



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:01 AM UTC

PDB ID : 3M9B / pdb_00003m9b
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

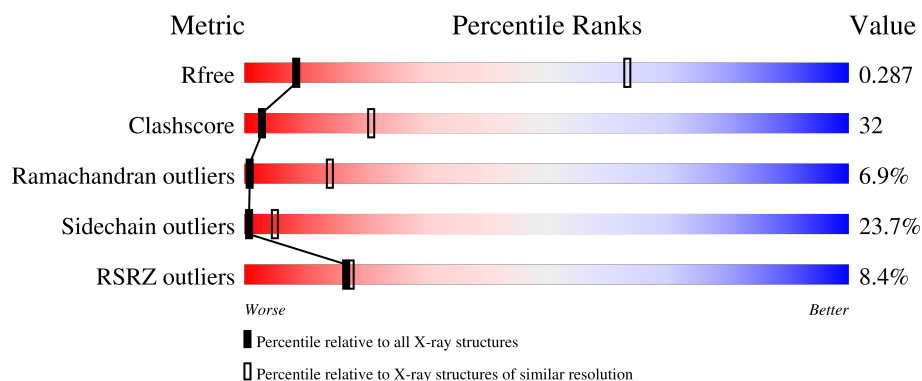
1 Overall quality at a glance

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}	180053	1022 (4.12-3.76)
Clashscore	190562	1000 (4.10-3.78)
Ramachandran outliers	187476	1009 (4.12-3.76)
Sidechain outliers	187428	1002 (4.12-3.76)
RSRZ outliers	180081	1022 (4.12-3.76)

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

Mol	Chain	Length	Quality of chain
1	A	251	
1	B	251	
1	C	251	
1	D	251	
1	E	251	

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Mol	Chain	Length	Quality of chain
1	F	251	
1	G	251	
1	H	251	
1	I	251	
1	J	251	
1	K	251	
1	L	251	

2 Entry composition

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

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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
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

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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

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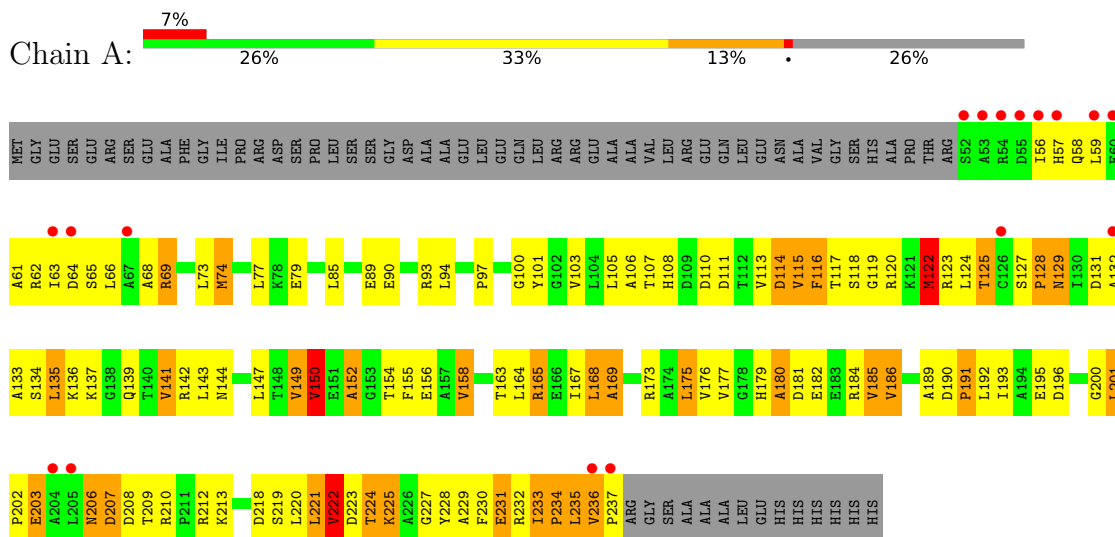
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Chain	Residue	Modelled	Actual	Comment	Reference
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K	239	GLY	-	expression tag	UNP P63345
K	240	SER	-	expression tag	UNP P63345
K	241	ALA	-	expression tag	UNP P63345
K	242	ALA	-	expression tag	UNP P63345
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
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L	251	HIS	-	expression tag	UNP P63345

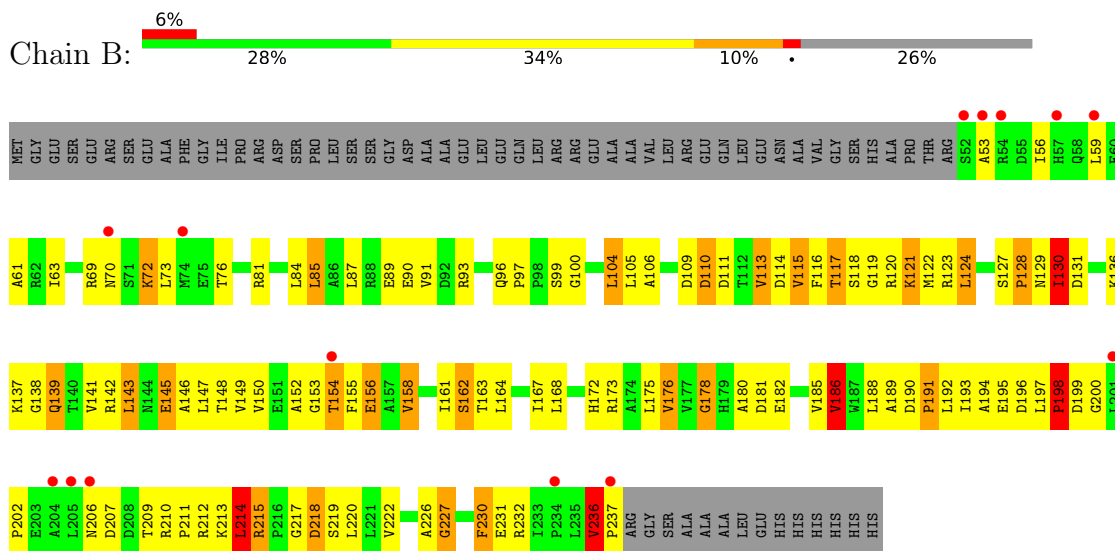
3 Residue-property plots

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

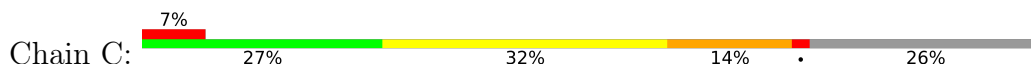
- Molecule 1: Proteasome-associated ATPase

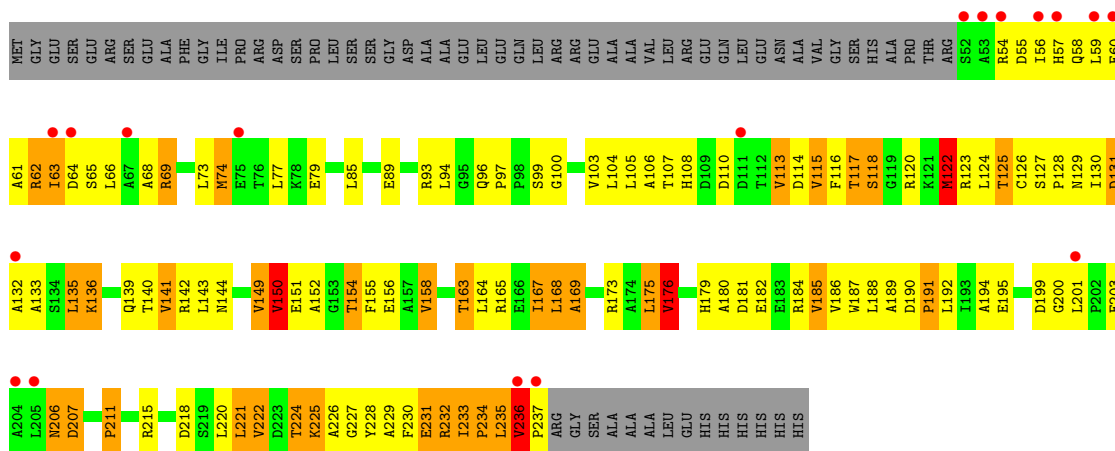


- Molecule 1: Proteasome-associated ATPase

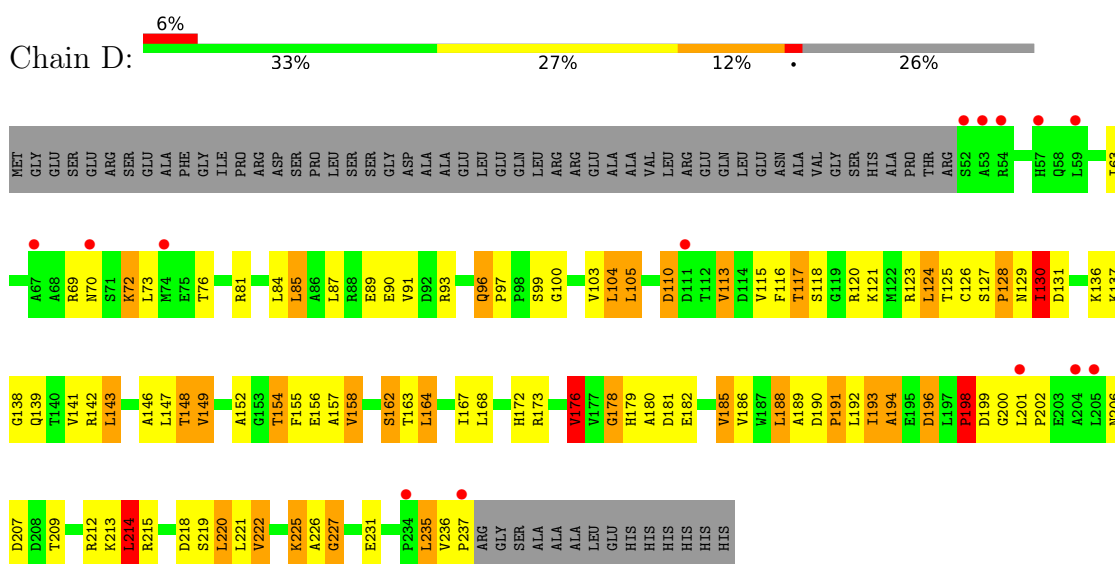


- Molecule 1: Proteasome-associated ATPase

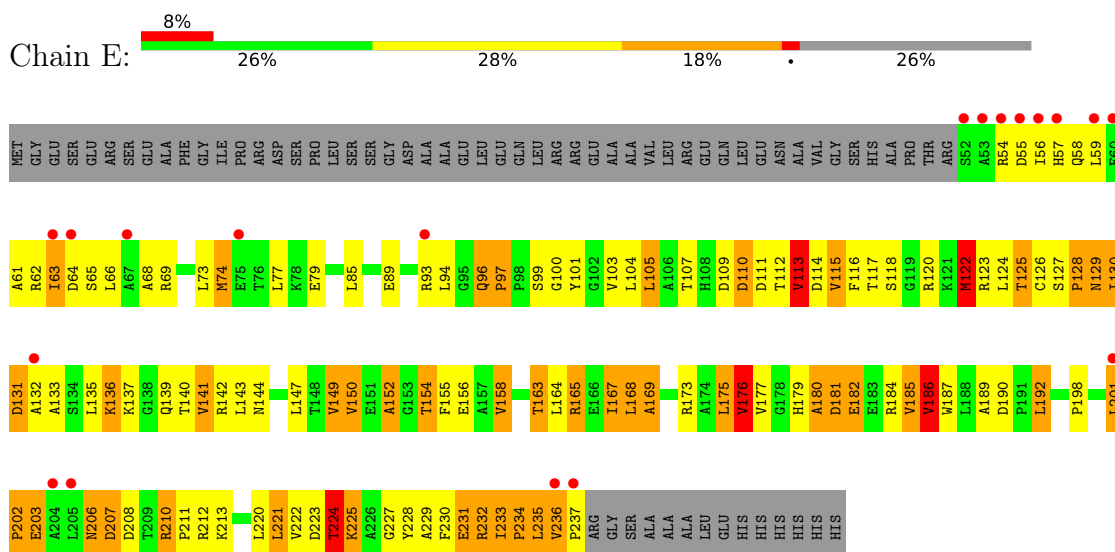




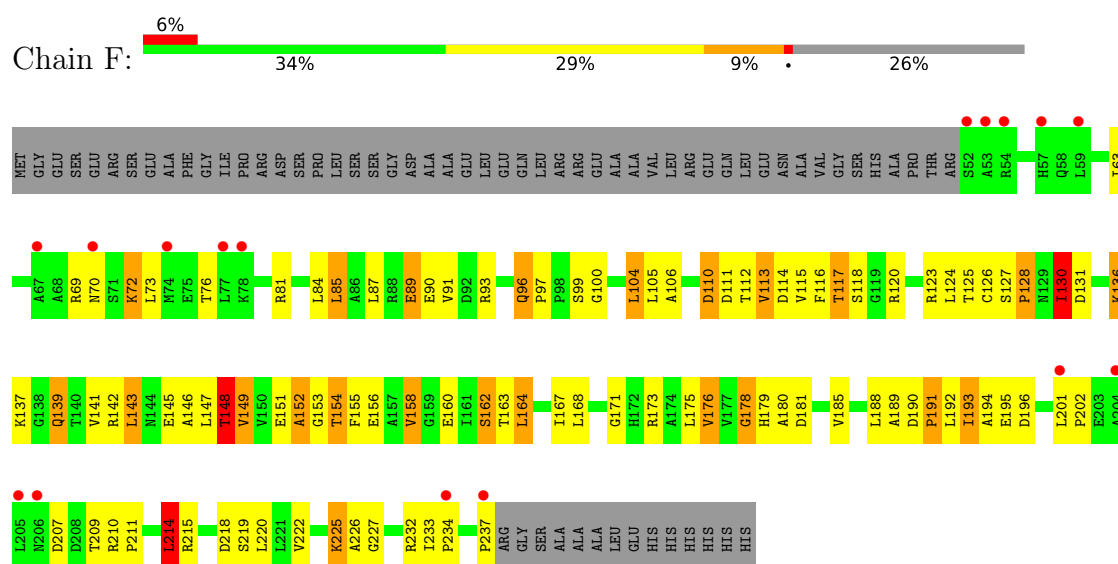
- Molecule 1: Proteasome-associated ATPase



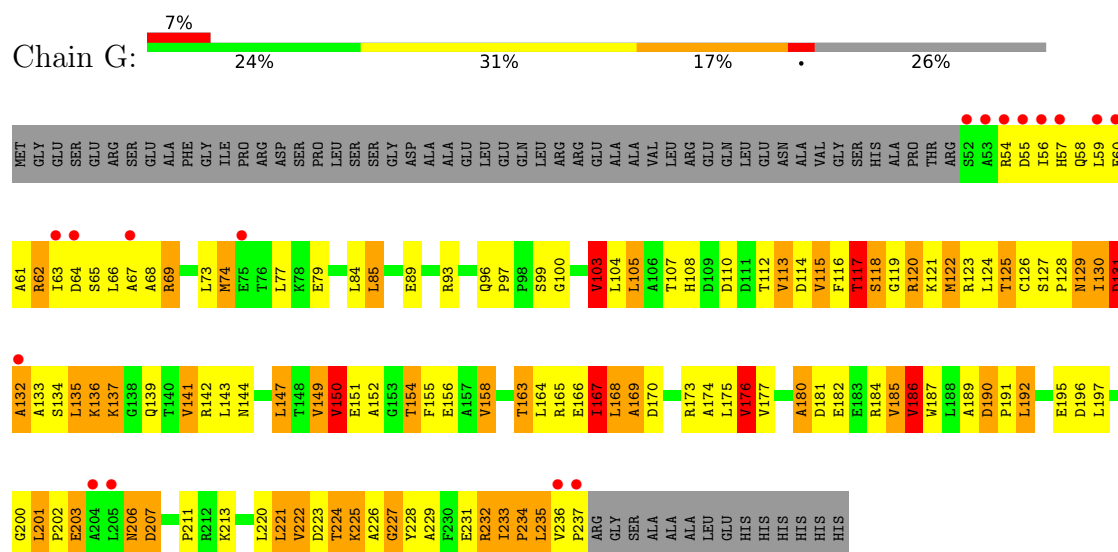
- Molecule 1: Proteasome-associated ATPase



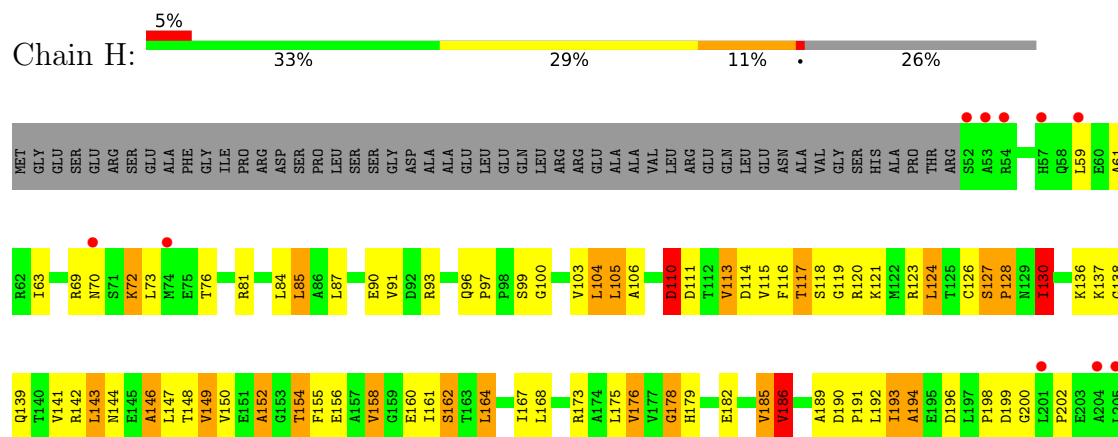
- Molecule 1: Proteasome-associated ATPase



- Molecule 1: Proteasome-associated ATPase

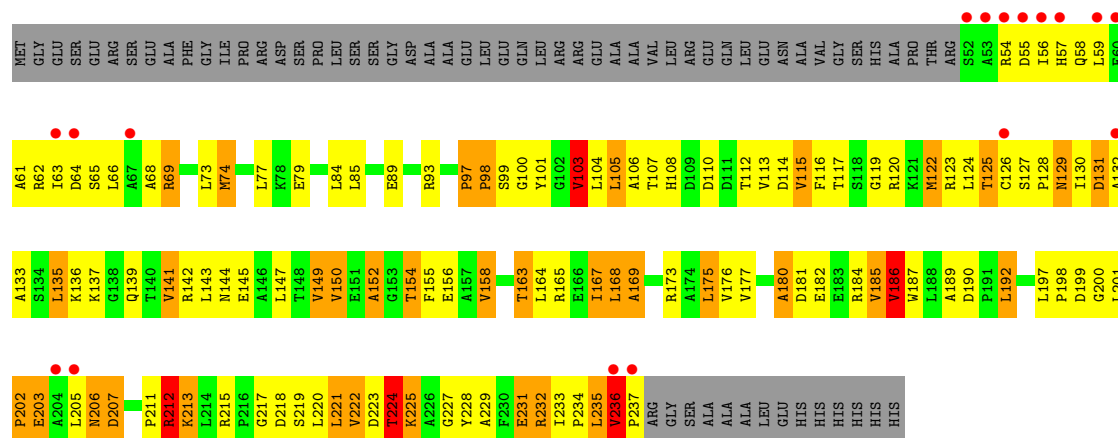
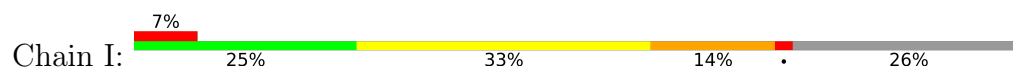


- Molecule 1: Proteasome-associated ATPase

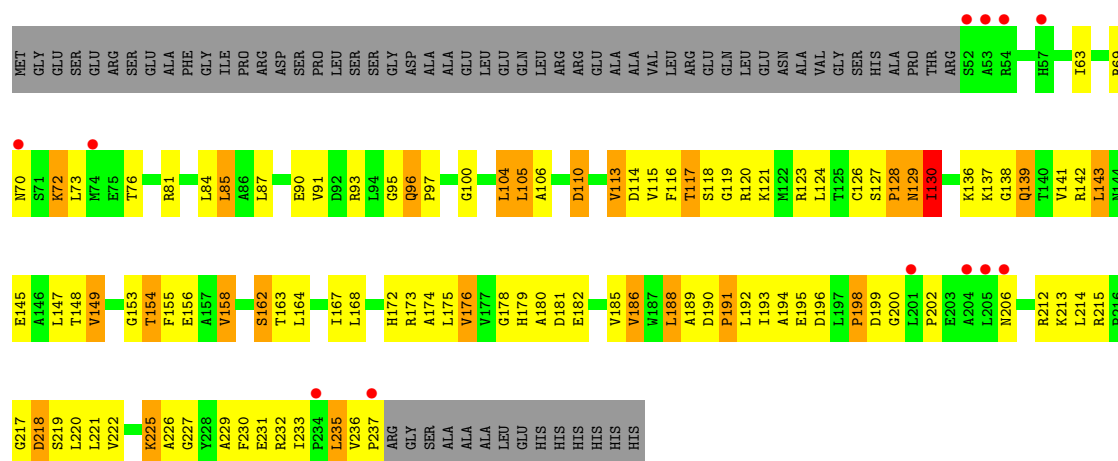




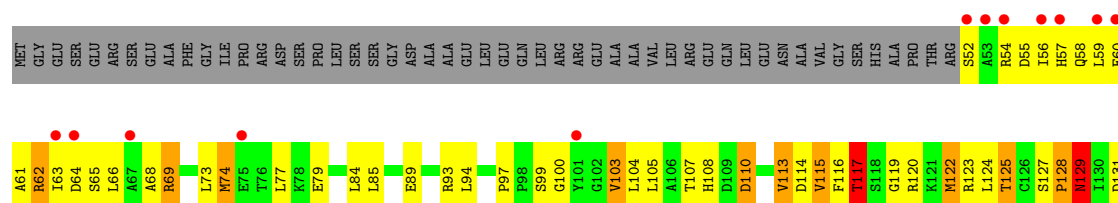
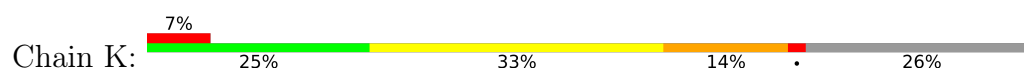
• Molecule 1: Proteasome-associated ATPase

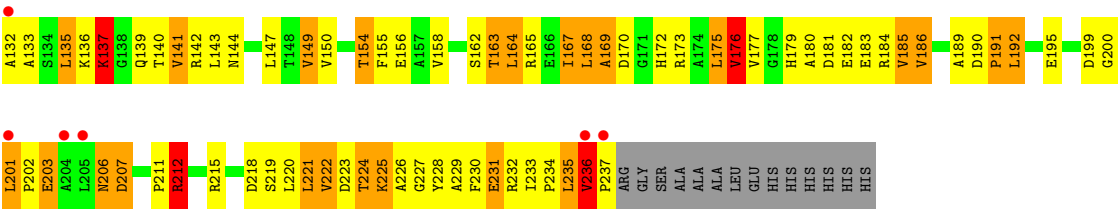


• Molecule 1: Proteasome-associated ATPase

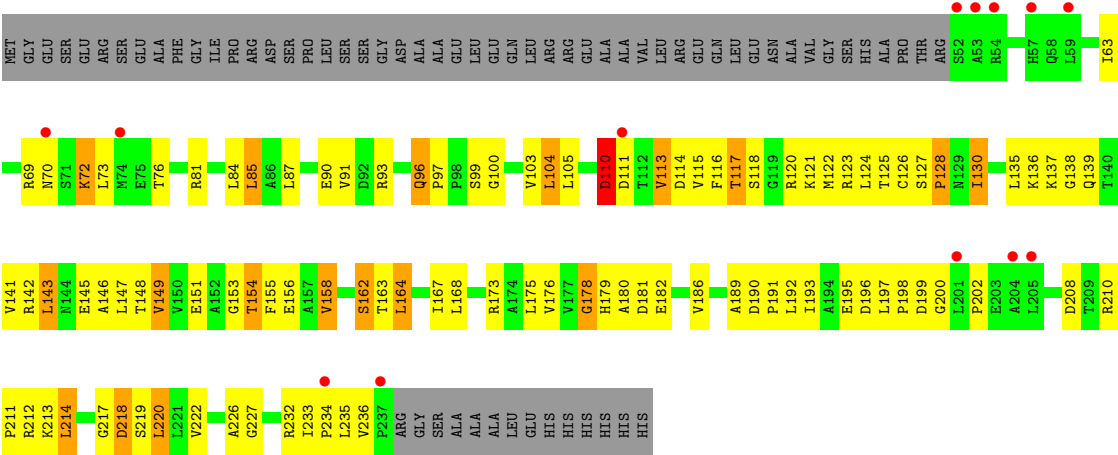


• Molecule 1: Proteasome-associated ATPase





● Molecule 1: Proteasome-associated ATPase



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 – 3.94	Depositor EDS
% Data completeness (in resolution range)	99.7 (25.00-3.94) 99.3 (25.00-3.94)	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	5010 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	152.3	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 186.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
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
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, 0.333 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	1.46	8/1451 (0.6%)	1.43	16/1969 (0.8%)
1	B	1.27	2/1451 (0.1%)	1.39	14/1969 (0.7%)
1	C	1.49	7/1451 (0.5%)	1.45	21/1969 (1.1%)
1	D	1.28	3/1451 (0.2%)	1.40	13/1969 (0.7%)
1	E	1.49	10/1451 (0.7%)	1.49	27/1969 (1.4%)
1	F	1.26	3/1451 (0.2%)	1.38	10/1969 (0.5%)
1	G	1.47	10/1451 (0.7%)	1.48	25/1969 (1.3%)
1	H	1.28	3/1451 (0.2%)	1.37	9/1969 (0.5%)
1	I	1.42	6/1451 (0.4%)	1.44	15/1969 (0.8%)
1	J	1.30	2/1451 (0.1%)	1.40	11/1969 (0.6%)
1	K	1.44	6/1451 (0.4%)	1.42	13/1969 (0.7%)
1	L	1.26	1/1451 (0.1%)	1.37	11/1969 (0.6%)
All	All	1.37	61/17412 (0.4%)	1.42	185/23628 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	D	0	1
1	I	0	1
1	K	0	1
All	All	0	5

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	117	THR	CA-C	11.68	1.58	1.52
1	C	117	THR	CA-C	10.40	1.57	1.52
1	A	93	ARG	CZ-NH1	8.64	1.44	1.32
1	G	236	VAL	CA-CB	8.61	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	236	VAL	CA-CB	8.57	1.65	1.54
1	K	236	VAL	CA-CB	8.40	1.65	1.54
1	E	93	ARG	CZ-NH1	8.26	1.44	1.32
1	C	93	ARG	CZ-NH1	8.25	1.44	1.32
1	A	196	ASP	CA-C	8.23	1.61	1.53
1	C	236	VAL	CA-CB	8.20	1.64	1.54
1	K	117	THR	CA-C	8.14	1.56	1.52
1	I	236	VAL	CA-CB	8.03	1.64	1.54
1	A	236	VAL	CA-CB	7.91	1.64	1.54
1	K	93	ARG	CZ-NH1	7.91	1.43	1.32
1	I	93	ARG	CZ-NH1	7.65	1.43	1.32
1	G	93	ARG	CZ-NH1	7.57	1.43	1.32
1	C	236	VAL	CA-C	7.39	1.60	1.52
1	G	236	VAL	CA-C	7.16	1.60	1.52
1	E	236	VAL	CA-C	7.15	1.60	1.52
1	I	236	VAL	CA-C	6.83	1.60	1.52
1	A	236	VAL	CA-C	6.72	1.59	1.52
1	F	176	VAL	CA-CB	-6.54	1.46	1.54
1	K	236	VAL	CA-C	6.40	1.59	1.52
1	K	93	ARG	NE-CZ	6.19	1.39	1.33
1	D	196	ASP	C-O	6.13	1.32	1.23
1	E	198	PRO	CA-C	6.12	1.59	1.52
1	G	118	SER	CA-C	-6.00	1.46	1.53
1	C	226	ALA	CA-CB	-6.00	1.44	1.54
1	B	176	VAL	CA-CB	-5.91	1.47	1.54
1	H	176	VAL	CA-CB	-5.90	1.46	1.54
1	E	182	GLU	CA-C	-5.88	1.45	1.52
1	C	93	ARG	NE-CZ	5.83	1.39	1.33
1	E	93	ARG	NE-CZ	5.80	1.39	1.33
1	F	237	PRO	N-CA	5.78	1.55	1.47
1	J	237	PRO	N-CA	5.75	1.55	1.47
1	H	160	GLU	CG-CD	5.73	1.66	1.52
1	J	176	VAL	CA-CB	-5.71	1.47	1.54
1	D	176	VAL	CA-CB	-5.71	1.47	1.54
1	G	226	ALA	CA-CB	-5.67	1.45	1.53
1	G	93	ARG	NE-CZ	5.63	1.39	1.33
1	I	93	ARG	NE-CZ	5.54	1.39	1.33
1	A	93	ARG	NE-CZ	5.52	1.39	1.33
1	B	236	VAL	CA-CB	5.52	1.59	1.53
1	E	186	VAL	CA-C	-5.34	1.46	1.52
1	G	103	VAL	CA-C	-5.32	1.47	1.52
1	E	105	LEU	N-CA	-5.31	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	121	LYS	CA-C	-5.28	1.46	1.52
1	K	226	ALA	CA-CB	-5.25	1.45	1.54
1	L	176	VAL	CA-CB	-5.20	1.47	1.54
1	E	165	ARG	N-CA	-5.17	1.40	1.46
1	F	160	GLU	CG-CD	5.15	1.65	1.52
1	H	237	PRO	N-CA	5.13	1.54	1.47
1	I	105	LEU	N-CA	-5.13	1.39	1.46
1	D	157	ALA	CA-CB	-5.11	1.47	1.54
1	A	165	ARG	N-CA	-5.10	1.40	1.46
1	C	118	SER	CA-C	-5.10	1.47	1.53
1	E	176	VAL	CA-CB	-5.05	1.47	1.55
1	A	90	GLU	CD-OE1	5.03	1.34	1.25
1	A	116	PHE	CA-C	-5.03	1.47	1.52
1	G	105	LEU	N-CA	-5.01	1.39	1.46
1	I	103	VAL	CA-C	-5.01	1.47	1.52

All (185) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	96	GLN	CA-C-N	9.28	126.43	119.66
1	D	96	GLN	C-N-CA	9.28	126.43	119.66
1	G	97	PRO	CA-C-N	8.97	131.06	119.84
1	G	97	PRO	C-N-CA	8.97	131.06	119.84
1	B	96	GLN	CA-C-N	8.89	126.15	119.66
1	B	96	GLN	C-N-CA	8.89	126.15	119.66
1	I	97	PRO	CA-C-N	8.87	130.93	119.84
1	I	97	PRO	C-N-CA	8.87	130.93	119.84
1	J	96	GLN	CA-C-N	8.71	126.02	119.66
1	J	96	GLN	C-N-CA	8.71	126.02	119.66
1	F	96	GLN	CA-C-N	8.69	126.00	119.66
1	F	96	GLN	C-N-CA	8.69	126.00	119.66
1	E	97	PRO	CA-C-N	8.44	130.40	119.84
1	E	97	PRO	C-N-CA	8.44	130.40	119.84
1	K	97	PRO	CA-C-N	8.17	130.05	119.84
1	K	97	PRO	C-N-CA	8.17	130.05	119.84
1	L	96	GLN	CA-C-N	8.09	125.57	119.66
1	L	96	GLN	C-N-CA	8.09	125.57	119.66
1	J	130	ILE	N-CA-C	7.98	119.37	107.80
1	K	180	ALA	N-CA-C	-7.93	98.48	110.14
1	A	97	PRO	CA-C-N	7.88	129.69	119.84
1	A	97	PRO	C-N-CA	7.88	129.69	119.84
1	H	96	GLN	CA-C-N	7.85	125.39	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	96	GLN	C-N-CA	7.85	125.39	119.66
1	E	180	ALA	N-CA-C	-7.75	97.62	109.95
1	B	130	ILE	N-CA-C	7.40	118.53	108.17
1	I	180	ALA	N-CA-C	-7.40	98.67	110.14
1	C	180	ALA	N-CA-C	-7.33	99.62	110.46
1	C	97	PRO	CA-C-N	7.26	128.91	119.84
1	C	97	PRO	C-N-CA	7.26	128.91	119.84
1	D	130	ILE	N-CA-C	7.25	118.26	108.11
1	J	176	VAL	CB-CA-C	-7.05	101.17	111.68
1	D	176	VAL	CB-CA-C	-7.04	101.20	111.68
1	D	163	THR	CA-C-N	-7.02	112.41	122.94
1	D	163	THR	C-N-CA	-7.02	112.41	122.94
1	G	233	ILE	CA-C-N	6.99	128.57	119.84
1	G	233	ILE	C-N-CA	6.99	128.57	119.84
1	L	163	THR	CA-C-N	-6.96	112.50	122.94
1	L	163	THR	C-N-CA	-6.96	112.50	122.94
1	H	130	ILE	N-CA-C	6.86	117.71	108.11
1	C	206	ASN	N-CA-C	6.72	120.56	110.14
1	F	176	VAL	CB-CA-C	-6.69	101.21	111.31
1	G	186	VAL	CB-CA-C	-6.61	100.65	110.82
1	A	180	ALA	N-CA-C	-6.56	99.97	110.14
1	E	97	PRO	O-C-N	6.43	124.27	121.31
1	B	176	VAL	CB-CA-C	-6.40	101.95	110.98
1	I	212	ARG	N-CA-C	6.35	116.95	108.38
1	E	186	VAL	CB-CA-C	-6.25	101.20	110.82
1	C	176	VAL	CB-CA-C	-6.24	100.91	110.95
1	H	176	VAL	CB-CA-C	-6.24	101.89	111.31
1	B	163	THR	CA-C-N	-6.23	113.14	122.74
1	B	163	THR	C-N-CA	-6.23	113.14	122.74
1	B	146	ALA	N-CA-C	-6.22	101.07	110.28
1	C	195	GLU	N-CA-C	6.22	117.86	111.14
1	B	214	LEU	N-CA-C	6.21	119.64	109.76
1	E	152	ALA	N-CA-C	-6.20	100.76	109.69
1	G	117	THR	N-CA-C	6.20	117.98	108.12
1	J	206	ASN	N-CA-C	6.18	119.40	109.02
1	C	69	ARG	N-CA-C	-6.17	103.87	112.45
1	E	233	ILE	CA-C-N	6.14	127.52	119.84
1	E	233	ILE	C-N-CA	6.14	127.52	119.84
1	G	206	ASN	N-CA-C	6.13	119.47	109.59
1	I	69	ARG	N-CA-C	-6.08	104.00	112.45
1	D	220	LEU	N-CA-C	6.07	119.59	109.95
1	J	163	THR	CA-C-N	-6.05	113.31	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	163	THR	C-N-CA	-6.05	113.31	122.81
1	C	122	MET	N-CA-C	6.04	119.39	109.85
1	E	69	ARG	N-CA-C	-6.01	104.10	112.45
1	E	206	ASN	N-CA-C	5.98	118.98	109.24
1	G	69	ARG	N-CA-C	-5.96	104.16	112.45
1	E	176	VAL	CB-CA-C	-5.93	101.69	110.82
1	A	69	ARG	N-CA-C	-5.93	104.21	112.45
1	F	148	THR	N-CA-C	-5.90	98.23	110.80
1	A	93	ARG	NE-CZ-NH2	-5.89	113.90	119.20
1	C	150	VAL	CB-CA-C	-5.87	101.66	111.29
1	C	233	ILE	CA-C-N	5.87	127.18	119.84
1	C	233	ILE	C-N-CA	5.87	127.18	119.84
1	I	206	ASN	N-CA-C	5.87	119.21	110.52
1	L	176	VAL	CB-CA-C	-5.87	101.50	110.95
1	K	69	ARG	N-CA-C	-5.87	104.30	112.45
1	J	235	LEU	CA-CB-CG	5.85	136.78	116.30
1	I	152	ALA	N-CA-C	-5.80	101.34	109.69
1	B	139	GLN	N-CA-C	-5.79	99.21	109.06
1	H	220	LEU	N-CA-C	5.79	119.16	109.95
1	B	206	ASN	N-CA-C	5.79	119.97	109.32
1	H	146	ALA	N-CA-C	-5.76	101.76	110.28
1	E	212	ARG	N-CA-C	5.75	116.14	108.38
1	B	197	LEU	CA-C-N	5.73	127.00	119.84
1	B	197	LEU	C-N-CA	5.73	127.00	119.84
1	E	93	ARG	NE-CZ-NH2	-5.73	114.04	119.20
1	L	220	LEU	N-CA-C	5.70	119.01	109.95
1	K	206	ASN	N-CA-C	5.69	119.33	110.17
1	C	97	PRO	O-C-N	5.67	123.92	121.31
1	F	163	THR	CA-C-N	-5.67	113.74	122.87
1	F	163	THR	C-N-CA	-5.67	113.74	122.87
1	D	206	ASN	N-CA-C	5.64	119.70	109.32
1	K	176	VAL	CB-CA-C	-5.63	102.14	110.82
1	F	146	ALA	N-CA-C	-5.63	101.52	109.96
1	A	212	ARG	N-CA-C	5.62	116.50	108.74
1	G	122	MET	N-CA-C	5.62	118.24	109.52
1	G	97	PRO	O-C-N	5.62	123.89	121.31
1	F	214	LEU	N-CA-C	5.61	118.68	109.76
1	G	192	LEU	N-CA-C	-5.60	106.80	113.97
1	B	186	VAL	CB-CA-C	-5.58	101.97	110.95
1	I	232	ARG	CA-C-N	-5.58	118.00	122.85
1	I	232	ARG	C-N-CA	-5.58	118.00	122.85
1	J	214	LEU	N-CA-C	5.58	118.72	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	192	LEU	N-CA-C	-5.57	107.12	114.31
1	G	195	GLU	N-CA-C	5.57	117.15	111.14
1	L	214	LEU	N-CA-C	5.54	118.57	109.76
1	A	206	ASN	N-CA-C	5.53	119.11	110.32
1	K	212	ARG	N-CA-C	5.52	115.83	108.38
1	G	118	SER	N-CA-C	-5.51	100.63	109.39
1	J	139	GLN	N-CA-C	-5.49	100.72	109.23
1	A	97	PRO	O-C-N	5.49	123.83	121.31
1	L	146	ALA	N-CA-C	-5.48	102.17	110.28
1	D	214	LEU	N-CA-C	5.47	118.17	109.96
1	F	152	ALA	N-CA-C	-5.47	101.44	109.81
1	D	235	LEU	CA-CB-CG	5.47	135.45	116.30
1	K	129	ASN	N-CA-C	5.47	120.65	112.94
1	K	195	GLU	N-CA-C	5.47	117.05	111.14
1	A	193	ILE	CB-CA-C	-5.46	104.99	111.65
1	E	232	ARG	CA-C-N	-5.46	118.10	122.85
1	E	232	ARG	C-N-CA	-5.46	118.10	122.85
1	I	186	VAL	CB-CA-C	-5.43	102.46	110.82
1	J	186	VAL	CB-CA-C	-5.38	102.28	110.95
1	F	130	ILE	N-CA-C	5.38	115.70	108.17
1	C	117	THR	CA-C-O	5.37	122.83	119.77
1	E	96	GLN	CA-C-N	5.37	123.58	119.66
1	E	96	GLN	C-N-CA	5.37	123.58	119.66
1	I	167	ILE	N-CA-C	-5.36	104.15	110.21
1	B	152	ALA	N-CA-C	-5.36	101.98	109.69
1	A	129	ASN	N-CA-C	5.34	119.66	113.20
1	A	152	ALA	N-CA-C	-5.34	102.00	109.69
1	C	117	THR	N-CA-C	5.34	116.63	108.30
1	D	148	THR	N-CA-C	-5.29	99.53	110.80
1	C	232	ARG	CA-C-N	-5.29	118.25	122.85
1	C	232	ARG	C-N-CA	-5.29	118.25	122.85
1	A	222	VAL	N-CA-C	5.27	116.61	108.44
1	K	62	ARG	N-CA-C	-5.25	104.99	111.40
1	E	122	MET	N-CA-C	5.24	118.28	109.95
1	I	150	VAL	CB-CA-C	-5.24	102.70	111.29
1	L	130	ILE	N-CA-C	5.24	115.64	107.99
1	D	146	ALA	N-CA-C	-5.23	102.54	110.28
1	C	118	SER	N-CA-C	-5.22	102.61	110.70
1	A	195	GLU	N-CA-C	5.22	117.88	111.82
1	D	152	ALA	N-CA-C	-5.21	101.84	109.81
1	E	129	ASN	N-CA-C	5.21	119.48	113.18
1	E	210	ARG	CA-C-N	5.21	126.35	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	210	ARG	C-N-CA	5.21	126.35	119.84
1	G	150	VAL	CB-CA-C	-5.21	102.75	111.29
1	E	167	ILE	N-CA-C	-5.19	104.35	110.21
1	C	96	GLN	CA-C-N	5.17	123.44	119.66
1	C	96	GLN	C-N-CA	5.17	123.44	119.66
1	I	176	VAL	CB-CA-C	-5.17	103.45	110.90
1	K	117	THR	N-CA-C	5.17	116.34	108.12
1	K	150	VAL	CB-CA-C	-5.17	102.81	111.29
1	L	110	ASP	N-CA-C	5.17	119.15	113.21
1	G	180	ALA	N-CA-C	-5.16	101.86	110.17
1	A	122	MET	N-CA-C	5.16	118.13	110.14
1	H	186	VAL	CB-CA-C	-5.14	102.68	110.95
1	G	197	LEU	CA-C-N	5.13	125.14	119.90
1	G	197	LEU	C-N-CA	5.13	125.14	119.90
1	H	152	ALA	N-CA-C	-5.12	101.62	109.41
1	E	192	LEU	N-CA-C	-5.12	107.42	113.97
1	E	93	ARG	NE-CZ-NH1	5.10	126.60	121.50
1	G	176	VAL	CB-CA-C	-5.10	102.96	110.82
1	A	213	LYS	N-CA-C	-5.10	102.21	110.32
1	G	62	ARG	N-CA-C	-5.10	105.18	111.40
1	L	186	VAL	CB-CA-C	-5.08	102.77	110.95
1	G	196	ASP	N-CA-C	5.06	117.40	108.24
1	C	62	ARG	N-CA-C	-5.05	105.24	111.40
1	H	110	ASP	N-CA-C	5.05	118.32	112.97
1	E	150	VAL	CB-CA-C	-5.04	103.02	111.29
1	C	93	ARG	NE-CZ-NH2	-5.04	114.66	119.20
1	E	113	VAL	N-CA-C	5.04	117.07	108.86
1	I	213	LYS	N-CA-C	-5.04	103.03	110.48
1	G	232	ARG	CA-C-N	-5.03	118.47	122.85
1	G	232	ARG	C-N-CA	-5.03	118.47	122.85
1	E	130	ILE	N-CA-C	5.03	117.00	109.20
1	G	96	GLN	CA-C-N	5.02	123.33	119.66
1	G	96	GLN	C-N-CA	5.02	123.33	119.66
1	K	192	LEU	N-CA-C	-5.02	107.54	113.97
1	A	150	VAL	CB-CA-C	-5.02	103.06	111.29
1	G	167	ILE	N-CA-C	-5.00	104.56	110.21

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	198	PRO	Peptide

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Mol	Chain	Res	Type	Group
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	119	0
1	B	1431	0	1443	86	0
1	C	1431	0	1443	124	0
1	D	1431	0	1443	77	0
1	E	1431	0	1443	113	0
1	F	1431	0	1443	84	0
1	G	1431	0	1443	109	0
1	H	1431	0	1443	84	0
1	I	1431	0	1443	128	0
1	J	1431	0	1443	79	0
1	K	1431	0	1443	112	0
1	L	1431	0	1443	69	0
All	All	17172	0	17316	1116	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 32.

All (1116) 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:C:120:ARG:HE	1:C:122:MET:HE2	1.09	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:120:ARG:HE	1:E:122:MET:HE3	1.20	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:120:ARG:HH21	1:C:122:MET:HE1	1.31	0.94
1:E:120:ARG:NE	1:E:122:MET:HE3	1.82	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:C:120:ARG:NE	1:C:122:MET:HE2	1.85	0.91
1:L:220:LEU:HD12	1:L:220:LEU:N	1.85	0.90
1:F:154:THR:HG22	1:F:155:PHE:H	1.38	0.89
1:J:220:LEU:HD12	1:J:220:LEU:N	1.86	0.89
1:K:120:ARG:HE	1:K:122:MET:HE2	1.37	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: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:L:155:PHE:HE2	1:L:191:PRO:HG2	1.38	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:186:VAL:HG12	1:H:227:GLY:C	2.05	0.81
1:B:220:LEU:HD12	1:B:220:LEU:N	1.95	0.81
1:H:162:SER:HB3	1:H:178:GLY:HA2	1.61	0.81
1:I:125:THR:HG23	1:L:97:PRO:HG3	1.63	0.81
1:A:235:LEU:CD1	1:A:237:PRO:HD3	2.11	0.81
1:H:116:PHE:HD1	1:H:120:ARG:O	1.63	0.80
1:H:139:GLN:NE2	1:H:152:ALA:HB1	1.96	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:168:LEU:HB2	1:A:173:ARG:O	1.81	0.80
1:I:168:LEU:HB2	1:I:173:ARG:O	1.81	0.80
1:I:184:ARG:HD3	1:I:224:THR:CG2	2.11	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:A:120:ARG:HE	1:A:122:MET:HE2	1.46	0.78
1:F:220:LEU:N	1:F:220:LEU:HD12	1.98	0.77
1:H:147:LEU:HD12	1:H:147:LEU:H	1.49	0.77
1:K:221:LEU:C	1:K:221:LEU:HD23	2.09	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:K:202:PRO:O	1:K:203:GLU:HB2	1.83	0.77
1:I:139:GLN:HE21	1:I:152:ALA:HB1	1.49	0.77
1:L:168:LEU:HD12	1:L:173:ARG:HB2	1.65	0.77

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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:D:168:LEU:HD12	1:D:173:ARG:HB2	1.67	0.76
1:H:168:LEU:HD12	1:H:173:ARG:HB2	1.65	0.76
1:E:220:LEU:HD12	1:E:229:ALA:HB1	1.65	0.76
1:C:186:VAL:CG1	1:C:227:GLY:O	2.33	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:J:155:PHE:CE2	1:J:191:PRO:HG2	2.20	0.76
1:G:125:THR:HG23	1:J:97:PRO:CG	2.16	0.76
1:K:186:VAL:CG1	1:K:227:GLY:O	2.31	0.76
1:I:120:ARG:NE	1:I:122:MET:HE3	2.00	0.76
1:L:116:PHE:HD1	1:L:120:ARG:O	1.69	0.76
1:D:220:LEU:N	1:D:220:LEU:HD12	2.01	0.76
1:I:189:ALA:H	1:I:192:LEU:HD12	1.51	0.76
1:I:115:VAL:HG22	1:I:124:LEU:HD21	1.67	0.76
1:I:120:ARG:HE	1:I:122:MET:HE3	1.51	0.76
1:K:235:LEU:HD22	1:K:236:VAL:H	1.50	0.76
1:E:105:LEU:HB2	1:E:114:ASP:O	1.84	0.76
1:K:120:ARG:NE	1:K:122:MET:HE2	2.01	0.75
1:I:105:LEU:HB2	1:I:114:ASP:O	1.85	0.75
1:F:147:LEU:HD12	1:F:147:LEU:H	1.49	0.75
1:L:155:PHE:CE2	1:L:191:PRO:HG2	2.20	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: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:J:126:CYS:HB3	1:J:149:VAL:CG2	2.16	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:A:220:LEU:HD12	1:A:229:ALA:HB1	1.69	0.73
1:H:116:PHE:CE2	1:H:226:ALA:HA	2.23	0.73
1:J:154:THR:CG2	1:J:155:PHE:H	1.99	0.73
1:F:162:SER:HB3	1:F:178:GLY:HA2	1.68	0.73
1:K:165:ARG:HG2	1:K:165:ARG:HH11	1.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ALA:H	1:A:192:LEU:HD12	1.54	0.73
1:G:124:LEU:HD11	1:G:143:LEU:CD2	2.18	0.73
1:E:168:LEU:HB2	1:E:173:ARG:O	1.89	0.73
1:K:105:LEU:HB2	1:K:114:ASP:O	1.88	0.73
1:K:189:ALA:N	1:K:192:LEU:HD12	2.03	0.72
1:F:126:CYS:HB3	1:F:149:VAL:CG2	2.18	0.72
1:K:135:LEU:HB2	1:K:139:GLN:NE2	2.04	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:B:219:SER:C	1:B:220:LEU:HD12	2.14	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:A:58:GLN:HE22	1:I:235:LEU:HG	1.55	0.71
1:G:163:THR:O	1:G:176:VAL:HG12	1.90	0.71
1:B:90:GLU:HA	1:B:93:ARG:HD3	1.71	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:C:221:LEU:C	1:C:221:LEU:HD23	2.15	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:K:177:VAL:HG12	1:K:183:GLU:HG2	1.73	0.71
1:L:116:PHE:CE2	1:L:226:ALA:HA	2.25	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:E:154:THR:HG22	1:E:155:PHE:H	1.56	0.70
1:F:116:PHE:CD2	1:F:226:ALA:HA	2.27	0.70
1:G:232:ARG:O	1:G:233:ILE:HD13	1.91	0.70
1:D:90:GLU:HA	1:D:93:ARG:HD3	1.72	0.70
1:E:202:PRO:O	1:E:203:GLU:HB2	1.92	0.70
1:C:77:LEU:HD13	1:C:77:LEU:O	1.92	0.70
1:C:127:SER:O	1:C:129:ASN:N	2.22	0.70
1:I:212:ARG:HE	1:I:215:ARG:HD3	1.57	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:HD13	1:I:77:LEU:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:206:ASN:O	1:G:207:ASP:HB2	1.91	0.69
1:J:116:PHE:HD1	1:J:120:ARG:O	1.75	0.69
1:J:219:SER:C	1:J:220:LEU:HD12	2.16	0.69
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:A:77:LEU:HD13	1:A:77:LEU:O	1.94	0.68
1:G:158:VAL:HG12	1:H:185:VAL:O	1.93	0.68
1:H:116:PHE:CD1	1:H:120:ARG:O	2.45	0.68
1:G:180:ALA:O	1:G:182:GLU:N	2.26	0.68
1:I:184:ARG:HD3	1:I:224:THR:HG21	1.75	0.68
1:K:165:ARG:HG2	1:K:165:ARG:NH1	2.08	0.68
1:G:221:LEU:HD23	1:G:221:LEU:O	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:I:221:LEU:HD23	1:I:221:LEU:C	2.19	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:H:97:PRO:CG	1:K:125:THR:HG23	2.24	0.67
1:J:138:GLY:O	1:J:155:PHE:CE1	2.48	0.67
1:A:120:ARG:NE	1:A:122:MET:HE2	2.10	0.67
1:K:235:LEU:HD13	1:K:237:PRO:HD3	1.72	0.67
1:L:219:SER:C	1:L:220:LEU:HD12	2.19	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:100:GLY:O	1:B:143:LEU:HD12	1.95	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: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:G:105:LEU:O	1:G:228:TYR:OH	2.14	0.66
1:H:219:SER:C	1:H:220:LEU:HD12	2.21	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:J:220:LEU:N	1:J:220:LEU:CD1	2.59	0.66
1:E:77:LEU:HD13	1:E:77:LEU:O	1.96	0.66
1:A:177:VAL:HG23	1:A:177:VAL:O	1.93	0.66
1:I:186:VAL:HG12	1:I:227:GLY:C	2.20	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:G:221:LEU:HD23	1:G:221:LEU:C	2.20	0.65
1:I:117:THR:O	1:I:119:GLY:N	2.29	0.65
1:A:139:GLN:HE21	1:A:152:ALA:HB1	1.59	0.65
1:G:62:ARG:HD2	1:H:63:ILE:HD11	1.78	0.65
1:I:124:LEU:HD11	1:I:143:LEU:CD2	2.25	0.65
1:J:116:PHE:CE2	1:J:226:ALA:HA	2.30	0.65
1:K:165:ARG:HB3	1:K:175:LEU:HD23	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:F:100:GLY:O	1:F:143:LEU:HD12	1.97	0.65
1:I:62:ARG:HD2	1:J:63:ILE:HD11	1.79	0.65
1:B:124:LEU:HD11	1:B:147:LEU:HB3	1.79	0.65
1:L:126:CYS:HB3	1:L:149:VAL:CG2	2.27	0.64
1:L:138:GLY:O	1:L:155:PHE:CE1	2.50	0.64
1:D:130:ILE:HD12	1:D:131:ASP:H	1.61	0.64
1:A:105:LEU:O	1:A:106:ALA:HB2	1.98	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: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:E:221:LEU:C	1:E:221:LEU:HD23	2.22	0.64
1:L:232:ARG:O	1:L:233:ILE:HG12	1.97	0.64
1:E:139:GLN:HE21	1:E:152:ALA:HB1	1.62	0.64
1:G:105:LEU:HD13	1:G:116:PHE:HB2	1.80	0.64
1:K:77:LEU:HD13	1:K:77:LEU:O	1.98	0.64
1:A:232:ARG:O	1:A:233:ILE:HD13	1.98	0.64
1:A:221:LEU:C	1:A:221:LEU:HD23	2.23	0.64
1:D:116:PHE:CE2	1:D:226:ALA:HA	2.33	0.64
1:I:235:LEU:CD1	1:I:237:PRO:HD3	2.28	0.64
1:J:154:THR:HG22	1:J:155:PHE:N	2.06	0.64
1:B:198:PRO:O	1:B:200:GLY:N	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:147:LEU:HD12	1:H:147:LEU:N	2.12	0.63
1:I:235:LEU:HD22	1:I:236:VAL:H	1.63	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
1:A:185:VAL:O	1:A:185:VAL:HG12	1.97	0.63
1:C:235:LEU:C	1:C:235:LEU:HD13	2.24	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: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:K:142:ARG:HD2	1:L:123:ARG:HD3	1.81	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:164:LEU:HD12	1:E:165:ARG:N	2.13	0.62
1:E:206:ASN:O	1:E:207:ASP:HB2	1.99	0.62
1:B:104:LEU:HD13	1:B:113:VAL:CG1	2.29	0.62
1:H:218:ASP:OD1	1:H:218:ASP:N	2.33	0.62
1:I:139:GLN:NE2	1:I:152:ALA:HB1	2.13	0.62
1:J:90:GLU:HA	1:J:93:ARG:HD3	1.81	0.62
1:K:164:LEU:HD12	1:K:164:LEU:C	2.24	0.62
1:F:104:LEU:HG	1:F:104:LEU:O	1.97	0.62
1:I:101:TYR:CE1	1:I:142:ARG:HG3	2.33	0.62
1:K:186:VAL:HG12	1:K:227:GLY:C	2.21	0.62
1:C:175:LEU:C	1:C:175:LEU:HD12	2.25	0.62
1:F:147:LEU:HD12	1:F:147:LEU:N	2.12	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:164:LEU:HD12	1:A:164:LEU:C	2.24	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: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:L:104:LEU:O	1:L:104:LEU:HG	2.00	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:E:168:LEU:HD22	1:E:169:ALA:H	1.65	0.61
1:F:219:SER:C	1:F:220:LEU:HD12	2.23	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:232:ARG:O	1:F:233:ILE:HG12	1.99	0.61
1:G:165:ARG:HG2	1:G:165:ARG:HH11	1.66	0.61
1:H:154:THR:CG2	1:H:155:PHE:H	2.07	0.61
1:A:158:VAL:HG12	1:B:185:VAL:O	2.00	0.61
1:B:138:GLY:O	1:B:155:PHE:CE1	2.53	0.61
1:D:116:PHE:HD1	1:D:120:ARG:O	1.82	0.61
1:H:90:GLU:HA	1:H:93:ARG:HD3	1.80	0.61
1:F:139:GLN:HB2	1:F:155:PHE:CE1	2.35	0.61
1:I:115:VAL:HG21	1:I:124:LEU:HD21	1.79	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: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:K:105:LEU:O	1:K:228:TYR:OH	2.18	0.61
1:A:125:THR:HG23	1:D:97:PRO:CG	2.30	0.61
1:K:62:ARG:HD2	1:L:63:ILE:HD11	1.83	0.61
1:L:220:LEU:N	1:L:220:LEU:CD1	2.60	0.61
1:I:235:LEU:HD13	1:I:237:PRO:HD3	1.82	0.61
1:A:177:VAL:O	1:A:177:VAL:CG2	2.48	0.61
1:C:220:LEU:HD12	1:C:229:ALA:HB1	1.81	0.61
1:I:189:ALA:N	1:I:192:LEU:HD12	2.15	0.61
1:B:154:THR:CG2	1:B:155:PHE:H	2.00	0.60
1:G:141:VAL:HG21	1:G:149:VAL:CG1	2.30	0.60
1:G:184:ARG:HD3	1:G:224:THR:HG21	1.83	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:A:108:HIS:C	1:A:110:ASP:H	2.09	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: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:K:235:LEU:HD22	1:K:236:VAL:N	2.16	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:120:ARG:HE	1:C:122:MET:HE3	1.59	0.60
1:A:117:THR:O	1:A:119:GLY:N	2.33	0.60
1:A:182:GLU:HB3	1:D:179:HIS:CD2	2.37	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:E:177:VAL:O	1:E:177:VAL:HG23	2.00	0.60
1:C:150:VAL:O	1:C:151:GLU:HB2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:ARG:HH11	1:E:165:ARG:HG2	1.65	0.60
1:E:235:LEU:C	1:E:235:LEU:HD13	2.25	0.60
1:C:139:GLN:NE2	1:C:152:ALA:HB1	2.17	0.59
1:H:110:ASP:OD1	1:H:110:ASP:O	2.21	0.59
1:C:120:ARG:NH2	1:C:122:MET:HE1	2.12	0.59
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:D:198:PRO:O	1:D:200:GLY:N	2.36	0.59
1:J:116:PHE:CD1	1:J:120:ARG:O	2.54	0.59
1:B:158:VAL:HG12	1:E:185:VAL:O	2.03	0.59
1:D:189:ALA:C	1:D:191:PRO:HD2	2.28	0.59
1:A:190:ASP:O	1:A:192:LEU:N	2.35	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: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:A:120:ARG:HH21	1:A:122:MET:HE1	1.68	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:C:141:VAL:HG21	1:C:149:VAL:CG1	2.34	0.58
1:K:105:LEU:HG	1:K:228:TYR:HE2	1.68	0.58
1:L:117:THR:O	1:L:118:SER:C	2.46	0.58
1:E:141:VAL:HG21	1:E:149:VAL:CG1	2.33	0.58
1:L:124:LEU:HD11	1:L:147:LEU:HB3	1.86	0.58
1:I:155:PHE:O	1:I:156:GLU:C	2.46	0.58
1:A:101:TYR:HD1	1:A:142:ARG:HA	1.69	0.58
1:G:105:LEU:HB2	1:G:114:ASP:O	2.03	0.58
1:C:189:ALA:O	1:C:190:ASP:C	2.46	0.57
1:K:108:HIS:C	1:K:110:ASP:H	2.11	0.57
1:B:122:MET:HE1	1:B:147:LEU:HD22	1.86	0.57
1:G:120:ARG:HH21	1:G:122:MET:HE1	1.68	0.57
1:B:220:LEU:N	1:B:220:LEU:CD1	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:105:LEU:O	1:E:228:TYR:OH	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:VAL:HG12	1:A:227:GLY:C	2.29	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:H:162:SER:HB2	1:H:176:VAL:HG12	1.86	0.57
1:F:210:ARG:HG2	1:F:211:PRO:HD2	1.85	0.57
1:G:168:LEU:HB2	1:G:173:ARG:O	2.04	0.57
1:D:219:SER:C	1:D:220:LEU:HD12	2.30	0.57
1:I:164:LEU:HD12	1:I:165:ARG:N	2.20	0.57
1:E:110:ASP:HB3	1:E:112:THR:HG23	1.87	0.57
1:I:168:LEU:HD22	1:I:169:ALA:H	1.70	0.57
1:L:154:THR:HG22	1:L:155:PHE:N	2.11	0.57
1:G:155:PHE:O	1:G:156:GLU:C	2.47	0.56
1:K:185:VAL:O	1:K:185:VAL:HG12	2.05	0.56
1:K:190:ASP:O	1:K:192:LEU:N	2.38	0.56
1:C:144:ASN:OD1	1:C:144:ASN:C	2.46	0.56
1:C:155:PHE:O	1:C:156:GLU:C	2.46	0.56
1:C:184:ARG:HD3	1:C:224:THR:CG2	2.35	0.56
1:L:116:PHE:CD2	1:L:226:ALA:HA	2.40	0.56
1:A:105:LEU:HG	1:A:228:TYR:HE2	1.71	0.56
1:H:198:PRO:O	1:H:200:GLY:N	2.39	0.56
1:K:220:LEU:HD23	1:K:220:LEU:H	1.70	0.56
1:C:168:LEU:O	1:C:169:ALA:C	2.48	0.56
1:I:127:SER:C	1:I:129:ASN:H	2.13	0.56
1:I:186:VAL:CG1	1:I:227:GLY:O	2.42	0.56
1:C:163:THR:O	1:C:176:VAL:HG12	2.06	0.56
1:H:138:GLY:O	1:H:155:PHE:CE1	2.58	0.56
1:B:172:HIS:O	1:B:188:LEU:HD12	2.04	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:124:LEU:HD21	1:B:147:LEU:O	2.05	0.56
1:E:94:LEU:HD11	1:F:128:PRO:HD2	1.88	0.55
1:F:99:SER:CB	1:F:142:ARG:HH11	2.18	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:J:139:GLN:HB2	1:J:155:PHE:HE1	1.71	0.55
1:C:141:VAL:HG21	1:C:149:VAL:HG13	1.89	0.55
1:I:177:VAL:HG23	1:I:177:VAL:O	2.06	0.55
1:G:124:LEU:HD11	1:G:143:LEU:HD21	1.88	0.55
1:H:117:THR:O	1:H:118:SER:C	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:GLN:HA	1:B:155:PHE:CE1	2.41	0.55
1:E:104:LEU:HD11	1:E:113:VAL:HG11	1.89	0.55
1:J:180:ALA:O	1:J:181:ASP:C	2.50	0.55
1:E:144:ASN:OD1	1:E:144:ASN:C	2.50	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:H:232:ARG:C	1:H:233:ILE:HG12	2.32	0.54
1:I:131:ASP:O	1:I:133:ALA:N	2.41	0.54
1:K:168:LEU:O	1:K:169:ALA:C	2.50	0.54
1:L:191:PRO:C	1:L:192:LEU:HD12	2.32	0.54
1:J:117:THR:O	1:J:118:SER:C	2.46	0.54
1:J:198:PRO:O	1:J:200:GLY:N	2.40	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:A:144:ASN:OD1	1:A:144:ASN:C	2.50	0.54
1:L:180:ALA:O	1:L:181:ASP:C	2.51	0.54
1:C:142:ARG:HD2	1:D:123:ARG:HD3	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:I:175:LEU:HD12	1:I:175:LEU:C	2.33	0.54
1:C:73:LEU:O	1:C:74:MET:C	2.50	0.54
1:E:190:ASP:O	1:E:192:LEU:N	2.41	0.54
1:E:73:LEU:O	1:E:74:MET:C	2.49	0.54
1:K:117:THR:C	1:K:119:GLY:H	2.16	0.54
1:A:73:LEU:O	1:A:74:MET:C	2.50	0.54
1:D:172:HIS:O	1:D:188:LEU:HD12	2.08	0.54
1:K:221:LEU:HD23	1:K:221:LEU:O	2.08	0.54
1:A:168:LEU:O	1:A:169:ALA:C	2.50	0.53
1:E:164:LEU:HD12	1:E:164:LEU:C	2.33	0.53
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:I:144:ASN:C	1:I:144:ASN:OD1	2.49	0.53
1:A:189:ALA:O	1:A:190:ASP:C	2.50	0.53
1:E:155:PHE:O	1:E:156:GLU:C	2.51	0.53
1:E:182:GLU:O	1:E:182:GLU:HG3	2.06	0.53
1:C:126:CYS:HB3	1:C:130:ILE:HD11	1.89	0.53
1:E:103:VAL:O	1:E:115:VAL:HG12	2.07	0.53
1:J:189:ALA:C	1:J:191:PRO:HD2	2.34	0.53
1:B:153:GLY:O	1:B:154:THR:O	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:124:LEU:N	1:I:124:LEU:HD23	2.24	0.53
1:J:104:LEU:HG	1:J:104:LEU:O	2.08	0.53
1:G:165:ARG:HG2	1:G:165:ARG:NH1	2.20	0.53
1:A:62:ARG:HD2	1:B:63:ILE:HD11	1.91	0.53
1:C:185:VAL:O	1:C:185:VAL:HG12	2.09	0.53
1:D:113:VAL:O	1:D:123:ARG:HA	2.08	0.53
1:I:189:ALA:H	1:I:192:LEU:CD1	2.21	0.53
1:J:110:ASP:OD1	1:J:110:ASP:O	2.26	0.53
1:K:164:LEU:HD12	1:K:165:ARG:H	1.74	0.53
1:F:191:PRO:C	1:F:192:LEU:HD12	2.33	0.53
1:F:220:LEU:N	1:F:220:LEU:CD1	2.70	0.53
1:G:189:ALA:O	1:G:190:ASP:C	2.52	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:207:ASP:OD1	1:B:209:THR:CG2	2.57	0.53
1:K:57:HIS:O	1:K:58:GLN:C	2.52	0.53
1:D:154:THR:CG2	1:D:155:PHE:N	2.65	0.53
1:E:124:LEU:HD23	1:E:124:LEU:N	2.24	0.53
1:K:167:ILE:HG22	1:K:168:LEU:H	1.74	0.53
1:I:235:LEU:HD22	1:I:236:VAL:N	2.24	0.52
1:C:182:GLU:HB3	1:F:179:HIS:CD2	2.43	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
1:C:131:ASP:O	1:C:133:ALA:N	2.42	0.52
1:G:144:ASN:C	1:G:144:ASN:OD1	2.51	0.52
1:I:185:VAL:O	1:I:185:VAL:HG12	2.10	0.52
1:J:137:LYS:HB2	1:J:190:ASP:OD2	2.08	0.52
1:I:190:ASP:O	1:I:192:LEU:N	2.41	0.52
1:D:191:PRO:C	1:D:192:LEU:HD12	2.34	0.52
1:E:105:LEU:HG	1:E:228:TYR:HE2	1.75	0.52
1:H:220:LEU:N	1:H:220:LEU:CD1	2.65	0.52
1:I:105:LEU:HD13	1:I:116:PHE:HB2	1.90	0.52
1:A:141:VAL:HG21	1:A:149:VAL:CG1	2.40	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:A:165:ARG:HG2	1:A:165:ARG:HH11	1.75	0.52
1:D:116:PHE:CD2	1:D:226:ALA:HA	2.45	0.52
1:I:116:PHE:CZ	1:I:225:LYS:O	2.63	0.52
1:J:232:ARG:O	1:J:233:ILE:HG12	2.10	0.52
1:E:131:ASP:O	1:E:133:ALA:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:TYR:CE1	1:A:142:ARG:HG3	2.45	0.52
1:C:117:THR:HG23	1:C:118:SER:H	1.75	0.52
1:F:180:ALA:O	1:F:181:ASP:C	2.50	0.52
1:I:142:ARG:HH11	1:J:123:ARG:HD3	1.74	0.52
1:K:144:ASN:C	1:K:144:ASN:OD1	2.51	0.52
1:K:220:LEU:HD23	1:K:220:LEU:N	2.24	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:G:73:LEU:O	1:G:74:MET:C	2.51	0.52
1:A:56:ILE:O	1:A:56:ILE:CG2	2.57	0.51
1:B:99:SER:CB	1:B:142:ARG:HH11	2.23	0.51
1:B:189:ALA:C	1:B:191:PRO:HD2	2.35	0.51
1:E:56:ILE:O	1:E:56:ILE:CG2	2.58	0.51
1:K:189:ALA:O	1:K:190:ASP:C	2.53	0.51
1:L:104:LEU:HD13	1:L:113:VAL:HG11	1.91	0.51
1:I:182:GLU:HB3	1:L:179:HIS:CD2	2.45	0.51
1:D:110:ASP:O	1:D:110:ASP:OD1	2.29	0.51
1:I:168:LEU:O	1:I:169:ALA:C	2.53	0.51
1:F:148:THR:O	1:F:148:THR:HG22	2.10	0.51
1:A:127:SER:O	1:A:128:PRO:C	2.54	0.51
1:E:101:TYR:HD1	1:E:142:ARG:HA	1.75	0.51
1:G:174:ALA:O	1:G:185:VAL:HA	2.10	0.51
1:H:104:LEU:HG	1:H:104:LEU:O	2.10	0.51
1:I:221:LEU:HD23	1:I:221:LEU:O	2.10	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:F:105:LEU:N	1:F:114:ASP:O	2.43	0.51
1:I:231:GLU:HG3	1:I:232:ARG:N	2.26	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:E:168:LEU:O	1:E:169:ALA:C	2.54	0.51
1:H:191:PRO:C	1:H:192:LEU:HD12	2.36	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:H:179:HIS:CD2	1:K:182:GLU:HB3	2.46	0.50
1:I:108:HIS:HB2	1:I:112:THR:O	2.10	0.50
1:D:180:ALA:O	1:D:181:ASP:C	2.54	0.50
1:I:105:LEU:O	1:I:106:ALA:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:190:ASP:C	1:I:192:LEU:H	2.19	0.50
1:K:184:ARG:HD3	1:K:224:THR:HG21	1.93	0.50
1:B:105:LEU:N	1:B:114:ASP:O	2.44	0.50
1:B:110:ASP:O	1:B:111:ASP:HB2	2.11	0.50
1:B:147:LEU:HD12	1:B:147:LEU:H	1.75	0.50
1:B:186:VAL:HG12	1:B:227:GLY:C	2.35	0.50
1:F:117:THR:O	1:F:118:SER:C	2.55	0.50
1:I:73:LEU:O	1:I:74:MET:C	2.53	0.50
1:K:168:LEU:HD22	1:K:169:ALA:H	1.77	0.50
1:D:190:ASP:N	1:D:191:PRO:CD	2.74	0.50
1:H:126:CYS:HB3	1:H:149:VAL:CG2	2.42	0.50
1:I:105:LEU:O	1:I:228:TYR:OH	2.28	0.50
1:I:124:LEU:HD11	1:I:143:LEU:HD22	1.93	0.50
1:I:158:VAL:HG12	1:J:185:VAL:O	2.11	0.50
1:C:56:ILE:O	1:C:56:ILE:CG2	2.59	0.50
1:G:167:ILE:HD12	1:G:167:ILE:H	1.76	0.50
1:H:139:GLN:HA	1:H:155:PHE:CE1	2.47	0.50
1:I:115:VAL:CG2	1:I:124:LEU:CD2	2.77	0.50
1:L:198:PRO:O	1:L:200:GLY:N	2.45	0.50
1:C:59:LEU:C	1:C:61:ALA:H	2.19	0.50
1:E:62:ARG:HD2	1:F:63:ILE:HD11	1.93	0.50
1:G:170:ASP:OD2	1:G:170:ASP:N	2.43	0.50
1:I:56:ILE:CG2	1:I:56:ILE:O	2.60	0.50
1:K:221:LEU:C	1:K:221:LEU:CD2	2.79	0.50
1:A:230:PHE:O	1:A:231:GLU:HB3	2.11	0.50
1:B:230:PHE:O	1:B:231:GLU:HB3	2.12	0.50
1:E:235:LEU:HD11	1:E:237:PRO:HD3	1.94	0.50
1:F:232:ARG:C	1:F:233:ILE:HG12	2.36	0.50
1:G:62:ARG:HD2	1:H:63:ILE:CD1	2.42	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:A:190:ASP:C	1:A:192:LEU:H	2.20	0.50
1:C:127:SER:C	1:C:129:ASN:H	2.14	0.50
1:H:99:SER:CB	1:H:142:ARG:HH11	2.24	0.50
1:I:57:HIS:O	1:I:58:GLN:C	2.55	0.50
1:A:155:PHE:O	1:A:156:GLU:C	2.55	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:73:LEU:O	1:K:74:MET:C	2.53	0.50
1:G:131:ASP:O	1:G:133:ALA:N	2.45	0.49
1:K:56:ILE:CG2	1:K:56:ILE:O	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:VAL:CG2	1:E:149:VAL:CG1	2.90	0.49
1:K:124:LEU:HD11	1:K:143:LEU:HD22	1.93	0.49
1:A:94:LEU:HD11	1:B:128:PRO:HD2	1.94	0.49
1:A:120:ARG:HE	1:A:122:MET:CE	2.22	0.49
1:A:235:LEU:HD22	1:A:236:VAL:N	2.27	0.49
1:G:116:PHE:CZ	1:G:225:LYS:O	2.66	0.49
1:H:189:ALA:C	1:H:191:PRO:HD2	2.38	0.49
1:I:115:VAL:HG22	1:I:124:LEU:CD2	2.41	0.49
1:E:124:LEU:HD11	1:E:143:LEU:HD22	1.95	0.49
1:H:110:ASP:O	1:H:111:ASP:HB2	2.11	0.49
1:J:124:LEU:HD11	1:J:147:LEU:HB3	1.94	0.49
1:J:153:GLY:O	1:J:154:THR:O	2.30	0.49
1:E:186:VAL:HG12	1:E:227:GLY:C	2.35	0.49
1:F:110:ASP:OD1	1:F:110:ASP:O	2.30	0.49
1:H:147:LEU:H	1:H:147:LEU:CD1	2.24	0.49
1:K:127:SER:C	1:K:129:ASN:H	2.21	0.49
1:H:100:GLY:O	1:H:143:LEU:HD12	2.12	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:I:165:ARG:HG2	1:I:165:ARG:NH1	2.28	0.49
1:L:124:LEU:HD21	1:L:147:LEU:O	2.13	0.49
1:L:210:ARG:HG2	1:L:211:PRO:HD2	1.95	0.49
1:A:164:LEU:HA	1:A:176:VAL:HG12	1.93	0.49
1:D:190:ASP:HB2	1:D:191:PRO:HD3	1.95	0.49
1:E:165:ARG:HG2	1:E:165:ARG:NH1	2.27	0.49
1:G:187:TRP:O	1:G:228:TYR:HA	2.12	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:K:103:VAL:O	1:K:115:VAL:HG12	2.13	0.49
1:L:85:LEU:HD23	1:L:85:LEU:O	2.12	0.49
1:C:62:ARG:HD2	1:D:63:ILE:HD11	1.95	0.49
1:E:189:ALA:H	1:E:192:LEU:CD1	2.25	0.49
1:L:122:MET:HE1	1:L:147:LEU:HD22	1.95	0.49
1:A:155:PHE:CE2	1:A:191:PRO:HG2	2.48	0.48
1:C:124:LEU:HD23	1:C:124:LEU:N	2.28	0.48
1:D:99:SER:HB2	1:D:142:ARG:HH11	1.78	0.48
1:D:104:LEU:HD13	1:D:113:VAL:HG11	1.95	0.48
1:F:85:LEU:O	1:F:85:LEU:HD23	2.13	0.48
1:G:124:LEU:N	1:G:124:LEU:HD23	2.28	0.48
1:H:191:PRO:HB2	1:H:192:LEU:HD12	1.95	0.48
1:L:110:ASP:O	1:L:110:ASP:OD1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LEU:HD11	1:A:143:LEU:HD22	1.94	0.48
1:G:168:LEU:O	1:G:169:ALA:C	2.56	0.48
1:G:177:VAL:HG23	1:G:177:VAL:O	2.13	0.48
1:H:85:LEU:O	1:H:85:LEU:HD23	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:I:108:HIS:C	1:I:110:ASP:H	2.21	0.48
1:A:57:HIS:O	1:A:58:GLN:C	2.57	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:184:ARG:CD	1:I:224:THR:HG22	2.41	0.48
1:L:139:GLN:HA	1:L:155:PHE:CE1	2.48	0.48
1:A:206:ASN:O	1:A:207:ASP:HB2	2.12	0.48
1:I:127:SER:C	1:I:129:ASN:N	2.70	0.48
1:C:105:LEU:HD13	1:C:116:PHE:HB2	1.95	0.48
1:C:135:LEU:H	1:C:135:LEU:CD2	2.26	0.48
1:C:187:TRP:O	1:C:228:TYR:HA	2.13	0.48
1:D:85:LEU:O	1:D:85:LEU:HD23	2.14	0.48
1:E:189:ALA:N	1:E:192:LEU:HD12	2.25	0.48
1:G:57:HIS:O	1:G:58:GLN:C	2.55	0.48
1:I:123:ARG:NH1	1:L:151:GLU:OE1	2.46	0.48
1:J:85:LEU:HD23	1:J:85:LEU:O	2.13	0.48
1:D:100:GLY:O	1:D:143:LEU:HD12	2.12	0.48
1:D:128:PRO:O	1:D:130:ILE:N	2.47	0.48
1:D:220:LEU:N	1:D:220:LEU:CD1	2.75	0.48
1:E:141:VAL:HG21	1:E:149:VAL:HG13	1.95	0.48
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:E:168:LEU:HD22	1:E:169:ALA:N	2.29	0.48
1:H:103:VAL:O	1:H:116:PHE:N	2.42	0.48
1:C:221:LEU:CD2	1:C:230:PHE:HB2	2.41	0.48
1:E:190:ASP:C	1:E:192:LEU:H	2.21	0.48
1:L:124:LEU:HD23	1:L:125:THR:H	1.79	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:D:139:GLN:HA	1:D:155:PHE:CE1	2.48	0.48
1:E:158:VAL:HG12	1:F:185:VAL:O	2.14	0.48
1:E:177:VAL:O	1:E:177:VAL:CG2	2.61	0.48
1:I:222:VAL:HG23	1:I:223:ASP:N	2.29	0.48
1:K:59:LEU:C	1:K:61:ALA:H	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:69:ARG:O	1:L:73:LEU:HG	2.13	0.48
1:C:59:LEU:O	1:C:61:ALA:N	2.46	0.47
1:C:235:LEU:HD22	1:C:236:VAL:N	2.29	0.47
1:E:59:LEU:C	1:E:61:ALA:H	2.21	0.47
1:E:59:LEU:C	1:E:61:ALA:N	2.72	0.47
1:G:84:LEU:HD13	1:G:84:LEU:O	2.14	0.47
1:G:124:LEU:HD11	1:G:143:LEU:HD22	1.93	0.47
1:G:168:LEU:HD12	1:G:173:ARG:HB2	1.96	0.47
1:H:130:ILE:HD12	1:H:130:ILE:HA	1.75	0.47
1:K:222:VAL:HG23	1:K:223:ASP:N	2.29	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:A:108:HIS:C	1:A:110:ASP:N	2.72	0.47
1:A:165:ARG:HG2	1:A:165:ARG:NH1	2.29	0.47
1:C:115:VAL:HG21	1:C:124:LEU:HD21	1.89	0.47
1:E:57:HIS:O	1:E:58:GLN:C	2.56	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:A:218:ASP:OD2	1:A:232:ARG:NH1	2.47	0.47
1:B:137:LYS:HB2	1:B:190:ASP:OD2	2.13	0.47
1:C:59:LEU:C	1:C:61:ALA:N	2.71	0.47
1:C:113:VAL:O	1:C:123:ARG:HA	2.13	0.47
1:G:59:LEU:C	1:G:61:ALA:H	2.23	0.47
1:G:141:VAL:CG2	1:G:149:VAL:CG1	2.92	0.47
1:K:59:LEU:C	1:K:61:ALA:N	2.72	0.47
1:K:155:PHE:O	1:K:156:GLU:C	2.58	0.47
1:E:74:MET:O	1:E:74:MET:HE3	2.14	0.47
1:G:150:VAL:O	1:G:151:GLU:HB2	2.14	0.47
1:I:212:ARG:HG3	1:I:213:LYS:O	2.15	0.47
1:K:100:GLY:O	1:K:143:LEU:N	2.48	0.47
1:B:116:PHE:HE1	1:B:119:GLY:C	2.23	0.47
1:B:176:VAL:HG21	1:B:186:VAL:HG22	1.95	0.47
1:I:59:LEU:C	1:I:61:ALA:H	2.23	0.47
1:B:210:ARG:HG2	1:B:211:PRO:CD	2.45	0.47
1:D:186:VAL:HB	1:D:227:GLY:O	2.14	0.47
1:E:141:VAL:CG2	1:E:149:VAL:HG13	2.45	0.47
1:G:56:ILE:CG2	1:G:56:ILE:O	2.62	0.47
1:G:176:VAL:CG2	1:G:186:VAL:CG2	2.93	0.47
1:H:124:LEU:HD23	1:H:124:LEU:HA	1.61	0.47
1:I:200:GLY:O	1:I:201:LEU:HB2	2.14	0.47
1:J:100:GLY:O	1:J:143:LEU:HD12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:139:GLN:HB2	1:J:155:PHE:CE1	2.50	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:L:189:ALA:C	1:L:191:PRO:HD2	2.40	0.47
1:E:59:LEU:O	1:E:61:ALA:N	2.48	0.47
1:G:175:LEU:CD2	1:J:235:LEU:HD12	2.36	0.47
1:G:222:VAL:HG23	1:G:223:ASP:N	2.30	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:A:180:ALA:O	1:A:182:GLU:N	2.47	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:C:99:SER:HB2	1:D:123:ARG:HB3	1.96	0.47
1:C:120:ARG:NH2	1:C:122:MET:CE	2.73	0.47
1:L:124:LEU:HD23	1:L:124:LEU:HA	1.67	0.47
1:D:124:LEU:HD21	1:D:147:LEU:O	2.14	0.46
1:G:66:LEU:O	1:G:69:ARG:N	2.43	0.46
1:H:186:VAL:HG12	1:H:227:GLY:O	2.13	0.46
1:K:231:GLU:HG3	1:K:232:ARG:N	2.31	0.46
1:C:57:HIS:O	1:C:58:GLN:C	2.58	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:J:191:PRO:HB2	1:J:192:LEU:HD12	1.97	0.46
1:K:190:ASP:C	1:K:192:LEU:H	2.23	0.46
1:K:221:LEU:CD2	1:K:230:PHE:HB2	2.45	0.46
1:B:214:LEU:HD12	1:B:215:ARG:H	1.81	0.46
1:D:128:PRO:C	1:D:130:ILE:H	2.23	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:G:235:LEU:HD13	1:G:235:LEU:C	2.40	0.46
1:H:72:LYS:O	1:H:76:THR:HG23	2.15	0.46
1:I:84:LEU:HD13	1:I:84:LEU:O	2.16	0.46
1:I:137:LYS:HB2	1:I:190:ASP:OD1	2.16	0.46
1:K:66:LEU:O	1:K:68:ALA:N	2.48	0.46
1:K:202:PRO:O	1:K:203:GLU:CB	2.60	0.46
1:C:66:LEU:O	1:C:68:ALA:N	2.49	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:A:59:LEU:C	1:A:61:ALA:N	2.73	0.46
1:A:131:ASP:O	1:A:133:ALA:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:HIS:C	1:B:188:LEU:HD12	2.41	0.46
1:B:190:ASP:N	1:B:191:PRO:HD2	2.31	0.46
1:C:74:MET:HE3	1:C:74:MET:O	2.15	0.46
1:F:136:LYS:N	1:F:139:GLN:OE1	2.38	0.46
1:I:100:GLY:O	1:I:143:LEU:N	2.45	0.46
1:A:221:LEU:C	1:A:222:VAL:HG12	2.41	0.46
1:B:106:ALA:H	1:B:114:ASP:HB2	1.81	0.46
1:E:189:ALA:O	1:E:190:ASP:C	2.57	0.46
1:F:124:LEU:HA	1:F:124:LEU:HD23	1.67	0.46
1:G:66:LEU:O	1:G:68:ALA:N	2.49	0.46
1:G:100:GLY:O	1:G:143:LEU:N	2.47	0.46
1:I:62:ARG:HD2	1:J:63:ILE:CD1	2.44	0.46
1:I:212:ARG:NE	1:I:215:ARG:HD3	2.28	0.46
1:L:99:SER:CB	1:L:142:ARG:HH11	2.28	0.46
1:A:59:LEU:C	1:A:61:ALA:H	2.23	0.46
1:A:74:MET:HE3	1:A:74:MET:O	2.15	0.46
1:A:105:LEU:N	1:A:114:ASP:O	2.45	0.46
1:B:113:VAL:O	1:B:123:ARG:HA	2.16	0.46
1:D:127:SER:HA	1:D:128:PRO:HD2	1.70	0.46
1:D:189:ALA:O	1:D:190:ASP:C	2.58	0.46
1:E:168:LEU:HD23	1:E:168:LEU:HA	1.74	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:72:LYS:O	1:J:76:THR:HG23	2.16	0.46
1:J:106:ALA:H	1:J:114:ASP:HB2	1.80	0.46
1:J:190:ASP:N	1:J:191:PRO:HD2	2.31	0.46
1:K:113:VAL:O	1:K:123:ARG:HA	2.16	0.46
1:K:127:SER:C	1:K:129:ASN:N	2.73	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:B:110:ASP:O	1:B:110:ASP:OD1	2.32	0.46
1:B:155:PHE:O	1:B:156:GLU:C	2.57	0.46
1:G:176:VAL:HG21	1:G:186:VAL:HG21	1.98	0.46
1:H:127:SER:HA	1:H:128:PRO:HD2	1.73	0.46
1:A:233:ILE:HA	1:A:234:PRO:HD2	1.63	0.46
1:I:59:LEU:C	1:I:61:ALA:N	2.73	0.46
1:I:233:ILE:HA	1:I:234:PRO:HD2	1.57	0.46
1:K:137:LYS:HB2	1:K:190:ASP:OD1	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:ASN:O	1:C:207:ASP:HB2	2.16	0.45
1:D:212:ARG:HG3	1:D:213:LYS:O	2.16	0.45
1:J:130:ILE:HD12	1:J:130:ILE:HA	1.77	0.45
1:K:66:LEU:O	1:K:69:ARG:N	2.44	0.45
1:K:206:ASN:O	1:K:207:ASP:CB	2.63	0.45
1:B:128:PRO:O	1:B:130:ILE:N	2.50	0.45
1:C:100:GLY:O	1:C:143:LEU:N	2.47	0.45
1:A:141:VAL:CG2	1:A:149:VAL:CG1	2.95	0.45
1:B:128:PRO:C	1:B:130:ILE:H	2.24	0.45
1:C:66:LEU:O	1:C:69:ARG:N	2.45	0.45
1:C:158:VAL:HA	1:D:185:VAL:HG12	1.98	0.45
1:D:162:SER:HB2	1:D:176:VAL:HG12	1.98	0.45
1:D:207:ASP:OD1	1:D:209:THR:HG22	2.17	0.45
1:E:113:VAL:O	1:E:123:ARG:HA	2.17	0.45
1:F:214:LEU:HD12	1:F:214:LEU:HA	1.46	0.45
1:I:187:TRP:O	1:I:228:TYR:HA	2.16	0.45
1:L:105:LEU:N	1:L:114:ASP:O	2.46	0.45
1:L:233:ILE:HA	1:L:234:PRO:HD2	1.83	0.45
1:A:120:ARG:HH21	1:A:122:MET:CE	2.27	0.45
1:E:124:LEU:HD11	1:E:143:LEU:HD21	1.98	0.45
1:E:235:LEU:CD1	1:E:237:PRO:HD3	2.47	0.45
1:H:69:ARG:O	1:H:73:LEU:HG	2.15	0.45
1:K:184:ARG:HD3	1:K:224:THR:CG2	2.46	0.45
1:A:66:LEU:O	1:A:69:ARG:N	2.46	0.45
1:E:201:LEU:HB3	1:E:202:PRO:CD	2.46	0.45
1:G:151:GLU:HG2	1:G:152:ALA:O	2.17	0.45
1:J:104:LEU:HD13	1:J:113:VAL:HG11	1.97	0.45
1:C:127:SER:C	1:C:129:ASN:N	2.74	0.45
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:B:236:VAL:HA	1:B:237:PRO:HD3	1.79	0.45
1:F:104:LEU:HD13	1:F:113:VAL:HG11	1.99	0.45
1:F:110:ASP:O	1:F:111:ASP:HB2	2.16	0.45
1:G:233:ILE:HA	1:G:234:PRO:HD2	1.48	0.45
1:J:124:LEU:HD21	1:J:147:LEU:O	2.16	0.45
1:K:108:HIS:C	1:K:110:ASP:N	2.75	0.45
1:D:235:LEU:HD23	1:D:237:PRO:HG3	1.98	0.45
1:F:136:LYS:O	1:F:139:GLN:HB3	2.17	0.45
1:I:97:PRO:HG3	1:I:145:GLU:OE1	2.17	0.45
1:J:113:VAL:O	1:J:123:ARG:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:54:ARG:O	1:K:55:ASP:C	2.59	0.45
1:K:120:ARG:HE	1:K:122:MET:CE	2.18	0.45
1:C:164:LEU:HD12	1:C:164:LEU:C	2.40	0.45
1:D:117:THR:O	1:D:118:SER:C	2.59	0.45
1:F:154:THR:HG22	1:F:155:PHE:N	2.19	0.45
1:I:164:LEU:HD12	1:I:164:LEU:C	2.39	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:180:ALA:O	1:E:181:ASP:C	2.59	0.44
1:I:66:LEU:O	1:I:69:ARG:N	2.45	0.44
1:L:232:ARG:C	1:L:233:ILE:HG12	2.42	0.44
1:C:141:VAL:CG2	1:C:149:VAL:CG1	2.95	0.44
1:D:137:LYS:HB2	1:D:190:ASP:OD2	2.17	0.44
1:F:139:GLN:HA	1:F:155:PHE:CE1	2.53	0.44
1:G:155:PHE:CE2	1:G:191:PRO:HG2	2.52	0.44
1:H:139:GLN:HB2	1:H:155:PHE:HE1	1.82	0.44
1:K:94:LEU:HD11	1:L:128:PRO:HD2	1.99	0.44
1:A:141:VAL:CG2	1:A:149:VAL:HG13	2.47	0.44
1:A:208:ASP:O	1:A:210:ARG:N	2.50	0.44
1:B:176:VAL:CG2	1:B:186:VAL:HG22	2.47	0.44
1:E:184:ARG:CD	1:E:224:THR:HG22	2.47	0.44
1:H:144:ASN:OD1	1:H:146:ALA:O	2.35	0.44
1:A:105:LEU:O	1:A:106:ALA:CB	2.63	0.44
1:E:184:ARG:NE	1:E:224:THR:HG22	2.32	0.44
1:F:130:ILE:HD12	1:F:131:ASP:H	1.82	0.44
1:G:225:LYS:HE2	1:G:225:LYS:HB2	1.65	0.44
1:L:212:ARG:HG3	1:L:213:LYS:O	2.17	0.44
1:A:101:TYR:CD1	1:A:142:ARG:HA	2.52	0.44
1:C:105:LEU:HG	1:C:228:TYR:HE2	1.82	0.44
1:C:189:ALA:H	1:C:192:LEU:CD1	2.27	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:F:153:GLY:O	1:F:154:THR:O	2.35	0.44
1:G:176:VAL:CG2	1:G:186:VAL:HG21	2.48	0.44
1:I:66:LEU:O	1:I:68:ALA:N	2.51	0.44
1:I:225:LYS:HB2	1:I:225:LYS:HE2	1.56	0.44
1:A:66:LEU:O	1:A:68:ALA:N	2.51	0.44
1:H:189:ALA:O	1:H:191:PRO:N	2.51	0.44
1:J:190:ASP:N	1:J:191:PRO:CD	2.80	0.44
1:K:117:THR:C	1:K:119:GLY:N	2.74	0.44
1:A:139:GLN:HB3	1:A:155:PHE:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LYS:HE2	1:A:225:LYS:HB2	1.28	0.44
1:C:108:HIS:C	1:C:110:ASP:H	2.25	0.44
1:I:54:ARG:O	1:I:55:ASP:C	2.61	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:C:139:GLN:HA	1:C:155:PHE:CE1	2.53	0.43
1:D:193:ILE:O	1:D:194:ALA:C	2.61	0.43
1:E:63:ILE:O	1:E:65:SER:N	2.51	0.43
1:E:223:ASP:HB2	1:E:230:PHE:HE2	1.83	0.43
1:G:59:LEU:C	1:G:61:ALA:N	2.74	0.43
1:K:104:LEU:HD11	1:K:113:VAL:HG11	1.99	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: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: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:K:117:THR:O	1:K:119:GLY:N	2.45	0.43
1:L:139:GLN:HA	1:L:155:PHE:HE1	1.84	0.43
1:H:164:LEU:HA	1:H:176:VAL:HA	1.99	0.43
1:I:164:LEU:HB2	1:I:220:LEU:CD2	2.49	0.43
1:B:104:LEU:HA	1:B:115:VAL:HG12	2.01	0.43
1:C:225:LYS:HE2	1:C:225:LYS:HB2	1.27	0.43
1:H:117:THR:O	1:H:119:GLY:N	2.51	0.43
1:I:217:GLY:O	1:I:218:ASP:C	2.60	0.43
1:J:117:THR:O	1:J:119:GLY:N	2.51	0.43
1:C:139:GLN:CB	1:C:155:PHE:HE1	2.31	0.43
1:C:141:VAL:HG23	1:C:142:ARG:N	2.33	0.43
1:C:168:LEU:HD23	1:C:168:LEU:HA	1.74	0.43
1:E:100:GLY:O	1:E:143:LEU:N	2.49	0.43
1:E:136:LYS:N	1:E:139:GLN:OE1	2.35	0.43
1:H:104:LEU:C	1:H:104:LEU:HD12	2.44	0.43
1:I:220:LEU:CD1	1:I:229:ALA:CB	2.97	0.43
1:A:164:LEU:HB2	1:A:220:LEU:CD2	2.48	0.43
1:D:164:LEU:HD12	1:D:220:LEU:HD11	2.00	0.43
1:F:128:PRO:O	1:F:130:ILE:N	2.52	0.43
1:F:139:GLN:NE2	1:F:152:ALA:HB1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:139:GLN:HA	1:I:155:PHE:CE1	2.54	0.43
1:A:221:LEU:HD22	1:A:230:PHE:HB2	2.01	0.43
1:B:105:LEU:HD13	1:B:116:PHE:HB2	2.01	0.43
1:C:175:LEU:C	1:C:175:LEU:CD1	2.92	0.43
1:G:122:MET:HE3	1:G:147:LEU:HD22	2.00	0.43
1:I:108:HIS:C	1:I:110:ASP:N	2.77	0.43
1:J:69:ARG:O	1:J:73:LEU:HG	2.17	0.43
1:B:180:ALA:O	1:B:181:ASP:C	2.61	0.43
1:F:127:SER:HA	1:F:128:PRO:HD2	1.78	0.43
1:F:171:GLY:O	1:F:193:ILE:HG21	2.19	0.43
1:F:233:ILE:HA	1:F:234:PRO:HD2	1.87	0.43
1:G:127:SER:C	1:G:129:ASN:N	2.77	0.43
1:G:139:GLN:HA	1:G:155:PHE:CE1	2.54	0.43
1:J:191:PRO:C	1:J:192:LEU:HD12	2.44	0.43
1:A:58:GLN:HE22	1:I:235:LEU:CG	2.28	0.42
1:A:141:VAL:HG21	1:A:149:VAL:HG13	2.00	0.42
1:C:120:ARG:CZ	1:C:122:MET:CE	2.97	0.42
1:E:62:ARG:HD2	1:F:63:ILE:CD1	2.49	0.42
1:E:101:TYR:CD1	1:E:142:ARG:HA	2.54	0.42
1:H:189:ALA:O	1:H:190:ASP:C	2.61	0.42
1:J:147:LEU:HD12	1:J:147:LEU:N	2.35	0.42
1:J:172:HIS:C	1:J:188:LEU:HD12	2.45	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:D:191:PRO:HB2	1:D:192:LEU:HD12	2.00	0.42
1:E:117:THR:HG23	1:E:118:SER:H	1.83	0.42
1:E:187:TRP:O	1:E:228:TYR:HA	2.19	0.42
1:F:96:GLN:HA	1:F:97:PRO:HD2	1.82	0.42
1:F:162:SER:HB2	1:F:176:VAL:HG12	2.01	0.42
1:F:191:PRO:HB2	1:F:192:LEU:HD12	2.01	0.42
1:G:142:ARG:HD2	1:H:123:ARG:HD3	2.00	0.42
1:H:154:THR:CG2	1:H:155:PHE:N	2.80	0.42
1:H:162:SER:HB3	1:H:178:GLY:CA	2.41	0.42
1:H:210:ARG:HG2	1:H:211:PRO:HD3	2.01	0.42
1:H:222:VAL:HA	1:H:228:TYR:O	2.19	0.42
1:K:131:ASP:O	1:K:133:ALA:N	2.52	0.42
1:B:155:PHE:HE2	1:B:191:PRO:CG	2.15	0.42
1:C:221:LEU:C	1:C:222:VAL:HG12	2.44	0.42
1:F:125:THR:O	1:F:148:THR:HA	2.19	0.42
1:H:164:LEU:HD22	1:H:164:LEU:C	2.44	0.42
1:J:225:LYS:HD2	1:J:225:LYS:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ASN:O	1:A:207:ASP:CB	2.67	0.42
1:B:117:THR:O	1:B:118:SER:C	2.60	0.42
1:B:147:LEU:N	1:B:147:LEU:CD1	2.82	0.42
1:C:221:LEU:C	1:C:221:LEU:CD2	2.84	0.42
1:E:184:ARG:CD	1:E:224:THR:CG2	2.93	0.42
1:G:200:GLY:O	1:G:201:LEU:HB2	2.18	0.42
1:I:222:VAL:CG2	1:I:223:ASP:N	2.77	0.42
1:A:100:GLY:O	1:A:143:LEU:N	2.51	0.42
1:B:214:LEU:HD12	1:B:214:LEU:HA	1.64	0.42
1:C:139:GLN:HB3	1:C:155:PHE:CE1	2.54	0.42
1:E:176:VAL:HG21	1:E:186:VAL:HG21	2.02	0.42
1:F:69:ARG:O	1:F:73:LEU:HG	2.19	0.42
1:I:105:LEU:CD1	1:I:116:PHE:HB2	2.48	0.42
1:I:141:VAL:HG21	1:I:149:VAL:HG13	2.01	0.42
1:I:168:LEU:HD22	1:I:169:ALA:N	2.32	0.42
1:J:232:ARG:C	1:J:233:ILE:HG12	2.45	0.42
1:K:99:SER:HB2	1:L:123:ARG:HB3	2.01	0.42
1:A:63:ILE:O	1:A:65:SER:N	2.53	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:124:LEU:N	1:A:124:LEU:HD23	2.34	0.42
1:A:131:ASP:HB3	1:A:134:SER:OG	2.19	0.42
1:B:130:ILE:HD12	1:B:131:ASP:H	1.84	0.42
1:B:215:ARG:HB2	1:B:218:ASP:OD1	2.20	0.42
1:C:63:ILE:C	1:C:65:SER:N	2.76	0.42
1:C:105:LEU:CB	1:C:114:ASP:O	2.67	0.42
1:D:96:GLN:HA	1:D:97:PRO:HD2	1.82	0.42
1:E:120:ARG:HE	1:E:122:MET:CE	2.09	0.42
1:E:165:ARG:NH1	1:E:165:ARG:CG	2.83	0.42
1:F:207:ASP:OD1	1:F:209:THR:CG2	2.67	0.42
1:I:135:LEU:H	1:I:135:LEU:CD2	2.33	0.42
1:I:154:THR:CG2	1:I:155:PHE:H	2.30	0.42
1:J:139:GLN:HA	1:J:155:PHE:CE1	2.55	0.42
1:K:63:ILE:O	1:K:65:SER:N	2.53	0.42
1:L:135:LEU:HA	1:L:135:LEU:HD23	1.86	0.42
1:F:189:ALA:O	1:F:190:ASP:C	2.61	0.42
1:H:193:ILE:O	1:H:194:ALA:C	2.63	0.42
1:J:128:PRO:O	1:J:130:ILE:N	2.52	0.42
1:K:155:PHE:CE2	1:K:191:PRO:HG2	2.54	0.42
1:A:117:THR:OG1	1:A:118:SER:N	2.53	0.42
1:D:69:ARG:O	1:D:73:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:LEU:N	1:F:147:LEU:CD1	2.78	0.42
1:G:220:LEU:CD1	1:G:229:ALA:HB1	2.39	0.42
1:H:128:PRO:C	1:H:130:ILE:H	2.27	0.42
1:J:128:PRO:C	1:J:130:ILE:H	2.28	0.42
1:J:154:THR:CG2	1:J:155:PHE:N	2.71	0.42
1:K:62:ARG:HD2	1:L:63:ILE:CD1	2.49	0.42
1:D:100:GLY:O	1:D:143:LEU:N	2.52	0.42
1:E:66:LEU:O	1:E:68:ALA:N	2.52	0.42
1:F:128:PRO:C	1:F:130:ILE:H	2.28	0.42
1:F:139:GLN:HB2	1:F:155:PHE:HE1	1.81	0.42
1:G:85:LEU:HD13	1:G:85:LEU:HA	2.00	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:I:197:LEU:HA	1:I:198:PRO:HD3	1.92	0.42
1:L:103:VAL:O	1:L:116:PHE:N	2.42	0.42
1:B:124:LEU:HA	1:B:124:LEU:HD23	1.70	0.41
1:F:189:ALA:O	1:F:191:PRO:N	2.53	0.41
1:H:207:ASP:OD1	1:H:209:THR:CG2	2.67	0.41
1:J:100:GLY:O	1:J:143:LEU:N	2.51	0.41
1:K:233:ILE:HA	1:K:234:PRO:HD2	1.61	0.41
1:C:105:LEU:O	1:C:106:ALA:HB2	2.20	0.41
1:F:147:LEU:H	1:F:147:LEU:CD1	2.24	0.41
1:H:106:ALA:H	1:H:114:ASP:HB2	1.85	0.41
1:H:179:HIS:CG	1:K:182:GLU:HB3	2.55	0.41
1:I:221:LEU:C	1:I:221:LEU:CD2	2.88	0.41
1:A:186:VAL:CG1	1:A:227:GLY:O	2.53	0.41
1:B:207:ASP:OD1	1:B:209:THR:HG23	2.20	0.41
1:D:124:LEU:HD23	1:D:125:THR:H	1.84	0.41
1:D:172:HIS:C	1:D:188:LEU:HD12	2.46	0.41
1:E:54:ARG:O	1:E:55:ASP:C	2.63	0.41
1:E:127:SER:O	1:E:128:PRO:C	2.62	0.41
1:G:130:ILE:O	1:G:132:ALA:N	2.53	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:K:168:LEU:HD23	1:K:168:LEU:HA	1.69	0.41
1:B:189:ALA:O	1:B:190:ASP:C	2.63	0.41
1:C:108:HIS:C	1:C:110:ASP:N	2.79	0.41
1:D:214:LEU:HD12	1:D:214:LEU:HA	1.59	0.41
1:E:165:ARG:HB3	1:E:175:LEU:HD23	2.02	0.41
1:G:108:HIS:HB2	1:G:112:THR:O	2.20	0.41
1:I:103:VAL:HG12	1:I:104:LEU:H	1.84	0.41

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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:A:135:LEU:H	1:A:135:LEU:CD2	2.34	0.41
1:D:105:LEU:HD12	1:D:105:LEU:HA	1.72	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:I:141:VAL:HG21	1:I:149:VAL:CG1	2.50	0.41
1:J:127:SER:HA	1:J:128:PRO:HD2	1.79	0.41
1:K:56:ILE:O	1:K:56:ILE:HG22	2.20	0.41
1:L:197:LEU:HA	1:L:198:PRO:HD3	1.91	0.41
1:A:221:LEU:HD23	1:A:221:LEU:O	2.21	0.41
1:B:53:ALA:HA	1:B:56:ILE:HD12	2.03	0.41
1:B:190:ASP:N	1:B:191:PRO:CD	2.84	0.41
1:C:63:ILE:C	1:C:65:SER:H	2.28	0.41
1:D:225:LYS:HD2	1:D:225:LYS:HA	1.91	0.41
1:E:164:LEU:HD12	1:E:165:ARG:H	1.84	0.41
1:F:72:LYS:O	1:F:76:THR:HG23	2.19	0.41
1:G:104:LEU:HD11	1:G:113:VAL:HG11	2.03	0.41
1:H:214:LEU:HD12	1:H:214:LEU:HA	1.50	0.41
1:J:96:GLN:HA	1:J:97:PRO:HD2	1.81	0.41
1:B:127:SER:HA	1:B:128:PRO:HD2	1.78	0.41
1:E:142:ARG:HD2	1:F:123:ARG:CD	2.49	0.41
1:G:105:LEU:HG	1:G:228:TYR:HE2	1.85	0.41
1:I:74:MET:HE3	1:I:74:MET:O	2.21	0.41
1:L:96:GLN:HA	1:L:97:PRO:HD2	1.80	0.41
1:B:59:LEU:C	1:B:61:ALA:N	2.79	0.41
1:E:233:ILE:HA	1:E:234:PRO:HD2	1.51	0.41
1:F:139:GLN:HA	1:F:155:PHE:CD1	2.55	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:I:168:LEU:HD12	1:I:173:ARG:HB2	2.02	0.41
1:A:63:ILE:C	1:A:65:SER:N	2.79	0.41
1:A:233:ILE:HD13	1:A:233:ILE:HA	1.94	0.41
1:B:214:LEU:HD12	1:B:215:ARG:N	2.35	0.41
1:D:117:THR:O	1:D:117:THR:HG23	2.20	0.41
1:D:130:ILE:HD13	1:D:130:ILE:HA	1.84	0.41
1:E:154:THR:CG2	1:E:155:PHE:H	2.25	0.41
1:E:168:LEU:CD2	1:E:169:ALA:H	2.33	0.41
1:E:208:ASP:O	1:E:210:ARG:N	2.54	0.41
1:F:89:GLU:O	1:F:93:ARG:HG3	2.21	0.41
1:F:116:PHE:CE2	1:F:225:LYS:O	2.73	0.41
1:G:63:ILE:O	1:G:65:SER:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:135:LEU:H	1:G:135:LEU:HD22	1.84	0.41
1:I:105:LEU:HG	1:I:228:TYR:HE2	1.86	0.41
1:I:165:ARG:HG2	1:I:165:ARG:HH11	1.86	0.41
1:J:124:LEU:HD23	1:J:124:LEU:HA	1.48	0.41
1:K:170:ASP:OD1	1:K:172:HIS:HB2	2.21	0.41
1:K:218:ASP:OD2	1:K:232:ARG:NH1	2.51	0.41
1:A:56:ILE:O	1:A:56:ILE:HG22	2.21	0.41
1:H:161:ILE:HD13	1:H:161:ILE:HA	1.78	0.41
1:I:184:ARG:CD	1:I:224:THR:CG2	2.90	0.41
1:L:153:GLY:O	1:L:154:THR:O	2.39	0.41
1:B:191:PRO:C	1:B:192:LEU:HD12	2.46	0.40
1:C:54:ARG:O	1:C:55:ASP:C	2.63	0.40
1:C:190:ASP:C	1:C:192:LEU:H	2.29	0.40
1:E:63:ILE:C	1:E:65:SER:N	2.78	0.40
1:F:164:LEU:HD22	1:F:164:LEU:C	2.46	0.40
1:G:54:ARG:O	1:G:55:ASP:C	2.62	0.40
1:H:128:PRO:O	1:H:130:ILE:N	2.53	0.40
1:I:126:CYS:HB3	1:I:130:ILE:HD11	2.03	0.40
1:J:189:ALA:O	1:J:190:ASP:C	2.63	0.40
1:B:89:GLU:O	1:B:93:ARG:HG3	2.21	0.40
1:H:59:LEU:C	1:H:61:ALA:N	2.79	0.40
1:L:208:ASP:C	1:L:210:ARG:H	2.29	0.40
1:B:69:ARG:O	1:B:73:LEU:HG	2.22	0.40
1:G:135:LEU:H	1:G:135:LEU:CD2	2.34	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:I:63:ILE:O	1:I:65:SER:N	2.55	0.40
1:J:188:LEU:HA	1:J:229:ALA:HB3	2.02	0.40
1:E:96:GLN:HA	1:E:97:PRO:HD2	1.92	0.40
1:G:154:THR:CG2	1:G:155:PHE:H	2.31	0.40
1:I:168:LEU:HD23	1:I:168:LEU:HA	1.74	0.40
1:K:190:ASP:C	1:K:192:LEU:N	2.80	0.40
1:A:62:ARG:HD2	1:B:63:ILE:CD1	2.49	0.40
1:B:100:GLY:O	1:B:143:LEU:N	2.55	0.40
1:C:206:ASN:O	1:C:207:ASP:CB	2.68	0.40
1:C:233:ILE:HA	1:C:234:PRO:HD2	1.48	0.40
1:G:117:THR:OG1	1:G:118:SER:N	2.54	0.40
1:G:136:LYS:HB3	1:G:190:ASP:HB2	2.03	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:I:190:ASP:C	1:I:192:LEU:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:127:SER:HA	1:K:128:PRO:HD2	1.85	0.40
1:L:164:LEU:C	1:L:164:LEU:HD22	2.47	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	13
1	B	184/251 (73%)	148 (80%)	21 (11%)	15 (8%)	0	11
1	C	184/251 (73%)	139 (76%)	31 (17%)	14 (8%)	1	13
1	D	184/251 (73%)	147 (80%)	27 (15%)	10 (5%)	1	18
1	E	184/251 (73%)	139 (76%)	31 (17%)	14 (8%)	1	13
1	F	184/251 (73%)	152 (83%)	23 (12%)	9 (5%)	1	19
1	G	184/251 (73%)	138 (75%)	28 (15%)	18 (10%)	0	8
1	H	184/251 (73%)	148 (80%)	27 (15%)	9 (5%)	1	19
1	I	184/251 (73%)	136 (74%)	34 (18%)	14 (8%)	1	13
1	J	184/251 (73%)	147 (80%)	24 (13%)	13 (7%)	1	14
1	K	184/251 (73%)	135 (73%)	36 (20%)	13 (7%)	1	14
1	L	184/251 (73%)	147 (80%)	27 (15%)	10 (5%)	1	18
All	All	2208/3012 (73%)	1713 (78%)	342 (16%)	153 (7%)	1	14

All (153) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	ALA
1	A	169	ALA

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Mol	Chain	Res	Type
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
1	F	194	ALA

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Mol	Chain	Res	Type
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
1	D	198	PRO

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Mol	Chain	Res	Type
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
1	J	198	PRO

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Mol	Chain	Res	Type
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%)	119 (77%)	35 (23%)	1	6
1	B	154/204 (76%)	117 (76%)	37 (24%)	1	5
1	C	154/204 (76%)	119 (77%)	35 (23%)	1	6
1	D	154/204 (76%)	113 (73%)	41 (27%)	0	4
1	E	154/204 (76%)	115 (75%)	39 (25%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	154/204 (76%)	120 (78%)	34 (22%)	1	6
1	G	154/204 (76%)	117 (76%)	37 (24%)	1	5
1	H	154/204 (76%)	116 (75%)	38 (25%)	1	4
1	I	154/204 (76%)	121 (79%)	33 (21%)	1	6
1	J	154/204 (76%)	117 (76%)	37 (24%)	1	5
1	K	154/204 (76%)	113 (73%)	41 (27%)	0	4
1	L	154/204 (76%)	123 (80%)	31 (20%)	1	9
All	All	1848/2448 (76%)	1410 (76%)	438 (24%)	1	5

All (438) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	MET
1	A	79	GLU
1	A	85	LEU
1	A	89	GLU
1	A	103	VAL
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	137	LYS
1	A	141	VAL
1	A	149	VAL
1	A	150	VAL
1	A	154	THR
1	A	158	VAL
1	A	163	THR
1	A	167	ILE
1	A	168	LEU
1	A	175	LEU
1	A	179	HIS
1	A	185	VAL
1	A	186	VAL

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Mol	Chain	Res	Type
1	A	219	SER
1	A	221	LEU
1	A	222	VAL
1	A	225	LYS
1	A	231	GLU
1	A	233	ILE
1	A	235	LEU
1	B	70	ASN
1	B	72	LYS
1	B	81	ARG
1	B	84	LEU
1	B	85	LEU
1	B	87	LEU
1	B	91	VAL
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	136	LYS
1	B	141	VAL
1	B	143	LEU
1	B	145	GLU
1	B	148	THR
1	B	149	VAL
1	B	156	GLU
1	B	158	VAL
1	B	161	ILE
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	193	ILE
1	B	196	ASP
1	B	214	LEU
1	B	215	ARG

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Mol	Chain	Res	Type
1	B	218	ASP
1	B	222	VAL
1	C	74	MET
1	C	79	GLU
1	C	85	LEU
1	C	89	GLU
1	C	107	THR
1	C	113	VAL
1	C	115	VAL
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	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	179	HIS
1	C	185	VAL
1	C	199	ASP
1	C	203	GLU
1	C	211	PRO
1	C	215	ARG
1	C	221	LEU
1	C	222	VAL
1	C	225	LYS
1	C	231	GLU
1	C	235	LEU
1	C	236	VAL
1	D	70	ASN
1	D	72	LYS
1	D	81	ARG
1	D	84	LEU
1	D	85	LEU

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Mol	Chain	Res	Type
1	D	87	LEU
1	D	89	GLU
1	D	91	VAL
1	D	104	LEU
1	D	105	LEU
1	D	110	ASP
1	D	113	VAL
1	D	115	VAL
1	D	117	THR
1	D	121	LYS
1	D	124	LEU
1	D	130	ILE
1	D	136	LYS
1	D	141	VAL
1	D	143	LEU
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	176	VAL
1	D	182	GLU
1	D	185	VAL
1	D	188	LEU
1	D	193	ILE
1	D	196	ASP
1	D	201	LEU
1	D	214	LEU
1	D	215	ARG
1	D	218	ASP
1	D	222	VAL
1	D	225	LYS
1	D	231	GLU
1	D	236	VAL
1	E	74	MET
1	E	79	GLU
1	E	85	LEU
1	E	89	GLU
1	E	107	THR
1	E	109	ASP

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Mol	Chain	Res	Type
1	E	110	ASP
1	E	111	ASP
1	E	113	VAL
1	E	115	VAL
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	137	LYS
1	E	140	THR
1	E	141	VAL
1	E	149	VAL
1	E	154	THR
1	E	158	VAL
1	E	163	THR
1	E	167	ILE
1	E	168	LEU
1	E	175	LEU
1	E	176	VAL
1	E	179	HIS
1	E	181	ASP
1	E	185	VAL
1	E	186	VAL
1	E	213	LYS
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	E	236	VAL
1	F	70	ASN
1	F	72	LYS
1	F	81	ARG
1	F	84	LEU
1	F	85	LEU
1	F	87	LEU
1	F	89	GLU
1	F	91	VAL
1	F	104	LEU

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Mol	Chain	Res	Type
1	F	110	ASP
1	F	113	VAL
1	F	115	VAL
1	F	117	THR
1	F	130	ILE
1	F	136	LYS
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	193	ILE
1	F	196	ASP
1	F	214	LEU
1	F	215	ARG
1	F	222	VAL
1	F	225	LYS
1	G	74	MET
1	G	79	GLU
1	G	85	LEU
1	G	89	GLU
1	G	103	VAL
1	G	107	THR
1	G	113	VAL
1	G	115	VAL
1	G	117	THR
1	G	120	ARG
1	G	125	THR
1	G	129	ASN
1	G	130	ILE
1	G	131	ASP
1	G	135	LEU
1	G	136	LYS
1	G	137	LYS

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Mol	Chain	Res	Type
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	185	VAL
1	G	186	VAL
1	G	190	ASP
1	G	213	LYS
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	85	LEU
1	H	87	LEU
1	H	91	VAL
1	H	104	LEU
1	H	105	LEU
1	H	110	ASP
1	H	113	VAL
1	H	115	VAL
1	H	117	THR
1	H	121	LYS
1	H	124	LEU
1	H	127	SER
1	H	130	ILE
1	H	136	LYS
1	H	141	VAL
1	H	143	LEU
1	H	148	THR
1	H	149	VAL

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Mol	Chain	Res	Type
1	H	156	GLU
1	H	158	VAL
1	H	162	SER
1	H	164	LEU
1	H	167	ILE
1	H	175	LEU
1	H	182	GLU
1	H	185	VAL
1	H	186	VAL
1	H	193	ILE
1	H	196	ASP
1	H	214	LEU
1	H	215	ARG
1	H	218	ASP
1	H	222	VAL
1	H	236	VAL
1	I	74	MET
1	I	79	GLU
1	I	85	LEU
1	I	89	GLU
1	I	103	VAL
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	149	VAL
1	I	154	THR
1	I	158	VAL
1	I	163	THR
1	I	167	ILE
1	I	168	LEU
1	I	175	LEU
1	I	185	VAL
1	I	186	VAL
1	I	205	LEU
1	I	212	ARG

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Mol	Chain	Res	Type
1	I	219	SER
1	I	221	LEU
1	I	222	VAL
1	I	224	THR
1	I	225	LYS
1	I	231	GLU
1	I	235	LEU
1	J	70	ASN
1	J	72	LYS
1	J	81	ARG
1	J	84	LEU
1	J	85	LEU
1	J	87	LEU
1	J	91	VAL
1	J	104	LEU
1	J	105	LEU
1	J	110	ASP
1	J	113	VAL
1	J	115	VAL
1	J	117	THR
1	J	121	LYS
1	J	129	ASN
1	J	130	ILE
1	J	136	LYS
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	175	LEU
1	J	182	GLU
1	J	186	VAL
1	J	188	LEU
1	J	193	ILE
1	J	196	ASP
1	J	215	ARG
1	J	221	LEU
1	J	222	VAL

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Mol	Chain	Res	Type
1	J	225	LYS
1	J	236	VAL
1	K	52	SER
1	K	74	MET
1	K	79	GLU
1	K	85	LEU
1	K	89	GLU
1	K	103	VAL
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	125	THR
1	K	129	ASN
1	K	135	LEU
1	K	136	LYS
1	K	137	LYS
1	K	140	THR
1	K	141	VAL
1	K	149	VAL
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	185	VAL
1	K	186	VAL
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

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Mol	Chain	Res	Type
1	K	236	VAL
1	L	70	ASN
1	L	72	LYS
1	L	81	ARG
1	L	84	LEU
1	L	85	LEU
1	L	87	LEU
1	L	91	VAL
1	L	104	LEU
1	L	110	ASP
1	L	113	VAL
1	L	115	VAL
1	L	117	THR
1	L	121	LYS
1	L	130	ILE
1	L	136	LYS
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	175	LEU
1	L	182	GLU
1	L	193	ILE
1	L	196	ASP
1	L	214	LEU
1	L	222	VAL
1	L	236	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	96	GLN
1	A	206	ASN
1	B	129	ASN
1	C	96	GLN
1	D	129	ASN

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Mol	Chain	Res	Type
1	E	96	GLN
1	F	179	HIS
1	H	108	HIS
1	H	129	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 oligosaccharides 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%)	0.67	17 (9%)	15 16	166, 225, 345, 406	0
1	B	186/251 (74%)	0.53	14 (7%)	20 19	158, 212, 412, 527	0
1	C	186/251 (74%)	0.66	18 (9%)	13 15	168, 226, 338, 403	0
1	D	186/251 (74%)	0.52	14 (7%)	20 19	155, 210, 417, 544	0
1	E	186/251 (74%)	0.65	19 (10%)	12 14	164, 220, 340, 398	0
1	F	186/251 (74%)	0.49	16 (8%)	16 17	156, 212, 419, 539	0
1	G	186/251 (74%)	0.67	17 (9%)	15 16	167, 224, 343, 406	0
1	H	186/251 (74%)	0.48	13 (6%)	22 20	157, 210, 406, 520	0
1	I	186/251 (74%)	0.63	17 (9%)	15 16	166, 222, 339, 402	0
1	J	186/251 (74%)	0.53	12 (6%)	25 21	156, 210, 417, 538	0
1	K	186/251 (74%)	0.64	18 (9%)	13 15	165, 223, 335, 409	0
1	L	186/251 (74%)	0.51	13 (6%)	22 20	157, 213, 423, 548	0
All	All	2232/3012 (74%)	0.58	188 (8%)	17 17	155, 218, 384, 548	0

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	52	SER	8.0
1	E	204	ALA	7.8
1	A	204	ALA	7.5
1	E	52	SER	7.2
1	K	204	ALA	7.2
1	G	52	SER	6.9
1	I	204	ALA	6.8
1	I	52	SER	6.5
1	B	205	LEU	6.4
1	G	204	ALA	6.4
1	G	236	VAL	6.2

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Mol	Chain	Res	Type	RSRZ
1	C	52	SER	6.0
1	C	236	VAL	6.0
1	K	205	LEU	6.0
1	H	205	LEU	5.9
1	K	52	SER	5.9
1	F	205	LEU	5.8
1	E	236	VAL	5.7
1	C	204	ALA	5.7
1	J	205	LEU	5.7
1	E	132	ALA	5.5
1	A	205	LEU	5.4
1	D	205	LEU	5.4
1	B	204	ALA	5.3
1	E	205	LEU	5.3
1	K	236	VAL	5.1
1	G	205	LEU	5.1
1	I	205	LEU	5.1
1	K	132	ALA	5.0
1	C	132	ALA	5.0
1	L	205	LEU	4.9
1	I	236	VAL	4.7
1	G	132	ALA	4.7
1	C	205	LEU	4.6
1	A	236	VAL	4.6
1	A	132	ALA	4.5
1	A	56	ILE	4.5
1	E	53	ALA	4.5
1	G	56	ILE	4.5
1	I	56	ILE	4.4
1	J	53	ALA	4.4
1	I	53	ALA	4.3
1	F	52	SER	4.3
1	D	204	ALA	4.3
1	I	132	ALA	4.3
1	G	53	ALA	4.3
1	A	53	ALA	4.2
1	L	53	ALA	4.2
1	E	56	ILE	4.2
1	K	237	PRO	4.2
1	H	204	ALA	4.2
1	C	56	ILE	4.2
1	J	52	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	G	237	PRO	4.1
1	C	53	ALA	4.0
1	K	56	ILE	4.0
1	D	53	ALA	3.9
1	H	52	SER	3.9
1	B	53	ALA	3.9
1	L	204	ALA	3.9
1	D	52	SER	3.8
1	B	52	SER	3.8
1	I	60	GLU	3.8
1	A	64	ASP	3.7
1	F	204	ALA	3.6
1	F	74	MET	3.6
1	K	53	ALA	3.6
1	C	237	PRO	3.5
1	L	52	SER	3.5
1	F	53	ALA	3.5
1	J	204	ALA	3.4
1	L	74	MET	3.4
1	K	60	GLU	3.4
1	G	64	ASP	3.4
1	I	237	PRO	3.4
1	J	54	ARG	3.4
1	L	54	ARG	3.4
1	J	74	MET	3.3
1	A	60	GLU	3.3
1	H	53	ALA	3.3
1	A	237	PRO	3.2
1	E	237	PRO	3.2
1	J	237	PRO	3.2
1	D	74	MET	3.2
1	G	60	GLU	3.2
1	E	201	LEU	3.2
1	B	234	PRO	3.2
1	D	54	ARG	3.1
1	D	237	PRO	3.1
1	L	57	HIS	3.1
1	C	60	GLU	3.1
1	D	70	ASN	3.1
1	A	54	ARG	3.1
1	B	54	ARG	3.1
1	B	201	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	67	ALA	3.0
1	I	64	ASP	3.0
1	B	74	MET	3.0
1	C	67	ALA	2.9
1	I	67	ALA	2.9
1	J	57	HIS	2.9
1	J	70	ASN	2.9
1	H	54	ARG	2.9
1	J	201	LEU	2.9
1	L	237	PRO	2.9
1	F	54	ARG	2.9
1	H	234	PRO	2.8
1	D	57	HIS	2.8
1	E	64	ASP	2.8
1	K	64	ASP	2.8
1	L	70	ASN	2.8
1	H	74	MET	2.8
1	F	70	ASN	2.8
1	B	237	PRO	2.8
1	F	237	PRO	2.7
1	B	70	ASN	2.7
1	H	237	PRO	2.7
1	E	67	ALA	2.7
1	E	54	ARG	2.7
1	G	67	ALA	2.7
1	H	201	LEU	2.6
1	E	75	GLU	2.6
1	G	59	LEU	2.6
1	H	70	ASN	2.6
1	F	234	PRO	2.6
1	E	60	GLU	2.6
1	L	234	PRO	2.6
1	E	59	LEU	2.6
1	I	59	LEU	2.6
1	C	64	ASP	2.6
1	G	63	ILE	2.6
1	C	54	ARG	2.6
1	F	206	ASN	2.6
1	J	206	ASN	2.6
1	A	59	LEU	2.6
1	H	57	HIS	2.5
1	I	54	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	126	CYS	2.5
1	J	234	PRO	2.5
1	G	54	ARG	2.5
1	G	57	HIS	2.5
1	G	75	GLU	2.5
1	D	234	PRO	2.5
1	A	63	ILE	2.5
1	F	201	LEU	2.5
1	K	57	HIS	2.5
1	E	55	ASP	2.5
1	K	54	ARG	2.5
1	L	111	ASP	2.5
1	I	63	ILE	2.4
1	K	67	ALA	2.4
1	K	59	LEU	2.4
1	A	55	ASP	2.4
1	I	55	ASP	2.4
1	E	57	HIS	2.3
1	I	57	HIS	2.3
1	D	201	LEU	2.3
1	F	57	HIS	2.3
1	C	59	LEU	2.3
1	I	126	CYS	2.3
1	D	111	ASP	2.3
1	C	63	ILE	2.3
1	C	75	GLU	2.3
1	H	206	ASN	2.2
1	E	63	ILE	2.2
1	B	59	LEU	2.2
1	L	201	LEU	2.2
1	K	63	ILE	2.2
1	A	57	HIS	2.2
1	B	57	HIS	2.2
1	K	75	GLU	2.2
1	C	111	ASP	2.2
1	L	59	LEU	2.2
1	D	59	LEU	2.1
1	C	201	LEU	2.1
1	F	59	LEU	2.1
1	C	57	HIS	2.1
1	G	55	ASP	2.1
1	K	201	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	101	TYR	2.1
1	F	78	LYS	2.1
1	B	206	ASN	2.1
1	F	77	LEU	2.1
1	F	67	ALA	2.0
1	E	93	ARG	2.0
1	B	154	THR	2.0
1	D	67	ALA	2.0
1	H	59	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.