Full wwPDB X-ray Structure Validation Report (i)

Jan 8, 2024 – 06:34 am GMT

PDB ID	:	5MSJ
Title	:	Mouse PA28alpha
Authors	:	Huber, E.M.; Groll, M.
Deposited on	:	2017-01-05
Resolution	:	3.50 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 (i) 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 (1)) were used in the production of this report:

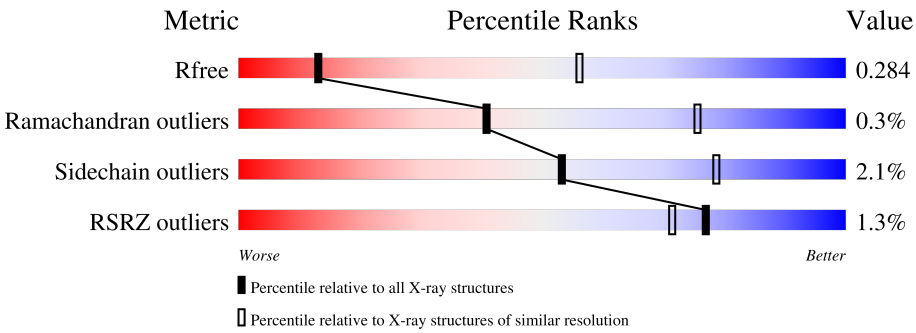
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	249	.% 81% • 16%
1	B	249	.% 81% • 18%
1	C	249	2% 80% • 18%
1	D	249	.% 80% • 18%
1	E	249	.% 81% • 16%
1	F	249	.% 79% • 19%

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Mol	Chain	Length	Quality of chain
1	G	249	.% 81% • 18%
1	H	249	.% 82% • 16%
1	I	249	.% 78% • 22%
1	J	249	2% 77% • 19%
1	K	249	82% • 17%
1	L	249	2% 82% • 16%
1	M	249	2% 78% • 19%
1	N	249	2% 82% • 16%
1	O	249	.% 79% • 18%
1	P	249	82% • 16%
1	Q	249	80% • 18%
1	R	249	.% 78% • 20%
1	S	249	.% 78% • 20%
1	T	249	80% • 17%
1	U	249	2% 84% • 15%
1	V	249	.% 80% • 19%
1	W	249	.% 82% 18%
1	X	249	79% • 20%
1	Y	249	2% 79% • 19%
1	Z	249	.% 81% • 18%
1	a	249	83% • 16%
1	b	249	.% 82% • 17%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 46128 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 activator complex subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	210	1690	1081	288	315	6	0	0	0
			Total	C	N	O	S			
1	B	204	1646	1051	282	307	6	0	0	0
			Total	C	N	O	S			
1	C	205	1653	1056	283	308	6	0	0	0
			Total	C	N	O	S			
1	D	203	1635	1045	278	306	6	0	0	0
			Total	C	N	O	S			
1	E	208	1675	1070	286	313	6	0	0	0
			Total	C	N	O	S			
1	F	201	1619	1037	274	302	6	0	0	0
			Total	C	N	O	S			
1	G	205	1649	1054	280	309	6	0	0	0
			Total	C	N	O	S			
1	H	208	1676	1071	286	313	6	0	0	0
			Total	C	N	O	S			
1	I	195	1577	1006	269	297	5	0	0	0
			Total	C	N	O	S			
1	J	202	1635	1047	280	303	5	0	0	0
			Total	C	N	O	S			
1	K	207	1667	1066	285	310	6	0	0	0
			Total	C	N	O	S			
1	L	209	1682	1075	287	314	6	0	0	0
			Total	C	N	O	S			
1	M	201	1622	1038	276	302	6	0	0	0
			Total	C	N	O	S			
1	N	208	1675	1071	286	312	6	0	0	0
			Total	C	N	O	S			
1	O	203	1632	1044	276	306	6	0	0	0
			Total	C	N	O	S			
1	P	208	1675	1071	286	312	6	0	0	0

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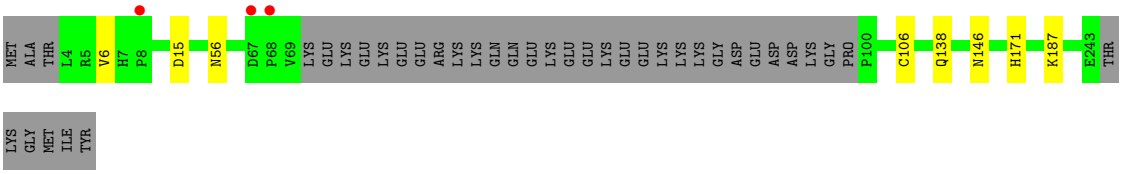
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	203	1635	1045	278	306	6	0	0	0
			Total	C	N	O	S			
1	R	200	1612	1032	273	301	6	0	0	0
			Total	C	N	O	S			
1	S	199	1602	1024	272	300	6	0	0	0
			Total	C	N	O	S			
1	T	206	1661	1062	284	309	6	0	0	0
			Total	C	N	O	S			
1	U	212	1711	1092	290	323	6	0	0	0
			Total	C	N	O	S			
1	V	202	1625	1039	275	305	6	0	0	0
			Total	C	N	O	S			
1	W	204	1647	1053	282	307	5	0	0	0
			Total	C	N	O	S			
1	X	200	1612	1031	273	303	5	0	0	0
			Total	C	N	O	S			
1	Y	201	1622	1037	276	304	5	0	0	0
			Total	C	N	O	S			
1	Z	204	1651	1057	282	307	5	0	0	0
			Total	C	N	O	S			
1	a	209	1683	1076	287	314	6	0	0	0
			Total	C	N	O	S			
1	b	206	1659	1062	284	307	6	0	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 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.

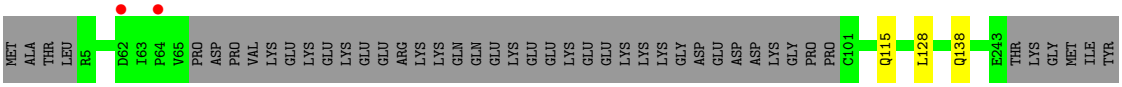
• Molecule 1: Proteasome activator complex subunit 1

Chain A:



• Molecule 1: Proteasome activator complex subunit 1

Chain B:

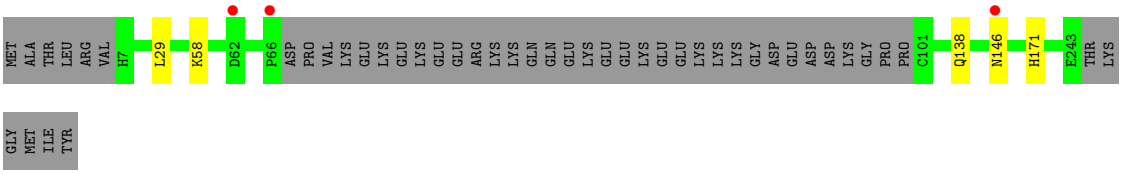


• Molecule 1: Proteasome activator complex subunit 1

Chain C:

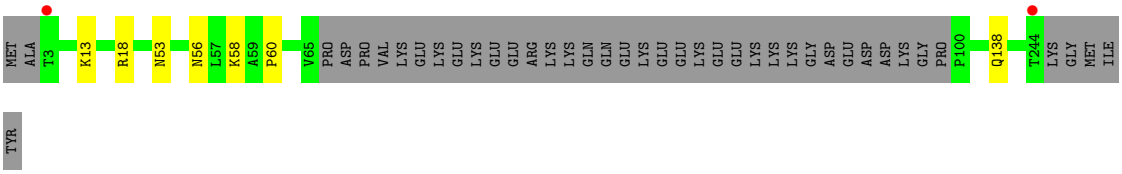
• Molecule 1: Proteasome activator complex subunit 1

Chain D:



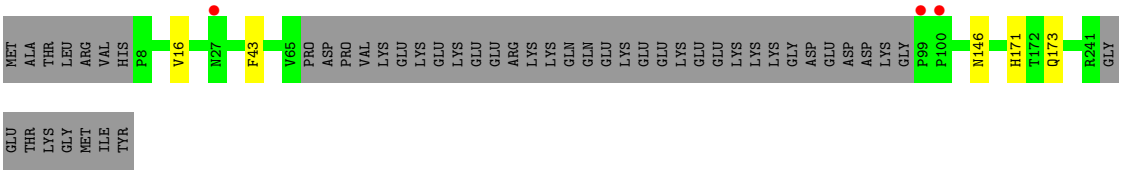
• Molecule 1: Proteasome activator complex subunit 1

Chain E:



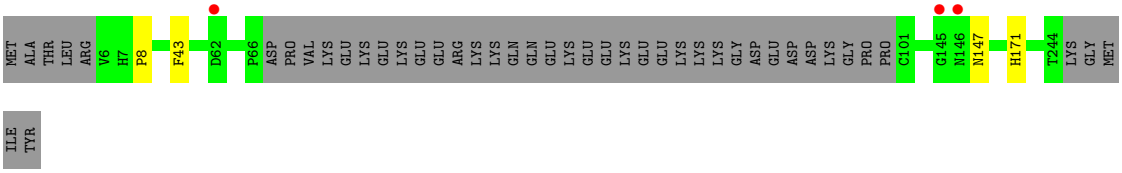
• Molecule 1: Proteasome activator complex subunit 1

Chain F:



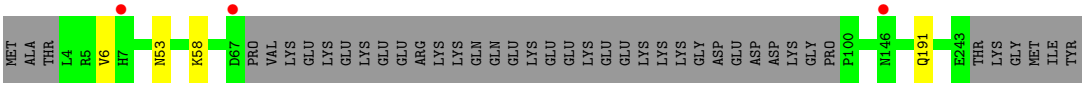
• Molecule 1: Proteasome activator complex subunit 1

Chain G:



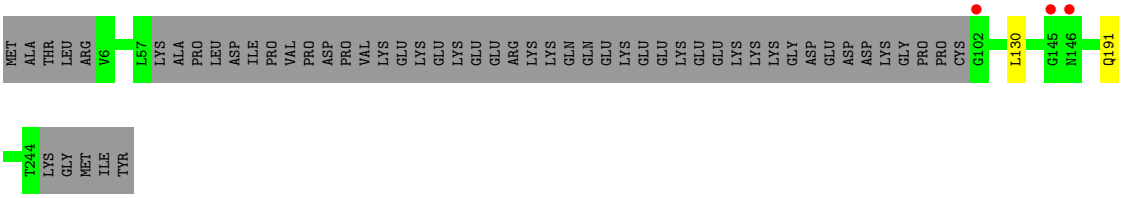
• Molecule 1: Proteasome activator complex subunit 1

Chain H:



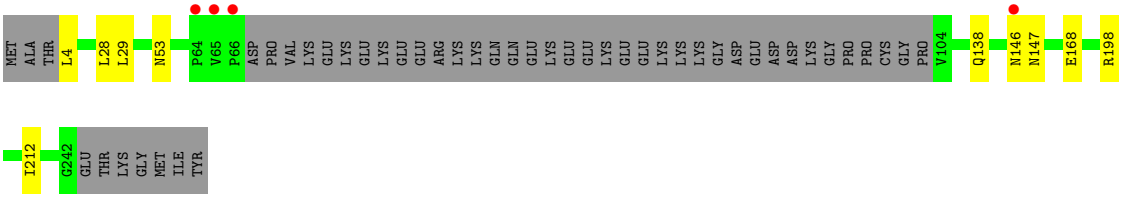
• Molecule 1: Proteasome activator complex subunit 1

Chain I:



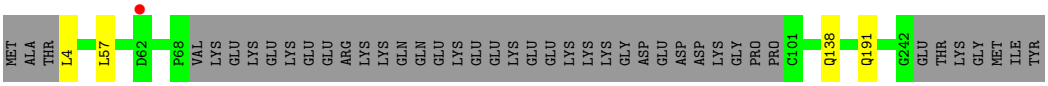
• Molecule 1: Proteasome activator complex subunit 1

Chain J:



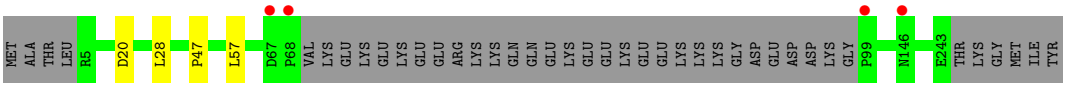
• Molecule 1: Proteasome activator complex subunit 1

Chain K:



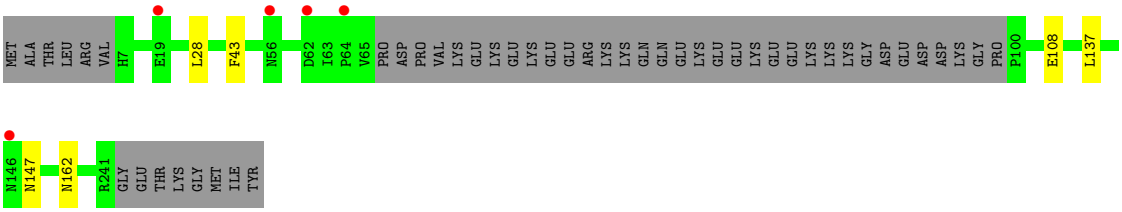
• Molecule 1: Proteasome activator complex subunit 1

Chain L:



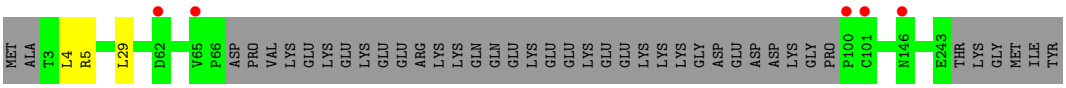
• Molecule 1: Proteasome activator complex subunit 1

Chain M:



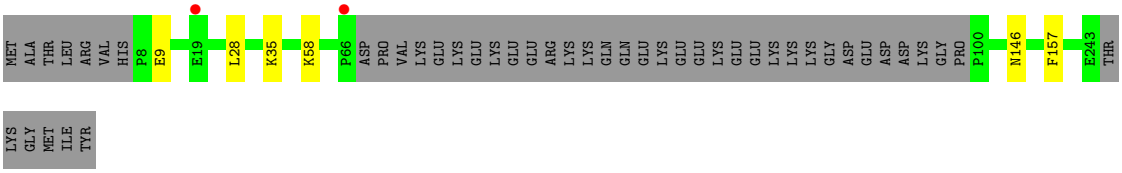
• Molecule 1: Proteasome activator complex subunit 1

Chain N:



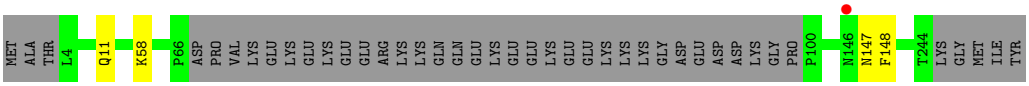
• Molecule 1: Proteasome activator complex subunit 1

Chain O:



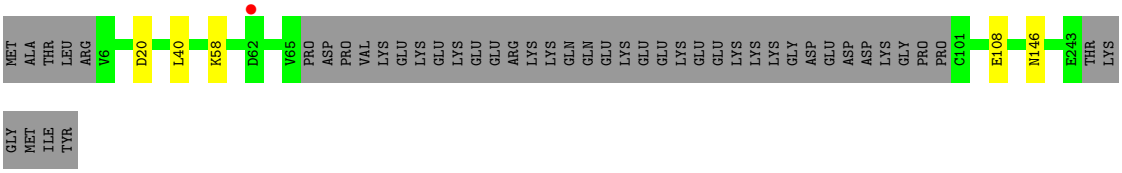
• Molecule 1: Proteasome activator complex subunit 1

Chain P:



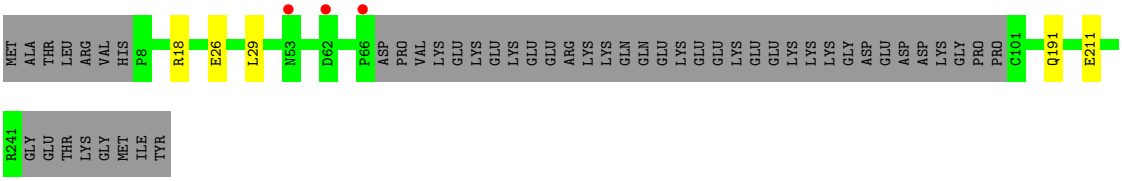
• Molecule 1: Proteasome activator complex subunit 1

Chain Q:



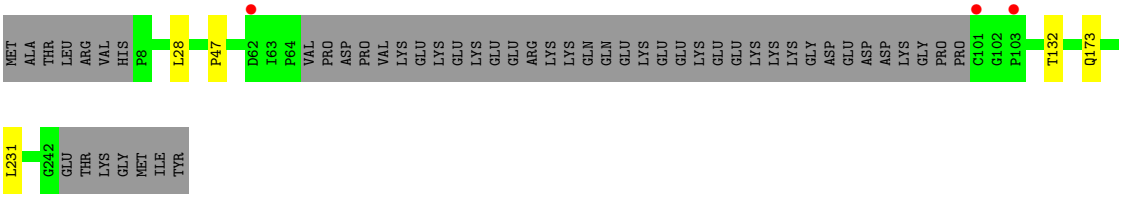
• Molecule 1: Proteasome activator complex subunit 1

Chain R:



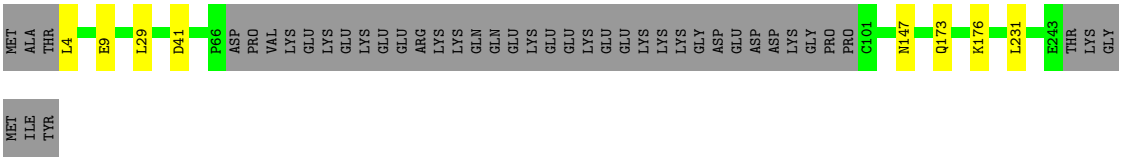
• Molecule 1: Proteasome activator complex subunit 1

Chain S:



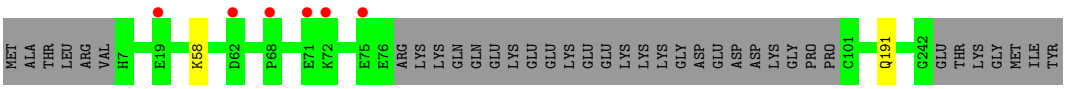
• Molecule 1: Proteasome activator complex subunit 1

Chain T:



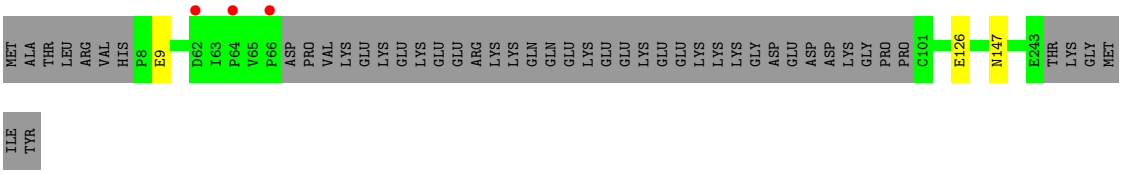
• Molecule 1: Proteasome activator complex subunit 1

Chain U:



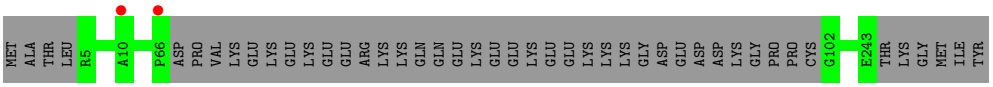
• Molecule 1: Proteasome activator complex subunit 1

Chain V:



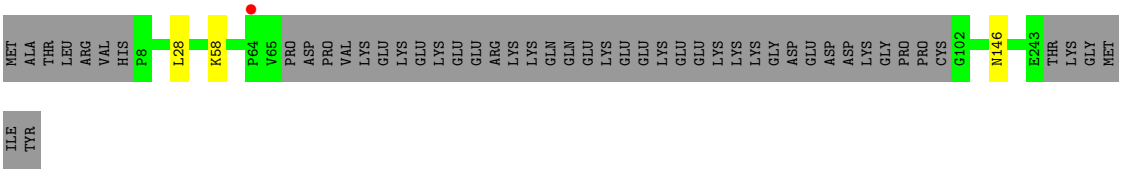
• Molecule 1: Proteasome activator complex subunit 1

Chain W:



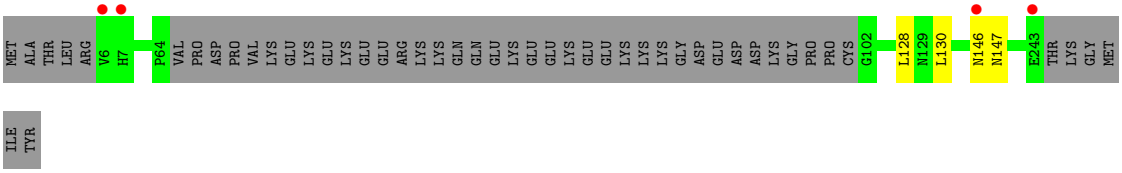
• Molecule 1: Proteasome activator complex subunit 1

Chain X:



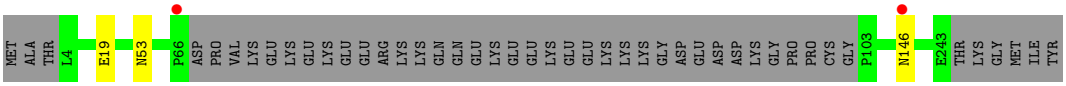
• Molecule 1: Proteasome activator complex subunit 1

Chain Y:



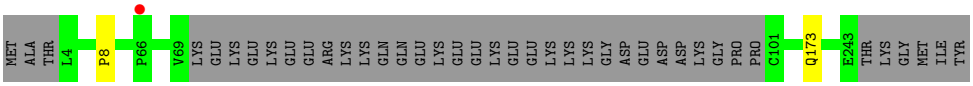
• Molecule 1: Proteasome activator complex subunit 1

Chain Z:



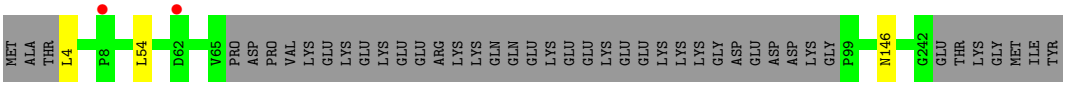
• Molecule 1: Proteasome activator complex subunit 1

Chain a:



• Molecule 1: Proteasome activator complex subunit 1

Chain b:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	87.79Å 119.80Å 196.67Å 94.21° 98.52° 87.98°	Depositor
Resolution (Å)	29.65 – 3.50 29.65 – 3.50	Depositor EDS
% Data completeness (in resolution range)	93.1 (29.65-3.50) 93.2 (29.65-3.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 3.47Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.250 , 0.283 0.251 , 0.284	Depositor DCC
R_{free} test set	4638 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	91.5	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 33.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	46128	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.36	0/1722	0.52	0/2329
1	B	0.37	0/1675	0.52	0/2262
1	C	0.36	0/1683	0.52	0/2274
1	D	0.36	0/1665	0.51	0/2250
1	E	0.36	0/1705	0.53	0/2304
1	F	0.36	0/1649	0.53	0/2228
1	G	0.36	0/1679	0.53	0/2270
1	H	0.37	0/1707	0.52	0/2307
1	I	0.37	0/1604	0.51	0/2165
1	J	0.37	0/1664	0.55	0/2248
1	K	0.36	0/1698	0.52	0/2296
1	L	0.37	0/1715	0.53	0/2320
1	M	0.37	0/1652	0.50	0/2232
1	N	0.36	0/1706	0.53	0/2306
1	O	0.36	0/1662	0.51	0/2245
1	P	0.37	0/1706	0.53	0/2306
1	Q	0.36	0/1664	0.51	0/2248
1	R	0.36	0/1641	0.51	0/2217
1	S	0.36	0/1630	0.51	0/2200
1	T	0.36	0/1691	0.52	0/2285
1	U	0.36	0/1742	0.50	0/2352
1	V	0.37	0/1654	0.51	0/2234
1	W	0.36	0/1677	0.52	0/2266
1	X	0.36	0/1640	0.51	0/2214
1	Y	0.36	0/1651	0.49	0/2230
1	Z	0.36	0/1681	0.51	0/2271
1	a	0.36	0/1714	0.51	0/2318
1	b	0.36	0/1690	0.53	0/2284
All	All	0.36	0/46967	0.52	0/63461

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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 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	206/249 (83%)	201 (98%)	4 (2%)	1 (0%)	29	68
1	B	200/249 (80%)	194 (97%)	6 (3%)	0	100	100
1	C	201/249 (81%)	197 (98%)	3 (2%)	1 (0%)	29	68
1	D	199/249 (80%)	195 (98%)	3 (2%)	1 (0%)	29	68
1	E	204/249 (82%)	199 (98%)	3 (2%)	2 (1%)	15	54
1	F	197/249 (79%)	190 (96%)	7 (4%)	0	100	100
1	G	201/249 (81%)	199 (99%)	1 (0%)	1 (0%)	29	68
1	H	204/249 (82%)	199 (98%)	3 (2%)	2 (1%)	15	54
1	I	191/249 (77%)	189 (99%)	2 (1%)	0	100	100
1	J	198/249 (80%)	194 (98%)	4 (2%)	0	100	100
1	K	203/249 (82%)	200 (98%)	3 (2%)	0	100	100
1	L	205/249 (82%)	200 (98%)	5 (2%)	0	100	100
1	M	197/249 (79%)	194 (98%)	3 (2%)	0	100	100
1	N	204/249 (82%)	201 (98%)	3 (2%)	0	100	100
1	O	199/249 (80%)	195 (98%)	3 (2%)	1 (0%)	29	68
1	P	204/249 (82%)	200 (98%)	3 (2%)	1 (0%)	29	68
1	Q	199/249 (80%)	195 (98%)	3 (2%)	1 (0%)	29	68
1	R	196/249 (79%)	192 (98%)	4 (2%)	0	100	100
1	S	195/249 (78%)	190 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T	202/249 (81%)	198 (98%)	4 (2%)	0	100	100
1	U	208/249 (84%)	203 (98%)	4 (2%)	1 (0%)	29	68
1	V	198/249 (80%)	193 (98%)	5 (2%)	0	100	100
1	W	200/249 (80%)	196 (98%)	4 (2%)	0	100	100
1	X	196/249 (79%)	192 (98%)	2 (1%)	2 (1%)	15	54
1	Y	197/249 (79%)	192 (98%)	4 (2%)	1 (0%)	29	68
1	Z	200/249 (80%)	199 (100%)	1 (0%)	0	100	100
1	a	205/249 (82%)	196 (96%)	8 (4%)	1 (0%)	29	68
1	b	202/249 (81%)	198 (98%)	3 (2%)	1 (0%)	29	68
All	All	5611/6972 (80%)	5491 (98%)	103 (2%)	17 (0%)	41	75

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	146	ASN
1	D	58	LYS
1	H	58	LYS
1	Y	147	ASN
1	b	146	ASN
1	A	6	VAL
1	C	58	LYS
1	P	58	LYS
1	U	58	LYS
1	E	58	LYS
1	O	58	LYS
1	Q	58	LYS
1	X	58	LYS
1	a	8	PRO
1	G	8	PRO
1	E	60	PRO
1	H	6	VAL

5.3.2 Protein sidechains (i)

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	188/223 (84%)	181 (96%)	7 (4%)	34	65
1	B	182/223 (82%)	179 (98%)	3 (2%)	62	83
1	C	183/223 (82%)	179 (98%)	4 (2%)	52	78
1	D	181/223 (81%)	177 (98%)	4 (2%)	52	78
1	E	186/223 (83%)	181 (97%)	5 (3%)	44	73
1	F	180/223 (81%)	175 (97%)	5 (3%)	43	72
1	G	183/223 (82%)	180 (98%)	3 (2%)	62	83
1	H	186/223 (83%)	184 (99%)	2 (1%)	73	88
1	I	174/223 (78%)	172 (99%)	2 (1%)	73	88
1	J	181/223 (81%)	171 (94%)	10 (6%)	21	54
1	K	185/223 (83%)	181 (98%)	4 (2%)	52	78
1	L	187/223 (84%)	183 (98%)	4 (2%)	53	79
1	M	180/223 (81%)	174 (97%)	6 (3%)	38	68
1	N	186/223 (83%)	183 (98%)	3 (2%)	62	83
1	O	181/223 (81%)	176 (97%)	5 (3%)	43	72
1	P	186/223 (83%)	183 (98%)	3 (2%)	62	83
1	Q	181/223 (81%)	177 (98%)	4 (2%)	52	78
1	R	179/223 (80%)	174 (97%)	5 (3%)	43	72
1	S	177/223 (79%)	172 (97%)	5 (3%)	43	72
1	T	184/223 (82%)	176 (96%)	8 (4%)	29	62
1	U	190/223 (85%)	189 (100%)	1 (0%)	88	94
1	V	180/223 (81%)	177 (98%)	3 (2%)	60	82
1	W	182/223 (82%)	182 (100%)	0	100	100
1	X	178/223 (80%)	177 (99%)	1 (1%)	86	94
1	Y	179/223 (80%)	176 (98%)	3 (2%)	60	82
1	Z	183/223 (82%)	180 (98%)	3 (2%)	62	83
1	a	187/223 (84%)	186 (100%)	1 (0%)	88	94
1	b	184/223 (82%)	182 (99%)	2 (1%)	73	88
All	All	5113/6244 (82%)	5007 (98%)	106 (2%)	53	79

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	56	ASN
1	A	106	CYS
1	A	138	GLN
1	A	146	ASN
1	A	171	HIS
1	A	187	LYS
1	B	115	GLN
1	B	128	LEU
1	B	138	GLN
1	C	19	GLU
1	C	62	ASP
1	C	138	GLN
1	C	171	HIS
1	D	29	LEU
1	D	138	GLN
1	D	146	ASN
1	D	171	HIS
1	E	13	LYS
1	E	18	ARG
1	E	53	ASN
1	E	56	ASN
1	E	138	GLN
1	F	16	VAL
1	F	43	PHE
1	F	146	ASN
1	F	171	HIS
1	F	173	GLN
1	G	43	PHE
1	G	147	ASN
1	G	171	HIS
1	H	53	ASN
1	H	191	GLN
1	I	130	LEU
1	I	191	GLN
1	J	4	LEU
1	J	28	LEU
1	J	29	LEU
1	J	53	ASN
1	J	138	GLN
1	J	146	ASN
1	J	147	ASN
1	J	168	GLU

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Mol	Chain	Res	Type
1	J	198	ARG
1	J	212	ILE
1	K	4	LEU
1	K	57	LEU
1	K	138	GLN
1	K	191	GLN
1	L	20	ASP
1	L	28	LEU
1	L	47	PRO
1	L	57	LEU
1	M	28	LEU
1	M	43	PHE
1	M	108	GLU
1	M	137	LEU
1	M	147	ASN
1	M	162	ASN
1	N	4	LEU
1	N	5	ARG
1	N	29	LEU
1	O	9	GLU
1	O	28	LEU
1	O	35	LYS
1	O	146	ASN
1	O	157	PHE
1	P	11	GLN
1	P	147	ASN
1	P	148	PHE
1	Q	20	ASP
1	Q	40	LEU
1	Q	108	GLU
1	Q	146	ASN
1	R	18	ARG
1	R	26	GLU
1	R	29	LEU
1	R	191	GLN
1	R	211	GLU
1	S	28	LEU
1	S	47	PRO
1	S	132	THR
1	S	173	GLN
1	S	231	LEU
1	T	4	LEU

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Mol	Chain	Res	Type
1	T	9	GLU
1	T	29	LEU
1	T	41	ASP
1	T	147	ASN
1	T	173	GLN
1	T	176	LYS
1	T	231	LEU
1	U	191	GLN
1	V	9	GLU
1	V	126	GLU
1	V	147	ASN
1	X	28	LEU
1	Y	128	LEU
1	Y	130	LEU
1	Y	146	ASN
1	Z	19	GLU
1	Z	53	ASN
1	Z	146	ASN
1	a	173	GLN
1	b	4	LEU
1	b	54	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	210	GLN
1	B	56	ASN
1	B	115	GLN
1	B	162	ASN
1	B	171	HIS
1	B	191	GLN
1	D	53	ASN
1	D	146	ASN
1	E	53	ASN
1	E	56	ASN
1	E	147	ASN
1	E	162	ASN
1	E	191	GLN
1	F	105	ASN
1	F	136	GLN
1	F	146	ASN

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Mol	Chain	Res	Type
1	F	191	GLN
1	F	202	HIS
1	H	53	ASN
1	H	105	ASN
1	H	171	HIS
1	H	191	GLN
1	I	53	ASN
1	I	191	GLN
1	J	27	ASN
1	J	105	ASN
1	J	146	ASN
1	K	191	GLN
1	L	129	ASN
1	L	147	ASN
1	M	53	ASN
1	M	136	GLN
1	M	162	ASN
1	N	105	ASN
1	N	136	GLN
1	N	146	ASN
1	N	147	ASN
1	N	191	GLN
1	N	210	GLN
1	O	115	GLN
1	O	146	ASN
1	P	136	GLN
1	P	191	GLN
1	Q	146	ASN
1	Q	199	GLN
1	R	115	GLN
1	R	136	GLN
1	R	191	GLN
1	S	115	GLN
1	T	115	GLN
1	T	147	ASN
1	T	210	GLN
1	U	191	GLN
1	V	147	ASN
1	W	105	ASN
1	W	153	GLN
1	X	50	ASN
1	X	129	ASN

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Mol	Chain	Res	Type
1	X	191	GLN
1	Y	105	ASN
1	Y	191	GLN
1	Z	191	GLN
1	b	56	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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	210/249 (84%)	-0.33	3 (1%)	75	69	66, 89, 122, 152	0
1	B	204/249 (81%)	-0.26	2 (0%)	82	77	70, 95, 136, 141	0
1	C	205/249 (82%)	-0.21	4 (1%)	65	60	71, 97, 133, 149	0
1	D	203/249 (81%)	-0.21	3 (1%)	73	68	76, 100, 148, 160	0
1	E	208/249 (83%)	-0.26	2 (0%)	82	77	82, 105, 135, 148	0
1	F	201/249 (80%)	-0.22	3 (1%)	73	68	73, 95, 137, 152	0
1	G	205/249 (82%)	-0.34	3 (1%)	73	68	71, 88, 122, 138	0
1	H	208/249 (83%)	-0.26	3 (1%)	75	69	79, 100, 134, 162	0
1	I	195/249 (78%)	-0.20	3 (1%)	73	68	79, 105, 143, 158	0
1	J	202/249 (81%)	-0.23	4 (1%)	65	60	75, 98, 143, 154	0
1	K	207/249 (83%)	-0.27	1 (0%)	91	88	75, 101, 144, 157	0
1	L	209/249 (83%)	-0.25	4 (1%)	66	61	76, 106, 137, 165	0
1	M	201/249 (80%)	-0.13	5 (2%)	57	51	75, 107, 145, 157	0
1	N	208/249 (83%)	-0.21	5 (2%)	59	53	73, 98, 137, 147	0
1	O	203/249 (81%)	-0.29	2 (0%)	82	77	71, 93, 125, 147	0
1	P	208/249 (83%)	-0.28	1 (0%)	91	88	72, 95, 132, 144	0
1	Q	203/249 (81%)	-0.25	1 (0%)	91	88	76, 100, 129, 135	0
1	R	200/249 (80%)	-0.27	3 (1%)	73	68	81, 100, 140, 171	0
1	S	199/249 (79%)	-0.28	3 (1%)	73	68	69, 94, 137, 159	0
1	T	206/249 (82%)	-0.35	0	100	100	70, 93, 131, 139	0
1	U	212/249 (85%)	-0.30	6 (2%)	53	47	69, 92, 144, 174	0
1	V	202/249 (81%)	-0.25	3 (1%)	73	68	76, 95, 134, 161	0
1	W	204/249 (81%)	-0.28	2 (0%)	82	77	73, 95, 137, 150	0
1	X	200/249 (80%)	-0.31	1 (0%)	91	88	69, 94, 128, 136	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	Y	201/249 (80%)	-0.28	4 (1%)	65	60	67, 96, 136, 162	0
1	Z	204/249 (81%)	-0.29	2 (0%)	82	77	68, 95, 134, 159	0
1	a	209/249 (83%)	-0.28	1 (0%)	91	88	71, 98, 133, 155	0
1	b	206/249 (82%)	-0.32	2 (0%)	82	77	71, 97, 133, 148	0
All	All	5723/6972 (82%)	-0.27	76 (1%)	77	71	66, 97, 137, 174	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	100	PRO	4.2
1	O	66	PRO	3.9
1	V	66	PRO	3.8
1	I	146	ASN	3.7
1	U	68	PRO	3.7
1	H	7	HIS	3.6
1	S	62	ASP	3.6
1	Y	146	ASN	3.6
1	N	62	ASP	3.4
1	U	75	GLU	3.4
1	Z	66	PRO	3.3
1	M	146	ASN	3.3
1	B	62	ASP	3.2
1	D	62	ASP	3.2
1	J	146	ASN	3.2
1	H	146	ASN	3.2
1	J	64	PRO	3.1
1	a	66	PRO	3.1
1	F	99	PRO	3.1
1	E	3	THR	3.0
1	F	27	ASN	3.0
1	J	66	PRO	3.0
1	E	244	THR	2.9
1	R	66	PRO	2.9
1	A	68	PRO	2.8
1	K	62	ASP	2.8
1	L	67	ASP	2.8
1	C	66	PRO	2.8
1	S	103	PRO	2.8
1	L	146	ASN	2.7
1	Z	146	ASN	2.7
1	L	68	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	Q	62	ASP	2.7
1	G	146	ASN	2.6
1	C	243	GLU	2.6
1	R	53	ASN	2.6
1	Y	243	GLU	2.5
1	C	101	CYS	2.5
1	C	146	ASN	2.5
1	G	62	ASP	2.5
1	U	72	LYS	2.5
1	Y	7	HIS	2.5
1	M	64	PRO	2.5
1	b	62	ASP	2.5
1	H	67	ASP	2.4
1	S	101	CYS	2.4
1	N	65	VAL	2.4
1	V	64	PRO	2.4
1	W	66	PRO	2.4
1	X	64	PRO	2.4
1	D	146	ASN	2.4
1	D	66	PRO	2.3
1	U	62	ASP	2.3
1	N	101	CYS	2.3
1	I	145	GLY	2.3
1	M	62	ASP	2.3
1	N	146	ASN	2.3
1	L	99	PRO	2.3
1	F	100	PRO	2.2
1	A	8	PRO	2.2
1	M	19	GLU	2.2
1	U	19	GLU	2.2
1	P	146	ASN	2.2
1	A	67	ASP	2.2
1	U	71	GLU	2.2
1	I	102	GLY	2.2
1	O	19	GLU	2.1
1	R	62	ASP	2.1
1	M	56	ASN	2.1
1	B	64	PRO	2.1
1	J	65	VAL	2.1
1	V	62	ASP	2.1
1	W	10	ALA	2.0
1	b	8	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	Y	6	VAL	2.0
1	G	145	GLY	2.0

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 monosaccharides 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.