



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jul 24, 2017 – 02:18 PM EDT

PDB ID : 5MPA  
EMDB ID: : EMD-3535  
Title : 26S proteasome in presence of ATP (s2)  
Authors : Wehmer, M.; Rudack, T.; Beck, F.; Aufderheide, A.; Pfeifer, G.; Plitzko, J.M.;  
Foerster, F.; Schulten, K.; Baumeister, W.; Sakata, E.  
Deposited on : unknown  
Resolution : 4.50 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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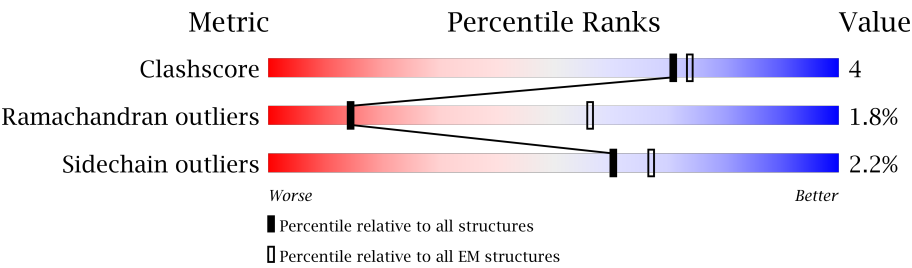
MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	252	80% 13% . .
1	a	252	81% 14% . .
2	B	250	77% 20% .
2	b	250	86% 13% .
3	C	258	74% 20% . 5%
3	c	258	83% 12% 5%
4	D	254	72% 20% . 6%
4	d	254	85% 9% 6%
5	E	260	75% 15% . . 7%

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Mol	Chain	Length	Quality of chain
5	e	260	
6	F	234	
6	f	234	
7	G	288	
7	g	288	
8	1	215	
8	h	215	
9	2	261	
9	i	261	
10	3	205	
10	j	205	
11	4	198	
11	k	198	
12	5	287	
12	l	287	
13	6	241	
13	m	241	
14	7	266	
14	n	266	
15	H	467	
16	I	437	
17	K	428	
18	L	437	
19	M	434	
20	J	405	

## 2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 67883 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	241	Total	C	N	O	S	0	0
			1907	1214	320	365	8		
1	A	241	Total	C	N	O	S	0	0
			1907	1214	320	365	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	250	Total	C	N	O	S	0	0
			1915	1219	315	377	4		
2	B	250	Total	C	N	O	S	0	0
			1915	1219	315	377	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		
3	C	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	240	Total	C	N	O	S	0	0
			1881	1176	329	372	4		
4	D	240	Total	C	N	O	S	0	0
			1881	1176	329	372	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	242	Total	C	N	O	S	0	0
			1861	1162	314	378	7		
5	E	242	Total	C	N	O	S	0	0
			1861	1162	314	378	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	231	Total	C	N	O	S	0	0
			1773	1114	307	348	4		
6	F	233	Total	C	N	O	S	0	0
			1795	1129	312	350	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	243	Total	C	N	O	S	0	0
			1892	1203	329	356	4		
7	G	243	Total	C	N	O	S	0	0
			1892	1203	329	356	4		

- Molecule 8 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		
8	1	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		

- Molecule 9 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	226	Total	C	N	O	S	0	0
			1719	1082	298	332	7		
9	2	226	Total	C	N	O	S	0	0
			1719	1082	298	332	7		

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	3	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

- Molecule 11 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	195	Total	C	N	O	S	0	0
			1561	992	264	299	6		
11	4	195	Total	C	N	O	S	0	0
			1561	992	264	299	6		

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		
12	5	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		

- Molecule 13 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		
13	6	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		

- Molecule 14 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	232	Total	C	N	O	S	0	0
			1815	1148	311	349	7		
14	7	229	Total	C	N	O	S	0	0
			1790	1133	306	344	7		

- Molecule 15 is a protein called 26S protease regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	390	Total	C	N	O	S	0	0
			3053	1920	546	570	17		

- Molecule 16 is a protein called 26S protease regulatory subunit 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	385	Total	C	N	O	S	0	0
			3022	1899	508	598	17		

- Molecule 17 is a protein called 26S protease regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	389	Total	C	N	O	S	0	0
			3078	1933	540	595	10		

- Molecule 18 is a protein called 26S protease subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	388	Total	C	N	O	S	0	0
			3082	1942	548	580	12		

- Molecule 19 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	381	Total	C	N	O	S	0	0
			2986	1870	524	580	12		

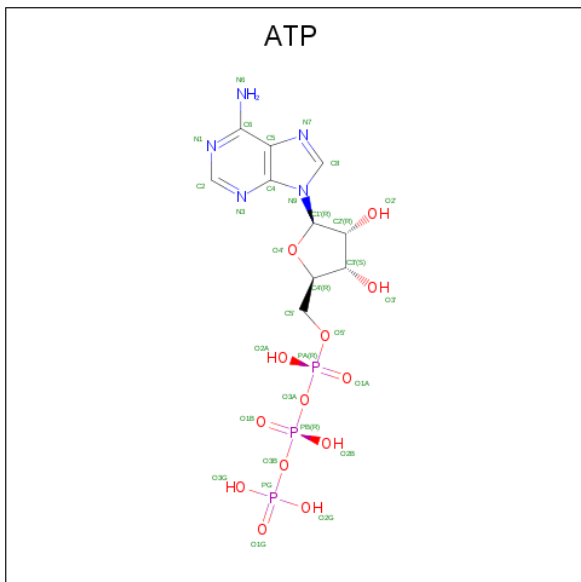
- Molecule 20 is a protein called 26S protease regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	J	386	Total	C	N	O	S	0	0
			3033	1906	543	567	17		

- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
21	J	1	Total	Mg	0
			1	1	
21	K	1	Total	Mg	0
			1	1	
21	H	1	Total	Mg	0
			1	1	
21	I	1	Total	Mg	0
			1	1	
21	L	1	Total	Mg	0
			1	1	
21	M	1	Total	Mg	0
			1	1	

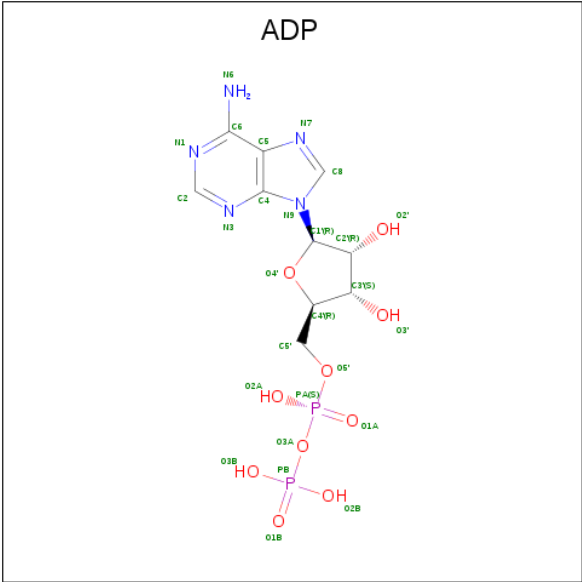
- Molecule 22 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
22	H	1	Total	C	N	O	P	0
			31	10	5	13	3	
22	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
22	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
22	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
22	M	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 23 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



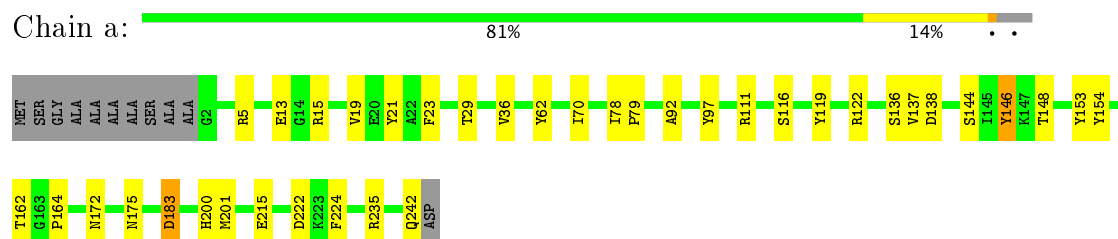


Mol	Chain	Residues	Atoms					AltConf
23	J	1	Total	C	N	O	P	0
			27	10	5	10	2	

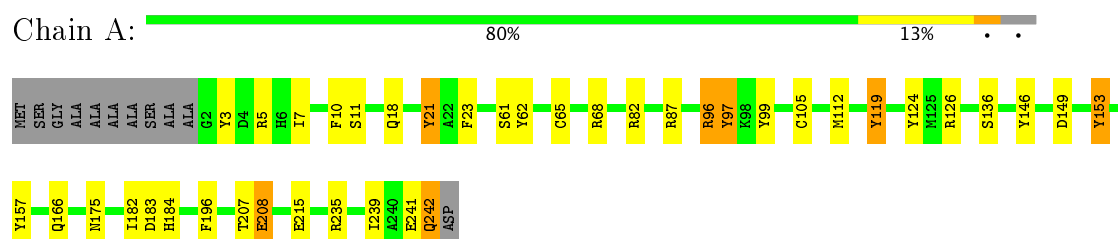
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

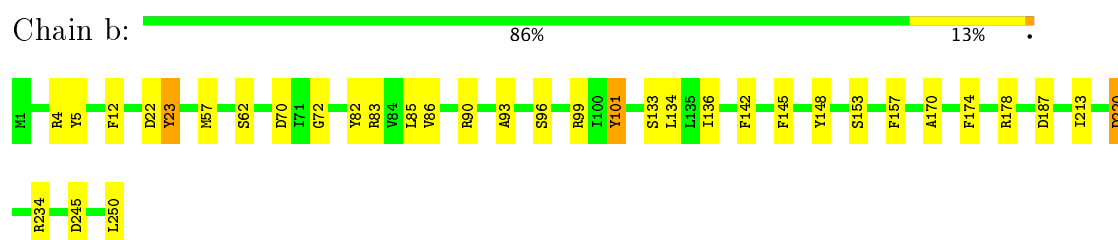
- Molecule 1: Proteasome subunit alpha type-1



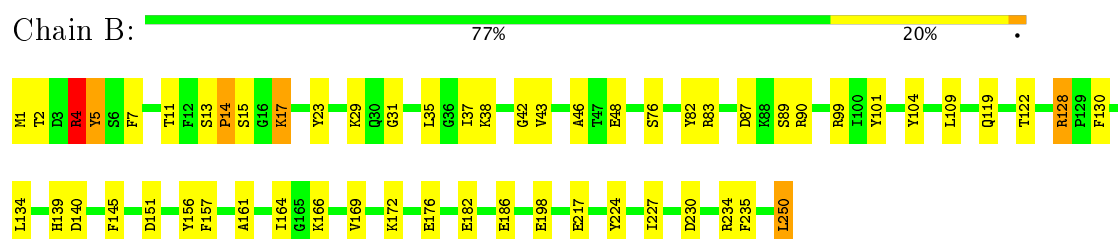
- Molecule 1: Proteasome subunit alpha type-1




- Molecule 2: Proteasome subunit alpha type-2

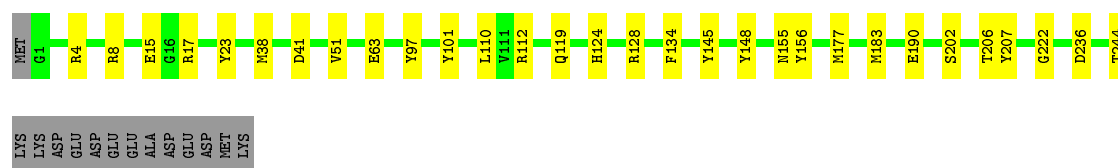


- Molecule 2: Proteasome subunit alpha type-2



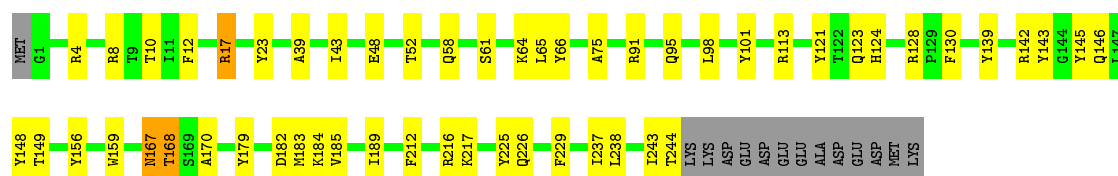
- Molecule 3: Proteasome subunit alpha type-3

Chain c: 




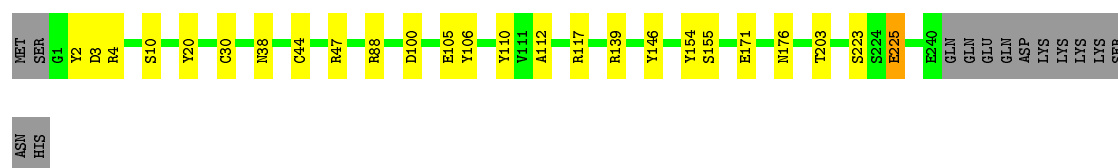
- Molecule 3: Proteasome subunit alpha type-3

Chain C: 



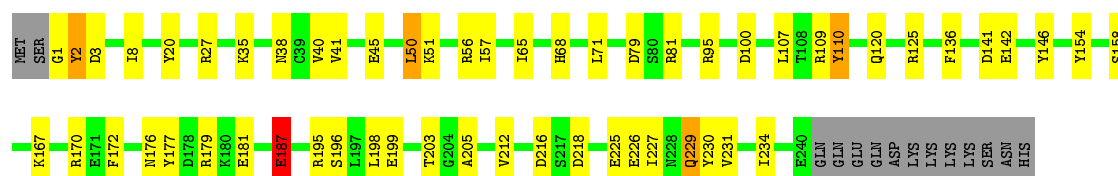
- Molecule 4: Proteasome subunit alpha type-4

Chain d: 




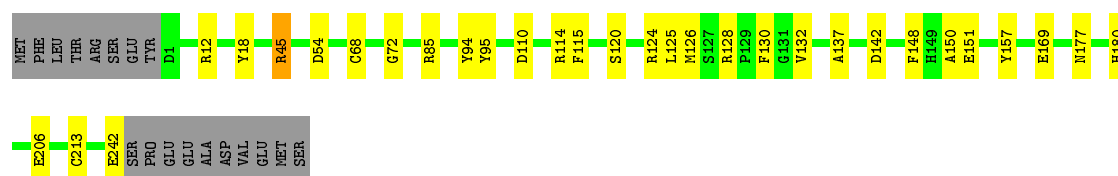
- Molecule 4: Proteasome subunit alpha type-4

Chain D: 



- Molecule 5: Proteasome subunit alpha type-5

Chain e: 



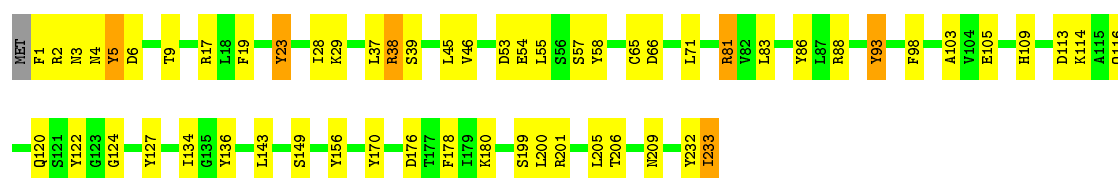
- Molecule 5: Proteasome subunit alpha type-5

Chain E: 

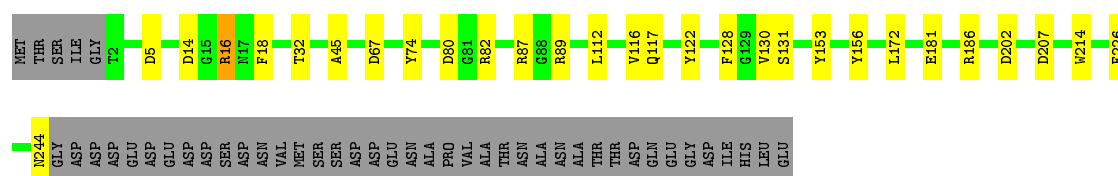
- Molecule 6: Proteasome subunit alpha type-6



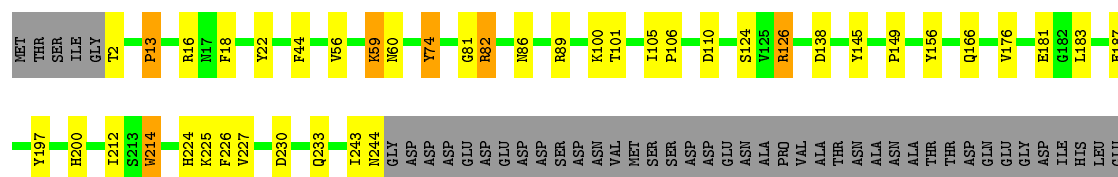
- Molecule 6: Proteasome subunit alpha type-6



- Molecule 7: Probable proteasome subunit alpha type-7



- Molecule 7: Probable proteasome subunit alpha type-7



- Molecule 8: Proteasome subunit beta type-1





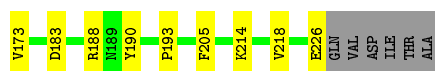
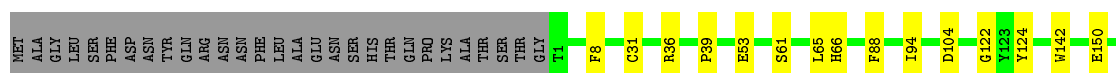
• Molecule 8: Proteasome subunit beta type-1

Chain 1: 79% 10% 9%



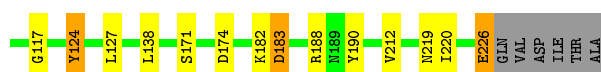
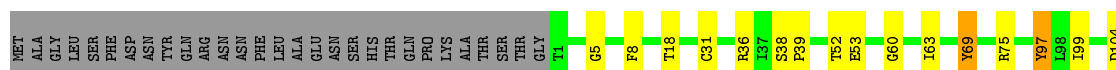
• Molecule 9: Proteasome subunit beta type-2

Chain i: 77% 9% 13%



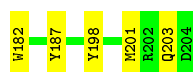
• Molecule 9: Proteasome subunit beta type-2

Chain 2: 75% 10% 13%



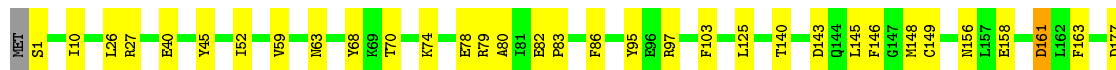
• Molecule 10: Proteasome subunit beta type-3

Chain j: 82% 17%



• Molecule 10: Proteasome subunit beta type-3

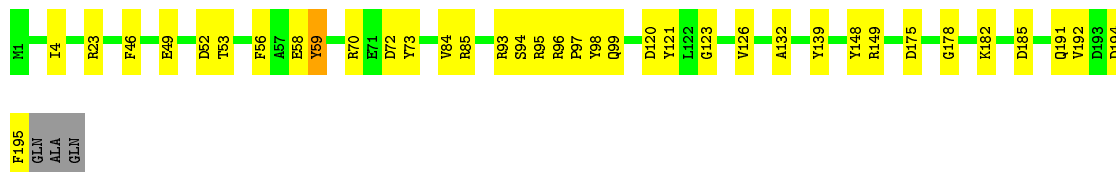
Chain 3: 80% 18%





• Molecule 11: Proteasome subunit beta type-4

Chain k: 80% 18% ..



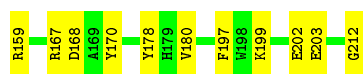
• Molecule 11: Proteasome subunit beta type-4

Chain 4: 85% 12% ..



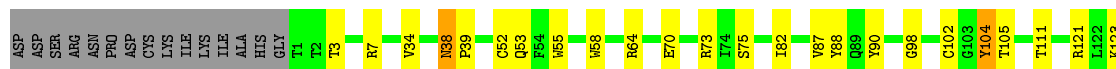
• Molecule 12: Proteasome subunit beta type-5

Chain l: 62% 11% 26%



• Molecule 12: Proteasome subunit beta type-5

Chain 5: 60% 13% 26%



• Molecule 13: Proteasome subunit beta type-6

Chain m: 79% 12% 8%











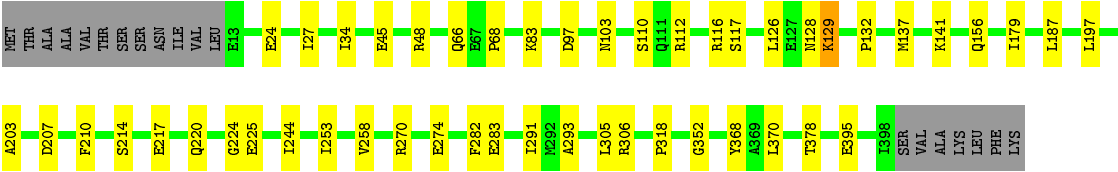
● Molecule 20: 26S protease regulatory subunit 8 homolog

Chain J: 

83%

12%

5%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	193337	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, ADP

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	1.34	7/1945 (0.4%)	1.49	26/2634 (1.0%)
1	a	1.34	6/1945 (0.3%)	1.51	31/2634 (1.2%)
10	3	1.33	6/1611 (0.4%)	1.43	16/2174 (0.7%)
10	j	1.50	16/1611 (1.0%)	1.49	16/2174 (0.7%)
11	4	1.34	3/1589 (0.2%)	1.40	13/2142 (0.6%)
11	k	1.50	10/1589 (0.6%)	1.61	24/2142 (1.1%)
12	5	1.49	13/1681 (0.8%)	1.56	20/2274 (0.9%)
12	l	1.50	13/1681 (0.8%)	1.59	24/2274 (1.1%)
13	6	1.41	9/1795 (0.5%)	1.49	23/2420 (1.0%)
13	m	1.50	14/1795 (0.8%)	1.55	18/2420 (0.7%)
14	7	1.41	7/1821 (0.4%)	1.49	14/2470 (0.6%)
14	n	1.49	19/1846 (1.0%)	1.48	23/2503 (0.9%)
15	H	1.06	5/3102 (0.2%)	1.05	13/4175 (0.3%)
16	I	1.10	11/3061 (0.4%)	1.03	7/4121 (0.2%)
17	K	1.07	9/3121 (0.3%)	1.06	14/4213 (0.3%)
18	L	1.04	8/3128 (0.3%)	1.02	10/4204 (0.2%)
19	M	1.06	11/3023 (0.4%)	1.01	6/4070 (0.1%)
2	B	1.34	8/1952 (0.4%)	1.45	22/2642 (0.8%)
2	b	1.41	11/1952 (0.6%)	1.49	26/2642 (1.0%)
20	J	1.04	4/3073 (0.1%)	1.02	11/4129 (0.3%)
3	C	1.36	3/1934 (0.2%)	1.49	23/2618 (0.9%)
3	c	1.41	8/1934 (0.4%)	1.44	18/2618 (0.7%)
4	D	1.32	11/1910 (0.6%)	1.39	14/2586 (0.5%)
4	d	1.36	10/1910 (0.5%)	1.45	20/2586 (0.8%)
5	E	1.43	10/1886 (0.5%)	1.52	24/2541 (0.9%)
5	e	1.41	12/1886 (0.6%)	1.51	18/2541 (0.7%)
6	F	1.39	7/1823 (0.4%)	1.47	24/2463 (1.0%)
6	f	1.37	7/1800 (0.4%)	1.50	21/2433 (0.9%)
7	G	1.28	4/1932 (0.2%)	1.36	15/2609 (0.6%)
7	g	1.41	7/1932 (0.4%)	1.41	15/2609 (0.6%)
8	l	1.45	4/1541 (0.3%)	1.59	23/2087 (1.1%)
8	h	1.50	10/1541 (0.6%)	1.55	15/2087 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
9	2	1.36	6/1750 (0.3%)	1.39	8/2373 (0.3%)
9	i	1.48	11/1750 (0.6%)	1.45	8/2373 (0.3%)
All	All	1.32	300/68850 (0.4%)	1.38	603/92981 (0.6%)

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	7
1	a	0	2
10	3	0	1
10	j	0	1
11	4	0	4
11	k	0	1
12	l	0	2
13	6	0	2
13	m	0	1
14	7	0	4
14	n	0	2
15	H	0	1
16	I	0	4
17	K	0	1
18	L	0	5
19	M	0	1
2	B	0	5
2	b	0	4
20	J	0	1
3	C	0	4
3	c	0	3
4	D	0	2
5	E	0	5
6	F	0	8
6	f	0	7
7	G	0	2
7	g	0	1
8	1	0	2
9	2	0	4
9	i	0	1
All	All	0	88

The worst 5 of 300 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	7	229	GLY	C-O	-14.51	1.00	1.23
12	5	212	GLY	C-O	-14.49	1.00	1.23
12	1	212	GLY	C-O	-14.48	1.00	1.23
7	G	244	ASN	C-O	-12.11	1.00	1.23
6	f	233	ILE	C-OXT	-12.08	1.00	1.23

The worst 5 of 603 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	7	187	ARG	NE-CZ-NH2	16.79	128.70	120.30
12	5	104	TYR	CB-CG-CD2	-13.38	112.97	121.00
12	5	187	TYR	CB-CG-CD1	12.91	128.75	121.00
12	5	121	ARG	NE-CZ-NH1	12.88	126.74	120.30
12	1	159	ARG	NE-CZ-NH1	12.35	126.48	120.30

There are no chirality outliers.

5 of 88 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a	146	TYR	Sidechain
1	a	148	THR	Peptide
2	b	134	LEU	Peptide
2	b	23	TYR	Sidechain
2	b	83	ARG	Sidechain

## 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	1907	0	1901	8	0
1	a	1907	0	1901	0	0
2	B	1915	0	1929	39	0
2	b	1915	0	1928	0	0
3	C	1904	0	1904	28	0
3	c	1904	0	1904	0	0
4	D	1881	0	1895	29	0
4	d	1881	0	1895	0	0
5	E	1861	0	1839	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	e	1861	0	1839	0	0
6	F	1795	0	1800	22	0
6	f	1773	0	1775	0	0
7	G	1892	0	1883	27	0
7	g	1892	0	1883	0	0
8	1	1512	0	1481	5	0
8	h	1512	0	1481	0	0
9	2	1719	0	1719	14	0
9	i	1719	0	1719	0	0
10	3	1581	0	1574	15	0
10	j	1581	0	1574	0	0
11	4	1561	0	1569	8	0
11	k	1561	0	1569	0	0
12	5	1644	0	1595	13	0
12	l	1644	0	1595	0	0
13	6	1757	0	1711	12	0
13	m	1757	0	1711	0	0
14	7	1790	0	1793	13	0
14	n	1815	0	1821	0	0
15	H	3053	0	3126	24	0
16	I	3022	0	3090	40	0
17	K	3078	0	3141	27	0
18	L	3082	0	3156	43	0
19	M	2986	0	3054	54	0
20	J	3033	0	3153	26	0
21	H	1	0	0	0	0
21	I	1	0	0	0	0
21	J	1	0	0	0	0
21	K	1	0	0	0	0
21	L	1	0	0	0	0
21	M	1	0	0	0	0
22	H	31	0	12	4	0
22	I	31	0	12	0	0
22	K	31	0	12	6	0
22	L	31	0	12	8	0
22	M	31	0	12	3	0
23	J	27	0	11	6	0
All	All	67883	0	67979	440	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 440 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)
18:L:183:ILE:CD1	22:L:501:ATP:N6	1.74	1.49
18:L:183:ILE:HD13	22:L:501:ATP:N6	1.41	1.17
20:J:197:LEU:HD11	23:J:501:ADP:H2'	1.24	1.15
19:M:374:ILE:HG21	19:M:376:TRP:CZ2	1.81	1.15
20:J:197:LEU:CD1	23:J:501:ADP:H2'	1.80	1.11

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 PDB entries followed by that with respect to all EM entries.

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	239/252 (95%)	218 (91%)	20 (8%)	1 (0%)	38	77
1	a	239/252 (95%)	221 (92%)	17 (7%)	1 (0%)	38	77
2	B	248/250 (99%)	232 (94%)	14 (6%)	2 (1%)	22	66
2	b	248/250 (99%)	223 (90%)	24 (10%)	1 (0%)	38	77
3	C	242/258 (94%)	225 (93%)	14 (6%)	3 (1%)	15	58
3	c	242/258 (94%)	217 (90%)	21 (9%)	4 (2%)	11	52
4	D	238/254 (94%)	215 (90%)	17 (7%)	6 (2%)	6	43
4	d	238/254 (94%)	221 (93%)	15 (6%)	2 (1%)	22	66
5	E	240/260 (92%)	223 (93%)	9 (4%)	8 (3%)	4	37
5	e	240/260 (92%)	222 (92%)	14 (6%)	4 (2%)	11	52
6	F	231/234 (99%)	211 (91%)	15 (6%)	5 (2%)	8	46
6	f	229/234 (98%)	207 (90%)	21 (9%)	1 (0%)	38	77
7	G	241/288 (84%)	223 (92%)	17 (7%)	1 (0%)	38	77
7	g	241/288 (84%)	221 (92%)	17 (7%)	3 (1%)	15	58
8	l	194/215 (90%)	186 (96%)	8 (4%)	0	100	100
8	h	194/215 (90%)	176 (91%)	17 (9%)	1 (0%)	32	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	2	224/261 (86%)	204 (91%)	18 (8%)	2 (1%)	20	63
9	i	224/261 (86%)	200 (89%)	17 (8%)	7 (3%)	5	39
10	3	202/205 (98%)	187 (93%)	12 (6%)	3 (2%)	12	54
10	j	202/205 (98%)	174 (86%)	23 (11%)	5 (2%)	6	43
11	4	193/198 (98%)	175 (91%)	13 (7%)	5 (3%)	6	42
11	k	193/198 (98%)	169 (88%)	19 (10%)	5 (3%)	6	42
12	5	210/287 (73%)	194 (92%)	14 (7%)	2 (1%)	18	61
12	l	210/287 (73%)	193 (92%)	17 (8%)	0	100	100
13	6	220/241 (91%)	193 (88%)	23 (10%)	4 (2%)	10	50
13	m	220/241 (91%)	196 (89%)	18 (8%)	6 (3%)	6	42
14	7	227/266 (85%)	202 (89%)	19 (8%)	6 (3%)	6	42
14	n	230/266 (86%)	205 (89%)	21 (9%)	4 (2%)	11	52
15	H	386/467 (83%)	333 (86%)	33 (8%)	20 (5%)	2	27
16	I	383/437 (88%)	345 (90%)	32 (8%)	6 (2%)	11	53
17	K	387/428 (90%)	350 (90%)	28 (7%)	9 (2%)	7	45
18	L	386/437 (88%)	343 (89%)	36 (9%)	7 (2%)	10	50
19	M	377/434 (87%)	339 (90%)	27 (7%)	11 (3%)	5	40
20	J	384/405 (95%)	347 (90%)	30 (8%)	7 (2%)	10	50
All	All	8602/9546 (90%)	7790 (91%)	660 (8%)	152 (2%)	14	50

5 of 152 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	d	203	THR
9	i	39	PRO
9	i	104	ASP
10	j	6	ILE
10	j	203	GLN

### 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 PDB entries followed by that with respect to all EM entries.

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	206/210 (98%)	203 (98%)	3 (2%)	70	86
1	a	206/210 (98%)	197 (96%)	9 (4%)	33	65
2	B	209/209 (100%)	205 (98%)	4 (2%)	62	82
2	b	209/209 (100%)	203 (97%)	6 (3%)	48	73
3	C	203/216 (94%)	202 (100%)	1 (0%)	91	95
3	c	203/216 (94%)	195 (96%)	8 (4%)	37	67
4	D	212/226 (94%)	206 (97%)	6 (3%)	49	74
4	d	212/226 (94%)	209 (99%)	3 (1%)	71	86
5	E	198/215 (92%)	193 (98%)	5 (2%)	53	77
5	e	198/215 (92%)	191 (96%)	7 (4%)	41	70
6	F	192/193 (100%)	190 (99%)	2 (1%)	80	90
6	f	190/193 (98%)	179 (94%)	11 (6%)	23	57
7	G	201/239 (84%)	198 (98%)	3 (2%)	70	86
7	g	201/239 (84%)	192 (96%)	9 (4%)	32	64
8	1	162/178 (91%)	161 (99%)	1 (1%)	89	94
8	h	162/178 (91%)	159 (98%)	3 (2%)	62	82
9	2	185/214 (86%)	184 (100%)	1 (0%)	91	95
9	i	185/214 (86%)	182 (98%)	3 (2%)	68	85
10	3	172/173 (99%)	171 (99%)	1 (1%)	89	94
10	j	172/173 (99%)	168 (98%)	4 (2%)	56	79
11	4	173/175 (99%)	171 (99%)	2 (1%)	75	88
11	k	173/175 (99%)	168 (97%)	5 (3%)	48	73
12	5	169/235 (72%)	167 (99%)	2 (1%)	75	88
12	l	169/235 (72%)	159 (94%)	10 (6%)	23	57
13	6	185/201 (92%)	184 (100%)	1 (0%)	91	95
13	m	185/201 (92%)	181 (98%)	4 (2%)	57	79
14	7	195/224 (87%)	192 (98%)	3 (2%)	70	86
14	n	198/224 (88%)	191 (96%)	7 (4%)	41	70
15	H	330/399 (83%)	326 (99%)	4 (1%)	75	88
16	I	342/385 (89%)	333 (97%)	9 (3%)	51	76
17	K	342/374 (91%)	338 (99%)	4 (1%)	75	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	L	332/377 (88%)	328 (99%)	4 (1%)	75	88
19	M	329/375 (88%)	322 (98%)	7 (2%)	59	80
20	J	336/352 (96%)	330 (98%)	6 (2%)	64	84
All	All	7336/8078 (91%)	7178 (98%)	158 (2%)	60	79

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	l	36	GLU
14	n	208	PHE
19	M	162	GLU
12	l	86	LEU
13	m	135	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	123	GLN
4	D	176	ASN
17	K	238	ASN
3	C	96	ASN
5	E	149	HIS

### 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

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
22	ATP	H	502	21	27,33,33	1.26	3 (11%)	25,52,52	3.68	9 (36%)
22	ATP	I	501	21	27,33,33	1.65	6 (22%)	25,52,52	2.86	8 (32%)
23	ADP	J	501	21	25,29,29	1.80	4 (16%)	24,45,45	3.37	6 (25%)
22	ATP	K	501	21	27,33,33	1.54	5 (18%)	25,52,52	3.21	6 (24%)
22	ATP	L	501	21	27,33,33	1.34	3 (11%)	25,52,52	2.67	8 (32%)
22	ATP	M	501	21	27,33,33	1.05	1 (3%)	25,52,52	3.14	8 (32%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	ATP	H	502	21	-	0/18/38/38	0/3/3/3
22	ATP	I	501	21	-	0/18/38/38	0/3/3/3
23	ADP	J	501	21	-	0/12/32/32	0/3/3/3
22	ATP	K	501	21	-	0/18/38/38	0/3/3/3
22	ATP	L	501	21	-	0/18/38/38	0/3/3/3
22	ATP	M	501	21	-	0/18/38/38	0/3/3/3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	H	502	ATP	C2-N3	2.06	1.35	1.32
23	J	501	ADP	C5-C4	2.10	1.45	1.40
22	H	502	ATP	C4-N3	2.18	1.38	1.35
22	K	501	ATP	C5-C4	2.31	1.45	1.40
23	J	501	ADP	C4-N3	2.44	1.39	1.35

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
22	H	502	ATP	N3-C2-N1	-15.89	115.02	128.86
23	J	501	ADP	N3-C2-N1	-15.17	115.64	128.86
22	K	501	ATP	N3-C2-N1	-14.39	116.32	128.86
22	M	501	ATP	N3-C2-N1	-13.52	117.09	128.86
22	L	501	ATP	N3-C2-N1	-10.78	119.47	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	H	502	ATP	4	0
23	J	501	ADP	6	0
22	K	501	ATP	6	0
22	L	501	ATP	8	0
22	M	501	ATP	3	0

## 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.