



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:50 AM GMT

PDB ID : 3JRM
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 : 2009-09-08
Resolution : 2.90 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

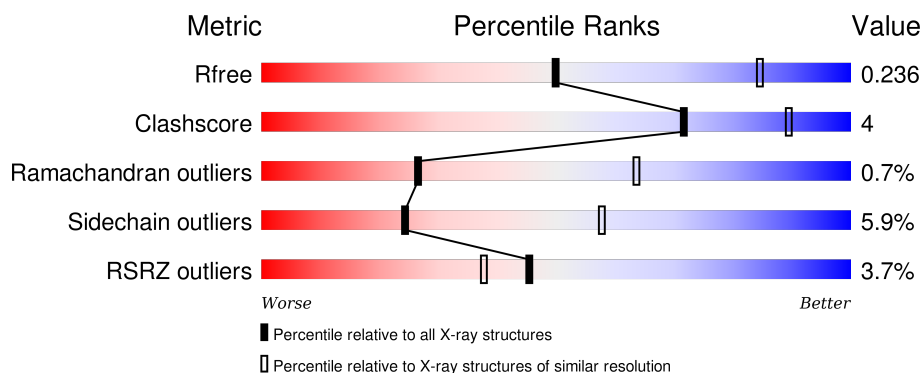
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	227	<div> <div>7%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>
1	B	227	<div> <div>6%</div> <div>86%</div> <div>11%</div> <div>.</div> </div>
1	C	227	<div> <div>4%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>
1	D	227	<div> <div>6%</div> <div>89%</div> <div>7%</div> <div>.</div> </div>
1	E	227	<div> <div>5%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	227	
1	G	227	
2	H	203	
2	I	203	
2	J	203	
2	K	203	
2	L	203	
2	M	203	
2	N	203	
3	O	228	
3	P	228	
3	Q	228	
3	R	228	
3	S	228	
3	T	228	
3	U	228	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 35035 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
1	A	227	Total	C	N	O	S	0	0	0
			1768	1123	299	343	3			
1	B	227	Total	C	N	O	S	0	0	0
			1768	1123	299	343	3			
1	C	227	Total	C	N	O	S	0	0	0
			1768	1123	299	343	3			
1	D	227	Total	C	N	O	S	0	0	0
			1768	1123	299	343	3			
1	E	227	Total	C	N	O	S	0	0	0
			1768	1123	299	343	3			
1	F	227	Total	C	N	O	S	0	0	0
			1768	1123	299	343	3			
1	G	227	Total	C	N	O	S	0	0	0
			1768	1123	299	343	3			

- Molecule 2 is a protein called Proteasome subunit beta.

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

- 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
			1680	1054	296	324	6			
3	P	218	Total	C	N	O	S	0	0	0
			1680	1054	296	324	6			
3	Q	218	Total	C	N	O	S	0	0	0
			1680	1054	296	324	6			
3	R	218	Total	C	N	O	S	0	0	0
			1680	1054	296	324	6			
3	S	218	Total	C	N	O	S	0	0	0
			1680	1054	296	324	6			
3	T	218	Total	C	N	O	S	0	0	0
			1680	1054	296	324	6			
3	U	218	Total	C	N	O	S	0	0	0
			1680	1054	296	324	6			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	49	VAL	THR	VARIANT	UNP Q9U8G2
O	102	ALA	GLU	ENGINEERED	UNP Q9U8G2
O	230	TYR	VAL	ENGINEERED	UNP Q9U8G2
O	226	THR	SER	ENGINEERED	UNP Q9U8G2
P	49	VAL	THR	VARIANT	UNP Q9U8G2
P	102	ALA	GLU	ENGINEERED	UNP Q9U8G2
P	230	TYR	VAL	ENGINEERED	UNP Q9U8G2
O	226	THR	SER	ENGINEERED	UNP Q9U8G2
Q	49	VAL	THR	VARIANT	UNP Q9U8G2
Q	102	ALA	GLU	ENGINEERED	UNP Q9U8G2
Q	230	TYR	VAL	ENGINEERED	UNP Q9U8G2
O	226	THR	SER	ENGINEERED	UNP Q9U8G2
R	49	VAL	THR	VARIANT	UNP Q9U8G2
R	102	ALA	GLU	ENGINEERED	UNP Q9U8G2
R	230	TYR	VAL	ENGINEERED	UNP Q9U8G2
O	226	THR	SER	ENGINEERED	UNP Q9U8G2
S	49	VAL	THR	VARIANT	UNP Q9U8G2
S	102	ALA	GLU	ENGINEERED	UNP Q9U8G2
S	230	TYR	VAL	ENGINEERED	UNP Q9U8G2
O	226	THR	SER	ENGINEERED	UNP Q9U8G2
T	49	VAL	THR	VARIANT	UNP Q9U8G2
T	102	ALA	GLU	ENGINEERED	UNP Q9U8G2
T	230	TYR	VAL	ENGINEERED	UNP Q9U8G2
O	226	THR	SER	ENGINEERED	UNP Q9U8G2

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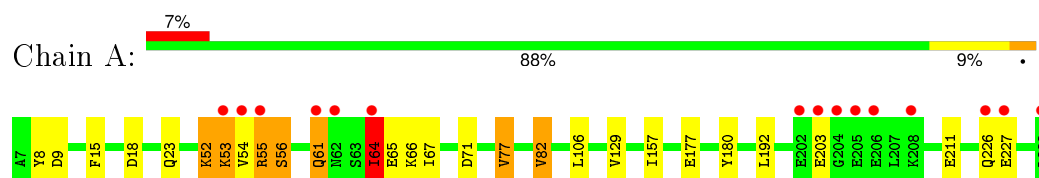
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Chain	Residue	Modelled	Actual	Comment	Reference
U	49	VAL	THR	VARIANT	UNP Q9U8G2
U	102	ALA	GLU	ENGINEERED	UNP Q9U8G2
U	230	TYR	VAL	ENGINEERED	UNP Q9U8G2

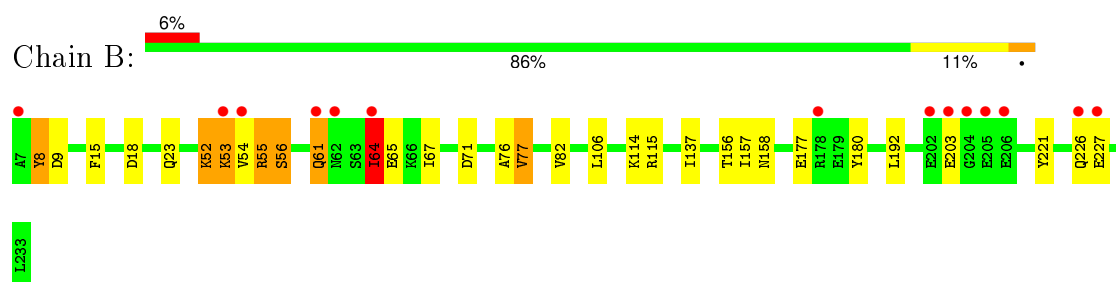
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

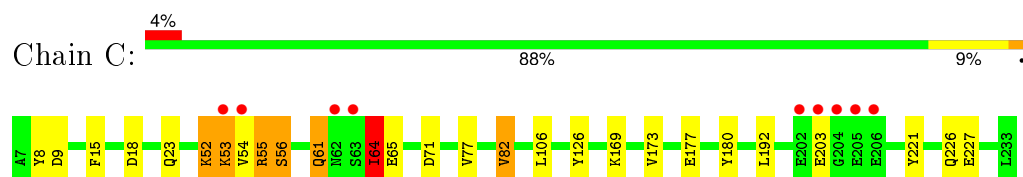
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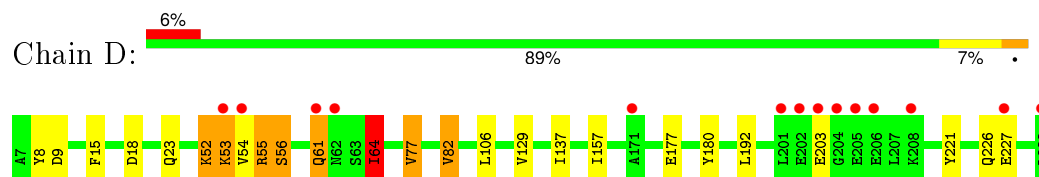
- Molecule 1: Proteasome subunit alpha



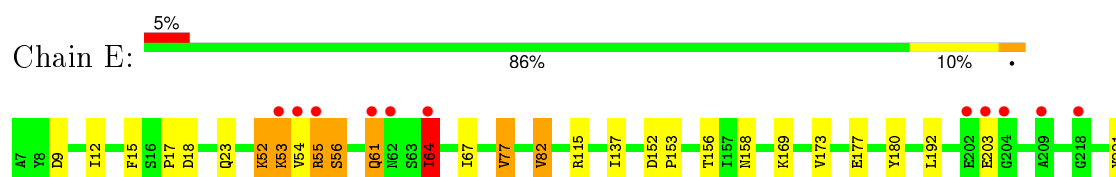
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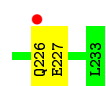


- Molecule 1: Proteasome subunit alpha

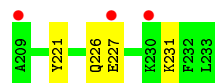
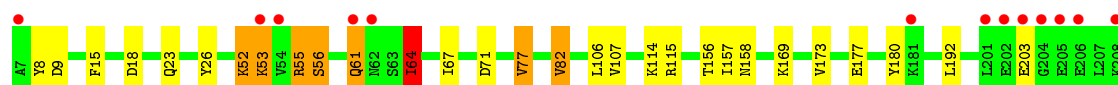
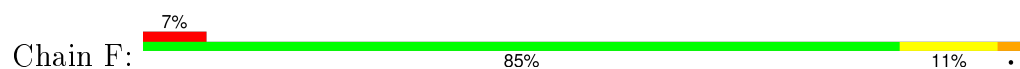


- Molecule 1: Proteasome subunit alpha

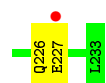
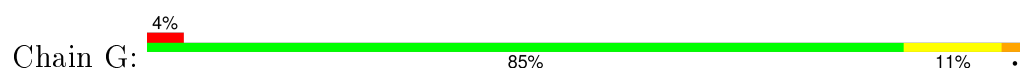




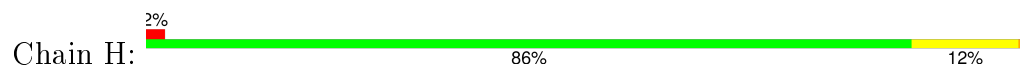
- Molecule 1: Proteasome subunit alpha



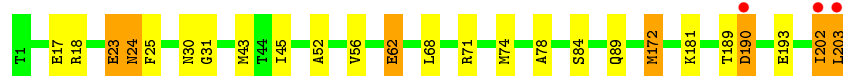
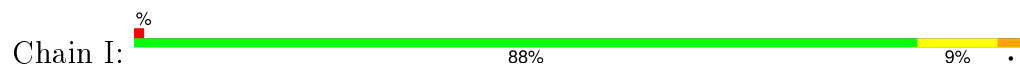
- Molecule 1: Proteasome subunit alpha



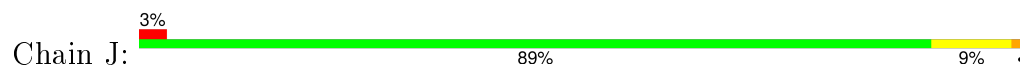
- Molecule 2: Proteasome subunit beta



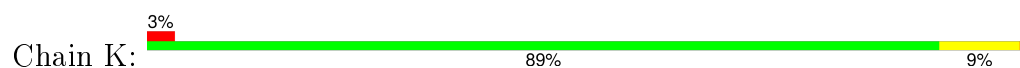
- Molecule 2: Proteasome subunit beta

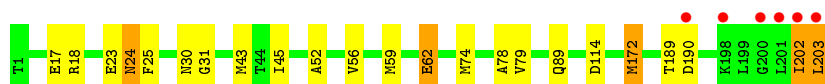


- Molecule 2: Proteasome subunit beta

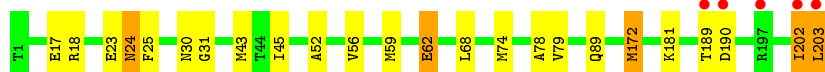
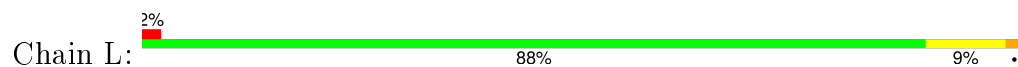


- Molecule 2: Proteasome subunit beta

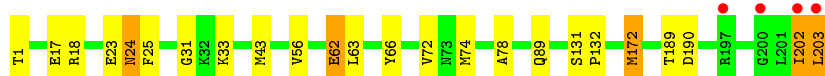
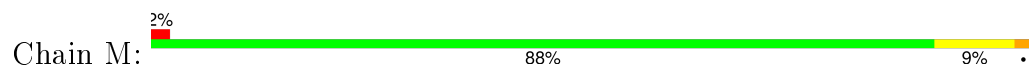




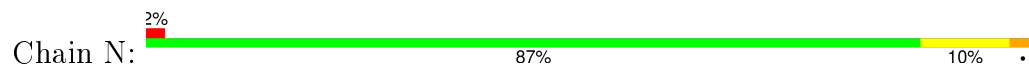
- Molecule 2: Proteasome subunit beta



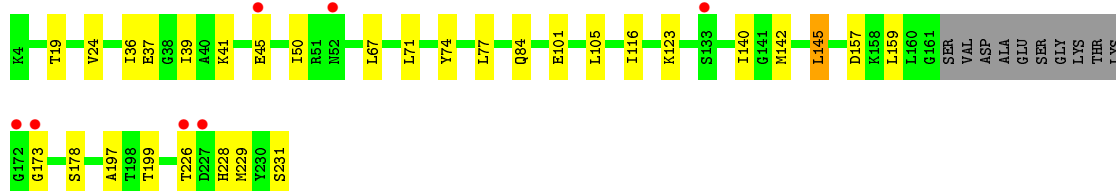
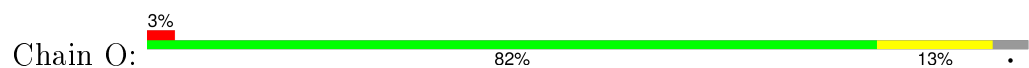
- Molecule 2: Proteasome subunit beta



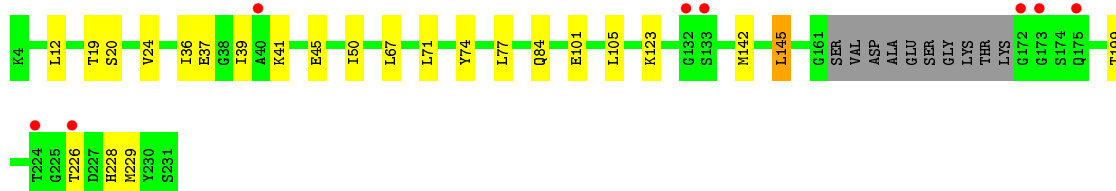
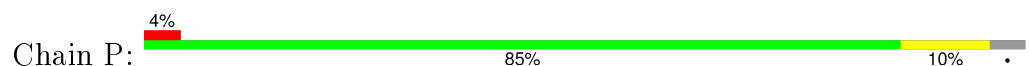
- Molecule 2: Proteasome subunit beta



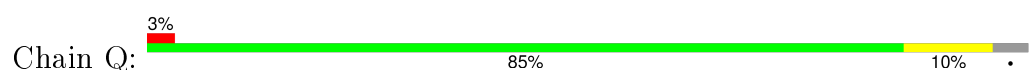
- Molecule 3: Proteasome activator protein PA26

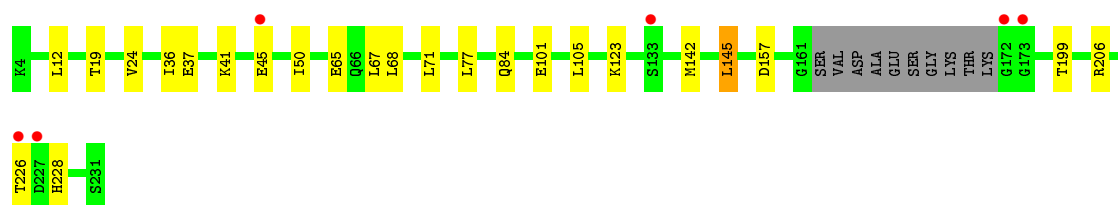


- Molecule 3: Proteasome activator protein PA26

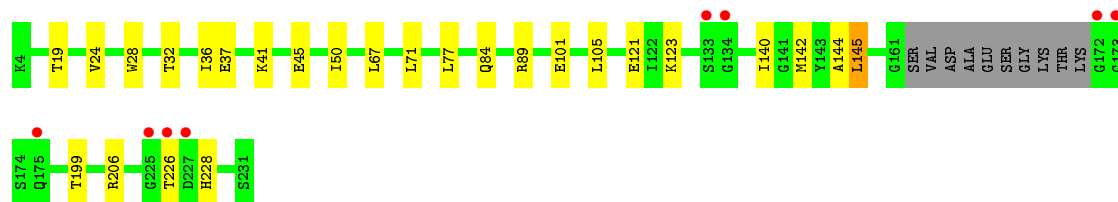
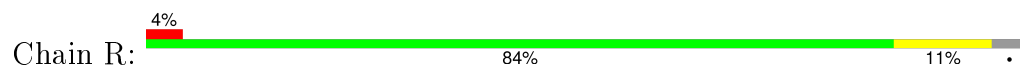


- Molecule 3: Proteasome activator protein PA26

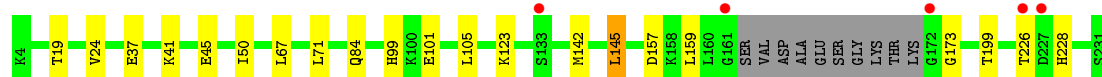
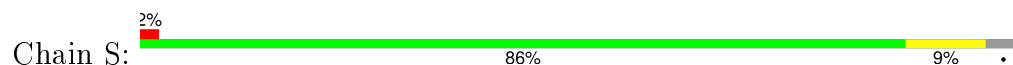




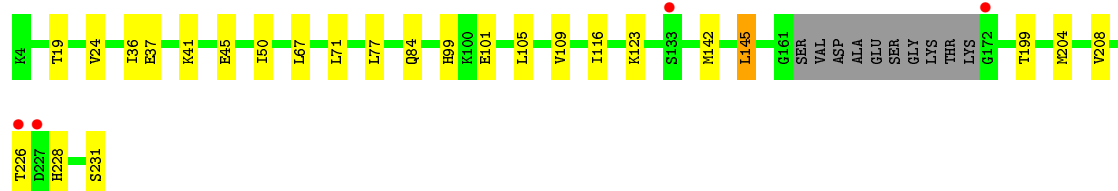
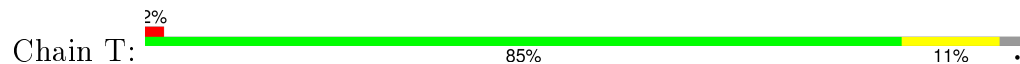
• Molecule 3: Proteasome activator protein PA26



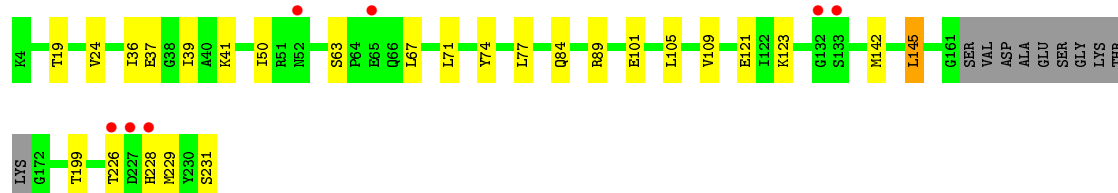
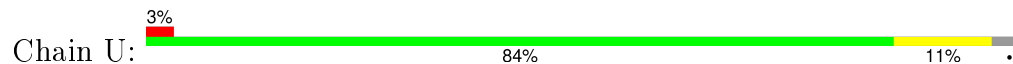
• Molecule 3: Proteasome activator protein PA26



• Molecule 3: Proteasome activator protein PA26



• Molecule 3: Proteasome activator protein PA26



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	255.07Å 126.36Å 180.78Å 90.00° 92.54° 90.00°	Depositor
Resolution (Å)	29.82 – 2.90 29.82 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.82-2.90) 98.6 (29.82-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.201 , 0.233 0.207 , 0.236	Depositor DCC
R_{free} test set	2516 reflections (2.05%)	DCC
Wilson B-factor (Å ²)	46.3	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 24.8	EDS
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	2 of 125182 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	35035	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [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	0.71	0/1792	0.70	0/2416
1	B	0.72	0/1792	0.71	1/2416 (0.0%)
1	C	0.72	0/1792	0.71	0/2416
1	D	0.72	0/1792	0.70	0/2416
1	E	0.70	0/1792	0.71	1/2416 (0.0%)
1	F	0.71	0/1792	0.73	1/2416 (0.0%)
1	G	0.73	0/1792	0.70	0/2416
2	H	0.71	1/1576 (0.1%)	0.73	0/2129
2	I	0.73	2/1576 (0.1%)	0.74	0/2129
2	J	0.73	0/1576	0.74	0/2129
2	K	0.73	2/1576 (0.1%)	0.72	0/2129
2	L	0.72	2/1576 (0.1%)	0.73	0/2129
2	M	0.72	2/1576 (0.1%)	0.73	1/2129 (0.0%)
2	N	0.73	1/1576 (0.1%)	0.73	1/2129 (0.0%)
3	O	0.65	0/1704	0.67	0/2304
3	P	0.64	0/1704	0.66	0/2304
3	Q	0.66	0/1704	0.65	0/2304
3	R	0.65	0/1704	0.67	0/2304
3	S	0.65	0/1704	0.67	0/2304
3	T	0.66	0/1704	0.68	0/2304
3	U	0.64	0/1704	0.67	0/2304
All	All	0.70	10/35504 (0.0%)	0.70	5/47943 (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
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	F	0	1
1	G	0	2
All	All	0	12

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	62	GLU	CG-CD	5.95	1.60	1.51
2	I	62	GLU	CG-CD	5.77	1.60	1.51
2	N	62	GLU	CG-CD	5.62	1.60	1.51
2	K	203	LEU	N-CA	5.50	1.57	1.46
2	H	203	LEU	N-CA	5.35	1.57	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	115	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	B	115	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	E	115	ARG	NE-CZ-NH1	5.13	122.87	120.30
2	N	203	LEU	CA-CB-CG	5.08	126.98	115.30
2	M	203	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	54	VAL	Peptide
1	A	8	TYR	Peptide
1	B	54	VAL	Peptide
1	B	8	TYR	Peptide
1	C	8	TYR	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	1768	0	1800	17	0
1	B	1768	0	1800	18	0
1	C	1768	0	1800	17	0
1	D	1768	0	1800	19	0
1	E	1768	0	1800	24	0
1	F	1768	0	1800	28	0
1	G	1768	0	1800	21	0
2	H	1557	0	1609	17	0
2	I	1557	0	1609	16	0
2	J	1557	0	1609	15	0
2	K	1557	0	1609	12	0
2	L	1557	0	1609	15	0
2	M	1557	0	1609	15	0
2	N	1557	0	1609	15	0
3	O	1680	0	1701	19	0
3	P	1680	0	1701	15	0
3	Q	1680	0	1701	13	0
3	R	1680	0	1701	14	0
3	S	1680	0	1701	13	0
3	T	1680	0	1701	21	0
3	U	1680	0	1701	19	0
All	All	35035	0	35770	305	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 4.

The worst 5 of 305 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)
3:R:50:ILE:HD11	3:R:67:LEU:HD21	1.64	0.77
3:Q:50:ILE:HD11	3:Q:67:LEU:HD21	1.67	0.77
2:I:43:MET:CE	2:I:56:VAL:HG22	2.15	0.76
3:S:50:ILE:HD11	3:S:67:LEU:HD21	1.67	0.76
3:O:50:ILE:HD11	3:O:67:LEU:HD21	1.69	0.75

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	215 (96%)	7 (3%)	3 (1%)	15	46
1	B	225/227 (99%)	216 (96%)	6 (3%)	3 (1%)	15	46
1	C	225/227 (99%)	215 (96%)	7 (3%)	3 (1%)	15	46
1	D	225/227 (99%)	215 (96%)	7 (3%)	3 (1%)	15	46
1	E	225/227 (99%)	213 (95%)	9 (4%)	3 (1%)	15	46
1	F	225/227 (99%)	215 (96%)	6 (3%)	4 (2%)	11	37
1	G	225/227 (99%)	213 (95%)	9 (4%)	3 (1%)	15	46
2	H	201/203 (99%)	193 (96%)	7 (4%)	1 (0%)	34	71
2	I	201/203 (99%)	193 (96%)	6 (3%)	2 (1%)	19	54
2	J	201/203 (99%)	192 (96%)	7 (4%)	2 (1%)	19	54
2	K	201/203 (99%)	193 (96%)	7 (4%)	1 (0%)	34	71
2	L	201/203 (99%)	193 (96%)	7 (4%)	1 (0%)	34	71
2	M	201/203 (99%)	192 (96%)	8 (4%)	1 (0%)	34	71
2	N	201/203 (99%)	193 (96%)	6 (3%)	2 (1%)	19	54
3	O	214/228 (94%)	210 (98%)	4 (2%)	0	100	100
3	P	214/228 (94%)	210 (98%)	4 (2%)	0	100	100
3	Q	214/228 (94%)	210 (98%)	4 (2%)	0	100	100
3	R	214/228 (94%)	210 (98%)	4 (2%)	0	100	100
3	S	214/228 (94%)	210 (98%)	4 (2%)	0	100	100
3	T	214/228 (94%)	210 (98%)	4 (2%)	0	100	100
3	U	214/228 (94%)	210 (98%)	4 (2%)	0	100	100
All	All	4480/4606 (97%)	4321 (96%)	127 (3%)	32 (1%)	26	63

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	SER
1	B	56	SER
1	C	56	SER
1	D	56	SER
1	E	56	SER

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	188/188 (100%)	176 (94%)	12 (6%)	22	53
1	B	188/188 (100%)	175 (93%)	13 (7%)	19	48
1	C	188/188 (100%)	175 (93%)	13 (7%)	19	48
1	D	188/188 (100%)	175 (93%)	13 (7%)	19	48
1	E	188/188 (100%)	176 (94%)	12 (6%)	22	53
1	F	188/188 (100%)	175 (93%)	13 (7%)	19	48
1	G	188/188 (100%)	175 (93%)	13 (7%)	19	48
2	H	170/170 (100%)	159 (94%)	11 (6%)	21	52
2	I	170/170 (100%)	158 (93%)	12 (7%)	18	47
2	J	170/170 (100%)	159 (94%)	11 (6%)	21	52
2	K	170/170 (100%)	160 (94%)	10 (6%)	24	58
2	L	170/170 (100%)	159 (94%)	11 (6%)	21	52
2	M	170/170 (100%)	160 (94%)	10 (6%)	24	58
2	N	170/170 (100%)	160 (94%)	10 (6%)	24	58
3	O	178/186 (96%)	169 (95%)	9 (5%)	29	65
3	P	178/186 (96%)	169 (95%)	9 (5%)	29	65
3	Q	178/186 (96%)	169 (95%)	9 (5%)	29	65
3	R	178/186 (96%)	170 (96%)	8 (4%)	34	70
3	S	178/186 (96%)	169 (95%)	9 (5%)	29	65
3	T	178/186 (96%)	170 (96%)	8 (4%)	34	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	U	178/186 (96%)	171 (96%)	7 (4%)	39 75
All	All	3752/3808 (98%)	3529 (94%)	223 (6%)	24 58

5 of 223 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	17	GLU
2	K	23	GLU
3	S	157	ASP
2	I	25	PHE
2	J	23	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	24	ASN
3	O	79	HIS
3	T	228	HIS
2	M	24	ASN
2	N	24	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	227/227 (100%)	-0.00	15 (6%)	22 16	26, 37, 61, 65	0
1	B	227/227 (100%)	0.05	14 (6%)	24 17	26, 37, 61, 65	0
1	C	227/227 (100%)	0.02	9 (3%)	42 35	26, 37, 61, 65	0
1	D	227/227 (100%)	0.05	14 (6%)	24 17	26, 37, 61, 65	0
1	E	227/227 (100%)	0.02	12 (5%)	30 23	26, 37, 61, 65	0
1	F	227/227 (100%)	0.03	16 (7%)	19 13	26, 37, 61, 65	0
1	G	227/227 (100%)	0.04	9 (3%)	42 35	26, 37, 61, 65	0
2	H	203/203 (100%)	-0.14	4 (1%)	68 64	25, 33, 47, 61	0
2	I	203/203 (100%)	-0.24	3 (1%)	76 74	25, 33, 47, 61	0
2	J	203/203 (100%)	-0.15	7 (3%)	49 41	25, 33, 47, 61	0
2	K	203/203 (100%)	-0.17	6 (2%)	54 47	25, 33, 47, 61	0
2	L	203/203 (100%)	-0.20	5 (2%)	61 55	25, 33, 47, 61	0
2	M	203/203 (100%)	-0.22	4 (1%)	68 64	25, 33, 47, 61	0
2	N	203/203 (100%)	-0.26	5 (2%)	61 55	25, 33, 47, 61	0
3	O	218/228 (95%)	-0.00	7 (3%)	51 43	31, 40, 51, 60	0
3	P	218/228 (95%)	-0.07	8 (3%)	45 38	30, 40, 51, 60	0
3	Q	218/228 (95%)	-0.06	6 (2%)	56 50	31, 40, 51, 60	0
3	R	218/228 (95%)	-0.01	8 (3%)	45 38	30, 40, 51, 60	0
3	S	218/228 (95%)	-0.13	5 (2%)	64 59	30, 40, 51, 60	0
3	T	218/228 (95%)	-0.05	4 (1%)	71 68	30, 40, 51, 60	0
3	U	218/228 (95%)	-0.07	7 (3%)	51 43	30, 40, 51, 60	0
All	All	4536/4606 (98%)	-0.07	168 (3%)	45 38	25, 37, 54, 65	0

The worst 5 of 168 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	202	ILE	10.2
2	J	202	ILE	7.3
2	K	202	ILE	7.0
2	M	202	ILE	6.4
2	H	202	ILE	6.3

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.