



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:42 am BST

PDB ID : 3M9D
Title : Crystal structure of the prokaryotic ubiquitin-like protein Pup complexed with the hexameric proteasomal ATPase Mpa which includes the amino terminal coiled coil domain and the inter domain
Authors : Li, H.; Wang, T.
Deposited on : 2010-03-22
Resolution : 4.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

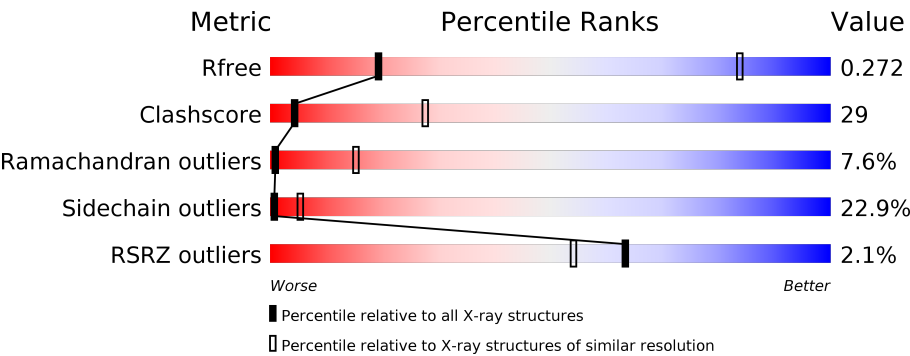
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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}	130704	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

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

Mol	Chain	Length	Quality of chain
1	A	251	<div><div>%</div><div><div></div><div>26%</div><div>32%</div><div>14%</div><div>•</div><div>26%</div></div></div>
1	B	251	<div><div>%</div><div><div></div><div>37%</div><div>25%</div><div>10%</div><div>•</div><div>26%</div></div></div>
1	C	251	<div><div>%</div><div><div></div><div>29%</div><div>30%</div><div>14%</div><div>•</div><div>26%</div></div></div>
1	D	251	<div><div>%</div><div><div></div><div>35%</div><div>27%</div><div>11%</div><div>•</div><div>26%</div></div></div>
1	E	251	<div><div>%</div><div><div></div><div>31%</div><div>30%</div><div>13%</div><div>•</div><div>26%</div></div></div>
1	F	251	<div><div>%</div><div><div></div><div>36%</div><div>29%</div><div>8%</div><div>•</div><div>26%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	J	251	
1	K	251	
1	L	251	
1	M	251	
1	N	251	
1	O	251	
2	G	68	
2	H	68	
2	I	68	
2	P	68	
2	Q	68	
2	R	68	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18636 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 Proteasome-associated ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1431	888	259	281	3			
1	B	186	Total	C	N	O	S	0	0	0
			1431	888	259	281	3			
1	C	186	Total	C	N	O	S	0	0	0
			1431	888	259	281	3			
1	D	186	Total	C	N	O	S	0	0	0
			1431	888	259	281	3			
1	E	186	Total	C	N	O	S	0	0	0
			1431	888	259	281	3			
1	F	186	Total	C	N	O	S	0	0	0
			1431	888	259	281	3			
1	J	186	Total	C	N	O	S	0	0	0
			1431	888	259	281	3			
1	K	186	Total	C	N	O	S	0	0	0
			1431	888	259	281	3			
1	L	186	Total	C	N	O	S	0	0	0
			1431	888	259	281	3			
1	M	186	Total	C	N	O	S	0	0	0
			1431	888	259	281	3			
1	N	186	Total	C	N	O	S	0	0	0
			1431	888	259	281	3			
1	O	186	Total	C	N	O	S	0	0	0
			1431	888	259	281	3			

There are 204 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	LEU	-	EXPRESSION TAG	UNP P63345
A	236	VAL	-	EXPRESSION TAG	UNP P63345
A	237	PRO	-	EXPRESSION TAG	UNP P63345
A	238	ARG	-	EXPRESSION TAG	UNP P63345
A	239	GLY	-	EXPRESSION TAG	UNP P63345

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Chain	Residue	Modelled	Actual	Comment	Reference
A	240	SER	-	EXPRESSION TAG	UNP P63345
A	241	ALA	-	EXPRESSION TAG	UNP P63345
A	242	ALA	-	EXPRESSION TAG	UNP P63345
A	243	ALA	-	EXPRESSION TAG	UNP P63345
A	244	LEU	-	EXPRESSION TAG	UNP P63345
A	245	GLU	-	EXPRESSION TAG	UNP P63345
A	246	HIS	-	EXPRESSION TAG	UNP P63345
A	247	HIS	-	EXPRESSION TAG	UNP P63345
A	248	HIS	-	EXPRESSION TAG	UNP P63345
A	249	HIS	-	EXPRESSION TAG	UNP P63345
A	250	HIS	-	EXPRESSION TAG	UNP P63345
A	251	HIS	-	EXPRESSION TAG	UNP P63345
B	235	LEU	-	EXPRESSION TAG	UNP P63345
B	236	VAL	-	EXPRESSION TAG	UNP P63345
B	237	PRO	-	EXPRESSION TAG	UNP P63345
B	238	ARG	-	EXPRESSION TAG	UNP P63345
B	239	GLY	-	EXPRESSION TAG	UNP P63345
B	240	SER	-	EXPRESSION TAG	UNP P63345
B	241	ALA	-	EXPRESSION TAG	UNP P63345
B	242	ALA	-	EXPRESSION TAG	UNP P63345
B	243	ALA	-	EXPRESSION TAG	UNP P63345
B	244	LEU	-	EXPRESSION TAG	UNP P63345
B	245	GLU	-	EXPRESSION TAG	UNP P63345
B	246	HIS	-	EXPRESSION TAG	UNP P63345
B	247	HIS	-	EXPRESSION TAG	UNP P63345
B	248	HIS	-	EXPRESSION TAG	UNP P63345
B	249	HIS	-	EXPRESSION TAG	UNP P63345
B	250	HIS	-	EXPRESSION TAG	UNP P63345
B	251	HIS	-	EXPRESSION TAG	UNP P63345
C	235	LEU	-	EXPRESSION TAG	UNP P63345
C	236	VAL	-	EXPRESSION TAG	UNP P63345
C	237	PRO	-	EXPRESSION TAG	UNP P63345
C	238	ARG	-	EXPRESSION TAG	UNP P63345
C	239	GLY	-	EXPRESSION TAG	UNP P63345
C	240	SER	-	EXPRESSION TAG	UNP P63345
C	241	ALA	-	EXPRESSION TAG	UNP P63345
C	242	ALA	-	EXPRESSION TAG	UNP P63345
C	243	ALA	-	EXPRESSION TAG	UNP P63345
C	244	LEU	-	EXPRESSION TAG	UNP P63345
C	245	GLU	-	EXPRESSION TAG	UNP P63345
C	246	HIS	-	EXPRESSION TAG	UNP P63345
C	247	HIS	-	EXPRESSION TAG	UNP P63345

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Chain	Residue	Modelled	Actual	Comment	Reference
C	248	HIS	-	EXPRESSION TAG	UNP P63345
C	249	HIS	-	EXPRESSION TAG	UNP P63345
C	250	HIS	-	EXPRESSION TAG	UNP P63345
C	251	HIS	-	EXPRESSION TAG	UNP P63345
D	235	LEU	-	EXPRESSION TAG	UNP P63345
D	236	VAL	-	EXPRESSION TAG	UNP P63345
D	237	PRO	-	EXPRESSION TAG	UNP P63345
D	238	ARG	-	EXPRESSION TAG	UNP P63345
D	239	GLY	-	EXPRESSION TAG	UNP P63345
D	240	SER	-	EXPRESSION TAG	UNP P63345
D	241	ALA	-	EXPRESSION TAG	UNP P63345
D	242	ALA	-	EXPRESSION TAG	UNP P63345
D	243	ALA	-	EXPRESSION TAG	UNP P63345
D	244	LEU	-	EXPRESSION TAG	UNP P63345
D	245	GLU	-	EXPRESSION TAG	UNP P63345
D	246	HIS	-	EXPRESSION TAG	UNP P63345
D	247	HIS	-	EXPRESSION TAG	UNP P63345
D	248	HIS	-	EXPRESSION TAG	UNP P63345
D	249	HIS	-	EXPRESSION TAG	UNP P63345
D	250	HIS	-	EXPRESSION TAG	UNP P63345
D	251	HIS	-	EXPRESSION TAG	UNP P63345
E	235	LEU	-	EXPRESSION TAG	UNP P63345
E	236	VAL	-	EXPRESSION TAG	UNP P63345
E	237	PRO	-	EXPRESSION TAG	UNP P63345
E	238	ARG	-	EXPRESSION TAG	UNP P63345
E	239	GLY	-	EXPRESSION TAG	UNP P63345
E	240	SER	-	EXPRESSION TAG	UNP P63345
E	241	ALA	-	EXPRESSION TAG	UNP P63345
E	242	ALA	-	EXPRESSION TAG	UNP P63345
E	243	ALA	-	EXPRESSION TAG	UNP P63345
E	244	LEU	-	EXPRESSION TAG	UNP P63345
E	245	GLU	-	EXPRESSION TAG	UNP P63345
E	246	HIS	-	EXPRESSION TAG	UNP P63345
E	247	HIS	-	EXPRESSION TAG	UNP P63345
E	248	HIS	-	EXPRESSION TAG	UNP P63345
E	249	HIS	-	EXPRESSION TAG	UNP P63345
E	250	HIS	-	EXPRESSION TAG	UNP P63345
E	251	HIS	-	EXPRESSION TAG	UNP P63345
F	235	LEU	-	EXPRESSION TAG	UNP P63345
F	236	VAL	-	EXPRESSION TAG	UNP P63345
F	237	PRO	-	EXPRESSION TAG	UNP P63345
F	238	ARG	-	EXPRESSION TAG	UNP P63345

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Chain	Residue	Modelled	Actual	Comment	Reference
F	239	GLY	-	EXPRESSION TAG	UNP P63345
F	240	SER	-	EXPRESSION TAG	UNP P63345
F	241	ALA	-	EXPRESSION TAG	UNP P63345
F	242	ALA	-	EXPRESSION TAG	UNP P63345
F	243	ALA	-	EXPRESSION TAG	UNP P63345
F	244	LEU	-	EXPRESSION TAG	UNP P63345
F	245	GLU	-	EXPRESSION TAG	UNP P63345
F	246	HIS	-	EXPRESSION TAG	UNP P63345
F	247	HIS	-	EXPRESSION TAG	UNP P63345
F	248	HIS	-	EXPRESSION TAG	UNP P63345
F	249	HIS	-	EXPRESSION TAG	UNP P63345
F	250	HIS	-	EXPRESSION TAG	UNP P63345
F	251	HIS	-	EXPRESSION TAG	UNP P63345
J	235	LEU	-	EXPRESSION TAG	UNP P63345
J	236	VAL	-	EXPRESSION TAG	UNP P63345
J	237	PRO	-	EXPRESSION TAG	UNP P63345
J	238	ARG	-	EXPRESSION TAG	UNP P63345
J	239	GLY	-	EXPRESSION TAG	UNP P63345
J	240	SER	-	EXPRESSION TAG	UNP P63345
J	241	ALA	-	EXPRESSION TAG	UNP P63345
J	242	ALA	-	EXPRESSION TAG	UNP P63345
J	243	ALA	-	EXPRESSION TAG	UNP P63345
J	244	LEU	-	EXPRESSION TAG	UNP P63345
J	245	GLU	-	EXPRESSION TAG	UNP P63345
J	246	HIS	-	EXPRESSION TAG	UNP P63345
J	247	HIS	-	EXPRESSION TAG	UNP P63345
J	248	HIS	-	EXPRESSION TAG	UNP P63345
J	249	HIS	-	EXPRESSION TAG	UNP P63345
J	250	HIS	-	EXPRESSION TAG	UNP P63345
J	251	HIS	-	EXPRESSION TAG	UNP P63345
K	235	LEU	-	EXPRESSION TAG	UNP P63345
K	236	VAL	-	EXPRESSION TAG	UNP P63345
K	237	PRO	-	EXPRESSION TAG	UNP P63345
K	238	ARG	-	EXPRESSION TAG	UNP P63345
K	239	GLY	-	EXPRESSION TAG	UNP P63345
K	240	SER	-	EXPRESSION TAG	UNP P63345
K	241	ALA	-	EXPRESSION TAG	UNP P63345
K	242	ALA	-	EXPRESSION TAG	UNP P63345
K	243	ALA	-	EXPRESSION TAG	UNP P63345
K	244	LEU	-	EXPRESSION TAG	UNP P63345
K	245	GLU	-	EXPRESSION TAG	UNP P63345
K	246	HIS	-	EXPRESSION TAG	UNP P63345

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Chain	Residue	Modelled	Actual	Comment	Reference
K	247	HIS	-	EXPRESSION TAG	UNP P63345
K	248	HIS	-	EXPRESSION TAG	UNP P63345
K	249	HIS	-	EXPRESSION TAG	UNP P63345
K	250	HIS	-	EXPRESSION TAG	UNP P63345
K	251	HIS	-	EXPRESSION TAG	UNP P63345
L	235	LEU	-	EXPRESSION TAG	UNP P63345
L	236	VAL	-	EXPRESSION TAG	UNP P63345
L	237	PRO	-	EXPRESSION TAG	UNP P63345
L	238	ARG	-	EXPRESSION TAG	UNP P63345
L	239	GLY	-	EXPRESSION TAG	UNP P63345
L	240	SER	-	EXPRESSION TAG	UNP P63345
L	241	ALA	-	EXPRESSION TAG	UNP P63345
L	242	ALA	-	EXPRESSION TAG	UNP P63345
L	243	ALA	-	EXPRESSION TAG	UNP P63345
L	244	LEU	-	EXPRESSION TAG	UNP P63345
L	245	GLU	-	EXPRESSION TAG	UNP P63345
L	246	HIS	-	EXPRESSION TAG	UNP P63345
L	247	HIS	-	EXPRESSION TAG	UNP P63345
L	248	HIS	-	EXPRESSION TAG	UNP P63345
L	249	HIS	-	EXPRESSION TAG	UNP P63345
L	250	HIS	-	EXPRESSION TAG	UNP P63345
L	251	HIS	-	EXPRESSION TAG	UNP P63345
M	235	LEU	-	EXPRESSION TAG	UNP P63345
M	236	VAL	-	EXPRESSION TAG	UNP P63345
M	237	PRO	-	EXPRESSION TAG	UNP P63345
M	238	ARG	-	EXPRESSION TAG	UNP P63345
M	239	GLY	-	EXPRESSION TAG	UNP P63345
M	240	SER	-	EXPRESSION TAG	UNP P63345
M	241	ALA	-	EXPRESSION TAG	UNP P63345
M	242	ALA	-	EXPRESSION TAG	UNP P63345
M	243	ALA	-	EXPRESSION TAG	UNP P63345
M	244	LEU	-	EXPRESSION TAG	UNP P63345
M	245	GLU	-	EXPRESSION TAG	UNP P63345
M	246	HIS	-	EXPRESSION TAG	UNP P63345
M	247	HIS	-	EXPRESSION TAG	UNP P63345
M	248	HIS	-	EXPRESSION TAG	UNP P63345
M	249	HIS	-	EXPRESSION TAG	UNP P63345
M	250	HIS	-	EXPRESSION TAG	UNP P63345
M	251	HIS	-	EXPRESSION TAG	UNP P63345
N	235	LEU	-	EXPRESSION TAG	UNP P63345
N	236	VAL	-	EXPRESSION TAG	UNP P63345
N	237	PRO	-	EXPRESSION TAG	UNP P63345

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Chain	Residue	Modelled	Actual	Comment	Reference
N	238	ARG	-	EXPRESSION TAG	UNP P63345
N	239	GLY	-	EXPRESSION TAG	UNP P63345
N	240	SER	-	EXPRESSION TAG	UNP P63345
N	241	ALA	-	EXPRESSION TAG	UNP P63345
N	242	ALA	-	EXPRESSION TAG	UNP P63345
N	243	ALA	-	EXPRESSION TAG	UNP P63345
N	244	LEU	-	EXPRESSION TAG	UNP P63345
N	245	GLU	-	EXPRESSION TAG	UNP P63345
N	246	HIS	-	EXPRESSION TAG	UNP P63345
N	247	HIS	-	EXPRESSION TAG	UNP P63345
N	248	HIS	-	EXPRESSION TAG	UNP P63345
N	249	HIS	-	EXPRESSION TAG	UNP P63345
N	250	HIS	-	EXPRESSION TAG	UNP P63345
N	251	HIS	-	EXPRESSION TAG	UNP P63345
O	235	LEU	-	EXPRESSION TAG	UNP P63345
O	236	VAL	-	EXPRESSION TAG	UNP P63345
O	237	PRO	-	EXPRESSION TAG	UNP P63345
O	238	ARG	-	EXPRESSION TAG	UNP P63345
O	239	GLY	-	EXPRESSION TAG	UNP P63345
O	240	SER	-	EXPRESSION TAG	UNP P63345
O	241	ALA	-	EXPRESSION TAG	UNP P63345
O	242	ALA	-	EXPRESSION TAG	UNP P63345
O	243	ALA	-	EXPRESSION TAG	UNP P63345
O	244	LEU	-	EXPRESSION TAG	UNP P63345
O	245	GLU	-	EXPRESSION TAG	UNP P63345
O	246	HIS	-	EXPRESSION TAG	UNP P63345
O	247	HIS	-	EXPRESSION TAG	UNP P63345
O	248	HIS	-	EXPRESSION TAG	UNP P63345
O	249	HIS	-	EXPRESSION TAG	UNP P63345
O	250	HIS	-	EXPRESSION TAG	UNP P63345
O	251	HIS	-	EXPRESSION TAG	UNP P63345

- Molecule 2 is a protein called Prokaryotic ubiquitin-like protein pup.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	31	Total	C	N	O	0	0	0
			244	143	40	61			
2	H	31	Total	C	N	O	0	0	0
			244	143	40	61			
2	I	31	Total	C	N	O	0	0	0
			244	143	40	61			
2	P	31	Total	C	N	O	0	0	0
			244	143	40	61			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Q	31	Total	C	N	O	0	0	0
			244	143	40	61			
2	R	31	Total	C	N	O	0	0	0
			244	143	40	61			

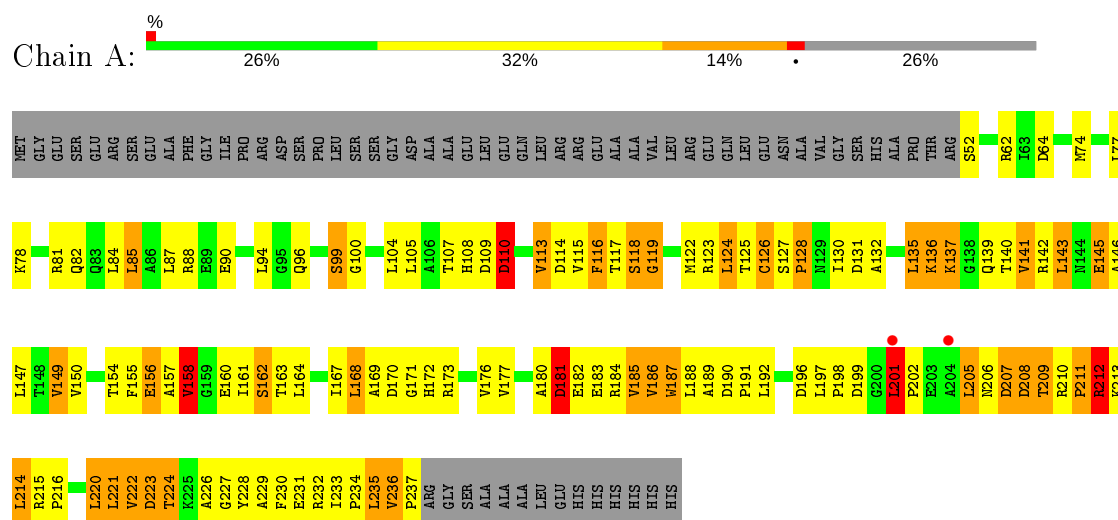
There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	GLY	-	EXPRESSION TAG	UNP O33246
G	-2	SER	-	EXPRESSION TAG	UNP O33246
G	-1	HIS	-	EXPRESSION TAG	UNP O33246
G	0	MET	-	EXPRESSION TAG	UNP O33246
G	64	GLU	GLN	ENGINEERED MUTATION	UNP O33246
H	-3	GLY	-	EXPRESSION TAG	UNP O33246
H	-2	SER	-	EXPRESSION TAG	UNP O33246
H	-1	HIS	-	EXPRESSION TAG	UNP O33246
H	0	MET	-	EXPRESSION TAG	UNP O33246
H	64	GLU	GLN	ENGINEERED MUTATION	UNP O33246
I	-3	GLY	-	EXPRESSION TAG	UNP O33246
I	-2	SER	-	EXPRESSION TAG	UNP O33246
I	-1	HIS	-	EXPRESSION TAG	UNP O33246
I	0	MET	-	EXPRESSION TAG	UNP O33246
I	64	GLU	GLN	ENGINEERED MUTATION	UNP O33246
P	-3	GLY	-	EXPRESSION TAG	UNP O33246
P	-2	SER	-	EXPRESSION TAG	UNP O33246
P	-1	HIS	-	EXPRESSION TAG	UNP O33246
P	0	MET	-	EXPRESSION TAG	UNP O33246
P	64	GLU	GLN	ENGINEERED MUTATION	UNP O33246
Q	-3	GLY	-	EXPRESSION TAG	UNP O33246
Q	-2	SER	-	EXPRESSION TAG	UNP O33246
Q	-1	HIS	-	EXPRESSION TAG	UNP O33246
Q	0	MET	-	EXPRESSION TAG	UNP O33246
Q	64	GLU	GLN	ENGINEERED MUTATION	UNP O33246
R	-3	GLY	-	EXPRESSION TAG	UNP O33246
R	-2	SER	-	EXPRESSION TAG	UNP O33246
R	-1	HIS	-	EXPRESSION TAG	UNP O33246
R	0	MET	-	EXPRESSION TAG	UNP O33246
R	64	GLU	GLN	ENGINEERED MUTATION	UNP O33246

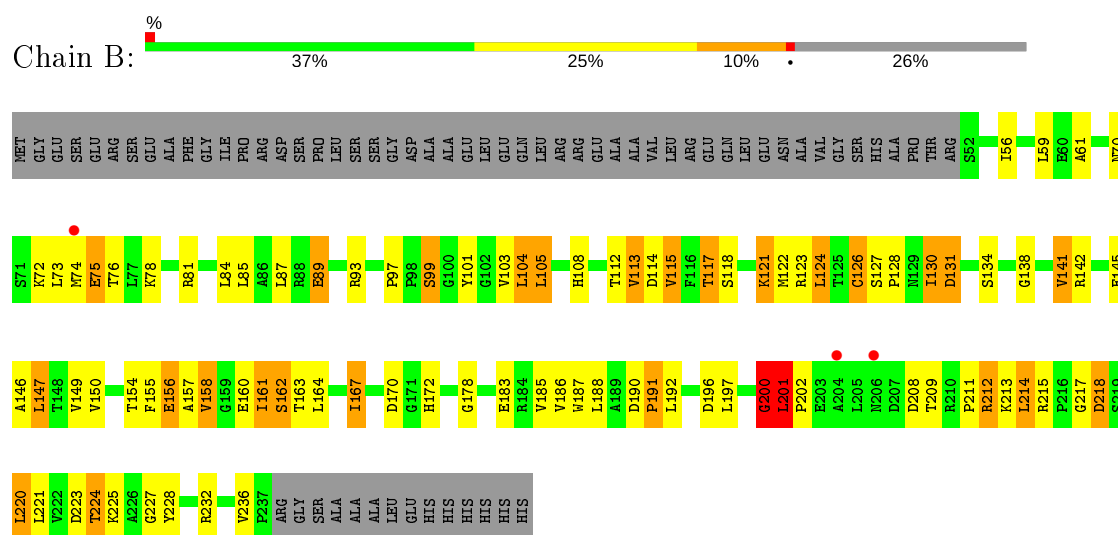
3 Residue-property plots

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

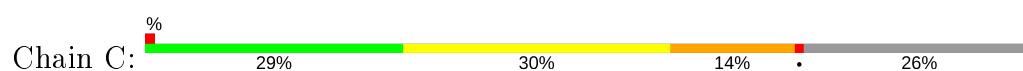
• Molecule 1: Proteasome-associated ATPase

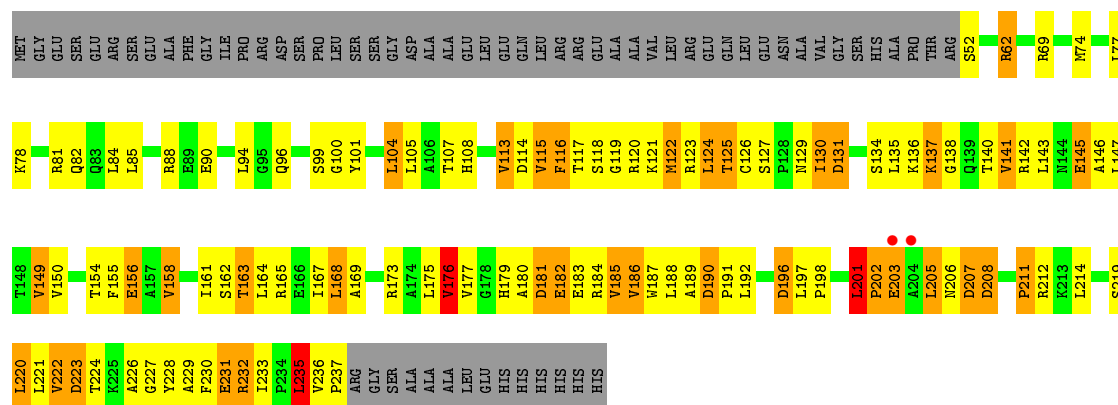


• Molecule 1: Proteasome-associated ATPase

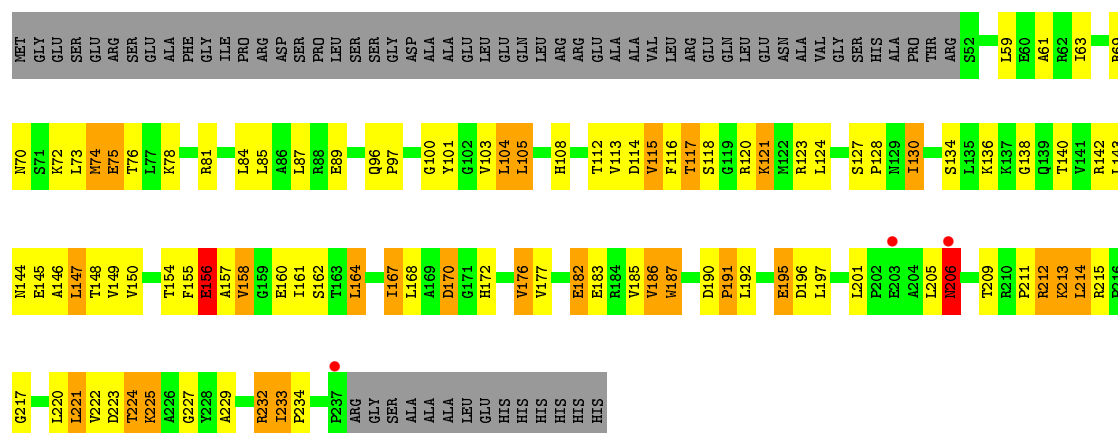


• Molecule 1: Proteasome-associated ATPase

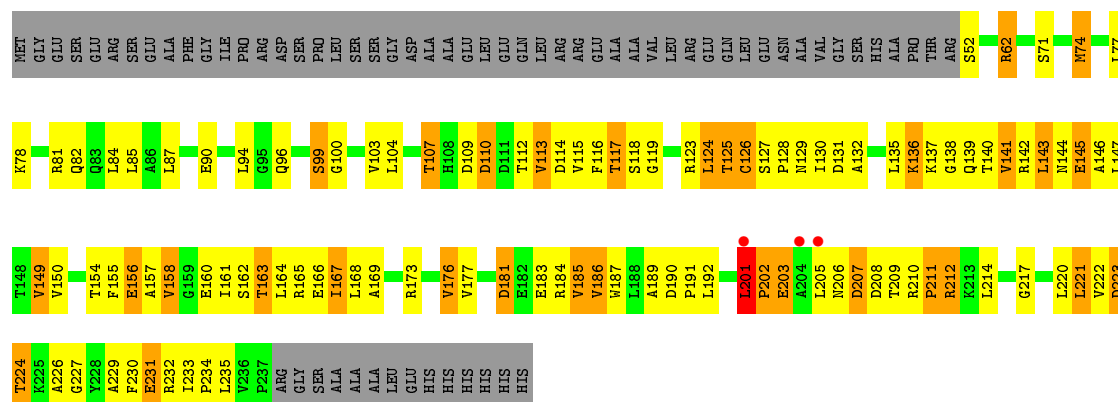
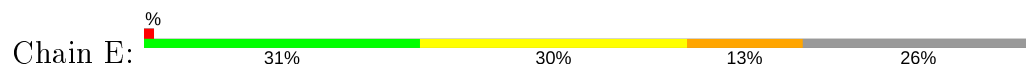




● Molecule 1: Proteasome-associated ATPase

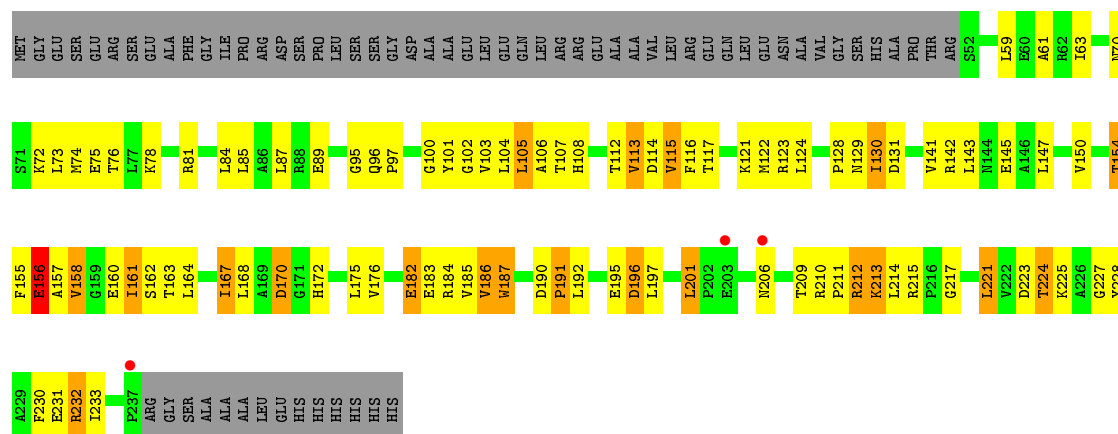


● Molecule 1: Proteasome-associated ATPase

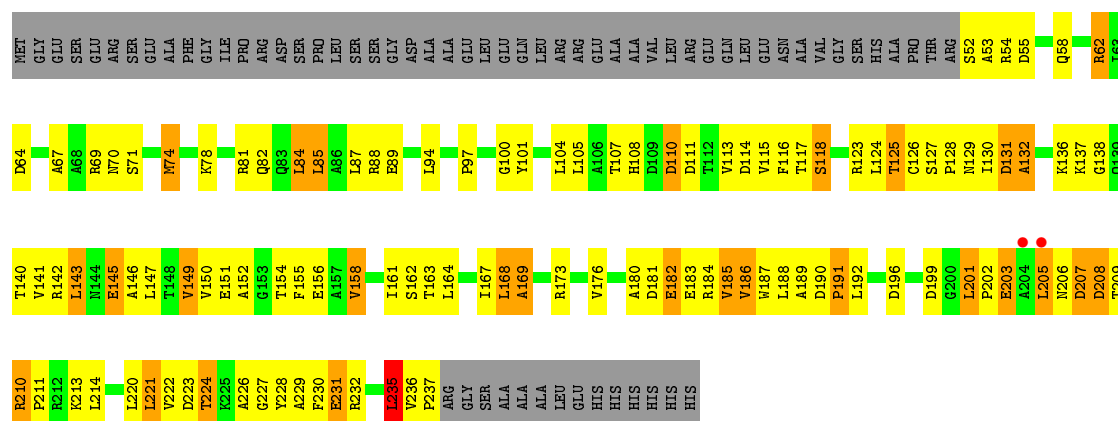
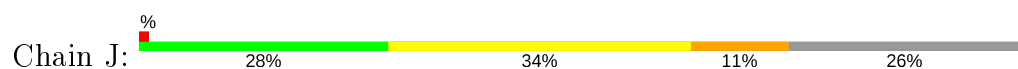


● Molecule 1: Proteasome-associated ATPase

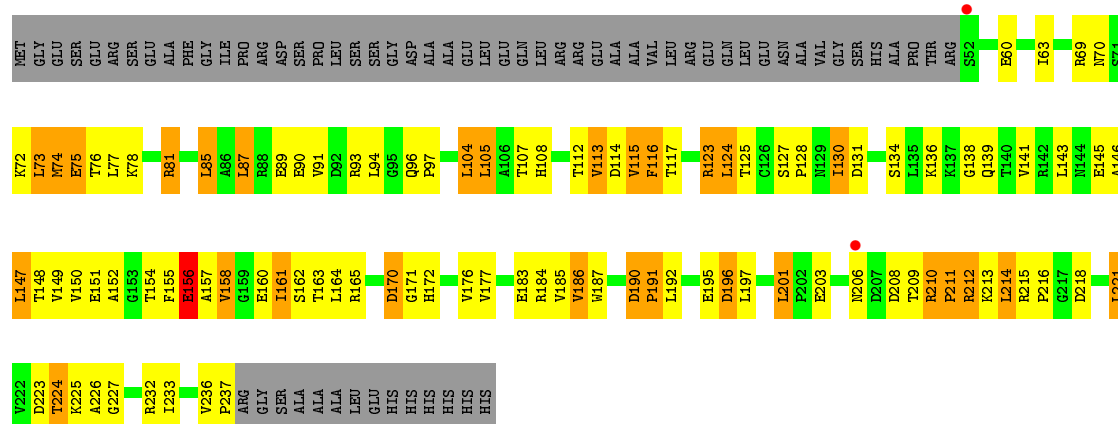




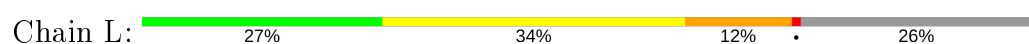
• Molecule 1: Proteasome-associated ATPase

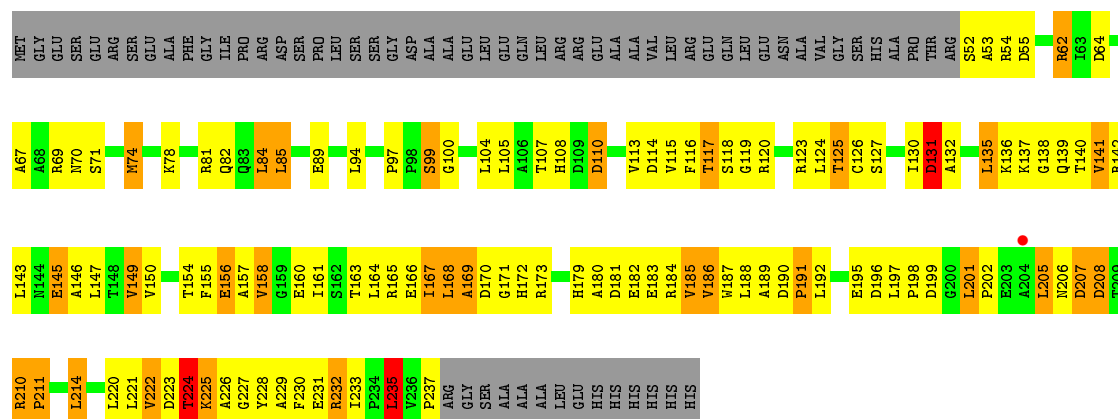


• Molecule 1: Proteasome-associated ATPase

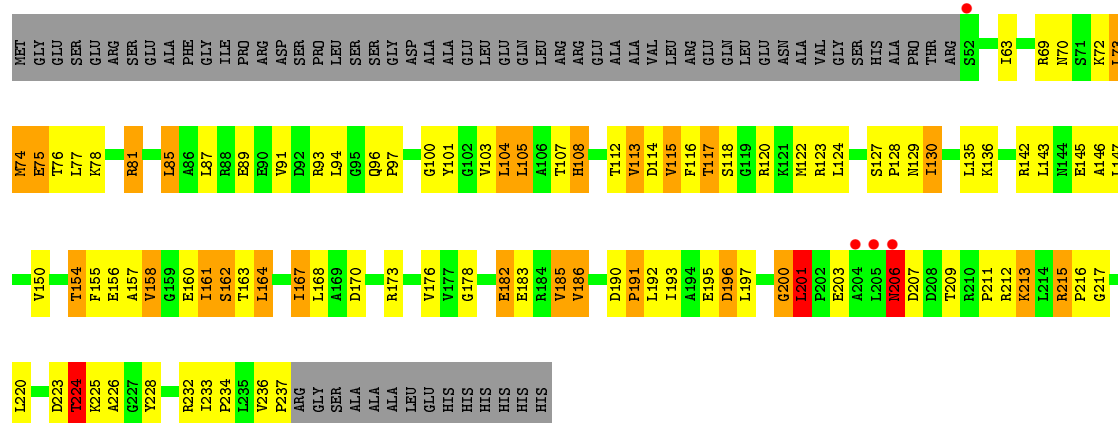


• Molecule 1: Proteasome-associated ATPase

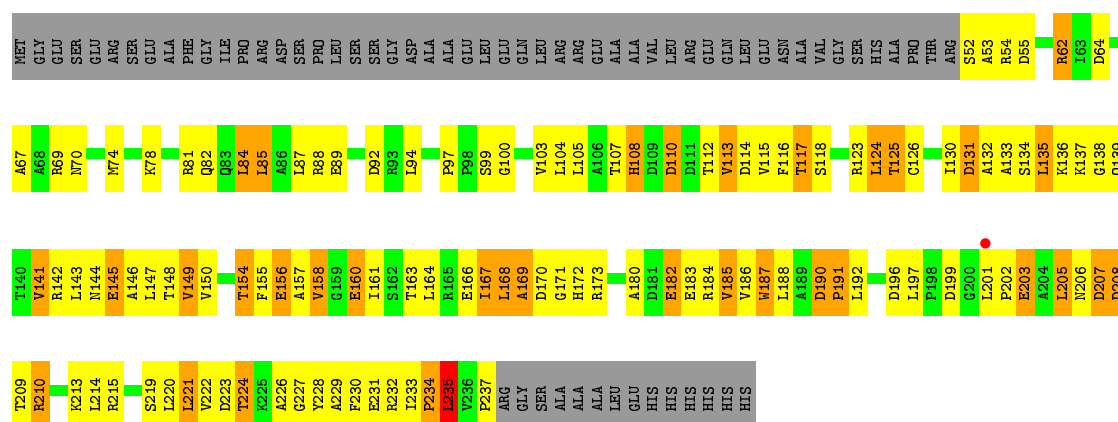
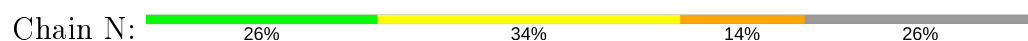




• Molecule 1: Proteasome-associated ATPase

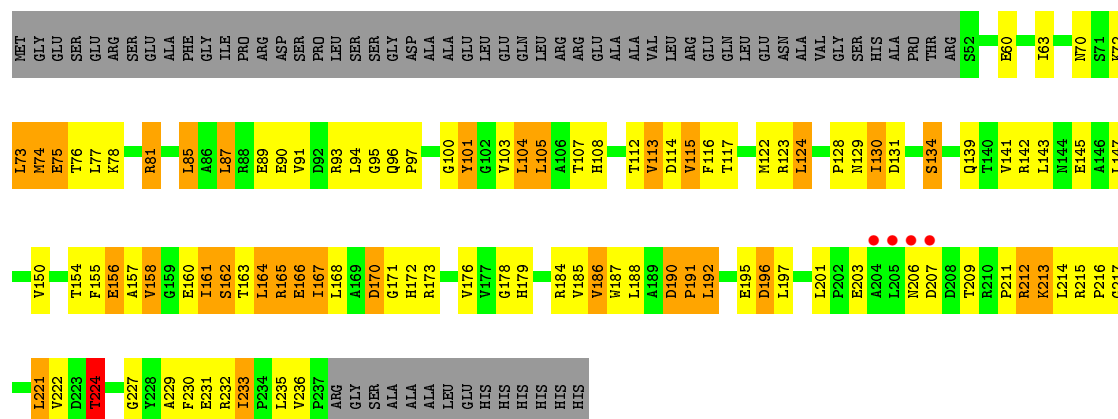


• Molecule 1: Proteasome-associated ATPase

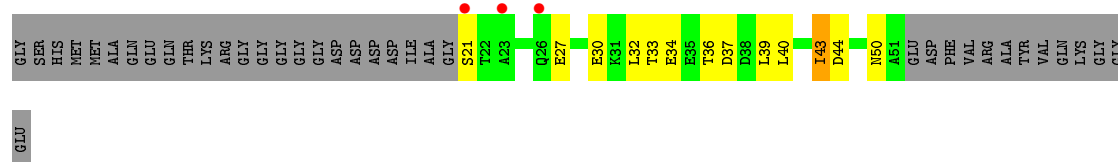


• Molecule 1: Proteasome-associated ATPase

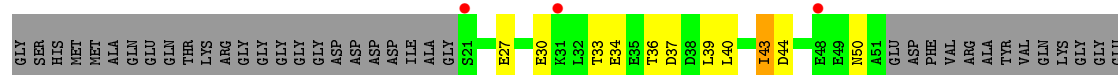
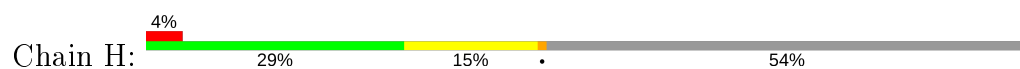




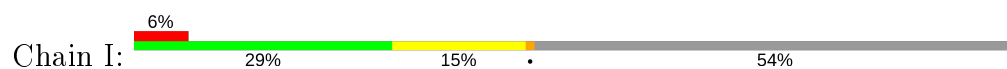
- Molecule 2: Prokaryotic ubiquitin-like protein pup



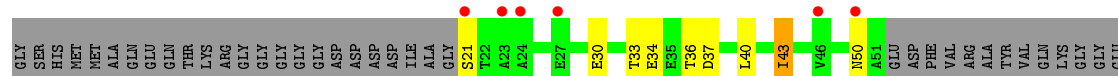
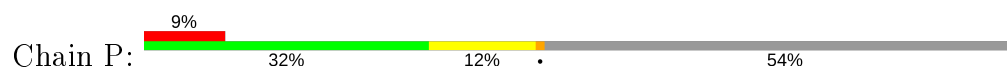
- Molecule 2: Prokaryotic ubiquitin-like protein pup



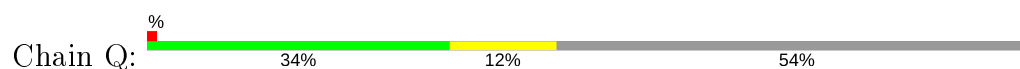
- Molecule 2: Prokaryotic ubiquitin-like protein pup

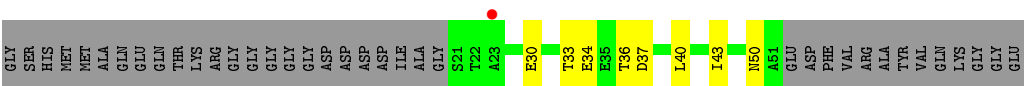


- Molecule 2: Prokaryotic ubiquitin-like protein pup

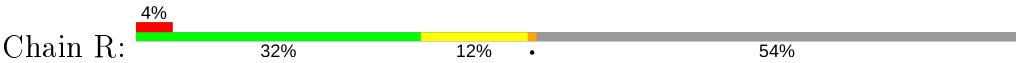


- Molecule 2: Prokaryotic ubiquitin-like protein pup





● Molecule 2: Prokaryotic ubiquitin-like protein pup



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	176.58Å 176.96Å 176.61Å 90.00° 89.94° 90.00°	Depositor
Resolution (Å)	25.00 – 4.50 25.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (25.00-4.50) 98.6 (25.00-3.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.85Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.264 , 0.292 0.246 , 0.272	Depositor DCC
R_{free} test set	5286 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	171.7	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 96.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.187 for -h,-l,-k 0.186 for -h,l,k 0.188 for -k,-h,-l 0.186 for k,h,-l 0.186 for -l,k,h 0.349 for -l,-h,k 0.350 for -k,l,-h 0.349 for -k,-l,h 0.350 for l,h,k 0.358 for h,-k,-l 0.187 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18636	wwPDB-VP
Average B, all atoms (Å ²)	153.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.96	7/1451 (0.5%)	0.93	4/1969 (0.2%)
1	B	0.82	2/1451 (0.1%)	0.90	1/1969 (0.1%)
1	C	0.98	5/1451 (0.3%)	0.96	5/1969 (0.3%)
1	D	0.83	2/1451 (0.1%)	0.89	1/1969 (0.1%)
1	E	0.95	5/1451 (0.3%)	0.96	3/1969 (0.2%)
1	F	0.81	2/1451 (0.1%)	0.90	1/1969 (0.1%)
1	J	0.94	4/1451 (0.3%)	0.95	4/1969 (0.2%)
1	K	0.81	3/1451 (0.2%)	0.90	1/1969 (0.1%)
1	L	0.91	5/1451 (0.3%)	0.95	4/1969 (0.2%)
1	M	0.85	2/1451 (0.1%)	0.91	1/1969 (0.1%)
1	N	0.93	4/1451 (0.3%)	0.94	5/1969 (0.3%)
1	O	0.81	2/1451 (0.1%)	0.90	1/1969 (0.1%)
2	G	0.65	0/243	0.66	0/327
2	H	0.64	0/243	0.65	0/327
2	I	0.65	0/243	0.64	0/327
2	P	0.65	0/243	0.66	0/327
2	Q	0.66	0/243	0.66	0/327
2	R	0.64	0/243	0.65	0/327
All	All	0.87	43/18870 (0.2%)	0.91	31/25590 (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	A	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	M	0	1
All	All	0	5

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	203	GLU	CD-OE2	11.77	1.38	1.25
1	J	208	ASP	CB-CG	7.66	1.67	1.51
1	A	212	ARG	CZ-NH1	-7.20	1.23	1.33
1	E	203	GLU	CG-CD	6.98	1.62	1.51
1	E	208	ASP	CB-CG	6.83	1.66	1.51
1	O	160	GLU	CB-CG	6.79	1.65	1.52
1	L	208	ASP	CB-CG	6.79	1.66	1.51
1	N	203	GLU	CD-OE2	6.66	1.32	1.25
1	A	208	ASP	CB-CG	6.50	1.65	1.51
1	D	160	GLU	CB-CG	6.41	1.64	1.52
1	M	160	GLU	CB-CG	6.29	1.64	1.52
1	J	208	ASP	CG-OD1	6.28	1.39	1.25
1	E	203	GLU	CD-OE1	6.25	1.32	1.25
1	F	160	GLU	CB-CG	6.16	1.63	1.52
1	E	208	ASP	CG-OD1	6.08	1.39	1.25
1	O	160	GLU	CG-CD	6.05	1.61	1.51
1	N	208	ASP	CB-CG	5.98	1.64	1.51
1	D	160	GLU	CG-CD	5.83	1.60	1.51
1	C	208	ASP	CB-CG	5.83	1.64	1.51
1	L	232	ARG	NE-CZ	5.80	1.40	1.33
1	J	64	ASP	CB-CG	5.79	1.64	1.51
1	B	160	GLU	CG-CD	5.78	1.60	1.51
1	C	232	ARG	NE-CZ	5.77	1.40	1.33
1	B	160	GLU	CB-CG	5.75	1.63	1.52
1	F	160	GLU	CG-CD	5.72	1.60	1.51
1	A	160	GLU	CB-CG	5.70	1.62	1.52
1	A	208	ASP	CG-OD1	5.66	1.38	1.25
1	M	160	GLU	CG-CD	5.63	1.60	1.51
1	C	126	CYS	CB-SG	-5.62	1.72	1.81
1	A	126	CYS	CB-SG	-5.58	1.72	1.81
1	N	64	ASP	CB-CG	5.57	1.63	1.51
1	L	208	ASP	CG-OD1	5.55	1.38	1.25
1	K	160	GLU	CB-CG	5.39	1.62	1.52
1	K	160	GLU	CG-CD	5.38	1.60	1.51
1	C	208	ASP	CG-OD1	5.35	1.37	1.25
1	N	160	GLU	CB-CG	5.31	1.62	1.52
1	L	64	ASP	CB-CG	5.24	1.62	1.51
1	E	160	GLU	CB-CG	5.21	1.62	1.52
1	L	160	GLU	CB-CG	5.21	1.62	1.52
1	J	203	GLU	CD-OE1	-5.11	1.20	1.25
1	K	203	GLU	CB-CG	5.10	1.61	1.52
1	A	209	THR	CA-CB	5.02	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	ASP	CB-CG	5.02	1.62	1.51

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	203	GLU	OE1-CD-OE2	8.52	133.53	123.30
1	J	205	LEU	CA-CB-CG	7.72	133.07	115.30
1	L	205	LEU	CA-CB-CG	7.40	132.32	115.30
1	E	205	LEU	CA-CB-CG	7.25	131.99	115.30
1	E	212	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	E	84	LEU	CA-CB-CG	6.70	130.70	115.30
1	C	84	LEU	CA-CB-CG	6.50	130.25	115.30
1	N	203	GLU	OE1-CD-OE2	6.45	131.04	123.30
1	A	84	LEU	CA-CB-CG	6.27	129.72	115.30
1	N	205	LEU	CA-CB-CG	6.12	129.38	115.30
1	A	205	LEU	CA-CB-CG	6.07	129.26	115.30
1	J	84	LEU	CA-CB-CG	5.90	128.88	115.30
1	N	235	LEU	CA-CB-CG	5.88	128.81	115.30
1	L	235	LEU	CA-CB-CG	5.82	128.69	115.30
1	L	232	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	N	84	LEU	CA-CB-CG	5.64	128.28	115.30
1	C	205	LEU	CA-CB-CG	5.58	128.13	115.30
1	L	84	LEU	CA-CB-CG	5.55	128.08	115.30
1	B	200	GLY	N-CA-C	5.50	126.84	113.10
1	O	206	ASN	N-CA-C	5.44	125.70	111.00
1	J	235	LEU	CA-CB-CG	5.44	127.81	115.30
1	J	64	ASP	CB-CG-OD1	5.41	123.17	118.30
1	M	206	ASN	N-CA-C	5.38	125.51	111.00
1	D	206	ASN	N-CA-C	5.37	125.49	111.00
1	C	235	LEU	CA-CB-CG	5.32	127.54	115.30
1	A	235	LEU	CA-CB-CG	5.26	127.40	115.30
1	F	116	PHE	N-CA-C	-5.24	96.86	111.00
1	K	116	PHE	N-CA-C	-5.23	96.89	111.00
1	A	235	LEU	CB-CG-CD2	5.10	119.67	111.00
1	C	176	VAL	CB-CA-C	-5.08	101.74	111.40
1	N	187	TRP	CA-CB-CG	5.04	123.28	113.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	234	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	C	236	VAL	Peptide
1	D	205	LEU	Peptide
1	E	234	PRO	Peptide
1	M	206	ASN	Peptide

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	1431	0	1443	116	0
1	B	1431	0	1443	74	0
1	C	1431	0	1443	98	0
1	D	1431	0	1443	95	0
1	E	1431	0	1443	96	0
1	F	1431	0	1443	90	0
1	J	1431	0	1443	95	0
1	K	1431	0	1443	84	0
1	L	1431	0	1443	107	0
1	M	1431	0	1443	99	0
1	N	1431	0	1443	99	0
1	O	1431	0	1443	98	0
2	G	244	0	222	20	0
2	H	244	0	222	12	0
2	I	244	0	222	17	0
2	P	244	0	222	15	0
2	Q	244	0	222	11	0
2	R	244	0	222	14	0
All	All	18636	0	18648	1081	0

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 29.

All (1081) 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:O:114:ASP:OD1	1:O:123:ARG:HG3	1.41	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:191:PRO:O	1:O:192:LEU:HG	1.46	1.13
1:J:236:VAL:HG12	1:J:237:PRO:HD2	1.27	1.11
1:D:115:VAL:HG21	1:D:124:LEU:HD12	1.30	1.08
1:F:114:ASP:OD1	1:F:123:ARG:HG3	1.56	1.05
1:A:236:VAL:HG12	1:A:237:PRO:HD2	1.36	1.03
1:A:125:THR:HG23	1:D:97:PRO:HG2	1.41	1.03
1:L:117:THR:HG23	1:L:118:SER:H	1.19	1.02
1:M:197:LEU:HB2	1:M:213:LYS:HE3	1.39	1.02
1:F:130:ILE:HD12	1:F:131:ASP:H	1.28	0.99
1:A:236:VAL:HG12	1:A:237:PRO:CD	1.93	0.98
1:E:117:THR:HG23	1:E:118:SER:H	1.27	0.98
1:E:164:LEU:HB2	1:E:220:LEU:HD21	1.46	0.98
1:J:190:ASP:O	1:J:192:LEU:N	1.97	0.97
1:A:190:ASP:O	1:A:192:LEU:N	1.96	0.97
1:N:190:ASP:O	1:N:192:LEU:N	2.00	0.94
1:A:164:LEU:HB2	1:A:220:LEU:HD21	1.50	0.92
1:C:117:THR:HG23	1:C:118:SER:H	1.34	0.91
1:C:190:ASP:O	1:C:192:LEU:N	2.02	0.91
1:E:190:ASP:O	1:E:192:LEU:N	2.03	0.91
1:N:104:LEU:HA	1:N:115:VAL:HG12	1.51	0.91
1:L:190:ASP:O	1:L:192:LEU:N	2.04	0.90
1:A:125:THR:HG23	1:D:97:PRO:CG	2.01	0.89
1:A:232:ARG:O	1:A:233:ILE:HG12	1.69	0.89
1:M:190:ASP:HB2	1:M:191:PRO:CD	2.03	0.88
1:A:104:LEU:HA	1:A:115:VAL:HG12	1.57	0.87
1:C:115:VAL:HG21	1:C:124:LEU:HD21	1.55	0.87
1:E:114:ASP:OD1	1:E:123:ARG:HG3	1.75	0.87
1:C:115:VAL:CG2	1:C:124:LEU:HD21	2.05	0.87
1:L:104:LEU:HA	1:L:115:VAL:HG12	1.57	0.87
1:E:220:LEU:HD12	1:E:229:ALA:HB1	1.59	0.85
1:E:94:LEU:HD11	1:F:128:PRO:HD2	1.59	0.84
1:J:230:PHE:O	1:J:231:GLU:HB3	1.77	0.84
1:D:115:VAL:CG2	1:D:124:LEU:HD12	2.06	0.84
1:L:117:THR:HG23	1:L:118:SER:N	1.91	0.84
1:A:114:ASP:OD1	1:A:123:ARG:HG3	1.78	0.84
1:A:183:GLU:O	1:D:161:ILE:HB	1.76	0.84
1:B:157:ALA:HB1	1:E:173:ARG:NH1	1.93	0.83
1:J:173:ARG:NH1	1:M:157:ALA:HB1	1.94	0.83
1:M:168:LEU:HD12	1:M:173:ARG:HB2	1.61	0.82
1:D:190:ASP:O	1:D:192:LEU:N	2.12	0.82
1:L:186:VAL:HG12	1:L:227:GLY:O	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:114:ASP:OD1	1:K:123:ARG:HG3	1.80	0.82
1:C:117:THR:HG23	1:C:118:SER:N	1.94	0.82
1:B:115:VAL:HG21	1:B:124:LEU:HD13	1.62	0.82
1:M:114:ASP:OD1	1:M:123:ARG:HG3	1.80	0.81
1:D:197:LEU:HB2	1:D:213:LYS:HE3	1.62	0.81
1:O:105:LEU:N	1:O:114:ASP:O	2.13	0.81
1:K:236:VAL:HG22	1:N:166:GLU:OE1	1.80	0.81
1:L:232:ARG:O	1:L:233:ILE:HD13	1.80	0.81
1:M:190:ASP:HB2	1:M:191:PRO:HD3	1.62	0.81
1:A:184:ARG:NH2	1:A:224:THR:O	2.14	0.81
1:C:105:LEU:HA	1:C:228:TYR:HE2	1.44	0.81
1:L:158:VAL:HA	1:M:185:VAL:HG12	1.64	0.80
1:J:236:VAL:CG1	1:J:237:PRO:HD2	2.09	0.79
1:N:126:CYS:HB3	1:N:130:ILE:HD11	1.62	0.79
1:C:117:THR:CG2	1:C:118:SER:H	1.93	0.79
1:J:185:VAL:O	1:M:158:VAL:HG12	1.81	0.79
1:K:157:ALA:HB1	1:N:173:ARG:NH1	1.96	0.79
1:N:192:LEU:HD22	1:N:214:LEU:HD21	1.65	0.79
1:F:197:LEU:HB2	1:F:213:LYS:HE3	1.65	0.79
1:C:185:VAL:HG12	1:F:158:VAL:HA	1.65	0.78
1:J:125:THR:HG23	1:M:97:PRO:HG2	1.63	0.78
1:A:94:LEU:HD11	1:B:128:PRO:HD2	1.66	0.78
1:L:161:ILE:HB	1:M:183:GLU:O	1.83	0.78
1:A:173:ARG:NH1	1:D:157:ALA:HB1	1.99	0.77
1:E:116:PHE:CE1	1:E:226:ALA:HA	2.20	0.77
1:J:104:LEU:HA	1:J:115:VAL:HG12	1.65	0.77
1:L:183:GLU:O	1:O:161:ILE:HB	1.84	0.77
1:E:162:SER:HB3	1:E:177:VAL:O	1.85	0.77
1:L:164:LEU:HB2	1:L:220:LEU:HD21	1.65	0.77
1:D:155:PHE:HE2	1:D:191:PRO:HG2	1.49	0.77
1:L:114:ASP:OD1	1:L:123:ARG:HG3	1.83	0.77
1:C:183:GLU:O	1:F:161:ILE:HB	1.84	0.77
1:E:230:PHE:O	1:E:231:GLU:HB3	1.84	0.77
1:A:168:LEU:HB2	1:A:173:ARG:O	1.85	0.76
1:C:125:THR:O	1:C:149:VAL:HG23	1.85	0.76
1:B:161:ILE:HD13	1:B:221:LEU:HA	1.67	0.76
1:J:186:VAL:HG12	1:J:227:GLY:O	1.84	0.76
1:J:184:ARG:NH2	1:J:224:THR:O	2.17	0.76
1:C:220:LEU:HD12	1:C:229:ALA:HB1	1.66	0.76
1:M:105:LEU:N	1:M:114:ASP:O	2.18	0.75
1:D:190:ASP:HB2	1:D:191:PRO:HD3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LEU:HD21	2:G:40:LEU:HD21	1.67	0.75
1:L:185:VAL:O	1:O:158:VAL:HG12	1.87	0.75
1:M:190:ASP:O	1:M:192:LEU:N	2.19	0.75
1:B:114:ASP:OD1	1:B:123:ARG:HG3	1.86	0.75
1:A:124:LEU:HA	1:D:97:PRO:HB3	1.68	0.75
1:E:186:VAL:HG12	1:E:227:GLY:O	1.87	0.75
1:F:104:LEU:HA	1:F:115:VAL:HA	1.68	0.74
1:K:162:SER:HB3	1:K:176:VAL:HG12	1.69	0.74
1:C:230:PHE:O	1:C:231:GLU:HB3	1.85	0.74
1:J:158:VAL:HA	1:K:185:VAL:HG12	1.68	0.74
1:A:168:LEU:HD12	1:A:173:ARG:HB2	1.67	0.74
1:A:173:ARG:HH12	1:D:157:ALA:HB1	1.53	0.74
1:E:168:LEU:HD12	1:E:173:ARG:HB2	1.69	0.74
1:J:180:ALA:O	1:J:182:GLU:N	2.20	0.74
1:A:161:ILE:HB	1:B:183:GLU:O	1.87	0.74
1:B:190:ASP:O	1:B:192:LEU:N	2.19	0.74
1:K:146:ALA:HB2	2:P:21:SER:HB2	1.67	0.73
1:N:62:ARG:HD2	1:O:63:ILE:HD11	1.69	0.73
1:K:197:LEU:HB2	1:K:213:LYS:HE3	1.71	0.73
1:C:141:VAL:HG23	1:C:142:ARG:N	2.04	0.73
1:N:186:VAL:HG12	1:N:227:GLY:O	1.88	0.73
1:A:186:VAL:HG12	1:A:227:GLY:C	2.09	0.73
1:K:186:VAL:HG12	1:K:227:GLY:C	2.10	0.72
1:K:155:PHE:CE2	1:K:191:PRO:HG2	2.23	0.72
1:J:221:LEU:HD23	1:J:230:PHE:HB2	1.71	0.72
1:J:105:LEU:HA	1:J:228:TYR:HE2	1.52	0.72
1:L:188:LEU:HD23	1:L:192:LEU:HD13	1.72	0.72
1:L:173:ARG:NH1	1:O:157:ALA:HB1	2.04	0.72
1:O:113:VAL:O	1:O:123:ARG:HA	1.89	0.72
1:F:232:ARG:O	1:F:233:ILE:HG12	1.90	0.71
1:J:141:VAL:HG23	1:J:142:ARG:N	2.05	0.71
1:F:105:LEU:N	1:F:114:ASP:O	2.22	0.71
1:A:201:LEU:HB3	1:A:202:PRO:CD	2.21	0.71
1:E:117:THR:HG23	1:E:118:SER:N	2.04	0.71
1:L:114:ASP:OD1	1:L:123:ARG:CG	2.39	0.71
1:B:158:VAL:HG12	1:E:185:VAL:O	1.90	0.71
1:C:206:ASN:O	1:C:207:ASP:HB2	1.89	0.71
1:B:97:PRO:HB3	1:E:124:LEU:HA	1.73	0.71
1:O:197:LEU:HB2	1:O:213:LYS:HE3	1.72	0.71
1:D:127:SER:O	1:D:130:ILE:HB	1.91	0.70
1:D:232:ARG:O	1:D:233:ILE:HG12	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LEU:HD12	1:A:229:ALA:HB1	1.72	0.70
1:F:155:PHE:HE2	1:F:191:PRO:HG2	1.54	0.70
1:A:185:VAL:HG12	1:D:158:VAL:HG12	1.74	0.70
1:E:221:LEU:HD23	1:E:230:PHE:HB2	1.74	0.70
1:L:69:ARG:HH11	1:M:74:MET:CE	2.05	0.70
1:E:186:VAL:HG12	1:E:227:GLY:C	2.11	0.70
1:L:168:LEU:HB2	1:L:173:ARG:O	1.92	0.70
1:O:114:ASP:OD1	1:O:123:ARG:CG	2.30	0.70
1:J:105:LEU:HA	1:J:228:TYR:CE2	2.27	0.70
1:K:158:VAL:HA	1:N:185:VAL:HG12	1.73	0.70
1:B:113:VAL:O	1:B:123:ARG:HA	1.92	0.69
1:E:161:ILE:HB	1:F:183:GLU:O	1.92	0.69
1:M:114:ASP:OD1	1:M:123:ARG:CG	2.41	0.69
1:C:105:LEU:N	1:C:114:ASP:O	2.24	0.69
1:D:124:LEU:HD21	1:D:147:LEU:HB2	1.73	0.69
1:F:114:ASP:OD1	1:F:123:ARG:CG	2.38	0.69
1:L:185:VAL:HG12	1:O:158:VAL:HA	1.75	0.69
1:A:206:ASN:O	1:A:207:ASP:HB2	1.93	0.69
1:A:214:LEU:N	1:A:214:LEU:HD23	2.08	0.68
1:J:125:THR:O	1:J:149:VAL:HG23	1.94	0.68
1:A:185:VAL:HG12	1:D:158:VAL:HA	1.74	0.68
1:M:113:VAL:O	1:M:123:ARG:HA	1.93	0.68
1:N:220:LEU:HD12	1:N:229:ALA:HB1	1.75	0.68
1:M:176:VAL:HG21	1:M:186:VAL:HG11	1.75	0.68
1:O:162:SER:HB2	1:O:176:VAL:HG12	1.76	0.68
1:O:130:ILE:HD12	1:O:131:ASP:H	1.59	0.68
1:B:101:TYR:CE2	1:B:142:ARG:HG3	2.29	0.67
1:F:113:VAL:O	1:F:123:ARG:HA	1.94	0.67
1:C:235:LEU:HD13	1:C:237:PRO:HD3	1.77	0.67
1:J:137:LYS:O	1:J:189:ALA:HB1	1.95	0.67
1:C:124:LEU:HD12	1:C:147:LEU:O	1.94	0.67
1:O:104:LEU:HA	1:O:115:VAL:HA	1.77	0.67
1:M:155:PHE:CE2	1:M:191:PRO:HG2	2.29	0.67
1:C:185:VAL:HG12	1:F:158:VAL:HG12	1.75	0.67
1:N:135:LEU:H	1:N:135:LEU:HD23	1.59	0.67
1:E:78:LYS:O	1:E:81:ARG:N	2.21	0.67
1:L:208:ASP:HB3	1:L:232:ARG:NH2	2.09	0.67
1:B:105:LEU:N	1:B:114:ASP:O	2.24	0.66
1:J:104:LEU:O	1:J:138:GLY:HA2	1.95	0.66
1:J:125:THR:HG23	1:M:97:PRO:CG	2.25	0.66
1:K:236:VAL:HB	1:K:237:PRO:HD2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:206:ASN:O	1:L:207:ASP:HB2	1.93	0.66
1:O:155:PHE:HE2	1:O:191:PRO:HG2	1.59	0.66
1:C:221:LEU:CD2	1:C:230:PHE:HB2	2.24	0.66
1:N:69:ARG:HH11	1:O:74:MET:CE	2.08	0.66
1:L:164:LEU:HB2	1:L:220:LEU:CD2	2.25	0.66
1:F:155:PHE:CE2	1:F:191:PRO:HG2	2.30	0.66
1:E:184:ARG:NH2	1:E:224:THR:O	2.29	0.66
1:A:221:LEU:HD23	1:A:230:PHE:HB2	1.78	0.66
1:F:128:PRO:C	1:F:130:ILE:H	2.00	0.66
1:C:78:LYS:O	1:C:81:ARG:N	2.21	0.66
1:J:168:LEU:HB2	1:J:173:ARG:O	1.96	0.66
1:O:176:VAL:HG21	1:O:186:VAL:HG11	1.77	0.66
1:A:230:PHE:O	1:A:231:GLU:HB3	1.96	0.65
1:J:185:VAL:HG12	1:M:158:VAL:HA	1.78	0.65
1:N:141:VAL:HG23	1:N:142:ARG:N	2.11	0.65
1:J:124:LEU:HA	1:M:97:PRO:HB3	1.77	0.65
1:C:221:LEU:HD23	1:C:230:PHE:HB2	1.79	0.65
1:D:105:LEU:N	1:D:114:ASP:O	2.28	0.65
1:L:221:LEU:HD22	1:L:230:PHE:HB2	1.79	0.65
1:K:212:ARG:HD2	1:K:215:ARG:HG3	1.79	0.65
1:L:124:LEU:HA	1:O:97:PRO:HB3	1.77	0.65
1:A:125:THR:O	1:A:149:VAL:HG23	1.97	0.65
1:J:183:GLU:O	1:M:161:ILE:HB	1.97	0.65
1:L:221:LEU:CD2	1:L:230:PHE:HB2	2.26	0.65
1:F:162:SER:HB3	1:F:176:VAL:HG12	1.79	0.64
1:O:176:VAL:HG21	1:O:186:VAL:CG1	2.27	0.64
1:K:192:LEU:HB3	1:K:214:LEU:CD2	2.28	0.64
1:F:130:ILE:CD1	1:F:131:ASP:H	2.07	0.64
1:C:125:THR:HG23	1:F:97:PRO:HG2	1.80	0.64
1:L:223:ASP:O	1:L:224:THR:C	2.36	0.64
1:B:155:PHE:O	1:B:156:GLU:C	2.36	0.64
1:A:236:VAL:HG12	1:A:237:PRO:HD3	1.80	0.64
1:A:168:LEU:CD1	1:A:173:ARG:HB2	2.28	0.63
1:D:191:PRO:O	1:D:192:LEU:HG	1.98	0.63
1:F:115:VAL:HG21	1:F:124:LEU:HD13	1.79	0.63
1:N:190:ASP:C	1:N:192:LEU:H	2.00	0.63
1:A:114:ASP:OD1	1:A:123:ARG:CG	2.47	0.63
1:A:185:VAL:O	1:D:158:VAL:HG12	1.98	0.63
1:C:124:LEU:HD23	1:C:124:LEU:N	2.14	0.63
1:E:104:LEU:HA	1:E:115:VAL:HG12	1.80	0.63
1:M:104:LEU:HA	1:M:115:VAL:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LEU:HD13	1:A:77:LEU:O	1.98	0.63
1:B:158:VAL:HA	1:E:185:VAL:HG12	1.79	0.63
1:B:192:LEU:HB3	1:B:214:LEU:HD22	1.80	0.63
1:C:116:PHE:HA	1:C:120:ARG:O	1.98	0.63
1:N:186:VAL:CG1	1:N:227:GLY:O	2.47	0.63
1:E:145:GLU:O	1:E:147:LEU:N	2.31	0.63
1:L:186:VAL:CG1	1:L:227:GLY:O	2.47	0.63
1:A:158:VAL:HA	1:B:185:VAL:HG12	1.81	0.63
1:N:126:CYS:HB3	1:N:130:ILE:CD1	2.28	0.63
1:O:170:ASP:C	1:O:172:HIS:H	2.02	0.63
1:F:190:ASP:O	1:F:192:LEU:N	2.32	0.62
1:L:104:LEU:O	1:L:138:GLY:HA2	2.00	0.62
1:O:128:PRO:C	1:O:130:ILE:H	2.01	0.62
1:B:187:TRP:N	1:B:227:GLY:O	2.31	0.62
1:D:192:LEU:HB3	1:D:214:LEU:HD22	1.81	0.62
1:N:116:PHE:CE1	1:N:226:ALA:HA	2.35	0.62
1:O:164:LEU:O	1:O:164:LEU:HD13	1.98	0.62
1:B:157:ALA:HB1	1:E:173:ARG:HH11	1.64	0.62
1:L:190:ASP:C	1:L:192:LEU:H	2.02	0.62
1:B:190:ASP:HB2	1:B:191:PRO:HD2	1.81	0.62
1:C:168:LEU:HB2	1:C:173:ARG:O	1.99	0.62
1:J:94:LEU:HD11	1:K:128:PRO:HD2	1.81	0.62
1:L:173:ARG:HH12	1:O:157:ALA:HB1	1.63	0.62
1:C:201:LEU:HB3	1:C:202:PRO:CD	2.30	0.61
1:C:173:ARG:NH1	1:F:157:ALA:HB1	2.15	0.61
1:J:114:ASP:OD1	1:J:123:ARG:HG3	1.99	0.61
1:M:162:SER:HB3	1:M:178:GLY:HA2	1.82	0.61
1:A:232:ARG:C	1:A:233:ILE:HG12	2.20	0.61
1:D:209:THR:HA	1:D:232:ARG:HH21	1.64	0.61
1:E:77:LEU:HD13	1:E:77:LEU:O	2.00	0.61
1:N:117:THR:O	1:N:118:SER:C	2.38	0.61
1:N:69:ARG:HH11	1:O:74:MET:HE3	1.64	0.61
1:E:164:LEU:HB2	1:E:220:LEU:CD2	2.27	0.61
1:M:157:ALA:O	1:M:158:VAL:HG13	2.00	0.61
1:D:104:LEU:HA	1:D:115:VAL:HA	1.82	0.61
1:D:232:ARG:O	1:D:233:ILE:CG1	2.48	0.61
1:L:230:PHE:O	1:L:231:GLU:HB3	2.00	0.61
1:M:108:HIS:HB3	1:M:112:THR:OG1	2.01	0.61
1:A:117:THR:O	1:A:118:SER:C	2.39	0.61
1:C:105:LEU:HA	1:C:228:TYR:CE2	2.32	0.61
1:C:163:THR:O	1:C:176:VAL:HG12	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:LEU:HA	1:A:228:TYR:HE2	1.65	0.61
1:C:158:VAL:HA	1:D:185:VAL:HG12	1.83	0.61
1:F:128:PRO:O	1:F:130:ILE:N	2.33	0.61
1:K:161:ILE:HD13	1:K:221:LEU:HA	1.83	0.61
1:O:190:ASP:HB2	1:O:191:PRO:HD3	1.81	0.61
1:F:161:ILE:HD13	1:F:221:LEU:HA	1.83	0.60
1:L:69:ARG:HH11	1:M:74:MET:HE3	1.65	0.60
1:C:235:LEU:CD1	1:C:237:PRO:HD3	2.31	0.60
1:J:173:ARG:HH12	1:M:157:ALA:HB1	1.66	0.60
1:K:73:LEU:HD11	2:P:50:ASN:ND2	2.17	0.60
1:K:158:VAL:HG12	1:N:185:VAL:O	2.02	0.60
1:O:162:SER:HB3	1:O:178:GLY:HA2	1.84	0.60
1:O:72:LYS:O	1:O:76:THR:HG23	2.01	0.60
1:A:81:ARG:HH21	2:G:43:ILE:HG12	1.66	0.60
1:N:84:LEU:HD13	1:N:84:LEU:O	2.01	0.60
1:C:221:LEU:HD23	1:C:221:LEU:O	2.02	0.60
1:E:201:LEU:HB3	1:E:202:PRO:CD	2.32	0.60
1:A:78:LYS:O	1:A:81:ARG:N	2.26	0.59
1:C:114:ASP:OD1	1:C:123:ARG:HG3	2.01	0.59
1:M:162:SER:HB2	1:M:176:VAL:HG12	1.84	0.59
1:N:100:GLY:O	1:N:143:LEU:N	2.34	0.59
1:J:117:THR:O	1:J:118:SER:C	2.40	0.59
1:M:116:PHE:CE1	1:M:226:ALA:HA	2.37	0.59
1:D:155:PHE:CE2	1:D:191:PRO:HG2	2.34	0.59
1:M:91:VAL:HA	1:M:94:LEU:HD12	1.82	0.59
1:K:209:THR:HA	1:K:232:ARG:HH21	1.68	0.59
1:M:104:LEU:HD21	1:M:136:LYS:O	2.02	0.59
1:M:190:ASP:C	1:M:192:LEU:H	2.06	0.59
1:O:157:ALA:O	1:O:158:VAL:HG13	2.03	0.59
1:B:212:ARG:HG3	1:B:213:LYS:N	2.18	0.59
2:I:33:THR:HA	2:I:36:THR:HB	1.85	0.59
1:A:236:VAL:CG1	1:A:237:PRO:HD2	2.20	0.59
1:F:190:ASP:HB2	1:F:191:PRO:HD3	1.84	0.59
1:B:190:ASP:HB2	1:B:191:PRO:CD	2.33	0.59
1:N:168:LEU:HB2	1:N:173:ARG:O	2.03	0.59
1:O:209:THR:HA	1:O:232:ARG:HH21	1.68	0.59
1:J:168:LEU:CD1	1:J:173:ARG:HB2	2.33	0.59
1:J:206:ASN:O	1:J:207:ASP:HB2	2.01	0.59
1:K:125:THR:O	1:K:148:THR:HG23	2.03	0.59
1:M:72:LYS:O	1:M:76:THR:HG23	2.02	0.59
1:F:155:PHE:O	1:F:156:GLU:C	2.41	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:LYS:HB3	1:D:190:ASP:OD2	2.02	0.58
1:L:124:LEU:HD23	1:L:124:LEU:N	2.18	0.58
1:L:141:VAL:HG23	1:L:142:ARG:N	2.17	0.58
1:A:186:VAL:HG12	1:A:227:GLY:O	2.03	0.58
1:K:162:SER:HB3	1:K:176:VAL:CG1	2.32	0.58
1:K:91:VAL:HA	1:K:94:LEU:HD12	1.84	0.58
1:L:185:VAL:O	1:L:185:VAL:HG12	2.02	0.58
1:N:94:LEU:HD11	1:O:128:PRO:HD2	1.86	0.58
1:C:62:ARG:HD2	1:D:63:ILE:HD11	1.84	0.58
1:O:203:GLU:OE2	1:O:212:ARG:NH2	2.37	0.58
2:P:36:THR:HG22	2:P:37:ASP:N	2.18	0.58
1:B:104:LEU:HA	1:B:115:VAL:HA	1.86	0.58
1:K:190:ASP:O	1:K:192:LEU:N	2.33	0.58
1:N:235:LEU:HD11	1:N:237:PRO:HG3	1.86	0.58
1:L:84:LEU:O	1:L:84:LEU:HD13	2.03	0.58
1:L:125:THR:HG23	1:O:97:PRO:HG2	1.85	0.58
1:N:85:LEU:HD21	2:Q:40:LEU:HD21	1.85	0.58
1:A:208:ASP:C	1:A:210:ARG:H	2.07	0.57
1:L:180:ALA:O	1:L:182:GLU:HG3	2.03	0.57
1:A:208:ASP:O	1:A:210:ARG:N	2.37	0.57
1:B:108:HIS:CE1	1:B:123:ARG:HD2	2.38	0.57
1:K:157:ALA:HB1	1:N:173:ARG:HH11	1.67	0.57
1:M:127:SER:O	1:M:130:ILE:HB	2.04	0.57
1:N:223:ASP:O	1:N:224:THR:C	2.42	0.57
1:L:185:VAL:HG12	1:O:158:VAL:HG12	1.86	0.57
1:D:128:PRO:C	1:D:130:ILE:H	2.07	0.57
2:I:36:THR:HG22	2:I:37:ASP:N	2.20	0.57
1:N:203:GLU:OE2	1:N:208:ASP:OD2	2.22	0.57
2:P:30:GLU:O	2:P:34:GLU:HB2	2.05	0.57
1:D:155:PHE:O	1:D:156:GLU:C	2.42	0.57
1:N:232:ARG:O	1:N:233:ILE:HD13	2.04	0.57
2:Q:30:GLU:O	2:Q:34:GLU:HB2	2.05	0.57
1:L:161:ILE:HD13	1:L:221:LEU:HA	1.86	0.57
1:C:116:PHE:CE1	1:C:226:ALA:HA	2.40	0.57
1:B:161:ILE:CD1	1:B:221:LEU:HA	2.34	0.56
1:F:103:VAL:HG12	1:F:104:LEU:N	2.21	0.56
1:K:170:ASP:C	1:K:172:HIS:H	2.07	0.56
1:F:232:ARG:O	1:F:233:ILE:CG1	2.54	0.56
1:K:72:LYS:O	1:K:76:THR:HG23	2.04	0.56
1:E:135:LEU:HD23	1:E:135:LEU:H	1.70	0.56
1:K:97:PRO:HB3	1:N:124:LEU:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:36:THR:HG22	2:R:37:ASP:N	2.21	0.56
1:A:105:LEU:O	1:A:228:TYR:OH	2.20	0.56
1:C:185:VAL:CG1	1:F:158:VAL:HA	2.33	0.56
1:K:69:ARG:HD3	2:P:50:ASN:HA	1.87	0.56
1:A:125:THR:HG23	1:D:97:PRO:HG3	1.86	0.56
1:A:141:VAL:HG23	1:A:142:ARG:N	2.20	0.56
1:C:115:VAL:CG2	1:C:124:LEU:CD2	2.83	0.56
1:D:186:VAL:HG12	1:D:227:GLY:C	2.25	0.56
2:H:33:THR:HA	2:H:36:THR:HB	1.88	0.56
1:L:184:ARG:NH2	1:L:224:THR:O	2.36	0.56
1:E:117:THR:CG2	1:E:118:SER:H	2.10	0.56
1:O:73:LEU:C	1:O:75:GLU:H	2.09	0.56
1:J:186:VAL:CG1	1:J:227:GLY:O	2.54	0.56
1:N:157:ALA:O	1:N:158:VAL:HG13	2.06	0.56
1:D:192:LEU:HB3	1:D:214:LEU:CD2	2.35	0.55
2:G:36:THR:HG22	2:G:37:ASP:N	2.21	0.55
1:J:220:LEU:HD12	1:J:229:ALA:HB1	1.87	0.55
1:D:72:LYS:O	1:D:76:THR:HG23	2.05	0.55
1:L:126:CYS:HB3	1:L:130:ILE:HD11	1.87	0.55
1:K:136:LYS:HB3	1:K:190:ASP:OD2	2.06	0.55
1:O:161:ILE:HD13	1:O:221:LEU:HA	1.88	0.55
2:Q:33:THR:HA	2:Q:36:THR:OG1	2.06	0.55
1:C:114:ASP:OD1	1:C:123:ARG:CG	2.54	0.55
1:F:95:GLY:O	1:F:142:ARG:NH2	2.38	0.55
1:F:209:THR:HG22	1:F:232:ARG:HH21	1.70	0.55
1:C:127:SER:O	1:C:130:ILE:HD12	2.06	0.55
1:F:213:LYS:O	1:F:215:ARG:HG2	2.07	0.55
1:J:85:LEU:HD21	2:P:40:LEU:HD21	1.88	0.55
1:A:124:LEU:N	1:A:124:LEU:HD23	2.21	0.55
1:F:128:PRO:C	1:F:130:ILE:N	2.59	0.55
1:M:100:GLY:N	1:M:143:LEU:O	2.30	0.55
2:R:30:GLU:O	2:R:34:GLU:HB2	2.07	0.55
1:E:127:SER:O	1:E:130:ILE:HD12	2.07	0.55
1:O:91:VAL:HA	1:O:94:LEU:HD12	1.87	0.55
1:E:158:VAL:HG12	1:F:185:VAL:HG12	1.87	0.55
1:F:72:LYS:O	1:F:76:THR:HG23	2.07	0.55
1:L:192:LEU:HD22	1:L:214:LEU:HD11	1.89	0.55
1:A:125:THR:CG2	1:D:97:PRO:HG2	2.28	0.55
1:B:97:PRO:HG2	1:E:125:THR:HG23	1.88	0.55
1:F:170:ASP:C	1:F:172:HIS:H	2.09	0.55
1:J:188:LEU:HD23	1:J:192:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:128:PRO:C	1:M:130:ILE:H	2.10	0.55
1:N:155:PHE:O	1:N:156:GLU:C	2.45	0.55
1:N:105:LEU:HG	1:N:228:TYR:HE2	1.72	0.55
1:B:220:LEU:HD12	1:B:220:LEU:N	2.22	0.54
1:C:184:ARG:NH2	1:C:224:THR:O	2.40	0.54
1:D:167:ILE:HG22	1:D:168:LEU:H	1.72	0.54
1:E:168:LEU:HB2	1:E:173:ARG:O	2.07	0.54
1:E:190:ASP:C	1:E:192:LEU:H	2.03	0.54
1:E:90:GLU:O	1:E:94:LEU:HG	2.07	0.54
1:D:69:ARG:HB3	2:I:50:ASN:ND2	2.21	0.54
1:J:127:SER:N	1:J:130:ILE:HD11	2.22	0.54
1:M:115:VAL:HG21	1:M:124:LEU:HD12	1.89	0.54
1:J:185:VAL:HG12	1:M:158:VAL:HG12	1.89	0.54
1:L:166:GLU:OE1	1:O:236:VAL:HG22	2.08	0.54
1:B:161:ILE:HB	1:E:183:GLU:O	2.06	0.54
1:C:94:LEU:HD11	1:D:128:PRO:HD2	1.90	0.54
1:J:116:PHE:CE1	1:J:226:ALA:HA	2.43	0.54
1:K:130:ILE:HD12	1:K:131:ASP:H	1.71	0.54
1:L:221:LEU:HD23	1:L:221:LEU:C	2.28	0.54
1:B:73:LEU:C	1:B:75:GLU:H	2.10	0.54
1:E:145:GLU:C	1:E:147:LEU:H	2.11	0.54
1:E:164:LEU:HD12	1:E:165:ARG:N	2.22	0.54
1:J:100:GLY:O	1:J:143:LEU:N	2.39	0.54
1:K:116:PHE:CE1	1:K:226:ALA:HA	2.42	0.54
1:J:84:LEU:O	1:J:84:LEU:HD13	2.08	0.54
1:J:69:ARG:HH11	1:K:74:MET:CE	2.20	0.54
1:L:69:ARG:HH11	1:M:74:MET:HE1	1.72	0.54
1:O:100:GLY:N	1:O:143:LEU:O	2.33	0.54
1:A:214:LEU:HD23	1:A:214:LEU:H	1.70	0.54
1:B:104:LEU:HD23	1:B:138:GLY:H	1.72	0.54
1:F:176:VAL:HG21	1:F:186:VAL:CG2	2.38	0.54
1:B:114:ASP:OD1	1:B:123:ARG:CG	2.55	0.54
1:M:195:GLU:O	1:M:197:LEU:N	2.40	0.54
1:B:157:ALA:HB1	1:E:173:ARG:HH12	1.71	0.54
1:D:116:PHE:CZ	1:D:225:LYS:O	2.61	0.54
1:E:135:LEU:HB2	1:E:139:GLN:NE2	2.23	0.54
1:B:209:THR:HA	1:B:232:ARG:HH21	1.72	0.53
1:E:155:PHE:O	1:E:156:GLU:C	2.45	0.53
1:C:101:TYR:HE2	1:D:123:ARG:HB2	1.72	0.53
2:R:33:THR:HA	2:R:36:THR:OG1	2.09	0.53
1:B:72:LYS:O	1:B:76:THR:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:VAL:HG22	1:E:166:GLU:OE1	2.09	0.53
2:G:33:THR:HA	2:G:36:THR:HB	1.91	0.53
1:N:221:LEU:HD23	1:N:221:LEU:O	2.08	0.53
1:M:73:LEU:HD11	2:R:50:ASN:HD21	1.73	0.53
1:L:222:VAL:HG23	1:L:223:ASP:N	2.24	0.53
1:F:175:LEU:HD21	1:J:54:ARG:HH22	1.73	0.53
1:F:73:LEU:C	1:F:75:GLU:H	2.11	0.53
1:L:166:GLU:HG3	1:L:167:ILE:O	2.08	0.53
1:N:124:LEU:HD23	1:N:124:LEU:N	2.24	0.53
1:F:187:TRP:N	1:F:227:GLY:O	2.34	0.53
1:J:192:LEU:HB3	1:J:214:LEU:HD11	1.91	0.53
1:K:190:ASP:C	1:K:192:LEU:H	2.11	0.53
1:L:155:PHE:CE2	1:L:191:PRO:HG2	2.44	0.53
1:N:188:LEU:HD23	1:N:192:LEU:HD13	1.91	0.53
1:C:135:LEU:HD23	1:C:135:LEU:H	1.74	0.53
1:F:162:SER:CB	1:F:176:VAL:HG12	2.38	0.53
1:M:162:SER:HB2	1:M:176:VAL:CG1	2.38	0.53
1:F:100:GLY:O	1:F:143:LEU:N	2.34	0.53
1:L:145:GLU:O	1:L:147:LEU:N	2.32	0.53
1:B:117:THR:O	1:B:118:SER:C	2.46	0.52
1:D:73:LEU:C	1:D:75:GLU:H	2.13	0.52
1:E:103:VAL:HG11	1:E:230:PHE:HZ	1.75	0.52
1:J:162:SER:HB3	1:J:176:VAL:HB	1.91	0.52
1:M:73:LEU:C	1:M:75:GLU:H	2.12	0.52
1:A:188:LEU:HD23	1:A:192:LEU:HD13	1.91	0.52
1:J:127:SER:C	1:J:129:ASN:H	2.13	0.52
1:L:105:LEU:O	1:L:228:TYR:OH	2.14	0.52
1:A:220:LEU:HD23	1:A:220:LEU:N	2.24	0.52
1:C:180:ALA:O	1:C:182:GLU:N	2.43	0.52
1:C:90:GLU:O	1:C:94:LEU:HG	2.10	0.52
1:J:190:ASP:C	1:J:192:LEU:H	2.05	0.52
1:K:155:PHE:HE2	1:K:191:PRO:HG2	1.68	0.52
1:O:155:PHE:O	1:O:156:GLU:C	2.47	0.52
2:P:50:ASN:O	2:P:50:ASN:OD1	2.28	0.52
2:R:33:THR:HA	2:R:36:THR:CB	2.39	0.52
1:B:73:LEU:O	1:B:75:GLU:N	2.43	0.52
1:C:77:LEU:O	1:C:77:LEU:HD13	2.08	0.52
1:O:100:GLY:O	1:O:101:TYR:HD2	1.93	0.52
1:O:230:PHE:O	1:O:231:GLU:HB3	2.10	0.52
1:J:168:LEU:HD13	1:J:173:ARG:HB2	1.90	0.52
1:A:126:CYS:HB3	1:A:130:ILE:CD1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LEU:C	1:A:77:LEU:HD13	2.30	0.52
1:E:223:ASP:O	1:E:224:THR:C	2.48	0.52
1:J:53:ALA:O	1:J:54:ARG:C	2.47	0.52
1:K:155:PHE:O	1:K:156:GLU:C	2.46	0.52
1:L:116:PHE:CE1	1:L:226:ALA:HA	2.44	0.52
1:N:167:ILE:HG22	1:N:168:LEU:H	1.75	0.52
1:C:208:ASP:HB3	1:C:232:ARG:NH2	2.24	0.52
1:E:158:VAL:HA	1:F:185:VAL:HG12	1.91	0.52
1:L:94:LEU:HD11	1:M:128:PRO:HD2	1.92	0.52
1:N:221:LEU:HD23	1:N:230:PHE:HB2	1.91	0.52
1:O:73:LEU:O	1:O:75:GLU:N	2.43	0.52
2:P:33:THR:HA	2:P:36:THR:OG1	2.10	0.52
1:B:103:VAL:HG12	1:B:104:LEU:N	2.25	0.52
1:B:190:ASP:C	1:B:192:LEU:H	2.12	0.52
2:G:30:GLU:O	2:G:34:GLU:HB2	2.09	0.52
1:J:137:LYS:O	1:J:189:ALA:CB	2.58	0.52
1:K:139:GLN:O	1:K:141:VAL:HG13	2.10	0.52
1:M:164:LEU:HD13	1:M:164:LEU:O	2.10	0.52
1:C:125:THR:HG23	1:F:97:PRO:CG	2.39	0.51
1:C:190:ASP:C	1:C:192:LEU:H	2.08	0.51
1:F:162:SER:HB2	1:F:176:VAL:CG1	2.41	0.51
2:I:30:GLU:O	2:I:34:GLU:HB2	2.10	0.51
1:O:168:LEU:HD12	1:O:173:ARG:HB2	1.92	0.51
1:C:104:LEU:O	1:C:104:LEU:HG	2.10	0.51
1:E:206:ASN:O	1:E:207:ASP:HB2	2.11	0.51
1:F:230:PHE:O	1:F:231:GLU:HB3	2.09	0.51
1:J:69:ARG:HH11	1:K:74:MET:HE3	1.74	0.51
1:M:117:THR:O	1:M:118:SER:C	2.48	0.51
1:M:223:ASP:O	1:M:225:LYS:N	2.43	0.51
1:O:134:SER:O	1:O:134:SER:OG	2.28	0.51
1:M:73:LEU:HD11	2:R:50:ASN:ND2	2.25	0.51
1:F:115:VAL:HG23	1:F:122:MET:O	2.11	0.51
1:C:131:ASP:HB3	1:C:134:SER:OG	2.10	0.51
1:N:104:LEU:O	1:N:138:GLY:HA2	2.11	0.51
1:L:182:GLU:HB3	1:O:179:HIS:HB3	1.92	0.51
1:A:170:ASP:O	1:A:172:HIS:N	2.44	0.51
1:J:124:LEU:N	1:J:124:LEU:HD23	2.26	0.51
1:L:118:SER:O	1:L:120:ARG:N	2.43	0.51
1:O:190:ASP:O	1:O:192:LEU:N	2.42	0.51
1:F:73:LEU:O	1:F:75:GLU:N	2.43	0.51
1:N:158:VAL:HA	1:O:185:VAL:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:33:THR:HA	2:Q:36:THR:CB	2.41	0.51
2:Q:50:ASN:O	2:Q:50:ASN:OD1	2.29	0.51
1:C:168:LEU:HD12	1:C:173:ARG:HB2	1.93	0.51
1:K:115:VAL:HG21	1:K:124:LEU:HD13	1.93	0.51
1:L:127:SER:O	1:L:130:ILE:CD1	2.59	0.51
1:L:126:CYS:HB3	1:L:130:ILE:CD1	2.41	0.51
1:N:53:ALA:O	1:N:54:ARG:C	2.49	0.51
1:K:73:LEU:C	1:K:75:GLU:H	2.13	0.51
1:A:162:SER:OG	1:A:222:VAL:HG11	2.11	0.51
1:C:232:ARG:O	1:C:233:ILE:HD13	2.11	0.51
1:F:190:ASP:C	1:F:192:LEU:H	2.14	0.51
2:H:40:LEU:HA	2:H:43:ILE:HB	1.92	0.51
1:J:105:LEU:O	1:J:228:TYR:OH	2.27	0.51
1:D:108:HIS:HB2	1:D:112:THR:O	2.10	0.51
1:B:218:ASP:N	1:B:218:ASP:OD1	2.45	0.50
1:J:161:ILE:HB	1:K:183:GLU:O	2.11	0.50
1:N:110:ASP:HB2	1:N:112:THR:HG23	1.93	0.50
1:N:126:CYS:CB	1:N:130:ILE:HD11	2.38	0.50
1:N:78:LYS:O	1:N:81:ARG:N	2.43	0.50
1:A:135:LEU:HD23	1:A:135:LEU:H	1.76	0.50
1:D:144:ASN:OD1	1:D:148:THR:HB	2.11	0.50
1:D:157:ALA:O	1:D:158:VAL:HG13	2.11	0.50
1:E:163:THR:O	1:E:176:VAL:HG12	2.12	0.50
1:E:192:LEU:HB3	1:E:214:LEU:HD11	1.93	0.50
1:B:197:LEU:HB2	1:B:213:LYS:HE3	1.91	0.50
1:J:192:LEU:HD22	1:J:214:LEU:HD11	1.93	0.50
1:J:220:LEU:HD23	1:J:220:LEU:N	2.26	0.50
1:J:223:ASP:O	1:J:224:THR:C	2.49	0.50
1:K:108:HIS:HB2	1:K:112:THR:O	2.12	0.50
1:N:158:VAL:HG12	1:O:185:VAL:HG12	1.93	0.50
1:O:85:LEU:O	1:O:89:GLU:HB2	2.11	0.50
1:A:208:ASP:HB3	1:A:232:ARG:HH21	1.76	0.50
1:A:232:ARG:HG2	1:A:233:ILE:H	1.76	0.50
1:E:232:ARG:C	1:E:233:ILE:HG12	2.32	0.50
1:N:208:ASP:HB3	1:N:232:ARG:NH2	2.27	0.50
1:N:92:ASP:OD1	2:Q:33:THR:HG21	2.11	0.50
1:O:155:PHE:CE2	1:O:191:PRO:HG2	2.43	0.50
1:A:136:LYS:H	1:A:139:GLN:NE2	2.09	0.50
2:H:36:THR:HG22	2:H:37:ASP:N	2.27	0.50
1:L:192:LEU:HB3	1:L:214:LEU:CD1	2.40	0.50
1:L:220:LEU:HD12	1:L:229:ALA:HB1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:89:GLU:O	1:O:93:ARG:HG3	2.11	0.50
2:Q:36:THR:HG22	2:Q:37:ASP:N	2.25	0.50
2:R:50:ASN:O	2:R:50:ASN:OD1	2.30	0.50
1:E:141:VAL:HG23	1:E:142:ARG:N	2.26	0.50
1:K:97:PRO:HG2	1:N:125:THR:HG23	1.93	0.50
1:O:128:PRO:C	1:O:130:ILE:N	2.64	0.50
1:A:105:LEU:HA	1:A:228:TYR:CE2	2.44	0.50
1:B:200:GLY:HA3	1:B:215:ARG:NH1	2.26	0.50
1:D:146:ALA:HB2	2:I:21:SER:HB2	1.94	0.50
1:E:192:LEU:HD22	1:E:214:LEU:HD11	1.94	0.50
2:I:40:LEU:HA	2:I:43:ILE:HB	1.94	0.50
1:J:220:LEU:H	1:J:220:LEU:HD23	1.76	0.50
1:L:99:SER:HB3	1:L:142:ARG:HH11	1.77	0.50
1:N:180:ALA:O	1:N:182:GLU:N	2.41	0.50
1:O:170:ASP:C	1:O:172:HIS:N	2.63	0.50
1:A:100:GLY:O	1:A:143:LEU:N	2.42	0.50
1:E:220:LEU:HD12	1:E:229:ALA:CB	2.37	0.50
1:C:168:LEU:HD21	1:F:233:ILE:HD12	1.94	0.50
2:H:30:GLU:O	2:H:34:GLU:HB2	2.11	0.50
1:L:125:THR:O	1:L:149:VAL:HG23	2.11	0.50
1:N:158:VAL:HG12	1:O:185:VAL:O	2.11	0.50
1:O:170:ASP:O	1:O:172:HIS:N	2.45	0.50
1:C:186:VAL:HG12	1:C:227:GLY:O	2.11	0.49
1:C:69:ARG:HD2	1:D:74:MET:HE3	1.94	0.49
1:K:192:LEU:HB3	1:K:214:LEU:HD22	1.94	0.49
1:M:85:LEU:O	1:M:89:GLU:HB2	2.12	0.49
1:O:235:LEU:HG	1:O:236:VAL:N	2.27	0.49
1:E:136:LYS:HD3	1:E:136:LYS:N	2.28	0.49
1:E:223:ASP:O	1:E:226:ALA:N	2.45	0.49
1:L:235:LEU:CD1	1:L:237:PRO:HD3	2.42	0.49
1:A:88:ARG:HD3	2:G:36:THR:HG21	1.95	0.49
1:F:162:SER:HB2	1:F:176:VAL:HG11	1.94	0.49
1:L:62:ARG:HD2	1:M:63:ILE:HD11	1.95	0.49
1:D:103:VAL:HG12	1:D:104:LEU:N	2.27	0.49
1:K:97:PRO:CG	1:N:125:THR:HG23	2.41	0.49
1:L:208:ASP:HB3	1:L:232:ARG:HH22	1.75	0.49
1:N:144:ASN:HD21	1:N:148:THR:HB	1.77	0.49
1:O:128:PRO:O	1:O:130:ILE:N	2.45	0.49
1:K:105:LEU:N	1:K:114:ASP:O	2.21	0.49
1:L:235:LEU:HD13	1:L:237:PRO:HD3	1.94	0.49
1:M:115:VAL:HG23	1:M:122:MET:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:223:ASP:O	1:M:224:THR:C	2.50	0.49
1:A:192:LEU:HB3	1:A:214:LEU:HD11	1.94	0.49
1:C:188:LEU:HD23	1:C:192:LEU:HD13	1.95	0.49
1:D:190:ASP:CB	1:D:191:PRO:HD3	2.42	0.49
1:E:77:LEU:C	1:E:77:LEU:HD13	2.33	0.49
1:M:212:ARG:HD2	1:M:215:ARG:HG3	1.95	0.49
1:N:112:THR:HG21	1:N:123:ARG:HH21	1.77	0.49
1:O:191:PRO:O	1:O:192:LEU:CG	2.39	0.49
1:O:187:TRP:N	1:O:227:GLY:O	2.43	0.49
1:O:73:LEU:C	1:O:75:GLU:N	2.65	0.49
1:D:118:SER:O	1:D:120:ARG:HG2	2.12	0.49
1:J:78:LYS:O	1:J:81:ARG:N	2.45	0.49
1:O:232:ARG:O	1:O:233:ILE:HG12	2.12	0.49
1:C:124:LEU:HA	1:F:97:PRO:HB3	1.94	0.49
1:K:162:SER:CB	1:K:176:VAL:CG1	2.91	0.49
1:L:220:LEU:N	1:L:220:LEU:HD23	2.28	0.49
1:L:167:ILE:HG22	1:L:168:LEU:H	1.78	0.49
1:O:101:TYR:CE2	1:O:142:ARG:HG3	2.47	0.49
1:D:100:GLY:N	1:D:143:LEU:O	2.31	0.49
2:I:33:THR:HA	2:I:36:THR:CB	2.43	0.49
1:K:128:PRO:C	1:K:130:ILE:H	2.16	0.49
1:A:113:VAL:O	1:A:123:ARG:HA	2.13	0.48
1:A:124:LEU:H	1:A:124:LEU:HD23	1.78	0.48
1:A:208:ASP:C	1:A:210:ARG:N	2.66	0.48
1:C:104:LEU:O	1:C:138:GLY:HA2	2.13	0.48
2:H:33:THR:HA	2:H:36:THR:CB	2.43	0.48
1:J:67:ALA:O	1:J:70:ASN:HB3	2.13	0.48
1:L:53:ALA:O	1:L:54:ARG:C	2.51	0.48
1:O:176:VAL:CG2	1:O:186:VAL:CG1	2.91	0.48
1:O:176:VAL:CG2	1:O:186:VAL:HG13	2.43	0.48
1:A:155:PHE:O	1:A:156:GLU:C	2.51	0.48
1:A:190:ASP:C	1:A:192:LEU:H	2.06	0.48
1:A:211:PRO:O	1:A:212:ARG:HB3	2.13	0.48
1:A:158:VAL:HG12	1:B:185:VAL:O	2.13	0.48
1:D:73:LEU:O	1:D:75:GLU:N	2.46	0.48
1:K:161:ILE:HB	1:N:183:GLU:O	2.13	0.48
1:L:232:ARG:O	1:L:233:ILE:CD1	2.57	0.48
1:D:170:ASP:C	1:D:172:HIS:H	2.16	0.48
1:F:130:ILE:HD12	1:F:131:ASP:N	2.11	0.48
1:K:73:LEU:HD11	2:P:50:ASN:HD21	1.77	0.48
1:M:164:LEU:HB3	1:M:220:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:85:LEU:O	1:K:89:GLU:HB2	2.14	0.48
1:M:69:ARG:HB3	2:R:50:ASN:ND2	2.28	0.48
1:N:145:GLU:C	1:N:147:LEU:H	2.17	0.48
1:A:90:GLU:O	1:A:94:LEU:HG	2.14	0.48
1:B:146:ALA:HB2	2:G:21:SER:HB2	1.94	0.48
1:K:113:VAL:O	1:K:123:ARG:HA	2.13	0.48
1:L:168:LEU:HD12	1:L:173:ARG:HB2	1.95	0.48
1:M:130:ILE:HD13	1:M:130:ILE:HA	1.69	0.48
1:F:105:LEU:HD22	1:F:121:LYS:NZ	2.29	0.48
1:K:89:GLU:O	1:K:93:ARG:HG3	2.14	0.48
1:L:125:THR:HG23	1:O:97:PRO:CG	2.44	0.48
1:L:225:LYS:O	1:L:226:ALA:C	2.48	0.48
2:P:33:THR:HA	2:P:36:THR:CB	2.43	0.48
1:A:136:LYS:N	1:A:136:LYS:HD3	2.28	0.48
1:A:201:LEU:HB3	1:A:202:PRO:HD3	1.96	0.48
1:L:155:PHE:O	1:L:156:GLU:C	2.52	0.48
2:R:33:THR:HA	2:R:36:THR:HB	1.95	0.48
1:A:208:ASP:HB3	1:A:232:ARG:NH2	2.28	0.48
1:A:184:ARG:HE	1:A:224:THR:HG22	1.79	0.48
1:C:155:PHE:O	1:C:156:GLU:C	2.52	0.48
1:D:190:ASP:HB2	1:D:191:PRO:CD	2.42	0.48
1:E:158:VAL:HG12	1:F:185:VAL:O	2.12	0.48
1:J:230:PHE:O	1:J:231:GLU:CB	2.54	0.48
1:L:117:THR:CG2	1:L:118:SER:N	2.64	0.48
1:L:124:LEU:HA	1:O:97:PRO:CB	2.42	0.48
1:M:232:ARG:O	1:M:233:ILE:HG12	2.14	0.48
1:A:188:LEU:N	1:A:188:LEU:HD12	2.29	0.48
1:A:81:ARG:HE	2:G:43:ILE:CG1	2.26	0.48
1:E:166:GLU:HG3	1:E:167:ILE:O	2.14	0.48
2:I:50:ASN:O	2:I:50:ASN:OD1	2.32	0.48
1:C:221:LEU:HD23	1:C:221:LEU:C	2.34	0.48
1:D:117:THR:O	1:D:118:SER:C	2.53	0.48
2:G:33:THR:HA	2:G:36:THR:CB	2.44	0.48
2:H:39:LEU:O	2:H:43:ILE:HB	2.14	0.48
1:M:73:LEU:O	1:M:75:GLU:N	2.47	0.48
1:O:101:TYR:CD2	1:O:142:ARG:HG3	2.49	0.48
1:C:223:ASP:O	1:C:224:THR:C	2.52	0.47
1:E:135:LEU:HB2	1:E:139:GLN:HE21	1.78	0.47
1:E:167:ILE:H	1:E:167:ILE:HD12	1.79	0.47
1:J:87:LEU:HD12	1:K:87:LEU:HD12	1.95	0.47
1:M:101:TYR:CE2	1:M:142:ARG:HG3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LEU:HD12	1:A:173:ARG:CB	2.41	0.47
1:B:158:VAL:HG12	1:E:185:VAL:HG12	1.96	0.47
1:C:192:LEU:HD22	1:C:214:LEU:HD11	1.96	0.47
1:F:223:ASP:O	1:F:225:LYS:N	2.47	0.47
1:J:164:LEU:HB2	1:J:220:LEU:CD2	2.44	0.47
1:M:186:VAL:HG23	1:M:228:TYR:HA	1.96	0.47
1:E:96:GLN:HG3	1:E:96:GLN:O	2.12	0.47
1:M:73:LEU:C	1:M:75:GLU:N	2.67	0.47
1:O:165:ARG:O	1:O:166:GLU:HB3	2.14	0.47
1:J:124:LEU:HD12	1:J:147:LEU:O	2.15	0.47
1:N:81:ARG:HE	2:Q:43:ILE:HG12	1.80	0.47
1:A:117:THR:HG23	1:A:118:SER:N	2.30	0.47
1:E:157:ALA:O	1:E:158:VAL:HG13	2.15	0.47
1:F:212:ARG:HD2	1:F:215:ARG:HG3	1.94	0.47
2:G:40:LEU:HA	2:G:43:ILE:HB	1.96	0.47
1:E:217:GLY:O	1:J:58:GLN:HG3	2.14	0.47
1:A:236:VAL:CG1	1:A:237:PRO:CD	2.81	0.47
1:C:137:LYS:O	1:C:189:ALA:HB1	2.15	0.47
1:D:161:ILE:HD13	1:D:221:LEU:HA	1.97	0.47
1:F:161:ILE:HD13	1:F:161:ILE:HA	1.69	0.47
1:F:184:ARG:NH2	1:F:224:THR:O	2.48	0.47
1:C:88:ARG:CZ	2:I:36:THR:HG23	2.45	0.47
1:N:221:LEU:CD2	1:N:230:PHE:HB2	2.44	0.47
1:B:187:TRP:O	1:B:228:TYR:HA	2.14	0.47
1:D:162:SER:HB2	1:D:176:VAL:CG1	2.44	0.47
1:E:124:LEU:CD2	1:E:124:LEU:N	2.78	0.47
1:M:89:GLU:O	1:M:93:ARG:HG3	2.14	0.47
1:A:184:ARG:NE	1:A:224:THR:HG22	2.30	0.47
1:N:233:ILE:HA	1:N:234:PRO:HD2	1.68	0.47
1:B:97:PRO:CG	1:E:125:THR:HG23	2.44	0.47
1:A:185:VAL:CG1	1:D:158:VAL:HG12	2.42	0.47
1:F:209:THR:HG22	1:F:232:ARG:NH2	2.29	0.47
1:F:73:LEU:C	1:F:75:GLU:N	2.68	0.47
1:A:81:ARG:HE	2:G:43:ILE:HG12	1.79	0.47
1:J:114:ASP:OD1	1:J:123:ARG:CG	2.62	0.47
1:M:155:PHE:O	1:M:156:GLU:C	2.54	0.47
1:M:190:ASP:O	1:M:193:ILE:N	2.46	0.47
1:N:190:ASP:HB2	1:N:191:PRO:HD3	1.95	0.47
1:C:127:SER:O	1:C:130:ILE:CD1	2.63	0.47
1:D:162:SER:HB3	1:D:176:VAL:HG12	1.97	0.47
1:J:189:ALA:O	1:J:190:ASP:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:78:LYS:O	1:L:81:ARG:N	2.48	0.47
1:N:67:ALA:O	1:N:70:ASN:HB3	2.15	0.47
1:A:124:LEU:N	1:A:124:LEU:CD2	2.78	0.46
1:B:73:LEU:C	1:B:75:GLU:N	2.68	0.46
1:L:139:GLN:HB3	1:L:155:PHE:CE1	2.50	0.46
1:N:185:VAL:HG12	1:N:185:VAL:O	2.14	0.46
1:A:99:SER:HB2	1:B:123:ARG:HB2	1.97	0.46
1:B:162:SER:HB3	1:B:178:GLY:HA2	1.98	0.46
1:C:188:LEU:HB3	1:C:192:LEU:HD12	1.96	0.46
1:D:195:GLU:O	1:D:213:LYS:NZ	2.35	0.46
1:E:107:THR:HA	1:E:113:VAL:HG12	1.97	0.46
1:E:62:ARG:HD2	1:F:63:ILE:HD11	1.97	0.46
1:F:186:VAL:HG12	1:F:227:GLY:C	2.35	0.46
1:K:73:LEU:C	1:K:75:GLU:N	2.68	0.46
1:K:73:LEU:O	1:K:75:GLU:N	2.48	0.46
1:O:222:VAL:HG12	1:O:229:ALA:HA	1.96	0.46
1:A:96:GLN:HG3	1:A:96:GLN:O	2.14	0.46
1:E:136:LYS:HD3	1:E:136:LYS:H	1.80	0.46
2:I:39:LEU:O	2:I:43:ILE:HB	2.15	0.46
1:L:127:SER:N	1:L:130:ILE:HD11	2.30	0.46
1:L:222:VAL:CG2	1:L:223:ASP:N	2.77	0.46
1:A:185:VAL:HG12	1:A:185:VAL:O	2.16	0.46
1:F:157:ALA:O	1:F:158:VAL:HG13	2.15	0.46
1:J:131:ASP:O	1:J:132:ALA:C	2.54	0.46
1:K:151:GLU:HG2	1:K:152:ALA:N	2.31	0.46
1:K:221:LEU:HG	1:K:221:LEU:O	2.13	0.46
1:J:190:ASP:CB	1:J:191:PRO:HD3	2.46	0.46
1:L:85:LEU:HD21	2:R:40:LEU:HD21	1.97	0.46
1:C:100:GLY:O	1:C:143:LEU:N	2.45	0.46
1:L:164:LEU:HD12	1:L:165:ARG:N	2.30	0.46
1:J:126:CYS:HB3	1:J:130:ILE:HD11	1.97	0.46
1:N:124:LEU:HD12	1:N:147:LEU:O	2.15	0.46
1:O:130:ILE:HA	1:O:130:ILE:HD13	1.72	0.46
1:C:123:ARG:HD2	1:F:101:TYR:OH	2.16	0.46
1:D:187:TRP:CD1	1:D:187:TRP:N	2.83	0.46
1:M:203:GLU:OE2	1:M:212:ARG:NH2	2.49	0.46
1:O:108:HIS:HB2	1:O:112:THR:O	2.16	0.46
1:L:145:GLU:C	1:L:147:LEU:H	2.18	0.46
1:A:124:LEU:HA	1:D:97:PRO:CB	2.43	0.46
1:D:103:VAL:O	1:D:116:PHE:N	2.49	0.46
1:D:162:SER:HB2	1:D:176:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:ILE:HB	1:D:183:GLU:O	2.15	0.46
1:K:130:ILE:HD13	1:K:130:ILE:HA	1.67	0.46
1:L:170:ASP:O	1:L:172:HIS:N	2.49	0.46
1:L:197:LEU:HA	1:L:198:PRO:HD3	1.89	0.46
1:M:127:SER:HA	1:M:128:PRO:HD2	1.83	0.46
1:C:77:LEU:HD13	1:C:77:LEU:C	2.36	0.45
1:D:191:PRO:C	1:D:192:LEU:HG	2.34	0.45
1:K:146:ALA:O	1:K:147:LEU:C	2.54	0.45
1:M:167:ILE:H	1:M:167:ILE:HG13	1.52	0.45
1:O:213:LYS:O	1:O:215:ARG:HG2	2.16	0.45
1:K:69:ARG:HB3	2:P:50:ASN:ND2	2.30	0.45
1:A:110:ASP:N	1:A:110:ASP:OD2	2.48	0.45
1:A:223:ASP:O	1:A:226:ALA:N	2.48	0.45
1:C:161:ILE:HD13	1:C:161:ILE:HA	1.73	0.45
1:C:81:ARG:NE	2:I:43:ILE:HG23	2.31	0.45
1:B:97:PRO:CB	1:E:124:LEU:HA	2.45	0.45
1:F:101:TYR:HB3	1:F:102:GLY:H	1.57	0.45
1:F:162:SER:CB	1:F:176:VAL:CG1	2.95	0.45
1:J:155:PHE:O	1:J:156:GLU:C	2.53	0.45
1:N:206:ASN:O	1:N:207:ASP:CB	2.64	0.45
2:P:40:LEU:HA	2:P:43:ILE:HB	1.97	0.45
1:J:168:LEU:O	1:J:169:ALA:C	2.55	0.45
1:J:185:VAL:HG12	1:M:158:VAL:CG1	2.45	0.45
1:B:212:ARG:HD2	1:B:215:ARG:HG3	1.98	0.45
1:C:220:LEU:CD1	1:C:229:ALA:HB1	2.40	0.45
1:D:96:GLN:HA	1:D:97:PRO:HD2	1.80	0.45
1:K:151:GLU:HG2	1:K:152:ALA:H	1.82	0.45
1:N:145:GLU:O	1:N:147:LEU:N	2.47	0.45
1:B:130:ILE:HD12	1:B:131:ASP:H	1.82	0.45
1:E:100:GLY:O	1:E:143:LEU:N	2.50	0.45
1:L:137:LYS:O	1:L:189:ALA:HB1	2.17	0.45
1:N:114:ASP:OD1	1:N:123:ARG:HG3	2.17	0.45
2:P:33:THR:C	2:P:36:THR:HB	2.37	0.45
1:A:197:LEU:HA	1:A:198:PRO:HD3	1.86	0.45
1:E:144:ASN:OD1	1:E:147:LEU:N	2.50	0.45
1:L:67:ALA:O	1:L:70:ASN:HB3	2.16	0.45
1:D:73:LEU:C	1:D:75:GLU:N	2.70	0.45
1:N:131:ASP:O	1:N:133:ALA:N	2.49	0.45
1:B:223:ASP:O	1:B:224:THR:C	2.56	0.45
1:F:182:GLU:HG2	1:F:182:GLU:O	2.17	0.45
1:F:192:LEU:HB3	1:F:214:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:208:ASP:C	1:J:210:ARG:H	2.21	0.45
1:K:232:ARG:O	1:K:233:ILE:HG12	2.17	0.45
1:M:186:VAL:HG23	1:M:228:TYR:CA	2.47	0.45
1:N:135:LEU:HB2	1:N:139:GLN:HE21	1.80	0.45
2:R:33:THR:C	2:R:36:THR:HB	2.37	0.45
1:D:164:LEU:HD13	1:D:164:LEU:O	2.16	0.45
1:E:127:SER:O	1:E:130:ILE:CD1	2.65	0.45
1:E:104:LEU:HD23	1:E:138:GLY:H	1.82	0.45
1:E:220:LEU:N	1:E:220:LEU:HD23	2.32	0.45
1:F:108:HIS:HB2	1:F:112:THR:O	2.17	0.45
1:F:186:VAL:HG12	1:F:228:TYR:N	2.32	0.45
1:J:62:ARG:HD2	1:K:63:ILE:HD11	1.98	0.45
1:L:161:ILE:CD1	1:L:221:LEU:HA	2.47	0.45
1:C:104:LEU:HD23	1:C:138:GLY:H	1.82	0.44
1:D:127:SER:HA	1:D:128:PRO:HD2	1.83	0.44
1:D:162:SER:CB	1:D:176:VAL:HG12	2.47	0.44
1:D:176:VAL:CG2	1:D:186:VAL:HG22	2.47	0.44
1:E:168:LEU:HD13	1:E:173:ARG:HH21	1.82	0.44
1:J:101:TYR:OH	1:K:123:ARG:HD2	2.17	0.44
1:M:154:THR:HB	1:M:155:PHE:H	1.16	0.44
1:N:230:PHE:O	1:N:231:GLU:HB3	2.17	0.44
1:A:137:LYS:O	1:A:189:ALA:HA	2.18	0.44
2:G:33:THR:C	2:G:36:THR:HB	2.37	0.44
1:J:101:TYR:HH	1:K:123:ARG:HD2	1.81	0.44
1:M:233:ILE:HA	1:M:234:PRO:HD2	1.75	0.44
1:L:124:LEU:HD23	1:L:124:LEU:H	1.82	0.44
1:N:190:ASP:CB	1:N:191:PRO:HD3	2.48	0.44
1:A:124:LEU:HD12	1:A:147:LEU:O	2.18	0.44
1:B:172:HIS:O	1:B:188:LEU:HD12	2.17	0.44
1:D:128:PRO:C	1:D:130:ILE:N	2.70	0.44
1:E:114:ASP:OD1	1:E:123:ARG:CG	2.58	0.44
1:J:124:LEU:HA	1:M:97:PRO:CB	2.47	0.44
1:L:100:GLY:O	1:L:143:LEU:N	2.43	0.44
1:L:124:LEU:N	1:L:124:LEU:CD2	2.80	0.44
1:M:115:VAL:HG21	1:M:124:LEU:CD1	2.47	0.44
1:J:158:VAL:HG12	1:K:185:VAL:O	2.18	0.44
1:M:225:LYS:HA	1:M:225:LYS:HD2	1.89	0.44
1:N:164:LEU:HB2	1:N:220:LEU:CD2	2.48	0.44
1:E:124:LEU:HD12	1:E:147:LEU:O	2.18	0.44
1:J:221:LEU:CD2	1:J:230:PHE:HB2	2.44	0.44
1:O:184:ARG:NH2	1:O:224:THR:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:96:GLN:HA	1:O:97:PRO:HD2	1.67	0.44
1:C:164:LEU:HB2	1:C:220:LEU:CD2	2.47	0.44
1:D:104:LEU:HD23	1:D:138:GLY:H	1.82	0.44
1:L:235:LEU:HD21	1:L:237:PRO:HG3	2.00	0.44
1:O:214:LEU:HD12	1:O:214:LEU:HA	1.73	0.44
1:A:223:ASP:O	1:A:224:THR:C	2.55	0.44
1:B:141:VAL:HG23	1:B:142:ARG:N	2.33	0.44
1:D:59:LEU:C	1:D:61:ALA:N	2.71	0.44
1:F:192:LEU:HB3	1:F:214:LEU:CD2	2.47	0.44
1:L:131:ASP:O	1:L:132:ALA:C	2.56	0.44
1:D:147:LEU:H	1:D:147:LEU:HG	1.49	0.44
1:M:215:ARG:HA	1:M:216:PRO:HD3	1.81	0.44
2:P:33:THR:HA	2:P:36:THR:HB	2.00	0.44
1:A:187:TRP:HD1	1:A:187:TRP:H	1.66	0.43
1:C:96:GLN:HG3	1:C:96:GLN:O	2.18	0.43
2:G:39:LEU:O	2:G:43:ILE:HB	2.18	0.43
1:K:161:ILE:HD13	1:K:161:ILE:HA	1.73	0.43
1:M:100:GLY:O	1:M:101:TYR:HD2	2.01	0.43
1:M:195:GLU:C	1:M:197:LEU:H	2.21	0.43
1:N:69:ARG:HH11	1:O:74:MET:HE1	1.80	0.43
1:D:222:VAL:HG12	1:D:229:ALA:HA	1.99	0.43
1:E:137:LYS:O	1:E:189:ALA:HB1	2.17	0.43
1:F:191:PRO:C	1:F:192:LEU:HG	2.39	0.43
1:J:236:VAL:CG1	1:J:237:PRO:CD	2.90	0.43
1:K:104:LEU:HD23	1:K:138:GLY:H	1.83	0.43
1:M:197:LEU:HD13	1:M:212:ARG:O	2.18	0.43
1:N:105:LEU:O	1:N:228:TYR:OH	2.24	0.43
1:N:154:THR:HB	1:N:155:PHE:H	1.19	0.43
1:N:87:LEU:HD12	1:O:87:LEU:HD12	1.98	0.43
1:A:162:SER:HB3	1:A:177:VAL:O	2.18	0.43
1:D:212:ARG:HD2	1:D:215:ARG:HG3	1.99	0.43
1:L:114:ASP:OD1	1:L:123:ARG:HD2	2.19	0.43
1:N:168:LEU:HA	1:N:168:LEU:HD23	1.79	0.43
1:N:206:ASN:O	1:N:207:ASP:HB2	2.18	0.43
1:B:108:HIS:HB3	1:B:112:THR:OG1	2.17	0.43
1:B:191:PRO:C	1:B:192:LEU:HG	2.38	0.43
1:B:214:LEU:HD12	1:B:214:LEU:HA	1.73	0.43
1:D:103:VAL:HG12	1:D:104:LEU:H	1.83	0.43
1:F:154:THR:HB	1:F:155:PHE:H	1.17	0.43
1:L:168:LEU:O	1:L:169:ALA:C	2.57	0.43
1:A:180:ALA:O	1:A:181:ASP:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:LEU:HD11	1:C:143:LEU:HD22	2.00	0.43
1:C:145:GLU:O	1:C:147:LEU:N	2.49	0.43
1:C:122:MET:HB3	1:F:100:GLY:HA2	2.01	0.43
1:K:190:ASP:HB2	1:K:191:PRO:HD3	2.00	0.43
1:L:116:PHE:CZ	1:L:226:ALA:HA	2.53	0.43
1:A:135:LEU:N	1:A:135:LEU:HD23	2.33	0.43
1:D:130:ILE:HD13	1:D:130:ILE:HA	1.60	0.43
1:E:202:PRO:HB2	1:E:203:GLU:H	1.72	0.43
1:E:184:ARG:NE	1:E:224:THR:HG22	2.33	0.43
1:K:157:ALA:HB1	1:N:173:ARG:HH12	1.78	0.43
1:L:135:LEU:HB2	1:L:139:GLN:HE21	1.83	0.43
1:N:124:LEU:CD2	1:N:124:LEU:N	2.81	0.43
1:A:186:VAL:HG12	1:A:228:TYR:N	2.33	0.43
1:D:176:VAL:HG21	1:D:186:VAL:HG22	2.00	0.43
1:E:104:LEU:O	1:E:138:GLY:HA2	2.19	0.43
1:F:130:ILE:HD13	1:F:130:ILE:HA	1.73	0.43
2:G:50:ASN:OD1	2:G:50:ASN:O	2.37	0.43
1:O:212:ARG:NH2	1:O:232:ARG:HH22	2.16	0.43
2:Q:33:THR:HA	2:Q:36:THR:HB	1.99	0.43
1:B:112:THR:C	1:B:113:VAL:HG22	2.39	0.43
1:B:59:LEU:C	1:B:61:ALA:N	2.72	0.43
1:C:185:VAL:HG12	1:F:158:VAL:CG1	2.44	0.43
1:D:209:THR:HG21	1:D:234:PRO:HB3	2.00	0.43
1:E:211:PRO:O	1:E:212:ARG:HB3	2.17	0.43
1:E:214:LEU:HA	1:E:214:LEU:HD23	1.78	0.43
1:J:88:ARG:HD3	2:P:36:THR:HG21	2.00	0.43
1:A:188:LEU:HB3	1:A:192:LEU:HD12	2.01	0.43
1:C:117:THR:CG2	1:C:118:SER:N	2.57	0.43
1:C:222:VAL:HG23	1:C:223:ASP:N	2.32	0.43
1:E:112:THR:HB	1:E:123:ARG:HE	1.84	0.43
1:D:69:ARG:HD3	2:I:50:ASN:HA	2.01	0.43
1:F:176:VAL:CG2	1:F:186:VAL:CG2	2.97	0.43
1:J:173:ARG:HH11	1:M:157:ALA:HB1	1.80	0.43
1:M:96:GLN:HA	1:M:97:PRO:HD2	1.69	0.43
1:O:212:ARG:HD2	1:O:215:ARG:HG3	1.99	0.43
1:F:168:LEU:HA	1:F:168:LEU:HD23	1.80	0.42
1:K:143:LEU:CD2	1:K:147:LEU:HB3	2.49	0.42
1:K:77:LEU:HD23	1:K:81:ARG:HB2	2.00	0.42
1:K:87:LEU:O	1:K:90:GLU:HB2	2.18	0.42
1:N:208:ASP:C	1:N:210:ARG:H	2.21	0.42
1:N:220:LEU:CD1	1:N:229:ALA:HB1	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:192:LEU:HB3	1:O:214:LEU:HD22	2.01	0.42
1:A:173:ARG:NH1	1:D:157:ALA:CB	2.76	0.42
1:A:180:ALA:O	1:A:182:GLU:N	2.52	0.42
1:D:59:LEU:C	1:D:61:ALA:H	2.22	0.42
1:J:180:ALA:O	1:J:182:GLU:HG3	2.19	0.42
1:K:210:ARG:O	1:K:211:PRO:C	2.57	0.42
1:O:95:GLY:O	1:O:142:ARG:NH2	2.52	0.42
1:B:89:GLU:O	1:B:93:ARG:HG3	2.19	0.42
1:C:124:LEU:CD2	1:C:124:LEU:N	2.83	0.42
1:C:180:ALA:O	1:C:182:GLU:HG3	2.19	0.42
1:C:189:ALA:O	1:C:190:ASP:C	2.57	0.42
1:C:197:LEU:HA	1:C:198:PRO:HD3	1.76	0.42
1:C:81:ARG:HE	2:I:43:ILE:CG2	2.32	0.42
2:I:43:ILE:HG22	2:I:44:ASP:N	2.34	0.42
1:M:157:ALA:C	1:M:158:VAL:HG22	2.40	0.42
1:M:77:LEU:HD23	1:M:81:ARG:HB2	2.01	0.42
2:I:33:THR:C	2:I:36:THR:HB	2.40	0.42
1:J:158:VAL:HA	1:K:185:VAL:CG1	2.43	0.42
1:K:223:ASP:O	1:K:225:LYS:N	2.52	0.42
1:L:157:ALA:O	1:L:158:VAL:HG13	2.19	0.42
1:M:236:VAL:HA	1:M:237:PRO:HD3	1.88	0.42
1:N:124:LEU:H	1:N:124:LEU:HD23	1.82	0.42
1:O:232:ARG:O	1:O:233:ILE:CG1	2.67	0.42
1:A:87:LEU:HD13	1:A:87:LEU:O	2.19	0.42
1:C:165:ARG:HG2	1:C:165:ARG:NH1	2.33	0.42
1:D:101:TYR:HE2	1:D:142:ARG:HD3	1.85	0.42
1:D:220:LEU:HD12	1:D:220:LEU:N	2.34	0.42
1:F:59:LEU:C	1:F:61:ALA:N	2.73	0.42
2:I:33:THR:CA	2:I:36:THR:HB	2.48	0.42
1:L:210:ARG:HA	1:L:211:PRO:HD2	1.84	0.42
1:N:103:VAL:HG11	1:N:230:PHE:HZ	1.84	0.42
1:N:108:HIS:HB3	1:N:112:THR:OG1	2.20	0.42
1:O:108:HIS:CE1	1:O:123:ARG:HD2	2.55	0.42
1:O:212:ARG:HH11	1:O:215:ARG:HG3	1.83	0.42
1:A:214:LEU:CD2	1:A:214:LEU:N	2.76	0.42
2:H:50:ASN:OD1	2:H:50:ASN:O	2.38	0.42
1:K:170:ASP:C	1:K:172:HIS:N	2.73	0.42
1:M:233:ILE:HD13	1:M:233:ILE:HA	1.87	0.42
1:A:185:VAL:HG12	1:D:158:VAL:CG1	2.47	0.42
1:D:185:VAL:O	1:D:185:VAL:HG12	2.20	0.42
1:D:223:ASP:O	1:D:224:THR:C	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:59:LEU:C	1:F:61:ALA:H	2.23	0.42
1:J:127:SER:H	1:J:130:ILE:HD11	1.84	0.42
1:J:145:GLU:O	1:J:147:LEU:N	2.42	0.42
1:J:235:LEU:HD22	1:J:236:VAL:O	2.20	0.42
1:L:182:GLU:HB3	1:O:179:HIS:CB	2.50	0.42
1:M:108:HIS:CB	1:M:112:THR:OG1	2.68	0.42
1:N:160:GLU:O	1:N:161:ILE:HD13	2.19	0.42
1:O:124:LEU:HD11	1:O:143:LEU:HD21	2.02	0.42
1:O:130:ILE:CD1	1:O:131:ASP:H	2.30	0.42
1:A:157:ALA:O	1:A:158:VAL:HG13	2.19	0.42
1:B:127:SER:HA	1:B:128:PRO:HD2	1.85	0.42
1:B:223:ASP:O	1:B:225:LYS:N	2.53	0.42
1:E:112:THR:HG21	1:E:123:ARG:HH21	1.84	0.42
1:E:125:THR:O	1:E:149:VAL:HG23	2.20	0.42
1:E:155:PHE:O	1:E:157:ALA:N	2.53	0.42
1:M:190:ASP:HB2	1:M:191:PRO:HD2	1.93	0.42
1:J:164:LEU:HB2	1:J:220:LEU:HD21	2.02	0.42
1:L:210:ARG:HB3	1:L:210:ARG:HE	1.69	0.42
1:O:87:LEU:O	1:O:90:GLU:HB2	2.19	0.42
1:C:230:PHE:O	1:C:231:GLU:CB	2.59	0.42
1:D:75:GLU:HG3	1:D:76:THR:N	2.34	0.42
1:E:164:LEU:C	1:E:164:LEU:HD12	2.39	0.42
2:G:43:ILE:HG22	2:G:44:ASP:N	2.34	0.42
1:M:212:ARG:HG3	1:M:213:LYS:O	2.20	0.42
1:N:113:VAL:O	1:N:123:ARG:HA	2.20	0.42
1:N:184:ARG:NH2	1:N:224:THR:O	2.51	0.42
1:M:69:ARG:HD3	2:R:50:ASN:HA	2.01	0.42
1:C:121:LYS:HG2	1:F:101:TYR:HD1	1.84	0.41
1:F:106:ALA:O	1:F:113:VAL:HG12	2.19	0.41
2:G:32:LEU:O	2:G:36:THR:OG1	2.26	0.41
2:H:43:ILE:HG22	2:H:44:ASP:N	2.35	0.41
1:J:190:ASP:HB2	1:J:191:PRO:HD3	2.01	0.41
1:L:131:ASP:OD1	1:L:131:ASP:N	2.43	0.41
1:L:168:LEU:HD13	1:L:173:ARG:HH21	1.84	0.41
1:L:179:HIS:CG	1:M:182:GLU:HB2	2.55	0.41
1:M:168:LEU:HA	1:M:168:LEU:HD23	1.72	0.41
1:N:99:SER:HB3	1:N:142:ARG:HH11	1.85	0.41
1:N:158:VAL:CG1	1:O:185:VAL:HG12	2.50	0.41
1:O:77:LEU:HD23	1:O:81:ARG:HB2	2.01	0.41
1:A:88:ARG:CZ	2:G:36:THR:OG1	2.68	0.41
1:E:126:CYS:SG	1:E:130:ILE:HD13	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:33:THR:C	2:H:36:THR:HB	2.41	0.41
1:K:96:GLN:HA	1:K:97:PRO:HD2	1.67	0.41
1:M:135:LEU:HA	1:M:135:LEU:HD23	1.80	0.41
1:O:115:VAL:HG23	1:O:122:MET:O	2.21	0.41
1:B:126:CYS:HB2	1:B:149:VAL:HB	2.02	0.41
1:E:185:VAL:HG12	1:E:185:VAL:O	2.20	0.41
1:E:221:LEU:CD2	1:E:230:PHE:HB2	2.46	0.41
1:F:96:GLN:HA	1:F:97:PRO:HD2	1.77	0.41
1:J:151:GLU:HG2	1:J:152:ALA:O	2.20	0.41
1:J:168:LEU:HD12	1:J:173:ARG:HB2	2.00	0.41
1:K:127:SER:HA	1:K:128:PRO:HD2	1.88	0.41
1:M:200:GLY:O	1:M:201:LEU:HB2	2.19	0.41
1:A:116:PHE:CE1	1:A:226:ALA:HA	2.55	0.41
1:A:117:THR:O	1:A:119:GLY:N	2.53	0.41
1:B:146:ALA:O	1:B:147:LEU:C	2.59	0.41
1:F:176:VAL:HG21	1:F:186:VAL:HG22	2.01	0.41
1:F:184:ARG:HD3	1:F:224:THR:HG22	2.01	0.41
2:G:27:GLU:O	2:G:27:GLU:HG2	2.21	0.41
1:N:170:ASP:O	1:N:172:HIS:N	2.52	0.41
1:C:113:VAL:O	1:C:123:ARG:HA	2.20	0.41
1:C:179:HIS:CG	1:D:182:GLU:HB2	2.56	0.41
1:D:105:LEU:HD22	1:D:121:LYS:NZ	2.36	0.41
1:E:87:LEU:O	1:E:87:LEU:HD13	2.21	0.41
1:F:187:TRP:O	1:F:228:TYR:HA	2.21	0.41
1:J:81:ARG:O	1:J:85:LEU:HB2	2.20	0.41
1:M:176:VAL:CG2	1:M:186:VAL:CG1	2.98	0.41
1:A:189:ALA:O	1:A:190:ASP:C	2.59	0.41
1:B:115:VAL:HG23	1:B:122:MET:O	2.21	0.41
1:C:100:GLY:O	1:C:142:ARG:HA	2.20	0.41
2:H:27:GLU:O	2:H:27:GLU:HG2	2.20	0.41
1:L:71:SER:O	1:L:74:MET:HB2	2.21	0.41
2:Q:33:THR:C	2:Q:36:THR:HB	2.41	0.41
1:D:161:ILE:CD1	1:D:221:LEU:HA	2.50	0.41
1:E:168:LEU:HA	1:E:168:LEU:HD23	1.72	0.41
1:J:141:VAL:HG23	1:J:142:ARG:H	1.83	0.41
1:N:235:LEU:CD1	1:N:237:PRO:HD3	2.50	0.41
1:O:104:LEU:CD2	1:O:139:GLN:H	2.34	0.41
1:O:215:ARG:HA	1:O:216:PRO:HD3	1.80	0.41
1:F:187:TRP:HD1	1:F:227:GLY:O	2.04	0.41
2:G:33:THR:CA	2:G:36:THR:HB	2.51	0.41
1:J:180:ALA:C	1:J:182:GLU:H	2.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:208:ASP:HB3	1:J:232:ARG:NH2	2.35	0.41
1:O:212:ARG:HG3	1:O:213:LYS:N	2.35	0.41
1:N:88:ARG:NE	2:Q:36:THR:OG1	2.54	0.41
2:R:40:LEU:HA	2:R:43:ILE:HB	2.02	0.41
1:A:127:SER:HA	1:A:128:PRO:HD2	1.91	0.41
1:B:59:LEU:C	1:B:61:ALA:H	2.23	0.41
1:C:162:SER:HB3	1:C:177:VAL:O	2.21	0.41
1:F:170:ASP:C	1:F:172:HIS:N	2.74	0.41
1:M:176:VAL:HG21	1:M:186:VAL:CG1	2.46	0.41
1:M:206:ASN:HB3	1:M:207:ASP:H	1.59	0.41
1:N:168:LEU:O	1:N:169:ALA:C	2.59	0.41
1:N:168:LEU:HD12	1:N:173:ARG:HB2	2.01	0.41
1:A:145:GLU:O	1:A:147:LEU:N	2.42	0.41
1:A:215:ARG:HA	1:A:216:PRO:HD3	1.95	0.41
1:B:161:ILE:HA	1:B:161:ILE:HD13	1.70	0.41
1:C:115:VAL:HG23	1:C:124:LEU:HD21	1.95	0.41
1:D:187:TRP:H	1:D:187:TRP:HD1	1.68	0.41
1:F:176:VAL:CG2	1:F:186:VAL:HG22	2.50	0.41
1:J:71:SER:O	1:J:74:MET:HB2	2.21	0.41
1:K:215:ARG:HA	1:K:216:PRO:HD3	1.87	0.41
1:K:184:ARG:NH2	1:K:224:THR:O	2.54	0.41
1:L:99:SER:HB2	1:M:123:ARG:HB2	2.02	0.41
1:M:146:ALA:HB2	2:R:21:SER:HB2	2.03	0.41
1:N:223:ASP:O	1:N:226:ALA:N	2.54	0.41
1:O:141:VAL:HG23	1:O:142:ARG:N	2.36	0.41
1:B:56:ILE:H	1:B:56:ILE:HG13	1.76	0.41
1:D:142:ARG:O	1:D:149:VAL:HA	2.22	0.41
1:K:161:ILE:HG22	1:K:161:ILE:O	2.20	0.41
1:M:190:ASP:C	1:M:192:LEU:N	2.72	0.41
1:K:97:PRO:CB	1:N:124:LEU:HA	2.51	0.41
1:O:103:VAL:O	1:O:116:PHE:N	2.53	0.41
1:O:104:LEU:HD23	1:O:139:GLN:H	1.86	0.41
1:A:105:LEU:HG	1:A:228:TYR:HE2	1.86	0.40
1:B:190:ASP:CB	1:B:191:PRO:CD	2.97	0.40
1:L:192:LEU:CD2	1:L:214:LEU:HD11	2.51	0.40
1:B:75:GLU:HG3	1:B:76:THR:N	2.35	0.40
1:M:103:VAL:HG12	1:M:104:LEU:N	2.36	0.40
1:N:197:LEU:O	1:N:213:LYS:NZ	2.49	0.40
1:O:212:ARG:HG3	1:O:213:LYS:O	2.21	0.40
1:A:88:ARG:CD	2:G:36:THR:HG21	2.51	0.40
1:B:97:PRO:HA	1:B:99:SER:OG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:PRO:O	1:C:212:ARG:HB3	2.21	0.40
1:E:99:SER:HB3	1:E:142:ARG:NH1	2.36	0.40
1:E:71:SER:O	1:E:74:MET:HB2	2.21	0.40
1:N:131:ASP:HB3	1:N:134:SER:OG	2.20	0.40
1:B:105:LEU:HD22	1:B:121:LYS:NZ	2.37	0.40
1:B:201:LEU:HD23	1:B:202:PRO:HD2	2.02	0.40
1:C:81:ARG:HE	2:I:43:ILE:HG23	1.86	0.40
2:H:33:THR:CA	2:H:36:THR:HB	2.51	0.40
1:K:124:LEU:HD21	1:K:147:LEU:C	2.42	0.40
1:L:136:LYS:H	1:L:136:LYS:HD3	1.86	0.40
1:E:81:ARG:HH21	2:H:43:ILE:HG12	1.86	0.40
1:K:127:SER:O	1:K:130:ILE:HB	2.22	0.40
1:L:192:LEU:HB3	1:L:214:LEU:HD11	2.03	0.40
1:N:125:THR:O	1:N:149:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	184/251 (73%)	128 (70%)	35 (19%)	21 (11%)	0	7
1	B	184/251 (73%)	148 (80%)	25 (14%)	11 (6%)	1	19
1	C	184/251 (73%)	136 (74%)	32 (17%)	16 (9%)	1	13
1	D	184/251 (73%)	142 (77%)	33 (18%)	9 (5%)	2	23
1	E	184/251 (73%)	133 (72%)	32 (17%)	19 (10%)	0	9
1	F	184/251 (73%)	144 (78%)	29 (16%)	11 (6%)	1	19
1	J	184/251 (73%)	131 (71%)	35 (19%)	18 (10%)	0	10
1	K	184/251 (73%)	145 (79%)	28 (15%)	11 (6%)	1	19
1	L	184/251 (73%)	126 (68%)	37 (20%)	21 (11%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	184/251 (73%)	142 (77%)	31 (17%)	11 (6%)	1	19
1	N	184/251 (73%)	132 (72%)	34 (18%)	18 (10%)	0	10
1	O	184/251 (73%)	142 (77%)	26 (14%)	16 (9%)	1	13
2	G	29/68 (43%)	28 (97%)	1 (3%)	0	100	100
2	H	29/68 (43%)	28 (97%)	1 (3%)	0	100	100
2	I	29/68 (43%)	28 (97%)	1 (3%)	0	100	100
2	P	29/68 (43%)	28 (97%)	1 (3%)	0	100	100
2	Q	29/68 (43%)	28 (97%)	1 (3%)	0	100	100
2	R	29/68 (43%)	28 (97%)	1 (3%)	0	100	100
All	All	2382/3420 (70%)	1817 (76%)	383 (16%)	182 (8%)	1	15

All (182) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	ASP
1	A	201	LEU
1	A	207	ASP
1	A	209	THR
1	B	191	PRO
1	C	196	ASP
1	C	207	ASP
1	D	145	GLU
1	D	196	ASP
1	D	206	ASN
1	E	110	ASP
1	E	145	GLU
1	E	201	LEU
1	E	207	ASP
1	F	129	ASN
1	F	145	GLU
1	F	196	ASP
1	J	118	SER
1	J	196	ASP
1	J	207	ASP
1	K	145	GLU
1	K	206	ASN
1	L	119	GLY
1	L	145	GLU
1	L	196	ASP

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Mol	Chain	Res	Type
1	L	207	ASP
1	M	145	GLU
1	M	191	PRO
1	M	196	ASP
1	M	206	ASN
1	M	211	PRO
1	N	110	ASP
1	N	132	ALA
1	N	145	GLU
1	N	201	LEU
1	N	207	ASP
1	O	145	GLU
1	O	192	LEU
1	A	119	GLY
1	A	132	ALA
1	A	145	GLU
1	A	169	ALA
1	A	171	GLY
1	A	181	ASP
1	A	196	ASP
1	A	211	PRO
1	B	74	MET
1	B	145	GLU
1	B	196	ASP
1	B	200	GLY
1	B	211	PRO
1	C	145	GLU
1	C	181	ASP
1	C	201	LEU
1	C	231	GLU
1	D	74	MET
1	E	129	ASN
1	E	146	ALA
1	E	181	ASP
1	E	202	PRO
1	E	209	THR
1	F	74	MET
1	F	224	THR
1	J	145	GLU
1	J	169	ALA
1	J	181	ASP
1	J	191	PRO

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Mol	Chain	Res	Type
1	J	201	LEU
1	J	231	GLU
1	K	156	GLU
1	K	196	ASP
1	K	211	PRO
1	L	110	ASP
1	L	146	ALA
1	L	169	ALA
1	L	171	GLY
1	L	181	ASP
1	L	201	LEU
1	L	225	LYS
1	M	200	GLY
1	M	224	THR
1	N	137	LYS
1	N	169	ALA
1	N	191	PRO
1	O	196	ASP
1	O	207	ASP
1	O	224	THR
1	A	74	MET
1	A	156	GLU
1	A	191	PRO
1	B	156	GLU
1	C	74	MET
1	C	156	GLU
1	C	211	PRO
1	D	191	PRO
1	D	211	PRO
1	D	224	THR
1	E	74	MET
1	E	169	ALA
1	E	231	GLU
1	F	156	GLU
1	J	74	MET
1	J	110	ASP
1	J	128	PRO
1	J	132	ALA
1	J	209	THR
1	K	74	MET
1	K	191	PRO
1	K	224	THR

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Mol	Chain	Res	Type
1	L	74	MET
1	L	131	ASP
1	L	211	PRO
1	M	74	MET
1	N	74	MET
1	N	156	GLU
1	N	196	ASP
1	N	209	THR
1	O	74	MET
1	O	129	ASN
1	O	166	GLU
1	O	211	PRO
1	A	137	LYS
1	A	146	ALA
1	A	212	ARG
1	B	201	LEU
1	C	119	GLY
1	C	129	ASN
1	C	146	ALA
1	C	191	PRO
1	D	156	GLU
1	D	217	GLY
1	E	117	THR
1	E	132	ALA
1	F	191	PRO
1	F	211	PRO
1	F	217	GLY
1	J	146	ALA
1	J	202	PRO
1	K	60	GLU
1	L	156	GLU
1	L	191	PRO
1	L	202	PRO
1	O	156	GLU
1	O	171	GLY
1	O	191	PRO
1	O	217	GLY
1	A	128	PRO
1	B	217	GLY
1	B	224	THR
1	C	169	ALA
1	E	128	PRO

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Mol	Chain	Res	Type
1	E	156	GLU
1	E	191	PRO
1	E	211	PRO
1	F	167	ILE
1	K	171	GLY
1	L	224	THR
1	M	129	ASN
1	M	217	GLY
1	N	146	ALA
1	N	171	GLY
1	N	234	PRO
1	A	118	SER
1	L	117	THR
1	L	195	GLU
1	N	202	PRO
1	O	60	GLU
1	A	158	VAL
1	B	167	ILE
1	J	97	PRO
1	L	97	PRO
1	M	201	LEU
1	N	190	ASP
1	O	167	ILE
1	C	190	ASP
1	F	201	LEU
1	O	201	LEU
1	C	202	PRO
1	J	211	PRO
1	E	119	GLY
1	K	201	LEU
1	N	97	PRO

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	154/204 (76%)	110 (71%)	44 (29%)	0	3
1	B	154/204 (76%)	116 (75%)	38 (25%)	0	4
1	C	154/204 (76%)	111 (72%)	43 (28%)	0	3
1	D	154/204 (76%)	114 (74%)	40 (26%)	0	4
1	E	154/204 (76%)	119 (77%)	35 (23%)	1	6
1	F	154/204 (76%)	118 (77%)	36 (23%)	1	5
1	J	154/204 (76%)	117 (76%)	37 (24%)	0	5
1	K	154/204 (76%)	113 (73%)	41 (27%)	0	4
1	L	154/204 (76%)	120 (78%)	34 (22%)	1	6
1	M	154/204 (76%)	119 (77%)	35 (23%)	1	6
1	N	154/204 (76%)	119 (77%)	35 (23%)	1	6
1	O	154/204 (76%)	116 (75%)	38 (25%)	0	4
2	G	27/52 (52%)	26 (96%)	1 (4%)	34	59
2	H	27/52 (52%)	26 (96%)	1 (4%)	34	59
2	I	27/52 (52%)	26 (96%)	1 (4%)	34	59
2	P	27/52 (52%)	26 (96%)	1 (4%)	34	59
2	Q	27/52 (52%)	27 (100%)	0	100	100
2	R	27/52 (52%)	26 (96%)	1 (4%)	34	59
All	All	2010/2760 (73%)	1549 (77%)	461 (23%)	1	5

All (461) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	SER
1	A	62	ARG
1	A	82	GLN
1	A	85	LEU
1	A	99	SER
1	A	107	THR
1	A	108	HIS
1	A	109	ASP
1	A	110	ASP
1	A	113	VAL
1	A	116	PHE

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Mol	Chain	Res	Type
1	A	122	MET
1	A	124	LEU
1	A	131	ASP
1	A	135	LEU
1	A	136	LYS
1	A	140	THR
1	A	141	VAL
1	A	143	LEU
1	A	149	VAL
1	A	150	VAL
1	A	154	THR
1	A	158	VAL
1	A	162	SER
1	A	163	THR
1	A	167	ILE
1	A	168	LEU
1	A	176	VAL
1	A	181	ASP
1	A	185	VAL
1	A	186	VAL
1	A	187	TRP
1	A	199	ASP
1	A	201	LEU
1	A	205	LEU
1	A	213	LYS
1	A	214	LEU
1	A	220	LEU
1	A	221	LEU
1	A	222	VAL
1	A	223	ASP
1	A	224	THR
1	A	235	LEU
1	A	236	VAL
1	B	70	ASN
1	B	75	GLU
1	B	78	LYS
1	B	81	ARG
1	B	84	LEU
1	B	85	LEU
1	B	87	LEU
1	B	89	GLU
1	B	99	SER

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Mol	Chain	Res	Type
1	B	104	LEU
1	B	105	LEU
1	B	113	VAL
1	B	115	VAL
1	B	117	THR
1	B	121	LYS
1	B	124	LEU
1	B	126	CYS
1	B	130	ILE
1	B	131	ASP
1	B	134	SER
1	B	141	VAL
1	B	147	LEU
1	B	150	VAL
1	B	154	THR
1	B	158	VAL
1	B	161	ILE
1	B	162	SER
1	B	163	THR
1	B	164	LEU
1	B	167	ILE
1	B	170	ASP
1	B	186	VAL
1	B	201	LEU
1	B	208	ASP
1	B	212	ARG
1	B	214	LEU
1	B	218	ASP
1	B	220	LEU
1	C	52	SER
1	C	62	ARG
1	C	82	GLN
1	C	85	LEU
1	C	99	SER
1	C	104	LEU
1	C	107	THR
1	C	108	HIS
1	C	113	VAL
1	C	115	VAL
1	C	116	PHE
1	C	122	MET
1	C	124	LEU

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Mol	Chain	Res	Type
1	C	125	THR
1	C	130	ILE
1	C	131	ASP
1	C	136	LYS
1	C	137	LYS
1	C	140	THR
1	C	141	VAL
1	C	149	VAL
1	C	150	VAL
1	C	154	THR
1	C	158	VAL
1	C	163	THR
1	C	167	ILE
1	C	168	LEU
1	C	175	LEU
1	C	176	VAL
1	C	181	ASP
1	C	182	GLU
1	C	185	VAL
1	C	186	VAL
1	C	187	TRP
1	C	196	ASP
1	C	201	LEU
1	C	203	GLU
1	C	205	LEU
1	C	219	SER
1	C	220	LEU
1	C	222	VAL
1	C	223	ASP
1	C	235	LEU
1	D	70	ASN
1	D	75	GLU
1	D	78	LYS
1	D	81	ARG
1	D	84	LEU
1	D	85	LEU
1	D	87	LEU
1	D	89	GLU
1	D	104	LEU
1	D	105	LEU
1	D	113	VAL
1	D	115	VAL

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Mol	Chain	Res	Type
1	D	117	THR
1	D	121	LYS
1	D	130	ILE
1	D	134	SER
1	D	140	THR
1	D	147	LEU
1	D	150	VAL
1	D	154	THR
1	D	156	GLU
1	D	158	VAL
1	D	164	LEU
1	D	167	ILE
1	D	170	ASP
1	D	176	VAL
1	D	177	VAL
1	D	182	GLU
1	D	186	VAL
1	D	187	TRP
1	D	195	GLU
1	D	201	LEU
1	D	206	ASN
1	D	212	ARG
1	D	213	LYS
1	D	214	LEU
1	D	221	LEU
1	D	225	LYS
1	D	232	ARG
1	D	233	ILE
1	E	52	SER
1	E	62	ARG
1	E	82	GLN
1	E	85	LEU
1	E	99	SER
1	E	107	THR
1	E	109	ASP
1	E	110	ASP
1	E	113	VAL
1	E	124	LEU
1	E	125	THR
1	E	126	CYS
1	E	131	ASP
1	E	136	LYS

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Mol	Chain	Res	Type
1	E	140	THR
1	E	141	VAL
1	E	143	LEU
1	E	149	VAL
1	E	150	VAL
1	E	154	THR
1	E	158	VAL
1	E	163	THR
1	E	167	ILE
1	E	176	VAL
1	E	181	ASP
1	E	185	VAL
1	E	186	VAL
1	E	187	TRP
1	E	201	LEU
1	E	210	ARG
1	E	221	LEU
1	E	222	VAL
1	E	223	ASP
1	E	224	THR
1	E	235	LEU
1	F	70	ASN
1	F	78	LYS
1	F	81	ARG
1	F	84	LEU
1	F	85	LEU
1	F	87	LEU
1	F	89	GLU
1	F	105	LEU
1	F	107	THR
1	F	113	VAL
1	F	115	VAL
1	F	117	THR
1	F	130	ILE
1	F	141	VAL
1	F	147	LEU
1	F	150	VAL
1	F	154	THR
1	F	156	GLU
1	F	158	VAL
1	F	161	ILE
1	F	163	THR

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Mol	Chain	Res	Type
1	F	164	LEU
1	F	167	ILE
1	F	170	ASP
1	F	182	GLU
1	F	186	VAL
1	F	187	TRP
1	F	195	GLU
1	F	196	ASP
1	F	201	LEU
1	F	206	ASN
1	F	210	ARG
1	F	212	ARG
1	F	213	LYS
1	F	221	LEU
1	F	232	ARG
2	G	43	ILE
2	H	43	ILE
2	I	43	ILE
1	J	52	SER
1	J	55	ASP
1	J	62	ARG
1	J	82	GLN
1	J	85	LEU
1	J	89	GLU
1	J	107	THR
1	J	108	HIS
1	J	110	ASP
1	J	111	ASP
1	J	113	VAL
1	J	125	THR
1	J	131	ASP
1	J	136	LYS
1	J	140	THR
1	J	143	LEU
1	J	149	VAL
1	J	150	VAL
1	J	154	THR
1	J	158	VAL
1	J	163	THR
1	J	167	ILE
1	J	168	LEU
1	J	182	GLU

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Mol	Chain	Res	Type
1	J	185	VAL
1	J	186	VAL
1	J	187	TRP
1	J	199	ASP
1	J	201	LEU
1	J	203	GLU
1	J	205	LEU
1	J	210	ARG
1	J	213	LYS
1	J	221	LEU
1	J	222	VAL
1	J	224	THR
1	J	235	LEU
1	K	70	ASN
1	K	73	LEU
1	K	75	GLU
1	K	78	LYS
1	K	81	ARG
1	K	85	LEU
1	K	87	LEU
1	K	104	LEU
1	K	105	LEU
1	K	107	THR
1	K	113	VAL
1	K	115	VAL
1	K	117	THR
1	K	123	ARG
1	K	124	LEU
1	K	130	ILE
1	K	134	SER
1	K	147	LEU
1	K	149	VAL
1	K	150	VAL
1	K	154	THR
1	K	156	GLU
1	K	158	VAL
1	K	161	ILE
1	K	163	THR
1	K	164	LEU
1	K	165	ARG
1	K	170	ASP
1	K	177	VAL

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Mol	Chain	Res	Type
1	K	186	VAL
1	K	187	TRP
1	K	190	ASP
1	K	195	GLU
1	K	196	ASP
1	K	201	LEU
1	K	208	ASP
1	K	210	ARG
1	K	212	ARG
1	K	214	LEU
1	K	218	ASP
1	K	221	LEU
1	L	52	SER
1	L	55	ASP
1	L	62	ARG
1	L	82	GLN
1	L	85	LEU
1	L	89	GLU
1	L	99	SER
1	L	107	THR
1	L	108	HIS
1	L	110	ASP
1	L	113	VAL
1	L	125	THR
1	L	131	ASP
1	L	135	LEU
1	L	140	THR
1	L	141	VAL
1	L	149	VAL
1	L	150	VAL
1	L	154	THR
1	L	158	VAL
1	L	163	THR
1	L	167	ILE
1	L	168	LEU
1	L	185	VAL
1	L	186	VAL
1	L	187	TRP
1	L	199	ASP
1	L	201	LEU
1	L	205	LEU
1	L	210	ARG

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Mol	Chain	Res	Type
1	L	214	LEU
1	L	222	VAL
1	L	224	THR
1	L	235	LEU
1	M	70	ASN
1	M	73	LEU
1	M	75	GLU
1	M	78	LYS
1	M	81	ARG
1	M	85	LEU
1	M	87	LEU
1	M	104	LEU
1	M	105	LEU
1	M	107	THR
1	M	108	HIS
1	M	113	VAL
1	M	115	VAL
1	M	117	THR
1	M	120	ARG
1	M	130	ILE
1	M	147	LEU
1	M	150	VAL
1	M	154	THR
1	M	158	VAL
1	M	161	ILE
1	M	162	SER
1	M	163	THR
1	M	164	LEU
1	M	167	ILE
1	M	170	ASP
1	M	182	GLU
1	M	185	VAL
1	M	186	VAL
1	M	196	ASP
1	M	201	LEU
1	M	209	THR
1	M	213	LYS
1	M	215	ARG
1	M	224	THR
1	N	52	SER
1	N	55	ASP
1	N	62	ARG

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Mol	Chain	Res	Type
1	N	82	GLN
1	N	85	LEU
1	N	89	GLU
1	N	107	THR
1	N	108	HIS
1	N	113	VAL
1	N	117	THR
1	N	124	LEU
1	N	125	THR
1	N	131	ASP
1	N	135	LEU
1	N	136	LYS
1	N	141	VAL
1	N	149	VAL
1	N	150	VAL
1	N	154	THR
1	N	158	VAL
1	N	163	THR
1	N	167	ILE
1	N	168	LEU
1	N	182	GLU
1	N	185	VAL
1	N	187	TRP
1	N	199	ASP
1	N	205	LEU
1	N	210	ARG
1	N	215	ARG
1	N	219	SER
1	N	221	LEU
1	N	222	VAL
1	N	224	THR
1	N	235	LEU
1	O	70	ASN
1	O	73	LEU
1	O	75	GLU
1	O	78	LYS
1	O	81	ARG
1	O	85	LEU
1	O	87	LEU
1	O	101	TYR
1	O	104	LEU
1	O	105	LEU

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Mol	Chain	Res	Type
1	O	107	THR
1	O	113	VAL
1	O	115	VAL
1	O	117	THR
1	O	124	LEU
1	O	130	ILE
1	O	134	SER
1	O	147	LEU
1	O	150	VAL
1	O	154	THR
1	O	158	VAL
1	O	161	ILE
1	O	162	SER
1	O	163	THR
1	O	164	LEU
1	O	165	ARG
1	O	167	ILE
1	O	170	ASP
1	O	186	VAL
1	O	188	LEU
1	O	190	ASP
1	O	195	GLU
1	O	196	ASP
1	O	212	ARG
1	O	213	LYS
1	O	221	LEU
1	O	224	THR
1	O	233	ILE
2	P	43	ILE
2	R	43	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	139	GLN
1	B	108	HIS
1	E	139	GLN
2	G	50	ASN
2	H	50	ASN
2	I	50	ASN
1	J	139	GLN

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Mol	Chain	Res	Type
1	L	139	GLN
1	M	70	ASN
1	N	139	GLN
2	P	50	ASN
2	Q	50	ASN
2	R	50	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	186/251 (74%)	0.23	2 (1%) 80 72	125, 145, 183, 213	0
1	B	186/251 (74%)	0.25	3 (1%) 72 62	127, 147, 186, 212	0
1	C	186/251 (74%)	0.26	2 (1%) 80 72	126, 146, 185, 216	0
1	D	186/251 (74%)	0.26	3 (1%) 72 62	129, 149, 186, 211	0
1	E	186/251 (74%)	0.27	3 (1%) 72 62	125, 145, 184, 215	0
1	F	186/251 (74%)	0.20	3 (1%) 72 62	127, 147, 183, 206	0
1	J	186/251 (74%)	0.26	2 (1%) 80 72	125, 144, 182, 216	0
1	K	186/251 (74%)	0.22	2 (1%) 80 72	126, 147, 187, 213	0
1	L	186/251 (74%)	0.24	1 (0%) 91 85	125, 145, 182, 214	0
1	M	186/251 (74%)	0.23	4 (2%) 62 52	126, 148, 184, 211	0
1	N	186/251 (74%)	0.26	1 (0%) 91 85	125, 144, 182, 212	0
1	O	186/251 (74%)	0.20	4 (2%) 62 52	128, 148, 185, 212	0
2	G	31/68 (45%)	0.87	3 (9%) 7 7	170, 194, 222, 240	0
2	H	31/68 (45%)	0.85	3 (9%) 7 7	170, 191, 223, 241	0
2	I	31/68 (45%)	1.03	4 (12%) 3 4	172, 192, 222, 240	0
2	P	31/68 (45%)	0.68	6 (19%) 1 1	170, 191, 220, 238	0
2	Q	31/68 (45%)	0.61	1 (3%) 47 38	172, 191, 223, 237	0
2	R	31/68 (45%)	0.92	3 (9%) 7 7	173, 193, 225, 244	0
All	All	2418/3420 (70%)	0.29	50 (2%) 63 54	125, 147, 198, 244	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	R	21	SER	7.6
2	I	21	SER	7.4
2	G	21	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	204	ALA	4.0
2	H	21	SER	3.8
1	D	206	ASN	3.7
1	A	204	ALA	3.7
1	C	204	ALA	3.6
1	F	206	ASN	3.4
1	B	204	ALA	3.4
1	L	204	ALA	3.4
1	M	205	LEU	3.3
1	M	52	SER	3.2
1	M	206	ASN	3.1
1	K	206	ASN	3.1
1	M	204	ALA	3.1
1	O	206	ASN	3.1
2	I	46	VAL	3.1
1	A	201	LEU	3.0
2	G	23	ALA	3.0
2	P	46	VAL	3.0
1	J	205	LEU	2.9
1	E	201	LEU	2.8
1	J	204	ALA	2.8
2	R	27	GLU	2.8
1	O	207	ASP	2.7
2	H	48	GLU	2.7
1	D	203	GLU	2.6
2	P	23	ALA	2.5
1	F	237	PRO	2.5
1	E	205	LEU	2.5
1	O	205	LEU	2.5
1	O	204	ALA	2.4
2	P	21	SER	2.4
1	C	203	GLU	2.4
1	D	237	PRO	2.3
2	P	50	ASN	2.3
1	B	74	MET	2.3
2	H	31	LYS	2.2
2	P	27	GLU	2.2
2	G	26	GLN	2.2
2	Q	23	ALA	2.1
1	B	206	ASN	2.1
2	P	24	ALA	2.1
1	F	203	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	52	SER	2.1
1	N	201	LEU	2.0
2	I	24	ALA	2.0
2	I	42	GLU	2.0
2	R	49	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.