



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2025 – 01:20 pm BST

PDB ID : 9QD2 / pdb\_00009qd2  
Title : Yeast 20S proteasome mutant: beta1\_G128V (b1-propeptide deleted) in complex with MG132  
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.  
Deposited on : 2025-03-05  
Resolution : 2.70 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](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	:	<b>FAILED</b>
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	<b>FAILED</b>
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

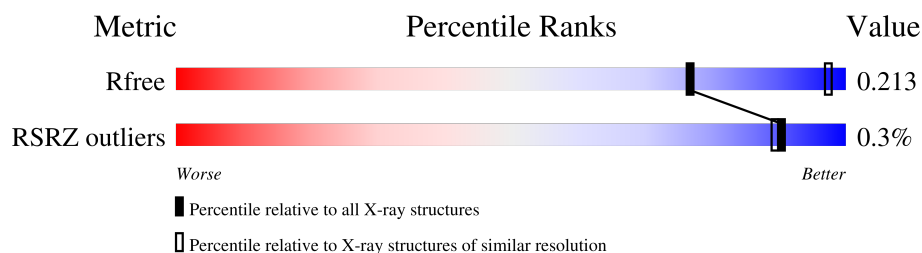
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	164625	3333 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49779 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 type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			
2	P	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			
3	Q	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			
4	R	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			
5	S	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			

- Molecule 6 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			
6	T	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			
7	U	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			

- Molecule 8 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	221	Total	C	N	O	S	0	0	0
			1677	1057	292	321	7			
8	V	221	Total	C	N	O	S	0	0	0
			1677	1057	292	321	7			

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1637	1041	279	310	7			
11	Y	211	Total	C	N	O	S	0	0	0
			1637	1041	279	310	7			

- Molecule 12 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 13 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	a	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	195	Total	C	N	O	S	0	0	0
			1508	954	249	298	7			
14	b	195	Total	C	N	O	S	0	0	0
			1508	954	249	298	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	128	VAL	GLY	engineered mutation	UNP P38624
b	128	VAL	GLY	engineered mutation	UNP P38624

- Molecule 15 is a protein called 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-C]PYRAZ

OLE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	d	4	Total 41	C 30	N 4	O 7	0	0	0
15	e	4	Total 41	C 30	N 4	O 7	0	0	0
15	f	4	Total 41	C 30	N 4	O 7	0	0	0
15	g	4	Total 41	C 30	N 4	O 7	0	0	0
15	h	4	Total 41	C 30	N 4	O 7	0	0	0
15	i	4	Total 41	C 30	N 4	O 7	0	0	0

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total 1	Mg 1	0	0
16	I	1	Total 1	Mg 1	0	0
16	J	1	Total 1	Mg 1	0	0
16	Z	1	Total 1	Mg 1	0	0

- Molecule 17 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	G	2	Total 2	Cl 2	0	0
17	N	1	Total 1	Cl 1	0	0
17	U	1	Total 1	Cl 1	0	0
17	b	1	Total 1	Cl 1	0	0

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	a	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	6	Total	O	0	0
			6	6		
19	B	13	Total	O	0	0
			13	13		
19	C	12	Total	O	0	0
			12	12		
19	D	9	Total	O	0	0
			9	9		
19	E	4	Total	O	0	0
			4	4		
19	F	6	Total	O	0	0
			6	6		
19	G	7	Total	O	0	0
			7	7		
19	H	16	Total	O	0	0
			16	16		
19	I	8	Total	O	0	0
			8	8		
19	J	13	Total	O	0	0
			13	13		
19	K	9	Total	O	0	0
			9	9		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	L	18	Total O 18 18	0	0
19	M	9	Total O 9 9	0	0
19	N	5	Total O 5 5	0	0
19	O	5	Total O 5 5	0	0
19	P	5	Total O 5 5	0	0
19	Q	8	Total O 8 8	0	0
19	R	3	Total O 3 3	0	0
19	S	4	Total O 4 4	0	0
19	T	8	Total O 8 8	0	0
19	U	11	Total O 11 11	0	0
19	V	9	Total O 9 9	0	0
19	W	9	Total O 9 9	0	0
19	X	14	Total O 14 14	0	0
19	Y	11	Total O 11 11	0	0
19	Z	7	Total O 7 7	0	0
19	a	9	Total O 9 9	0	0
19	b	9	Total O 9 9	0	0
19	d	1	Total O 1 1	0	0
19	e	1	Total O 1 1	0	0
19	g	1	Total O 1 1	0	0
19	h	2	Total O 2 2	0	0



MolProbity failed to run properly - this section is therefore empty.

### 3 Data and refinement statistics

Xtriage (Phenix) failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.23Å 300.11Å 145.77Å 90.00° 113.25° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.2 (15.00-2.70) 97.2 (15.00-2.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.176 , 0.214 (Not available) , 0.213	Depositor DCC
$R_{free}$ test set	14253 reflections (5.00%)	wwPDB-VP
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 58.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	49779	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

validation-pack failed to run properly - this section is therefore empty.

### 4.5 Carbohydrates [i](#)

validation-pack failed to run properly - this section is therefore empty.

### 4.6 Ligand geometry [i](#)

validation-pack failed to run properly - this section is therefore empty.

### 4.7 Other polymers [i](#)

validation-pack failed to run properly - this section is therefore empty.

## 4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 5 Fit of model and data ⓘ

### 5.1 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, 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	250/250 (100%)	-0.78	1 (0%) 89 88	54, 70, 101, 177	0
1	O	250/250 (100%)	-0.73	1 (0%) 89 88	59, 77, 115, 172	0
2	B	244/258 (94%)	-0.61	3 (1%) 76 76	56, 74, 121, 169	0
2	P	244/258 (94%)	-0.58	2 (0%) 82 82	61, 79, 124, 173	0
3	C	240/254 (94%)	-0.66	1 (0%) 89 88	56, 77, 131, 156	0
3	Q	240/254 (94%)	-0.53	4 (1%) 69 68	60, 90, 152, 178	0
4	D	235/260 (90%)	-0.72	0 100 100	58, 79, 110, 151	0
4	R	235/260 (90%)	-0.63	1 (0%) 89 88	56, 80, 115, 151	0
5	E	231/234 (98%)	-0.71	0 100 100	59, 82, 114, 139	0
5	S	231/234 (98%)	-0.62	0 100 100	62, 86, 120, 157	0
6	F	243/288 (84%)	-0.69	0 100 100	55, 77, 117, 140	0
6	T	243/288 (84%)	-0.64	0 100 100	58, 83, 128, 147	0
7	G	241/252 (95%)	-0.74	0 100 100	54, 70, 100, 134	0
7	U	241/252 (95%)	-0.74	0 100 100	58, 73, 104, 143	0
8	H	221/231 (95%)	-0.84	0 100 100	54, 66, 89, 120	0
8	V	221/231 (95%)	-0.80	0 100 100	56, 69, 91, 135	0
9	I	204/205 (99%)	-0.85	0 100 100	50, 65, 90, 117	0
9	W	204/205 (99%)	-0.87	0 100 100	51, 68, 96, 116	0
10	J	195/198 (98%)	-0.66	1 (0%) 87 86	52, 68, 95, 128	0
10	X	195/198 (98%)	-0.66	1 (0%) 87 86	55, 72, 94, 138	0
11	K	211/211 (100%)	-0.77	0 100 100	53, 66, 91, 177	0
11	Y	211/211 (100%)	-0.71	0 100 100	52, 67, 96, 181	0
12	L	222/222 (100%)	-0.66	1 (0%) 87 86	52, 70, 101, 121	0
12	Z	222/222 (100%)	-0.69	1 (0%) 87 86	53, 67, 99, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/246 (94%)	-0.80	1 (0%) 89 88	53, 71, 91, 111	0
13	a	233/246 (94%)	-0.83	0 100 100	51, 69, 91, 111	0
14	N	195/195 (100%)	-0.66	1 (0%) 87 86	53, 69, 117, 149	0
14	b	195/195 (100%)	-0.67	0 100 100	52, 69, 118, 151	0
15	d	2/4 (50%)	-0.09	0 100 100	87, 87, 87, 96	0
15	e	2/4 (50%)	-0.81	0 100 100	71, 71, 71, 71	0
15	f	2/4 (50%)	-0.41	0 100 100	86, 86, 86, 89	0
15	g	2/4 (50%)	0.78	0 100 100	92, 92, 92, 101	0
15	h	2/4 (50%)	-1.26	0 100 100	77, 77, 77, 77	0
15	i	2/4 (50%)	-0.19	0 100 100	81, 81, 81, 84	0
All	All	6342/6632 (95%)	-0.71	19 (0%) 90 89	50, 73, 114, 181	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	205	ALA	4.0
10	X	1	MET	3.7
14	N	135	TYR	3.4
1	A	1	MET	3.3
2	B	219	ALA	3.2
1	O	1	MET	3.2
2	P	219	ALA	3.2
3	Q	50	LEU	2.7
3	Q	51	LYS	2.7
10	J	1	MET	2.6
13	M	1	THR	2.5
12	Z	160	TYR	2.4
2	B	218	GLY	2.4
2	B	51	VAL	2.4
2	P	51	VAL	2.4
4	R	113	LEU	2.3
3	C	205	ALA	2.3
3	Q	49	THR	2.2
12	L	136	CYS	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
15	A1I48	f	4	15/16	0.94	0.11	69,75,88,93	0
15	A1I48	d	4	15/16	0.95	0.11	62,76,89,90	0
15	A1I48	h	4	15/16	0.95	0.09	67,71,73,74	0
15	A1I48	g	4	15/16	0.96	0.09	66,77,86,90	0
15	A1I48	i	4	15/16	0.97	0.09	71,80,84,84	0
15	A1I48	e	4	15/16	0.98	0.06	62,67,70,71	0

## 5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
16	MG	I	301	1/1	0.85	0.17	109,109,109,109	0
18	MES	a	301	12/12	0.87	0.14	122,130,143,149	0
16	MG	Z	301	1/1	0.93	0.13	99,99,99,99	0
16	MG	G	301	1/1	0.93	0.11	82,82,82,82	0
16	MG	J	201	1/1	0.94	0.10	30,30,30,30	0
17	CL	G	303	1/1	0.95	0.21	30,30,30,30	0
17	CL	U	301	1/1	0.97	0.04	70,70,70,70	0
17	CL	G	302	1/1	0.98	0.03	64,64,64,64	0
17	CL	b	201	1/1	0.98	0.06	81,81,81,81	0
17	CL	N	201	1/1	0.98	0.04	79,79,79,79	0

## 5.5 Other polymers [i](#)

There are no such residues in this entry.