



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:28 AM GMT

PDB ID : 2H6J
Title : Crystal Structure of the Beta F145A Rhodococcus Proteasome (CASP Target)
Authors : Kwon, Y.D.
Deposited on : 2006-05-31
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
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

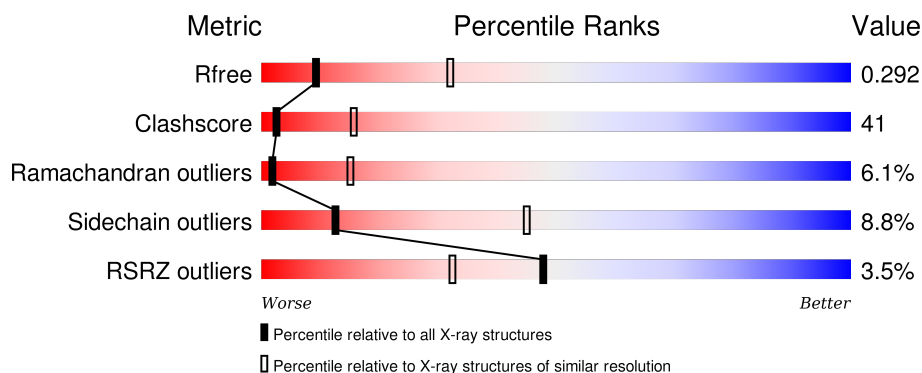
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	259	<div> <div>4%</div> <div>34% 44% 7% 15%</div> </div>
1	B	259	<div> <div>%</div> <div>37% 38% 10% 15%</div> </div>
1	C	259	<div> <div>36% 43% 5% 15%</div> </div>
1	D	259	<div> <div>%</div> <div>31% 46% 7% 15%</div> </div>
1	E	259	<div> <div>4%</div> <div>32% 45% 8% 15%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	259	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>34%</div><div>44%</div><div>7%</div><div>15%</div></div></div>
1	G	259	<div><div><div></div><div></div><div></div><div></div></div><div><div>5%</div><div>32%</div><div>46%</div><div>6%</div><div>15%</div></div></div>
2	H	294	<div><div><div></div><div></div><div></div><div></div></div><div><div>3%</div><div>42%</div><div>33%</div><div>7%</div><div>18%</div></div></div>
2	I	294	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>43%</div><div>34%</div><div><div></div><div></div></div><div>18%</div></div></div>
2	J	294	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>41%</div><div>35%</div><div>5%</div><div>18%</div></div></div>
2	K	294	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>39%</div><div>37%</div><div>6%</div><div>18%</div></div></div>
2	L	294	<div><div><div></div><div></div><div></div><div></div></div><div><div>3%</div><div>41%</div><div>35%</div><div>5%</div><div>18%</div></div></div>
2	M	294	<div><div><div></div><div></div><div></div><div></div></div><div><div>4%</div><div>43%</div><div>33%</div><div>6%</div><div>18%</div></div></div>
2	N	294	<div><div><div></div><div></div><div></div><div></div></div><div><div>6%</div><div>41%</div><div>34%</div><div>7%</div><div>18%</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22218 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 alpha-type subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1523	960	264	294	5			
1	B	219	Total	C	N	O	S	0	0	0
			1523	960	264	294	5			
1	C	219	Total	C	N	O	S	0	0	0
			1523	960	264	294	5			
1	D	219	Total	C	N	O	S	0	0	0
			1523	960	264	294	5			
1	E	219	Total	C	N	O	S	0	0	0
			1523	960	264	294	5			
1	F	219	Total	C	N	O	S	0	0	0
			1523	960	264	294	5			
1	G	219	Total	C	N	O	S	0	0	0
			1523	960	264	294	5			

- Molecule 2 is a protein called Proteasome beta-type subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	242	Total	C	N	O	S	0	0	0
			1601	1004	273	322	2			
2	I	242	Total	C	N	O	S	0	0	0
			1601	1004	273	322	2			
2	J	242	Total	C	N	O	S	0	0	0
			1601	1004	273	322	2			
2	K	242	Total	C	N	O	S	0	0	0
			1601	1004	273	322	2			
2	L	242	Total	C	N	O	S	0	0	0
			1601	1004	273	322	2			
2	M	242	Total	C	N	O	S	0	0	0
			1601	1004	273	322	2			
2	N	242	Total	C	N	O	S	0	0	0
			1601	1004	273	322	2			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	145	ALA	PHE	ENGINEERED	UNP Q53079
I	145	ALA	PHE	ENGINEERED	UNP Q53079
J	145	ALA	PHE	ENGINEERED	UNP Q53079
K	145	ALA	PHE	ENGINEERED	UNP Q53079
L	145	ALA	PHE	ENGINEERED	UNP Q53079
M	145	ALA	PHE	ENGINEERED	UNP Q53079
N	145	ALA	PHE	ENGINEERED	UNP Q53079

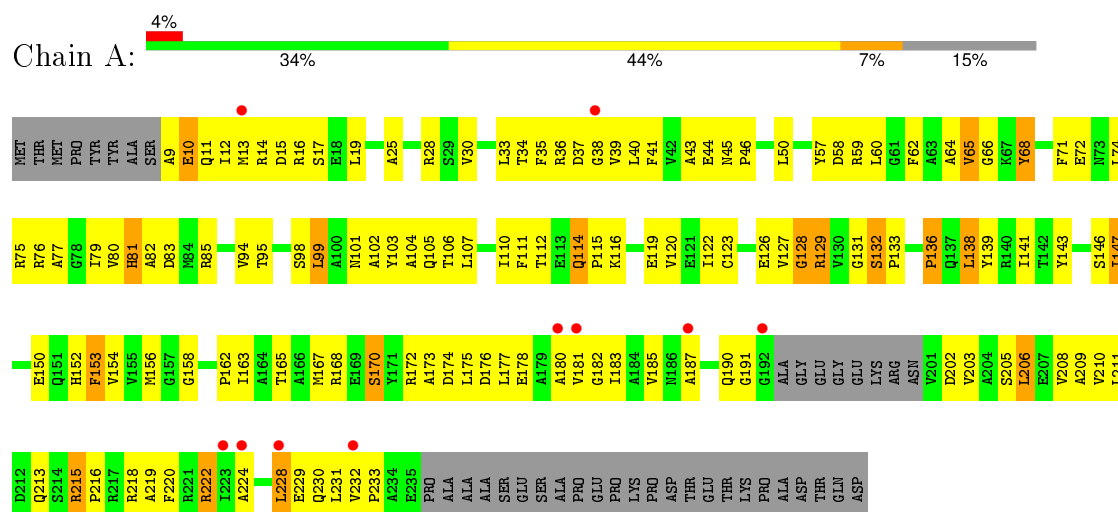
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	17	Total O 17 17	0	0
3	B	25	Total O 25 25	0	0
3	C	31	Total O 31 31	0	0
3	D	29	Total O 29 29	0	0
3	E	27	Total O 27 27	0	0
3	F	21	Total O 21 21	0	0
3	G	21	Total O 21 21	0	0
3	H	25	Total O 25 25	0	0
3	I	30	Total O 30 30	0	0
3	J	24	Total O 24 24	0	0
3	K	26	Total O 26 26	0	0
3	L	24	Total O 24 24	0	0
3	M	34	Total O 34 34	0	0
3	N	16	Total O 16 16	0	0

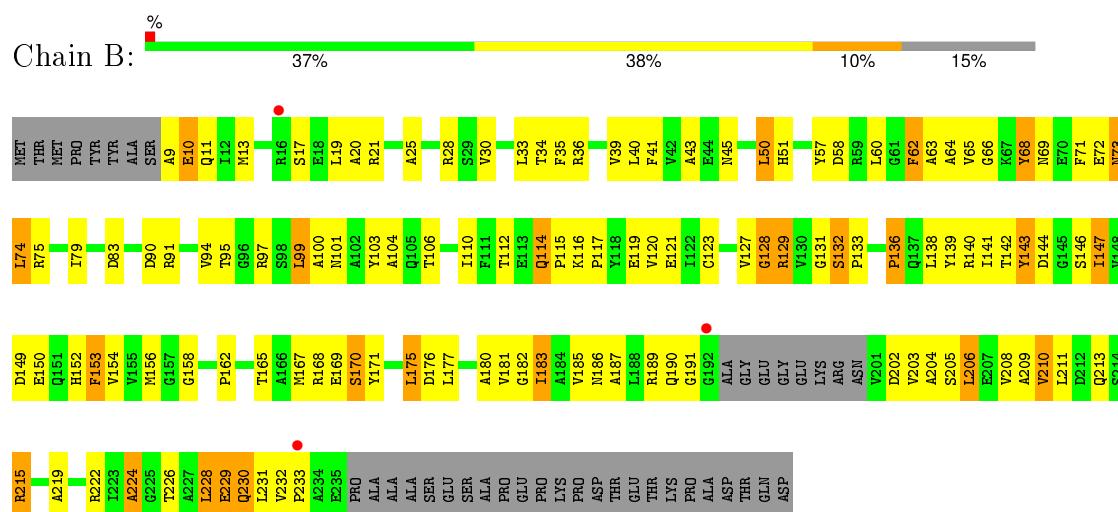
3 Residue-property plots

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.

• Molecule 1: Proteasome alpha-type subunit 1

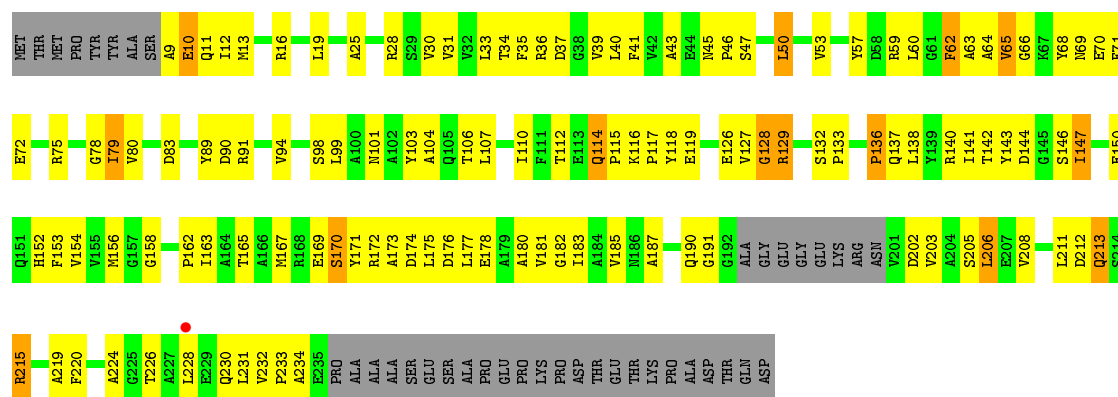


• Molecule 1: Proteasome alpha-type subunit 1

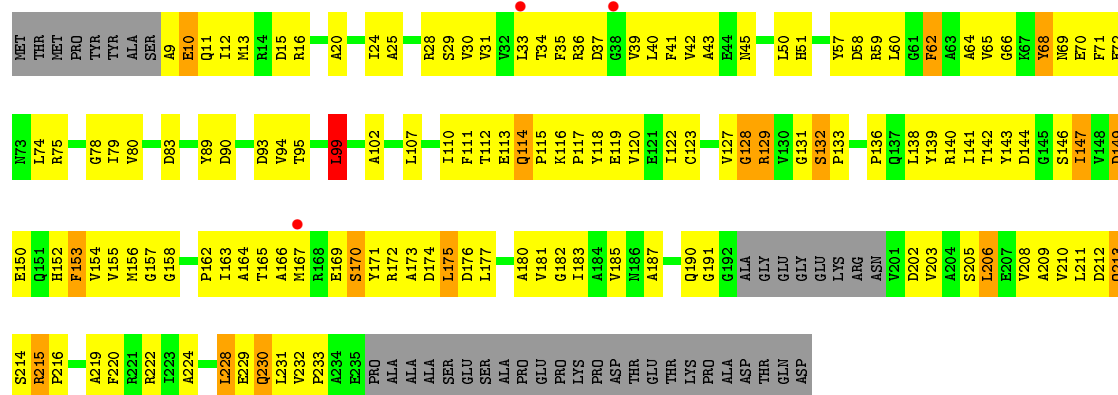


• Molecule 1: Proteasome alpha-type subunit 1

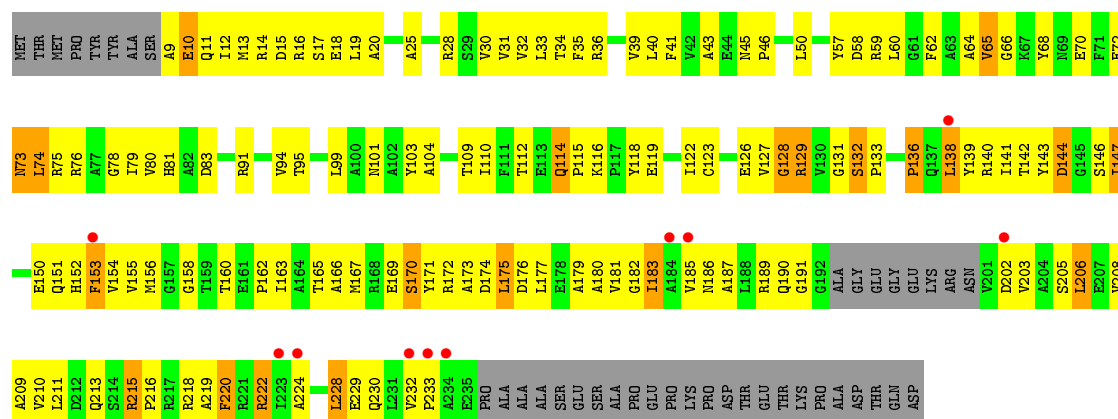




• Molecule 1: Proteasome alpha-type subunit 1

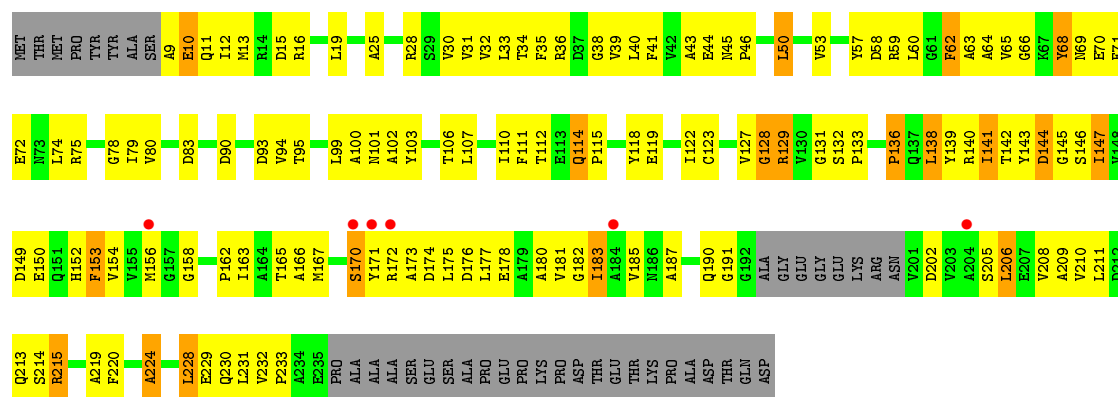


• Molecule 1: Proteasome alpha-type subunit 1

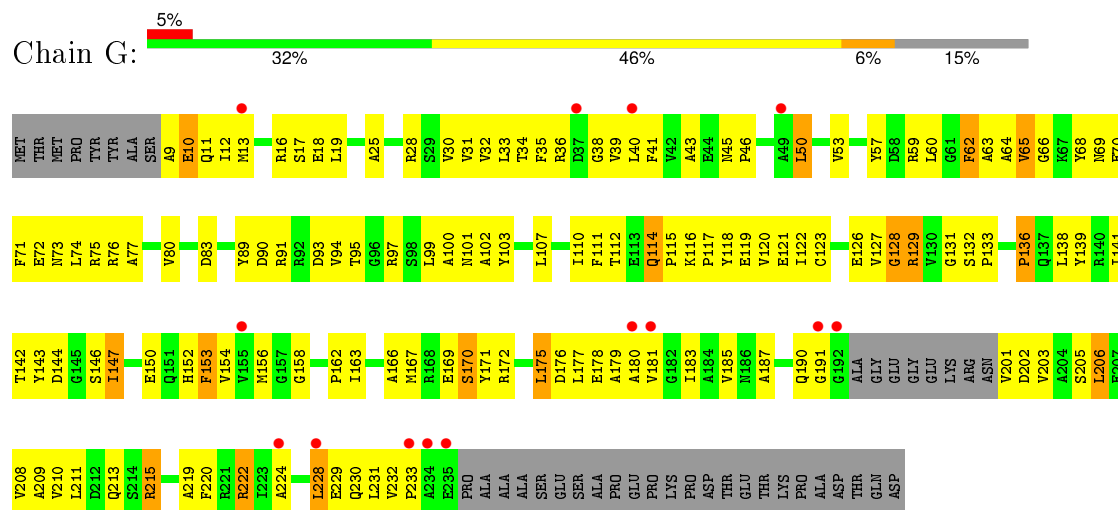


• Molecule 1: Proteasome alpha-type subunit 1

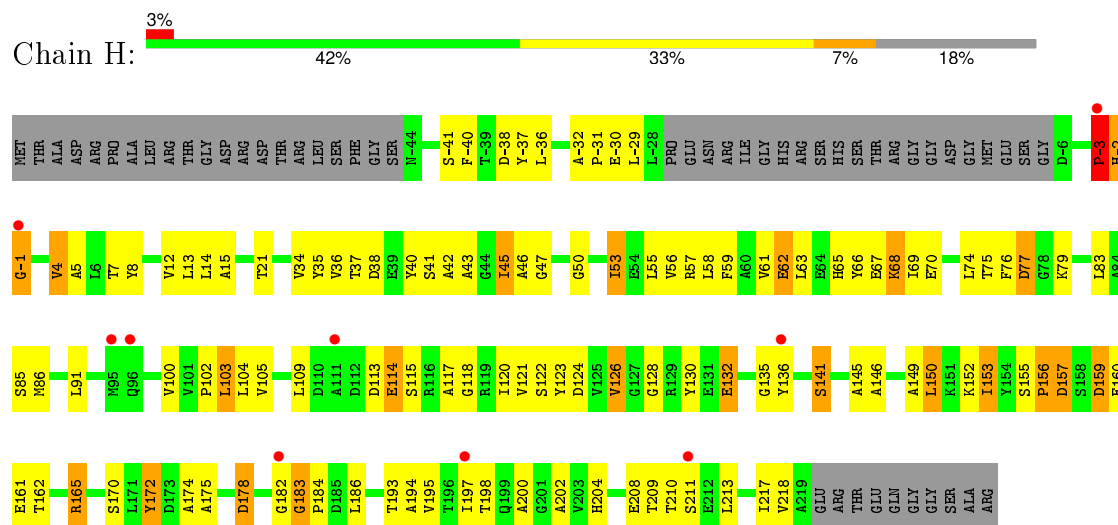




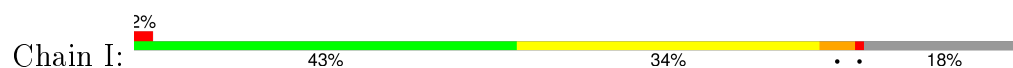
• Molecule 1: Proteasome alpha-type subunit 1

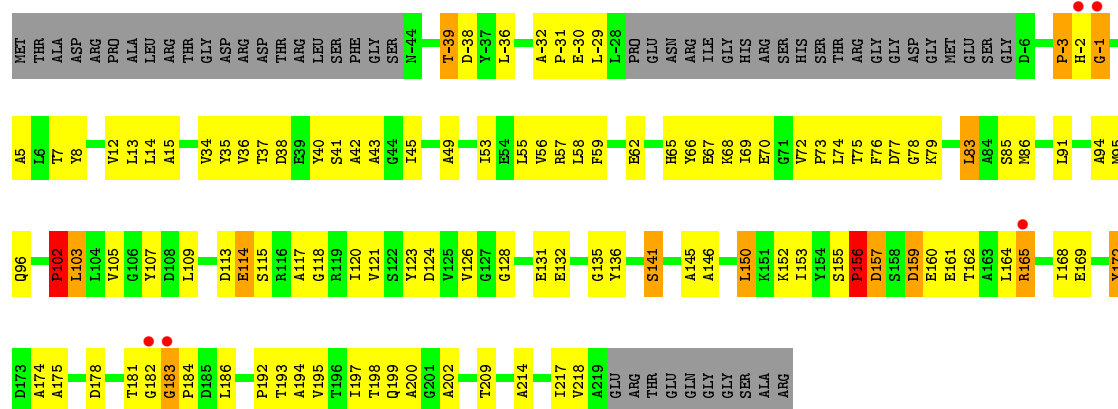


• Molecule 2: Proteasome beta-type subunit 1



• Molecule 2: Proteasome beta-type subunit 1

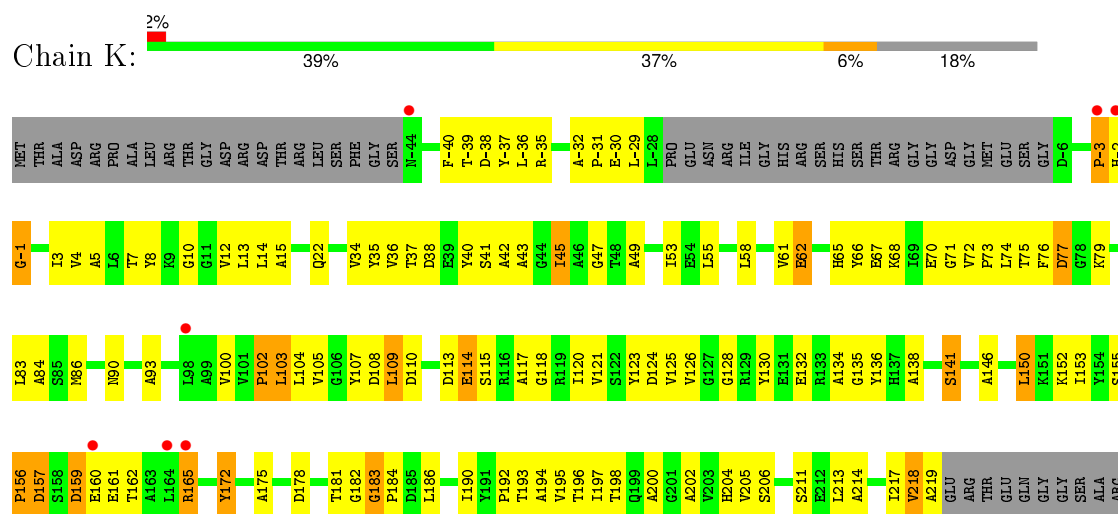




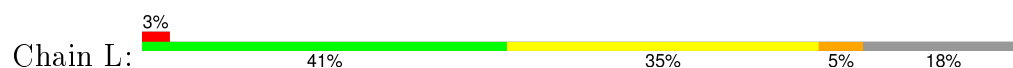
• Molecule 2: Proteasome beta-type subunit 1



• Molecule 2: Proteasome beta-type subunit 1



• Molecule 2: Proteasome beta-type subunit 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	149.44Å 210.71Å 248.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 3.20 49.06 – 3.11	Depositor EDS
% Data completeness (in resolution range)	76.9 (19.98-3.20) 83.0 (49.06-3.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.262 , 0.290 0.264 , 0.292	Depositor DCC
R_{free} test set	2823 reflections (5.13%)	DCC
Wilson B-factor (Å ²)	89.2	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 100.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 66425 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	22218	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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 ⓘ

5.1 Standard geometry ⓘ

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	0.56	0/1547	0.78	0/2116
1	B	0.63	0/1547	0.82	0/2116
1	C	0.63	0/1547	0.82	0/2116
1	D	0.61	0/1547	0.80	1/2116 (0.0%)
1	E	0.59	0/1547	0.79	0/2116
1	F	0.51	0/1547	0.75	0/2116
1	G	0.50	0/1547	0.75	0/2116
2	H	0.62	2/1622 (0.1%)	0.78	1/2223 (0.0%)
2	I	0.68	2/1622 (0.1%)	0.81	2/2223 (0.1%)
2	J	0.67	2/1622 (0.1%)	0.80	1/2223 (0.0%)
2	K	0.67	2/1622 (0.1%)	0.81	1/2223 (0.0%)
2	L	0.63	2/1622 (0.1%)	0.80	1/2223 (0.0%)
2	M	0.64	2/1622 (0.1%)	0.80	1/2223 (0.0%)
2	N	0.59	2/1622 (0.1%)	0.76	1/2223 (0.0%)
All	All	0.61	14/22183 (0.1%)	0.79	9/30373 (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	C	0	1
1	D	0	1
1	G	0	1
2	H	0	2
2	I	0	2
2	J	0	2
2	K	0	1
2	L	0	2
2	N	0	1
All	All	0	13

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	-1	GLY	C-N	14.62	1.67	1.34
2	J	-1	GLY	C-N	13.26	1.64	1.34
2	H	-1	GLY	C-N	12.49	1.62	1.34
2	N	-1	GLY	C-N	12.18	1.62	1.34
2	K	-1	GLY	C-N	11.96	1.61	1.34

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	-1	GLY	CA-C-N	-9.02	97.35	117.20
2	H	-1	GLY	CA-C-N	-8.37	98.78	117.20
2	K	-1	GLY	CA-C-N	-8.19	99.18	117.20
2	M	-1	GLY	CA-C-N	-8.17	99.22	117.20
2	L	-1	GLY	CA-C-N	-7.93	99.75	117.20

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	89	TYR	Sidechain
1	D	89	TYR	Sidechain
1	G	89	TYR	Sidechain
2	H	-1	GLY	Mainchain,Peptide
2	I	-1	GLY	Mainchain

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	1523	0	1395	147	0
1	B	1523	0	1395	142	0
1	C	1523	0	1395	155	0
1	D	1523	0	1395	167	0
1	E	1523	0	1395	173	0
1	F	1523	0	1395	154	0
1	G	1523	0	1395	153	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1601	0	1449	100	0
2	I	1601	0	1449	103	0
2	J	1601	0	1449	104	0
2	K	1601	0	1449	102	0
2	L	1601	0	1449	104	0
2	M	1601	0	1449	108	0
2	N	1601	0	1449	107	0
3	A	17	0	0	1	0
3	B	25	0	0	5	0
3	C	31	0	0	10	0
3	D	29	0	0	5	0
3	E	27	0	0	14	0
3	F	21	0	0	5	0
3	G	21	0	0	4	0
3	H	25	0	0	2	0
3	I	30	0	0	3	0
3	J	24	0	0	3	0
3	K	26	0	0	6	0
3	L	24	0	0	3	0
3	M	34	0	0	10	0
3	N	16	0	0	1	0
All	All	22218	0	19908	1733	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 41.

The worst 5 of 1733 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:M:-1:GLY:C	2:M:1:THR:N	1.67	1.45
1:G:114:GLN:HG3	1:G:115:PRO:HD2	1.29	1.11
2:J:124:ASP:HB2	2:J:128:GLY:H	1.14	1.11
2:J:175:ALA:HB2	2:J:183:GLY:H	1.18	1.09
1:E:114:GLN:HG3	1:E:115:PRO:HD2	1.34	1.07

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	215/259 (83%)	150 (70%)	47 (22%)	18 (8%)	1	6
1	B	215/259 (83%)	155 (72%)	42 (20%)	18 (8%)	1	6
1	C	215/259 (83%)	155 (72%)	45 (21%)	15 (7%)	1	10
1	D	215/259 (83%)	158 (74%)	41 (19%)	16 (7%)	1	9
1	E	215/259 (83%)	151 (70%)	46 (21%)	18 (8%)	1	6
1	F	215/259 (83%)	149 (69%)	49 (23%)	17 (8%)	1	8
1	G	215/259 (83%)	151 (70%)	51 (24%)	13 (6%)	2	16
2	H	238/294 (81%)	192 (81%)	34 (14%)	12 (5%)	3	21
2	I	238/294 (81%)	189 (79%)	39 (16%)	10 (4%)	3	26
2	J	238/294 (81%)	191 (80%)	36 (15%)	11 (5%)	3	23
2	K	238/294 (81%)	192 (81%)	34 (14%)	12 (5%)	3	21
2	L	238/294 (81%)	193 (81%)	34 (14%)	11 (5%)	3	23
2	M	238/294 (81%)	195 (82%)	33 (14%)	10 (4%)	3	26
2	N	238/294 (81%)	190 (80%)	35 (15%)	13 (6%)	2	18
All	All	3171/3871 (82%)	2411 (76%)	566 (18%)	194 (6%)	2	15

5 of 194 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	GLY
1	A	129	ARG
1	A	170	SER
1	A	224	ALA
1	B	128	GLY

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	137/205 (67%)	126 (92%)	11 (8%)	15	52
1	B	137/205 (67%)	124 (90%)	13 (10%)	11	40
1	C	137/205 (67%)	128 (93%)	9 (7%)	21	61
1	D	137/205 (67%)	126 (92%)	11 (8%)	15	52
1	E	137/205 (67%)	124 (90%)	13 (10%)	11	40
1	F	137/205 (67%)	125 (91%)	12 (9%)	12	45
1	G	137/205 (67%)	125 (91%)	12 (9%)	12	45
2	H	133/222 (60%)	119 (90%)	14 (10%)	8	35
2	I	133/222 (60%)	120 (90%)	13 (10%)	10	38
2	J	133/222 (60%)	120 (90%)	13 (10%)	10	38
2	K	133/222 (60%)	122 (92%)	11 (8%)	14	49
2	L	133/222 (60%)	120 (90%)	13 (10%)	10	38
2	M	133/222 (60%)	122 (92%)	11 (8%)	14	49
2	N	133/222 (60%)	122 (92%)	11 (8%)	14	49
All	All	1890/2989 (63%)	1723 (91%)	167 (9%)	12	45

5 of 167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	175	LEU
2	H	165	ARG
2	M	165	ARG
1	G	206	LEU
2	H	62	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	114	GLN

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Mol	Chain	Res	Type
1	G	114	GLN
2	K	-33	HIS
1	E	114	GLN
1	F	101	ASN

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 carbohydrates 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 ⓘ

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	219/259 (84%)	0.01	10 (4%) 36 23	28, 77, 133, 187	0
1	B	219/259 (84%)	-0.22	3 (1%) 78 65	18, 62, 122, 157	0
1	C	219/259 (84%)	-0.26	1 (0%) 91 87	13, 60, 121, 168	0
1	D	219/259 (84%)	-0.15	3 (1%) 78 65	17, 72, 136, 170	0
1	E	219/259 (84%)	-0.08	10 (4%) 36 23	23, 73, 128, 156	0
1	F	219/259 (84%)	0.08	6 (2%) 58 44	34, 90, 152, 194	0
1	G	219/259 (84%)	0.23	14 (6%) 23 13	39, 92, 148, 179	0
2	H	242/294 (82%)	0.08	9 (3%) 45 30	38, 86, 144, 192	0
2	I	242/294 (82%)	-0.03	5 (2%) 67 52	22, 69, 141, 177	0
2	J	242/294 (82%)	-0.11	5 (2%) 67 52	17, 66, 139, 194	0
2	K	242/294 (82%)	-0.11	7 (2%) 55 41	20, 67, 134, 177	0
2	L	242/294 (82%)	0.03	10 (4%) 41 27	22, 71, 129, 177	0
2	M	242/294 (82%)	0.14	13 (5%) 29 17	31, 81, 142, 181	0
2	N	242/294 (82%)	0.28	18 (7%) 17 10	31, 92, 154, 185	0
All	All	3227/3871 (83%)	-0.01	114 (3%) 48 32	13, 76, 141, 194	0

The worst 5 of 114 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	224	ALA	5.4
1	G	37	ASP	4.8
2	N	112	ASP	4.4
1	G	234	ALA	4.2
1	F	156	MET	4.1

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 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.