL:HG13	1:G:68:HIS:O	2.11	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:K:68:HIS:NE2	1:K:274:ASP:OD2	2.45	0.49
1:J:347:GLN:HG3	1:J:349:LYS:H	1.77	0.49
1:B:44:ILE:HG12	1:B:266:LEU:HD21	1.87	0.49
1:E:324:VAL:CG1	1:E:340:GLY:CA	2.82	0.49
1:E:6:ARG:CG	1:E:66:ILE:HD11	2.41	0.49
1:I:14:PRO:HD3	1:I:370:GLU:OE1	2.09	0.49
1:B:155:HIS:HD1	1:I:452:GLU:CG	2.24	0.49
1:E:46:ALA:C	1:E:392:ARG:CD	2.80	0.49
1:I:44:ILE:CD1	1:I:266:LEU:HD11	2.38	0.49
1:G:420:ARG:HG3	1:H:313:ASN:HB3	1.95	0.49
1:K:347:GLN:HG3	1:K:349:LYS:H	1.77	0.49
1:K:24:PHE:CE2	1:K:25:GLN:CG	2.87	0.49
1:D:420:ARG:CZ	1:I:313:ASN:OD1	2.60	0.49
1:F:347:GLN:HG3	1:F:349:LYS:H	1.77	0.49
1:E:347:GLN:HG3	1:E:349:LYS:H	1.77	0.49
1:D:347:GLN:HG3	1:D:349:LYS:H	1.77	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:I:11:TYR:CG	1:I:369:LYS:CE	2.95	0.49
1:K:68:HIS:NE2	1:K:274:ASP:OD1	2.46	0.49
1:H:72:ARG:HH22	1:H:265:HIS:HD2	1.59	0.49
1:K:327:MET:O	1:K:342:LEU:HD23	2.00	0.49
1:A:11:TYR:CE1	1:A:333:PRO:CB	2.95	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:K:24:PHE:O	1:K:28:GLU:HG3	2.13	0.49
1:G:347:GLN:HG3	1:G:349:LYS:H	1.77	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:A:24:PHE:O	1:A:28:GLU:HG3	2.13	0.49
1:B:24:PHE:O	1:B: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:I:24:PHE:O	1:I:28:GLU:HG3	2.13	0.48
1:A:10:SER:HA	1:A:273:ASN:O	2.12	0.48
1:L:44:ILE:CD1	1:L:266:LEU:HD21	2.43	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:G:70:VAL:HG21	1:G:72:ARG:NH2	2.28	0.48
1:L:70:VAL:HG21	1:L:72:ARG:NH2	2.28	0.48
1:A:324:VAL:HG11	1:A:331:LEU:CD2	2.43	0.48
1:J:46:ALA:CB	1:J:392:ARG:CD	2.89	0.48
1:I:11:TYR:CD1	1:I:369:LYS:HE3	2.49	0.48
1:B:46:ALA:HB1	1:B:392:ARG:HD3	1.95	0.48
1:I:70:VAL:HG13	1:I:269:VAL:HG11	1.94	0.48
1:B:452:GLU:CG	1:D:309:GLU:OE2	2.60	0.48
1:H:70:VAL:HG21	1:H:72:ARG:NH2	2.28	0.48
1:E:327:MET:CG	1:E:342:LEU:HD21	2.36	0.48
1:E:24:PHE:O	1:E:28:GLU:HG3	2.13	0.48
1:I:347:GLN:HG3	1:I:349:LYS:H	1.77	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:H:9:SER:O	1:H:273:ASN:HB3	2.14	0.48
1:E:68:HIS:NE2	1:E:270:THR:HG23	2.29	0.48
1:J:333:PRO:HB3	1:J:369:LYS:HE3	1.96	0.48
1:H:149:TYR:CD2	1:H:305[A]:ARG:HD3	2.49	0.48
1:C:70:VAL:HG21	1:C:72:ARG:NH2	2.28	0.48
1:F:24:PHE:O	1:F:28:GLU:HG3	2.13	0.48
1:H:24:PHE:CE2	1:H:25:GLN:CG	2.87	0.48
1:E:70:VAL:HG21	1:E:72:ARG:NH2	2.28	0.48
1:J:70:VAL:CG1	1:J:269:VAL:HG11	2.43	0.48
1:D:420:ARG:HE	1:I:313:ASN:CG	2.15	0.48
1:K:170:ARG:HE	1:L:199:PRO:HG3	1.78	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:F:70:VAL:HG21	1:F:72:ARG:NH2	2.28	0.48
1:E:24:PHE:CE2	1:E:25:GLN:CG	2.87	0.48
1:B:334:ARG:HA	1:B:335:PRO:HD3	1.77	0.48
1:I:149:TYR:CD2	1:I:305[A]:ARG:HD3	2.49	0.48
1:F:149:TYR:CD2	1:F:305[A]:ARG:HD3	2.49	0.48
1:E:149:TYR:CD2	1:E:305[A]:ARG:HD3	2.49	0.48
1:F:72:ARG:NH1	1:F:265:HIS:CD2	2.82	0.48
1:B:70:VAL:HG21	1:B:72:ARG:NH2	2.28	0.48
1:A:149:TYR:CD2	1:A:305[A]:ARG:HD3	2.49	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:L:327:MET:CG	1:L:342:LEU:HD21	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:9:SER:O	1:L:273:ASN:CA	2.62	0.48
1:H:24:PHE:O	1:H:28:GLU:HG3	2.13	0.48
1:K:70:VAL:HG21	1:K:72:ARG:NH2	2.28	0.48
1:F:324:VAL:CG1	1:F:340:GLY:HA3	2.40	0.48
1:J:149:TYR:CD2	1:J:305[A]:ARG:HD3	2.49	0.48
1:D:24:PHE:O	1:D:28:GLU:HG3	2.13	0.47
1:J:70:VAL:HG21	1:J:72:ARG:NH2	2.28	0.47
1:B:151:LYS:O	1:I:454:ASN:HB3	2.14	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:D:11:TYR:HE1	1:D:333:PRO:CA	2.15	0.47
1:K:333:PRO:HB3	1:K:369:LYS:HE3	1.96	0.47
1:J:302:HIS:HB3	1:J:305[B]:ARG:HH11	1.80	0.47
1:H:228:LEU:HG	1:H:303:HIS:CE1	2.50	0.47
1:J:46:ALA:CB	1:J:392:ARG:CZ	2.91	0.47
1:K:327:MET:SD	1:K:342:LEU:CD1	3.00	0.47
1:B:333:PRO:HB3	1:B:369:LYS:HE3	1.96	0.47
1:A:11:TYR:CD1	1:A:369:LYS:CE	2.98	0.47
1:G:42:ARG:HD2	1:G:49:GLU:OE1	2.15	0.47
1:K:40:GLN:O	1:K:72:ARG:N	2.34	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:F:228:LEU:HG	1:F:303:HIS:CE1	2.50	0.47
1:B:302:HIS:HB3	1:B:305[B]:ARG:HH11	1.80	0.47
1:F:46:ALA:CB	1:F:392:ARG:CZ	2.78	0.47
1:I:333:PRO:HB3	1:I:369:LYS:HE3	1.96	0.47
1:E:333:PRO:HB3	1:E:369:LYS:HE3	1.96	0.47
1:L:44:ILE:CG1	1:L:266:LEU:CD2	2.91	0.47
1:I:270:THR:HG21	1:I:392:ARG:HH12	1.79	0.47
1:L:228:LEU:HG	1:L:303:HIS:CE1	2.50	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:C:333:PRO:HB3	1:C:369:LYS:HE3	1.96	0.47
1:C:24:PHE:O	1:C:28:GLU:HG3	2.13	0.47
1:K:68:HIS:CE1	1:K:274:ASP:CG	2.88	0.47
1:B:452:GLU:HG3	1:D:155:HIS:CE1	2.49	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:D:228:LEU:HG	1:D:303:HIS:CE1	2.50	0.47
1:B:228:LEU:HG	1:B:303:HIS:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:ARG:HD2	1:D:49:GLU:OE1	2.15	0.47
1:L:325:LEU:HD11	1:L:331:LEU:HD11	1.96	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:A:228:LEU:HG	1:A:303:HIS:CE1	2.50	0.47
1:G:228:LEU:HG	1:G:303:HIS:CE1	2.50	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:A:333:PRO:HB3	1:A:369:LYS:HE3	1.96	0.47
1:E:40:GLN:O	1:E:72:ARG:N	2.34	0.47
1:D:302:HIS:HB3	1:D:305[B]:ARG:HH11	1.80	0.47
1:C:42:ARG:HD2	1:C:49:GLU:OE1	2.15	0.47
1:B:155:HIS:ND1	1:I:452:GLU:HG3	2.29	0.47
1:H:72:ARG:NH2	1:H:265:HIS:HD2	2.13	0.47
1:D:10:SER:HA	1:D:273:ASN:O	2.15	0.47
1:K:228:LEU:HG	1:K:303:HIS:CE1	2.50	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: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:H:42:ARG:HD2	1:H:49:GLU:OE1	2.15	0.47
1:E:302:HIS:HB3	1:E:305[B]:ARG:HH11	1.80	0.47
1:C:228:LEU:HG	1:C:303:HIS:CE1	2.50	0.47
1:K:149:TYR:CD2	1:K:305[A]:ARG:HD3	2.49	0.47
1:F:11:TYR:CZ	1:F:333:PRO:HB3	2.46	0.46
1:C:400:GLN:HA	1:E:396:ARG:HH12	1.78	0.46
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: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:F:42:ARG:HD2	1:F:49:GLU:OE1	2.15	0.46
1:L:302:HIS:HB3	1:L:305[B]:ARG:HH11	1.80	0.46
1:L:149:TYR:CD2	1:L:305[A]:ARG:HD3	2.49	0.46
1:A:40:GLN:O	1:A:72:ARG:N	2.34	0.46
1:K:327:MET:C	1:K:329:GLY:H	2.05	0.46
1:B:40:GLN:O	1:B:72:ARG:N	2.34	0.46
1:G:333:PRO:HB3	1:G:369:LYS:HE3	1.96	0.46
1:L:9:SER:O	1:L:273:ASN:CB	2.64	0.46
1:G:24:PHE:CE2	1:G:25:GLN:CG	2.87	0.46
1:A:327:MET:C	1:A:329:GLY:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:HIS:HB3	1:A:305[B]:ARG:HH11	1.80	0.46
1:K:302:HIS:HB3	1:K:305[B]:ARG:HH11	1.80	0.46
1:D:24:PHE:CE2	1:D:25:GLN:CG	2.86	0.46
1:C:302:HIS:HB3	1:C:305[B]:ARG:HH11	1.80	0.46
1:J:228:LEU:HG	1:J:303:HIS:CE1	2.50	0.46
1:G:454:ASN:HB3	1:H:151:LYS:O	2.16	0.46
1:K:42:ARG:HD2	1:K:49:GLU:OE1	2.15	0.46
1:E:27:LYS:O	1:E:31:ALA:N	2.49	0.46
1:J:329:GLY:HA3	1:J:343:PRO:HD2	1.98	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: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:I:42:ARG:HD2	1:I:49:GLU:OE1	2.15	0.46
1:C:436:CYS:HA	1:C:437:PRO:HD3	1.71	0.46
1:B:396:ARG:HD3	1:F:400:GLN:CG	2.46	0.46
1:J:42:ARG:HD2	1:J:49:GLU:OE1	2.15	0.46
1:I:271:ARG:NH1	1:I:392:ARG:NH1	2.63	0.46
1:H:334:ARG:HA	1:H:335:PRO:HD3	1.77	0.46
1:F:5:VAL:O	1:F:12:GLY:HA2	2.16	0.46
1:D:333:PRO:HB3	1:D:369:LYS:HE3	1.96	0.46
1:L:324:VAL:O	1:L:327:MET:HB2	2.16	0.46
1:B:199:PRO:CD	1:D:170:ARG:HG3	2.46	0.46
1:J:5:VAL:O	1:J:12:GLY:HA2	2.16	0.46
1:K:436:CYS:HA	1:K:437:PRO:HD3	1.71	0.46
1:C:11:TYR:CE1	1:C:333:PRO:HA	2.22	0.45
1:A:440:GLN:HB2	1:E:320:ALA:HB2	1.98	0.45
1:E:420:ARG:CZ	1:F:313:ASN:OD1	2.64	0.45
1:E:420:ARG:NH2	1:F:313:ASN:OD1	2.49	0.45
1:A:27:LYS:O	1:A:31:ALA:N	2.49	0.45
1:C:27:LYS:O	1:C:31:ALA:N	2.49	0.45
1:H:5:VAL:O	1:H:12:GLY:HA2	2.16	0.45
1:J:27:LYS:O	1:J:31:ALA:N	2.49	0.45
1:A:46:ALA:O	1:A:392:ARG:HD3	2.16	0.45
1:I:302:HIS:HB3	1:I:305[B]:ARG:HH11	1.80	0.45
1:B:11:TYR:CG	1:B:369:LYS:HE3	2.51	0.45
1:L:324:VAL:CG1	1:L:340:GLY:HA2	2.29	0.45
1:J:9:SER:O	1:J:273:ASN:HB3	2.17	0.45
1:C:396:ARG:HE	1:E:400:GLN:NE2	2.04	0.45
1:K:3:VAL:HG23	1:K:15:VAL:HB	1.99	0.45
1:H:46:ALA:CA	1:H:392:ARG:CD	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:ASN:HB3	1:H:420:ARG:HG3	1.99	0.45
1:B:320:ALA:CB	1:I:440:GLN:HB2	2.46	0.45
1:B:3:VAL:HG23	1:B:15:VAL:HB	1.99	0.45
1:L:5:VAL:O	1:L:12:GLY:HA2	2.16	0.45
1:E:5:VAL:O	1:E:12:GLY:HA2	2.16	0.45
1:B:5:VAL:O	1:B:12:GLY:HA2	2.16	0.45
1:F:436:CYS:HA	1:F:437:PRO:HD3	1.71	0.45
1:J:44:ILE:HG21	1:J:266:LEU:HD21	1.99	0.45
1:I:40:GLN:O	1:I:72:ARG:N	2.34	0.45
1:F:324:VAL:CG1	1:F:340:GLY:CA	2.93	0.45
1:A:155:HIS:HD1	1:F:452:GLU:CD	2.12	0.45
1:A:155:HIS:CE1	1:F:452:GLU:HG2	2.51	0.45
1:A:3:VAL:HG23	1:A:15:VAL:HB	1.99	0.45
1:H:68:HIS:CE1	1:H:273:ASN:CB	2.98	0.45
1:G:3:VAL:HG23	1:G:15:VAL:HB	1.99	0.45
1:B:11:TYR:CB	1:B:369:LYS:HE2	2.47	0.45
1:G:11:TYR:HE1	1:G:333:PRO:CA	2.26	0.45
1:J:325:LEU:HD23	1:J:331:LEU:CD1	2.40	0.45
1:I:3:VAL:HG23	1:I:15:VAL:HB	1.99	0.45
1:G:5:VAL:O	1:G:12:GLY:HA2	2.16	0.45
1:D:436:CYS:HA	1:D:437:PRO:HD3	1.71	0.45
1:B:199:PRO:CG	1:D:170:ARG:HG3	2.46	0.45
1:J:324:VAL:HG11	1:J:340:GLY:HA3	1.99	0.45
1:D:3:VAL:HG23	1:D:15:VAL:HB	1.99	0.45
1:A:5:VAL:O	1:A:12:GLY:HA2	2.16	0.45
1:K:297:LEU:HD23	1:K:297:LEU:HA	1.78	0.45
1:F:40:GLN:O	1:F:72:ARG:N	2.34	0.45
1:H:27:LYS:O	1:H:31:ALA:N	2.49	0.45
1:F:300:GLU:HB3	1:F:302:HIS:NE2	2.32	0.45
1:C:44:ILE:HG23	1:C:48:LYS:C	2.38	0.45
1:E:44:ILE:HG23	1:E:48:LYS:C	2.37	0.45
1:G:44:ILE:HG23	1:G:48:LYS:C	2.37	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:B:44:ILE:HG23	1:B:48:LYS:C	2.38	0.44
1:A:44:ILE:HG23	1:A:48:LYS:C	2.38	0.44
1:E:6:ARG:NH1	1:E:274:ASP:OD1	2.51	0.44
1:D:44:ILE:HG23	1:D:48:LYS:C	2.38	0.44
1:J:3:VAL:HG23	1:J:15:VAL:HB	1.99	0.44
1:E:300:GLU:HB3	1:E:302:HIS:NE2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:44:ILE:HG23	1:F:48:LYS:C	2.38	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:E:44:ILE:HD13	1:E:266:LEU:CD1	2.46	0.44
1:B:313:ASN:HB3	1:I:420:ARG:CG	2.33	0.44
1:L:3:VAL:HG23	1:L:15:VAL:HB	1.99	0.44
1:H:300:GLU:HB3	1:H:302:HIS:NE2	2.32	0.44
1:D:5:VAL:O	1:D:12:GLY:HA2	2.16	0.44
1:B:46:ALA:O	1:B:392:ARG:CD	2.32	0.44
1:J:199:PRO:HG2	1:L:170:ARG:HE	1.78	0.44
1:L:438:GLN:HB3	1:L:440:GLN:CD	2.38	0.44
1:B:438:GLN:HB3	1:B:440:GLN:CD	2.38	0.44
1:H:37:PRO:O	1:H:41:LEU:HG	2.18	0.44
1:A:300:GLU:HB3	1:A:302:HIS:NE2	2.32	0.44
1:K:5:VAL:O	1:K:12:GLY:HA2	2.16	0.44
1:J:44:ILE:HG23	1:J:48:LYS:C	2.38	0.44
1:G:11:TYR:HD1	1:G:369:LYS:CE	2.29	0.44
1:F:24:PHE:CE2	1:F:25:GLN:CG	2.87	0.44
1:A:24:PHE:CE2	1:A:25:GLN:CG	2.87	0.44
1:A:438:GLN:HB3	1:A:440:GLN:CD	2.38	0.44
1:D:37:PRO:O	1:D:41:LEU:HG	2.18	0.44
1:L:300:GLU:HB3	1:L:302:HIS:NE2	2.32	0.44
1:K:44:ILE:HG23	1:K:48:LYS:C	2.38	0.44
1:H:44:ILE:CB	1:H:266:LEU:HD21	2.47	0.44
1:H:44:ILE:HG23	1:H:48:LYS:C	2.38	0.44
1:F:11:TYR:HE1	1:F:333:PRO:HA	1.80	0.44
1:I:44:ILE:HG23	1:I:48:LYS:C	2.37	0.44
1:J:24:PHE:CE2	1:J:25:GLN:CG	2.87	0.44
1:E:37:PRO:O	1:E:41:LEU:HG	2.18	0.44
1:J:37:PRO:O	1:J:41:LEU:HG	2.18	0.44
1:D:27:LYS:O	1:D:31:ALA:N	2.49	0.44
1:L:37:PRO:O	1:L:41:LEU:HG	2.18	0.44
1:K:37:PRO:O	1:K:41:LEU:HG	2.18	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:D:438:GLN:HB3	1:D:440:GLN:CD	2.38	0.44
1:K:438:GLN:HB3	1:K:440:GLN:CD	2.38	0.44
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:J:329:GLY:O	1:J:366:ARG:NH2	2.50	0.44
1:H:40:GLN:O	1:H:72:ARG:N	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:VAL:HG23	1:E:15:VAL:HB	1.99	0.44
1:D:300:GLU:HB3	1:D:302:HIS:NE2	2.32	0.44
1:J:452:GLU:OE2	1:L:309:GLU:CG	2.66	0.44
1:C:438:GLN:HB3	1:C:440:GLN:CD	2.38	0.44
1:D:46:ALA:HA	1:D:392:ARG:HD2	1.99	0.44
1:C:37:PRO:O	1:C:41:LEU:HG	2.18	0.44
1:D:14:PRO:HD2	1:D:370:GLU:CD	2.38	0.44
1:F:3:VAL:HG23	1:F:15:VAL:HB	1.99	0.44
1:E:253:CYS:HB3	1:E:296:SER:HB3	2.00	0.44
1:G:205:ARG:HH21	1:G:207:GLU:CG	2.31	0.44
1:C:297:LEU:HD23	1:C:297:LEU:HA	1.78	0.44
1:F:46:ALA:H	1:F:392:ARG:NH1	2.12	0.43
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:K:11:TYR:CZ	1:K:333:PRO:C	2.85	0.43
1:F:11:TYR:OH	1:F:333:PRO:O	2.29	0.43
1:I:300:GLU:HB3	1:I:302:HIS:NE2	2.33	0.43
1:H:205:ARG:HH21	1:H:207:GLU:CG	2.31	0.43
1:E:44:ILE:HD13	1:E:266:LEU:CG	2.35	0.43
1:J:205:ARG:HH21	1:J:207:GLU:CG	2.31	0.43
1:L:44:ILE:HG23	1:L:48:LYS:C	2.38	0.43
1:E:70:VAL:CG1	1:E:269:VAL:HG11	2.48	0.43
1:I:438:GLN:HB3	1:I:440:GLN:CD	2.38	0.43
1:F:37:PRO:O	1:F:41:LEU:HG	2.17	0.43
1:K:205:ARG:HH21	1:K:207:GLU:CG	2.31	0.43
1:B:205:ARG:HH21	1:B:207:GLU:CG	2.31	0.43
1:F:11:TYR:CE1	1:F:369:LYS:CE	3.00	0.43
1:E:4:PHE:HB3	1:E:66:ILE:HD12	2.00	0.43
1:B:37:PRO:O	1:B:41:LEU:HG	2.18	0.43
1:J:300:GLU:HB3	1:J:302:HIS:NE2	2.32	0.43
1:C:205:ARG:HH21	1:C:207:GLU:CG	2.31	0.43
1:H:253:CYS:HB3	1:H:296:SER:HB3	2.00	0.43
1:G:438:GLN:HB3	1:G:440:GLN:CD	2.38	0.43
1:E:438:GLN:HB3	1:E:440:GLN:CD	2.38	0.43
1:D:455:ARG:CD	1:I:221:ASP:OD1	2.64	0.43
1:C:334:ARG:HA	1:C:335:PRO:HD3	1.77	0.43
1:C:253:CYS:HB3	1:C:296:SER:HB3	2.00	0.43
1:J:436:CYS:HA	1:J:437:PRO:HD3	1.71	0.43
1:D:334:ARG:HA	1:D:335:PRO:HD3	1.77	0.43
1:K:329:GLY:N	1:K:342:LEU:HD23	2.33	0.43
1:J:438:GLN:HB3	1:J:440:GLN:CD	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:VAL:HG22	1:C:69:ILE:HG12	2.01	0.43
1:B:43:VAL:HG22	1:B:69:ILE:HG12	2.01	0.43
1:H:3:VAL:HG23	1:H:15:VAL:HB	1.99	0.43
1:L:4:PHE:HB3	1:L:66:ILE:HD12	2.00	0.43
1:F:11:TYR:CE1	1:F:333:PRO:HB3	2.53	0.43
1:I:2:ILE:CD1	1:I:378:ASP:OD2	2.67	0.43
1:G:300:GLU:HB3	1:G:302:HIS:NE2	2.32	0.43
1:A:297:LEU:HD23	1:A:297:LEU:HA	1.78	0.43
1:F:220:LYS:HD3	1:F:220:LYS:HA	1.90	0.43
1:G:4:PHE:HB3	1:G:66:ILE:HD12	2.01	0.43
1:D:44:ILE:HD13	1:D:266:LEU:HD13	2.00	0.43
1:D:44:ILE:HD13	1:D:266:LEU:CG	2.41	0.43
1:H:438:GLN:HB3	1:H:440:GLN:CD	2.38	0.43
1:A:199:PRO:HG3	1:E:170:ARG:HE	1.83	0.43
1:G:27:LYS:O	1:G:31:ALA:N	2.49	0.43
1:J:68:HIS:NE2	1:J:270:THR:HG23	2.33	0.43
1:G:436:CYS:HA	1:G:437:PRO:HD3	1.71	0.43
1:A:362:PHE:CE2	1:A:364:PHE:HB3	2.54	0.43
1:L:205:ARG:HH21	1:L:207:GLU:CG	2.31	0.43
1:K:43:VAL:HG22	1:K:69:ILE:HG12	2.01	0.43
1:F:438:GLN:HB3	1:F:440:GLN:CD	2.38	0.43
1:J:362:PHE:CE2	1:J:364:PHE:HB3	2.54	0.43
1:A:37:PRO:O	1:A:41:LEU:HG	2.18	0.43
1:I:37:PRO:O	1:I:41:LEU:HG	2.18	0.43
1:G:37:PRO:O	1:G:41:LEU:HG	2.18	0.43
1:G:397:ALA:CA	1:G:400:GLN:HG2	2.49	0.43
1:G:43:VAL:HG22	1:G:69:ILE:HG12	2.01	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:F:205:ARG:HH21	1:F:207:GLU:CG	2.31	0.43
1:E:230:THR:HG22	1:E:231:ASN:O	2.19	0.43
1:I:362:PHE:CE2	1:I:364:PHE:HB3	2.54	0.43
1:B:220:LYS:HA	1:B:220:LYS:HD3	1.90	0.43
1:I:188:ILE:CG2	1:I:191:ARG:CB	2.86	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:J:253:CYS:HB3	1:J:296:SER:HB3	2.00	0.43
1:G:362:PHE:CE2	1:G:364:PHE:HB3	2.54	0.43
1:E:205:ARG:HH21	1:E:207:GLU:CG	2.31	0.43
1:D:230:THR:HG22	1:D:231:ASN:O	2.19	0.43
1:H:46:ALA:CA	1:H:392:ARG:HD3	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:GLN:OE1	1:F:396:ARG:CG	2.64	0.43
1:A:4:PHE:HB3	1:A:66:ILE:HD12	2.00	0.43
1:L:438:GLN:HA	1:L:439:PRO:HD3	1.87	0.43
1:C:155:HIS:HE1	1:H:452:GLU:HG3	1.81	0.43
1:I:43:VAL:HG22	1:I:69:ILE:HG12	2.01	0.43
1:K:362:PHE:CE2	1:K:364:PHE:HB3	2.54	0.43
1:F:362:PHE:CE2	1:F:364:PHE:HB3	2.54	0.43
1:A:253:CYS:HB3	1:A:296:SER:HB3	2.00	0.43
1:K:230:THR:HG22	1:K:231:ASN:O	2.19	0.43
1:A:205:ARG:HH21	1:A:207:GLU:CG	2.31	0.43
1:B:253:CYS:HB3	1:B:296:SER:HB3	2.00	0.43
1:H:11:TYR:HE1	1:H:333:PRO:HA	1.00	0.42
1:B:11:TYR:CE1	1:B:369:LYS:HE3	2.54	0.42
1:A:230:THR:HG22	1:A:231:ASN:O	2.19	0.42
1:L:362:PHE:CE2	1:L:364:PHE:HB3	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:L:24:PHE:CE2	1:L:25:GLN:CG	2.87	0.42
1:B:313:ASN:CB	1:I:420:ARG:HG3	2.34	0.42
1:L:27:LYS:O	1:L:31:ALA:N	2.49	0.42
1:K:13:PHE:CE2	1:K:33:ARG:CZ	3.03	0.42
1:A:166:CYS:HA	1:A:174:LEU:HD13	2.01	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:D:253:CYS:HB3	1:D:296:SER:HB3	2.00	0.42
1:I:27:LYS:O	1:I:31:ALA:N	2.49	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:B:230:THR:HG22	1:B:231:ASN:O	2.19	0.42
1:K:253:CYS:HB3	1:K:296:SER:HB3	2.00	0.42
1:B:362:PHE:CE2	1:B:364:PHE:HB3	2.54	0.42
1:D:438:GLN:HB3	1:D:440:GLN:NE2	2.35	0.42
1:F:438:GLN:HB3	1:F:440:GLN:NE2	2.35	0.42
1:K:438:GLN:HB3	1:K: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: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:J:230:THR:HG22	1:J:231:ASN:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:253:CYS:HB3	1:I:296:SER:HB3	2.00	0.42
1:C:166:CYS:HA	1:C:174:LEU:HD13	2.01	0.42
1:I:4:PHE:HB3	1:I:66:ILE:HD12	2.01	0.42
1:G:11:TYR:CE1	1:G:369:LYS:HE3	2.55	0.42
1:K:72:ARG:HH12	1:K:265:HIS:CD2	2.37	0.42
1:C:438:GLN:HB3	1:C:440:GLN:NE2	2.35	0.42
1:H:438:GLN:HB3	1:H:440:GLN:NE2	2.35	0.42
1:B:345:GLN:CD	1:B:345:GLN:N	2.73	0.42
1:L:43:VAL:HG22	1:L:69:ILE:HG12	2.01	0.42
1:J:13:PHE:CE2	1:J:33:ARG:CZ	3.03	0.42
1:E:362:PHE:CE2	1:E:364:PHE:HB3	2.54	0.42
1:L:166:CYS:HA	1:L:174:LEU:HD13	2.02	0.42
1:G:253:CYS:HB3	1:G:296:SER:HB3	2.00	0.42
1:C:362:PHE:CE2	1:C:364:PHE:HB3	2.54	0.42
1:K:166:CYS:HA	1:K:174:LEU:HD13	2.01	0.42
1:F:44:ILE:CD1	1:F:266:LEU:CD1	2.97	0.42
1:H:43:VAL:HG22	1:H:69:ILE:HG12	2.01	0.42
1:F:4:PHE:HB3	1:F:66:ILE:HD12	2.01	0.42
1:B:309:GLU:OE2	1:I:452:GLU:CB	2.67	0.42
1:J:438:GLN:HB3	1:J:440:GLN:NE2	2.35	0.42
1:F:43:VAL:HG22	1:F:69:ILE:HG12	2.01	0.42
1:G:68:HIS:CE1	1:G:274:ASP:OD1	2.73	0.42
1:H:13:PHE:CE2	1:H:33:ARG:CZ	3.03	0.42
1:G:13:PHE:CE2	1:G:33:ARG:CZ	3.03	0.42
1:L:59:CYS:SG	1:L:61:LEU:HB2	2.60	0.42
1:B:59:CYS:SG	1:B:61:LEU:HB2	2.60	0.42
1:I:205:ARG:HH21	1:I:207:GLU:CG	2.31	0.42
1:G:334:ARG:HA	1:G:335:PRO:HD3	1.77	0.42
1:C:220:LYS:HA	1:C:220:LYS:HD3	1.90	0.42
1:H:272:LEU:HA	1:H:272:LEU:HD23	1.91	0.42
1:L:253:CYS:HB3	1:L:296:SER:HB3	2.00	0.42
1:K:4:PHE:HB3	1:K:66:ILE:HD12	2.00	0.42
1:I:188:ILE:O	1:I:188:ILE:CG2	2.68	0.42
1:J:452:GLU:HG3	1:L:155:HIS:CE1	2.54	0.42
1:F:438:GLN:HA	1:F:439:PRO:HD3	1.87	0.42
1:B:438:GLN:HA	1:B:439:PRO:HD3	1.87	0.42
1:A:43:VAL:HG22	1:A:69:ILE:HG12	2.01	0.42
1:K:10:SER:HA	1:K:273:ASN:O	2.19	0.42
1:E:13:PHE:CE2	1:E:33:ARG:CZ	3.03	0.42
1:C:4:PHE:HB3	1:C:66:ILE:HD12	2.00	0.42
1:H:59:CYS:SG	1:H:61:LEU:HB2	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:4:PHE:HB3	1:H:66:ILE:HD12	2.00	0.42
1:H:230:THR:HG22	1:H:231:ASN:O	2.19	0.42
1:K:334:ARG:HA	1:K:335:PRO:HD3	1.77	0.42
1:J:166:CYS:HA	1:J:174:LEU:HD13	2.01	0.42
1:H:297:LEU:HD23	1:H:297:LEU:HA	1.78	0.42
1:B:297:LEU:HD23	1:B:297:LEU:HA	1.78	0.42
1:D:4:PHE:HB3	1:D:66:ILE:HD12	2.00	0.42
1:L:438:GLN:HB3	1:L:440:GLN:NE2	2.35	0.42
1:C:6:ARG:NH1	1:C:68:HIS:ND1	2.55	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:G:166:CYS:HA	1:G:174:LEU:HD13	2.02	0.42
1:D:205:ARG:HH21	1:D:207:GLU:CG	2.31	0.42
1:E:425:ILE:HD12	1:E:437:PRO:HD3	2.02	0.42
1:E:329:GLY:H	1:E:342:LEU:HD23	1.83	0.42
1:K:46:ALA:O	1:K:392:ARG:HA	2.19	0.42
1:A:438:GLN:HB3	1:A:440:GLN:NE2	2.35	0.42
1:C:13:PHE:CE2	1:C:33:ARG:CZ	3.03	0.42
1:B:13:PHE:CE2	1:B:33:ARG:CZ	3.03	0.42
1:H:166:CYS:HA	1:H:174:LEU:HD13	2.01	0.42
1:J:329:GLY:C	1:J:366:ARG:NH2	2.73	0.42
1:L:68:HIS:CD2	1:L:270:THR:HG23	2.55	0.42
1:L:13:PHE:CE2	1:L:33:ARG:CZ	3.03	0.42
1:D:13:PHE:CE2	1:D:33:ARG:CZ	3.03	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:H:425:ILE:HD12	1:H:437:PRO:HD3	2.02	0.42
1:E:174:LEU:HD22	1:E:206:ALA:HA	2.02	0.42
1:I:59:CYS:SG	1:I:61:LEU:HB2	2.60	0.41
1:B:425:ILE:HD12	1:B:437:PRO:HD3	2.02	0.41
1:B:309:GLU:CD	1:I:452:GLU:HG2	2.37	0.41
1:I:438:GLN:HB3	1:I:440:GLN:NE2	2.35	0.41
1:B:27:LYS:O	1:B:31:ALA:N	2.49	0.41
1:G:59:CYS:SG	1:G:61:LEU:HB2	2.60	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:B:307:LEU:HB3	1:B:311:GLN:HB2	2.03	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:E:46:ALA:CB	1:E:392:ARG:HD3	2.49	0.41
1:B:199:PRO:CG	1:D:170:ARG:HE	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:438:GLN:HB3	1:G:440:GLN:NE2	2.35	0.41
1:A:438:GLN:HA	1:A:439:PRO:HD3	1.87	0.41
1:K:438:GLN:HA	1:K:439:PRO:HD3	1.87	0.41
1:J:329:GLY:HA2	1:J:366:ARG:NH2	2.26	0.41
1:J:174:LEU:HD22	1:J:206:ALA:HA	2.02	0.41
1:F:162:LEU:HD12	1:F:163:ARG:H	1.86	0.41
1:H:220:LYS:HA	1:H:220:LYS:HD3	1.90	0.41
1:B:166:CYS:HA	1:B:174:LEU:HD13	2.01	0.41
1:J:4:PHE:HB3	1:J:66:ILE:HD12	2.01	0.41
1:B:452:GLU:OE2	1:D:155:HIS:ND1	2.32	0.41
1:F:13:PHE:CE2	1:F:33:ARG:CZ	3.03	0.41
1:A:13:PHE:CE2	1:A:33:ARG:CZ	3.03	0.41
1:K:59:CYS:SG	1:K:61:LEU:HB2	2.60	0.41
1:C:59:CYS:SG	1:C:61:LEU:HB2	2.60	0.41
1:H:307:LEU:HB3	1:H:311:GLN:HB2	2.03	0.41
1:K:425:ILE:HD12	1:K:437:PRO:HD3	2.02	0.41
1:G:162:LEU:HD12	1:G:163:ARG:H	1.86	0.41
1:K:162:LEU:HD12	1:K:163:ARG:H	1.86	0.41
1:A:275:ARG:HE	1:A:275:ARG:HB3	1.71	0.41
1:I:24:PHE:CE2	1:I:25:GLN:CG	2.87	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:G:174:LEU:HD22	1:G:206:ALA:HA	2.02	0.41
1:F:297:LEU:HA	1:F:297:LEU:HD23	1.78	0.41
1:B:44:ILE:CD1	1:B:266:LEU:CD1	2.95	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: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:B:309:GLU:OE2	1:I:452:GLU:CD	2.58	0.41
1:F:72:ARG:NH1	1:F:265:HIS:NE2	2.69	0.41
1:A:174:LEU:HD22	1:A:206:ALA:HA	2.02	0.41
1:F:174:LEU:HD22	1:F:206:ALA:HA	2.02	0.41
1:C:174:LEU:HD22	1:C:206:ALA:HA	2.02	0.41
1:C:45:PHE:HB2	1:C:67:VAL:HG12	2.03	0.41
1:G:45:PHE:HB2	1:G:67:VAL:HG12	2.03	0.41
1:C:162:LEU:HD12	1:C:163:ARG:H	1.86	0.41
1:I:174:LEU:HD22	1:I:206:ALA:HA	2.02	0.41
1:L:11:TYR:HH	1:L:333:PRO:C	2.21	0.41
1:F:327:MET:C	1:F:329:GLY:N	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:166:CYS:HA	1:I:174:LEU:HD13	2.02	0.41
1:H:45:PHE:HB2	1:H:67:VAL:HG12	2.03	0.41
1:F:46:ALA:C	1:F:392:ARG:HD3	2.40	0.41
1:H:11:TYR:OH	1:H:333:PRO:O	2.21	0.41
1:K:329:GLY:CA	1:K:341:LEU:O	2.61	0.41
1:J:199:PRO:HG3	1:L:170:ARG:NE	2.15	0.41
1:E:438:GLN:HB3	1:E:440:GLN:NE2	2.35	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:H:255:HIS:HB3	1:H:402:ARG:HG2	2.03	0.41
1:F:307:LEU:HB3	1:F:311:GLN:HB2	2.03	0.41
1:D:425:ILE:HD12	1:D:437:PRO:HD3	2.02	0.41
1:I:45:PHE:HB2	1:I:67:VAL:HG12	2.03	0.41
1:B:162:LEU:HD12	1:B:163:ARG:H	1.86	0.41
1:L:425:ILE:HD12	1:L:437:PRO:HD3	2.03	0.41
1:F:334:ARG:HA	1:F:335:PRO:HD3	1.77	0.41
1:A:255:HIS:HB3	1:A:402:ARG:HG2	2.03	0.41
1:K:45:PHE:HB2	1:K:67:VAL:HG12	2.03	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: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:F:42:ARG:CG	1:F:72:ARG:HG3	2.51	0.41
1:E:42:ARG:CG	1:E:72:ARG:HG3	2.51	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:A:45:PHE:HB2	1:A:67:VAL:HG12	2.03	0.41
1:I:162:LEU:HD12	1:I:163:ARG:H	1.86	0.41
1:D:45:PHE:HB2	1:D:67:VAL:HG12	2.03	0.41
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:C:307:LEU:HB3	1:C:311:GLN:HB2	2.02	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:L:174:LEU:HD22	1:L:206:ALA:HA	2.02	0.40
1:F:255:HIS:HB3	1:F:402:ARG:HG2	2.03	0.40
1:B:255:HIS:HB3	1:B:402:ARG:HG2	2.03	0.40
1:A:162:LEU:HD12	1:A:163:ARG:H	1.86	0.40
1:F:277:PHE:HB2	1:F:318:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:HIS:HB3	1:C:402:ARG:HG2	2.03	0.40
1:B:246:ASN:HA	1:B:247:PRO:HA	1.91	0.40
1:D:272:LEU:HD23	1:D:272:LEU:HA	1.91	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:J:72:ARG:NH1	1:J:265:HIS:CD2	2.90	0.40
1:G:72:ARG:HH22	1:G:265:HIS:CD2	2.35	0.40
1:G:42:ARG:CG	1:G:72:ARG:HG3	2.52	0.40
1:B:42:ARG:CG	1:B:72:ARG:HG3	2.52	0.40
1:A:425:ILE:HD12	1:A:437:PRO:HD3	2.02	0.40
1:L:277:PHE:HB2	1:L:318:TYR:CZ	2.56	0.40
1:I:255:HIS:HB3	1:I:402:ARG:HG2	2.03	0.40
1:J:255:HIS:HB3	1:J:402:ARG:HG2	2.03	0.40
1:A:277:PHE:HB2	1:A:318:TYR:CZ	2.56	0.40
1:F:45:PHE:HB2	1:F:67:VAL:HG12	2.03	0.40
1:D:162:LEU:HD12	1:D:163:ARG:H	1.86	0.40
1:D:220:LYS:HD3	1:D:220:LYS:HA	1.90	0.40
1:K:220:LYS:HA	1:K:220:LYS:HD3	1.90	0.40
1:B:396:ARG:CG	1:F:400:GLN:CD	2.89	0.40
1:I:42:ARG:CG	1:I:72:ARG:HG3	2.51	0.40
1:H:174:LEU:HD22	1:H:206:ALA:HA	2.02	0.40
1:B:45:PHE:HB2	1:B:67:VAL:HG12	2.03	0.40
1:A:307:LEU:HB3	1:A:311:GLN:HB2	2.03	0.40
1:K:307:LEU:HB3	1:K:311:GLN:HB2	2.03	0.40
1:C:425:ILE:HD12	1:C:437:PRO:HD3	2.02	0.40
1:B:174:LEU:HD22	1:B:206:ALA:HA	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:C:277:PHE:HB2	1:C:318:TYR:CZ	2.56	0.40
1:F:11:TYR:CD1	1:F:369:LYS:HE3	2.56	0.40
1:J:42:ARG:CG	1:J:72:ARG:HG3	2.51	0.40
1:K:313:ASN:CG	1:L:420:ARG:HE	2.25	0.40
1:J:330:VAL:HG21	1:J:364:PHE:HE2	1.87	0.40
1:H:42:ARG:CG	1:H:72:ARG:HG3	2.52	0.40
1:L:307:LEU:HB3	1:L:311:GLN:HB2	2.03	0.40
1:J:425:ILE:HD12	1:J:437:PRO:HD3	2.02	0.40
1:J:297:LEU:HA	1:J:297:LEU:HD23	1.78	0.40
1:L:297:LEU:HA	1:L:297:LEU:HD23	1.78	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
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:F:326:GLN:OE1	1:G:280:ASP:C[1_554]	2.19	0.01
1:C:326:GLN:O	1:E:282:GLN:CG[2_555]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	371/470 (79%)	361 (97%)	10 (3%)	0	100	100
1	B	371/470 (79%)	358 (96%)	12 (3%)	1 (0%)	46	83
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
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 ⓘ

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%)	327 (99%)	4 (1%)	78	90
1	B	331/403 (82%)	325 (98%)	6 (2%)	66	87
1	C	331/403 (82%)	327 (99%)	4 (1%)	78	90
1	D	331/403 (82%)	327 (99%)	4 (1%)	78	90
1	E	331/403 (82%)	326 (98%)	5 (2%)	72	88
1	F	331/403 (82%)	327 (99%)	4 (1%)	78	90
1	G	331/403 (82%)	327 (99%)	4 (1%)	78	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	331/403 (82%)	327 (99%)	4 (1%)	78	90
1	I	331/403 (82%)	327 (99%)	4 (1%)	78	90
1	J	331/403 (82%)	327 (99%)	4 (1%)	78	90
1	K	331/403 (82%)	327 (99%)	4 (1%)	78	90
1	L	331/403 (82%)	326 (98%)	5 (2%)	72	88
All	All	3972/4836 (82%)	3920 (99%)	52 (1%)	76	89

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	22	SER
1	A	32	LYS
1	A	52	ASN
1	B	8	ASN
1	B	22	SER
1	B	32	LYS
1	B	52	ASN
1	B	345	GLN
1	B	347	GLN
1	C	8	ASN
1	C	22	SER
1	C	32	LYS
1	C	52	ASN
1	D	8	ASN
1	D	22	SER
1	D	32	LYS
1	D	52	ASN
1	E	8	ASN
1	E	22	SER
1	E	32	LYS
1	E	52	ASN
1	E	327	MET
1	F	8	ASN
1	F	22	SER
1	F	32	LYS
1	F	52	ASN
1	G	8	ASN
1	G	22	SER
1	G	32	LYS

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Mol	Chain	Res	Type
1	G	52	ASN
1	H	8	ASN
1	H	22	SER
1	H	32	LYS
1	H	52	ASN
1	I	8	ASN
1	I	22	SER
1	I	32	LYS
1	I	52	ASN
1	J	8	ASN
1	J	22	SER
1	J	32	LYS
1	J	52	ASN
1	K	8	ASN
1	K	22	SER
1	K	32	LYS
1	K	52	ASN
1	L	8	ASN
1	L	22	SER
1	L	32	LYS
1	L	52	ASN
1	L	327	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	34	GLN
1	A	40	GLN
1	A	52	ASN
1	A	64	GLN
1	A	71	GLN
1	A	265	HIS
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	265	HIS
1	B	317	GLN
1	B	347	GLN

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Mol	Chain	Res	Type
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	265	HIS
1	D	8	ASN
1	D	34	GLN
1	D	40	GLN
1	D	52	ASN
1	D	64	GLN
1	D	71	GLN
1	D	265	HIS
1	D	317	GLN
1	D	400	GLN
1	E	8	ASN
1	E	34	GLN
1	E	40	GLN
1	E	52	ASN
1	E	64	GLN
1	E	71	GLN
1	E	265	HIS
1	E	317	GLN
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	265	HIS
1	G	34	GLN
1	G	40	GLN
1	G	52	ASN
1	G	64	GLN
1	G	71	GLN
1	G	265	HIS
1	G	400	GLN
1	H	34	GLN
1	H	40	GLN

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Mol	Chain	Res	Type
1	H	52	ASN
1	H	64	GLN
1	H	71	GLN
1	H	265	HIS
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	265	HIS
1	J	34	GLN
1	J	40	GLN
1	J	52	ASN
1	J	64	GLN
1	J	68	HIS
1	J	71	GLN
1	J	265	HIS
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	265	HIS
1	L	8	ASN
1	L	34	GLN
1	L	40	GLN
1	L	52	ASN
1	L	64	GLN
1	L	71	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	375/470 (79%)	0.56	31 (8%) 14 18	41, 41, 105, 105	0
1	B	375/470 (79%)	0.91	50 (13%) 4 10	71, 71, 152, 152	0
1	C	375/470 (79%)	0.54	28 (7%) 17 20	39, 39, 110, 110	0
1	D	375/470 (79%)	0.71	41 (10%) 7 12	55, 55, 154, 154	0
1	E	375/470 (79%)	0.60	35 (9%) 11 15	28, 28, 118, 118	0
1	F	375/470 (79%)	0.60	32 (8%) 13 17	38, 38, 116, 116	0
1	G	375/470 (79%)	0.86	55 (14%) 3 9	50, 50, 131, 131	0
1	H	375/470 (79%)	1.01	66 (17%) 2 7	75, 75, 206, 206	0
1	I	375/470 (79%)	0.72	43 (11%) 6 11	65, 65, 172, 172	0
1	J	375/470 (79%)	0.93	59 (15%) 3 8	102, 102, 172, 172	0
1	K	375/470 (79%)	0.85	57 (15%) 3 9	77, 77, 176, 176	0
1	L	375/470 (79%)	1.08	77 (20%) 1 6	140, 140, 214, 214	0
All	All	4500/5640 (79%)	0.78	574 (12%) 5 10	28, 75, 172, 214	0

All (574) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	330	VAL	7.7
1	L	340	GLY	7.7
1	L	330	VAL	7.3
1	D	330	VAL	7.0
1	G	350	VAL	6.6
1	L	162	LEU	6.5
1	H	369	LYS	6.5
1	H	351	THR	6.4
1	F	333	PRO	6.3
1	I	464[A]	ASP	6.2
1	H	333	PRO	6.1

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Mol	Chain	Res	Type	RSRZ
1	G	351	THR	6.0
1	F	206	ALA	6.0
1	D	465	VAL	5.9
1	K	330	VAL	5.9
1	H	180	PRO	5.9
1	I	393	VAL	5.8
1	F	464[A]	ASP	5.8
1	J	340	GLY	5.7
1	E	428	ASN	5.7
1	L	465	VAL	5.6
1	B	141	PRO	5.6
1	B	330	VAL	5.6
1	J	333	PRO	5.6
1	L	249	LEU	5.6
1	D	464[A]	ASP	5.6
1	J	331	LEU	5.5
1	H	462	TRP	5.5
1	L	176	LEU	5.5
1	L	250	VAL	5.5
1	D	340	GLY	5.5
1	K	340	GLY	5.4
1	G	453	TRP	5.4
1	D	378	ASP	5.2
1	B	340	GLY	5.1
1	J	145	SER	5.1
1	D	343	PRO	5.1
1	L	333	PRO	5.0
1	H	350	VAL	4.9
1	G	464[A]	ASP	4.9
1	H	11	TYR	4.9
1	A	351	THR	4.9
1	L	403	TRP	4.9
1	G	330	VAL	4.9
1	K	464[A]	ASP	4.8
1	K	465	VAL	4.8
1	K	206	ALA	4.8
1	A	378	ASP	4.8
1	H	397	ALA	4.8
1	H	342	LEU	4.7
1	B	355	GLY	4.7
1	G	435	LYS	4.7
1	H	179	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
1	I	369	LYS	4.7
1	L	331	LEU	4.7
1	K	333	PRO	4.7
1	I	179	GLY	4.7
1	I	433	HIS	4.6
1	G	340	GLY	4.6
1	H	160	GLY	4.6
1	G	145	SER	4.6
1	A	465	VAL	4.6
1	G	366	ARG	4.6
1	L	145	SER	4.5
1	H	453	TRP	4.5
1	K	208	PHE	4.5
1	J	341	LEU	4.5
1	H	162	LEU	4.5
1	K	193	SER	4.5
1	B	341	LEU	4.4
1	B	464[A]	ASP	4.4
1	B	162	LEU	4.4
1	L	392	ARG	4.4
1	I	178	GLN	4.4
1	E	333	PRO	4.4
1	H	239	ILE	4.4
1	G	341	LEU	4.3
1	I	258	VAL	4.3
1	A	403	TRP	4.3
1	H	433	HIS	4.3
1	H	349	LYS	4.3
1	D	341	LEU	4.3
1	G	433	HIS	4.3
1	F	330	VAL	4.2
1	C	330	VAL	4.2
1	I	206	ALA	4.2
1	F	465	VAL	4.2
1	E	330	VAL	4.2
1	B	333	PRO	4.2
1	H	206	ALA	4.2
1	L	341	LEU	4.2
1	C	340	GLY	4.1
1	G	462	TRP	4.1
1	B	363	VAL	4.1
1	J	425	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	L	286	SER	4.0
1	B	426	GLU	4.0
1	J	426	GLU	4.0
1	F	258	VAL	4.0
1	H	330	VAL	3.9
1	B	375	GLY	3.9
1	G	349	LYS	3.9
1	L	462	TRP	3.9
1	G	458	MET	3.9
1	G	465	VAL	3.9
1	H	393	VAL	3.9
1	D	333	PRO	3.8
1	H	22	SER	3.8
1	K	331	LEU	3.8
1	G	364	PHE	3.8
1	C	464[A]	ASP	3.8
1	H	394	ASP	3.8
1	H	193	SER	3.7
1	H	205	ARG	3.7
1	A	393	VAL	3.7
1	I	445	TRP	3.7
1	D	342	LEU	3.6
1	I	348	ARG	3.6
1	D	329	GLY	3.6
1	I	330	VAL	3.6
1	L	277	PHE	3.6
1	J	393	VAL	3.6
1	B	356	ASN	3.6
1	B	343	PRO	3.6
1	F	340	GLY	3.5
1	K	448	ASN	3.5
1	I	249	LEU	3.5
1	A	162	LEU	3.5
1	H	178	GLN	3.5
1	K	2	ILE	3.5
1	D	331	LEU	3.5
1	D	162	LEU	3.5
1	L	424	PRO	3.5
1	I	259	ILE	3.4
1	L	164	VAL	3.4
1	J	445	TRP	3.4
1	G	444	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	145	SER	3.4
1	J	50	LEU	3.4
1	L	258	VAL	3.4
1	G	378	ASP	3.4
1	I	333	PRO	3.4
1	B	433	HIS	3.4
1	H	367	ASP	3.4
1	J	350	VAL	3.4
1	L	163	ARG	3.4
1	E	340	GLY	3.4
1	L	254	ASN	3.4
1	D	403	TRP	3.3
1	E	160	GLY	3.3
1	F	145	SER	3.3
1	H	176	LEU	3.3
1	E	331	LEU	3.3
1	I	180	PRO	3.3
1	K	174	LEU	3.3
1	H	194	GLY	3.3
1	H	343	PRO	3.3
1	J	146	PHE	3.3
1	K	433	HIS	3.3
1	L	206	ALA	3.3
1	B	50	LEU	3.3
1	L	146	PHE	3.3
1	D	230	THR	3.3
1	I	434	MET	3.3
1	H	146	PHE	3.3
1	L	230	THR	3.3
1	E	378	ASP	3.3
1	E	180	PRO	3.3
1	G	461	HIS	3.3
1	I	349	LYS	3.3
1	I	239	ILE	3.3
1	J	258	VAL	3.3
1	I	432	MET	3.2
1	J	342	LEU	3.2
1	D	143	TYR	3.2
1	D	339	ALA	3.2
1	B	350	VAL	3.2
1	H	347	GLN	3.2
1	C	428	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	462	TRP	3.2
1	G	258	VAL	3.2
1	H	425	ILE	3.2
1	B	11	TYR	3.2
1	J	369	LYS	3.2
1	G	331	LEU	3.2
1	K	3	VAL	3.2
1	E	145	SER	3.2
1	F	378	ASP	3.2
1	F	341	LEU	3.2
1	B	364	PHE	3.2
1	K	164	VAL	3.2
1	B	206	ALA	3.1
1	K	369	LYS	3.1
1	A	206	ALA	3.1
1	L	452	GLU	3.1
1	K	194	GLY	3.1
1	J	461	HIS	3.1
1	J	453	TRP	3.1
1	D	344	GLU	3.1
1	I	366	ARG	3.1
1	G	434	MET	3.1
1	J	452	GLU	3.1
1	L	228	LEU	3.1
1	H	204	THR	3.1
1	L	425	ILE	3.1
1	J	231	ASN	3.1
1	E	206	ALA	3.1
1	I	462	TRP	3.1
1	H	291	ALA	3.0
1	J	462	TRP	3.0
1	J	351	THR	3.0
1	E	146	PHE	3.0
1	L	236	ILE	3.0
1	E	211	LYS	3.0
1	J	329	GLY	3.0
1	H	398	ALA	3.0
1	L	366	ARG	3.0
1	B	145	SER	3.0
1	D	248	VAL	3.0
1	G	445	TRP	3.0
1	E	178	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	J	239	ILE	3.0
1	I	392	ARG	3.0
1	L	320	ALA	3.0
1	H	340	GLY	2.9
1	B	16	GLU	2.9
1	B	217	THR	2.9
1	K	364	PHE	2.9
1	K	440	GLN	2.9
1	G	146	PHE	2.9
1	J	400	GLN	2.9
1	L	43	VAL	2.9
1	J	356	ASN	2.9
1	J	143	TYR	2.9
1	L	362	PHE	2.9
1	D	356	ASN	2.9
1	G	231	ASN	2.9
1	I	394	ASP	2.9
1	G	361	GLY	2.9
1	J	144	HIS	2.9
1	I	347	GLN	2.8
1	I	350	VAL	2.8
1	J	364	PHE	2.8
1	F	351	THR	2.8
1	B	369	LYS	2.8
1	K	341	LEU	2.8
1	L	393	VAL	2.8
1	L	259	ILE	2.8
1	C	206	ALA	2.8
1	I	465	VAL	2.8
1	E	366	ARG	2.8
1	F	205	ARG	2.8
1	B	462	TRP	2.8
1	E	161	LYS	2.8
1	H	364	PHE	2.8
1	J	162	LEU	2.8
1	L	339	ALA	2.8
1	K	145	SER	2.8
1	K	453	TRP	2.8
1	G	454	ASN	2.8
1	H	167	GLY	2.8
1	H	395	GLN	2.8
1	K	425	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	295	ASN	2.8
1	H	53	HIS	2.8
1	B	366	ARG	2.8
1	E	231	ASN	2.8
1	B	15	VAL	2.7
1	B	285	TYR	2.7
1	K	15	VAL	2.7
1	K	366	ARG	2.7
1	B	465	VAL	2.7
1	L	434	MET	2.7
1	F	231	ASN	2.7
1	L	178	GLN	2.7
1	E	364	PHE	2.7
1	G	295	ASN	2.7
1	F	426	GLU	2.7
1	L	208	PHE	2.7
1	C	341	LEU	2.7
1	J	444	GLU	2.7
1	K	258	VAL	2.7
1	A	341	LEU	2.7
1	G	143	TYR	2.7
1	E	341	LEU	2.7
1	I	425	ILE	2.7
1	L	428	ASN	2.7
1	K	432	MET	2.7
1	D	355	GLY	2.7
1	B	205	ARG	2.7
1	H	435	LYS	2.7
1	E	464[A]	ASP	2.7
1	K	205	ARG	2.7
1	D	179	GLY	2.7
1	C	434	MET	2.6
1	F	403	TRP	2.6
1	D	39	ASP	2.6
1	L	251	PHE	2.6
1	F	350	VAL	2.6
1	A	350	VAL	2.6
1	K	444	GLU	2.6
1	A	340	GLY	2.6
1	G	363	VAL	2.6
1	I	395	GLN	2.6
1	L	16	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	L	69	ILE	2.6
1	I	11	TYR	2.6
1	J	11	TYR	2.6
1	G	426	GLU	2.6
1	E	162	LEU	2.6
1	F	428	ASN	2.6
1	C	247	PRO	2.6
1	A	248	VAL	2.6
1	A	208	PHE	2.6
1	H	396	ARG	2.6
1	B	344	GLU	2.6
1	K	447	TRP	2.6
1	I	428	ASN	2.6
1	G	369	LYS	2.6
1	B	435	LYS	2.6
1	I	162	LEU	2.6
1	E	465	VAL	2.6
1	C	347	GLN	2.6
1	J	339	ALA	2.6
1	L	287	LEU	2.6
1	A	363	VAL	2.6
1	I	463	PHE	2.6
1	A	258	VAL	2.6
1	L	177	ALA	2.6
1	K	414	THR	2.6
1	B	163	ARG	2.6
1	D	5	VAL	2.6
1	L	67	VAL	2.6
1	E	210	PHE	2.6
1	H	363	VAL	2.6
1	B	211	LYS	2.6
1	F	433	HIS	2.6
1	J	366	ARG	2.6
1	K	463	PHE	2.6
1	A	207	GLU	2.6
1	E	304	PHE	2.5
1	L	364	PHE	2.5
1	C	346	GLY	2.5
1	L	234	ARG	2.5
1	H	341	LEU	2.5
1	J	240	ALA	2.5
1	A	230	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	248	VAL	2.5
1	L	451	CYS	2.5
1	K	445	TRP	2.5
1	H	445	TRP	2.5
1	H	370	GLU	2.5
1	A	163	ARG	2.5
1	F	424	PRO	2.5
1	H	192	MET	2.5
1	D	249	LEU	2.5
1	J	304	PHE	2.5
1	L	324	VAL	2.5
1	A	400	GLN	2.5
1	K	462	TRP	2.5
1	J	307	LEU	2.5
1	L	369	LYS	2.5
1	D	259	ILE	2.5
1	E	462	TRP	2.5
1	K	162	LEU	2.5
1	C	143	TYR	2.5
1	F	11	TYR	2.5
1	C	331	LEU	2.5
1	E	355	GLY	2.5
1	C	144	HIS	2.5
1	B	210	PHE	2.5
1	D	393	VAL	2.5
1	G	347	GLN	2.5
1	C	447	TRP	2.4
1	E	425	ILE	2.4
1	B	425	ILE	2.4
1	E	176	LEU	2.4
1	F	393	VAL	2.4
1	J	464[A]	ASP	2.4
1	J	361	GLY	2.4
1	D	15	VAL	2.4
1	K	11	TYR	2.4
1	E	356	ASN	2.4
1	E	298	ILE	2.4
1	F	250	VAL	2.4
1	A	333	PRO	2.4
1	E	433	HIS	2.4
1	H	51	GLN	2.4
1	H	366	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	206	ALA	2.4
1	G	324	VAL	2.4
1	A	462	TRP	2.4
1	C	299	LYS	2.4
1	G	333	PRO	2.4
1	K	350	VAL	2.4
1	J	397	ALA	2.4
1	K	290	VAL	2.4
1	I	431	CYS	2.4
1	I	250	VAL	2.4
1	B	14	PRO	2.4
1	G	425	ILE	2.4
1	L	229	ILE	2.4
1	F	147	PHE	2.4
1	F	364	PHE	2.4
1	A	429	GLY	2.4
1	F	445	TRP	2.4
1	B	351	THR	2.4
1	A	428	ASN	2.4
1	H	378	ASP	2.4
1	A	364	PHE	2.3
1	F	210	PHE	2.3
1	H	415	THR	2.3
1	H	345	GLN	2.3
1	C	445	TRP	2.3
1	D	369	LYS	2.3
1	H	290	VAL	2.3
1	L	374	GLU	2.3
1	G	437	PRO	2.3
1	H	362	PHE	2.3
1	I	367	ASP	2.3
1	G	329	GLY	2.3
1	L	179	GLY	2.3
1	K	146	PHE	2.3
1	L	231	ASN	2.3
1	J	403	TRP	2.3
1	A	210	PHE	2.3
1	D	206	ALA	2.3
1	L	370	GLU	2.3
1	B	17	VAL	2.3
1	D	247	PRO	2.3
1	G	432	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	429	GLY	2.3
1	L	458	MET	2.3
1	A	356	ASN	2.3
1	H	458	MET	2.3
1	A	349	LYS	2.3
1	B	376	GLU	2.3
1	G	205	ARG	2.3
1	D	366	ARG	2.3
1	F	331	LEU	2.3
1	H	66	ILE	2.3
1	K	204	THR	2.2
1	A	355	GLY	2.2
1	D	346	GLY	2.2
1	L	22	SER	2.2
1	G	72	ARG	2.2
1	L	454	ASN	2.2
1	K	342	LEU	2.2
1	J	316[A]	GLN	2.2
1	K	143	TYR	2.2
1	D	180	PRO	2.2
1	I	414	THR	2.2
1	K	339	ALA	2.2
1	L	147	PHE	2.2
1	B	392	ARG	2.2
1	L	161	LYS	2.2
1	L	60	ASP	2.2
1	L	445	TRP	2.2
1	H	161	LYS	2.2
1	J	15	VAL	2.2
1	J	290	VAL	2.2
1	G	367	ASP	2.2
1	K	192	MET	2.2
1	L	459	GLY	2.2
1	L	44	ILE	2.2
1	J	189	PRO	2.2
1	G	348	ARG	2.2
1	H	52	ASN	2.2
1	G	141	PRO	2.2
1	G	335	PRO	2.2
1	C	350	VAL	2.2
1	D	463	PHE	2.2
1	L	453	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	250	VAL	2.2
1	K	49	GLU	2.2
1	G	343	PRO	2.2
1	B	445	TRP	2.2
1	L	264	PHE	2.2
1	D	145	SER	2.2
1	G	250	VAL	2.2
1	K	303	HIS	2.2
1	J	396	ARG	2.2
1	D	323	CYS	2.2
1	C	282	GLN	2.2
1	G	39	ASP	2.2
1	I	219	ASP	2.2
1	B	231	ASN	2.2
1	D	448	ASN	2.2
1	G	162	LEU	2.2
1	H	268	CYS	2.2
1	I	331	LEU	2.2
1	C	230	THR	2.1
1	B	193	SER	2.1
1	L	141	PRO	2.1
1	B	3	VAL	2.1
1	K	72	ARG	2.1
1	C	333	PRO	2.1
1	G	40	GLN	2.1
1	I	368	CYS	2.1
1	I	397	ALA	2.1
1	A	259	ILE	2.1
1	K	163	ARG	2.1
1	C	432	MET	2.1
1	G	342	LEU	2.1
1	D	217	THR	2.1
1	L	464[A]	ASP	2.1
1	J	347	GLN	2.1
1	C	199	PRO	2.1
1	F	208	PHE	2.1
1	L	336	GLY	2.1
1	A	372	TYR	2.1
1	K	426	GLU	2.1
1	A	342	LEU	2.1
1	K	372	TYR	2.1
1	K	403	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	331	LEU	2.1
1	G	204	THR	2.1
1	L	232	ASN	2.1
1	E	163	ARG	2.1
1	J	3	VAL	2.1
1	J	419	PRO	2.1
1	H	208	PHE	2.1
1	F	342	LEU	2.1
1	C	208	PHE	2.1
1	H	21	THR	2.1
1	C	210	PHE	2.1
1	F	434	MET	2.1
1	K	393	VAL	2.1
1	L	17	VAL	2.1
1	L	323	CYS	2.1
1	H	432	MET	2.1
1	J	199	PRO	2.1
1	J	416	LYS	2.1
1	F	295	ASN	2.1
1	J	414	THR	2.1
1	B	258	VAL	2.1
1	K	176	LEU	2.1
1	E	445	TRP	2.1
1	L	378	ASP	2.1
1	D	432	MET	2.1
1	F	207	GLU	2.1
1	B	230	THR	2.0
1	G	463	PHE	2.0
1	H	164	VAL	2.0
1	L	210	PHE	2.0
1	B	459	GLY	2.0
1	B	204	THR	2.0
1	G	164	VAL	2.0
1	K	343	PRO	2.0
1	L	321	GLU	2.0
1	I	362	PHE	2.0
1	C	336	GLY	2.0
1	E	440	GLN	2.0
1	I	378	ASP	2.0
1	J	355	GLY	2.0
1	K	210	PHE	2.0
1	G	315	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	447	TRP	2.0
1	J	315	TYR	2.0
1	H	231	ASN	2.0
1	J	65	SER	2.0
1	K	295	ASN	2.0
1	L	315	TYR	2.0
1	H	428	ASN	2.0
1	K	374	GLU	2.0
1	B	434	MET	2.0
1	C	49	GLU	2.0
1	I	364	PHE	2.0
1	C	433	HIS	2.0
1	J	398	ALA	2.0
1	D	176	LEU	2.0
1	E	287	LEU	2.0
1	J	64	GLN	2.0
1	J	291	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
2	ZN	F	501	1/1	0.93	0.28	-0.16	38,38,38,38	0
2	ZN	D	501	1/1	0.86	0.26	-0.32	54,54,54,54	0
2	ZN	J	501	1/1	0.95	0.29	-0.52	101,101,101,101	0
2	ZN	E	501	1/1	0.94	0.21	-0.56	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	I	506	1/1	0.75	0.51	-0.61	171,171,171,171	0
2	ZN	I	501	1/1	0.90	0.25	-0.62	65,65,65,65	0
2	ZN	C	503	1/1	0.97	0.17	-0.66	39,39,39,39	0
2	ZN	C	504	1/1	0.94	0.22	-0.74	39,39,39,39	0
2	ZN	J	508	1/1	0.72	0.29	-0.77	101,101,101,101	0
2	ZN	H	508	1/1	0.68	0.31	-0.82	75,75,75,75	0
2	ZN	J	503	1/1	0.91	0.12	-0.88	101,101,101,101	0
2	ZN	K	504	1/1	0.84	0.24	-0.91	77,77,77,77	0
2	ZN	B	506	1/1	0.90	0.37	-0.93	151,151,151,151	0
2	ZN	H	501	1/1	0.87	0.27	-0.94	75,75,75,75	0
2	ZN	C	508	1/1	0.61	0.22	-0.95	39,39,39,39	0
2	ZN	H	503	1/1	0.88	0.21	-0.95	75,75,75,75	0
2	ZN	A	505	1/1	0.66	0.22	-0.97	105,105,105,105	0
2	ZN	B	501	1/1	0.94	0.30	-0.97	70,70,70,70	0
2	ZN	K	501	1/1	0.93	0.17	-0.98	77,77,77,77	0
2	ZN	G	508	1/1	0.40	0.33	-0.98	49,49,49,49	0
2	ZN	H	505	1/1	0.31	0.27	-0.99	205,205,205,205	0
2	ZN	D	508	1/1	0.73	0.21	-1.00	54,54,54,54	0
2	ZN	A	501	1/1	0.81	0.17	-1.04	40,40,40,40	0
2	ZN	J	504	1/1	0.83	0.20	-1.06	101,101,101,101	0
2	ZN	G	505	1/1	0.60	0.30	-1.06	131,131,131,131	0
2	ZN	J	505	1/1	0.39	0.30	-1.09	171,171,171,171	0
2	ZN	H	504	1/1	0.94	0.17	-1.11	75,75,75,75	0
2	ZN	H	507	1/1	0.75	0.19	-1.11	75,75,75,75	0
2	ZN	E	503	1/1	0.92	0.18	-1.11	28,28,28,28	0
2	ZN	K	508	1/1	0.59	0.23	-1.15	77,77,77,77	0
2	ZN	E	508	1/1	0.77	0.17	-1.18	28,28,28,28	0
2	ZN	H	506	1/1	0.54	0.38	-1.20	205,205,205,205	0
2	ZN	I	504	1/1	0.92	0.14	-1.20	65,65,65,65	0
2	ZN	I	505	1/1	0.89	0.07	-1.21	171,171,171,171	0
2	ZN	A	503	1/1	0.77	0.16	-1.22	40,40,40,40	0
2	ZN	B	504	1/1	0.82	0.22	-1.22	70,70,70,70	0
2	ZN	A	507	1/1	0.86	0.14	-1.23	40,40,40,40	0
2	ZN	F	507	1/1	0.90	0.15	-1.25	38,38,38,38	0
2	ZN	C	506	1/1	0.93	0.06	-1.28	104,104,104,104	0
2	ZN	K	505	1/1	0.71	0.23	-1.28	176,176,176,176	0
2	ZN	L	507	1/1	0.67	0.07	-1.30	139,139,139,139	0
2	ZN	D	503	1/1	0.78	0.16	-1.35	54,54,54,54	0
2	ZN	F	505	1/1	0.71	0.12	-1.38	105,105,105,105	0
2	ZN	F	503	1/1	0.95	0.14	-1.38	38,38,38,38	0
2	ZN	C	501	1/1	0.92	0.20	-1.39	39,39,39,39	0
2	ZN	J	507	1/1	0.84	0.15	-1.40	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	L	504	1/1	0.75	0.11	-1.40	139,139,139,139	0
2	ZN	E	504	1/1	0.91	0.11	-1.42	28,28,28,28	0
2	ZN	I	507	1/1	0.90	0.14	-1.44	65,65,65,65	0
2	ZN	J	502	1/1	0.92	0.09	-1.44	101,101,101,101	0
2	ZN	B	505	1/1	0.87	0.10	-1.44	151,151,151,151	0
2	ZN	I	502	1/1	0.96	0.13	-1.48	65,65,65,65	0
2	ZN	E	505	1/1	0.37	0.15	-1.49	117,117,117,117	0
2	ZN	C	505	1/1	0.87	0.18	-1.51	104,104,104,104	0
2	ZN	A	504	1/1	0.88	0.10	-1.55	40,40,40,40	0
2	ZN	K	502	1/1	0.69	0.08	-1.57	77,77,77,77	0
2	ZN	F	504	1/1	0.92	0.16	-1.60	38,38,38,38	0
2	ZN	G	501	1/1	0.96	0.21	-1.60	49,49,49,49	0
2	ZN	G	503	1/1	0.93	0.17	-1.61	49,49,49,49	0
2	ZN	D	507	1/1	0.95	0.12	-1.64	54,54,54,54	0
2	ZN	G	504	1/1	0.90	0.21	-1.68	49,49,49,49	0
2	ZN	C	507	1/1	0.96	0.13	-1.71	39,39,39,39	0
2	ZN	B	508	1/1	0.61	0.16	-1.71	70,70,70,70	0
2	ZN	G	507	1/1	0.76	0.09	-1.75	49,49,49,49	0
2	ZN	G	502	1/1	0.85	0.09	-1.76	49,49,49,49	0
2	ZN	G	506	1/1	0.85	0.14	-1.76	131,131,131,131	0
2	ZN	E	502	1/1	0.96	0.05	-1.77	28,28,28,28	0
2	ZN	L	505	1/1	0.90	0.18	-1.82	213,213,213,213	0
2	ZN	K	507	1/1	0.96	0.11	-1.83	77,77,77,77	0
2	ZN	L	508	1/1	0.35	0.20	-1.83	139,139,139,139	0
2	ZN	B	503	1/1	0.95	0.15	-1.88	70,70,70,70	0
2	ZN	D	502	1/1	0.79	0.17	-1.91	54,54,54,54	0
2	ZN	D	505	1/1	0.88	0.10	-1.92	153,153,153,153	0
2	ZN	L	503	1/1	0.73	0.13	-1.94	139,139,139,139	0
2	ZN	D	504	1/1	0.96	0.05	-1.96	54,54,54,54	0
2	ZN	A	502	1/1	0.89	0.12	-1.97	40,40,40,40	0
2	ZN	L	502	1/1	0.93	0.10	-1.97	139,139,139,139	0
2	ZN	A	508	1/1	0.78	0.15	-1.97	40,40,40,40	0
2	ZN	E	507	1/1	0.90	0.10	-2.03	28,28,28,28	0
2	ZN	F	502	1/1	0.88	0.07	-2.10	38,38,38,38	0
2	ZN	E	506	1/1	0.82	0.20	-2.12	117,117,117,117	0
2	ZN	A	506	1/1	0.76	0.08	-2.30	105,105,105,105	0
2	ZN	L	506	1/1	0.85	0.18	-2.32	213,213,213,213	0
2	ZN	C	502	1/1	0.87	0.10	-2.35	39,39,39,39	0
2	ZN	H	502	1/1	0.84	0.07	-2.37	75,75,75,75	0
2	ZN	B	507	1/1	0.79	0.09	-2.38	70,70,70,70	0
2	ZN	F	508	1/1	0.76	0.17	-2.38	38,38,38,38	0
2	ZN	D	506	1/1	0.93	0.10	-2.40	153,153,153,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	K	506	1/1	0.43	0.15	-2.43	176,176,176,176	0
2	ZN	I	503	1/1	0.85	0.10	-2.45	65,65,65,65	0
2	ZN	I	508	1/1	0.90	0.16	-2.46	65,65,65,65	0
2	ZN	L	501	1/1	0.92	0.17	-2.47	139,139,139,139	0
2	ZN	J	506	1/1	0.75	0.23	-2.68	171,171,171,171	0
2	ZN	B	502	1/1	0.91	0.06	-2.72	70,70,70,70	0
2	ZN	K	503	1/1	0.92	0.11	-2.77	77,77,77,77	0
2	ZN	F	506	1/1	0.88	0.08	-3.08	105,105,105,105	0

6.5 Other polymers

There are no such residues in this entry.