



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 01:42 am BST

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

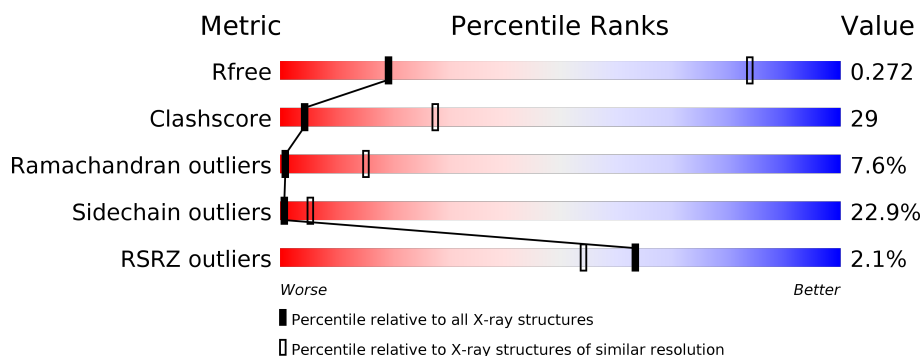
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

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

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

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

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18636 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

There are 204 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

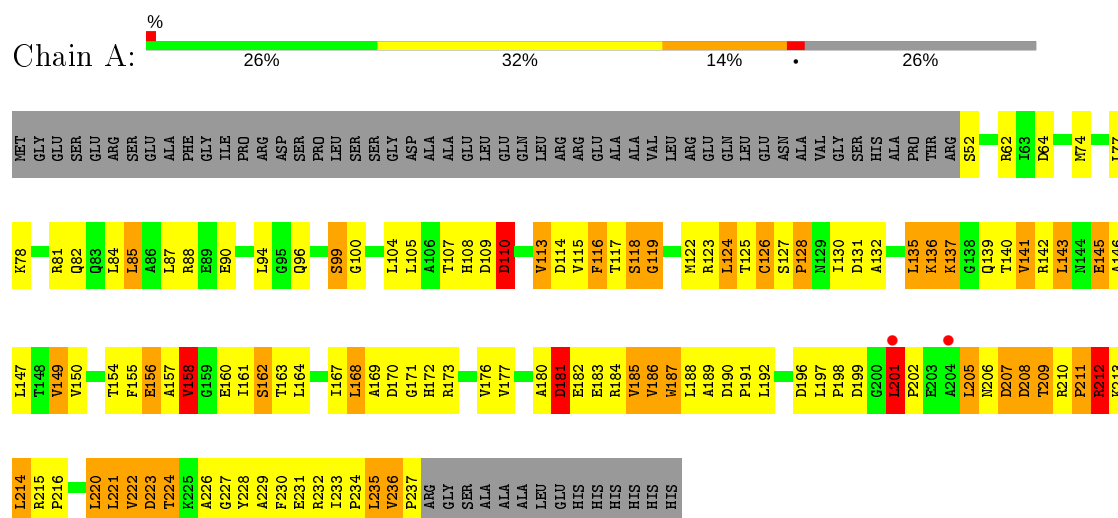
There are 30 discrepancies between the modelled and reference sequences:

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

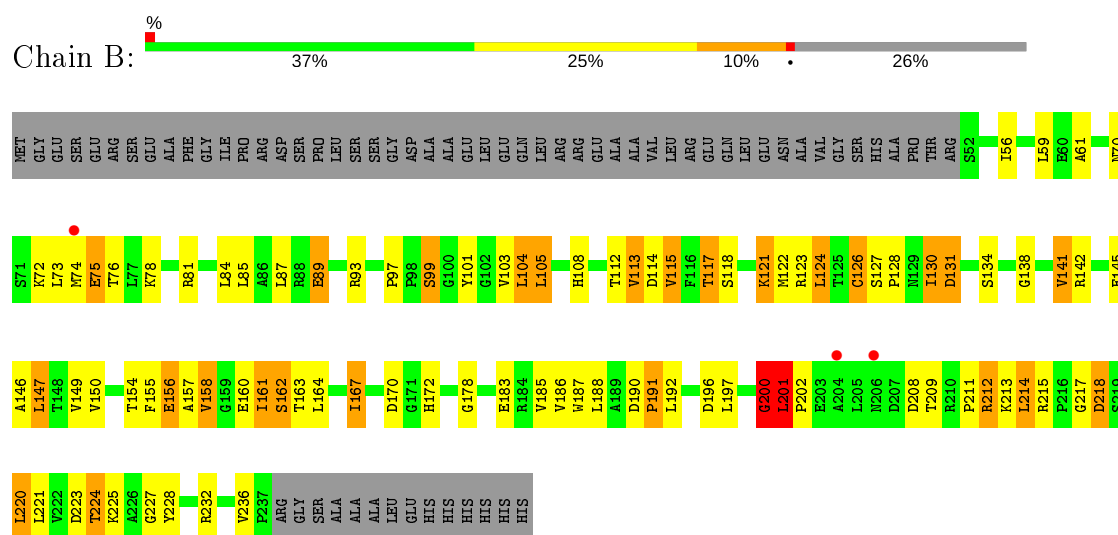
3 Residue-property plots

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

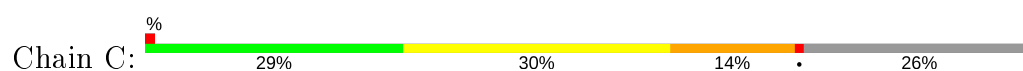
• Molecule 1: Proteasome-associated ATPase



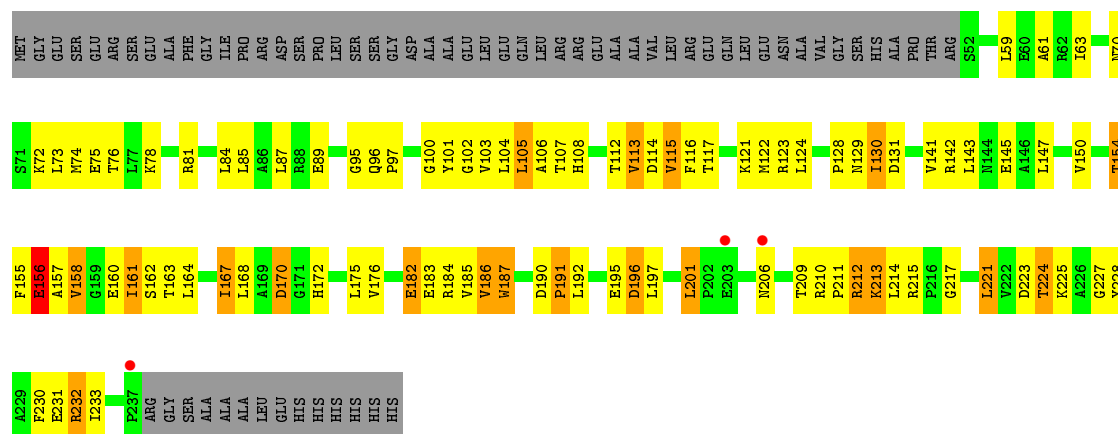
• Molecule 1: Proteasome-associated ATPase



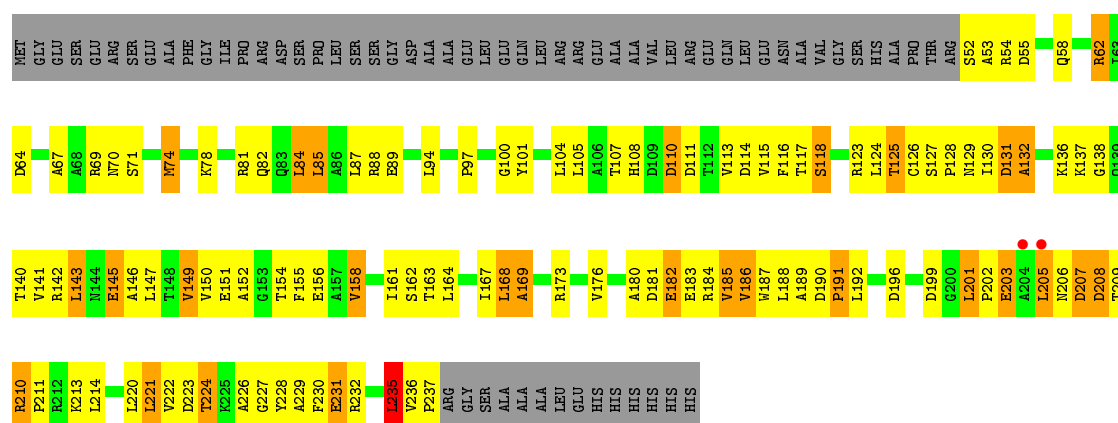
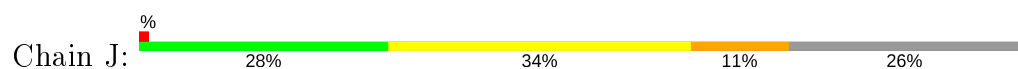
• Molecule 1: Proteasome-associated ATPase



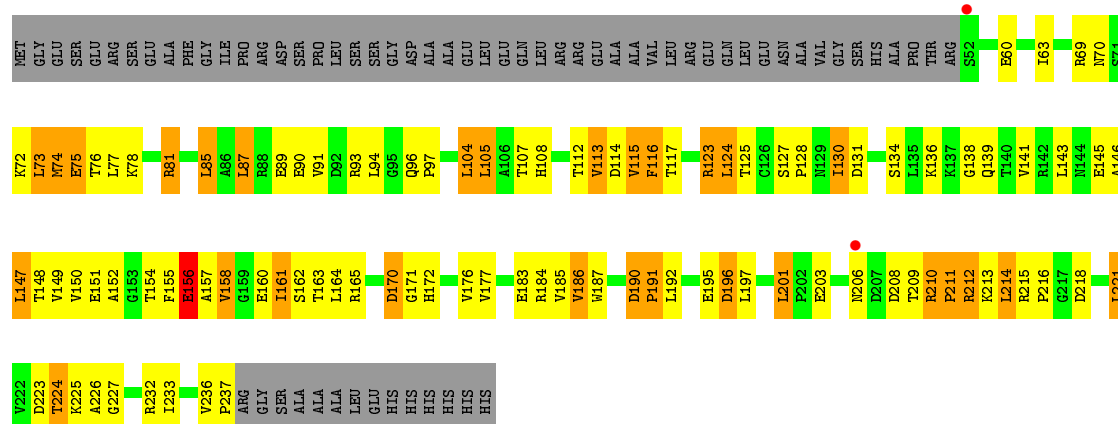
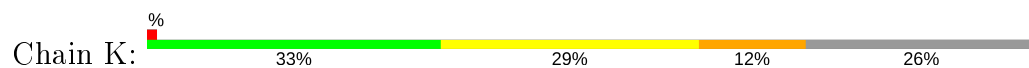




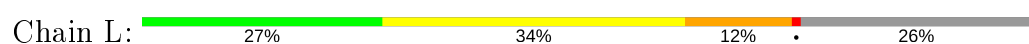
• Molecule 1: Proteasome-associated ATPase

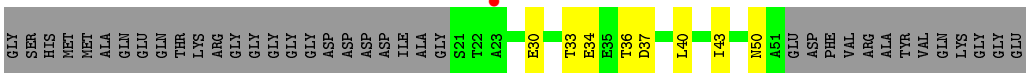


• Molecule 1: Proteasome-associated ATPase

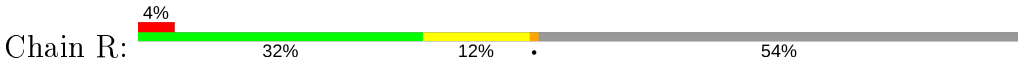


• Molecule 1: Proteasome-associated ATPase





● Molecule 2: Prokaryotic ubiquitin-like protein pup



4 Data and refinement statistics

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

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

¹ Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	M	0	1
All	All	0	5

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	203	GLU	CD-OE2	11.77	1.38	1.25
1	J	208	ASP	CB-CG	7.66	1.67	1.51
1	A	212	ARG	CZ-NH1	-7.20	1.23	1.33
1	E	203	GLU	CG-CD	6.98	1.62	1.51
1	E	208	ASP	CB-CG	6.83	1.66	1.51

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	203	GLU	OE1-CD-OE2	8.52	133.53	123.30
1	J	205	LEU	CA-CB-CG	7.72	133.07	115.30
1	L	205	LEU	CA-CB-CG	7.40	132.32	115.30
1	E	205	LEU	CA-CB-CG	7.25	131.99	115.30
1	E	212	ARG	NE-CZ-NH2	-7.01	116.79	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1431	0	1443	116	0
1	B	1431	0	1443	74	0
1	C	1431	0	1443	98	0
1	D	1431	0	1443	95	0
1	E	1431	0	1443	96	0
1	F	1431	0	1443	90	0
1	J	1431	0	1443	95	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	1431	0	1443	84	0
1	L	1431	0	1443	107	0
1	M	1431	0	1443	99	0
1	N	1431	0	1443	99	0
1	O	1431	0	1443	98	0
2	G	244	0	222	20	0
2	H	244	0	222	12	0
2	I	244	0	222	17	0
2	P	244	0	222	15	0
2	Q	244	0	222	11	0
2	R	244	0	222	14	0
All	All	18636	0	18648	1081	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

The worst 5 of 1081 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:114:ASP:OD1	1:O:123:ARG:HG3	1.41	1.16
1:O:191:PRO:O	1:O:192:LEU:HG	1.46	1.13
1:J:236:VAL:HG12	1:J:237:PRO:HD2	1.27	1.11
1:D:115:VAL:HG21	1:D:124:LEU:HD12	1.30	1.08
1:F:114:ASP:OD1	1:F:123:ARG:HG3	1.56	1.05

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	184/251 (73%)	128 (70%)	35 (19%)	21 (11%)	0 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	184/251 (73%)	148 (80%)	25 (14%)	11 (6%)	1	19
1	C	184/251 (73%)	136 (74%)	32 (17%)	16 (9%)	1	13
1	D	184/251 (73%)	142 (77%)	33 (18%)	9 (5%)	2	23
1	E	184/251 (73%)	133 (72%)	32 (17%)	19 (10%)	0	9
1	F	184/251 (73%)	144 (78%)	29 (16%)	11 (6%)	1	19
1	J	184/251 (73%)	131 (71%)	35 (19%)	18 (10%)	0	10
1	K	184/251 (73%)	145 (79%)	28 (15%)	11 (6%)	1	19
1	L	184/251 (73%)	126 (68%)	37 (20%)	21 (11%)	0	7
1	M	184/251 (73%)	142 (77%)	31 (17%)	11 (6%)	1	19
1	N	184/251 (73%)	132 (72%)	34 (18%)	18 (10%)	0	10
1	O	184/251 (73%)	142 (77%)	26 (14%)	16 (9%)	1	13
2	G	29/68 (43%)	28 (97%)	1 (3%)	0	100	100
2	H	29/68 (43%)	28 (97%)	1 (3%)	0	100	100
2	I	29/68 (43%)	28 (97%)	1 (3%)	0	100	100
2	P	29/68 (43%)	28 (97%)	1 (3%)	0	100	100
2	Q	29/68 (43%)	28 (97%)	1 (3%)	0	100	100
2	R	29/68 (43%)	28 (97%)	1 (3%)	0	100	100
All	All	2382/3420 (70%)	1817 (76%)	383 (16%)	182 (8%)	1	15

5 of 182 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	ASP
1	A	201	LEU
1	A	207	ASP
1	A	209	THR
1	B	191	PRO

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

5 of 461 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	107	THR
1	J	158	VAL
1	O	85	LEU
1	F	147	LEU
1	F	221	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	50	ASN
1	J	139	GLN
2	P	50	ASN
2	H	50	ASN

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Mol	Chain	Res	Type
1	N	139	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

The worst 5 of 50 RSRZ outliers are listed below:

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

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Mol	Chain	Res	Type	RSRZ
1	E	204	ALA	4.0
2	H	21	SER	3.8

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.