



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:32 AM GMT

PDB ID : 3M9B
Title : Crystal structure of the amino terminal coiled coil domain and the inter domain
of the Mycobacterium tuberculosis proteasomal ATPase Mpa
Authors : Li, H.; Wang, T.
Deposited on : 2010-03-21
Resolution : 3.94 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

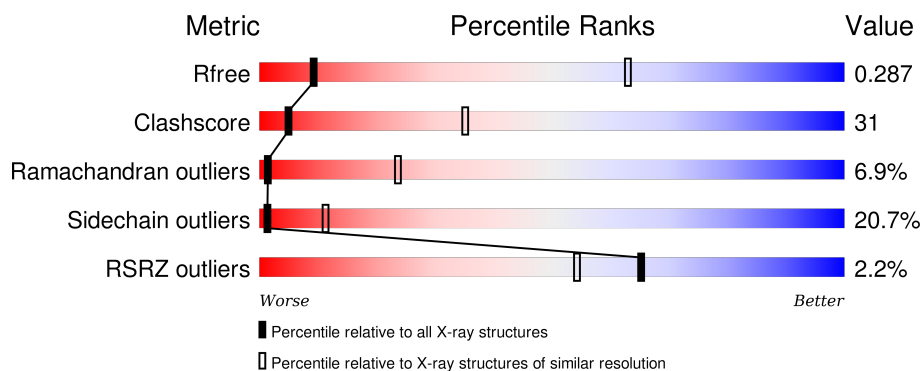
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.94 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1007 (4.34-3.54)
Clashscore	102246	1042 (4.30-3.58)
Ramachandran outliers	100387	1000 (4.30-3.58)
Sidechain outliers	100360	1021 (4.32-3.56)
RSRZ outliers	91569	1011 (4.34-3.54)

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

Mol	Chain	Length	Quality of chain
1	A	251	<div> <div>28%</div> <div>34%</div> <div>12%</div> <div>26%</div> </div>
1	B	251	<div> <div>2%</div> <div>35%</div> <div>29%</div> <div>10%</div> <div>26%</div> </div>
1	C	251	<div> <div>2%</div> <div>29%</div> <div>30%</div> <div>14%</div> <div>26%</div> </div>
1	D	251	<div> <div>2%</div> <div>37%</div> <div>29%</div> <div>8%</div> <div>26%</div> </div>
1	E	251	<div> <div>2%</div> <div>27%</div> <div>33%</div> <div>12%</div> <div>26%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	251	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>35%</div><div>30%</div><div>8%</div><div>26%</div></div></div>
1	G	251	<div><div><div></div><div></div><div></div><div></div></div><div><div>%</div><div>25%</div><div>33%</div><div>14%</div><div>26%</div></div></div>
1	H	251	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>35%</div><div>30%</div><div>9%</div><div>26%</div></div></div>
1	I	251	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>26%</div><div>36%</div><div>11%</div><div>26%</div></div></div>
1	J	251	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>35%</div><div>31%</div><div>8%</div><div>26%</div></div></div>
1	K	251	<div><div><div></div><div></div><div></div><div></div></div><div><div>%</div><div>26%</div><div>33%</div><div>14%</div><div>26%</div></div></div>
1	L	251	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>36%</div><div>32%</div><div>6%</div><div>26%</div></div></div>

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 17172 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	G	186	Total	C	N	O	S	0	0	0
			1431	888	259	281	3			
1	H	186	Total	C	N	O	S	0	0	0
			1431	888	259	281	3			
1	I	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			

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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
G	235	LEU	-	EXPRESSION TAG	UNP P63345
G	236	VAL	-	EXPRESSION TAG	UNP P63345
G	237	PRO	-	EXPRESSION TAG	UNP P63345
G	238	ARG	-	EXPRESSION TAG	UNP P63345
G	239	GLY	-	EXPRESSION TAG	UNP P63345
G	240	SER	-	EXPRESSION TAG	UNP P63345
G	241	ALA	-	EXPRESSION TAG	UNP P63345
G	242	ALA	-	EXPRESSION TAG	UNP P63345
G	243	ALA	-	EXPRESSION TAG	UNP P63345
G	244	LEU	-	EXPRESSION TAG	UNP P63345
G	245	GLU	-	EXPRESSION TAG	UNP P63345
G	246	HIS	-	EXPRESSION TAG	UNP P63345
G	247	HIS	-	EXPRESSION TAG	UNP P63345
G	248	HIS	-	EXPRESSION TAG	UNP P63345
G	249	HIS	-	EXPRESSION TAG	UNP P63345
G	250	HIS	-	EXPRESSION TAG	UNP P63345
G	251	HIS	-	EXPRESSION TAG	UNP P63345
H	235	LEU	-	EXPRESSION TAG	UNP P63345
H	236	VAL	-	EXPRESSION TAG	UNP P63345
H	237	PRO	-	EXPRESSION TAG	UNP P63345
H	238	ARG	-	EXPRESSION TAG	UNP P63345
H	239	GLY	-	EXPRESSION TAG	UNP P63345
H	240	SER	-	EXPRESSION TAG	UNP P63345
H	241	ALA	-	EXPRESSION TAG	UNP P63345
H	242	ALA	-	EXPRESSION TAG	UNP P63345
H	243	ALA	-	EXPRESSION TAG	UNP P63345
H	244	LEU	-	EXPRESSION TAG	UNP P63345
H	245	GLU	-	EXPRESSION TAG	UNP P63345
H	246	HIS	-	EXPRESSION TAG	UNP P63345

Continued on next page...

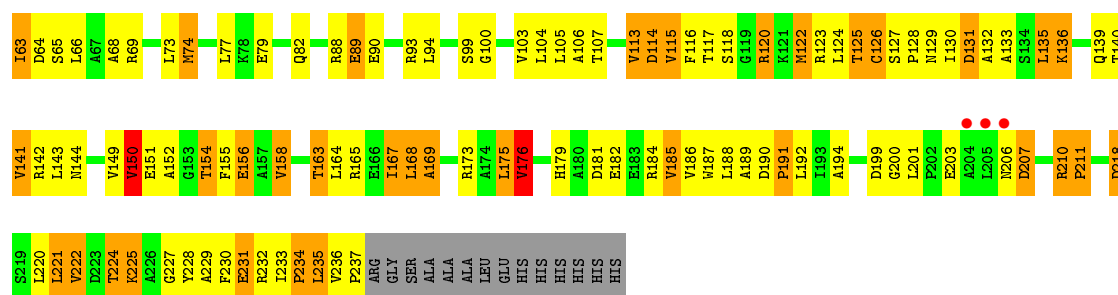
Continued from previous page...

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

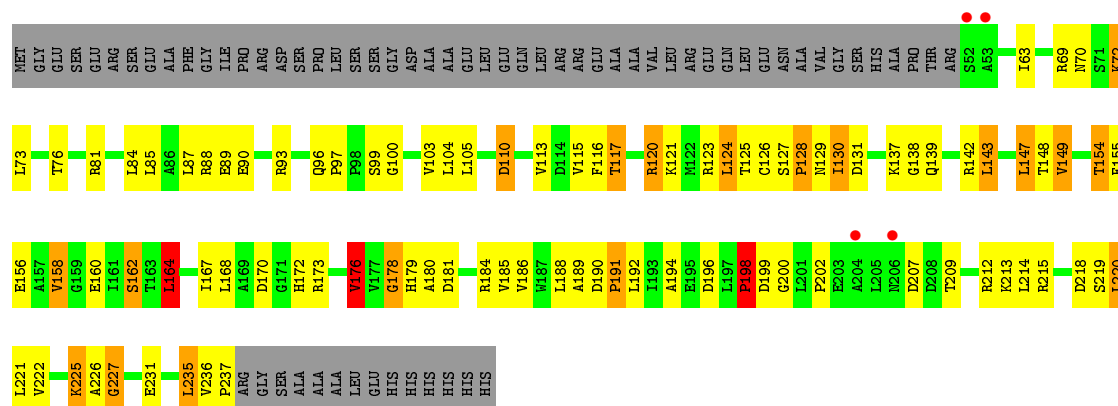
Continued on next page...

Continued from previous page...

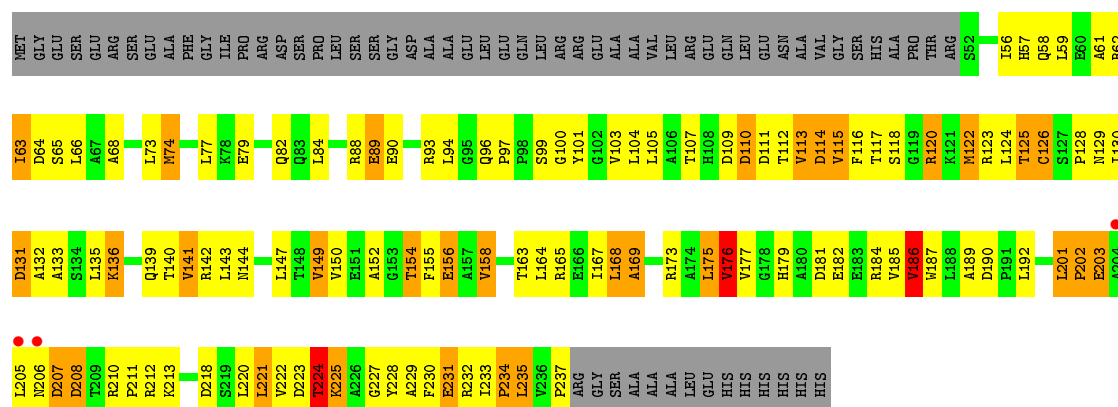
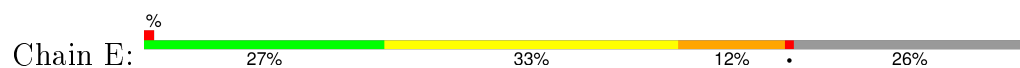
Chain	Residue	Modelled	Actual	Comment	Reference
K	238	ARG	-	EXPRESSION TAG	UNP P63345
K	239	GLY	-	EXPRESSION TAG	UNP P63345
K	240	SER	-	EXPRESSION TAG	UNP P63345
K	241	ALA	-	EXPRESSION TAG	UNP P63345
K	242	ALA	-	EXPRESSION TAG	UNP P63345
K	243	ALA	-	EXPRESSION TAG	UNP P63345
K	244	LEU	-	EXPRESSION TAG	UNP P63345
K	245	GLU	-	EXPRESSION TAG	UNP P63345
K	246	HIS	-	EXPRESSION TAG	UNP P63345
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



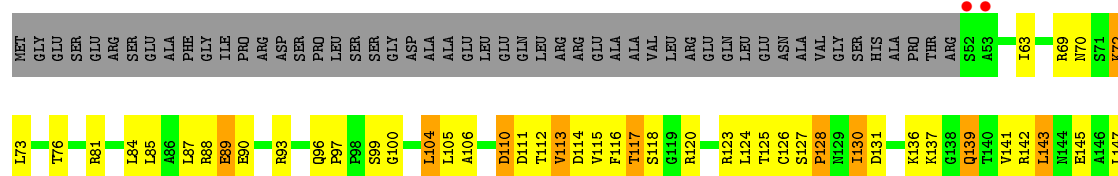
• Molecule 1: Proteasome-associated ATPase

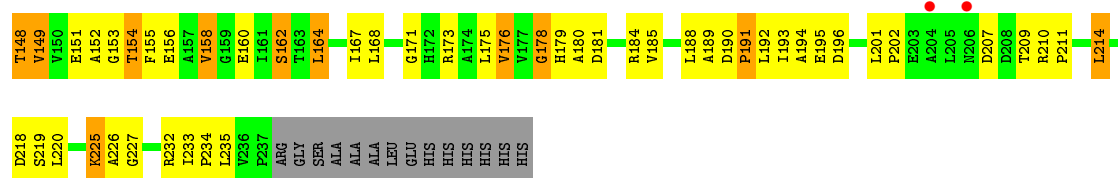


• Molecule 1: Proteasome-associated ATPase

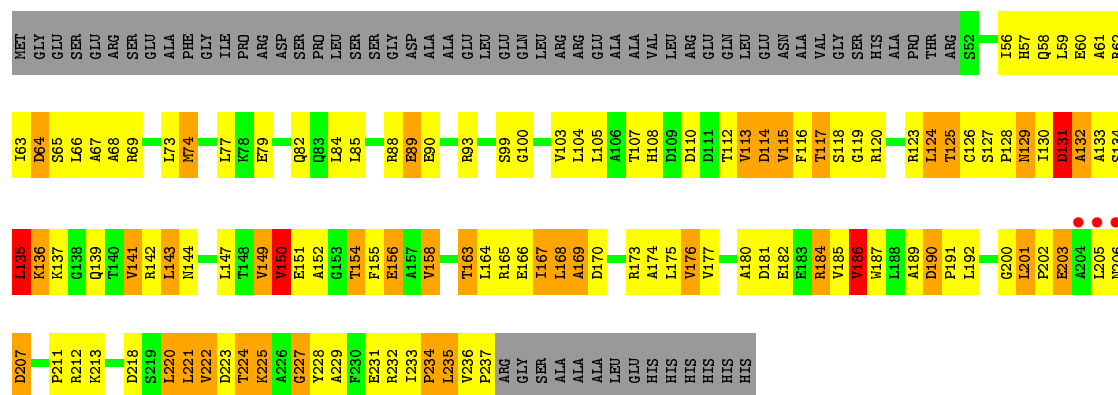
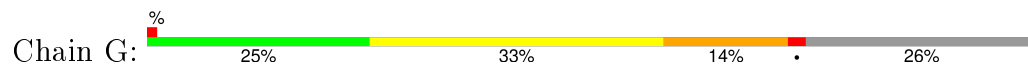


• Molecule 1: Proteasome-associated ATPase

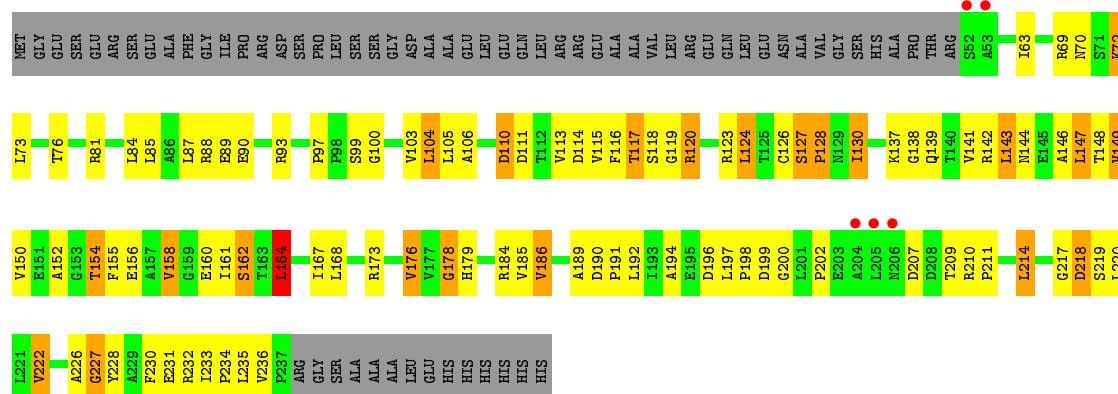




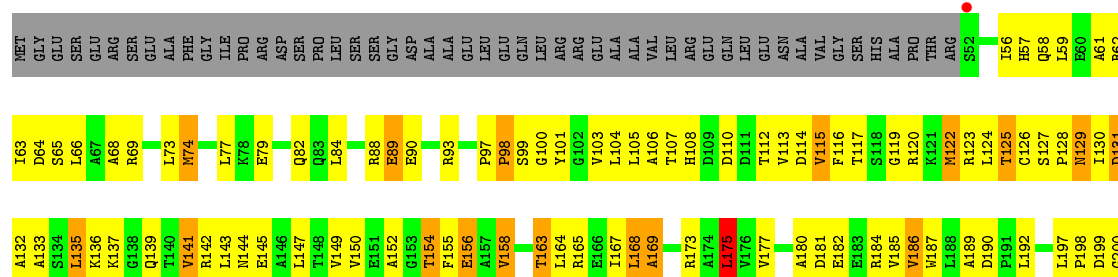
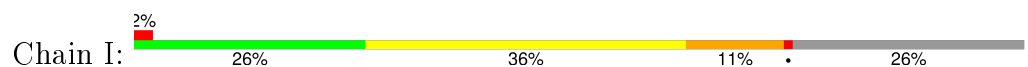
• Molecule 1: Proteasome-associated ATPase

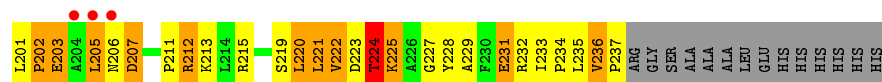


• Molecule 1: Proteasome-associated ATPase

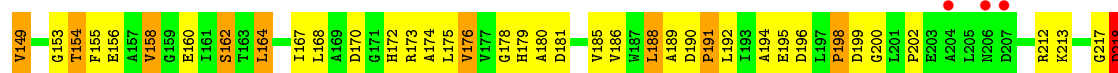
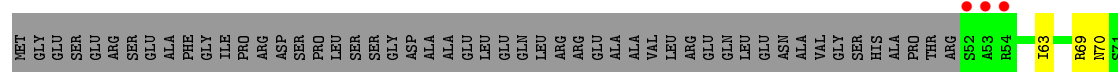


• Molecule 1: Proteasome-associated ATPase

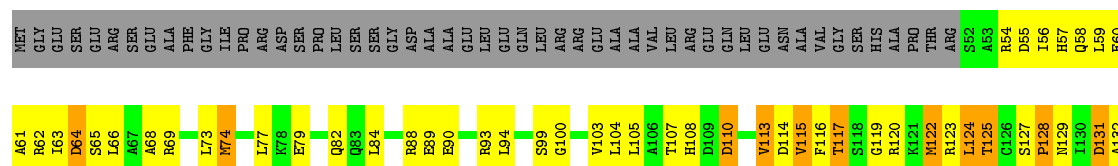
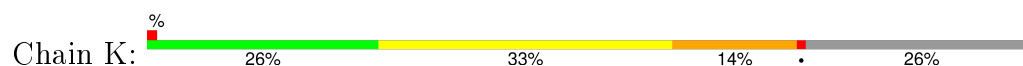




• Molecule 1: Proteasome-associated ATPase



• Molecule 1: Proteasome-associated ATPase



K225	E231	ARG
A226	R232	GLY
G227	I233	SER
	P234	ALA
	L235	ALA
	V236	LEU
	P237	GLU
		HIS
		HIS
		HIS
		HIS
		HIS
		HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	176.79Å 176.65Å 176.63Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	25.00 – 3.94 25.00 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (25.00-3.94) 99.7 (25.00-3.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.85Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.275 , 0.304 0.262 , 0.287	Depositor DCC
R_{free} test set	4860 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	152.3	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 147.3	EDS
Estimated twinning fraction	0.003 for k,h,l 0.007 for -k,-h,l 0.002 for l,k,-h 0.006 for -h,-l,-k 0.003 for -h,l,k 0.449 for l,h,k 0.449 for k,l,h 0.448 for -k,-l,h 0.448 for l,-h,-k 0.450 for -h,-k,l 0.005 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 98265 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17172	wwPDB-VP
Average B, all atoms (Å ²)	239.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	1.24	8/1451 (0.6%)	1.15	4/1969 (0.2%)
1	B	1.08	3/1451 (0.2%)	1.09	4/1969 (0.2%)
1	C	1.24	8/1451 (0.6%)	1.13	5/1969 (0.3%)
1	D	1.09	3/1451 (0.2%)	1.11	8/1969 (0.4%)
1	E	1.27	9/1451 (0.6%)	1.16	6/1969 (0.3%)
1	F	1.08	4/1451 (0.3%)	1.09	6/1969 (0.3%)
1	G	1.22	6/1451 (0.4%)	1.14	8/1969 (0.4%)
1	H	1.10	3/1451 (0.2%)	1.10	8/1969 (0.4%)
1	I	1.20	5/1451 (0.3%)	1.13	4/1969 (0.2%)
1	J	1.10	3/1451 (0.2%)	1.12	6/1969 (0.3%)
1	K	1.22	5/1451 (0.3%)	1.12	6/1969 (0.3%)
1	L	1.07	3/1451 (0.2%)	1.10	5/1969 (0.3%)
All	All	1.16	60/17412 (0.3%)	1.12	70/23628 (0.3%)

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	B	0	2
1	D	0	1
1	I	0	1
1	K	0	1
All	All	0	5

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	160	GLU	CG-CD	9.62	1.66	1.51
1	A	93	ARG	CZ-NH1	9.08	1.44	1.33
1	E	93	ARG	CZ-NH1	8.66	1.44	1.33
1	F	160	GLU	CG-CD	8.66	1.65	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	93	ARG	CZ-NH1	8.65	1.44	1.33
1	A	90	GLU	CD-OE1	8.41	1.34	1.25
1	J	160	GLU	CG-CD	8.33	1.64	1.51
1	K	93	ARG	CZ-NH1	8.28	1.43	1.33
1	D	160	GLU	CG-CD	8.12	1.64	1.51
1	I	93	ARG	CZ-NH1	8.01	1.43	1.33
1	E	90	GLU	CD-OE1	7.94	1.34	1.25
1	G	93	ARG	CZ-NH1	7.92	1.43	1.33
1	G	90	GLU	CD-OE1	7.90	1.34	1.25
1	B	160	GLU	CG-CD	7.71	1.63	1.51
1	C	90	GLU	CD-OE1	7.53	1.33	1.25
1	I	90	GLU	CD-OE1	7.38	1.33	1.25
1	L	160	GLU	CG-CD	7.16	1.62	1.51
1	K	90	GLU	CD-OE1	7.07	1.33	1.25
1	G	90	GLU	CD-OE2	6.89	1.33	1.25
1	H	160	GLU	CB-CG	6.71	1.64	1.52
1	B	160	GLU	CB-CG	6.67	1.64	1.52
1	E	90	GLU	CD-OE2	6.31	1.32	1.25
1	A	90	GLU	CD-OE2	6.29	1.32	1.25
1	E	156	GLU	CG-CD	6.16	1.61	1.51
1	F	89	GLU	CG-CD	6.03	1.61	1.51
1	I	156	GLU	CG-CD	5.84	1.60	1.51
1	E	126	CYS	CB-SG	-5.82	1.72	1.81
1	K	90	GLU	CD-OE2	5.82	1.32	1.25
1	I	90	GLU	CD-OE2	5.75	1.31	1.25
1	A	89	GLU	CG-CD	5.74	1.60	1.51
1	C	90	GLU	CD-OE2	5.69	1.31	1.25
1	J	160	GLU	CB-CG	5.66	1.62	1.52
1	C	126	CYS	CB-SG	-5.60	1.72	1.81
1	D	89	GLU	CG-CD	5.55	1.60	1.51
1	A	156	GLU	CG-CD	5.50	1.60	1.51
1	C	90	GLU	CG-CD	5.48	1.60	1.51
1	J	89	GLU	CG-CD	5.45	1.60	1.51
1	H	89	GLU	CG-CD	5.44	1.60	1.51
1	K	90	GLU	CG-CD	5.37	1.60	1.51
1	E	89	GLU	CD-OE2	5.34	1.31	1.25
1	A	90	GLU	CG-CD	5.29	1.59	1.51
1	A	89	GLU	CD-OE2	5.27	1.31	1.25
1	L	89	GLU	CG-CD	5.25	1.59	1.51
1	C	89	GLU	CG-CD	5.24	1.59	1.51
1	B	89	GLU	CG-CD	5.24	1.59	1.51
1	K	93	ARG	NE-CZ	5.24	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	160	GLU	CB-CG	5.20	1.62	1.52
1	G	156	GLU	CG-CD	5.17	1.59	1.51
1	G	89	GLU	CD-OE2	5.15	1.31	1.25
1	C	156	GLU	CG-CD	5.11	1.59	1.51
1	E	79	GLU	CD-OE2	5.09	1.31	1.25
1	A	126	CYS	CB-SG	-5.09	1.73	1.81
1	E	89	GLU	CG-CD	5.07	1.59	1.51
1	F	89	GLU	CB-CG	5.06	1.61	1.52
1	C	79	GLU	CD-OE2	5.06	1.31	1.25
1	I	89	GLU	CD-OE2	5.06	1.31	1.25
1	F	160	GLU	CD-OE2	5.03	1.31	1.25
1	L	160	GLU	CB-CG	5.02	1.61	1.52
1	G	236	VAL	CA-CB	5.01	1.65	1.54
1	E	90	GLU	CG-CD	5.00	1.59	1.51

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	ARG	NE-CZ-NH2	-12.81	113.90	120.30
1	E	93	ARG	NE-CZ-NH1	12.61	126.60	120.30
1	E	93	ARG	NE-CZ-NH2	-12.52	114.04	120.30
1	A	93	ARG	NE-CZ-NH1	12.34	126.47	120.30
1	C	93	ARG	NE-CZ-NH1	12.16	126.38	120.30
1	I	93	ARG	NE-CZ-NH1	11.67	126.14	120.30
1	G	93	ARG	NE-CZ-NH1	11.30	125.95	120.30
1	C	93	ARG	NE-CZ-NH2	-11.28	114.66	120.30
1	K	93	ARG	NE-CZ-NH1	11.02	125.81	120.30
1	I	93	ARG	NE-CZ-NH2	-10.65	114.97	120.30
1	G	93	ARG	NE-CZ-NH2	-10.14	115.23	120.30
1	K	93	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	J	235	LEU	CA-CB-CG	9.34	136.78	115.30
1	D	235	LEU	CA-CB-CG	8.76	135.45	115.30
1	B	235	LEU	CA-CB-CG	8.00	133.71	115.30
1	L	235	LEU	CA-CB-CG	7.43	132.40	115.30
1	H	235	LEU	CA-CB-CG	6.98	131.34	115.30
1	F	235	LEU	CA-CB-CG	6.75	130.82	115.30
1	H	235	LEU	CB-CG-CD2	6.63	122.27	111.00
1	J	235	LEU	CB-CG-CD2	6.57	122.17	111.00
1	D	235	LEU	CB-CG-CD2	6.56	122.16	111.00
1	I	205	LEU	CA-CB-CG	6.41	130.05	115.30
1	F	235	LEU	CB-CG-CD2	6.37	121.83	111.00
1	B	164	LEU	CA-CB-CG	6.29	129.76	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	164	LEU	CA-CB-CG	6.28	129.74	115.30
1	A	205	LEU	CA-CB-CG	6.19	129.54	115.30
1	E	205	LEU	CA-CB-CG	6.17	129.48	115.30
1	J	88	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	B	235	LEU	CB-CG-CD2	5.96	121.13	111.00
1	F	164	LEU	CA-CB-CG	5.88	128.82	115.30
1	G	205	LEU	CA-CB-CG	5.88	128.82	115.30
1	D	88	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	L	164	LEU	CA-CB-CG	5.85	128.76	115.30
1	L	235	LEU	CB-CG-CD2	5.84	120.94	111.00
1	H	88	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	J	124	LEU	CA-CB-CG	-5.68	102.23	115.30
1	G	186	VAL	CB-CA-C	-5.66	100.65	111.40
1	K	205	LEU	CA-CB-CG	5.66	128.31	115.30
1	C	176	VAL	CB-CA-C	-5.52	100.91	111.40
1	J	164	LEU	CA-CB-CG	5.50	127.95	115.30
1	H	147	LEU	CA-CB-CG	-5.47	102.72	115.30
1	H	184	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	L	88	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	D	147	LEU	CA-CB-CG	-5.46	102.75	115.30
1	K	135	LEU	CA-CB-CG	5.41	127.74	115.30
1	G	184	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	J	176	VAL	CB-CA-C	-5.38	101.17	111.40
1	D	176	VAL	CB-CA-C	-5.37	101.20	111.40
1	E	186	VAL	CB-CA-C	-5.37	101.20	111.40
1	F	176	VAL	CB-CA-C	-5.37	101.21	111.40
1	F	184	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	I	175	LEU	CA-CB-CG	5.26	127.41	115.30
1	F	88	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	K	64	ASP	CB-CG-OD1	5.22	123.00	118.30
1	D	184	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	L	176	VAL	CB-CA-C	-5.21	101.50	111.40
1	K	143	LEU	CA-CB-CG	5.14	127.13	115.30
1	G	143	LEU	CA-CB-CG	5.13	127.11	115.30
1	A	184	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	G	135	LEU	CA-CB-CG	5.13	127.10	115.30
1	C	150	VAL	CB-CA-C	-5.13	101.66	111.40
1	E	176	VAL	CB-CA-C	-5.11	101.69	111.40
1	H	197	LEU	CA-CB-CG	5.11	127.05	115.30
1	E	84	LEU	CA-CB-CG	5.07	126.97	115.30
1	B	147	LEU	CA-CB-CG	-5.06	103.67	115.30
1	D	220	LEU	CB-CG-CD2	-5.06	102.40	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	64	ASP	CB-CG-OD1	5.03	122.83	118.30
1	H	164	LEU	CA-CB-CG	5.03	126.86	115.30
1	C	210	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	H	176	VAL	CB-CA-C	-5.00	101.89	111.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	198	PRO	Peptide
1	B	236	VAL	Peptide
1	D	198	PRO	Peptide
1	I	236	VAL	Peptide
1	K	236	VAL	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	117	0
1	B	1431	0	1443	82	0
1	C	1431	0	1443	113	0
1	D	1431	0	1443	74	0
1	E	1431	0	1443	112	0
1	F	1431	0	1443	81	0
1	G	1431	0	1443	106	0
1	H	1431	0	1443	78	0
1	I	1431	0	1443	124	0
1	J	1431	0	1443	74	0
1	K	1431	0	1443	113	0
1	L	1431	0	1443	65	0
All	All	17172	0	17316	1071	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 31.

All (1071) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:ASP:OD1	1:E:123:ARG:HG3	1.44	1.16
1:K:186:VAL:HG12	1:K:227:GLY:O	1.48	1.13
1:C:120:ARG:HE	1:C:122:MET:CE	1.59	1.12
1:K:235:LEU:HD11	1:K:237:PRO:HD3	1.37	1.05
1:D:154:THR:HG22	1:D:155:PHE:H	1.15	1.04
1:E:115:VAL:CG2	1:E:124:LEU:HD21	1.87	1.04
1:I:186:VAL:HG12	1:I:227:GLY:O	1.55	1.04
1:K:235:LEU:CD1	1:K:237:PRO:HD3	1.88	1.03
1:B:154:THR:HG22	1:B:155:PHE:H	1.23	1.03
1:K:114:ASP:OD1	1:K:123:ARG:HG3	1.57	1.02
1:I:115:VAL:CG2	1:I:124:LEU:HD21	1.89	1.02
1:A:115:VAL:CG2	1:A:124:LEU:HD21	1.88	1.02
1:J:154:THR:HG22	1:J:155:PHE:H	1.23	1.02
1:C:120:ARG:HE	1:C:122:MET:HE3	1.25	1.01
1:I:114:ASP:OD1	1:I:123:ARG:HG3	1.61	1.00
1:E:186:VAL:HG12	1:E:227:GLY:O	1.63	0.98
1:G:186:VAL:HG12	1:G:227:GLY:O	1.64	0.97
1:B:155:PHE:HE2	1:B:191:PRO:HG2	1.29	0.97
1:L:154:THR:HG22	1:L:155:PHE:H	1.30	0.95
1:C:115:VAL:CG2	1:C:124:LEU:HD21	1.96	0.94
1:H:154:THR:HG22	1:H:155:PHE:H	1.33	0.94
1:D:155:PHE:HE2	1:D:191:PRO:HG2	1.31	0.93
1:K:189:ALA:H	1:K:192:LEU:HD12	1.32	0.93
1:K:168:LEU:HB2	1:K:173:ARG:O	1.68	0.92
1:C:168:LEU:HB2	1:C:173:ARG:O	1.70	0.91
1:I:220:LEU:HD12	1:I:229:ALA:HB1	1.52	0.91
1:A:186:VAL:HG12	1:A:227:GLY:O	1.68	0.91
1:L:220:LEU:HD12	1:L:220:LEU:N	1.85	0.90
1:J:220:LEU:N	1:J:220:LEU:HD12	1.86	0.89
1:F:154:THR:HG22	1:F:155:PHE:H	1.38	0.89
1:G:115:VAL:HG23	1:G:124:LEU:HD21	1.56	0.88
1:H:155:PHE:HE2	1:H:191:PRO:HG2	1.35	0.87
1:G:220:LEU:HD12	1:G:229:ALA:HB1	1.57	0.86
1:L:155:PHE:HE2	1:L:191:PRO:HG2	1.38	0.85
1:G:115:VAL:CG2	1:G:124:LEU:HD21	2.06	0.85
1:H:232:ARG:O	1:H:233:ILE:HG12	1.76	0.85
1:H:220:LEU:N	1:H:220:LEU:HD12	1.89	0.85
1:C:120:ARG:NE	1:C:122:MET:CE	2.40	0.85
1:K:115:VAL:CG2	1:K:124:LEU:HD21	2.07	0.84
1:C:120:ARG:HE	1:C:122:MET:HE2	1.42	0.84
1:C:115:VAL:HG23	1:C:124:LEU:HD21	1.58	0.84
1:F:155:PHE:HE2	1:F:191:PRO:HG2	1.41	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:PHE:CE2	1:B:191:PRO:HG2	2.12	0.83
1:G:125:THR:HG23	1:J:97:PRO:HG3	1.58	0.83
1:D:155:PHE:CE2	1:D:191:PRO:HG2	2.13	0.83
1:B:97:PRO:HG3	1:E:125:THR:HG23	1.59	0.82
1:F:116:PHE:CE2	1:F:226:ALA:HA	2.14	0.82
1:L:218:ASP:OD2	1:L:232:ARG:NH1	2.12	0.82
1:K:115:VAL:HG23	1:K:124:LEU:HD21	1.61	0.82
1:F:155:PHE:CE2	1:F:191:PRO:HG2	2.15	0.82
1:G:175:LEU:HD21	1:J:235:LEU:HD12	1.61	0.81
1:E:126:CYS:HB3	1:E:130:ILE:HD11	1.63	0.81
1:B:220:LEU:HD12	1:B:220:LEU:N	1.95	0.81
1:I:125:THR:HG23	1:L:97:PRO:HG3	1.63	0.81
1:H:162:SER:HB3	1:H:178:GLY:HA2	1.61	0.81
1:A:235:LEU:CD1	1:A:237:PRO:HD3	2.11	0.81
1:H:139:GLN:NE2	1:H:152:ALA:HB1	1.96	0.80
1:H:116:PHE:HD1	1:H:120:ARG:O	1.63	0.80
1:B:116:PHE:HD1	1:B:120:ARG:O	1.63	0.80
1:J:155:PHE:HE2	1:J:191:PRO:HG2	1.45	0.80
1:A:120:ARG:HH21	1:A:122:MET:HE1	1.46	0.80
1:A:168:LEU:HB2	1:A:173:ARG:O	1.81	0.80
1:I:184:ARG:HD3	1:I:224:THR:CG2	2.11	0.80
1:I:168:LEU:HB2	1:I:173:ARG:O	1.81	0.80
1:A:125:THR:HG23	1:D:97:PRO:HG3	1.64	0.80
1:E:115:VAL:HG23	1:E:124:LEU:HD21	1.62	0.79
1:A:115:VAL:HG22	1:A:124:LEU:HD21	1.62	0.79
1:C:125:THR:HG23	1:F:97:PRO:HG3	1.62	0.79
1:F:218:ASP:OD2	1:F:232:ARG:NH1	2.16	0.78
1:C:155:PHE:HE2	1:C:191:PRO:HG2	1.48	0.78
1:H:97:PRO:HG3	1:K:125:THR:HG23	1.64	0.78
1:D:154:THR:CG2	1:D:155:PHE:H	1.94	0.78
1:J:162:SER:HB3	1:J:178:GLY:HA2	1.65	0.78
1:K:154:THR:HG22	1:K:155:PHE:H	1.48	0.78
1:F:116:PHE:HD1	1:F:120:ARG:O	1.64	0.78
1:F:220:LEU:HD12	1:F:220:LEU:N	1.98	0.77
1:H:147:LEU:HD12	1:H:147:LEU:H	1.49	0.77
1:K:202:PRO:O	1:K:203:GLU:HB2	1.83	0.77
1:B:116:PHE:CE2	1:B:226:ALA:HA	2.18	0.77
1:I:202:PRO:O	1:I:203:GLU:HB2	1.84	0.77
1:J:95:GLY:O	1:J:142:ARG:NH2	2.17	0.77
1:L:168:LEU:HD12	1:L:173:ARG:HB2	1.65	0.77
1:I:139:GLN:HE21	1:I:152:ALA:HB1	1.49	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:168:LEU:HD12	1:J:173:ARG:HB2	1.65	0.77
1:H:168:LEU:HD12	1:H:173:ARG:HB2	1.65	0.76
1:D:168:LEU:HD12	1:D:173:ARG:HB2	1.67	0.76
1:H:186:VAL:HG12	1:H:227:GLY:C	2.05	0.76
1:E:220:LEU:HD12	1:E:229:ALA:HB1	1.65	0.76
1:J:155:PHE:CE2	1:J:191:PRO:HG2	2.20	0.76
1:E:163:THR:O	1:E:176:VAL:HG12	1.86	0.76
1:H:155:PHE:CE2	1:H:191:PRO:HG2	2.20	0.76
1:C:186:VAL:CG1	1:C:227:GLY:O	2.33	0.76
1:K:186:VAL:CG1	1:K:227:GLY:O	2.31	0.76
1:G:125:THR:HG23	1:J:97:PRO:CG	2.16	0.76
1:L:116:PHE:HD1	1:L:120:ARG:O	1.69	0.76
1:D:220:LEU:HD12	1:D:220:LEU:N	2.01	0.76
1:I:189:ALA:H	1:I:192:LEU:HD12	1.51	0.76
1:K:235:LEU:HD22	1:K:236:VAL:H	1.50	0.76
1:I:115:VAL:HG22	1:I:124:LEU:HD21	1.67	0.76
1:E:105:LEU:HB2	1:E:114:ASP:O	1.84	0.76
1:I:105:LEU:HB2	1:I:114:ASP:O	1.85	0.75
1:L:155:PHE:CE2	1:L:191:PRO:HG2	2.20	0.75
1:F:147:LEU:H	1:F:147:LEU:HD12	1.49	0.75
1:D:154:THR:HG22	1:D:155:PHE:N	1.98	0.75
1:K:164:LEU:HD12	1:K:165:ARG:N	2.01	0.75
1:A:235:LEU:HD13	1:A:237:PRO:HD3	1.68	0.75
1:E:184:ARG:HD3	1:E:224:THR:CG2	2.17	0.74
1:I:99:SER:HB2	1:J:123:ARG:HB3	1.69	0.74
1:J:126:CYS:HB3	1:J:149:VAL:CG2	2.16	0.74
1:F:126:CYS:HB3	1:F:149:VAL:HG23	1.68	0.74
1:G:202:PRO:O	1:G:203:GLU:HB2	1.86	0.74
1:A:202:PRO:O	1:A:203:GLU:HB2	1.87	0.74
1:J:126:CYS:HB3	1:J:149:VAL:HG23	1.70	0.73
1:J:154:THR:CG2	1:J:155:PHE:H	1.99	0.73
1:H:116:PHE:CE2	1:H:226:ALA:HA	2.23	0.73
1:A:220:LEU:HD12	1:A:229:ALA:HB1	1.69	0.73
1:K:165:ARG:HH11	1:K:165:ARG:HG2	1.53	0.73
1:F:162:SER:HB3	1:F:178:GLY:HA2	1.68	0.73
1:C:114:ASP:OD1	1:C:123:ARG:HG3	1.87	0.73
1:C:165:ARG:HG2	1:C:165:ARG:HH11	1.54	0.73
1:A:164:LEU:HD12	1:A:165:ARG:N	2.03	0.73
1:E:189:ALA:H	1:E:192:LEU:HD12	1.54	0.73
1:G:124:LEU:HD11	1:G:143:LEU:CD2	2.18	0.73
1:A:189:ALA:H	1:A:192:LEU:HD12	1.54	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:221:LEU:C	1:K:221:LEU:HD23	2.09	0.73
1:K:105:LEU:HB2	1:K:114:ASP:O	1.88	0.73
1:E:168:LEU:HB2	1:E:173:ARG:O	1.89	0.73
1:K:189:ALA:N	1:K:192:LEU:HD12	2.03	0.72
1:K:135:LEU:HB2	1:K:139:GLN:NE2	2.04	0.72
1:F:126:CYS:HB3	1:F:149:VAL:CG2	2.18	0.72
1:G:189:ALA:H	1:G:192:LEU:HD12	1.55	0.72
1:D:162:SER:HB3	1:D:178:GLY:HA2	1.71	0.72
1:E:120:ARG:HH21	1:E:122:MET:HE1	1.55	0.72
1:D:124:LEU:HD11	1:D:147:LEU:HB3	1.70	0.72
1:G:126:CYS:HB3	1:G:130:ILE:HD11	1.71	0.72
1:C:189:ALA:H	1:C:192:LEU:HD12	1.54	0.71
1:G:127:SER:O	1:G:129:ASN:N	2.22	0.71
1:A:124:LEU:HD11	1:A:143:LEU:CD2	2.20	0.71
1:E:184:ARG:HD3	1:E:224:THR:HG21	1.72	0.71
1:F:168:LEU:HD12	1:F:173:ARG:HB2	1.73	0.71
1:K:163:THR:O	1:K:176:VAL:HG12	1.91	0.71
1:G:163:THR:O	1:G:176:VAL:HG12	1.90	0.71
1:A:58:GLN:HE22	1:I:235:LEU:HG	1.55	0.71
1:C:103:VAL:O	1:C:115:VAL:HG12	1.91	0.71
1:K:189:ALA:H	1:K:192:LEU:CD1	2.03	0.71
1:B:90:GLU:HA	1:B:93:ARG:HD3	1.71	0.71
1:A:185:VAL:O	1:D:158:VAL:HG12	1.91	0.71
1:G:186:VAL:CG1	1:G:227:GLY:O	2.39	0.71
1:L:116:PHE:CE2	1:L:226:ALA:HA	2.25	0.71
1:K:177:VAL:HG12	1:K:183:GLU:HG2	1.73	0.71
1:B:104:LEU:O	1:B:104:LEU:HG	1.91	0.70
1:C:186:VAL:HG13	1:C:227:GLY:O	1.90	0.70
1:G:206:ASN:O	1:G:207:ASP:HB2	1.91	0.70
1:F:116:PHE:CD2	1:F:226:ALA:HA	2.27	0.70
1:E:154:THR:HG22	1:E:155:PHE:H	1.56	0.70
1:G:232:ARG:O	1:G:233:ILE:HD13	1.91	0.70
1:E:202:PRO:O	1:E:203:GLU:HB2	1.92	0.70
1:D:90:GLU:HA	1:D:93:ARG:HD3	1.72	0.70
1:I:212:ARG:HE	1:I:215:ARG:HD3	1.57	0.70
1:C:127:SER:O	1:C:129:ASN:N	2.22	0.70
1:C:77:LEU:O	1:C:77:LEU:HD13	1.92	0.70
1:I:184:ARG:HD3	1:I:224:THR:HG22	1.74	0.70
1:A:139:GLN:NE2	1:A:152:ALA:HB1	2.07	0.69
1:I:77:LEU:O	1:I:77:LEU:HD13	1.92	0.69
1:J:116:PHE:HD1	1:J:120:ARG:O	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:104:LEU:HD13	1:L:113:VAL:CG1	2.23	0.69
1:C:155:PHE:CE2	1:C:191:PRO:HG2	2.27	0.69
1:E:232:ARG:O	1:E:233:ILE:HD13	1.93	0.69
1:G:185:VAL:O	1:J:158:VAL:HG12	1.92	0.69
1:G:103:VAL:O	1:G:115:VAL:HG12	1.93	0.69
1:C:120:ARG:HH21	1:C:122:MET:CE	2.06	0.69
1:I:165:ARG:HH12	1:L:235:LEU:HD11	1.58	0.69
1:C:124:LEU:HD11	1:C:143:LEU:CD2	2.23	0.68
1:C:139:GLN:HE21	1:C:152:ALA:HB1	1.56	0.68
1:J:218:ASP:OD2	1:J:232:ARG:NH1	2.23	0.68
1:G:158:VAL:HG12	1:H:185:VAL:O	1.93	0.68
1:A:77:LEU:HD13	1:A:77:LEU:O	1.94	0.68
1:H:116:PHE:CD1	1:H:120:ARG:O	2.45	0.68
1:I:184:ARG:HD3	1:I:224:THR:HG21	1.75	0.68
1:K:165:ARG:NH1	1:K:165:ARG:HG2	2.08	0.68
1:G:180:ALA:O	1:G:182:GLU:N	2.26	0.68
1:G:221:LEU:O	1:G:221:LEU:HD23	1.93	0.68
1:H:158:VAL:HG12	1:K:185:VAL:O	1.93	0.68
1:A:142:ARG:HD2	1:B:123:ARG:HD3	1.74	0.68
1:L:162:SER:HB3	1:L:178:GLY:HA2	1.75	0.68
1:B:116:PHE:CD2	1:B:226:ALA:HA	2.29	0.68
1:B:97:PRO:CG	1:E:125:THR:HG23	2.24	0.67
1:E:230:PHE:O	1:E:231:GLU:HB3	1.94	0.67
1:C:120:ARG:HH21	1:C:122:MET:HE1	1.58	0.67
1:J:138:GLY:O	1:J:155:PHE:CE1	2.48	0.67
1:H:97:PRO:CG	1:K:125:THR:HG23	2.24	0.67
1:B:219:SER:C	1:B:220:LEU:HD12	2.14	0.67
1:K:235:LEU:HD13	1:K:237:PRO:HD3	1.72	0.67
1:C:120:ARG:NE	1:C:122:MET:HE2	2.08	0.67
1:L:126:CYS:HB3	1:L:149:VAL:HG23	1.76	0.67
1:I:125:THR:HG23	1:L:97:PRO:CG	2.25	0.66
1:B:154:THR:HG22	1:B:155:PHE:N	2.04	0.66
1:G:184:ARG:HD3	1:G:224:THR:CG2	2.25	0.66
1:B:100:GLY:O	1:B:143:LEU:HD12	1.95	0.66
1:C:221:LEU:HD23	1:C:221:LEU:C	2.15	0.66
1:G:105:LEU:O	1:G:228:TYR:OH	2.14	0.66
1:A:114:ASP:OD1	1:A:123:ARG:HG3	1.96	0.66
1:A:184:ARG:HD3	1:A:224:THR:HG21	1.78	0.66
1:J:220:LEU:N	1:J:220:LEU:CD1	2.59	0.66
1:C:235:LEU:HD11	1:C:237:PRO:HD3	1.77	0.66
1:F:90:GLU:HA	1:F:93:ARG:HD3	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:LEU:HD13	1:E:77:LEU:O	1.96	0.66
1:A:177:VAL:O	1:A:177:VAL:HG23	1.93	0.66
1:C:105:LEU:HB2	1:C:114:ASP:O	1.96	0.65
1:C:221:LEU:HD22	1:C:230:PHE:HB2	1.77	0.65
1:I:117:THR:O	1:I:119:GLY:N	2.29	0.65
1:E:120:ARG:HE	1:E:122:MET:CE	2.09	0.65
1:A:139:GLN:HE21	1:A:152:ALA:HB1	1.59	0.65
1:I:124:LEU:HD11	1:I:143:LEU:CD2	2.25	0.65
1:K:165:ARG:HB3	1:K:175:LEU:HD23	1.78	0.65
1:J:116:PHE:CE2	1:J:226:ALA:HA	2.30	0.65
1:G:62:ARG:HD2	1:H:63:ILE:HD11	1.78	0.65
1:G:77:LEU:O	1:G:77:LEU:HD13	1.95	0.65
1:I:185:VAL:O	1:L:158:VAL:HG12	1.95	0.65
1:E:115:VAL:HG21	1:E:124:LEU:HD21	1.77	0.65
1:C:165:ARG:HG2	1:C:165:ARG:NH1	2.07	0.65
1:I:62:ARG:HD2	1:J:63:ILE:HD11	1.79	0.65
1:F:100:GLY:O	1:F:143:LEU:HD12	1.97	0.65
1:B:124:LEU:HD11	1:B:147:LEU:HB3	1.79	0.65
1:L:138:GLY:O	1:L:155:PHE:CE1	2.50	0.64
1:L:126:CYS:HB3	1:L:149:VAL:CG2	2.27	0.64
1:J:219:SER:C	1:J:220:LEU:HD12	2.16	0.64
1:D:130:ILE:HD12	1:D:131:ASP:H	1.61	0.64
1:K:124:LEU:HD11	1:K:143:LEU:CD2	2.27	0.64
1:L:116:PHE:CD1	1:L:120:ARG:O	2.50	0.64
1:A:105:LEU:O	1:A:106:ALA:HB2	1.98	0.64
1:I:220:LEU:CD1	1:I:229:ALA:HB1	2.27	0.64
1:E:186:VAL:CG1	1:E:227:GLY:O	2.43	0.64
1:L:232:ARG:O	1:L:233:ILE:HG12	1.97	0.64
1:G:105:LEU:HD13	1:G:116:PHE:HB2	1.80	0.64
1:E:139:GLN:HE21	1:E:152:ALA:HB1	1.62	0.64
1:K:77:LEU:O	1:K:77:LEU:HD13	1.98	0.64
1:A:232:ARG:O	1:A:233:ILE:HD13	1.98	0.64
1:C:120:ARG:NE	1:C:122:MET:HE3	2.05	0.64
1:J:154:THR:HG22	1:J:155:PHE:N	2.06	0.64
1:I:235:LEU:CD1	1:I:237:PRO:HD3	2.28	0.64
1:D:116:PHE:CE2	1:D:226:ALA:HA	2.33	0.64
1:H:147:LEU:N	1:H:147:LEU:HD12	2.12	0.63
1:I:235:LEU:HD22	1:I:236:VAL:H	1.63	0.63
1:B:198:PRO:O	1:B:200:GLY:N	2.28	0.63
1:A:175:LEU:HD12	1:A:185:VAL:HG23	1.80	0.63
1:B:168:LEU:HD12	1:B:173:ARG:HB2	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:VAL:HG12	1:A:185:VAL:O	1.97	0.63
1:F:137:LYS:HB2	1:F:190:ASP:OD2	1.97	0.63
1:C:125:THR:HG23	1:F:97:PRO:CG	2.27	0.63
1:D:138:GLY:O	1:D:155:PHE:CE1	2.51	0.63
1:I:221:LEU:C	1:I:221:LEU:HD23	2.19	0.63
1:K:142:ARG:HD2	1:L:123:ARG:HD3	1.81	0.63
1:B:162:SER:HB3	1:B:178:GLY:HA2	1.79	0.63
1:F:104:LEU:HD13	1:F:113:VAL:CG1	2.28	0.63
1:E:124:LEU:HD11	1:E:143:LEU:CD2	2.28	0.63
1:H:104:LEU:HD13	1:H:113:VAL:CG1	2.28	0.63
1:A:165:ARG:HB3	1:A:175:LEU:HD23	1.80	0.63
1:E:206:ASN:O	1:E:207:ASP:HB2	1.99	0.62
1:E:164:LEU:HD12	1:E:165:ARG:N	2.13	0.62
1:H:218:ASP:N	1:H:218:ASP:OD1	2.33	0.62
1:I:139:GLN:NE2	1:I:152:ALA:HB1	2.13	0.62
1:B:104:LEU:HD13	1:B:113:VAL:CG1	2.29	0.62
1:J:90:GLU:HA	1:J:93:ARG:HD3	1.81	0.62
1:I:101:TYR:CE1	1:I:142:ARG:HG3	2.33	0.62
1:E:120:ARG:HE	1:E:122:MET:HE3	1.64	0.62
1:F:104:LEU:O	1:F:104:LEU:HG	1.97	0.62
1:F:147:LEU:N	1:F:147:LEU:HD12	2.12	0.62
1:L:219:SER:C	1:L:220:LEU:HD12	2.19	0.62
1:K:162:SER:HB3	1:K:177:VAL:O	2.00	0.62
1:H:124:LEU:HD11	1:H:147:LEU:HB3	1.81	0.62
1:K:220:LEU:HD12	1:K:229:ALA:HB1	1.81	0.62
1:A:120:ARG:HE	1:A:122:MET:HE2	1.64	0.62
1:C:154:THR:HG22	1:C:155:PHE:H	1.65	0.62
1:C:185:VAL:O	1:F:158:VAL:HG12	1.98	0.62
1:L:90:GLU:HA	1:L:93:ARG:HD3	1.82	0.62
1:L:104:LEU:HG	1:L:104:LEU:O	2.00	0.62
1:D:104:LEU:HD13	1:D:113:VAL:CG1	2.30	0.62
1:K:127:SER:O	1:K:129:ASN:N	2.33	0.62
1:K:235:LEU:HD11	1:K:237:PRO:CD	2.20	0.62
1:J:104:LEU:HD13	1:J:113:VAL:CG1	2.30	0.61
1:H:154:THR:CG2	1:H:155:PHE:H	2.07	0.61
1:F:232:ARG:O	1:F:233:ILE:HG12	1.99	0.61
1:E:168:LEU:HD22	1:E:169:ALA:H	1.65	0.61
1:G:165:ARG:HG2	1:G:165:ARG:HH11	1.66	0.61
1:B:138:GLY:O	1:B:155:PHE:CE1	2.53	0.61
1:H:219:SER:C	1:H:220:LEU:HD12	2.21	0.61
1:D:116:PHE:HD1	1:D:120:ARG:O	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:90:GLU:HA	1:H:93:ARG:HD3	1.80	0.61
1:A:158:VAL:HG12	1:B:185:VAL:O	2.00	0.61
1:I:115:VAL:HG21	1:I:124:LEU:HD21	1.79	0.61
1:F:139:GLN:HB2	1:F:155:PHE:CE1	2.35	0.61
1:K:221:LEU:HD22	1:K:230:PHE:HB2	1.82	0.61
1:K:232:ARG:O	1:K:233:ILE:HD13	2.00	0.61
1:K:105:LEU:O	1:K:228:TYR:OH	2.18	0.61
1:A:115:VAL:CG2	1:A:124:LEU:CD2	2.74	0.61
1:C:186:VAL:HG12	1:C:227:GLY:O	2.00	0.61
1:I:186:VAL:HG12	1:I:227:GLY:C	2.20	0.61
1:A:125:THR:HG23	1:D:97:PRO:CG	2.30	0.61
1:L:220:LEU:CD1	1:L:220:LEU:N	2.60	0.61
1:K:62:ARG:HD2	1:L:63:ILE:HD11	1.83	0.61
1:I:235:LEU:HD13	1:I:237:PRO:HD3	1.82	0.61
1:I:189:ALA:N	1:I:192:LEU:HD12	2.15	0.61
1:G:221:LEU:C	1:G:221:LEU:HD23	2.20	0.61
1:A:177:VAL:CG2	1:A:177:VAL:O	2.48	0.61
1:C:220:LEU:HD12	1:C:229:ALA:HB1	1.81	0.61
1:B:154:THR:CG2	1:B:155:PHE:H	2.00	0.60
1:G:184:ARG:HD3	1:G:224:THR:HG21	1.83	0.60
1:G:141:VAL:HG21	1:G:149:VAL:CG1	2.30	0.60
1:B:116:PHE:CD1	1:B:120:ARG:O	2.52	0.60
1:A:105:LEU:HB2	1:A:114:ASP:O	2.02	0.60
1:B:218:ASP:OD2	1:B:232:ARG:NH1	2.32	0.60
1:G:235:LEU:CD1	1:G:237:PRO:HD3	2.30	0.60
1:K:235:LEU:HD22	1:K:236:VAL:N	2.16	0.60
1:C:105:LEU:O	1:C:228:TYR:OH	2.19	0.60
1:E:142:ARG:HD2	1:F:123:ARG:HD3	1.83	0.60
1:E:115:VAL:HG23	1:E:124:LEU:CD2	2.32	0.60
1:F:116:PHE:CD1	1:F:120:ARG:O	2.52	0.60
1:C:136:LYS:N	1:C:139:GLN:OE1	2.33	0.60
1:E:139:GLN:NE2	1:E:152:ALA:HB1	2.17	0.60
1:A:182:GLU:HB3	1:D:179:HIS:CD2	2.37	0.60
1:A:117:THR:O	1:A:119:GLY:N	2.33	0.60
1:E:177:VAL:O	1:E:177:VAL:HG23	2.00	0.60
1:E:165:ARG:HH11	1:E:165:ARG:HG2	1.65	0.60
1:C:150:VAL:O	1:C:151:GLU:HB2	2.00	0.60
1:C:139:GLN:NE2	1:C:152:ALA:HB1	2.17	0.59
1:K:120:ARG:HH21	1:K:122:MET:HE1	1.66	0.59
1:H:110:ASP:OD1	1:H:110:ASP:O	2.21	0.59
1:E:221:LEU:HD23	1:E:221:LEU:C	2.22	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:235:LEU:HD11	1:G:237:PRO:HD3	1.84	0.59
1:I:127:SER:O	1:I:129:ASN:N	2.36	0.59
1:J:116:PHE:CD1	1:J:120:ARG:O	2.54	0.59
1:D:198:PRO:O	1:D:200:GLY:N	2.36	0.59
1:A:221:LEU:C	1:A:221:LEU:HD23	2.23	0.59
1:B:158:VAL:HG12	1:E:185:VAL:O	2.03	0.59
1:E:114:ASP:OD1	1:E:123:ARG:CG	2.36	0.59
1:L:154:THR:CG2	1:L:155:PHE:H	2.08	0.59
1:A:190:ASP:O	1:A:192:LEU:N	2.35	0.59
1:C:235:LEU:HD13	1:C:235:LEU:C	2.24	0.58
1:B:147:LEU:HD12	1:B:147:LEU:N	2.17	0.58
1:C:232:ARG:O	1:C:233:ILE:HD13	2.02	0.58
1:A:115:VAL:HG22	1:A:124:LEU:CD2	2.31	0.58
1:C:235:LEU:CD1	1:C:237:PRO:HD3	2.33	0.58
1:I:154:THR:HG22	1:I:155:PHE:H	1.67	0.58
1:I:232:ARG:O	1:I:233:ILE:HD13	2.04	0.58
1:G:182:GLU:HB3	1:J:179:HIS:CD2	2.38	0.58
1:K:105:LEU:HG	1:K:228:TYR:HE2	1.68	0.58
1:C:141:VAL:HG21	1:C:149:VAL:CG1	2.34	0.58
1:L:124:LEU:HD11	1:L:147:LEU:HB3	1.86	0.58
1:E:141:VAL:HG21	1:E:149:VAL:CG1	2.33	0.58
1:A:101:TYR:HD1	1:A:142:ARG:HA	1.69	0.58
1:K:186:VAL:HG12	1:K:227:GLY:C	2.21	0.58
1:G:105:LEU:HB2	1:G:114:ASP:O	2.03	0.58
1:C:175:LEU:C	1:C:175:LEU:HD12	2.25	0.57
1:E:105:LEU:O	1:E:228:TYR:OH	2.21	0.57
1:B:220:LEU:CD1	1:B:220:LEU:N	2.66	0.57
1:C:136:LYS:HB3	1:C:190:ASP:HB2	1.86	0.57
1:C:164:LEU:HD12	1:C:165:ARG:N	2.18	0.57
1:E:120:ARG:NH2	1:E:122:MET:HE1	2.20	0.57
1:K:206:ASN:O	1:K:207:ASP:HB2	2.04	0.57
1:D:126:CYS:HB3	1:D:149:VAL:HG23	1.85	0.57
1:A:115:VAL:HG21	1:A:124:LEU:HD21	1.80	0.57
1:H:162:SER:HB2	1:H:176:VAL:HG12	1.86	0.57
1:A:235:LEU:HD11	1:A:237:PRO:HD3	1.85	0.57
1:C:184:ARG:HD3	1:C:224:THR:HG21	1.87	0.57
1:K:164:LEU:C	1:K:164:LEU:HD12	2.24	0.57
1:E:120:ARG:NE	1:E:122:MET:HE3	2.19	0.57
1:G:168:LEU:HB2	1:G:173:ARG:O	2.04	0.57
1:F:210:ARG:HG2	1:F:211:PRO:HD2	1.85	0.57
1:I:164:LEU:HD12	1:I:165:ARG:N	2.20	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:219:SER:C	1:F:220:LEU:HD12	2.23	0.57
1:L:154:THR:HG22	1:L:155:PHE:N	2.11	0.57
1:I:168:LEU:HD22	1:I:169:ALA:H	1.70	0.57
1:A:164:LEU:HD12	1:A:164:LEU:C	2.24	0.57
1:E:110:ASP:HB3	1:E:112:THR:HG23	1.87	0.57
1:K:190:ASP:O	1:K:192:LEU:N	2.38	0.56
1:K:185:VAL:O	1:K:185:VAL:HG12	2.05	0.56
1:K:120:ARG:HE	1:K:122:MET:CE	2.18	0.56
1:L:116:PHE:CD2	1:L:226:ALA:HA	2.40	0.56
1:C:184:ARG:HD3	1:C:224:THR:CG2	2.35	0.56
1:A:105:LEU:HG	1:A:228:TYR:HE2	1.71	0.56
1:K:220:LEU:HD23	1:K:220:LEU:H	1.70	0.56
1:H:198:PRO:O	1:H:200:GLY:N	2.39	0.56
1:I:186:VAL:CG1	1:I:227:GLY:O	2.42	0.56
1:H:138:GLY:O	1:H:155:PHE:CE1	2.58	0.56
1:C:163:THR:O	1:C:176:VAL:HG12	2.06	0.56
1:C:115:VAL:HG23	1:C:124:LEU:CD2	2.35	0.56
1:C:141:VAL:CG2	1:C:149:VAL:HG13	2.36	0.56
1:B:172:HIS:O	1:B:188:LEU:HD12	2.04	0.56
1:A:108:HIS:C	1:A:110:ASP:H	2.09	0.56
1:B:124:LEU:HD21	1:B:147:LEU:O	2.05	0.56
1:F:99:SER:CB	1:F:142:ARG:HH11	2.18	0.55
1:E:94:LEU:HD11	1:F:128:PRO:HD2	1.88	0.55
1:J:139:GLN:HB2	1:J:155:PHE:HE1	1.71	0.55
1:A:184:ARG:HD3	1:A:224:THR:CG2	2.36	0.55
1:C:94:LEU:HD11	1:D:128:PRO:HD2	1.87	0.55
1:E:235:LEU:HD13	1:E:235:LEU:C	2.25	0.55
1:C:141:VAL:HG21	1:C:149:VAL:HG13	1.89	0.55
1:I:177:VAL:O	1:I:177:VAL:HG23	2.06	0.55
1:G:124:LEU:HD11	1:G:143:LEU:HD21	1.88	0.55
1:C:124:LEU:HD11	1:C:143:LEU:HD22	1.87	0.55
1:D:116:PHE:CD1	1:D:120:ARG:O	2.59	0.55
1:E:104:LEU:HD11	1:E:113:VAL:HG11	1.89	0.55
1:B:139:GLN:HA	1:B:155:PHE:CE1	2.41	0.55
1:D:104:LEU:O	1:D:104:LEU:HG	2.05	0.55
1:F:99:SER:HB2	1:F:142:ARG:HH11	1.72	0.55
1:F:124:LEU:HD11	1:F:147:LEU:HB3	1.89	0.55
1:G:154:THR:HG22	1:G:155:PHE:H	1.71	0.55
1:I:120:ARG:NE	1:I:122:MET:HE3	2.21	0.54
1:I:131:ASP:O	1:I:133:ALA:N	2.41	0.54
1:J:198:PRO:O	1:J:200:GLY:N	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:ALA:C	1:D:191:PRO:HD2	2.28	0.54
1:A:101:TYR:HD2	1:B:121:LYS:HB3	1.71	0.54
1:A:105:LEU:HD13	1:A:116:PHE:HB2	1.89	0.54
1:E:115:VAL:CG2	1:E:124:LEU:CD2	2.74	0.54
1:H:116:PHE:CD2	1:H:226:ALA:HA	2.42	0.54
1:C:142:ARG:HD2	1:D:123:ARG:HD3	1.89	0.54
1:E:190:ASP:O	1:E:192:LEU:N	2.41	0.54
1:D:172:HIS:O	1:D:188:LEU:HD12	2.08	0.54
1:K:221:LEU:O	1:K:221:LEU:HD23	2.08	0.54
1:E:184:ARG:HD3	1:E:224:THR:HG22	1.90	0.53
1:H:137:LYS:HB2	1:H:190:ASP:OD2	2.08	0.53
1:L:117:THR:O	1:L:118:SER:C	2.46	0.53
1:E:182:GLU:HG3	1:E:182:GLU:O	2.06	0.53
1:E:103:VAL:O	1:E:115:VAL:HG12	2.07	0.53
1:I:155:PHE:O	1:I:156:GLU:C	2.46	0.53
1:C:126:CYS:HB3	1:C:130:ILE:HD11	1.89	0.53
1:B:153:GLY:O	1:B:154:THR:O	2.26	0.53
1:I:124:LEU:HD23	1:I:124:LEU:N	2.24	0.53
1:J:104:LEU:O	1:J:104:LEU:HG	2.08	0.53
1:G:165:ARG:HG2	1:G:165:ARG:NH1	2.20	0.53
1:K:108:HIS:C	1:K:110:ASP:H	2.11	0.53
1:C:144:ASN:C	1:C:144:ASN:OD1	2.46	0.53
1:I:189:ALA:H	1:I:192:LEU:CD1	2.21	0.53
1:C:185:VAL:HG12	1:C:185:VAL:O	2.09	0.53
1:D:113:VAL:O	1:D:123:ARG:HA	2.08	0.53
1:A:62:ARG:HD2	1:B:63:ILE:HD11	1.91	0.53
1:K:164:LEU:HD12	1:K:165:ARG:H	1.74	0.53
1:J:110:ASP:OD1	1:J:110:ASP:O	2.26	0.53
1:C:189:ALA:O	1:C:190:ASP:C	2.46	0.53
1:F:220:LEU:N	1:F:220:LEU:CD1	2.70	0.53
1:J:212:ARG:HG3	1:J:213:LYS:O	2.09	0.53
1:K:212:ARG:HE	1:K:215:ARG:HD3	1.74	0.53
1:B:122:MET:HE1	1:B:147:LEU:HD22	1.90	0.53
1:B:207:ASP:OD1	1:B:209:THR:CG2	2.57	0.53
1:D:154:THR:CG2	1:D:155:PHE:N	2.65	0.53
1:E:124:LEU:N	1:E:124:LEU:HD23	2.24	0.53
1:K:167:ILE:HG22	1:K:168:LEU:H	1.74	0.53
1:A:186:VAL:HG12	1:A:227:GLY:C	2.29	0.52
1:I:235:LEU:HD22	1:I:236:VAL:N	2.24	0.52
1:E:99:SER:HB2	1:F:123:ARG:HB3	1.90	0.52
1:G:135:LEU:HB2	1:G:139:GLN:NE2	2.23	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:GLU:HB3	1:F:179:HIS:CD2	2.43	0.52
1:J:137:LYS:HB2	1:J:190:ASP:OD2	2.08	0.52
1:I:185:VAL:O	1:I:185:VAL:HG12	2.10	0.52
1:C:131:ASP:O	1:C:133:ALA:N	2.42	0.52
1:C:120:ARG:NH2	1:C:122:MET:CE	2.73	0.52
1:I:190:ASP:O	1:I:192:LEU:N	2.41	0.52
1:K:120:ARG:HE	1:K:122:MET:HE2	1.75	0.52
1:H:117:THR:O	1:H:118:SER:C	2.46	0.52
1:E:105:LEU:HG	1:E:228:TYR:HE2	1.75	0.52
1:I:105:LEU:HD13	1:I:116:PHE:HB2	1.90	0.52
1:H:220:LEU:CD1	1:H:220:LEU:N	2.65	0.52
1:D:219:SER:C	1:D:220:LEU:HD12	2.30	0.52
1:A:168:LEU:HD22	1:A:169:ALA:H	1.75	0.52
1:C:190:ASP:O	1:C:192:LEU:N	2.43	0.52
1:D:126:CYS:HB3	1:D:149:VAL:CG2	2.39	0.52
1:I:120:ARG:HE	1:I:122:MET:HE3	1.74	0.52
1:A:141:VAL:HG21	1:A:149:VAL:CG1	2.40	0.52
1:I:116:PHE:CZ	1:I:225:LYS:O	2.63	0.52
1:A:165:ARG:HG2	1:A:165:ARG:HH11	1.75	0.52
1:J:232:ARG:O	1:J:233:ILE:HG12	2.10	0.52
1:D:116:PHE:CD2	1:D:226:ALA:HA	2.45	0.52
1:G:155:PHE:O	1:G:156:GLU:C	2.47	0.52
1:E:131:ASP:O	1:E:133:ALA:N	2.43	0.52
1:C:155:PHE:O	1:C:156:GLU:C	2.46	0.52
1:I:142:ARG:HH11	1:J:123:ARG:HD3	1.74	0.52
1:A:101:TYR:CE1	1:A:142:ARG:HG3	2.45	0.52
1:K:220:LEU:N	1:K:220:LEU:HD23	2.24	0.52
1:I:127:SER:C	1:I:129:ASN:H	2.13	0.52
1:C:117:THR:HG23	1:C:118:SER:H	1.75	0.52
1:A:58:GLN:NE2	1:I:235:LEU:HG	2.23	0.52
1:A:116:PHE:CZ	1:A:225:LYS:O	2.63	0.52
1:D:99:SER:CB	1:D:142:ARG:HH11	2.22	0.52
1:A:56:ILE:O	1:A:56:ILE:CG2	2.57	0.51
1:L:104:LEU:HD13	1:L:113:VAL:HG11	1.91	0.51
1:B:99:SER:CB	1:B:142:ARG:HH11	2.23	0.51
1:E:56:ILE:O	1:E:56:ILE:CG2	2.58	0.51
1:C:168:LEU:O	1:C:169:ALA:C	2.48	0.51
1:I:182:GLU:HB3	1:L:179:HIS:CD2	2.45	0.51
1:D:110:ASP:OD1	1:D:110:ASP:O	2.29	0.51
1:F:148:THR:HG22	1:F:148:THR:O	2.10	0.51
1:G:174:ALA:O	1:G:185:VAL:HA	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:221:LEU:HD23	1:I:221:LEU:O	2.10	0.51
1:H:104:LEU:HG	1:H:104:LEU:O	2.10	0.51
1:E:101:TYR:HD1	1:E:142:ARG:HA	1.75	0.51
1:A:120:ARG:HE	1:A:122:MET:CE	2.22	0.51
1:C:139:GLN:CB	1:C:155:PHE:CE1	2.94	0.51
1:C:158:VAL:HG12	1:D:185:VAL:O	2.09	0.51
1:G:184:ARG:HD3	1:G:224:THR:HG22	1.93	0.51
1:A:222:VAL:HG23	1:A:223:ASP:N	2.24	0.51
1:I:231:GLU:HG3	1:I:232:ARG:N	2.26	0.51
1:I:120:ARG:HH21	1:I:122:MET:HE1	1.76	0.51
1:J:117:THR:O	1:J:118:SER:C	2.46	0.51
1:F:105:LEU:N	1:F:114:ASP:O	2.43	0.51
1:A:124:LEU:HD11	1:A:143:LEU:HD21	1.90	0.51
1:A:235:LEU:HD22	1:A:236:VAL:H	1.76	0.51
1:J:116:PHE:CD2	1:J:226:ALA:HA	2.46	0.51
1:H:126:CYS:HB3	1:H:149:VAL:HG23	1.94	0.50
1:I:108:HIS:HB2	1:I:112:THR:O	2.10	0.50
1:H:179:HIS:CD2	1:K:182:GLU:HB3	2.46	0.50
1:I:105:LEU:O	1:I:106:ALA:HB2	2.12	0.50
1:K:184:ARG:HD3	1:K:224:THR:HG21	1.93	0.50
1:K:168:LEU:HD22	1:K:169:ALA:H	1.77	0.50
1:B:105:LEU:N	1:B:114:ASP:O	2.44	0.50
1:B:147:LEU:HD12	1:B:147:LEU:H	1.75	0.50
1:B:110:ASP:O	1:B:111:ASP:HB2	2.11	0.50
1:D:190:ASP:N	1:D:191:PRO:CD	2.74	0.50
1:I:124:LEU:HD11	1:I:143:LEU:HD22	1.93	0.50
1:I:105:LEU:O	1:I:228:TYR:OH	2.28	0.50
1:H:126:CYS:HB3	1:H:149:VAL:CG2	2.42	0.50
1:J:180:ALA:O	1:J:181:ASP:C	2.50	0.50
1:I:158:VAL:HG12	1:J:185:VAL:O	2.11	0.50
1:I:115:VAL:CG2	1:I:124:LEU:CD2	2.77	0.50
1:H:139:GLN:HA	1:H:155:PHE:CE1	2.47	0.50
1:L:198:PRO:O	1:L:200:GLY:N	2.45	0.50
1:C:56:ILE:CG2	1:C:56:ILE:O	2.59	0.50
1:G:167:ILE:HD12	1:G:167:ILE:H	1.76	0.50
1:E:144:ASN:C	1:E:144:ASN:OD1	2.50	0.50
1:K:221:LEU:C	1:K:221:LEU:CD2	2.79	0.50
1:E:62:ARG:HD2	1:F:63:ILE:HD11	1.93	0.50
1:I:56:ILE:CG2	1:I:56:ILE:O	2.60	0.50
1:G:170:ASP:OD2	1:G:170:ASP:N	2.43	0.50
1:G:62:ARG:HD2	1:H:63:ILE:CD1	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:PHE:O	1:A:231:GLU:HB3	2.11	0.50
1:E:235:LEU:HD11	1:E:237:PRO:HD3	1.94	0.50
1:B:230:PHE:O	1:B:231:GLU:HB3	2.12	0.50
1:L:110:ASP:O	1:L:111:ASP:HB2	2.11	0.50
1:A:105:LEU:O	1:A:228:TYR:OH	2.29	0.50
1:H:99:SER:CB	1:H:142:ARG:HH11	2.24	0.50
1:C:104:LEU:HD11	1:C:113:VAL:HG11	1.94	0.50
1:C:167:ILE:HD12	1:C:167:ILE:H	1.77	0.50
1:K:168:LEU:O	1:K:169:ALA:C	2.50	0.49
1:K:56:ILE:O	1:K:56:ILE:CG2	2.60	0.49
1:G:131:ASP:O	1:G:133:ALA:N	2.45	0.49
1:L:191:PRO:C	1:L:192:LEU:HD12	2.32	0.49
1:F:191:PRO:C	1:F:192:LEU:HD12	2.33	0.49
1:K:124:LEU:HD11	1:K:143:LEU:HD22	1.93	0.49
1:E:141:VAL:CG2	1:E:149:VAL:CG1	2.90	0.49
1:A:206:ASN:O	1:A:207:ASP:HB2	2.12	0.49
1:I:115:VAL:HG22	1:I:124:LEU:CD2	2.41	0.49
1:G:116:PHE:CZ	1:G:225:LYS:O	2.66	0.49
1:A:235:LEU:HD22	1:A:236:VAL:N	2.27	0.49
1:A:144:ASN:C	1:A:144:ASN:OD1	2.50	0.49
1:A:94:LEU:HD11	1:B:128:PRO:HD2	1.94	0.49
1:E:124:LEU:HD11	1:E:143:LEU:HD22	1.95	0.49
1:J:153:GLY:O	1:J:154:THR:O	2.30	0.49
1:H:110:ASP:O	1:H:111:ASP:HB2	2.11	0.49
1:L:180:ALA:O	1:L:181:ASP:C	2.51	0.49
1:J:124:LEU:HD11	1:J:147:LEU:HB3	1.94	0.49
1:H:147:LEU:H	1:H:147:LEU:CD1	2.24	0.49
1:C:73:LEU:O	1:C:74:MET:C	2.50	0.49
1:F:110:ASP:OD1	1:F:110:ASP:O	2.30	0.49
1:H:100:GLY:O	1:H:143:LEU:HD12	2.12	0.49
1:K:117:THR:C	1:K:119:GLY:H	2.16	0.49
1:E:73:LEU:O	1:E:74:MET:C	2.49	0.49
1:I:165:ARG:HG2	1:I:165:ARG:NH1	2.28	0.49
1:A:120:ARG:NH2	1:A:122:MET:HE1	2.21	0.49
1:E:164:LEU:C	1:E:164:LEU:HD12	2.33	0.49
1:L:124:LEU:HD21	1:L:147:LEU:O	2.13	0.49
1:F:106:ALA:H	1:F:114:ASP:HB2	1.78	0.49
1:H:230:PHE:O	1:H:231:GLU:HB3	2.11	0.49
1:L:210:ARG:HG2	1:L:211:PRO:HD2	1.95	0.49
1:D:190:ASP:HB2	1:D:191:PRO:HD3	1.95	0.49
1:G:187:TRP:O	1:G:228:TYR:HA	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LEU:HA	1:A:176:VAL:HG12	1.93	0.49
1:E:165:ARG:HG2	1:E:165:ARG:NH1	2.27	0.49
1:I:144:ASN:C	1:I:144:ASN:OD1	2.49	0.49
1:I:175:LEU:C	1:I:175:LEU:HD12	2.33	0.49
1:A:73:LEU:O	1:A:74:MET:C	2.50	0.49
1:K:103:VAL:O	1:K:115:VAL:HG12	2.13	0.49
1:A:168:LEU:O	1:A:169:ALA:C	2.50	0.49
1:F:210:ARG:HG2	1:F:211:PRO:CD	2.43	0.49
1:K:59:LEU:O	1:K:61:ALA:N	2.45	0.49
1:L:85:LEU:HD23	1:L:85:LEU:O	2.12	0.49
1:E:189:ALA:H	1:E:192:LEU:CD1	2.25	0.49
1:E:155:PHE:O	1:E:156:GLU:C	2.51	0.49
1:C:62:ARG:HD2	1:D:63:ILE:HD11	1.95	0.49
1:C:124:LEU:HD23	1:C:124:LEU:N	2.28	0.48
1:H:191:PRO:HB2	1:H:192:LEU:HD12	1.95	0.48
1:G:124:LEU:HD23	1:G:124:LEU:N	2.28	0.48
1:A:189:ALA:O	1:A:190:ASP:C	2.50	0.48
1:A:155:PHE:CE2	1:A:191:PRO:HG2	2.48	0.48
1:D:104:LEU:HD13	1:D:113:VAL:HG11	1.95	0.48
1:D:99:SER:HB2	1:D:142:ARG:HH11	1.78	0.48
1:L:110:ASP:O	1:L:110:ASP:OD1	2.31	0.48
1:F:85:LEU:O	1:F:85:LEU:HD23	2.13	0.48
1:A:124:LEU:HD11	1:A:143:LEU:HD22	1.94	0.48
1:J:189:ALA:C	1:J:191:PRO:HD2	2.34	0.48
1:H:85:LEU:O	1:H:85:LEU:HD23	2.13	0.48
1:G:177:VAL:HG23	1:G:177:VAL:O	2.13	0.48
1:B:104:LEU:HD13	1:B:113:VAL:HG11	1.94	0.48
1:G:131:ASP:HB3	1:G:134:SER:OG	2.12	0.48
1:L:139:GLN:HA	1:L:155:PHE:CE1	2.48	0.48
1:I:184:ARG:CD	1:I:224:THR:HG22	2.41	0.48
1:G:189:ALA:O	1:G:190:ASP:C	2.52	0.48
1:C:218:ASP:OD2	1:C:232:ARG:NH1	2.46	0.48
1:D:221:LEU:HD12	1:D:222:VAL:N	2.29	0.48
1:I:123:ARG:NH1	1:L:151:GLU:OE1	2.46	0.48
1:H:186:VAL:HG12	1:H:227:GLY:O	2.13	0.48
1:C:105:LEU:HD13	1:C:116:PHE:HB2	1.95	0.48
1:C:187:TRP:O	1:C:228:TYR:HA	2.13	0.48
1:E:189:ALA:N	1:E:192:LEU:HD12	2.25	0.48
1:C:135:LEU:H	1:C:135:LEU:CD2	2.26	0.48
1:J:85:LEU:HD23	1:J:85:LEU:O	2.13	0.48
1:D:85:LEU:O	1:D:85:LEU:HD23	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:113:VAL:O	1:G:123:ARG:HA	2.14	0.48
1:G:114:ASP:OD1	1:G:123:ARG:HG3	2.14	0.48
1:K:124:LEU:N	1:K:124:LEU:HD23	2.29	0.48
1:D:220:LEU:N	1:D:220:LEU:CD1	2.75	0.48
1:D:128:PRO:O	1:D:130:ILE:N	2.47	0.48
1:E:141:VAL:HG21	1:E:149:VAL:HG13	1.95	0.48
1:D:100:GLY:O	1:D:143:LEU:HD12	2.12	0.48
1:K:57:HIS:O	1:K:58:GLN:C	2.52	0.48
1:H:232:ARG:C	1:H:233:ILE:HG12	2.32	0.48
1:H:103:VAL:O	1:H:116:PHE:N	2.42	0.48
1:E:168:LEU:HD22	1:E:169:ALA:N	2.29	0.48
1:C:221:LEU:CD2	1:C:230:PHE:HB2	2.41	0.48
1:L:124:LEU:HD23	1:L:125:THR:H	1.79	0.48
1:D:139:GLN:HA	1:D:155:PHE:CE1	2.48	0.48
1:E:177:VAL:CG2	1:E:177:VAL:O	2.61	0.48
1:E:158:VAL:HG12	1:F:185:VAL:O	2.14	0.48
1:I:222:VAL:HG23	1:I:223:ASP:N	2.29	0.48
1:L:69:ARG:O	1:L:73:LEU:HG	2.13	0.48
1:B:85:LEU:HD23	1:B:85:LEU:O	2.14	0.48
1:B:212:ARG:HG3	1:B:213:LYS:O	2.14	0.48
1:G:124:LEU:HD11	1:G:143:LEU:HD22	1.93	0.47
1:C:235:LEU:HD22	1:C:236:VAL:N	2.29	0.47
1:G:168:LEU:HD12	1:G:173:ARG:HB2	1.96	0.47
1:K:222:VAL:HG23	1:K:223:ASP:N	2.29	0.47
1:G:84:LEU:HD13	1:G:84:LEU:O	2.14	0.47
1:G:144:ASN:C	1:G:144:ASN:OD1	2.51	0.47
1:C:59:LEU:O	1:C:61:ALA:N	2.46	0.47
1:H:130:ILE:HD12	1:H:130:ILE:HA	1.75	0.47
1:H:176:VAL:HG21	1:H:186:VAL:CG2	2.44	0.47
1:K:116:PHE:CZ	1:K:225:LYS:O	2.67	0.47
1:D:191:PRO:C	1:D:192:LEU:HD12	2.34	0.47
1:C:115:VAL:HG21	1:C:124:LEU:HD21	1.89	0.47
1:A:165:ARG:HG2	1:A:165:ARG:NH1	2.29	0.47
1:J:230:PHE:O	1:J:231:GLU:HB3	2.13	0.47
1:K:84:LEU:HD13	1:K:84:LEU:O	2.14	0.47
1:B:137:LYS:HB2	1:B:190:ASP:OD2	2.13	0.47
1:C:113:VAL:O	1:C:123:ARG:HA	2.13	0.47
1:A:218:ASP:OD2	1:A:232:ARG:NH1	2.47	0.47
1:G:141:VAL:CG2	1:G:149:VAL:CG1	2.92	0.47
1:K:100:GLY:O	1:K:143:LEU:N	2.48	0.47
1:I:212:ARG:HG3	1:I:213:LYS:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:150:VAL:O	1:G:151:GLU:HB2	2.14	0.47
1:B:176:VAL:HG21	1:B:186:VAL:HG22	1.95	0.47
1:J:139:GLN:HB2	1:J:155:PHE:CE1	2.50	0.47
1:J:154:THR:CG2	1:J:155:PHE:N	2.71	0.47
1:G:176:VAL:CG2	1:G:186:VAL:CG2	2.93	0.47
1:J:162:SER:HB2	1:J:176:VAL:HG12	1.96	0.47
1:K:139:GLN:HA	1:K:155:PHE:CE1	2.49	0.47
1:H:124:LEU:HD23	1:H:124:LEU:HA	1.61	0.47
1:E:141:VAL:CG2	1:E:149:VAL:HG13	2.45	0.47
1:J:100:GLY:O	1:J:143:LEU:HD12	2.15	0.47
1:F:180:ALA:O	1:F:181:ASP:C	2.50	0.47
1:G:56:ILE:CG2	1:G:56:ILE:O	2.62	0.47
1:K:144:ASN:C	1:K:144:ASN:OD1	2.51	0.47
1:I:200:GLY:O	1:I:201:LEU:HB2	2.14	0.47
1:D:186:VAL:HB	1:D:227:GLY:O	2.14	0.47
1:B:210:ARG:HG2	1:B:211:PRO:CD	2.45	0.47
1:G:175:LEU:CD2	1:J:235:LEU:HD12	2.36	0.47
1:E:59:LEU:O	1:E:61:ALA:N	2.48	0.47
1:G:73:LEU:O	1:G:74:MET:C	2.51	0.47
1:G:222:VAL:HG23	1:G:223:ASP:N	2.30	0.47
1:B:189:ALA:C	1:B:191:PRO:HD2	2.35	0.47
1:K:189:ALA:O	1:K:190:ASP:C	2.53	0.47
1:G:185:VAL:O	1:G:185:VAL:HG12	2.15	0.47
1:J:172:HIS:O	1:J:188:LEU:HD12	2.15	0.47
1:L:100:GLY:O	1:L:143:LEU:HD12	2.14	0.47
1:C:99:SER:HB2	1:D:123:ARG:HB3	1.96	0.47
1:A:180:ALA:O	1:A:182:GLU:N	2.47	0.47
1:L:124:LEU:HD23	1:L:124:LEU:HA	1.67	0.47
1:A:200:GLY:O	1:A:201:LEU:HB2	2.15	0.47
1:C:63:ILE:O	1:C:65:SER:N	2.48	0.47
1:D:124:LEU:HD21	1:D:147:LEU:O	2.14	0.46
1:K:231:GLU:HG3	1:K:232:ARG:N	2.31	0.46
1:G:66:LEU:O	1:G:69:ARG:N	2.43	0.46
1:J:191:PRO:HB2	1:J:192:LEU:HD12	1.97	0.46
1:A:120:ARG:NE	1:A:122:MET:HE2	2.28	0.46
1:I:168:LEU:O	1:I:169:ALA:C	2.53	0.46
1:D:103:VAL:O	1:D:116:PHE:N	2.41	0.46
1:I:59:LEU:O	1:I:61:ALA:N	2.48	0.46
1:K:221:LEU:CD2	1:K:230:PHE:HB2	2.45	0.46
1:A:127:SER:O	1:A:128:PRO:C	2.54	0.46
1:H:191:PRO:C	1:H:192:LEU:HD12	2.36	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:202:PRO:O	1:K:203:GLU:CB	2.60	0.46
1:I:137:LYS:HB2	1:I:190:ASP:OD1	2.16	0.46
1:B:214:LEU:HD12	1:B:215:ARG:H	1.81	0.46
1:K:66:LEU:O	1:K:68:ALA:N	2.48	0.46
1:K:73:LEU:O	1:K:74:MET:C	2.53	0.46
1:G:59:LEU:O	1:G:61:ALA:N	2.48	0.46
1:G:117:THR:O	1:G:119:GLY:N	2.47	0.46
1:I:84:LEU:HD13	1:I:84:LEU:O	2.16	0.46
1:H:72:LYS:O	1:H:76:THR:HG23	2.15	0.46
1:E:105:LEU:HD13	1:E:116:PHE:HB2	1.96	0.46
1:G:105:LEU:CD1	1:G:116:PHE:HB2	2.43	0.46
1:C:66:LEU:O	1:C:68:ALA:N	2.49	0.46
1:B:190:ASP:N	1:B:191:PRO:HD2	2.31	0.46
1:I:100:GLY:O	1:I:143:LEU:N	2.45	0.46
1:F:136:LYS:N	1:F:139:GLN:OE1	2.38	0.46
1:I:222:VAL:CG2	1:I:223:ASP:N	2.77	0.46
1:I:73:LEU:O	1:I:74:MET:C	2.53	0.46
1:A:131:ASP:O	1:A:133:ALA:N	2.49	0.46
1:G:100:GLY:O	1:G:143:LEU:N	2.47	0.46
1:B:106:ALA:H	1:B:114:ASP:HB2	1.81	0.46
1:F:124:LEU:HA	1:F:124:LEU:HD23	1.67	0.46
1:I:212:ARG:NE	1:I:215:ARG:HD3	2.28	0.46
1:I:62:ARG:HD2	1:J:63:ILE:CD1	2.44	0.46
1:G:66:LEU:O	1:G:68:ALA:N	2.49	0.46
1:L:99:SER:CB	1:L:142:ARG:HH11	2.28	0.46
1:K:113:VAL:O	1:K:123:ARG:HA	2.16	0.46
1:J:190:ASP:N	1:J:191:PRO:HD2	2.31	0.46
1:E:168:LEU:HA	1:E:168:LEU:HD23	1.74	0.46
1:E:168:LEU:O	1:E:169:ALA:C	2.54	0.46
1:B:113:VAL:O	1:B:123:ARG:HA	2.16	0.46
1:A:105:LEU:N	1:A:114:ASP:O	2.45	0.46
1:D:127:SER:HA	1:D:128:PRO:HD2	1.70	0.46
1:H:113:VAL:O	1:H:123:ARG:HA	2.15	0.46
1:I:180:ALA:O	1:I:182:GLU:N	2.48	0.46
1:J:106:ALA:H	1:J:114:ASP:HB2	1.80	0.46
1:J:72:LYS:O	1:J:76:THR:HG23	2.16	0.46
1:K:200:GLY:O	1:K:201:LEU:HB2	2.16	0.46
1:L:72:LYS:O	1:L:76:THR:HG23	2.15	0.46
1:G:176:VAL:HG21	1:G:186:VAL:HG21	1.98	0.46
1:I:190:ASP:C	1:I:192:LEU:H	2.19	0.46
1:B:110:ASP:O	1:B:110:ASP:OD1	2.32	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:127:SER:HA	1:H:128:PRO:HD2	1.73	0.46
1:B:186:VAL:HG12	1:B:227:GLY:C	2.35	0.46
1:D:180:ALA:O	1:D:181:ASP:C	2.54	0.46
1:K:137:LYS:HB2	1:K:190:ASP:OD1	2.16	0.46
1:A:233:ILE:HA	1:A:234:PRO:HD2	1.63	0.46
1:I:233:ILE:HA	1:I:234:PRO:HD2	1.57	0.46
1:F:117:THR:O	1:F:118:SER:C	2.55	0.46
1:L:137:LYS:HB2	1:L:190:ASP:OD2	2.16	0.46
1:B:139:GLN:HA	1:B:155:PHE:HE1	1.77	0.45
1:C:123:ARG:NH1	1:F:151:GLU:OE1	2.39	0.45
1:K:206:ASN:O	1:K:207:ASP:CB	2.63	0.45
1:K:66:LEU:O	1:K:69:ARG:N	2.44	0.45
1:J:130:ILE:HA	1:J:130:ILE:HD12	1.77	0.45
1:D:212:ARG:HG3	1:D:213:LYS:O	2.16	0.45
1:C:206:ASN:O	1:C:207:ASP:HB2	2.16	0.45
1:C:100:GLY:O	1:C:143:LEU:N	2.47	0.45
1:B:128:PRO:O	1:B:130:ILE:N	2.50	0.45
1:E:113:VAL:O	1:E:123:ARG:HA	2.17	0.45
1:I:187:TRP:O	1:I:228:TYR:HA	2.16	0.45
1:L:233:ILE:HA	1:L:234:PRO:HD2	1.83	0.45
1:F:232:ARG:C	1:F:233:ILE:HG12	2.36	0.45
1:D:162:SER:HB2	1:D:176:VAL:HG12	1.98	0.45
1:A:141:VAL:CG2	1:A:149:VAL:CG1	2.95	0.45
1:C:158:VAL:HA	1:D:185:VAL:HG12	1.98	0.45
1:C:59:LEU:C	1:C:61:ALA:H	2.19	0.45
1:C:66:LEU:O	1:C:69:ARG:N	2.45	0.45
1:D:207:ASP:OD1	1:D:209:THR:HG22	2.17	0.45
1:L:105:LEU:N	1:L:114:ASP:O	2.46	0.45
1:F:214:LEU:HD12	1:F:214:LEU:HA	1.46	0.45
1:E:124:LEU:HD11	1:E:143:LEU:HD21	1.98	0.45
1:A:190:ASP:C	1:A:192:LEU:H	2.20	0.45
1:C:127:SER:C	1:C:129:ASN:H	2.14	0.45
1:E:235:LEU:CD1	1:E:237:PRO:HD3	2.47	0.45
1:K:184:ARG:HD3	1:K:224:THR:CG2	2.46	0.45
1:I:57:HIS:O	1:I:58:GLN:C	2.55	0.45
1:H:69:ARG:O	1:H:73:LEU:HG	2.15	0.45
1:J:104:LEU:HD13	1:J:113:VAL:HG11	1.97	0.45
1:E:201:LEU:HB3	1:E:202:PRO:CD	2.46	0.45
1:A:155:PHE:O	1:A:156:GLU:C	2.55	0.45
1:G:151:GLU:HG2	1:G:152:ALA:O	2.17	0.45
1:A:66:LEU:O	1:A:69:ARG:N	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:ASP:N	1:D:191:PRO:HD2	2.32	0.45
1:F:126:CYS:CB	1:F:149:VAL:HG23	2.43	0.45
1:I:206:ASN:O	1:I:207:ASP:HB2	2.16	0.45
1:G:233:ILE:HA	1:G:234:PRO:HD2	1.48	0.45
1:F:104:LEU:HD13	1:F:113:VAL:HG11	1.99	0.45
1:J:124:LEU:HD21	1:J:147:LEU:O	2.16	0.45
1:F:110:ASP:O	1:F:111:ASP:HB2	2.16	0.45
1:B:236:VAL:HA	1:B:237:PRO:HD3	1.79	0.45
1:H:189:ALA:C	1:H:191:PRO:HD2	2.38	0.45
1:F:136:LYS:O	1:F:139:GLN:HB3	2.17	0.45
1:J:113:VAL:O	1:J:123:ARG:HA	2.17	0.45
1:I:97:PRO:HG3	1:I:145:GLU:OE1	2.17	0.45
1:D:235:LEU:HD23	1:D:237:PRO:HG3	1.98	0.45
1:F:154:THR:HG22	1:F:155:PHE:N	2.19	0.45
1:K:135:LEU:HB2	1:K:139:GLN:HE21	1.77	0.45
1:L:113:VAL:O	1:L:123:ARG:HA	2.17	0.45
1:E:120:ARG:NE	1:E:122:MET:CE	2.75	0.44
1:K:127:SER:C	1:K:129:ASN:H	2.21	0.44
1:I:66:LEU:O	1:I:69:ARG:N	2.45	0.44
1:D:137:LYS:HB2	1:D:190:ASP:OD2	2.17	0.44
1:H:139:GLN:HB2	1:H:155:PHE:HE1	1.82	0.44
1:F:139:GLN:HA	1:F:155:PHE:CE1	2.53	0.44
1:C:141:VAL:CG2	1:C:149:VAL:CG1	2.95	0.44
1:G:155:PHE:CE2	1:G:191:PRO:HG2	2.52	0.44
1:K:94:LEU:HD11	1:L:128:PRO:HD2	1.99	0.44
1:E:184:ARG:CD	1:E:224:THR:HG22	2.47	0.44
1:A:141:VAL:CG2	1:A:149:VAL:HG13	2.47	0.44
1:B:176:VAL:CG2	1:B:186:VAL:HG22	2.47	0.44
1:H:144:ASN:OD1	1:H:146:ALA:O	2.35	0.44
1:A:208:ASP:O	1:A:210:ARG:N	2.50	0.44
1:G:225:LYS:HE2	1:G:225:LYS:HB2	1.65	0.44
1:E:184:ARG:NE	1:E:224:THR:HG22	2.32	0.44
1:A:105:LEU:O	1:A:106:ALA:CB	2.63	0.44
1:I:127:SER:C	1:I:129:ASN:N	2.70	0.44
1:F:130:ILE:HD12	1:F:131:ASP:H	1.82	0.44
1:L:212:ARG:HG3	1:L:213:LYS:O	2.17	0.44
1:I:225:LYS:HE2	1:I:225:LYS:HB2	1.56	0.44
1:G:176:VAL:CG2	1:G:186:VAL:HG21	2.48	0.44
1:F:153:GLY:O	1:F:154:THR:O	2.35	0.44
1:C:189:ALA:H	1:C:192:LEU:CD1	2.27	0.44
1:C:105:LEU:HG	1:C:228:TYR:HE2	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:TYR:CD1	1:A:142:ARG:HA	2.52	0.44
1:C:221:LEU:HD23	1:C:222:VAL:N	2.32	0.44
1:C:231:GLU:HG3	1:C:232:ARG:N	2.32	0.44
1:I:66:LEU:O	1:I:68:ALA:N	2.51	0.44
1:J:190:ASP:N	1:J:191:PRO:CD	2.80	0.44
1:H:189:ALA:O	1:H:191:PRO:N	2.51	0.44
1:A:66:LEU:O	1:A:68:ALA:N	2.51	0.44
1:A:139:GLN:HB3	1:A:155:PHE:CE1	2.53	0.44
1:A:225:LYS:HB2	1:A:225:LYS:HE2	1.28	0.44
1:G:168:LEU:O	1:G:169:ALA:C	2.56	0.44
1:C:59:LEU:C	1:C:61:ALA:N	2.71	0.44
1:G:222:VAL:CG2	1:G:223:ASP:N	2.81	0.44
1:A:57:HIS:HB3	1:I:163:THR:OG1	2.18	0.44
1:E:223:ASP:O	1:E:225:LYS:N	2.51	0.44
1:F:110:ASP:OD1	1:F:112:THR:HG23	2.18	0.44
1:J:105:LEU:N	1:J:114:ASP:O	2.46	0.44
1:A:168:LEU:HD23	1:A:168:LEU:HA	1.83	0.43
1:I:142:ARG:HD2	1:J:123:ARG:HD3	1.99	0.43
1:A:57:HIS:O	1:A:58:GLN:C	2.57	0.43
1:I:108:HIS:C	1:I:110:ASP:H	2.21	0.43
1:K:104:LEU:HD11	1:K:113:VAL:HG11	1.99	0.43
1:C:139:GLN:HA	1:C:155:PHE:CE1	2.53	0.43
1:E:223:ASP:HB2	1:E:230:PHE:HE2	1.83	0.43
1:L:100:GLY:O	1:L:143:LEU:N	2.49	0.43
1:L:127:SER:HA	1:L:128:PRO:HD2	1.78	0.43
1:E:63:ILE:O	1:E:65:SER:N	2.51	0.43
1:I:97:PRO:CB	1:I:98:PRO:HD2	2.48	0.43
1:I:141:VAL:CG2	1:I:149:VAL:HG13	2.49	0.43
1:G:57:HIS:O	1:G:58:GLN:C	2.55	0.43
1:L:139:GLN:HA	1:L:155:PHE:HE1	1.84	0.43
1:K:117:THR:O	1:K:119:GLY:N	2.45	0.43
1:A:59:LEU:O	1:A:61:ALA:N	2.50	0.43
1:H:105:LEU:N	1:H:114:ASP:O	2.47	0.43
1:B:154:THR:CG2	1:B:155:PHE:N	2.70	0.43
1:I:164:LEU:HB2	1:I:220:LEU:CD2	2.49	0.43
1:H:164:LEU:HA	1:H:176:VAL:HA	1.99	0.43
1:K:59:LEU:C	1:K:61:ALA:H	2.20	0.43
1:E:59:LEU:C	1:E:61:ALA:N	2.72	0.43
1:E:190:ASP:C	1:E:192:LEU:H	2.21	0.43
1:B:104:LEU:HA	1:B:115:VAL:HG12	2.01	0.43
1:H:117:THR:O	1:H:119:GLY:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:117:THR:O	1:J:119:GLY:N	2.51	0.43
1:C:225:LYS:HB2	1:C:225:LYS:HE2	1.27	0.43
1:E:100:GLY:O	1:E:143:LEU:N	2.49	0.43
1:C:168:LEU:HD23	1:C:168:LEU:HA	1.74	0.43
1:I:220:LEU:CD1	1:I:229:ALA:CB	2.97	0.43
1:C:139:GLN:CB	1:C:155:PHE:HE1	2.31	0.43
1:E:136:LYS:N	1:E:139:GLN:OE1	2.35	0.43
1:C:141:VAL:HG23	1:C:142:ARG:N	2.33	0.43
1:F:139:GLN:NE2	1:F:152:ALA:HB1	2.34	0.43
1:I:139:GLN:HA	1:I:155:PHE:CE1	2.54	0.43
1:D:164:LEU:HD12	1:D:220:LEU:HD11	2.00	0.43
1:A:164:LEU:HB2	1:A:220:LEU:CD2	2.48	0.43
1:F:128:PRO:O	1:F:130:ILE:N	2.52	0.43
1:B:105:LEU:HD13	1:B:116:PHE:HB2	2.01	0.43
1:A:221:LEU:HD22	1:A:230:PHE:HB2	2.01	0.43
1:E:59:LEU:C	1:E:61:ALA:H	2.21	0.43
1:J:69:ARG:O	1:J:73:LEU:HG	2.17	0.43
1:F:233:ILE:HA	1:F:234:PRO:HD2	1.87	0.43
1:F:127:SER:HA	1:F:128:PRO:HD2	1.78	0.43
1:G:139:GLN:HA	1:G:155:PHE:CE1	2.54	0.43
1:K:59:LEU:C	1:K:61:ALA:N	2.72	0.43
1:E:57:HIS:O	1:E:58:GLN:C	2.56	0.43
1:F:171:GLY:O	1:F:193:ILE:HG21	2.19	0.43
1:C:120:ARG:CZ	1:C:122:MET:CE	2.97	0.42
1:A:58:GLN:HE22	1:I:235:LEU:CG	2.28	0.42
1:E:101:TYR:CD1	1:E:142:ARG:HA	2.54	0.42
1:A:141:VAL:HG21	1:A:149:VAL:HG13	2.00	0.42
1:E:62:ARG:HD2	1:F:63:ILE:CD1	2.49	0.42
1:J:147:LEU:N	1:J:147:LEU:HD12	2.35	0.42
1:E:187:TRP:O	1:E:228:TYR:HA	2.19	0.42
1:D:191:PRO:HB2	1:D:192:LEU:HD12	2.00	0.42
1:H:154:THR:CG2	1:H:155:PHE:N	2.80	0.42
1:F:191:PRO:HB2	1:F:192:LEU:HD12	2.01	0.42
1:H:162:SER:HB3	1:H:178:GLY:CA	2.41	0.42
1:F:96:GLN:HA	1:F:97:PRO:HD2	1.82	0.42
1:K:155:PHE:O	1:K:156:GLU:C	2.58	0.42
1:F:162:SER:HB2	1:F:176:VAL:HG12	2.01	0.42
1:G:142:ARG:HD2	1:H:123:ARG:HD3	2.00	0.42
1:G:59:LEU:C	1:G:61:ALA:H	2.23	0.42
1:E:117:THR:HG23	1:E:118:SER:H	1.83	0.42
1:K:131:ASP:O	1:K:133:ALA:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:210:ARG:HG2	1:H:211:PRO:HD3	2.01	0.42
1:B:72:LYS:O	1:B:76:THR:HG23	2.19	0.42
1:C:200:GLY:O	1:C:201:LEU:HB2	2.19	0.42
1:H:222:VAL:HA	1:H:228:TYR:O	2.19	0.42
1:B:155:PHE:HE2	1:B:191:PRO:CG	2.15	0.42
1:A:108:HIS:C	1:A:110:ASP:N	2.72	0.42
1:F:125:THR:O	1:F:148:THR:HA	2.19	0.42
1:J:225:LYS:HA	1:J:225:LYS:HD2	1.88	0.42
1:E:184:ARG:CD	1:E:224:THR:CG2	2.93	0.42
1:B:147:LEU:N	1:B:147:LEU:CD1	2.82	0.42
1:A:206:ASN:O	1:A:207:ASP:CB	2.67	0.42
1:I:59:LEU:C	1:I:61:ALA:H	2.23	0.42
1:A:59:LEU:C	1:A:61:ALA:N	2.73	0.42
1:G:200:GLY:O	1:G:201:LEU:HB2	2.18	0.42
1:A:100:GLY:O	1:A:143:LEU:N	2.51	0.42
1:I:105:LEU:CD1	1:I:116:PHE:HB2	2.48	0.42
1:E:176:VAL:HG21	1:E:186:VAL:HG21	2.02	0.42
1:I:168:LEU:HD22	1:I:169:ALA:N	2.32	0.42
1:C:139:GLN:HB3	1:C:155:PHE:CE1	2.54	0.42
1:K:99:SER:HB2	1:L:123:ARG:HB3	2.01	0.42
1:B:214:LEU:HD12	1:B:214:LEU:HA	1.64	0.42
1:K:120:ARG:NH2	1:K:122:MET:HE1	2.33	0.42
1:I:141:VAL:HG21	1:I:149:VAL:HG13	2.01	0.42
1:F:69:ARG:O	1:F:73:LEU:HG	2.19	0.42
1:I:164:LEU:HD12	1:I:164:LEU:C	2.39	0.42
1:C:188:LEU:HD23	1:C:192:LEU:HD13	2.02	0.42
1:D:72:LYS:O	1:D:76:THR:HG23	2.20	0.42
1:A:63:ILE:O	1:A:65:SER:N	2.53	0.42
1:A:124:LEU:N	1:A:124:LEU:HD23	2.34	0.42
1:J:139:GLN:HA	1:J:155:PHE:CE1	2.55	0.42
1:D:96:GLN:HA	1:D:97:PRO:HD2	1.82	0.42
1:I:154:THR:CG2	1:I:155:PHE:H	2.30	0.42
1:C:105:LEU:CB	1:C:114:ASP:O	2.67	0.42
1:E:165:ARG:NH1	1:E:165:ARG:CG	2.83	0.42
1:B:215:ARG:HB2	1:B:218:ASP:OD1	2.20	0.42
1:B:130:ILE:HD12	1:B:131:ASP:H	1.84	0.42
1:A:131:ASP:HB3	1:A:134:SER:OG	2.19	0.42
1:K:63:ILE:O	1:K:65:SER:N	2.53	0.42
1:F:207:ASP:OD1	1:F:209:THR:CG2	2.67	0.42
1:I:135:LEU:CD2	1:I:135:LEU:H	2.33	0.42
1:L:135:LEU:HD23	1:L:135:LEU:HA	1.86	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:PHE:O	1:B:156:GLU:C	2.57	0.42
1:K:155:PHE:CE2	1:K:191:PRO:HG2	2.54	0.42
1:J:128:PRO:O	1:J:130:ILE:N	2.52	0.42
1:G:220:LEU:CD1	1:G:229:ALA:HB1	2.39	0.42
1:F:147:LEU:CD1	1:F:147:LEU:N	2.78	0.42
1:K:62:ARG:HD2	1:L:63:ILE:CD1	2.49	0.42
1:A:117:THR:OG1	1:A:118:SER:N	2.53	0.42
1:K:222:VAL:CG2	1:K:223:ASP:N	2.80	0.42
1:D:69:ARG:O	1:D:73:LEU:HG	2.20	0.42
1:K:190:ASP:C	1:K:192:LEU:H	2.23	0.42
1:F:139:GLN:HB2	1:F:155:PHE:HE1	1.81	0.42
1:G:164:LEU:HB2	1:G:220:LEU:CD2	2.50	0.42
1:H:233:ILE:HA	1:H:234:PRO:HD2	1.83	0.42
1:L:103:VAL:O	1:L:116:PHE:N	2.42	0.42
1:D:100:GLY:O	1:D:143:LEU:N	2.52	0.42
1:I:197:LEU:HA	1:I:198:PRO:HD3	1.92	0.42
1:E:66:LEU:O	1:E:68:ALA:N	2.52	0.42
1:G:85:LEU:HA	1:G:85:LEU:HD13	2.00	0.42
1:C:57:HIS:O	1:C:58:GLN:C	2.58	0.42
1:F:189:ALA:O	1:F:191:PRO:N	2.53	0.41
1:B:124:LEU:HA	1:B:124:LEU:HD23	1.70	0.41
1:K:233:ILE:HA	1:K:234:PRO:HD2	1.61	0.41
1:G:235:LEU:C	1:G:235:LEU:HD13	2.40	0.41
1:J:100:GLY:O	1:J:143:LEU:N	2.51	0.41
1:H:207:ASP:OD1	1:H:209:THR:CG2	2.67	0.41
1:L:189:ALA:C	1:L:191:PRO:HD2	2.40	0.41
1:F:147:LEU:CD1	1:F:147:LEU:H	2.24	0.41
1:C:105:LEU:O	1:C:106:ALA:HB2	2.20	0.41
1:E:189:ALA:O	1:E:190:ASP:C	2.57	0.41
1:H:179:HIS:CG	1:K:182:GLU:HB3	2.55	0.41
1:H:106:ALA:H	1:H:114:ASP:HB2	1.85	0.41
1:K:168:LEU:HA	1:K:168:LEU:HD23	1.69	0.41
1:A:186:VAL:CG1	1:A:227:GLY:O	2.53	0.41
1:D:124:LEU:HD23	1:D:125:THR:H	1.84	0.41
1:G:130:ILE:O	1:G:132:ALA:N	2.53	0.41
1:B:207:ASP:OD1	1:B:209:THR:HG23	2.20	0.41
1:I:56:ILE:O	1:I:56:ILE:HG22	2.20	0.41
1:K:141:VAL:CG2	1:K:149:VAL:HG13	2.50	0.41
1:B:116:PHE:HE1	1:B:119:GLY:C	2.23	0.41
1:E:165:ARG:HB3	1:E:175:LEU:HD23	2.02	0.41
1:B:172:HIS:C	1:B:188:LEU:HD12	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:174:ALA:O	1:J:185:VAL:HA	2.21	0.41
1:G:108:HIS:HB2	1:G:112:THR:O	2.20	0.41
1:D:214:LEU:HA	1:D:214:LEU:HD12	1.59	0.41
1:I:103:VAL:HG12	1:I:104:LEU:H	1.84	0.41
1:E:176:VAL:CG2	1:E:186:VAL:CG2	2.99	0.41
1:G:99:SER:HB2	1:H:123:ARG:HB3	2.02	0.41
1:A:221:LEU:C	1:A:222:VAL:HG12	2.41	0.41
1:L:197:LEU:HA	1:L:198:PRO:HD3	1.91	0.41
1:K:56:ILE:HG22	1:K:56:ILE:O	2.20	0.41
1:J:127:SER:HA	1:J:128:PRO:HD2	1.79	0.41
1:I:141:VAL:HG21	1:I:149:VAL:CG1	2.50	0.41
1:A:135:LEU:CD2	1:A:135:LEU:H	2.34	0.41
1:D:105:LEU:HA	1:D:105:LEU:HD12	1.72	0.41
1:D:189:ALA:O	1:D:190:ASP:C	2.58	0.41
1:B:190:ASP:N	1:B:191:PRO:CD	2.84	0.41
1:G:104:LEU:HD11	1:G:113:VAL:HG11	2.03	0.41
1:J:96:GLN:HA	1:J:97:PRO:HD2	1.81	0.41
1:E:164:LEU:HD12	1:E:165:ARG:H	1.84	0.41
1:K:127:SER:C	1:K:129:ASN:N	2.73	0.41
1:A:221:LEU:O	1:A:221:LEU:HD23	2.21	0.41
1:I:120:ARG:HE	1:I:122:MET:CE	2.33	0.41
1:F:72:LYS:O	1:F:76:THR:HG23	2.19	0.41
1:B:53:ALA:HA	1:B:56:ILE:HD12	2.03	0.41
1:H:214:LEU:HA	1:H:214:LEU:HD12	1.50	0.41
1:D:225:LYS:HA	1:D:225:LYS:HD2	1.91	0.41
1:E:186:VAL:HG12	1:E:227:GLY:C	2.35	0.41
1:G:105:LEU:HG	1:G:228:TYR:HE2	1.85	0.41
1:L:96:GLN:HA	1:L:97:PRO:HD2	1.80	0.41
1:E:142:ARG:HD2	1:F:123:ARG:CD	2.49	0.41
1:E:221:LEU:HD23	1:E:221:LEU:O	2.21	0.41
1:B:127:SER:HA	1:B:128:PRO:HD2	1.78	0.41
1:G:59:LEU:C	1:G:61:ALA:N	2.74	0.41
1:F:139:GLN:HA	1:F:155:PHE:CD1	2.55	0.41
1:I:168:LEU:HD12	1:I:173:ARG:HB2	2.02	0.41
1:G:189:ALA:H	1:G:192:LEU:CD1	2.29	0.41
1:G:190:ASP:O	1:G:192:LEU:N	2.53	0.41
1:E:233:ILE:HA	1:E:234:PRO:HD2	1.51	0.41
1:I:105:LEU:HG	1:I:228:TYR:HE2	1.86	0.41
1:I:165:ARG:HH11	1:I:165:ARG:HG2	1.86	0.41
1:F:116:PHE:CE2	1:F:225:LYS:O	2.73	0.41
1:E:168:LEU:CD2	1:E:169:ALA:H	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:THR:CG2	1:E:155:PHE:H	2.25	0.41
1:F:89:GLU:O	1:F:93:ARG:HG3	2.21	0.41
1:D:130:ILE:HD13	1:D:130:ILE:HA	1.84	0.41
1:A:233:ILE:HD13	1:A:233:ILE:HA	1.94	0.41
1:K:218:ASP:OD2	1:K:232:ARG:NH1	2.51	0.41
1:B:214:LEU:HD12	1:B:215:ARG:N	2.35	0.41
1:G:135:LEU:H	1:G:135:LEU:HD22	1.84	0.41
1:J:124:LEU:HD23	1:J:124:LEU:HA	1.48	0.41
1:E:208:ASP:O	1:E:210:ARG:N	2.54	0.41
1:G:63:ILE:O	1:G:65:SER:N	2.54	0.41
1:D:117:THR:HG23	1:D:117:THR:O	2.20	0.41
1:K:170:ASP:OD1	1:K:172:HIS:HB2	2.21	0.41
1:L:153:GLY:O	1:L:154:THR:O	2.39	0.41
1:I:184:ARG:CD	1:I:224:THR:CG2	2.90	0.41
1:A:56:ILE:O	1:A:56:ILE:HG22	2.21	0.41
1:K:117:THR:C	1:K:119:GLY:N	2.74	0.41
1:H:161:ILE:HA	1:H:161:ILE:HD13	1.78	0.41
1:B:128:PRO:C	1:B:130:ILE:H	2.24	0.40
1:H:128:PRO:O	1:H:130:ILE:N	2.53	0.40
1:I:59:LEU:C	1:I:61:ALA:N	2.73	0.40
1:A:59:LEU:C	1:A:61:ALA:H	2.23	0.40
1:I:126:CYS:HB3	1:I:130:ILE:HD11	2.03	0.40
1:B:89:GLU:O	1:B:93:ARG:HG3	2.21	0.40
1:D:128:PRO:C	1:D:130:ILE:H	2.23	0.40
1:G:141:VAL:HG21	1:G:149:VAL:HG11	2.02	0.40
1:G:168:LEU:HD23	1:G:168:LEU:HA	1.69	0.40
1:G:135:LEU:CD2	1:G:135:LEU:H	2.34	0.40
1:J:188:LEU:HA	1:J:229:ALA:HB3	2.02	0.40
1:B:69:ARG:O	1:B:73:LEU:HG	2.22	0.40
1:I:63:ILE:O	1:I:65:SER:N	2.55	0.40
1:I:168:LEU:HD23	1:I:168:LEU:HA	1.74	0.40
1:G:154:THR:CG2	1:G:155:PHE:H	2.31	0.40
1:K:54:ARG:O	1:K:55:ASP:C	2.59	0.40
1:E:96:GLN:HA	1:E:97:PRO:HD2	1.92	0.40
1:G:187:TRP:N	1:G:227:GLY:O	2.55	0.40
1:H:218:ASP:OD2	1:H:232:ARG:NH1	2.54	0.40
1:G:136:LYS:HB3	1:G:190:ASP:HB2	2.03	0.40
1:C:127:SER:C	1:C:129:ASN:N	2.74	0.40
1:B:100:GLY:O	1:B:143:LEU:N	2.55	0.40
1:K:127:SER:HA	1:K:128:PRO:HD2	1.85	0.40
1:C:233:ILE:HA	1:C:234:PRO:HD2	1.48	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:108:HIS:C	1:K:110:ASP:N	2.75	0.40
1:A:62:ARG:HD2	1:B:63:ILE:CD1	2.49	0.40
1:G:117:THR:OG1	1:G:118:SER:N	2.54	0.40
1:C:206:ASN:O	1:C:207:ASP:CB	2.68	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%)	137 (74%)	33 (18%)	14 (8%)	1	20
1	B	184/251 (73%)	148 (80%)	21 (11%)	15 (8%)	1	18
1	C	184/251 (73%)	139 (76%)	31 (17%)	14 (8%)	1	20
1	D	184/251 (73%)	147 (80%)	27 (15%)	10 (5%)	2	30
1	E	184/251 (73%)	139 (76%)	31 (17%)	14 (8%)	1	20
1	F	184/251 (73%)	152 (83%)	23 (12%)	9 (5%)	3	32
1	G	184/251 (73%)	138 (75%)	28 (15%)	18 (10%)	1	14
1	H	184/251 (73%)	148 (80%)	27 (15%)	9 (5%)	3	32
1	I	184/251 (73%)	136 (74%)	34 (18%)	14 (8%)	1	20
1	J	184/251 (73%)	147 (80%)	24 (13%)	13 (7%)	1	23
1	K	184/251 (73%)	135 (73%)	36 (20%)	13 (7%)	1	23
1	L	184/251 (73%)	147 (80%)	27 (15%)	10 (5%)	2	30
All	All	2208/3012 (73%)	1713 (78%)	342 (16%)	153 (7%)	1	24

All (153) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	ALA
1	A	169	ALA
1	A	203	GLU
1	A	207	ASP
1	B	128	PRO
1	B	154	THR
1	C	132	ALA
1	C	169	ALA
1	E	132	ALA
1	E	169	ALA
1	E	203	GLU
1	E	207	ASP
1	F	128	PRO
1	F	154	THR
1	G	132	ALA
1	G	169	ALA
1	G	181	ASP
1	G	203	GLU
1	G	207	ASP
1	H	154	THR
1	H	199	ASP
1	I	132	ALA
1	I	169	ALA
1	I	203	GLU
1	I	207	ASP
1	J	154	THR
1	J	199	ASP
1	K	128	PRO
1	K	132	ALA
1	K	169	ALA
1	K	203	GLU
1	K	207	ASP
1	L	154	THR
1	L	199	ASP
1	A	181	ASP
1	A	224	THR
1	C	207	ASP
1	D	128	PRO
1	D	154	THR
1	D	194	ALA
1	E	224	THR
1	E	234	PRO
1	F	178	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	194	ALA
1	F	195	GLU
1	G	131	ASP
1	H	128	PRO
1	H	178	GLY
1	H	194	ALA
1	I	128	PRO
1	I	181	ASP
1	J	145	GLU
1	L	218	ASP
1	A	128	PRO
1	A	209	THR
1	B	145	GLU
1	B	178	GLY
1	B	194	ALA
1	B	227	GLY
1	C	64	ASP
1	C	181	ASP
1	C	194	ALA
1	C	234	PRO
1	D	178	GLY
1	D	199	ASP
1	E	128	PRO
1	F	227	GLY
1	G	110	ASP
1	G	234	PRO
1	H	227	GLY
1	J	128	PRO
1	J	202	PRO
1	J	227	GLY
1	K	181	ASP
1	K	211	PRO
1	L	128	PRO
1	L	227	GLY
1	A	64	ASP
1	A	147	LEU
1	A	191	PRO
1	B	129	ASN
1	B	195	GLU
1	B	198	PRO
1	B	199	ASP
1	D	191	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	198	PRO
1	D	227	GLY
1	E	64	ASP
1	E	147	LEU
1	E	202	PRO
1	E	211	PRO
1	G	150	VAL
1	H	217	GLY
1	I	98	PRO
1	I	211	PRO
1	I	224	THR
1	J	194	ALA
1	J	217	GLY
1	K	64	ASP
1	K	137	LYS
1	K	147	LEU
1	K	191	PRO
1	L	202	PRO
1	B	191	PRO
1	C	60	GLU
1	C	128	PRO
1	C	191	PRO
1	C	224	THR
1	D	129	ASN
1	E	201	LEU
1	F	191	PRO
1	G	60	GLU
1	G	64	ASP
1	G	67	ALA
1	G	128	PRO
1	G	147	LEU
1	H	202	PRO
1	I	64	ASP
1	I	147	LEU
1	I	199	ASP
1	J	195	GLU
1	K	60	GLU
1	L	195	GLU
1	B	230	PHE
1	G	137	LYS
1	I	150	VAL
1	J	129	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	198	PRO
1	J	218	ASP
1	K	201	LEU
1	L	145	GLU
1	L	217	GLY
1	A	234	PRO
1	B	202	PRO
1	B	217	GLY
1	C	150	VAL
1	D	202	PRO
1	L	178	GLY
1	A	150	VAL
1	C	211	PRO
1	F	202	PRO
1	G	227	GLY
1	J	191	PRO
1	A	201	LEU
1	C	63	ILE
1	E	150	VAL
1	F	201	LEU
1	G	201	LEU
1	B	150	VAL
1	E	63	ILE
1	G	211	PRO
1	H	150	VAL
1	I	202	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	154/204 (76%)	121 (79%)	33 (21%)	1	10
1	B	154/204 (76%)	126 (82%)	28 (18%)	2	16
1	C	154/204 (76%)	118 (77%)	36 (23%)	1	8
1	D	154/204 (76%)	126 (82%)	28 (18%)	2	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	154/204 (76%)	114 (74%)	40 (26%)	0	6
1	F	154/204 (76%)	127 (82%)	27 (18%)	2	18
1	G	154/204 (76%)	115 (75%)	39 (25%)	1	6
1	H	154/204 (76%)	126 (82%)	28 (18%)	2	16
1	I	154/204 (76%)	123 (80%)	31 (20%)	1	13
1	J	154/204 (76%)	125 (81%)	29 (19%)	2	15
1	K	154/204 (76%)	115 (75%)	39 (25%)	1	6
1	L	154/204 (76%)	129 (84%)	25 (16%)	3	22
All	All	1848/2448 (76%)	1465 (79%)	383 (21%)	1	11

All (383) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	MET
1	A	79	GLU
1	A	82	GLN
1	A	88	ARG
1	A	89	GLU
1	A	107	THR
1	A	111	ASP
1	A	113	VAL
1	A	114	ASP
1	A	115	VAL
1	A	122	MET
1	A	125	THR
1	A	129	ASN
1	A	135	LEU
1	A	136	LYS
1	A	141	VAL
1	A	149	VAL
1	A	150	VAL
1	A	154	THR
1	A	158	VAL
1	A	167	ILE
1	A	168	LEU
1	A	179	HIS
1	A	185	VAL
1	A	186	VAL
1	A	199	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	210	ARG
1	A	219	SER
1	A	220	LEU
1	A	221	LEU
1	A	222	VAL
1	A	225	LYS
1	A	231	GLU
1	B	70	ASN
1	B	72	LYS
1	B	81	ARG
1	B	84	LEU
1	B	87	LEU
1	B	104	LEU
1	B	109	ASP
1	B	110	ASP
1	B	113	VAL
1	B	115	VAL
1	B	117	THR
1	B	121	LYS
1	B	124	LEU
1	B	130	ILE
1	B	141	VAL
1	B	143	LEU
1	B	145	GLU
1	B	148	THR
1	B	156	GLU
1	B	158	VAL
1	B	162	SER
1	B	164	LEU
1	B	167	ILE
1	B	175	LEU
1	B	182	GLU
1	B	186	VAL
1	B	196	ASP
1	B	218	ASP
1	C	74	MET
1	C	82	GLN
1	C	88	ARG
1	C	89	GLU
1	C	107	THR
1	C	113	VAL
1	C	114	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	115	VAL
1	C	120	ARG
1	C	122	MET
1	C	125	THR
1	C	131	ASP
1	C	135	LEU
1	C	136	LYS
1	C	140	THR
1	C	141	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	179	HIS
1	C	185	VAL
1	C	199	ASP
1	C	203	GLU
1	C	210	ARG
1	C	211	PRO
1	C	218	ASP
1	C	221	LEU
1	C	222	VAL
1	C	225	LYS
1	C	231	GLU
1	C	235	LEU
1	D	70	ASN
1	D	72	LYS
1	D	81	ARG
1	D	84	LEU
1	D	87	LEU
1	D	110	ASP
1	D	115	VAL
1	D	117	THR
1	D	120	ARG
1	D	121	LYS
1	D	124	LEU
1	D	130	ILE
1	D	143	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	148	THR
1	D	149	VAL
1	D	156	GLU
1	D	158	VAL
1	D	162	SER
1	D	164	LEU
1	D	167	ILE
1	D	170	ASP
1	D	176	VAL
1	D	196	ASP
1	D	215	ARG
1	D	218	ASP
1	D	225	LYS
1	D	231	GLU
1	D	236	VAL
1	E	74	MET
1	E	82	GLN
1	E	88	ARG
1	E	89	GLU
1	E	107	THR
1	E	109	ASP
1	E	110	ASP
1	E	111	ASP
1	E	113	VAL
1	E	114	ASP
1	E	115	VAL
1	E	120	ARG
1	E	122	MET
1	E	125	THR
1	E	129	ASN
1	E	131	ASP
1	E	135	LEU
1	E	136	LYS
1	E	140	THR
1	E	141	VAL
1	E	149	VAL
1	E	154	THR
1	E	158	VAL
1	E	167	ILE
1	E	168	LEU
1	E	175	LEU
1	E	176	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	179	HIS
1	E	181	ASP
1	E	186	VAL
1	E	208	ASP
1	E	212	ARG
1	E	213	LYS
1	E	218	ASP
1	E	221	LEU
1	E	222	VAL
1	E	224	THR
1	E	225	LYS
1	E	231	GLU
1	E	235	LEU
1	F	70	ASN
1	F	72	LYS
1	F	81	ARG
1	F	84	LEU
1	F	87	LEU
1	F	104	LEU
1	F	110	ASP
1	F	113	VAL
1	F	115	VAL
1	F	117	THR
1	F	130	ILE
1	F	139	GLN
1	F	141	VAL
1	F	143	LEU
1	F	145	GLU
1	F	148	THR
1	F	149	VAL
1	F	156	GLU
1	F	158	VAL
1	F	162	SER
1	F	164	LEU
1	F	167	ILE
1	F	175	LEU
1	F	188	LEU
1	F	196	ASP
1	F	214	LEU
1	F	225	LYS
1	G	74	MET
1	G	79	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	82	GLN
1	G	88	ARG
1	G	89	GLU
1	G	107	THR
1	G	113	VAL
1	G	114	ASP
1	G	115	VAL
1	G	117	THR
1	G	120	ARG
1	G	124	LEU
1	G	125	THR
1	G	129	ASN
1	G	131	ASP
1	G	135	LEU
1	G	136	LYS
1	G	141	VAL
1	G	149	VAL
1	G	150	VAL
1	G	154	THR
1	G	158	VAL
1	G	163	THR
1	G	166	GLU
1	G	167	ILE
1	G	168	LEU
1	G	176	VAL
1	G	186	VAL
1	G	190	ASP
1	G	212	ARG
1	G	213	LYS
1	G	218	ASP
1	G	220	LEU
1	G	221	LEU
1	G	222	VAL
1	G	224	THR
1	G	225	LYS
1	G	231	GLU
1	G	235	LEU
1	H	70	ASN
1	H	72	LYS
1	H	81	ARG
1	H	84	LEU
1	H	87	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	104	LEU
1	H	110	ASP
1	H	115	VAL
1	H	117	THR
1	H	120	ARG
1	H	124	LEU
1	H	127	SER
1	H	130	ILE
1	H	141	VAL
1	H	143	LEU
1	H	148	THR
1	H	149	VAL
1	H	156	GLU
1	H	158	VAL
1	H	162	SER
1	H	164	LEU
1	H	167	ILE
1	H	186	VAL
1	H	196	ASP
1	H	214	LEU
1	H	218	ASP
1	H	222	VAL
1	H	236	VAL
1	I	74	MET
1	I	79	GLU
1	I	82	GLN
1	I	88	ARG
1	I	89	GLU
1	I	107	THR
1	I	113	VAL
1	I	115	VAL
1	I	122	MET
1	I	125	THR
1	I	129	ASN
1	I	131	ASP
1	I	135	LEU
1	I	136	LYS
1	I	141	VAL
1	I	154	THR
1	I	158	VAL
1	I	163	THR
1	I	167	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	168	LEU
1	I	175	LEU
1	I	186	VAL
1	I	205	LEU
1	I	212	ARG
1	I	219	SER
1	I	220	LEU
1	I	221	LEU
1	I	222	VAL
1	I	224	THR
1	I	225	LYS
1	I	231	GLU
1	J	70	ASN
1	J	72	LYS
1	J	81	ARG
1	J	84	LEU
1	J	87	LEU
1	J	110	ASP
1	J	113	VAL
1	J	115	VAL
1	J	117	THR
1	J	121	LYS
1	J	130	ILE
1	J	141	VAL
1	J	143	LEU
1	J	148	THR
1	J	149	VAL
1	J	156	GLU
1	J	158	VAL
1	J	162	SER
1	J	164	LEU
1	J	167	ILE
1	J	170	ASP
1	J	175	LEU
1	J	186	VAL
1	J	188	LEU
1	J	196	ASP
1	J	218	ASP
1	J	221	LEU
1	J	222	VAL
1	J	225	LYS
1	K	74	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	79	GLU
1	K	82	GLN
1	K	88	ARG
1	K	89	GLU
1	K	107	THR
1	K	110	ASP
1	K	113	VAL
1	K	115	VAL
1	K	117	THR
1	K	122	MET
1	K	124	LEU
1	K	125	THR
1	K	131	ASP
1	K	135	LEU
1	K	136	LYS
1	K	140	THR
1	K	147	LEU
1	K	154	THR
1	K	158	VAL
1	K	163	THR
1	K	164	LEU
1	K	167	ILE
1	K	168	LEU
1	K	175	LEU
1	K	176	VAL
1	K	179	HIS
1	K	186	VAL
1	K	190	ASP
1	K	199	ASP
1	K	212	ARG
1	K	219	SER
1	K	221	LEU
1	K	222	VAL
1	K	224	THR
1	K	225	LYS
1	K	231	GLU
1	K	235	LEU
1	K	236	VAL
1	L	70	ASN
1	L	72	LYS
1	L	81	ARG
1	L	84	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	87	LEU
1	L	104	LEU
1	L	110	ASP
1	L	115	VAL
1	L	117	THR
1	L	121	LYS
1	L	130	ILE
1	L	141	VAL
1	L	143	LEU
1	L	148	THR
1	L	149	VAL
1	L	156	GLU
1	L	158	VAL
1	L	162	SER
1	L	164	LEU
1	L	167	ILE
1	L	196	ASP
1	L	214	LEU
1	L	225	LYS
1	L	231	GLU
1	L	236	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	70	ASN
1	A	96	GLN
1	B	70	ASN
1	C	70	ASN
1	C	96	GLN
1	D	70	ASN
1	E	70	ASN
1	E	96	GLN
1	F	70	ASN
1	G	70	ASN
1	H	70	ASN
1	I	70	ASN
1	J	70	ASN
1	K	70	ASN
1	L	70	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%)	-0.20	3 (1%) 74 63	166, 225, 345, 406	0
1	B	186/251 (74%)	-0.25	5 (2%) 58 46	158, 212, 412, 527	0
1	C	186/251 (74%)	-0.22	3 (1%) 74 63	168, 226, 338, 403	0
1	D	186/251 (74%)	-0.25	4 (2%) 65 54	155, 210, 417, 544	0
1	E	186/251 (74%)	-0.21	3 (1%) 74 63	164, 220, 340, 398	0
1	F	186/251 (74%)	-0.25	4 (2%) 65 54	156, 212, 419, 539	0
1	G	186/251 (74%)	-0.17	3 (1%) 74 63	167, 224, 343, 406	0
1	H	186/251 (74%)	-0.25	5 (2%) 58 46	157, 210, 406, 520	0
1	I	186/251 (74%)	-0.21	4 (2%) 65 54	166, 222, 339, 402	0
1	J	186/251 (74%)	-0.23	6 (3%) 51 38	156, 210, 417, 538	0
1	K	186/251 (74%)	-0.23	3 (1%) 74 63	165, 223, 335, 409	0
1	L	186/251 (74%)	-0.24	6 (3%) 51 38	157, 213, 423, 548	0
All	All	2232/3012 (74%)	-0.23	49 (2%) 65 54	155, 218, 384, 548	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	53	ALA	5.1
1	J	204	ALA	4.9
1	L	204	ALA	4.6
1	A	204	ALA	4.4
1	D	53	ALA	4.3
1	F	204	ALA	4.3
1	F	53	ALA	4.3
1	G	204	ALA	4.3
1	B	204	ALA	4.3
1	D	204	ALA	4.3
1	K	204	ALA	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	204	ALA	4.1
1	H	53	ALA	4.0
1	B	53	ALA	3.9
1	G	205	LEU	3.8
1	E	204	ALA	3.8
1	J	53	ALA	3.8
1	C	205	LEU	3.7
1	H	204	ALA	3.6
1	A	205	LEU	3.5
1	K	205	LEU	3.4
1	C	204	ALA	3.0
1	E	205	LEU	3.0
1	F	206	ASN	3.0
1	F	52	SER	2.9
1	I	205	LEU	2.8
1	L	206	ASN	2.8
1	J	206	ASN	2.7
1	L	52	SER	2.7
1	J	52	SER	2.7
1	D	52	SER	2.6
1	H	52	SER	2.6
1	H	206	ASN	2.6
1	B	206	ASN	2.6
1	E	206	ASN	2.6
1	B	52	SER	2.6
1	D	206	ASN	2.5
1	A	206	ASN	2.4
1	C	206	ASN	2.4
1	I	206	ASN	2.4
1	G	206	ASN	2.3
1	K	206	ASN	2.2
1	H	205	LEU	2.2
1	B	54	ARG	2.1
1	L	203	GLU	2.1
1	I	52	SER	2.1
1	L	54	ARG	2.1
1	J	54	ARG	2.0
1	J	207	ASP	2.0

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

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

6.3 Carbohydrates [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.