



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 28, 2023 – 07:02 AM EDT

PDB ID : 3JTL  
Title : Crystal structure of archaeal 20S proteasome in complex with mutated P26 activator  
Authors : Stadtmueller, B.M.; Whitby, F.G.; Hill, C.P.  
Deposited on : 2009-09-12  
Resolution : 3.20 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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 : 2.35  
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) : 2.35

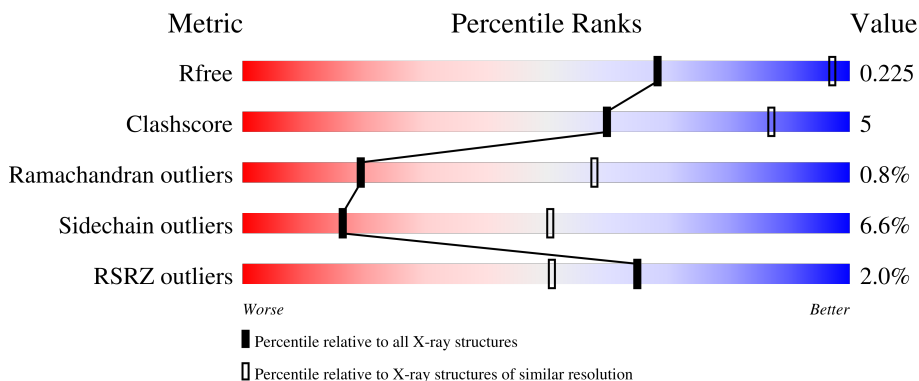
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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  $\geq 3$ , 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	227	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="text-align: center;">3%      82%      17%      .</p>
1	B	227	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="text-align: center;">4%      86%      12%      .</p>
1	C	227	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="text-align: center;">2%      85%      13%      .</p>
1	D	227	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="text-align: center;">4%      83%      15%      .</p>
1	E	227	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="text-align: center;">3%      82%      17%      .</p>

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Mol	Chain	Length	Quality of chain
1	F	227	 4% 82% 17% .
1	G	227	 3% 78% 20% .
2	H	203	 % 82% 15% .
2	I	203	 % 85% 14% .
2	J	203	 2% 83% 14% .
2	K	203	 % 84% 14% .
2	L	203	 % 84% 14% .
2	M	203	 % 84% 14% .
2	N	203	 % 84% 14% .
3	O	228	 % 84% 11% .
3	P	228	 2% 82% 12% . .
3	Q	228	 2% 83% 12% .
3	R	228	 % 84% 11% .
3	S	228	 % 84% 11% .
3	T	228	 2% 85% 10% .
3	U	228	 % 83% 11% . .

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 35140 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 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	227	Total 1769	C 1123	N 299	O 344	S 3	0	0	0
1	B	227	Total 1769	C 1123	N 299	O 344	S 3	0	0	0
1	C	227	Total 1769	C 1123	N 299	O 344	S 3	0	0	0
1	D	227	Total 1769	C 1123	N 299	O 344	S 3	0	0	0
1	E	227	Total 1769	C 1123	N 299	O 344	S 3	0	0	0
1	F	227	Total 1769	C 1123	N 299	O 344	S 3	0	0	0
1	G	227	Total 1769	C 1123	N 299	O 344	S 3	0	0	0

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	203	Total 1557	C 985	N 264	O 297	S 11	0	0	0
2	I	203	Total 1557	C 985	N 264	O 297	S 11	0	0	0
2	J	203	Total 1557	C 985	N 264	O 297	S 11	0	0	0
2	K	203	Total 1557	C 985	N 264	O 297	S 11	0	0	0
2	L	203	Total 1557	C 985	N 264	O 297	S 11	0	0	0
2	M	203	Total 1557	C 985	N 264	O 297	S 11	0	0	0
2	N	203	Total 1557	C 985	N 264	O 297	S 11	0	0	0

- Molecule 3 is a protein called Proteasome activator protein PA26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	O	218	Total	C	N	O	S	0	0	0
			1694	1065	299	325	5			
3	P	218	Total	C	N	O	S	0	0	0
			1694	1065	299	325	5			
3	Q	218	Total	C	N	O	S	0	0	0
			1694	1065	299	325	5			
3	R	218	Total	C	N	O	S	0	0	0
			1694	1065	299	325	5			
3	S	218	Total	C	N	O	S	0	0	0
			1694	1065	299	325	5			
3	T	218	Total	C	N	O	S	0	0	0
			1694	1065	299	325	5			
3	U	218	Total	C	N	O	S	0	0	0
			1694	1065	299	325	5			

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	49	VAL	THR	variant	UNP Q9U8G2
O	225	HIS	GLY	engineered mutation	UNP Q9U8G2
O	226	LEU	SER	engineered mutation	UNP Q9U8G2
O	228	VAL	HIS	engineered mutation	UNP Q9U8G2
O	229	LEU	MET	engineered mutation	UNP Q9U8G2
O	230	TYR	VAL	engineered mutation	UNP Q9U8G2
O	231	ARG	SER	engineered mutation	UNP Q9U8G2
P	49	VAL	THR	variant	UNP Q9U8G2
P	225	HIS	GLY	engineered mutation	UNP Q9U8G2
P	226	LEU	SER	engineered mutation	UNP Q9U8G2
P	228	VAL	HIS	engineered mutation	UNP Q9U8G2
P	229	LEU	MET	engineered mutation	UNP Q9U8G2
P	230	TYR	VAL	engineered mutation	UNP Q9U8G2
P	231	ARG	SER	engineered mutation	UNP Q9U8G2
Q	49	VAL	THR	variant	UNP Q9U8G2
Q	225	HIS	GLY	engineered mutation	UNP Q9U8G2
Q	226	LEU	SER	engineered mutation	UNP Q9U8G2
Q	228	VAL	HIS	engineered mutation	UNP Q9U8G2
Q	229	LEU	MET	engineered mutation	UNP Q9U8G2
Q	230	TYR	VAL	engineered mutation	UNP Q9U8G2
Q	231	ARG	SER	engineered mutation	UNP Q9U8G2
R	49	VAL	THR	variant	UNP Q9U8G2
R	225	HIS	GLY	engineered mutation	UNP Q9U8G2
R	226	LEU	SER	engineered mutation	UNP Q9U8G2

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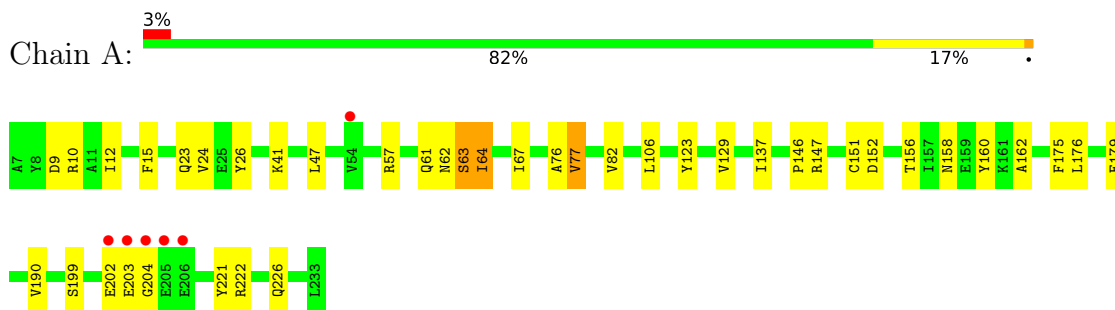
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Chain	Residue	Modelled	Actual	Comment	Reference
R	228	VAL	HIS	engineered mutation	UNP Q9U8G2
R	229	LEU	MET	engineered mutation	UNP Q9U8G2
R	230	TYR	VAL	engineered mutation	UNP Q9U8G2
R	231	ARG	SER	engineered mutation	UNP Q9U8G2
S	49	VAL	THR	variant	UNP Q9U8G2
S	225	HIS	GLY	engineered mutation	UNP Q9U8G2
S	226	LEU	SER	engineered mutation	UNP Q9U8G2
S	228	VAL	HIS	engineered mutation	UNP Q9U8G2
S	229	LEU	MET	engineered mutation	UNP Q9U8G2
S	230	TYR	VAL	engineered mutation	UNP Q9U8G2
S	231	ARG	SER	engineered mutation	UNP Q9U8G2
T	49	VAL	THR	variant	UNP Q9U8G2
T	225	HIS	GLY	engineered mutation	UNP Q9U8G2
T	226	LEU	SER	engineered mutation	UNP Q9U8G2
T	228	VAL	HIS	engineered mutation	UNP Q9U8G2
T	229	LEU	MET	engineered mutation	UNP Q9U8G2
T	230	TYR	VAL	engineered mutation	UNP Q9U8G2
T	231	ARG	SER	engineered mutation	UNP Q9U8G2
U	49	VAL	THR	variant	UNP Q9U8G2
U	225	HIS	GLY	engineered mutation	UNP Q9U8G2
U	226	LEU	SER	engineered mutation	UNP Q9U8G2
U	228	VAL	HIS	engineered mutation	UNP Q9U8G2
U	229	LEU	MET	engineered mutation	UNP Q9U8G2
U	230	TYR	VAL	engineered mutation	UNP Q9U8G2
U	231	ARG	SER	engineered mutation	UNP Q9U8G2

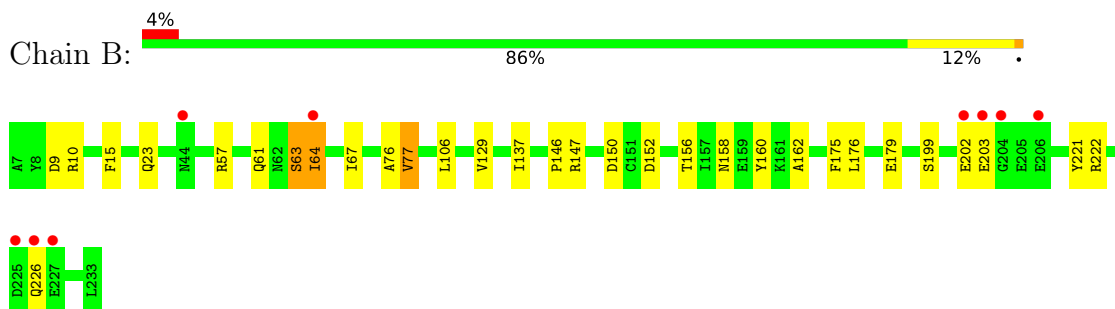
### 3 Residue-property plots [i](#)

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.

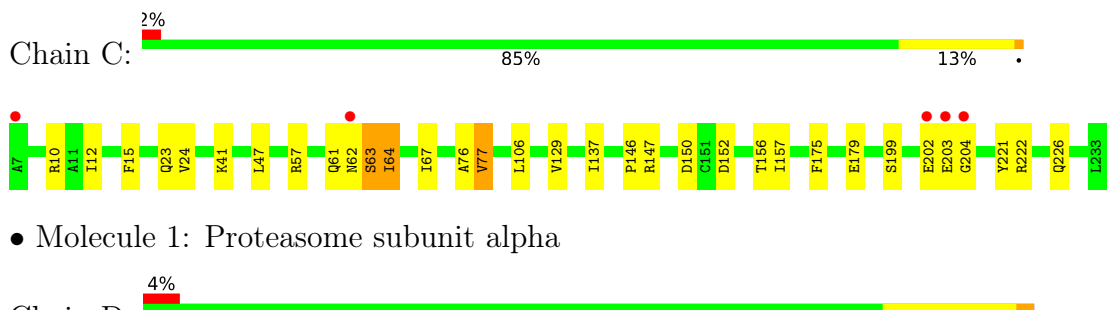
- Molecule 1: Proteasome subunit alpha



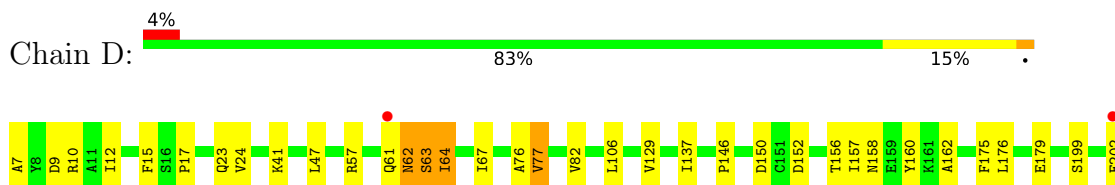
- Molecule 1: Proteasome subunit alpha

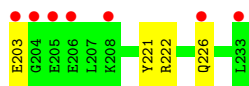


- Molecule 1: Proteasome subunit alpha

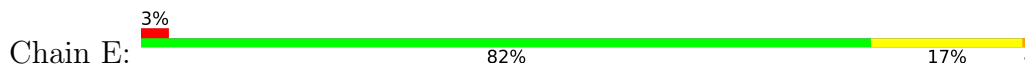


- Molecule 1: Proteasome subunit alpha

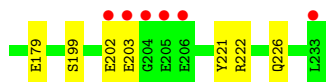
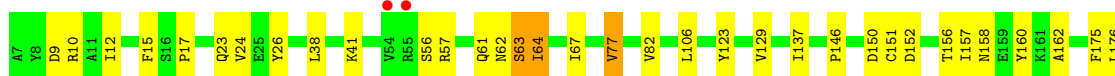
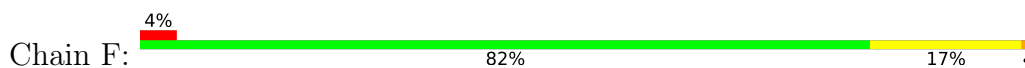




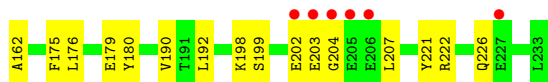
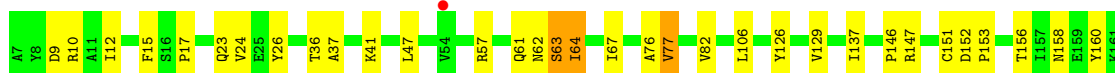
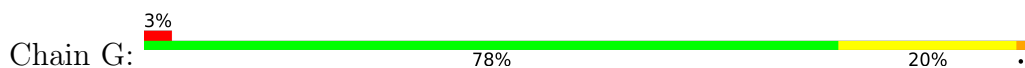
• Molecule 1: Proteasome subunit alpha



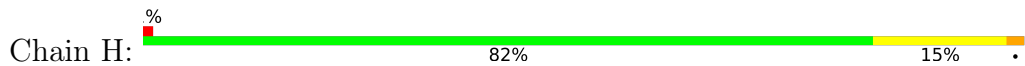
• Molecule 1: Proteasome subunit alpha



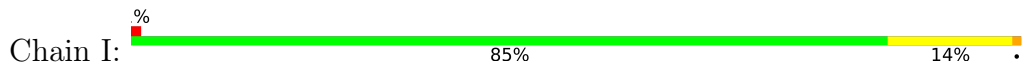
• Molecule 1: Proteasome subunit alpha



• Molecule 2: Proteasome subunit beta



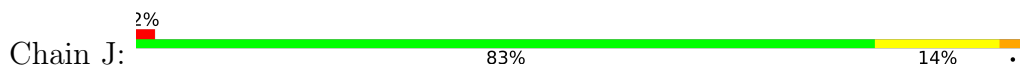
• Molecule 2: Proteasome subunit beta



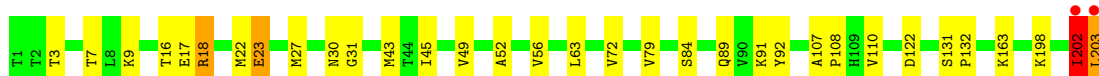
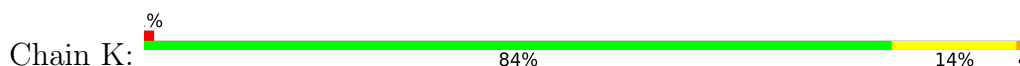




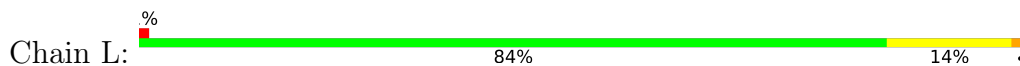
● Molecule 2: Proteasome subunit beta



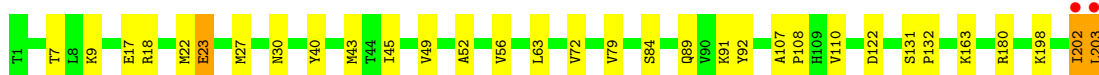
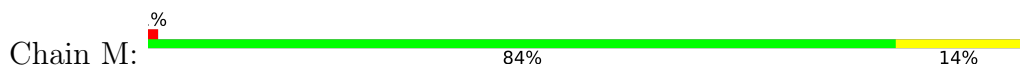
● Molecule 2: Proteasome subunit beta



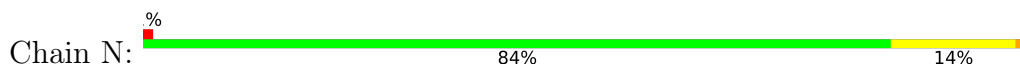
● Molecule 2: Proteasome subunit beta



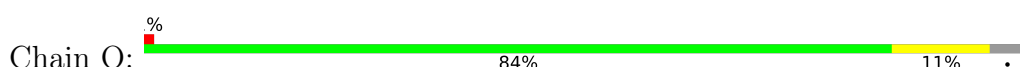
● Molecule 2: Proteasome subunit beta



● Molecule 2: Proteasome subunit beta

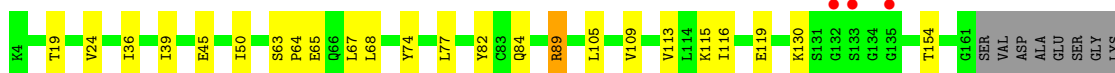
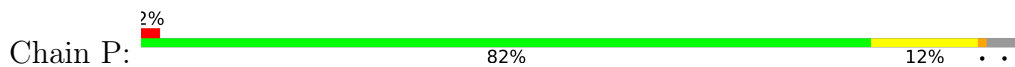


● Molecule 3: Proteasome activator protein PA26

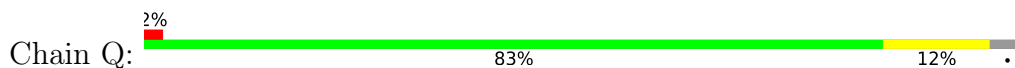




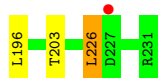
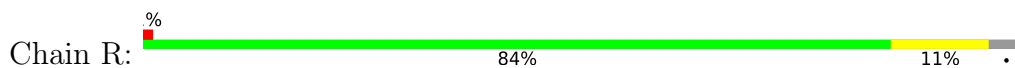
- Molecule 3: Proteasome activator protein PA26



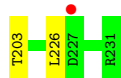
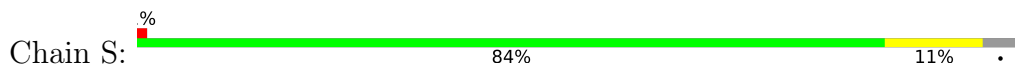
- Molecule 3: Proteasome activator protein PA26



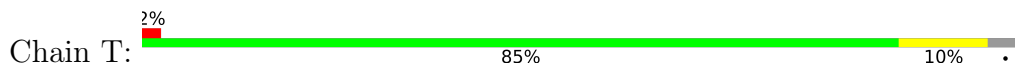
- Molecule 3: Proteasome activator protein PA26



- Molecule 3: Proteasome activator protein PA26

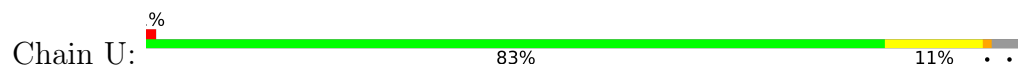


- Molecule 3: Proteasome activator protein PA26





● Molecule 3: Proteasome activator protein PA26



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	255.83Å 126.58Å 182.17Å 90.00° 92.95° 90.00°	Depositor
Resolution (Å)	29.85 – 3.20 29.85 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.85-3.20) 99.0 (29.85-3.20)	Depositor EDS
$R_{merge}$	0.26	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 3.18Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.194 , 0.226 0.199 , 0.225	Depositor DCC
$R_{free}$ test set	1905 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.0	Xtrriage
Anisotropy	0.050	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 21.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.002 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	35140	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [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	0.78	1/1793 (0.1%)	0.75	0/2416
1	B	0.77	0/1793	0.74	0/2416
1	C	0.77	0/1793	0.75	0/2416
1	D	0.81	1/1793 (0.1%)	0.75	0/2416
1	E	0.81	1/1793 (0.1%)	0.78	0/2416
1	F	0.77	1/1793 (0.1%)	0.77	0/2416
1	G	0.77	1/1793 (0.1%)	0.74	0/2416
2	H	0.83	1/1576 (0.1%)	0.80	0/2129
2	I	0.83	3/1576 (0.2%)	0.80	1/2129 (0.0%)
2	J	0.81	1/1576 (0.1%)	0.80	2/2129 (0.1%)
2	K	0.84	3/1576 (0.2%)	0.80	1/2129 (0.0%)
2	L	0.83	1/1576 (0.1%)	0.78	1/2129 (0.0%)
2	M	0.86	2/1576 (0.1%)	0.81	2/2129 (0.1%)
2	N	0.85	3/1576 (0.2%)	0.81	2/2129 (0.1%)
3	O	0.74	0/1718	0.72	0/2322
3	P	0.71	0/1718	0.73	2/2322 (0.1%)
3	Q	0.72	0/1718	0.72	0/2322
3	R	0.75	0/1718	0.72	1/2322 (0.0%)
3	S	0.74	0/1718	0.71	0/2322
3	T	0.73	0/1718	0.72	0/2322
3	U	0.77	1/1718 (0.1%)	0.72	1/2322 (0.0%)
All	All	0.78	20/35609 (0.1%)	0.76	13/48069 (0.0%)

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
3	T	0	1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	22	MET	CG-SD	6.40	1.97	1.81
3	U	35	GLU	CG-CD	6.27	1.61	1.51
1	E	7	ALA	CA-CB	6.17	1.65	1.52
1	A	151	CYS	CB-SG	-6.11	1.71	1.82
2	M	22	MET	CB-CG	5.91	1.70	1.51

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	184	ARG	NE-CZ-NH2	-5.66	117.47	120.30
2	J	22	MET	CG-SD-CE	5.59	109.15	100.20
2	M	22	MET	CB-CG-SD	5.54	129.01	112.40
2	N	22	MET	CG-SD-CE	5.52	109.03	100.20
2	N	22	MET	CB-CG-SD	5.50	128.89	112.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	T	223	ARG	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	1769	0	1800	19	0
1	B	1769	0	1800	12	0
1	C	1769	0	1800	13	0
1	D	1769	0	1800	24	0
1	E	1769	0	1800	25	2
1	F	1769	0	1800	28	0
1	G	1769	0	1800	25	0
2	H	1557	0	1609	18	0
2	I	1557	0	1609	17	0
2	J	1557	0	1609	16	0
2	K	1557	0	1609	16	0
2	L	1557	0	1609	16	0
2	M	1557	0	1609	15	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	1557	0	1609	15	0
3	O	1694	0	1722	19	0
3	P	1694	0	1722	18	0
3	Q	1694	0	1722	16	0
3	R	1694	0	1722	15	1
3	S	1694	0	1722	13	0
3	T	1694	0	1722	15	0
3	U	1694	0	1722	20	1
All	All	35140	0	35917	325	3

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 5.

The worst 5 of 325 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)
2:N:43:MET:CE	2:N:56:VAL:HG22	2.02	0.90
2:I:43:MET:CE	2:I:56:VAL:HG22	2.03	0.89
3:T:89:ARG:HD3	3:U:203:THR:HG21	1.54	0.86
2:J:43:MET:CE	2:J:56:VAL:HG22	2.06	0.85
3:S:89:ARG:HD3	3:T:203:THR:HG21	1.59	0.84

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:14:ASP:OD1	3:U:45:GLU:OE1[4_555]	1.98	0.22
1:E:181:LYS:NZ	2:M:180:ARG:O[4_546]	2.03	0.17
1:E:181:LYS:CE	2:M:180:ARG:O[4_546]	2.14	0.06

## 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	225/227 (99%)	213 (95%)	9 (4%)	3 (1%)	12	47
1	B	225/227 (99%)	214 (95%)	9 (4%)	2 (1%)	17	56
1	C	225/227 (99%)	215 (96%)	7 (3%)	3 (1%)	12	47
1	D	225/227 (99%)	215 (96%)	8 (4%)	2 (1%)	17	56
1	E	225/227 (99%)	215 (96%)	7 (3%)	3 (1%)	12	47
1	F	225/227 (99%)	214 (95%)	8 (4%)	3 (1%)	12	47
1	G	225/227 (99%)	215 (96%)	7 (3%)	3 (1%)	12	47
2	H	201/203 (99%)	187 (93%)	12 (6%)	2 (1%)	15	54
2	I	201/203 (99%)	187 (93%)	12 (6%)	2 (1%)	15	54
2	J	201/203 (99%)	185 (92%)	14 (7%)	2 (1%)	15	54
2	K	201/203 (99%)	187 (93%)	12 (6%)	2 (1%)	15	54
2	L	201/203 (99%)	187 (93%)	12 (6%)	2 (1%)	15	54
2	M	201/203 (99%)	188 (94%)	11 (6%)	2 (1%)	15	54
2	N	201/203 (99%)	186 (92%)	13 (6%)	2 (1%)	15	54
3	O	214/228 (94%)	208 (97%)	5 (2%)	1 (0%)	29	67
3	P	214/228 (94%)	206 (96%)	7 (3%)	1 (0%)	29	67
3	Q	214/228 (94%)	209 (98%)	4 (2%)	1 (0%)	29	67
3	R	214/228 (94%)	207 (97%)	6 (3%)	1 (0%)	29	67
3	S	214/228 (94%)	206 (96%)	8 (4%)	0	100	100
3	T	214/228 (94%)	208 (97%)	5 (2%)	1 (0%)	29	67
3	U	214/228 (94%)	208 (97%)	6 (3%)	0	100	100
All	All	4480/4606 (97%)	4260 (95%)	182 (4%)	38 (1%)	19	58

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	ILE
1	B	64	ILE
1	C	64	ILE
1	D	64	ILE
1	E	64	ILE



### 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	188/188 (100%)	175 (93%)	13 (7%)	15	49
1	B	188/188 (100%)	175 (93%)	13 (7%)	15	49
1	C	188/188 (100%)	174 (93%)	14 (7%)	13	46
1	D	188/188 (100%)	174 (93%)	14 (7%)	13	46
1	E	188/188 (100%)	175 (93%)	13 (7%)	15	49
1	F	188/188 (100%)	174 (93%)	14 (7%)	13	46
1	G	188/188 (100%)	175 (93%)	13 (7%)	15	49
2	H	170/170 (100%)	157 (92%)	13 (8%)	13	45
2	I	170/170 (100%)	157 (92%)	13 (8%)	13	45
2	J	170/170 (100%)	156 (92%)	14 (8%)	11	41
2	K	170/170 (100%)	157 (92%)	13 (8%)	13	45
2	L	170/170 (100%)	156 (92%)	14 (8%)	11	41
2	M	170/170 (100%)	157 (92%)	13 (8%)	13	45
2	N	170/170 (100%)	155 (91%)	15 (9%)	10	36
3	O	180/188 (96%)	172 (96%)	8 (4%)	28	64
3	P	180/188 (96%)	170 (94%)	10 (6%)	21	57
3	Q	180/188 (96%)	170 (94%)	10 (6%)	21	57
3	R	180/188 (96%)	173 (96%)	7 (4%)	32	67
3	S	180/188 (96%)	171 (95%)	9 (5%)	24	60
3	T	180/188 (96%)	173 (96%)	7 (4%)	32	67
3	U	180/188 (96%)	172 (96%)	8 (4%)	28	64
All	All	3766/3822 (98%)	3518 (93%)	248 (7%)	16	51

5 of 248 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	84	SER
3	R	119	GLU

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Mol	Chain	Res	Type
2	K	89	GLN
3	R	65	GLU
3	T	68	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	191	GLN
3	O	79	HIS
3	U	79	HIS
2	N	191	GLN
2	H	191	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	227/227 (100%)	-0.27	6 (2%) 56 40	23, 40, 69, 79	0
1	B	227/227 (100%)	-0.21	9 (3%) 38 25	23, 40, 69, 79	0
1	C	227/227 (100%)	-0.26	5 (2%) 62 48	23, 40, 69, 79	0
1	D	227/227 (100%)	-0.22	9 (3%) 38 25	23, 40, 69, 79	0
1	E	227/227 (100%)	-0.20	6 (2%) 56 40	23, 40, 69, 79	0
1	F	227/227 (100%)	-0.23	8 (3%) 44 28	23, 40, 69, 79	0
1	G	227/227 (100%)	-0.17	7 (3%) 49 32	23, 40, 69, 79	0
2	H	203/203 (100%)	-0.33	2 (0%) 82 72	24, 34, 54, 71	0
2	I	203/203 (100%)	-0.42	2 (0%) 82 72	24, 34, 54, 71	0
2	J	203/203 (100%)	-0.37	4 (1%) 65 51	24, 34, 54, 71	0
2	K	203/203 (100%)	-0.38	2 (0%) 82 72	24, 34, 54, 71	0
2	L	203/203 (100%)	-0.37	2 (0%) 82 72	24, 34, 54, 71	0
2	M	203/203 (100%)	-0.37	2 (0%) 82 72	24, 34, 54, 71	0
2	N	203/203 (100%)	-0.39	2 (0%) 82 72	24, 35, 54, 71	0
3	O	218/228 (95%)	-0.28	3 (1%) 75 63	25, 40, 55, 64	0
3	P	218/228 (95%)	-0.32	5 (2%) 60 47	26, 40, 55, 64	0
3	Q	218/228 (95%)	-0.35	5 (2%) 60 47	26, 40, 55, 64	0
3	R	218/228 (95%)	-0.30	3 (1%) 75 63	25, 40, 55, 64	0
3	S	218/228 (95%)	-0.40	3 (1%) 75 63	25, 40, 55, 64	0
3	T	218/228 (95%)	-0.31	4 (1%) 68 55	25, 40, 55, 64	0
3	U	218/228 (95%)	-0.34	3 (1%) 75 63	25, 40, 55, 64	0
All	All	4536/4606 (98%)	-0.31	92 (2%) 65 51	23, 38, 63, 79	0

The worst 5 of 92 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	202	ILE	7.4
2	K	202	ILE	6.1
2	H	202	ILE	5.4
2	J	202	ILE	5.3
2	N	202	ILE	5.1

## 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.