wwPDB X-ray Structure Validation Summary Report (i)

Jan 3, 2024 – 01:11 pm GMT

PDB ID	:	5CGF
Title	:	Yeast 20S proteasome beta5-G48C mutant
Authors	:	Dubiella, C.; Groll, M.
Deposited on	:	2015-07-09
Resolution	:	2.80 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
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:

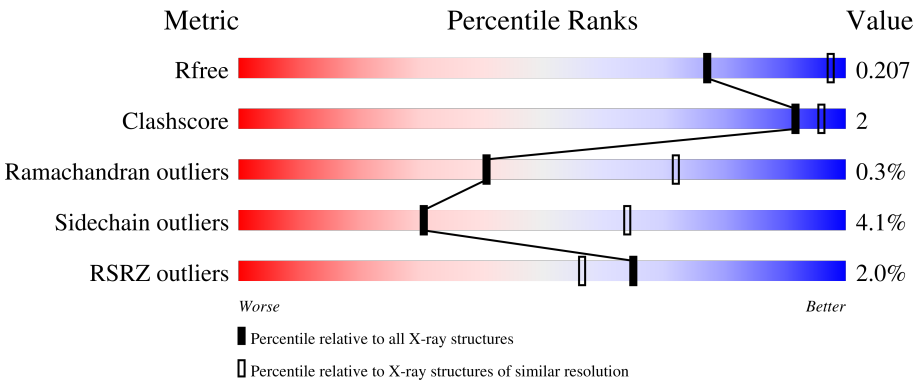
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	250	2%, 98%, •
1	O	250	2%, 97%, •
2	B	258	2%, 86%, 9%, 5%
2	P	258	3%, 86%, 8%, • 5%
3	C	254	4%, 86%, 7%, • 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	7% 86% 7% 6%
4	D	260	.% 85% 5% 10%
4	R	260	2% 84% 5% 10%
5	E	234	2% 90% 8%
5	S	234	6% 89% 9%
6	F	288	.% 80% 5% 16%
6	T	288	.% 80% 5% 16%
7	G	252	.% 88% 8%
7	U	252	.% 89% 6%
8	H	232	3% 89% 7%
8	V	232	3% 89% 7%
9	I	205	94% 6%
9	W	205	.% 93% 6%
10	J	198	.% 89% 8%
10	X	198	2% 90% 8%
11	K	212	92% 6%
11	Y	212	92% 6%
12	L	222	94% 5%
12	Z	222	94% 5%
13	M	246	88% 7% 5%
13	a	246	92% 5%
14	N	196	.% 94% 5%
14	b	196	.% 97%

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 49795 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	250	1915	1219	315	377	4	0	0	0
1	O	250	1915	1219	315	377	4	0	0	0

- Molecule 2 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	244	1904	1201	321	379	3	0	0	0
2	P	244	1904	1201	321	379	3	0	0	0

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	240	1881	1176	329	372	4	0	0	0
3	Q	240	1881	1176	329	372	4	0	0	0

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	235	1813	1136	304	366	7	0	0	0
4	R	235	1813	1136	304	366	7	0	0	0

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	231	1773	1114	307	348	4	0	0	0
5	S	231	1773	1114	307	348	4	0	0	0

- Molecule 6 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	243	1892	1203	329	356	4	0	0	0
6	T	243	1892	1203	329	356	4	0	0	0

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	241	1907	1214	320	365	8	0	0	0
7	U	241	1907	1214	320	365	8	0	0	0

- Molecule 8 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	226	1719	1082	298	332	7	0	0	0
8	V	226	1719	1082	298	332	7	0	0	0

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	204	1581	1010	258	305	8	0	0	0
9	W	204	1581	1010	258	305	8	0	0	0

- Molecule 10 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	195	1561	992	264	299	6	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	X	195	1561	992	264	299	6	0	0	0

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	212	1646	1046	280	312	8	0	0	0
11	Y	212	1646	1046	280	312	8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	48	CYS	GLY	engineered mutation	UNP P30656
Y	48	CYS	GLY	engineered mutation	UNP P30656

- Molecule 12 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	222	1757	1115	303	335	4	0	0	0
12	Z	222	1757	1115	303	335	4	0	0	0

- Molecule 13 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	233	1824	1154	312	351	7	0	0	0
13	a	233	1824	1154	312	351	7	0	0	0

- Molecule 14 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	N	196	1512	955	250	300	7	0	0	0
14	b	196	1512	955	250	300	7	0	0	0

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	G	1	Total Mg 1 1	0	0
15	I	2	Total Mg 2 2	0	0
15	K	1	Total Mg 1 1	0	0
15	L	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	W	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0

- Molecule 16 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	12	Total O 12 12	0	0
17	B	12	Total O 12 12	0	0
17	C	15	Total O 15 15	0	0
17	D	7	Total O 7 7	0	0
17	E	6	Total O 6 6	0	0
17	F	13	Total O 13 13	0	0
17	G	19	Total O 19 19	0	0
17	H	19	Total O 19 19	0	0
17	I	16	Total O 16 16	0	0
17	J	13	Total O 13 13	0	0

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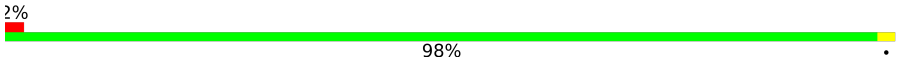
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	K	17	Total O 17 17	0	0
17	L	24	Total O 24 24	0	0
17	M	24	Total O 24 24	0	0
17	N	21	Total O 21 21	0	0
17	O	5	Total O 5 5	0	0
17	P	17	Total O 17 17	0	0
17	Q	11	Total O 11 11	0	0
17	R	10	Total O 10 10	0	0
17	S	8	Total O 8 8	0	0
17	T	9	Total O 9 9	0	0
17	U	18	Total O 18 18	0	0
17	V	16	Total O 16 16	0	0
17	W	12	Total O 12 12	0	0
17	X	13	Total O 13 13	0	0
17	Y	22	Total O 22 22	0	0
17	Z	16	Total O 16 16	0	0
17	a	21	Total O 21 21	0	0
17	b	20	Total O 20 20	0	0

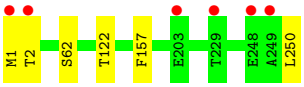
3 Residue-property plots (i)

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 subunit alpha type-2

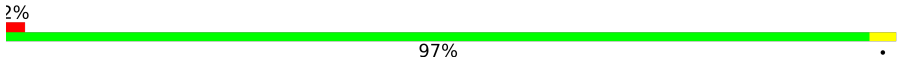
Chain A:

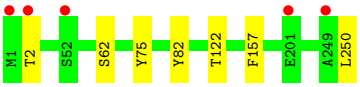




• Molecule 1: Proteasome subunit alpha type-2

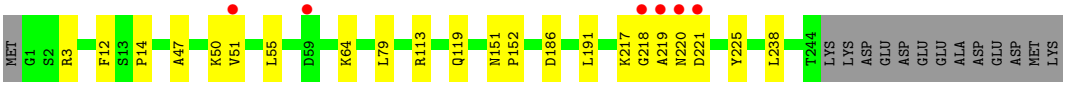
Chain O:





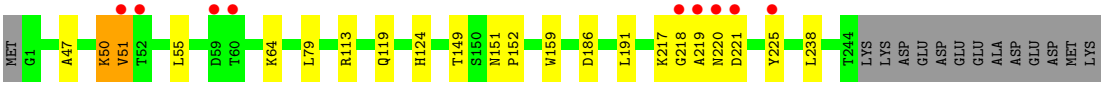
• Molecule 2: Proteasome subunit alpha type-3

Chain B:



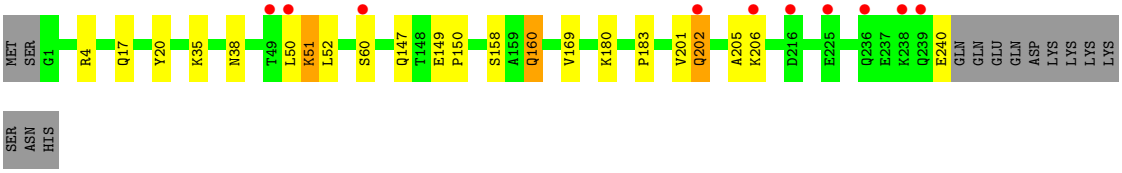
• Molecule 2: Proteasome subunit alpha type-3

Chain P:



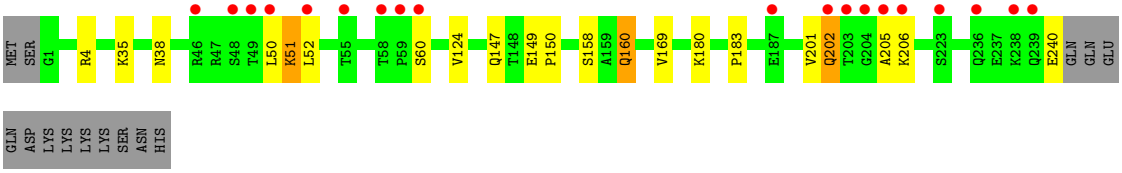
• Molecule 3: Proteasome subunit alpha type-4

Chain C:



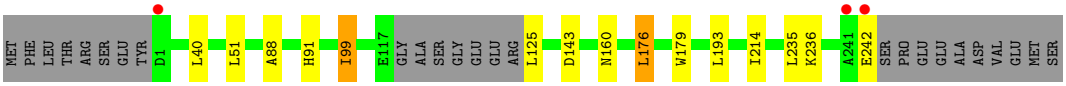
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



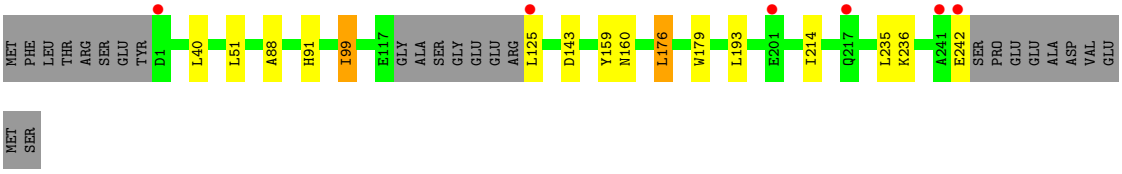
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



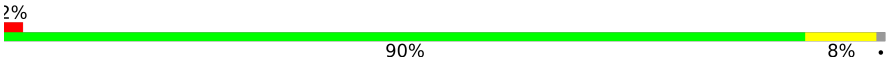
• Molecule 4: Proteasome subunit alpha type-5

Chain R:



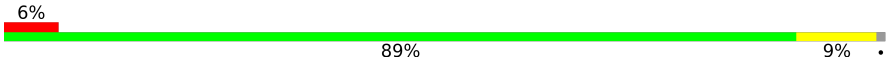
• Molecule 5: Proteasome subunit alpha type-6

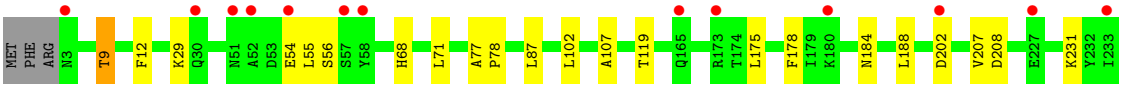
Chain E:



• Molecule 5: Proteasome subunit alpha type-6

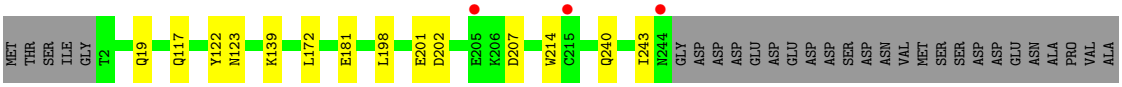
Chain S:

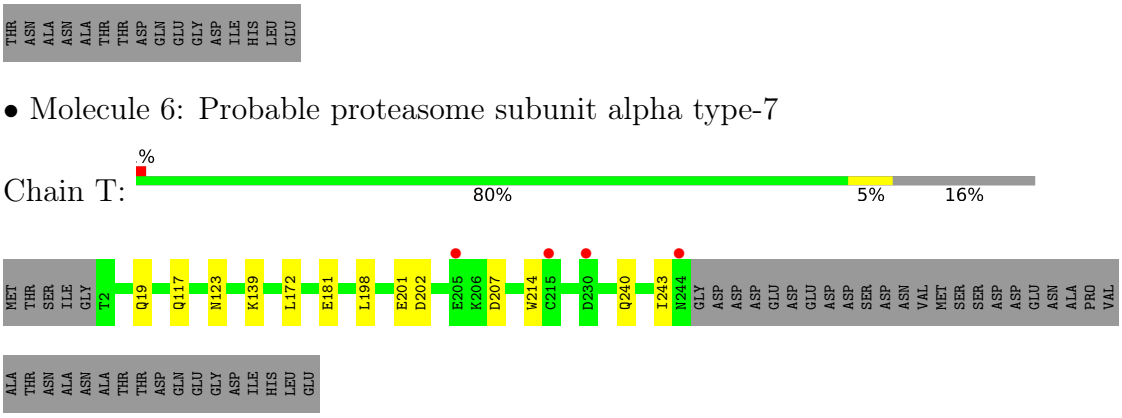




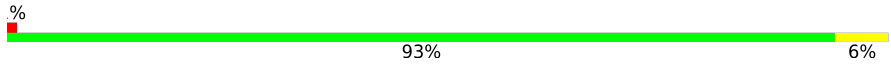
• Molecule 6: Probable proteasome subunit alpha type-7

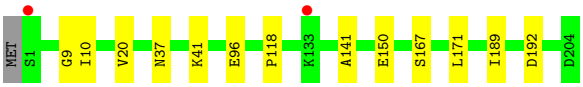
Chain F:




THR ASN ALA ASN ALA THR THR ASP GLN GLU GLY ASP ILE HIS LEU GLU
• Molecule 6: Probable proteasome subunit alpha type-7
Chain T:
%
80%
5%
16%
MET THR SER ILE GLY T2 Q19 Q117 N123 K139 L172 E181 L198 E201 D202 E205 K206 D207 W214 C215 D230 Q240 I243 N244 GLY ASP ASP ASP GLU ASP GLU ASP ASP SER ASP ASN VAL MET SER SER ASP ASP GLU ASN ALA PRO VAL
ALA THR ASN ALA ASN ALA THR THR ASP GLN GLU GLY ASP ILE HIS LEU GLU
• Molecule 7: Proteasome subunit alpha type-1
Chain G:
%
88%
8%
MET SER GLY ALA ALA ALA ALA SER ALA ALA G2 F23 T26 I63 R68 V73 V74 N75 I78 P79 N83 L115 S116 Q117 R122 M125 T133 K165 L205 E208 E215 D222 R235 L236 A240 E241 Q242 ASP
• Molecule 7: Proteasome subunit alpha type-1
Chain U:
%
89%
6%
MET SER GLY ALA ALA ALA ALA SER ALA ALA G2 F23 T26 P51 V73 V74 N75 I78 P79 N83 L115 S116 Q117 R122 M125 T133 K165 L205 E208 D222 R235 L236 Q242 ASP
• Molecule 8: Proteasome subunit beta type-2
Chain H:
3%
89%
7%
T1 T2 I3 N30 C43 T52 V55 T56 I63 L68 P74 L80 K84 I99 D104 P105 S112 I113 L125 S126 L127 R196 E197 E198 T210 C221 D222 I223 Q224 E225 E226 GLN VAL ASP ILE THR ALA
• Molecule 8: Proteasome subunit beta type-2
Chain V:
3%
89%
7%
T1 T2 I3 N30 C43 T52 V55 T56 I63 L68 P74 L80 K84 I99 D104 P105 S112 I113 L125 S126 L127 R196 T210 C221 D222 I223 Q224 E225 E226 GLN VAL ASP ILE THR ALA
• Molecule 9: Proteasome subunit beta type-3
Chain I:
94%
6%
MET S1 G9 I10 V20 N37 K41 E96 P118 A141 S167 L171 I189 D192 D204
• Molecule 9: Proteasome subunit beta type-3

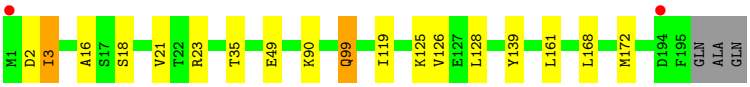
Chain W:





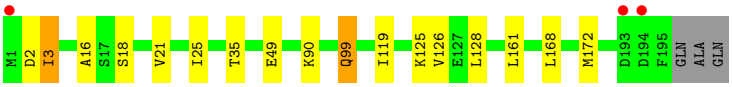
- Molecule 10: Proteasome subunit beta type-4

Chain J:



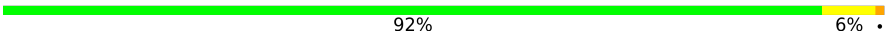
- Molecule 10: Proteasome subunit beta type-4

Chain X:



- Molecule 11: Proteasome subunit beta type-5

Chain K:

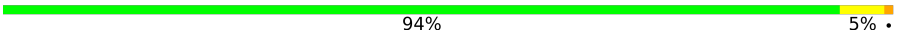


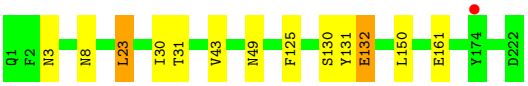
- Molecule 11: Proteasome subunit beta type-5

Chain Y:

- Molecule 12: Proteasome subunit beta type-6

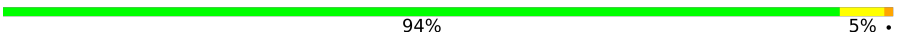
Chain L:

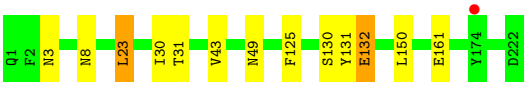




- Molecule 12: Proteasome subunit beta type-6

Chain Z:



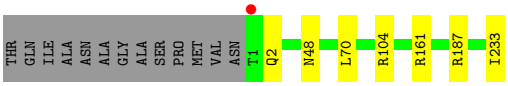


• Molecule 13: Proteasome subunit beta type-7

Chain M:

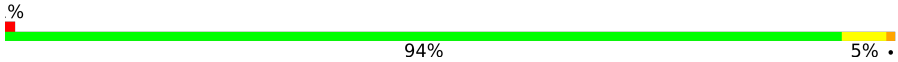
• Molecule 13: Proteasome subunit beta type-7

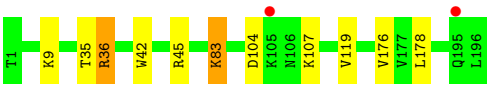
Chain a:



• Molecule 14: Proteasome subunit beta type-1

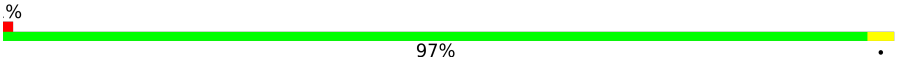
Chain N:

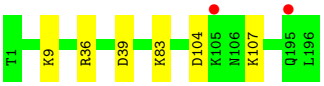




• Molecule 14: Proteasome subunit beta type-1

Chain b:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.46Å 300.96Å 143.86Å 90.00° 112.88° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (15.00-2.80) 98.7 (15.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.186 , 0.201 0.192 , 0.207	Depositor DCC
R_{free} test set	12725 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	54.3	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	49795	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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)

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

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	0.25	0/1952	0.47	0/2642
1	O	0.25	0/1952	0.47	0/2642
2	B	0.26	0/1934	0.50	0/2618
2	P	0.26	0/1934	0.50	0/2618
3	C	0.26	0/1910	0.51	0/2586
3	Q	0.26	0/1910	0.51	0/2586
4	D	0.25	0/1837	0.48	0/2475
4	R	0.25	0/1837	0.48	0/2475
5	E	0.25	0/1800	0.48	0/2433
5	S	0.25	0/1800	0.48	0/2433
6	F	0.26	0/1932	0.46	0/2609
6	T	0.25	0/1932	0.46	0/2609
7	G	0.26	0/1945	0.47	0/2634
7	U	0.26	0/1945	0.47	0/2634
8	H	0.28	0/1750	0.54	1/2373 (0.0%)
8	V	0.27	0/1750	0.52	0/2373
9	I	0.28	0/1611	0.54	0/2174
9	W	0.28	0/1611	0.54	0/2174
10	J	0.25	0/1589	0.48	0/2142
10	X	0.25	0/1589	0.48	0/2142
11	K	0.26	0/1683	0.53	1/2277 (0.0%)
11	Y	0.26	0/1683	0.53	1/2277 (0.0%)
12	L	0.30	0/1795	0.53	1/2420 (0.0%)
12	Z	0.30	0/1795	0.53	1/2420 (0.0%)
13	M	0.33	0/1855	0.54	0/2514
13	a	0.29	0/1855	0.54	0/2514
14	N	0.26	0/1541	0.51	0/2087
14	b	0.25	0/1541	0.51	0/2087
All	All	0.27	0/50268	0.50	5/67968 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	Z	132	GLU	CB-CG-CD	5.32	128.55	114.20
12	L	132	GLU	CB-CG-CD	5.31	128.53	114.20
11	Y	4	LEU	CA-CB-CG	5.21	127.28	115.30
11	K	4	LEU	CA-CB-CG	5.19	127.23	115.30
8	H	127	LEU	CB-CG-CD2	-5.16	102.24	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1915	0	1929	1	0
1	O	1915	0	1929	1	0
2	B	1904	0	1904	9	0
2	P	1904	0	1904	8	0
3	C	1881	0	1895	7	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	6	0
4	R	1813	0	1797	7	0
5	E	1773	0	1775	7	0
5	S	1773	0	1775	8	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	2	0
7	G	1907	0	1901	6	0
7	U	1907	0	1901	4	0
8	H	1719	0	1719	10	0
8	V	1719	0	1719	11	0
9	I	1581	0	1574	5	0
9	W	1581	0	1574	6	0
10	J	1561	0	1569	9	0
10	X	1561	0	1569	8	0
11	K	1646	0	1597	8	0
11	Y	1646	0	1597	6	0
12	L	1757	0	1711	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Z	1757	0	1711	3	0
13	M	1824	0	1832	6	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	7	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0
15	K	1	0	0	0	0
15	L	1	0	0	0	0
15	N	1	0	0	0	0
15	W	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
17	A	12	0	0	0	0
17	B	12	0	0	0	0
17	C	15	0	0	0	0
17	D	7	0	0	0	0
17	E	6	0	0	0	0
17	F	13	0	0	0	0
17	G	19	0	0	0	0
17	H	19	0	0	0	0
17	I	16	0	0	0	0
17	J	13	0	0	0	0
17	K	17	0	0	0	0
17	L	24	0	0	0	0
17	M	24	0	0	0	0
17	N	21	0	0	0	0
17	O	5	0	0	0	0
17	P	17	0	0	0	0
17	Q	11	0	0	0	0
17	R	10	0	0	0	0
17	S	8	0	0	0	0
17	T	9	0	0	0	0
17	U	18	0	0	0	0
17	V	16	0	0	0	0
17	W	12	0	0	0	0
17	X	13	0	0	0	0
17	Y	22	0	0	0	0
17	Z	16	0	0	0	0
17	a	21	0	0	0	0
17	b	20	0	0	0	0
All	All	49795	0	49134	140	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 2.

The worst 5 of 140 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)
11:K:31:VAL:HA	12:L:132:GLU:OE1	1.87	0.73
8:V:52:THR:O	8:V:56:THR:OG1	2.11	0.68
8:H:52:THR:O	8:H:56:THR:OG1	2.12	0.67
13:M:233:ILE:OXT	13:M:233:ILE:HG13	1.98	0.62
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.46	0.62

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 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	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	34	66
1	O	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	34	66
2	B	242/258 (94%)	236 (98%)	2 (1%)	4 (2%)	9	29
2	P	242/258 (94%)	236 (98%)	2 (1%)	4 (2%)	9	29
3	C	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	12	36
3	Q	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	12	36
4	D	231/260 (89%)	229 (99%)	2 (1%)	0	100	100
4	R	231/260 (89%)	229 (99%)	2 (1%)	0	100	100
5	E	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
5	S	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
6	F	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
6	T	241/288 (84%)	237 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
7	U	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
8	H	224/232 (97%)	217 (97%)	7 (3%)	0	100	100
8	V	224/232 (97%)	217 (97%)	7 (3%)	0	100	100
9	I	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
10	X	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	231/246 (94%)	222 (96%)	9 (4%)	0	100	100
13	a	231/246 (94%)	222 (96%)	9 (4%)	0	100	100
14	N	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
14	b	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
All	All	6284/6614 (95%)	6133 (98%)	135 (2%)	16 (0%)	41	72

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	221	ASP
3	C	202	GLN
2	P	51	VAL
2	P	221	ASP

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	209/209 (100%)	205 (98%)	4 (2%)	57	85
1	O	209/209 (100%)	205 (98%)	4 (2%)	57	85
2	B	203/216 (94%)	195 (96%)	8 (4%)	32	66
2	P	203/216 (94%)	195 (96%)	8 (4%)	32	66
3	C	212/226 (94%)	201 (95%)	11 (5%)	23	55
3	Q	212/226 (94%)	201 (95%)	11 (5%)	23	55
4	D	194/215 (90%)	183 (94%)	11 (6%)	20	50
4	R	194/215 (90%)	183 (94%)	11 (6%)	20	50
5	E	190/193 (98%)	180 (95%)	10 (5%)	22	54
5	S	190/193 (98%)	180 (95%)	10 (5%)	22	54
6	F	201/239 (84%)	191 (95%)	10 (5%)	24	56
6	T	201/239 (84%)	191 (95%)	10 (5%)	24	56
7	G	206/210 (98%)	196 (95%)	10 (5%)	25	57
7	U	206/210 (98%)	196 (95%)	10 (5%)	25	57
8	H	185/190 (97%)	177 (96%)	8 (4%)	29	62
8	V	185/190 (97%)	177 (96%)	8 (4%)	29	62
9	I	172/173 (99%)	168 (98%)	4 (2%)	50	82
9	W	172/173 (99%)	168 (98%)	4 (2%)	50	82
10	J	173/175 (99%)	168 (97%)	5 (3%)	42	76
10	X	173/175 (99%)	168 (97%)	5 (3%)	42	76
11	K	170/170 (100%)	162 (95%)	8 (5%)	26	59
11	Y	170/170 (100%)	162 (95%)	8 (5%)	26	59
12	L	185/185 (100%)	178 (96%)	7 (4%)	33	67
12	Z	185/185 (100%)	177 (96%)	8 (4%)	29	62
13	M	199/208 (96%)	192 (96%)	7 (4%)	36	70
13	a	199/208 (96%)	192 (96%)	7 (4%)	36	70
14	N	162/162 (100%)	157 (97%)	5 (3%)	40	74
14	b	162/162 (100%)	156 (96%)	6 (4%)	34	68
All	All	5322/5542 (96%)	5104 (96%)	218 (4%)	30	64

5 of 218 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	P	113	ARG
5	S	29	LYS
12	Z	31	THR
2	P	238	LEU
3	Q	240	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 122 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	179	ASN
11	Y	208	ASN
3	Q	147	GLN
11	Y	190	ASN
13	a	179	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)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	250/250 (100%)	-0.43	6 (2%)	59	49	36, 49, 84, 123	0
1	O	250/250 (100%)	-0.34	5 (2%)	65	56	41, 58, 103, 133	0
2	B	244/258 (94%)	-0.30	6 (2%)	57	47	37, 56, 98, 148	0
2	P	244/258 (94%)	-0.25	9 (3%)	41	31	41, 59, 101, 147	0
3	C	240/254 (94%)	-0.24	10 (4%)	36	26	37, 60, 122, 150	0
3	Q	240/254 (94%)	0.08	19 (7%)	12	7	45, 74, 159, 189	0
4	D	235/260 (90%)	-0.38	3 (1%)	77	72	42, 61, 95, 137	0
4	R	235/260 (90%)	-0.27	6 (2%)	56	46	44, 67, 109, 148	0
5	E	231/234 (98%)	-0.32	5 (2%)	62	52	45, 64, 102, 147	0
5	S	231/234 (98%)	-0.05	13 (5%)	24	16	47, 76, 122, 167	0
6	F	243/288 (84%)	-0.47	3 (1%)	79	73	39, 57, 110, 138	0
6	T	243/288 (84%)	-0.32	4 (1%)	72	66	43, 69, 125, 158	0
7	G	241/252 (95%)	-0.50	3 (1%)	79	73	32, 52, 85, 137	0
7	U	241/252 (95%)	-0.42	3 (1%)	79	73	40, 56, 86, 132	0
8	H	226/232 (97%)	-0.42	7 (3%)	49	39	33, 50, 82, 147	0
8	V	226/232 (97%)	-0.38	6 (2%)	54	44	38, 51, 83, 162	0
9	I	204/205 (99%)	-0.73	1 (0%)	91	88	34, 46, 70, 94	0
9	W	204/205 (99%)	-0.68	2 (0%)	82	77	35, 46, 75, 100	0
10	J	195/198 (98%)	-0.55	2 (1%)	82	77	34, 49, 74, 129	0
10	X	195/198 (98%)	-0.54	3 (1%)	73	68	34, 50, 73, 135	0
11	K	212/212 (100%)	-0.62	1 (0%)	91	88	30, 46, 67, 87	0
11	Y	212/212 (100%)	-0.60	1 (0%)	91	88	36, 49, 72, 93	0
12	L	222/222 (100%)	-0.58	1 (0%)	91	88	36, 51, 79, 114	0
12	Z	222/222 (100%)	-0.61	1 (0%)	91	88	35, 50, 82, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.68	1 (0%)	92	91	32, 49, 72, 88	0
13	a	233/246 (94%)	-0.64	1 (0%)	92	91	32, 48, 70, 86	0
14	N	196/196 (100%)	-0.70	2 (1%)	82	77	32, 43, 71, 98	0
14	b	196/196 (100%)	-0.67	2 (1%)	82	77	34, 45, 71, 104	0
All	All	6344/6614 (95%)	-0.44	126 (1%)	65	56	30, 54, 102, 189	0

The worst 5 of 126 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	49	THR	9.2
2	P	219	ALA	7.7
3	Q	50	LEU	7.7
8	V	224	GLN	7.4
2	B	221	ASP	6.4

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	MG	W	301	1/1	0.94	0.27	50,50,50,50	0
15	MG	Z	301	1/1	0.94	0.36	60,60,60,60	0
15	MG	N	201	1/1	0.95	0.12	51,51,51,51	0
15	MG	L	301	1/1	0.97	0.08	63,63,63,63	0
15	MG	G	301	1/1	0.98	0.04	47,47,47,47	0
15	MG	I	302	1/1	0.98	0.07	53,53,53,53	0
15	MG	I	301	1/1	0.99	0.19	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	MG	K	301	1/1	0.99	0.09	45,45,45,45	0
16	CL	G	302	1/1	0.99	0.12	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.