Full wwPDB X-ray Structure Validation Report (i)

Feb 14, 2024 – 12:53 PM EST

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

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

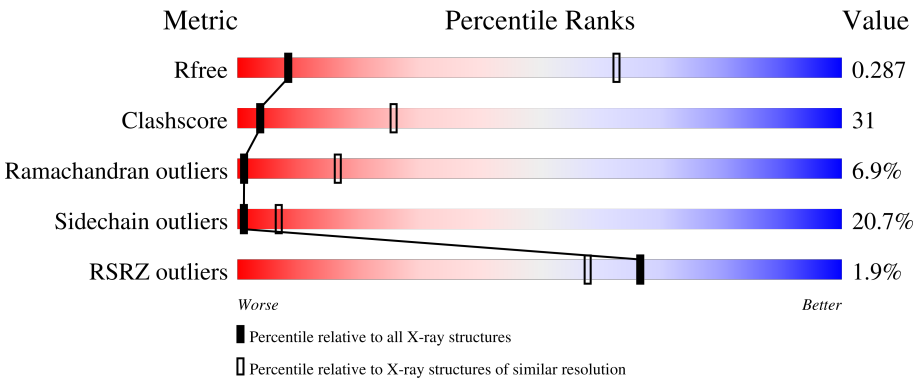
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1036 (4.20-3.68)
Clashscore	141614	1009 (4.18-3.70)
Ramachandran outliers	138981	1057 (4.20-3.68)
Sidechain outliers	138945	1049 (4.20-3.68)
RSRZ outliers	127900	1007 (4.24-3.64)

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

Mol	Chain	Length	Quality of chain
1	A	251	.% 28% 34% 12% 26%
1	B	251	3% 35% 29% 10% 26%
1	C	251	29% 30% 14% • 26%
1	D	251	2% 37% 29% 8% • 26%
1	E	251	27% 33% 12% • 26%

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

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 17172 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome-associated ATPase.

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

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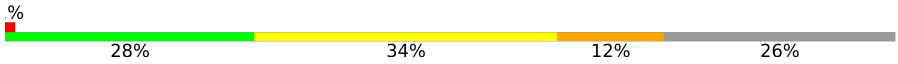
Chain	Residue	Modelled	Actual	Comment	Reference
K	238	ARG	-	expression tag	UNP P63345
K	239	GLY	-	expression tag	UNP P63345
K	240	SER	-	expression tag	UNP P63345
K	241	ALA	-	expression tag	UNP P63345
K	242	ALA	-	expression tag	UNP P63345
K	243	ALA	-	expression tag	UNP P63345
K	244	LEU	-	expression tag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

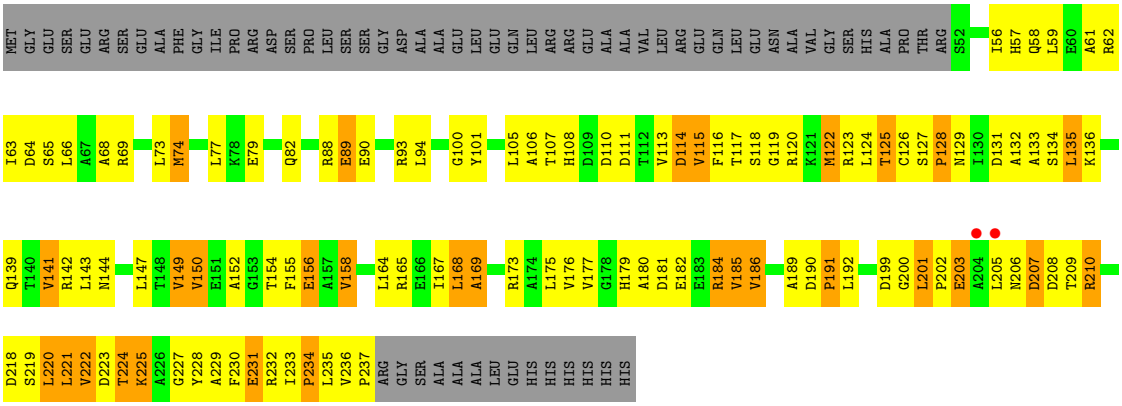
3 Residue-property plots (i)

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

• Molecule 1: Proteasome-associated ATPase

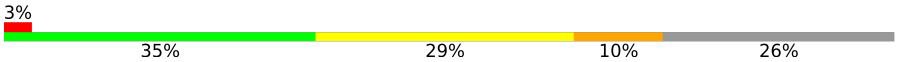
Chain A:

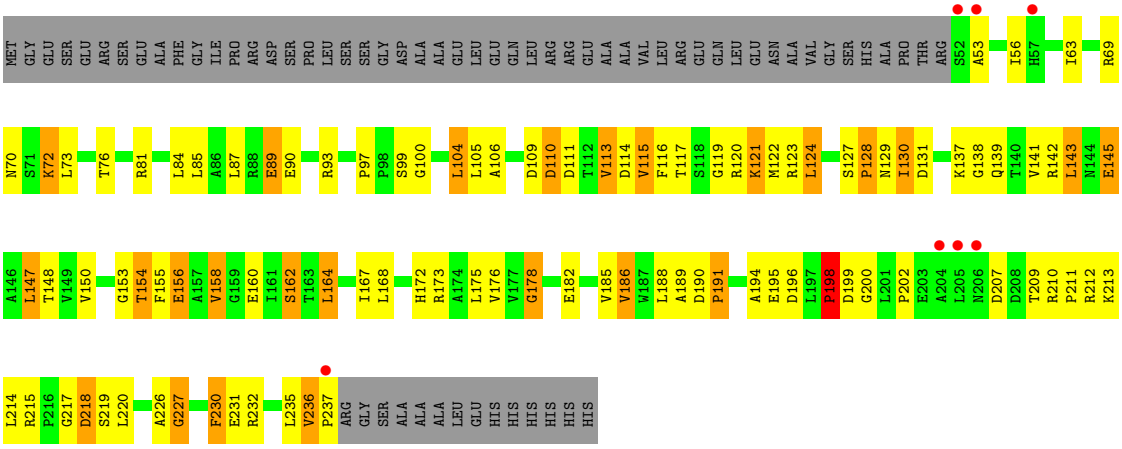




• Molecule 1: Proteasome-associated ATPase

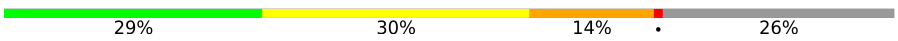
Chain B:

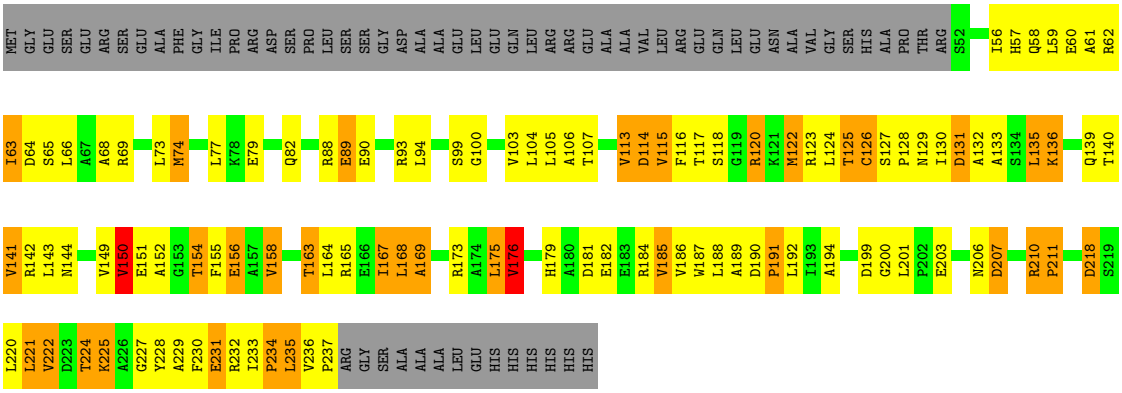




• Molecule 1: Proteasome-associated ATPase

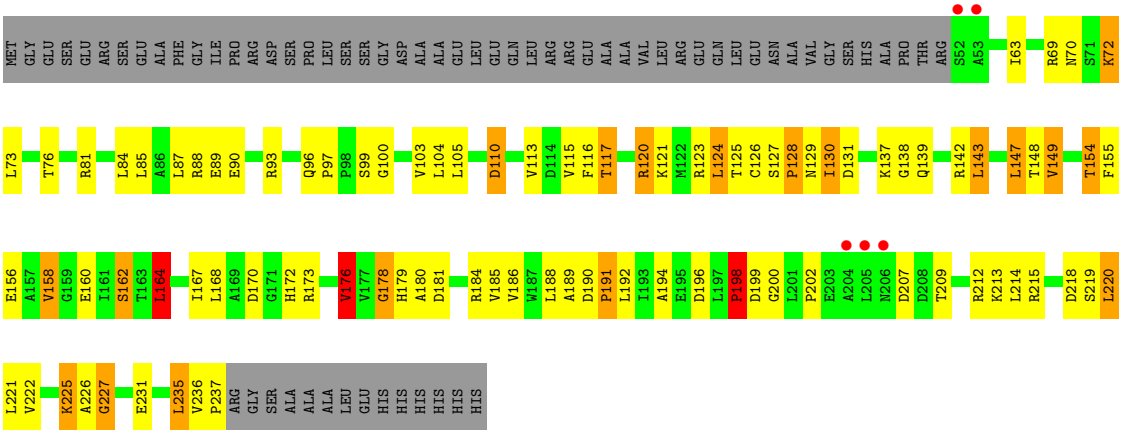
Chain C:





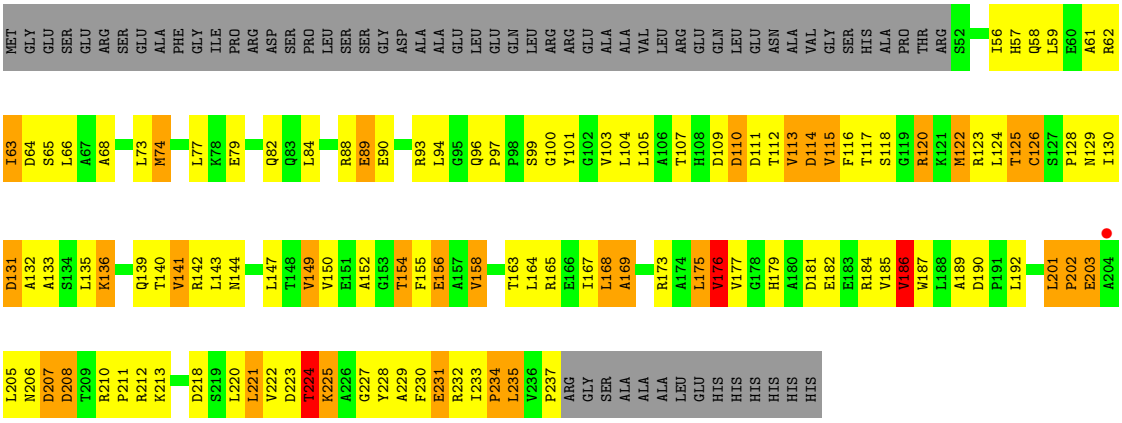
• Molecule 1: Proteasome-associated ATPase

Chain D: 2% 37% 29% 8% • 26%



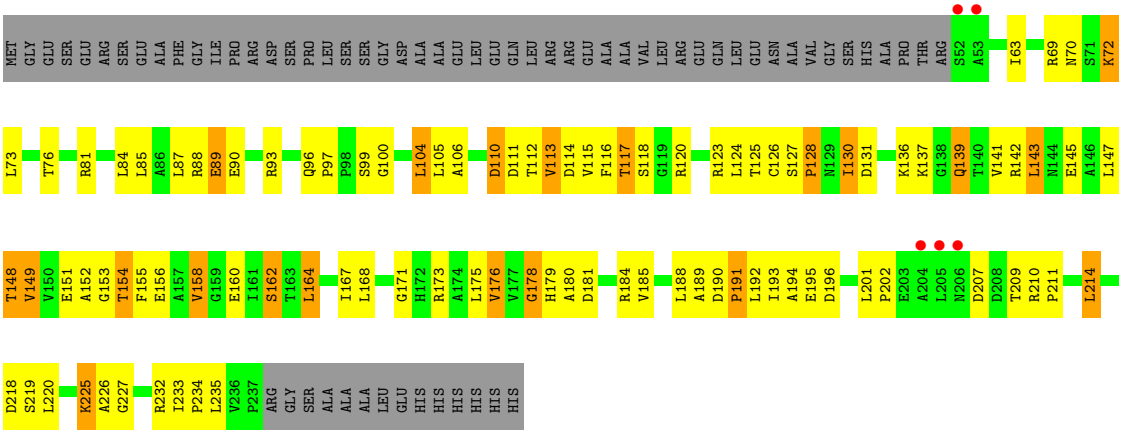
• Molecule 1: Proteasome-associated ATPase

Chain E: 27% 33% 12% • 26%



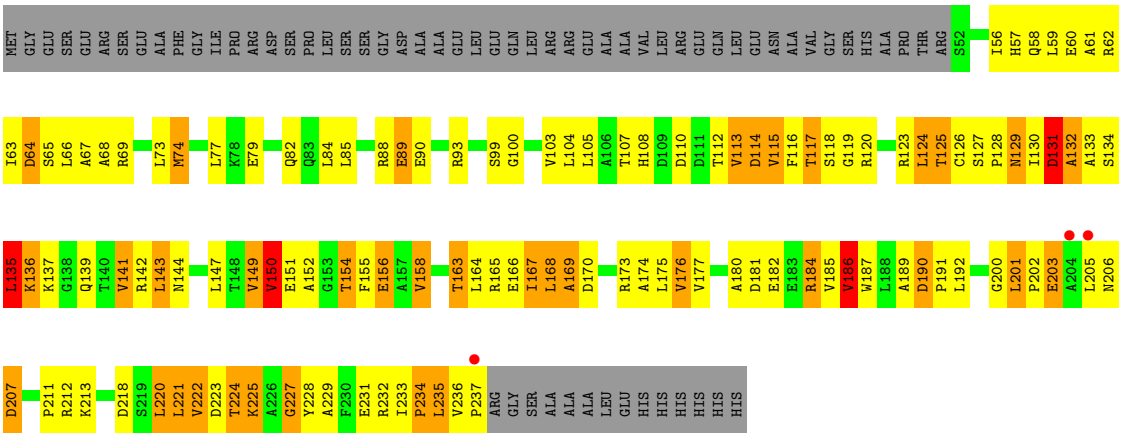
• Molecule 1: Proteasome-associated ATPase

Chain F: 2% 35% 30% 8% 26%



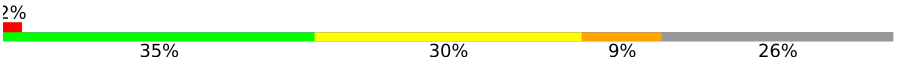
• Molecule 1: Proteasome-associated ATPase

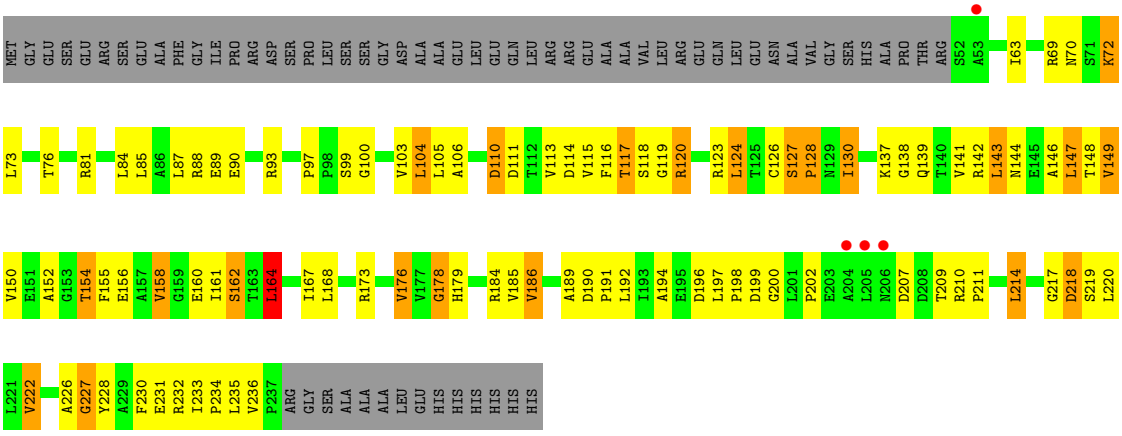
Chain G:



• Molecule 1: Proteasome-associated ATPase

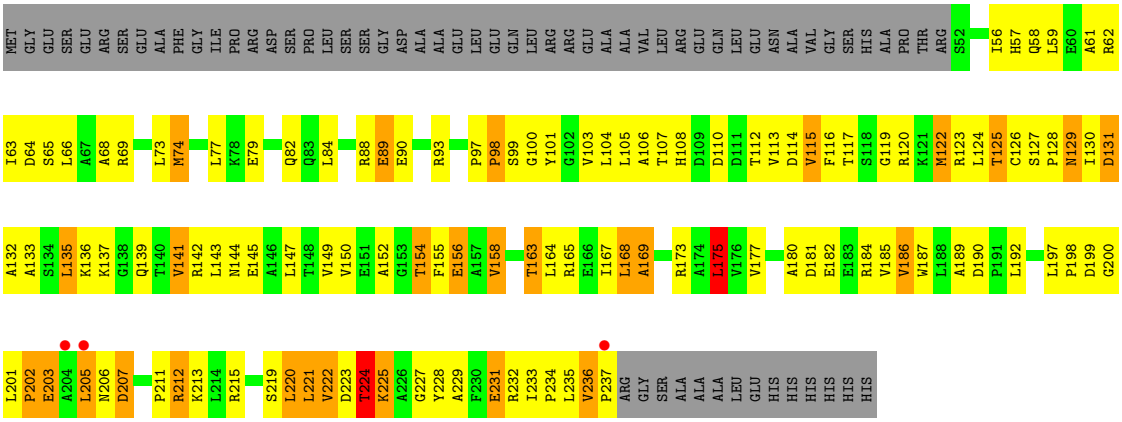
Chain H:





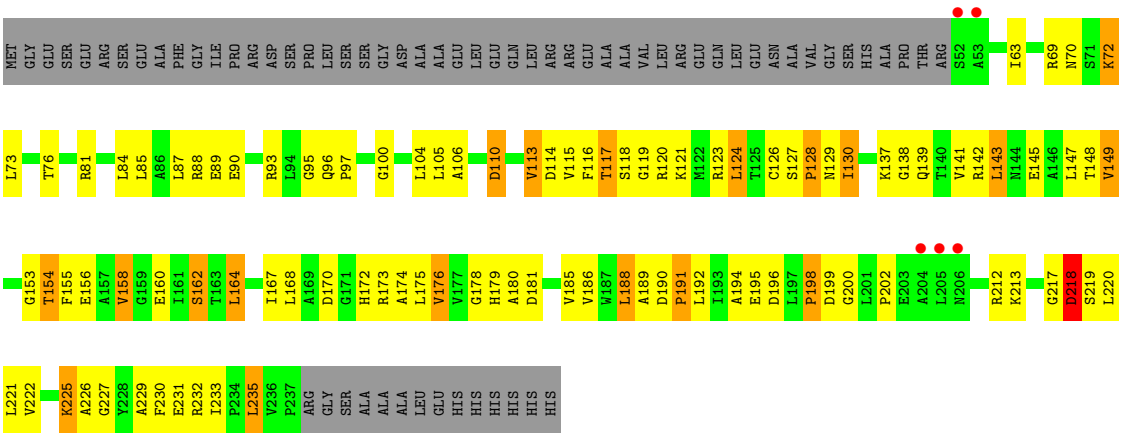
• Molecule 1: Proteasome-associated ATPase

Chain I:



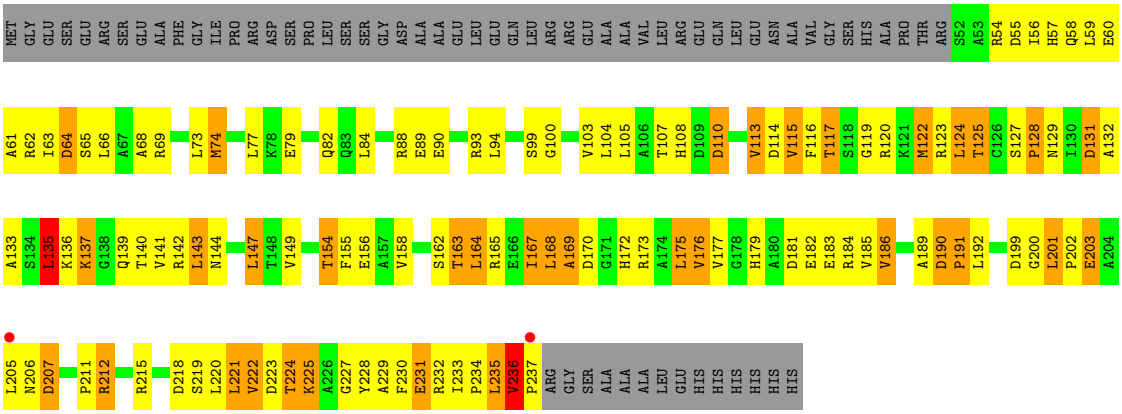
• Molecule 1: Proteasome-associated ATPase

Chain J: 2% 35% 31% 8% 26%



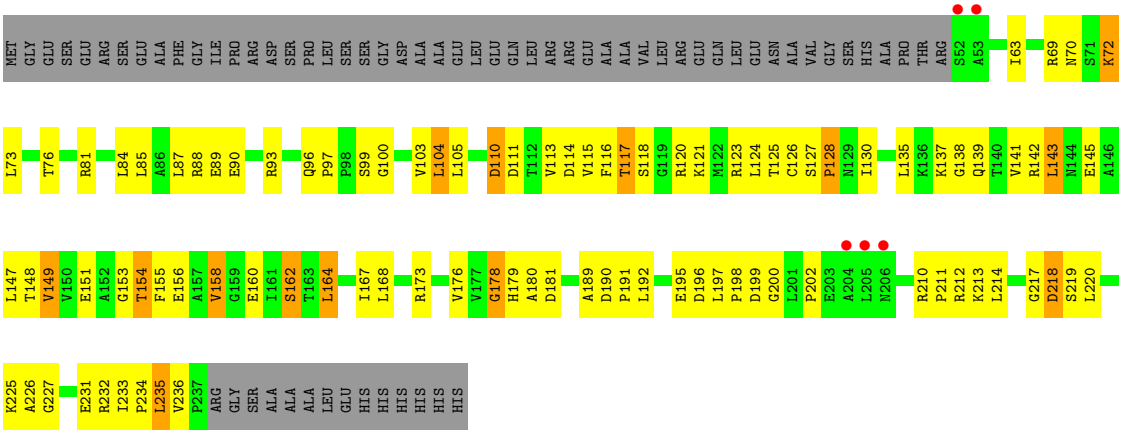
• Molecule 1: Proteasome-associated ATPase

Chain K: % 26% 33% 14% 26%



• Molecule 1: Proteasome-associated ATPase

Chain L: 2% 36% 32% 6% 26%


MET GLY GLU SER GLU ARG SER GLU ALA PHE GLY ILE PRO ARG ASP SER PRO LEU SER SER GLY ASP ALA ALA GLU LEU GLU GLN LEU ARG ARG GLU ALA ALA VAL LEU ARG GLU GLN LEU GLU ASN ALA VAL GLY SER HIS ALA PRO THR ARG S52 A53 I63 R69 N70 S71 K72
L73 T76 R81 L84 L85 A86 L87 R88 E89 E90 R93 Q96 P97 P98 S99 G100 V103 L104 L105 D110 D111 T112 V113 D114 V115 F116 T117 S118 G119 R120 K121 M122 R123 L124 T125 C126 S127 P128 N129 I130 L135 K136 K137 G138 Q139 T140 V141 R142 L143 N144 E145 A146
L147 T148 V149 V150 E151 A152 G153 T154 F155 E156 A157 V158 G159 E160 I161 S162 T163 L164 I167 L168 R173 V176 V177 G178 H179 A180 D181 A189 D190 P191 L192 E195 D196 L197 P198 D199 G200 L201 P202 E203 A204 L205 N206 R210 P211 R212 K213 L214 G217 D218 S219 L220
K225 A226 G227 E231 R232 I233 P234 L235 V236 P237 ARG GLY SER ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	176.79Å 176.65Å 176.63Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	25.00 – 3.94 25.00 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (25.00-3.94) 99.4 (25.00-3.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [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 (5.10%)	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)	0.23 , 152.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	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.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.24	8/1451 (0.6%)	1.15	4/1969 (0.2%)
1	B	1.08	3/1451 (0.2%)	1.09	4/1969 (0.2%)
1	C	1.24	8/1451 (0.6%)	1.13	5/1969 (0.3%)
1	D	1.09	3/1451 (0.2%)	1.11	8/1969 (0.4%)
1	E	1.27	9/1451 (0.6%)	1.16	6/1969 (0.3%)
1	F	1.08	4/1451 (0.3%)	1.09	6/1969 (0.3%)
1	G	1.22	6/1451 (0.4%)	1.14	8/1969 (0.4%)
1	H	1.10	3/1451 (0.2%)	1.10	8/1969 (0.4%)
1	I	1.20	5/1451 (0.3%)	1.13	4/1969 (0.2%)
1	J	1.10	3/1451 (0.2%)	1.12	6/1969 (0.3%)
1	K	1.22	5/1451 (0.3%)	1.12	6/1969 (0.3%)
1	L	1.07	3/1451 (0.2%)	1.10	5/1969 (0.3%)
All	All	1.16	60/17412 (0.3%)	1.12	70/23628 (0.3%)

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

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

All (60) bond length outliers are listed below:

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

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

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

All (70) bond angle outliers are listed below:

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

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

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

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	198	PRO	Peptide
1	B	236	VAL	Peptide
1	D	198	PRO	Peptide
1	I	236	VAL	Peptide
1	K	236	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1431	0	1443	117	0
1	B	1431	0	1443	82	0
1	C	1431	0	1443	113	0
1	D	1431	0	1443	74	0
1	E	1431	0	1443	112	0
1	F	1431	0	1443	81	0
1	G	1431	0	1443	106	0
1	H	1431	0	1443	78	0
1	I	1431	0	1443	124	0
1	J	1431	0	1443	74	0
1	K	1431	0	1443	113	0
1	L	1431	0	1443	65	0
All	All	17172	0	17316	1071	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:PHE:CE2	1:B:191:PRO:HG2	2.12	0.83
1:G:125:THR:HG23	1:J:97:PRO:HG3	1.58	0.83
1:D:155:PHE:CE2	1:D:191:PRO:HG2	2.13	0.83
1:B:97:PRO:HG3	1:E:125:THR:HG23	1.59	0.82
1:F:116:PHE:CE2	1:F:226:ALA:HA	2.14	0.82
1:L:218:ASP:OD2	1:L:232:ARG:NH1	2.12	0.82
1:K:115:VAL:HG23	1:K:124:LEU:HD21	1.61	0.82
1:F:155:PHE:CE2	1:F:191:PRO:HG2	2.15	0.82
1:G:175:LEU:HD21	1:J:235:LEU:HD12	1.61	0.81
1:E:126:CYS:HB3	1:E:130:ILE:HD11	1.63	0.81
1:B:220:LEU:HD12	1:B:220:LEU:N	1.95	0.81
1: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:A:120:ARG:HH21	1:A:122:MET:HE1	1.46	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: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:202:PRO:O	1:K:203:GLU:HB2	1.83	0.77
1:B:116:PHE:CE2	1:B:226:ALA:HA	2.18	0.77
1:I:202:PRO:O	1:I:203:GLU:HB2	1.84	0.77
1:J:95:GLY:O	1:J:142:ARG:NH2	2.17	0.77
1: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:H:186:VAL:HG12	1:H:227:GLY:C	2.05	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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:221:LEU:C	1:K:221:LEU:HD23	2.09	0.73
1: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:E:120:ARG:HH21	1:E:122:MET:HE1	1.55	0.72
1:D:124:LEU:HD11	1:D:147:LEU:HB3	1.70	0.72
1:G:126:CYS:HB3	1:G:130:ILE:HD11	1.71	0.72
1:C:189:ALA:H	1:C:192:LEU:HD12	1.54	0.71
1:G:127:SER:O	1:G:129:ASN:N	2.22	0.71
1:A:124:LEU:HD11	1:A:143:LEU:CD2	2.20	0.71
1:E:184:ARG:HD3	1:E:224:THR:HG21	1.72	0.71
1:F:168:LEU:HD12	1:F:173:ARG:HB2	1.73	0.71
1:K:163:THR:O	1:K:176:VAL:HG12	1.91	0.71
1: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: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:G:206:ASN:O	1:G:207:ASP:HB2	1.91	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
1:J:116:PHE:HD1	1:J:120:ARG:O	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:104:LEU:HD13	1:L:113:VAL:CG1	2.23	0.69
1:C:155:PHE:CE2	1:C:191:PRO:HG2	2.27	0.69
1:E:232:ARG:O	1:E:233:ILE:HD13	1.93	0.69
1:G:185:VAL:O	1:J:158:VAL:HG12	1.92	0.69
1:G:103:VAL:O	1:G:115:VAL:HG12	1.93	0.69
1:C:120:ARG:HH21	1:C:122:MET:CE	2.06	0.69
1:I:165:ARG:HH12	1:L:235:LEU:HD11	1.58	0.69
1:C:124:LEU:HD11	1:C:143:LEU:CD2	2.23	0.68
1:C:139:GLN:HE21	1:C:152:ALA:HB1	1.56	0.68
1:J:218:ASP:OD2	1:J:232:ARG:NH1	2.23	0.68
1: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:L:162:SER:HB3	1:L:178:GLY:HA2	1.75	0.68
1:B:116:PHE:CD2	1:B:226:ALA:HA	2.29	0.68
1:B:97:PRO:CG	1:E:125:THR:HG23	2.24	0.67
1:E:230:PHE:O	1:E:231:GLU:HB3	1.94	0.67
1:C:120:ARG:HH21	1:C:122:MET:HE1	1.58	0.67
1: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:B:219:SER:C	1:B:220:LEU:HD12	2.14	0.67
1:K:235:LEU:HD13	1:K:237:PRO:HD3	1.72	0.67
1:C:120:ARG:NE	1:C:122:MET:HE2	2.08	0.67
1:L:126:CYS:HB3	1:L:149:VAL:HG23	1.76	0.67
1:I:125:THR:HG23	1:L:97:PRO:CG	2.25	0.66
1:B: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:C:221:LEU:C	1:C:221:LEU:HD23	2.15	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:LEU:HD13	1:E:77:LEU:O	1.96	0.66
1:A:177:VAL:HG23	1:A:177:VAL:O	1.93	0.66
1:C:105:LEU:HB2	1:C:114:ASP:O	1.96	0.65
1:C:221:LEU:HD22	1:C:230:PHE:HB2	1.77	0.65
1:I:117:THR:O	1:I:119:GLY:N	2.29	0.65
1:A:139:GLN:HE21	1:A:152:ALA:HB1	1.59	0.65
1:E:120:ARG:HE	1:E:122:MET:CE	2.09	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:J:219:SER:C	1:J:220:LEU:HD12	2.16	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: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:C:120:ARG:NE	1:C:122:MET:HE3	2.05	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:VAL:O	1:A:185:VAL:HG12	1.97	0.63
1:F:137:LYS:HB2	1:F:190:ASP:OD2	1.97	0.63
1:C:125:THR:HG23	1:F:97:PRO:CG	2.27	0.63
1:D:138:GLY:O	1:D:155:PHE:CE1	2.51	0.63
1:I:221:LEU:HD23	1:I:221:LEU:C	2.19	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:E:120:ARG:HE	1:E:122:MET:HE3	1.64	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: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:L:219:SER:C	1:L:220:LEU:HD12	2.19	0.62
1:H:124:LEU:HD11	1:H:147:LEU:HB3	1.81	0.62
1:K:220:LEU:HD12	1:K:229:ALA:HB1	1.81	0.62
1:A:120:ARG:HE	1:A:122:MET:HE2	1.64	0.62
1:C:154:THR:HG22	1:C:155:PHE:H	1.65	0.62
1:C:185:VAL:O	1:F:158:VAL:HG12	1.98	0.62
1:L:90:GLU:HA	1:L:93:ARG:HD3	1.82	0.62
1: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:90:GLU:HA	1:H:93:ARG:HD3	1.80	0.61
1:H:219:SER:C	1:H:220:LEU:HD12	2.21	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:I:186:VAL:HG12	1:I:227:GLY:C	2.20	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:G:221:LEU:HD23	1:G:221:LEU:C	2.20	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: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: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
1:E:165:ARG:HH11	1:E:165:ARG:HG2	1.65	0.60
1:C:139:GLN:NE2	1:C:152:ALA:HB1	2.17	0.59
1:K:120:ARG:HH21	1:K:122:MET:HE1	1.66	0.59
1:H:110:ASP:OD1	1:H:110:ASP:O	2.21	0.59
1:E:221:LEU:C	1:E:221:LEU:HD23	2.22	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:235:LEU:HD11	1:G:237:PRO:HD3	1.84	0.59
1:I:127:SER:O	1:I:129:ASN:N	2.36	0.59
1: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:A:221:LEU:C	1:A:221:LEU:HD23	2.23	0.59
1:B:158:VAL:HG12	1:E:185:VAL:O	2.03	0.59
1: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:C:235:LEU:C	1:C:235:LEU:HD13	2.24	0.58
1:A:115:VAL:HG22	1:A:124:LEU:CD2	2.31	0.58
1:C:235:LEU:CD1	1:C:237:PRO:HD3	2.33	0.58
1:I:154:THR:HG22	1:I:155:PHE:H	1.67	0.58
1:I:232:ARG:O	1:I:233:ILE:HD13	2.04	0.58
1:G:182:GLU:HB3	1:J:179:HIS:CD2	2.38	0.58
1: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: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: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:K:186:VAL:HG12	1:K:227:GLY:C	2.21	0.58
1:C:175:LEU:C	1:C:175:LEU:HD12	2.25	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:E:120:ARG:NH2	1:E:122:MET:HE1	2.20	0.57
1:K:206:ASN:O	1:K:207:ASP:HB2	2.04	0.57
1:D:126:CYS:HB3	1:D:149:VAL:HG23	1.85	0.57
1:A:115:VAL:HG21	1:A:124:LEU:HD21	1.80	0.57
1: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:E:120:ARG:NE	1:E:122:MET:HE3	2.19	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:K:164:LEU:HD12	1:K:164:LEU:C	2.24	0.57
1:F:219:SER:C	1:F:220:LEU:HD12	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:164:LEU:HD12	1:I:165:ARG:N	2.20	0.57
1:A:164:LEU:HD12	1:A:164:LEU:C	2.24	0.57
1:E:110:ASP:HB3	1:E:112:THR:HG23	1.87	0.57
1: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:K:120:ARG:HE	1:K:122:MET:CE	2.18	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: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: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:A:108:HIS:C	1:A:110:ASP:H	2.09	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:E:235:LEU:C	1:E:235:LEU:HD13	2.25	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:C:124:LEU:HD11	1:C:143:LEU:HD22	1.87	0.55
1:D:116:PHE:CD1	1:D:120:ARG:O	2.59	0.55
1: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:D:104:LEU:O	1:D:104:LEU:HG	2.05	0.55
1:F:99:SER:HB2	1:F:142:ARG:HH11	1.72	0.55
1:F:124:LEU:HD11	1:F:147:LEU:HB3	1.89	0.55
1:G:154:THR:HG22	1:G:155:PHE:H	1.71	0.55
1:I:120:ARG:NE	1:I:122:MET:HE3	2.21	0.54
1:I:131:ASP:O	1:I:133:ALA:N	2.41	0.54
1:J:198:PRO:O	1:J:200:GLY:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:189:ALA:C	1:D:191:PRO:HD2	2.28	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:E:190:ASP:O	1:E:192:LEU:N	2.41	0.54
1:D:172:HIS:O	1:D:188:LEU:HD12	2.08	0.54
1:K:221:LEU:HD23	1:K:221:LEU:O	2.08	0.54
1:E:184:ARG:HD3	1:E:224:THR:HG22	1.90	0.53
1:H:137:LYS:HB2	1:H:190:ASP:OD2	2.08	0.53
1:L:117:THR:O	1:L:118:SER:C	2.46	0.53
1:E:182:GLU: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:I:155:PHE:O	1:I:156:GLU:C	2.46	0.53
1:B:153:GLY:O	1:B:154:THR:O	2.26	0.53
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:C:144:ASN:OD1	1:C:144:ASN:C	2.46	0.53
1:G:165:ARG:HG2	1:G:165:ARG:NH1	2.20	0.53
1:K:108:HIS:C	1:K:110:ASP:H	2.11	0.53
1: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:C:189:ALA:O	1:C:190:ASP:C	2.46	0.53
1:F:220:LEU:N	1:F:220:LEU:CD1	2.70	0.53
1:J:212:ARG:HG3	1:J:213:LYS:O	2.09	0.53
1:K:212:ARG:HE	1:K:215:ARG:HD3	1.74	0.53
1:B:122:MET:HE1	1:B:147:LEU:HD22	1.90	0.53
1:B:207:ASP:OD1	1:B:209:THR:CG2	2.57	0.53
1:D:154:THR:CG2	1:D:155:PHE:N	2.65	0.53
1:E:124:LEU: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:A:186:VAL:HG12	1:A:227:GLY:C	2.29	0.52
1:I:235:LEU:HD22	1:I:236:VAL:N	2.24	0.52
1: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:120:ARG:NH2	1:C:122:MET:CE	2.73	0.52
1:H:117:THR:O	1:H:118:SER:C	2.46	0.52
1:I:190:ASP:O	1:I:192:LEU:N	2.41	0.52
1:K:120:ARG:HE	1:K:122:MET:HE2	1.75	0.52
1:D:219:SER:C	1:D:220:LEU:HD12	2.30	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:I:120:ARG:HE	1:I:122:MET:HE3	1.74	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
1:G:155:PHE:O	1:G:156:GLU:C	2.47	0.52
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:C:155:PHE:O	1:C:156:GLU:C	2.46	0.52
1:I:127:SER:C	1:I:129:ASN:H	2.13	0.52
1:I:142:ARG:HH11	1:J:123:ARG:HD3	1.74	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: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:E:56:ILE:O	1:E:56:ILE:CG2	2.58	0.51
1:L:104:LEU:HD13	1:L:113:VAL:HG11	1.91	0.51
1:C:168:LEU:O	1:C:169:ALA:C	2.48	0.51
1:I:182:GLU:HB3	1:L:179:HIS:CD2	2.45	0.51
1:D:110:ASP:O	1:D:110:ASP:OD1	2.29	0.51
1:F:148:THR:O	1:F:148:THR:HG22	2.10	0.51
1:E:101:TYR:HD1	1:E:142:ARG:HA	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:120:ARG:HE	1:A:122:MET:CE	2.22	0.51
1:C:139:GLN:CB	1:C:155:PHE:CE1	2.94	0.51
1:C:158:VAL:HG12	1:D:185:VAL:O	2.09	0.51
1:G:184:ARG:HD3	1:G:224:THR:HG22	1.93	0.51
1:A:222:VAL:HG23	1:A:223:ASP:N	2.24	0.51
1:F:105:LEU:N	1:F:114:ASP:O	2.43	0.51
1:I:120:ARG:HH21	1:I:122:MET:HE1	1.76	0.51
1:I:231:GLU:HG3	1:I:232:ARG:N	2.26	0.51
1:J:117:THR:O	1:J:118:SER:C	2.46	0.51
1:A:124:LEU:HD11	1:A:143:LEU:HD21	1.90	0.51
1:A:235:LEU:HD22	1:A:236:VAL:H	1.76	0.51
1:J:116:PHE:CD2	1:J:226:ALA:HA	2.46	0.51
1:H:126:CYS:HB3	1:H:149:VAL:HG23	1.94	0.50
1: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:I:105:LEU:O	1:I:106:ALA:HB2	2.12	0.50
1:K:184:ARG:HD3	1:K:224:THR:HG21	1.93	0.50
1: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: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:J:180:ALA:O	1:J:181:ASP:C	2.50	0.50
1:C:56:ILE:O	1:C:56:ILE:CG2	2.59	0.50
1:E:144:ASN:OD1	1:E:144:ASN:C	2.50	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H:99:SER:CB	1:H:142:ARG:HH11	2.24	0.50
1:C:104:LEU:HD11	1:C:113:VAL:HG11	1.94	0.50
1:C:167:ILE:HD12	1:C:167:ILE:H	1.77	0.50
1: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
1:K:168:LEU:O	1:K:169:ALA:C	2.50	0.49
1:A:206:ASN:O	1:A:207:ASP:HB2	2.12	0.49
1:E:141:VAL:CG2	1:E:149:VAL:CG1	2.90	0.49
1:F:191:PRO:C	1:F:192:LEU:HD12	2.33	0.49
1:K:124:LEU:HD11	1:K:143:LEU:HD22	1.93	0.49
1:L:191:PRO:C	1:L:192:LEU:HD12	2.32	0.49
1:A:94:LEU:HD11	1:B:128:PRO:HD2	1.94	0.49
1:A:144:ASN:OD1	1:A:144:ASN:C	2.50	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: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:L:180:ALA:O	1:L:181:ASP:C	2.51	0.49
1:C:73:LEU:O	1:C:74:MET:C	2.50	0.49
1:F:110:ASP:OD1	1:F:110:ASP:O	2.30	0.49
1:H:147:LEU:H	1:H:147:LEU:CD1	2.24	0.49
1:E:73:LEU:O	1:E:74:MET:C	2.49	0.49
1:H:100:GLY:O	1:H:143:LEU:HD12	2.12	0.49
1:K:117:THR:C	1:K:119:GLY:H	2.16	0.49
1:A:120:ARG:NH2	1:A:122:MET:HE1	2.21	0.49
1:E:164:LEU:HD12	1:E:164:LEU:C	2.33	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:73:LEU:O	1:A:74:MET:C	2.50	0.49
1:A:164:LEU:HA	1:A:176:VAL:HG12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:144:ASN:C	1:I:144:ASN:OD1	2.49	0.49
1:I:175:LEU:HD12	1:I:175:LEU:C	2.33	0.49
1:A:168:LEU:O	1:A:169:ALA:C	2.50	0.49
1:F:210:ARG:HG2	1:F:211:PRO:CD	2.43	0.49
1:K:59:LEU:O	1:K:61:ALA:N	2.45	0.49
1: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:155:PHE:O	1:E:156:GLU:C	2.51	0.49
1:E:189:ALA:H	1:E:192:LEU:CD1	2.25	0.49
1:A:155:PHE:CE2	1:A:191:PRO:HG2	2.48	0.48
1:A:189:ALA:O	1:A:190:ASP:C	2.50	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
1:A:124:LEU:HD11	1:A:143:LEU:HD22	1.94	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:J:189:ALA:C	1:J:191:PRO:HD2	2.34	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: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:G:189:ALA:O	1:G:190:ASP:C	2.52	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: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:H:186:VAL:HG12	1:H:227:GLY:O	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:57:HIS:O	1:K:58:GLN:C	2.52	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:H:232:ARG:C	1:H:233:ILE:HG12	2.32	0.48
1:C:221:LEU:CD2	1:C:230:PHE:HB2	2.41	0.48
1:L:124:LEU:HD23	1:L:125:THR:H	1.79	0.48
1: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: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: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:144:ASN:C	1:G:144:ASN:OD1	2.51	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: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:D:191:PRO:C	1:D:192:LEU:HD12	2.34	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:113:VAL:O	1:C:123:ARG:HA	2.13	0.47
1:G:141:VAL:CG2	1:G:149:VAL:CG1	2.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:100:GLY:O	1:K:143:LEU:N	2.48	0.47
1:B:176:VAL:HG21	1:B:186:VAL:HG22	1.95	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:F:180:ALA:O	1:F:181:ASP:C	2.50	0.47
1:G:56:ILE:CG2	1:G:56:ILE:O	2.62	0.47
1: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
1:J:139:GLN:HB2	1:J:155:PHE:CE1	2.50	0.47
1:J:154:THR:CG2	1:J:155:PHE:N	2.71	0.47
1: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:K:144:ASN:C	1:K:144:ASN:OD1	2.51	0.47
1:E:59:LEU:O	1:E:61:ALA:N	2.48	0.47
1:G:73:LEU:O	1:G:74:MET:C	2.51	0.47
1:G: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:B:189:ALA:C	1:B:191:PRO:HD2	2.35	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:K:189:ALA:O	1:K:190:ASP:C	2.53	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: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:K:231:GLU:HG3	1:K:232:ARG:N	2.31	0.46
1:A:120:ARG:NE	1:A:122:MET:HE2	2.28	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:I:168:LEU:O	1:I:169:ALA:C	2.53	0.46
1:J:191:PRO:HB2	1:J:192:LEU:HD12	1.97	0.46
1:A:127:SER:O	1:A:128:PRO:C	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:72:LYS:O	1:H:76:THR:HG23	2.15	0.46
1:H:191:PRO:C	1:H:192:LEU:HD12	2.36	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:73:LEU:O	1:K:74:MET:C	2.53	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:131:ASP:O	1:A:133:ALA:N	2.49	0.46
1:B:190:ASP:N	1:B:191:PRO:HD2	2.31	0.46
1:F:136:LYS:N	1:F:139:GLN:OE1	2.38	0.46
1:I:73:LEU:O	1:I:74:MET:C	2.53	0.46
1:I:100:GLY:O	1:I:143:LEU:N	2.45	0.46
1:I:222:VAL:CG2	1:I:223:ASP:N	2.77	0.46
1:B:106:ALA:H	1:B:114:ASP:HB2	1.81	0.46
1:F:124:LEU:HA	1:F:124:LEU:HD23	1.67	0.46
1: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: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:E:168:LEU:HD23	1:E:168:LEU:HA	1.74	0.46
1:E:168:LEU:O	1:E:169:ALA:C	2.54	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: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:186:VAL:HG12	1:B:227:GLY:C	2.35	0.46
1:D:180:ALA:O	1:D:181:ASP:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:190:ASP:C	1:I:192:LEU:H	2.19	0.46
1:A:233:ILE:HA	1:A:234:PRO:HD2	1.63	0.46
1:F:117:THR:O	1:F:118:SER:C	2.55	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
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:C:59:LEU:C	1:C:61:ALA:H	2.19	0.45
1:C:66:LEU:O	1:C:69:ARG:N	2.45	0.45
1: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:F:232:ARG:C	1:F:233:ILE:HG12	2.36	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:190:ASP:C	1:A:192:LEU:H	2.20	0.45
1:C:127:SER:C	1:C:129:ASN:H	2.14	0.45
1:E: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:I:57:HIS:O	1:I:58:GLN:C	2.55	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:A:155:PHE:O	1:A:156:GLU:C	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:ASP:N	1:D:191:PRO:HD2	2.32	0.45
1:F:126:CYS:CB	1:F:149:VAL:HG23	2.43	0.45
1:I:206:ASN:O	1:I:207:ASP:HB2	2.16	0.45
1: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: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:H:189:ALA:C	1:H:191:PRO:HD2	2.38	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
1:F:154:THR:HG22	1:F:155:PHE:N	2.19	0.45
1:K:135:LEU:HB2	1:K:139:GLN:HE21	1.77	0.45
1:L:113:VAL:O	1:L:123:ARG:HA	2.17	0.45
1:E:120:ARG:NE	1:E:122:MET:CE	2.75	0.44
1:I:66:LEU:O	1:I:69:ARG:N	2.45	0.44
1:K:127:SER:C	1:K:129:ASN:H	2.21	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:I:127:SER:C	1:I:129:ASN:N	2.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:139:GLN:HB3	1:A:155:PHE:CE1	2.53	0.44
1:A:225:LYS:HE2	1:A:225:LYS:HB2	1.28	0.44
1:C:59:LEU:C	1:C:61:ALA:N	2.71	0.44
1:G:168:LEU:O	1:G:169:ALA:C	2.56	0.44
1:G:222:VAL:CG2	1:G:223:ASP:N	2.81	0.44
1:A:57:HIS:HB3	1:I:163:THR:OG1	2.18	0.44
1:E:223:ASP:O	1:E:225:LYS:N	2.51	0.44
1:F:110:ASP:OD1	1:F:112:THR:HG23	2.18	0.44
1:J:105:LEU:N	1:J:114:ASP:O	2.46	0.44
1:A:57:HIS:O	1:A:58:GLN:C	2.57	0.43
1:A:168:LEU:HD23	1:A:168:LEU:HA	1.83	0.43
1:I:108:HIS:C	1:I:110:ASP:H	2.21	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: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: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:G:57:HIS:O	1:G:58:GLN:C	2.55	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:B:154:THR:CG2	1:B:155:PHE:N	2.70	0.43
1:E:59:LEU:C	1:E:61:ALA:N	2.72	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:K:59:LEU:C	1:K:61:ALA:H	2.20	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:E:190:ASP:C	1:E:192:LEU:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:117:THR:O	1:H:119:GLY:N	2.51	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: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
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:E:59:LEU:C	1:E:61:ALA:H	2.21	0.43
1:J:69:ARG:O	1:J:73:LEU:HG	2.17	0.43
1:E:57:HIS:O	1:E:58:GLN:C	2.56	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:139:GLN:HA	1:G:155:PHE:CE1	2.54	0.43
1:K:59:LEU:C	1:K:61:ALA:N	2.72	0.43
1: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:J:147:LEU:HD12	1:J:147:LEU:N	2.35	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:59:LEU:C	1:G:61:ALA:H	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:210:ARG:HG2	1:H:211:PRO:HD3	2.01	0.42
1: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:K:155:PHE:O	1:K:156:GLU:C	2.58	0.42
1:A:108:HIS:C	1:A:110:ASP:N	2.72	0.42
1:B:155:PHE:HE2	1:B:191:PRO:CG	2.15	0.42
1:F:125:THR:O	1:F:148:THR:HA	2.19	0.42
1:J:225:LYS:HD2	1:J:225:LYS:HA	1.88	0.42
1:A:59:LEU:C	1:A:61:ALA:N	2.73	0.42
1:A:206:ASN:O	1:A:207:ASP:CB	2.67	0.42
1:B:147:LEU:N	1:B:147:LEU:CD1	2.82	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:59:LEU:C	1:I:61:ALA:H	2.23	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:K:99:SER:HB2	1:L:123:ARG:HB3	2.01	0.42
1:K:120:ARG:NH2	1:K:122:MET:HE1	2.33	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:I:164:LEU:HD12	1:I:164:LEU:C	2.39	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:PHE:O	1:B:156:GLU:C	2.57	0.42
1: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
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:K:62:ARG:HD2	1:L:63:ILE:CD1	2.49	0.42
1:K:222:VAL:CG2	1:K:223:ASP:N	2.80	0.42
1:C:57:HIS:O	1:C:58:GLN:C	2.58	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: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:K:190:ASP:C	1:K:192:LEU:H	2.23	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:G:235:LEU:HD13	1:G:235:LEU:C	2.40	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:E:189:ALA:O	1:E:190:ASP:C	2.57	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:L:189:ALA:C	1:L:191:PRO:HD2	2.40	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: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:116:PHE:HE1	1:B:119:GLY:C	2.23	0.41
1:B:172:HIS:C	1:B:188:LEU:HD12	2.41	0.41
1:D:214:LEU:HD12	1:D:214:LEU:HA	1.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:221:LEU:C	1:A:222:VAL:HG12	2.41	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:D:189:ALA:O	1:D:190:ASP:C	2.58	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:I:120:ARG:HE	1:I:122:MET:CE	2.33	0.41
1:J:96:GLN:HA	1:J:97:PRO:HD2	1.81	0.41
1:K:127:SER:C	1:K:129:ASN:N	2.73	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:E:186:VAL:HG12	1:E:227:GLY:C	2.35	0.41
1:E:221:LEU:HD23	1:E:221:LEU:O	2.21	0.41
1:G:59:LEU:C	1:G:61:ALA:N	2.74	0.41
1:G:105:LEU:HG	1:G:228:TYR:HE2	1.85	0.41
1:L:96:GLN:HA	1:L:97:PRO:HD2	1.80	0.41
1:E: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:THR:CG2	1:E:155:PHE:H	2.25	0.41
1: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
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:K:117:THR:C	1:K:119:GLY:N	2.74	0.41
1:L:153:GLY:O	1:L:154:THR:O	2.39	0.41
1:A:59:LEU:C	1:A:61:ALA:H	2.23	0.40
1:B:128:PRO:C	1:B:130:ILE:H	2.24	0.40
1:H:128:PRO:O	1:H:130:ILE:N	2.53	0.40
1:I:59:LEU:C	1:I:61:ALA:N	2.73	0.40
1:I:126:CYS:HB3	1:I:130:ILE:HD11	2.03	0.40
1:B:89:GLU:O	1:B:93:ARG:HG3	2.21	0.40
1:B:69:ARG:O	1:B:73:LEU:HG	2.22	0.40
1:D:128:PRO:C	1:D:130:ILE:H	2.23	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:54:ARG:O	1:K:55:ASP:C	2.59	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:127:SER:C	1:C:129:ASN:N	2.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:108:HIS:C	1:K:110:ASP:N	2.75	0.40
1:K:127:SER:HA	1:K:128:PRO:HD2	1.85	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	15
1	B	184/251 (73%)	148 (80%)	21 (11%)	15 (8%)	1	13
1	C	184/251 (73%)	139 (76%)	31 (17%)	14 (8%)	1	15
1	D	184/251 (73%)	147 (80%)	27 (15%)	10 (5%)	2	21
1	E	184/251 (73%)	139 (76%)	31 (17%)	14 (8%)	1	15
1	F	184/251 (73%)	152 (83%)	23 (12%)	9 (5%)	2	22
1	G	184/251 (73%)	138 (75%)	28 (15%)	18 (10%)	0	10
1	H	184/251 (73%)	148 (80%)	27 (15%)	9 (5%)	2	22
1	I	184/251 (73%)	136 (74%)	34 (18%)	14 (8%)	1	15
1	J	184/251 (73%)	147 (80%)	24 (13%)	13 (7%)	1	16
1	K	184/251 (73%)	135 (73%)	36 (20%)	13 (7%)	1	16
1	L	184/251 (73%)	147 (80%)	27 (15%)	10 (5%)	2	21
All	All	2208/3012 (73%)	1713 (78%)	342 (16%)	153 (7%)	1	16

All (153) Ramachandran outliers are listed below:

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

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

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

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	154/204 (76%)	121 (79%)	33 (21%)	1 6
1	B	154/204 (76%)	126 (82%)	28 (18%)	1 11
1	C	154/204 (76%)	118 (77%)	36 (23%)	1 5
1	D	154/204 (76%)	126 (82%)	28 (18%)	1 11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	154/204 (76%)	114 (74%)	40 (26%)	0 4
1	F	154/204 (76%)	127 (82%)	27 (18%)	2 13
1	G	154/204 (76%)	115 (75%)	39 (25%)	0 4
1	H	154/204 (76%)	126 (82%)	28 (18%)	1 11
1	I	154/204 (76%)	123 (80%)	31 (20%)	1 8
1	J	154/204 (76%)	125 (81%)	29 (19%)	1 10
1	K	154/204 (76%)	115 (75%)	39 (25%)	0 4
1	L	154/204 (76%)	129 (84%)	25 (16%)	2 15
All	All	1848/2448 (76%)	1465 (79%)	383 (21%)	1 7

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

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

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

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Mol	Chain	Res	Type
1	C	115	VAL
1	C	120	ARG
1	C	122	MET
1	C	125	THR
1	C	131	ASP
1	C	135	LEU
1	C	136	LYS
1	C	140	THR
1	C	141	VAL
1	C	150	VAL
1	C	154	THR
1	C	158	VAL
1	C	163	THR
1	C	167	ILE
1	C	168	LEU
1	C	175	LEU
1	C	176	VAL
1	C	179	HIS
1	C	185	VAL
1	C	199	ASP
1	C	203	GLU
1	C	210	ARG
1	C	211	PRO
1	C	218	ASP
1	C	221	LEU
1	C	222	VAL
1	C	225	LYS
1	C	231	GLU
1	C	235	LEU
1	D	70	ASN
1	D	72	LYS
1	D	81	ARG
1	D	84	LEU
1	D	87	LEU
1	D	110	ASP
1	D	115	VAL
1	D	117	THR
1	D	120	ARG
1	D	121	LYS
1	D	124	LEU
1	D	130	ILE
1	D	143	LEU

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

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

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

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

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

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

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

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

Mol	Chain	Res	Type
1	A	58	GLN
1	A	70	ASN
1	A	96	GLN
1	B	70	ASN
1	C	70	ASN
1	C	96	GLN
1	D	70	ASN
1	E	70	ASN
1	E	96	GLN
1	F	70	ASN
1	G	70	ASN
1	H	70	ASN
1	I	70	ASN
1	J	70	ASN
1	K	70	ASN
1	L	70	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.00	2 (1%)	80	72	166, 225, 345, 406	0
1	B	186/251 (74%)	0.03	7 (3%)	40	32	158, 212, 412, 527	0
1	C	186/251 (74%)	-0.03	0	100	100	168, 226, 338, 403	0
1	D	186/251 (74%)	0.01	5 (2%)	54	44	155, 210, 417, 544	0
1	E	186/251 (74%)	-0.04	1 (0%)	91	85	164, 220, 340, 398	0
1	F	186/251 (74%)	0.02	5 (2%)	54	44	156, 212, 419, 539	0
1	G	186/251 (74%)	0.00	3 (1%)	72	62	167, 224, 343, 406	0
1	H	186/251 (74%)	-0.02	4 (2%)	62	52	157, 210, 406, 520	0
1	I	186/251 (74%)	-0.01	3 (1%)	72	62	166, 222, 339, 402	0
1	J	186/251 (74%)	-0.03	5 (2%)	54	44	156, 210, 417, 538	0
1	K	186/251 (74%)	-0.04	2 (1%)	80	72	165, 223, 335, 409	0
1	L	186/251 (74%)	0.02	5 (2%)	54	44	157, 213, 423, 548	0
All	All	2232/3012 (74%)	-0.01	42 (1%)	66	58	155, 218, 384, 548	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	204	ALA	7.8
1	J	204	ALA	7.2
1	L	53	ALA	6.3
1	L	204	ALA	6.3
1	B	204	ALA	6.1
1	D	204	ALA	5.4
1	H	204	ALA	5.2
1	A	204	ALA	4.2
1	H	205	LEU	4.2
1	F	53	ALA	4.1
1	B	53	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	H	53	ALA	4.0
1	L	205	LEU	4.0
1	D	52	SER	3.8
1	F	206	ASN	3.6
1	D	53	ALA	3.6
1	J	53	ALA	3.6
1	F	205	LEU	3.6
1	L	52	SER	3.4
1	D	205	LEU	3.3
1	B	205	LEU	3.2
1	G	204	ALA	3.1
1	J	52	SER	3.1
1	L	206	ASN	3.1
1	B	206	ASN	3.0
1	I	237	PRO	3.0
1	I	204	ALA	2.9
1	G	237	PRO	2.9
1	G	205	LEU	2.9
1	J	205	LEU	2.9
1	A	205	LEU	2.7
1	B	237	PRO	2.6
1	D	206	ASN	2.5
1	H	206	ASN	2.5
1	I	205	LEU	2.4
1	B	57	HIS	2.3
1	B	52	SER	2.3
1	E	204	ALA	2.3
1	K	205	LEU	2.3
1	F	52	SER	2.2
1	K	237	PRO	2.2
1	J	206	ASN	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 monosaccharides 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.