



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2025 – 01:19 pm BST

PDB ID : 9QAI / pdb_00009qai
Title : Yeast 20S proteasome mutant: beta5_T3M in complex with MG132
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.
Deposited on : 2025-02-28
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	FAILED
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

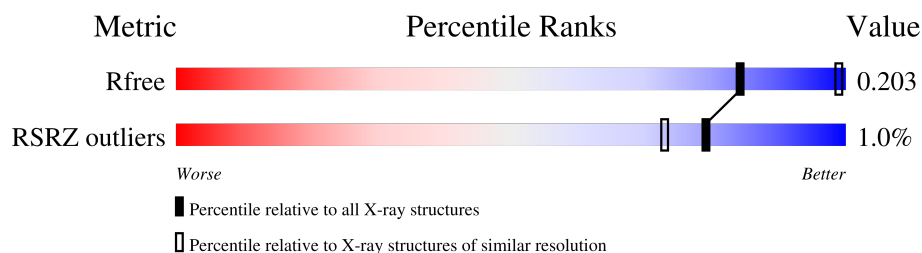
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3657 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49851 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	225	Total	C	N	O	S	0	0	0
			1712	1078	297	330	7			
8	V	225	Total	C	N	O	S	0	0	0
			1712	1078	297	330	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
			1638	1042	279	309	8			
11	Y	211	Total	C	N	O	S	0	0	0
			1638	1042	279	309	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	3	MET	THR	engineered mutation	UNP P30656
Y	3	MET	THR	engineered mutation	UNP P30656

- 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	231	Total	C	N	O	S	0	0	0
			1806	1142	309	348	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
			1505	951	249	298	7			
14	b	195	Total	C	N	O	S	0	0	0
			1505	951	249	298	7			

- 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	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
15	j	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	K	1	Total 1	Mg 1	0	0
16	M	1	Total 1	Mg 1	0	0
16	N	1	Total 1	Mg 1	0	0
16	V	1	Total 1	Mg 1	0	0
16	X	1	Total 1	Mg 1	0	0
16	Y	1	Total 1	Mg 1	0	0
16	Z	1	Total 1	Mg 1	0	0
16	b	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	1	Total Cl 1 1	0	0
17	N	1	Total Cl 1 1	0	0
17	U	1	Total Cl 1 1	0	0
17	b	1	Total Cl 1 1	0	0

- Molecule 18 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	11	Total O 11 11	0	0
18	B	15	Total O 15 15	0	0
18	C	10	Total O 10 10	0	0
18	D	8	Total O 8 8	0	0
18	E	6	Total O 6 6	0	0
18	F	16	Total O 16 16	0	0
18	G	9	Total O 9 9	0	0
18	H	14	Total O 14 14	0	0
18	I	8	Total O 8 8	0	0
18	J	11	Total O 11 11	0	0
18	K	10	Total O 10 10	0	0
18	L	15	Total O 15 15	0	0
18	M	16	Total O 16 16	0	0
18	N	5	Total O 5 5	0	0
18	O	6	Total O 6 6	0	0
18	P	8	Total O 8 8	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	Q	8	Total O 8 8	0	0
18	R	3	Total O 3 3	0	0
18	S	5	Total O 5 5	0	0
18	T	11	Total O 11 11	0	0
18	U	14	Total O 14 14	0	0
18	V	6	Total O 6 6	0	0
18	W	7	Total O 7 7	0	0
18	X	9	Total O 9 9	0	0
18	Y	10	Total O 10 10	0	0
18	Z	14	Total O 14 14	0	0
18	a	12	Total O 12 12	0	0
18	b	11	Total O 11 11	0	0
18	f	1	Total O 1 1	0	0
18	g	1	Total O 1 1	0	0
18	i	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, α , β , γ	136.13Å 300.28Å 145.70Å 90.00° 113.08° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.1 (15.00-2.80) 96.5 (15.00-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.187 , 0.205 (Not available) , 0.203	Depositor DCC
R_{free} test set	12695 reflections (5.00%)	wwPDB-VP
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 56.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49851	wwPDB-VP
Average B, all atoms (Å ²)	69.0	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, 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	250/250 (100%)	-0.54	1 (0%) 89 85	42, 57, 94, 133	0
1	O	250/250 (100%)	-0.53	2 (0%) 82 77	46, 66, 111, 146	0
2	B	244/258 (94%)	-0.37	4 (1%) 70 63	44, 65, 111, 169	0
2	P	244/258 (94%)	-0.37	4 (1%) 70 63	43, 69, 111, 169	0
3	C	240/254 (94%)	-0.35	2 (0%) 82 77	43, 69, 135, 167	0
3	Q	240/254 (94%)	-0.09	9 (3%) 44 36	53, 84, 170, 192	0
4	D	235/260 (90%)	-0.36	2 (0%) 81 75	50, 72, 106, 150	0
4	R	235/260 (90%)	-0.24	0 100 100	55, 75, 119, 154	0
5	E	231/234 (98%)	-0.38	1 (0%) 89 85	51, 73, 112, 154	0
5	S	231/234 (98%)	-0.22	0 100 100	52, 79, 125, 159	0
6	F	243/288 (84%)	-0.44	2 (0%) 82 77	41, 67, 117, 143	0
6	T	243/288 (84%)	-0.31	4 (1%) 70 63	40, 73, 134, 162	0
7	G	241/252 (95%)	-0.52	0 100 100	41, 61, 102, 158	0
7	U	241/252 (95%)	-0.54	0 100 100	45, 61, 97, 143	0
8	H	225/231 (97%)	-0.57	1 (0%) 89 85	40, 56, 94, 153	0
8	V	225/231 (97%)	-0.50	2 (0%) 81 75	43, 59, 93, 181	0
9	I	204/205 (99%)	-0.68	0 100 100	39, 55, 87, 114	0
9	W	204/205 (99%)	-0.69	0 100 100	40, 58, 90, 110	0
10	J	195/198 (98%)	-0.56	2 (1%) 79 73	40, 59, 89, 125	0
10	X	195/198 (98%)	-0.52	2 (1%) 79 73	40, 62, 89, 138	0
11	K	211/211 (100%)	-0.47	0 100 100	41, 60, 92, 114	0
11	Y	211/211 (100%)	-0.46	0 100 100	45, 60, 94, 113	0
12	L	222/222 (100%)	-0.31	8 (3%) 46 38	43, 61, 109, 139	0
12	Z	222/222 (100%)	-0.35	9 (4%) 42 34	45, 60, 108, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	231/246 (93%)	-0.58	2 (0%) 81 75	39, 59, 86, 105	0
13	a	233/246 (94%)	-0.62	1 (0%) 89 85	39, 57, 84, 108	0
14	N	195/195 (100%)	-0.66	0 100 100	38, 51, 83, 109	0
14	b	195/195 (100%)	-0.71	0 100 100	37, 52, 82, 112	0
15	e	2/4 (50%)	1.46	0 100 100	98, 98, 98, 99	0
15	f	2/4 (50%)	1.78	1 (50%) 0 1	99, 99, 99, 102	0
15	g	2/4 (50%)	0.66	0 100 100	69, 69, 69, 96	0
15	h	2/4 (50%)	2.38	2 (100%) 0 0	106, 106, 106, 110	0
15	i	2/4 (50%)	1.75	1 (50%) 0 1	105, 105, 105, 110	0
15	j	2/4 (50%)	-0.02	0 100 100	71, 71, 71, 86	0
All	All	6348/6632 (95%)	-0.45	62 (0%) 79 73	37, 64, 111, 192	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	Z	174	TYR	5.4
12	L	174	TYR	5.3
3	Q	50	LEU	5.1
12	L	165	ASN	3.8
13	a	1	THR	3.7
2	B	51	VAL	3.7
12	Z	168	VAL	3.6
3	Q	205	ALA	3.4
3	Q	49	THR	3.3
13	M	1	THR	3.2
10	X	1	MET	3.0
12	L	168	VAL	3.0
8	V	223	ILE	3.0
2	B	218	GLY	2.9
8	H	223	ILE	2.9
3	Q	206	LYS	2.9
4	D	240	ALA	2.9
15	f	3	LEU	2.8
2	P	51	VAL	2.8
12	L	170	LYS	2.8
2	P	218	GLY	2.8
6	F	202	ASP	2.7
10	X	2	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
12	L	136	CYS	2.7
2	B	219	ALA	2.6
15	h	3	LEU	2.6
12	Z	163	GLY	2.6
12	L	164	THR	2.6
12	Z	169	LYS	2.5
10	J	1	MET	2.5
8	V	224	GLN	2.5
12	L	169	LYS	2.5
12	Z	165	ASN	2.5
12	Z	170	LYS	2.5
12	Z	172	LEU	2.5
12	Z	173	LYS	2.4
2	B	1	GLY	2.4
13	M	47	ASP	2.4
3	Q	234	ILE	2.3
6	F	215	CYS	2.3
5	E	123	GLY	2.3
12	L	172	LEU	2.3
6	T	204	LYS	2.3
1	A	1	MET	2.2
3	Q	48	SER	2.2
15	i	3	LEU	2.2
3	C	58	THR	2.2
1	O	2	THR	2.2
2	P	219	ALA	2.2
4	D	241	ALA	2.2
3	Q	52	LEU	2.2
15	h	2	LEU	2.2
12	Z	166	GLY	2.1
3	Q	175	LYS	2.1
2	P	52	THR	2.1
3	C	186	VAL	2.1
1	O	1	MET	2.1
6	T	14	ASP	2.0
10	J	174	MET	2.0
3	Q	51	LYS	2.0
6	T	215	CYS	2.0
6	T	243	ILE	2.0

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, 95th 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 ²)	Q<0.9
15	A1I48	h	4	15/16	0.93	0.14	55,78,120,124	0
15	A1I48	i	4	15/16	0.94	0.14	59,79,124,127	0
15	A1I48	e	4	15/16	0.95	0.12	52,78,93,94	0
15	A1I48	g	4	15/16	0.95	0.15	53,93,114,118	0
15	A1I48	j	4	15/16	0.95	0.16	58,95,107,128	0
15	A1I48	f	4	15/16	0.96	0.11	57,79,96,96	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, 95th 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 ²)	Q<0.9
16	MG	V	301	1/1	0.93	0.15	76,76,76,76	0
16	MG	Y	301	1/1	0.94	0.06	61,61,61,61	0
16	MG	M	301	1/1	0.95	0.09	59,59,59,59	0
16	MG	I	301	1/1	0.96	0.07	65,65,65,65	0
16	MG	Z	301	1/1	0.96	0.07	74,74,74,74	0
16	MG	X	201	1/1	0.97	0.15	43,43,43,43	0
16	MG	G	301	1/1	0.97	0.04	59,59,59,59	0
16	MG	K	301	1/1	0.97	0.12	64,64,64,64	0
16	MG	J	201	1/1	0.98	0.17	47,47,47,47	0
16	MG	N	201	1/1	0.98	0.05	49,49,49,49	0
16	MG	b	201	1/1	0.98	0.03	48,48,48,48	0
17	CL	b	202	1/1	0.98	0.06	67,67,67,67	0
17	CL	N	202	1/1	0.99	0.06	55,55,55,55	0
17	CL	G	302	1/1	0.99	0.08	44,44,44,44	0
17	CL	U	301	1/1	1.00	0.07	45,45,45,45	0

5.5 Other polymers [i](#)

There are no such residues in this entry.