



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 07:11 PM GMT

PDB ID : 1PMA
Title : PROTEASOME FROM THERMOPLASMA ACIDOPHILUM
Authors : Loewe, J.; Stock, D.; Jap, B.; Zwickl, P.; Baumeister, W.; Huber, R.
Deposited on : 1994-12-19
Resolution : 3.40 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

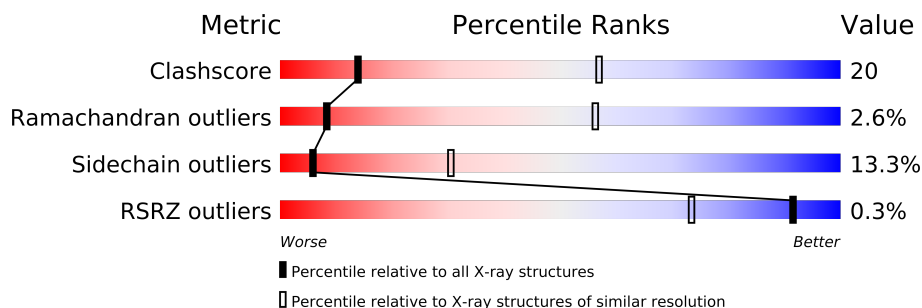
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.40 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.











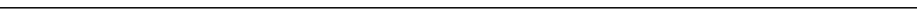



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RSRZ outliers	66119	1017 (3.52-3.28)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	233	
1	C	233	
1	D	233	
1	E	233	
1	F	233	
1	G	233	
1	H	233	
1	I	233	
1	J	233	
1	K	233	
1	L	233	
1	M	233	
1	N	233	
1	O	233	
2	1	211	
2	2	211	

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Mol	Chain	Length	Quality of chain
2	B	211	
2	P	211	
2	Q	211	
2	R	211	
2	S	211	
2	T	211	
2	U	211	
2	V	211	
2	W	211	
2	X	211	
2	Y	211	
2	Z	211	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 56294 atoms, of which 10402 are hydrogens and 0 are deuterium.

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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	C	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	D	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	E	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	F	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	G	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	H	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	I	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	J	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	K	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	L	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	M	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	N	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			
1	O	221	Total	C	H	N	O	S	0	0	0
			2113	1092	393	290	335	3			

- Molecule 2 is a protein called PROTEASOME.

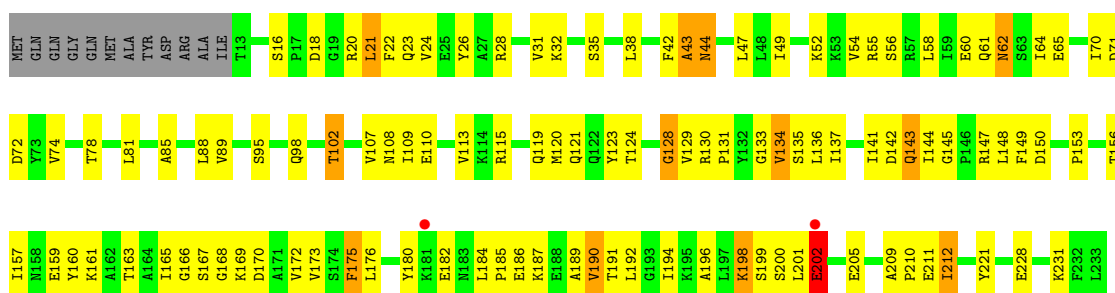
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	P	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	Q	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	R	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	S	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	T	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	U	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	V	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	W	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	X	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	Y	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	Z	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	1	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	0	0
2	2	203	Total 1908	C 985	H 350	N 264	O 298	S 11	0	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.

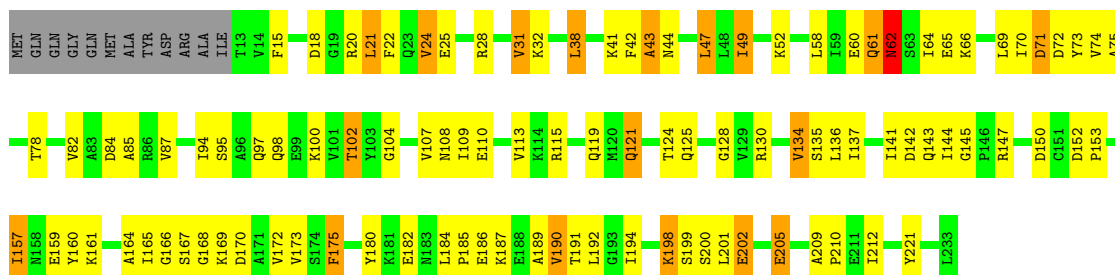
- Molecule 1: PROTEASOME

Chain A: 



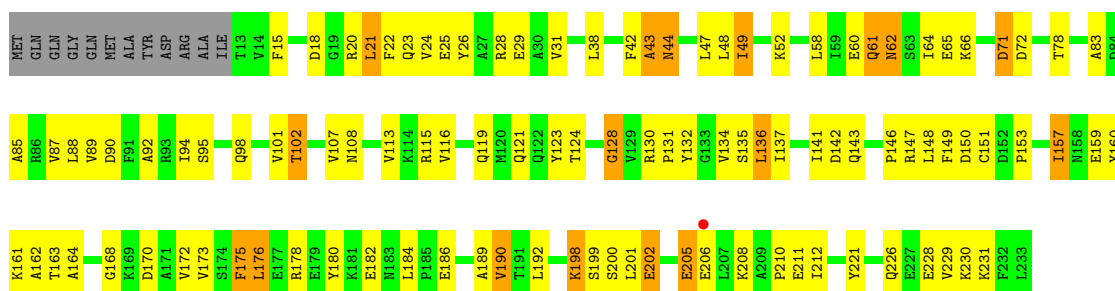
- Molecule 1: PROTEASOME

Chain C: 



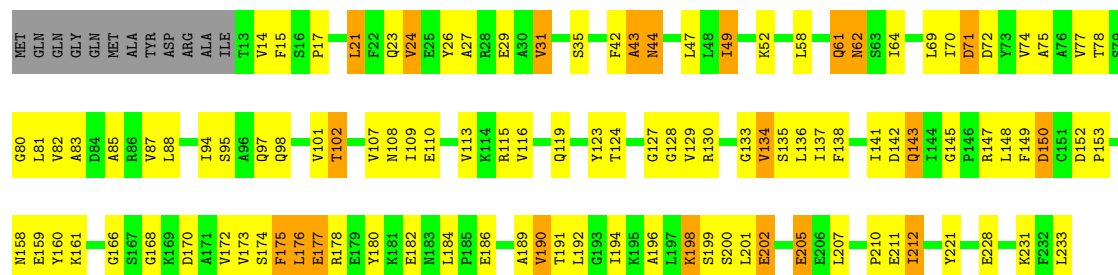
- Molecule 1: PROTEASOME

Chain D: 



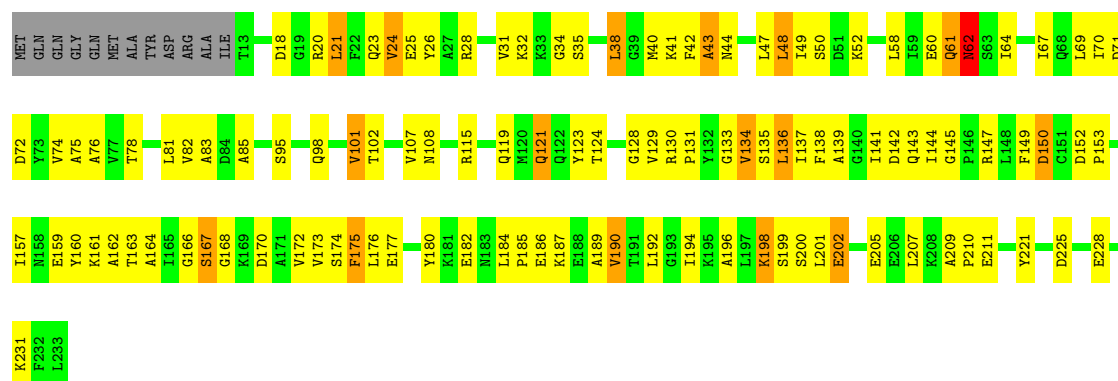
- Molecule 1: PROTEASOME

Chain E:



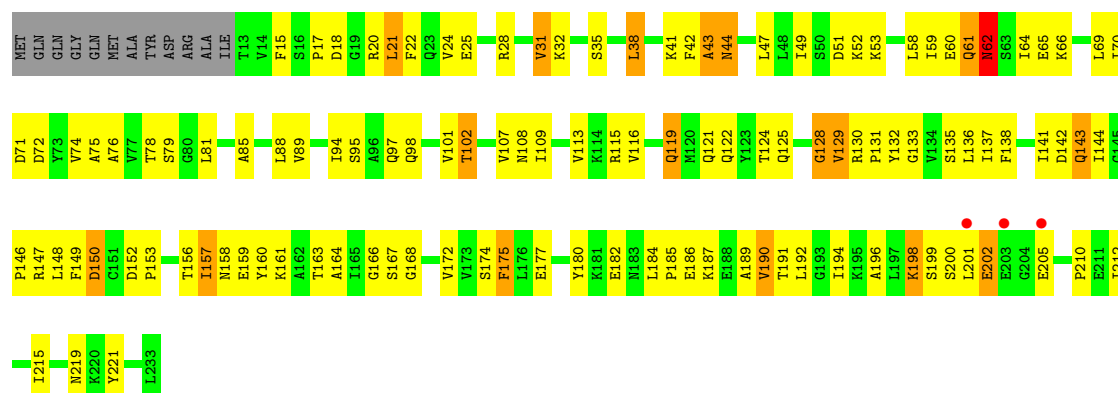
• Molecule 1: PROTEASOME

Chain F:



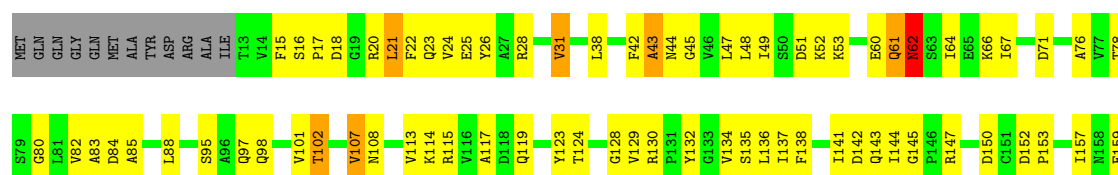
• Molecule 1: PROTEASOME

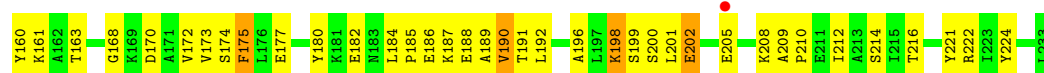
Chain G:



• Molecule 1: PROTEASOME

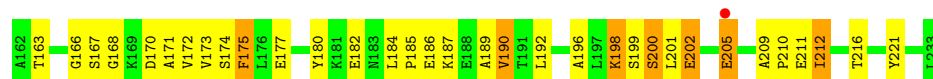
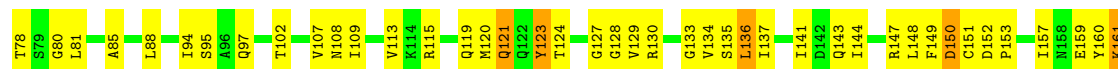
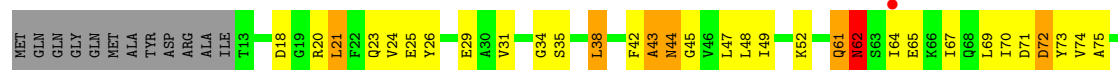
Chain H:





• Molecule 1: PROTEASOME

Chain I:



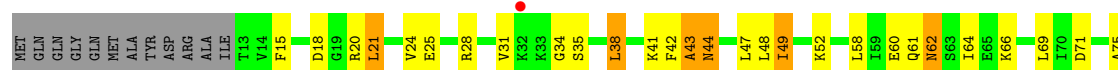
• Molecule 1: PROTEASOME

Chain J:



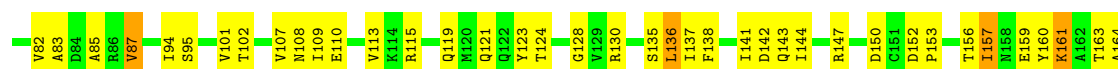
• Molecule 1: PROTEASOME

Chain K:

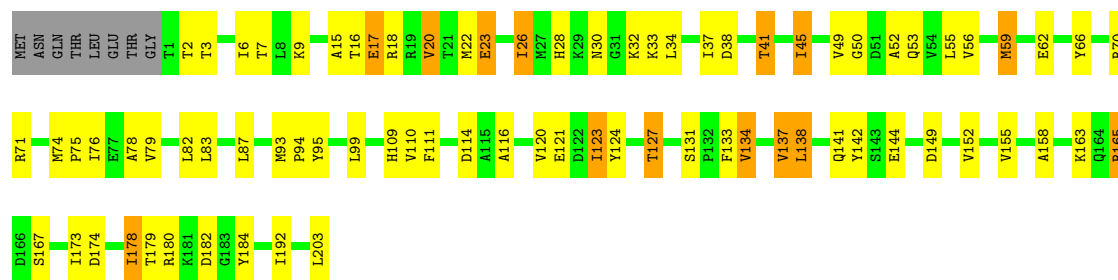


• Molecule 1: PROTEASOME

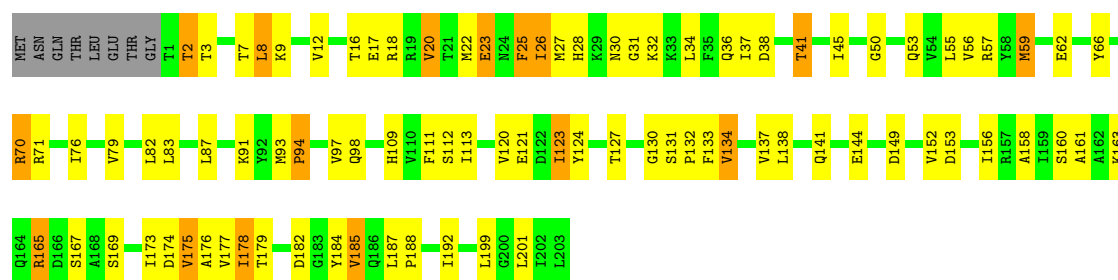
Chain L:



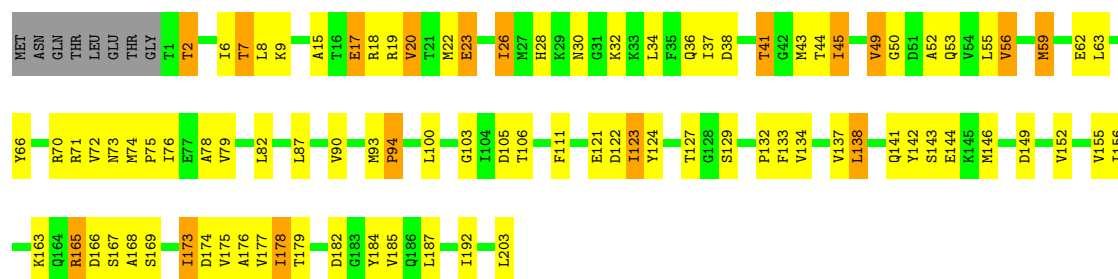
• Molecule 2: PROTEASOME

Chain T: 

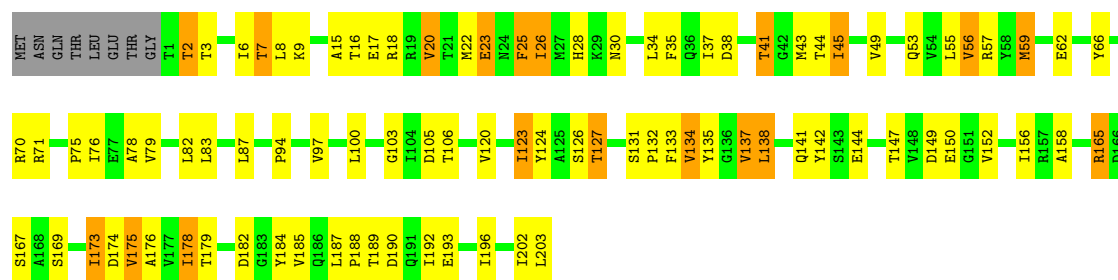
• Molecule 2: PROTEASOME

Chain U: 

• Molecule 2: PROTEASOME

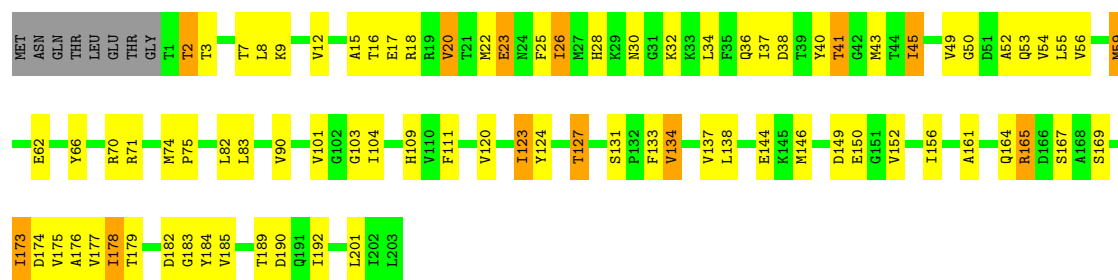
Chain V: 

• Molecule 2: PROTEASOME

Chain W: 

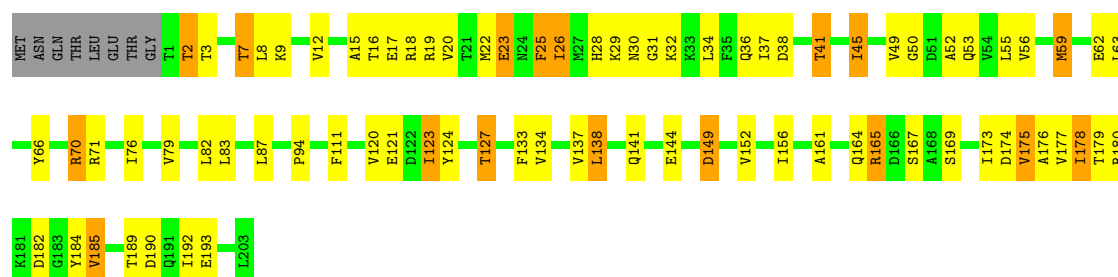
• Molecule 2: PROTEASOME

Chain X: 



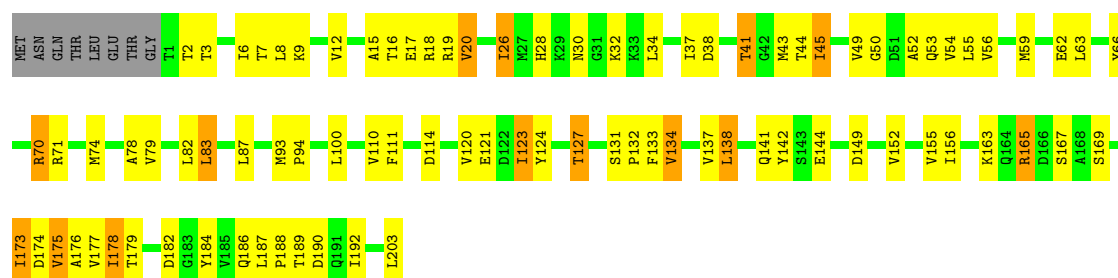
• Molecule 2: PROTEASOME

Chain Y:



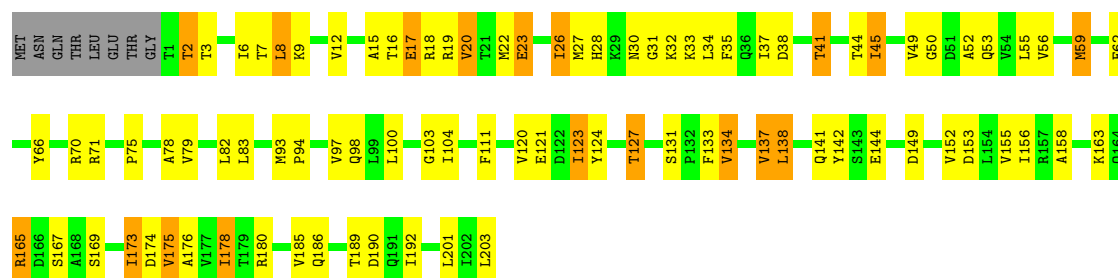
• Molecule 2: PROTEASOME

Chain Z:



• Molecule 2: PROTEASOME

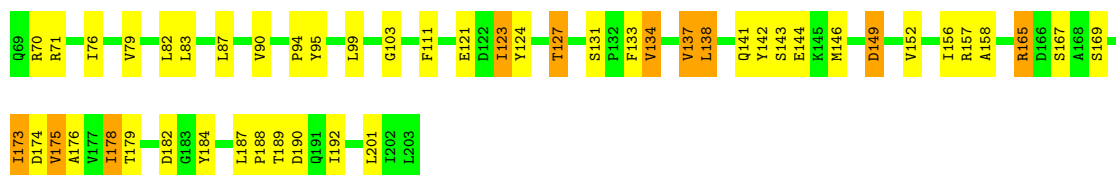
Chain 1:



• Molecule 2: PROTEASOME

Chain 2:





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	311.90Å 209.70Å 117.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.40 20.97 – 3.40	Depositor EDS
% Data completeness (in resolution range)	85.7 (10.00-3.40) 85.0 (20.97-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 3.37Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.221 , (Not available) 0.208 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	80.4	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 88.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 90045 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	56294	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.52	0/1743	0.71	1/2348 (0.0%)
1	C	0.51	0/1743	0.71	0/2348
1	D	0.52	0/1743	0.70	1/2348 (0.0%)
1	E	0.55	0/1743	0.72	0/2348
1	F	0.52	0/1743	0.70	0/2348
1	G	0.54	0/1743	0.69	0/2348
1	H	0.53	0/1743	0.70	0/2348
1	I	0.50	0/1743	0.70	0/2348
1	J	0.51	0/1743	0.69	0/2348
1	K	0.51	0/1743	0.69	1/2348 (0.0%)
1	L	0.53	0/1743	0.70	0/2348
1	M	0.51	0/1743	0.70	0/2348
1	N	0.54	0/1743	0.70	0/2348
1	O	0.52	0/1743	0.71	0/2348
2	1	0.55	0/1577	0.74	1/2129 (0.0%)
2	2	0.53	0/1577	0.75	1/2129 (0.0%)
2	B	0.56	0/1577	0.76	0/2129
2	P	0.57	0/1577	0.76	0/2129
2	Q	0.54	0/1577	0.75	0/2129
2	R	0.55	0/1577	0.77	2/2129 (0.1%)
2	S	0.57	0/1577	0.77	0/2129
2	T	0.55	0/1577	0.75	1/2129 (0.0%)
2	U	0.54	0/1577	0.74	0/2129
2	V	0.56	0/1577	0.77	0/2129
2	W	0.57	0/1577	0.75	1/2129 (0.0%)
2	X	0.54	0/1577	0.73	0/2129
2	Y	0.52	0/1577	0.74	0/2129
2	Z	0.54	0/1577	0.75	0/2129
All	All	0.53	0/46480	0.72	9/62678 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	95	TYR	N-CA-C	-5.91	95.06	111.00
2	1	8	LEU	CA-CB-CG	5.55	128.06	115.30
1	D	128	GLY	N-CA-C	5.36	126.49	113.10
2	W	8	LEU	CA-CB-CG	5.32	127.54	115.30
1	K	128	GLY	N-CA-C	5.31	126.39	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1720	393	1361	77	0
1	C	1720	393	1361	73	0
1	D	1720	393	1361	77	0
1	E	1720	393	1361	81	0
1	F	1720	393	1361	81	0
1	G	1720	393	1361	98	0
1	H	1720	393	1361	81	0
1	I	1720	393	1361	80	0
1	J	1720	393	1361	72	0
1	K	1720	393	1361	69	0
1	L	1720	393	1361	77	0
1	M	1720	393	1361	72	0
1	N	1720	393	1361	66	0
1	O	1720	393	1361	75	0
2	1	1558	350	1259	74	0
2	2	1558	350	1259	59	0
2	B	1558	350	1259	82	0
2	P	1558	350	1259	64	0
2	Q	1558	350	1259	53	0
2	R	1558	350	1259	69	0
2	S	1558	350	1259	78	0
2	T	1558	350	1259	59	0
2	U	1558	350	1259	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	V	1558	350	1259	74	0
2	W	1558	350	1259	69	0
2	X	1558	350	1259	61	0
2	Y	1558	350	1259	66	0
2	Z	1558	350	1259	67	0
All	All	45892	10402	36680	1849	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

The worst 5 of 1849 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:38:ASP:HB3	2:B:41:THR:HG23	1.38	1.03
2:T:38:ASP:HB3	2:T:41:THR:HG23	1.44	1.00
2:Q:45:ILE:HG12	2:Q:52:ALA:HB1	1.44	0.99
2:Q:38:ASP:HB3	2:Q:41:THR:HG23	1.46	0.98
2:R:38:ASP:HB3	2:R:41:THR:HG23	1.45	0.98

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	219/233 (94%)	184 (84%)	26 (12%)	9 (4%)	4	42
1	C	219/233 (94%)	185 (84%)	25 (11%)	9 (4%)	4	42
1	D	219/233 (94%)	184 (84%)	28 (13%)	7 (3%)	6	51
1	E	219/233 (94%)	188 (86%)	22 (10%)	9 (4%)	4	42
1	F	219/233 (94%)	183 (84%)	25 (11%)	11 (5%)	3	34
1	G	219/233 (94%)	186 (85%)	23 (10%)	10 (5%)	4	37
1	H	219/233 (94%)	186 (85%)	25 (11%)	8 (4%)	5	46
1	I	219/233 (94%)	188 (86%)	22 (10%)	9 (4%)	4	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	219/233 (94%)	182 (83%)	26 (12%)	11 (5%)	3	34
1	K	219/233 (94%)	187 (85%)	26 (12%)	6 (3%)	8	55
1	L	219/233 (94%)	186 (85%)	24 (11%)	9 (4%)	4	42
1	M	219/233 (94%)	184 (84%)	26 (12%)	9 (4%)	4	42
1	N	219/233 (94%)	187 (85%)	23 (10%)	9 (4%)	4	42
1	O	219/233 (94%)	188 (86%)	23 (10%)	8 (4%)	5	46
2	1	201/211 (95%)	184 (92%)	15 (8%)	2 (1%)	22	78
2	2	201/211 (95%)	181 (90%)	19 (10%)	1 (0%)	38	87
2	B	201/211 (95%)	185 (92%)	14 (7%)	2 (1%)	22	78
2	P	201/211 (95%)	183 (91%)	16 (8%)	2 (1%)	22	78
2	Q	201/211 (95%)	180 (90%)	20 (10%)	1 (0%)	38	87
2	R	201/211 (95%)	184 (92%)	15 (8%)	2 (1%)	22	78
2	S	201/211 (95%)	181 (90%)	16 (8%)	4 (2%)	11	62
2	T	201/211 (95%)	176 (88%)	23 (11%)	2 (1%)	22	78
2	U	201/211 (95%)	184 (92%)	15 (8%)	2 (1%)	22	78
2	V	201/211 (95%)	179 (89%)	20 (10%)	2 (1%)	22	78
2	W	201/211 (95%)	186 (92%)	13 (6%)	2 (1%)	22	78
2	X	201/211 (95%)	181 (90%)	18 (9%)	2 (1%)	22	78
2	Y	201/211 (95%)	183 (91%)	16 (8%)	2 (1%)	22	78
2	Z	201/211 (95%)	185 (92%)	14 (7%)	2 (1%)	22	78
All	All	5880/6216 (95%)	5150 (88%)	578 (10%)	152 (3%)	8	56

5 of 152 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	GLY
1	A	182	GLU
1	A	200	SER
1	C	128	GLY
1	C	200	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	184/193 (95%)	163 (89%)	21 (11%)	8	38
1	C	184/193 (95%)	160 (87%)	24 (13%)	6	31
1	D	184/193 (95%)	159 (86%)	25 (14%)	5	29
1	E	184/193 (95%)	159 (86%)	25 (14%)	5	29
1	F	184/193 (95%)	158 (86%)	26 (14%)	5	28
1	G	184/193 (95%)	162 (88%)	22 (12%)	7	35
1	H	184/193 (95%)	164 (89%)	20 (11%)	9	42
1	I	184/193 (95%)	162 (88%)	22 (12%)	7	35
1	J	184/193 (95%)	162 (88%)	22 (12%)	7	35
1	K	184/193 (95%)	160 (87%)	24 (13%)	6	31
1	L	184/193 (95%)	159 (86%)	25 (14%)	5	29
1	M	184/193 (95%)	162 (88%)	22 (12%)	7	35
1	N	184/193 (95%)	160 (87%)	24 (13%)	6	31
1	O	184/193 (95%)	157 (85%)	27 (15%)	4	26
2	1	170/177 (96%)	148 (87%)	22 (13%)	6	32
2	2	170/177 (96%)	144 (85%)	26 (15%)	4	24
2	B	170/177 (96%)	145 (85%)	25 (15%)	4	26
2	P	170/177 (96%)	148 (87%)	22 (13%)	6	32
2	Q	170/177 (96%)	143 (84%)	27 (16%)	4	22
2	R	170/177 (96%)	143 (84%)	27 (16%)	4	22
2	S	170/177 (96%)	146 (86%)	24 (14%)	5	28
2	T	170/177 (96%)	152 (89%)	18 (11%)	10	43
2	U	170/177 (96%)	146 (86%)	24 (14%)	5	28
2	V	170/177 (96%)	145 (85%)	25 (15%)	4	26
2	W	170/177 (96%)	145 (85%)	25 (15%)	4	26
2	X	170/177 (96%)	149 (88%)	21 (12%)	7	34
2	Y	170/177 (96%)	144 (85%)	26 (15%)	4	24
2	Z	170/177 (96%)	150 (88%)	20 (12%)	8	36
All	All	4956/5180 (96%)	4295 (87%)	661 (13%)	6	30

5 of 661 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	201	LEU
2	P	138	LEU
2	Z	173	ILE
1	N	49	ILE
1	O	71	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 120 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	23	GLN
1	N	98	GLN
2	Z	28	HIS
1	L	44	ASN
1	M	44	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	221/233 (94%)	-0.12	2 (0%) 81 47	17, 56, 117, 155	0
1	C	221/233 (94%)	-0.18	0 100 100	13, 53, 115, 154	0
1	D	221/233 (94%)	-0.17	1 (0%) 88 61	21, 53, 116, 153	0
1	E	221/233 (94%)	-0.19	0 100 100	17, 52, 115, 155	0
1	F	221/233 (94%)	-0.14	0 100 100	16, 57, 116, 153	0
1	G	221/233 (94%)	-0.08	3 (1%) 72 35	20, 56, 118, 155	0
1	H	221/233 (94%)	-0.12	1 (0%) 88 61	21, 57, 116, 154	0
1	I	221/233 (94%)	-0.12	2 (0%) 81 47	17, 55, 116, 155	0
1	J	221/233 (94%)	-0.12	2 (0%) 81 47	21, 55, 116, 156	0
1	K	221/233 (94%)	-0.17	1 (0%) 88 61	20, 55, 116, 153	0
1	L	221/233 (94%)	-0.19	1 (0%) 88 61	13, 53, 116, 153	0
1	M	221/233 (94%)	-0.16	0 100 100	17, 53, 117, 153	0
1	N	221/233 (94%)	-0.17	1 (0%) 88 61	19, 52, 116, 156	0
1	O	221/233 (94%)	-0.17	1 (0%) 88 61	18, 51, 116, 152	0
2	1	203/211 (96%)	-0.38	0 100 100	9, 33, 69, 85	0
2	2	203/211 (96%)	-0.38	0 100 100	6, 33, 69, 88	0
2	B	203/211 (96%)	-0.36	0 100 100	11, 34, 69, 90	0
2	P	203/211 (96%)	-0.36	0 100 100	8, 35, 69, 89	0
2	Q	203/211 (96%)	-0.41	0 100 100	8, 33, 71, 90	0
2	R	203/211 (96%)	-0.45	0 100 100	6, 32, 68, 86	0
2	S	203/211 (96%)	-0.42	0 100 100	7, 33, 68, 91	0
2	T	203/211 (96%)	-0.40	0 100 100	10, 35, 73, 90	0
2	U	203/211 (96%)	-0.39	0 100 100	14, 34, 70, 92	0
2	V	203/211 (96%)	-0.39	0 100 100	11, 32, 69, 89	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
2	W	203/211 (96%)	-0.41	0	100	100	11, 34, 69, 85	0
2	X	203/211 (96%)	-0.43	0	100	100	8, 32, 70, 90	0
2	Y	203/211 (96%)	-0.44	0	100	100	10, 32, 68, 92	0
2	Z	203/211 (96%)	-0.46	0	100	100	9, 32, 69, 91	0
All	All	5936/6216 (95%)	-0.27	15 (0%)	91	73	6, 43, 107, 156	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	205	GLU	2.8
1	G	205	GLU	2.8
1	G	201	LEU	2.7
1	L	55	ARG	2.4
1	I	205	GLU	2.4

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.