wwPDB X-ray Structure Validation Summary Report (i)

Oct 16, 2021 – 07:58 PM EDT

PDB ID	:	1Q5R
Title	:	The Rhodococcus 20S proteasome with unprocessed pro-peptides
Authors	:	Kwon, Y.D.; Nagy, I.; Adams, P.D.; Baumeister, W.; Jap, B.K.
Deposited on	:	2003-08-08
Resolution	:	3.10 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 following versions of software and data (see references (i)) were used in the production of this report:

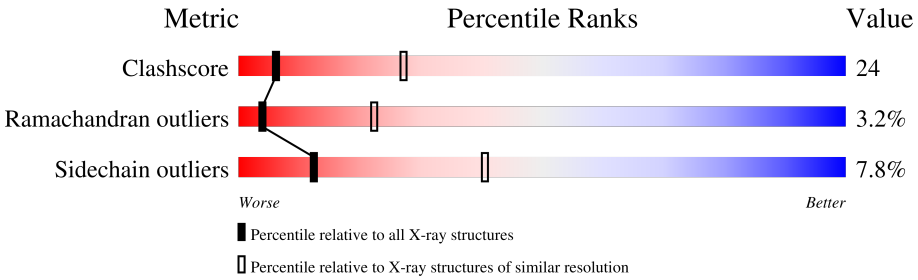
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.10 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	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	259	45% 34% 5% 15%
1	B	259	47% 31% 6% 15%
1	C	259	47% 31% 6% 15%
1	D	259	46% 33% 5% 15%
1	E	259	48% 30% 6% 15%
1	F	259	49% 30% 6% 15%
1	G	259	46% 34% 5% 15%
2	H	294	48% 33% • 15%

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Mol	Chain	Length	Quality of chain
2	I	294	48% 35% 15%
2	J	294	51% 31% 15%
2	K	294	49% 32% 15%
2	L	294	50% 32% 15%
2	M	294	48% 34% 15%
2	N	294	47% 34% 15%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 25013 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
			1695	1057	312	321	5			
1	B	219	Total	C	N	O	S	0	0	0
			1695	1057	312	321	5			
1	C	219	Total	C	N	O	S	0	0	0
			1695	1057	312	321	5			
1	D	219	Total	C	N	O	S	0	0	0
			1695	1057	312	321	5			
1	E	219	Total	C	N	O	S	0	0	0
			1695	1057	312	321	5			
1	F	219	Total	C	N	O	S	0	0	0
			1695	1057	312	321	5			
1	G	219	Total	C	N	O	S	0	0	0
			1695	1057	312	321	5			

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q53080
A	2	HIS	-	expression tag	UNP Q53080
A	3	HIS	-	expression tag	UNP Q53080
A	4	HIS	-	expression tag	UNP Q53080
A	5	HIS	-	expression tag	UNP Q53080
A	6	HIS	-	expression tag	UNP Q53080
A	7	HIS	-	expression tag	UNP Q53080
B	1	MET	-	initiating methionine	UNP Q53080
B	2	HIS	-	expression tag	UNP Q53080
B	3	HIS	-	expression tag	UNP Q53080
B	4	HIS	-	expression tag	UNP Q53080
B	5	HIS	-	expression tag	UNP Q53080
B	6	HIS	-	expression tag	UNP Q53080
B	7	HIS	-	expression tag	UNP Q53080
C	1	MET	-	initiating methionine	UNP Q53080

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2	HIS	-	expression tag	UNP Q53080
C	3	HIS	-	expression tag	UNP Q53080
C	4	HIS	-	expression tag	UNP Q53080
C	5	HIS	-	expression tag	UNP Q53080
C	6	HIS	-	expression tag	UNP Q53080
C	7	HIS	-	expression tag	UNP Q53080
D	1	MET	-	initiating methionine	UNP Q53080
D	2	HIS	-	expression tag	UNP Q53080
D	3	HIS	-	expression tag	UNP Q53080
D	4	HIS	-	expression tag	UNP Q53080
D	5	HIS	-	expression tag	UNP Q53080
D	6	HIS	-	expression tag	UNP Q53080
D	7	HIS	-	expression tag	UNP Q53080
E	1	MET	-	initiating methionine	UNP Q53080
E	2	HIS	-	expression tag	UNP Q53080
E	3	HIS	-	expression tag	UNP Q53080
E	4	HIS	-	expression tag	UNP Q53080
E	5	HIS	-	expression tag	UNP Q53080
E	6	HIS	-	expression tag	UNP Q53080
E	7	HIS	-	expression tag	UNP Q53080
F	1	MET	-	initiating methionine	UNP Q53080
F	2	HIS	-	expression tag	UNP Q53080
F	3	HIS	-	expression tag	UNP Q53080
F	4	HIS	-	expression tag	UNP Q53080
F	5	HIS	-	expression tag	UNP Q53080
F	6	HIS	-	expression tag	UNP Q53080
F	7	HIS	-	expression tag	UNP Q53080
G	1	MET	-	initiating methionine	UNP Q53080
G	2	HIS	-	expression tag	UNP Q53080
G	3	HIS	-	expression tag	UNP Q53080
G	4	HIS	-	expression tag	UNP Q53080
G	5	HIS	-	expression tag	UNP Q53080
G	6	HIS	-	expression tag	UNP Q53080
G	7	HIS	-	expression tag	UNP Q53080

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	251	Total	C	N	O	S	0	0	0
			1864	1164	323	375	2			
2	I	251	Total	C	N	O	S	0	0	0
			1864	1164	323	375	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	251	Total	C	N	O	S	0	0	0
			1864	1164	323	375	2			
2	K	251	Total	C	N	O	S	0	0	0
			1864	1164	323	375	2			
2	L	251	Total	C	N	O	S	0	0	0
			1864	1164	323	375	2			
2	M	251	Total	C	N	O	S	0	0	0
			1864	1164	323	375	2			
2	N	251	Total	C	N	O	S	0	0	0
			1864	1164	323	375	2			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-63	ALA	LYS	engineered mutation	UNP Q53079
I	-63	ALA	LYS	engineered mutation	UNP Q53079
J	-63	ALA	LYS	engineered mutation	UNP Q53079
K	-63	ALA	LYS	engineered mutation	UNP Q53079
L	-63	ALA	LYS	engineered mutation	UNP Q53079
M	-63	ALA	LYS	engineered mutation	UNP Q53079
N	-63	ALA	LYS	engineered mutation	UNP Q53079

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	5	Total	O	0	0
			5	5		
3	C	3	Total	O	0	0
			3	3		
3	D	6	Total	O	0	0
			6	6		
3	E	5	Total	O	0	0
			5	5		
3	F	2	Total	O	0	0
			2	2		
3	G	1	Total	O	0	0
			1	1		
3	H	13	Total	O	0	0
			13	13		
3	I	14	Total	O	0	0
			14	14		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	13	Total O 13 13	0	0
3	K	8	Total O 8 8	0	0
3	L	12	Total O 12 12	0	0
3	M	6	Total O 6 6	0	0
3	N	8	Total O 8 8	0	0

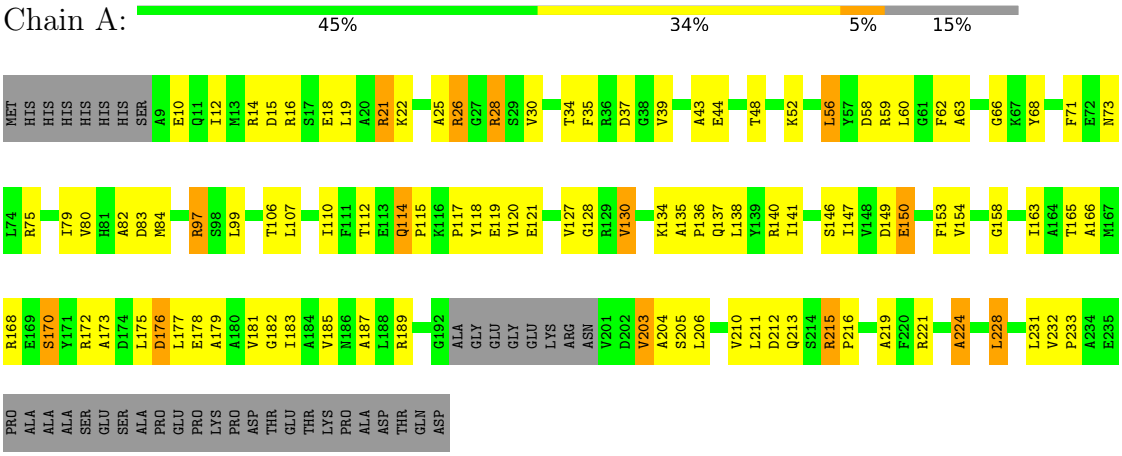
3 Residue-property plots (i)

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

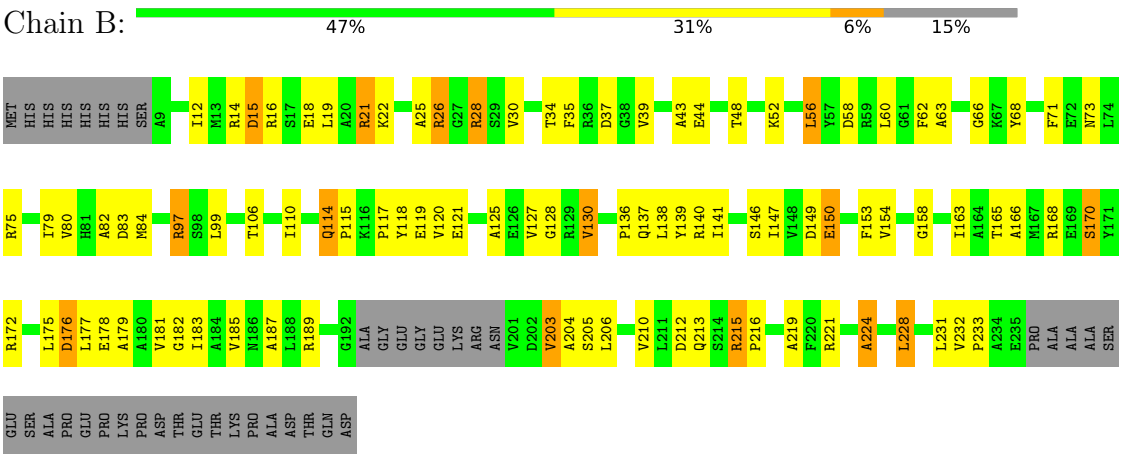
• Molecule 1: proteasome alpha-type subunit 1

Chain A:



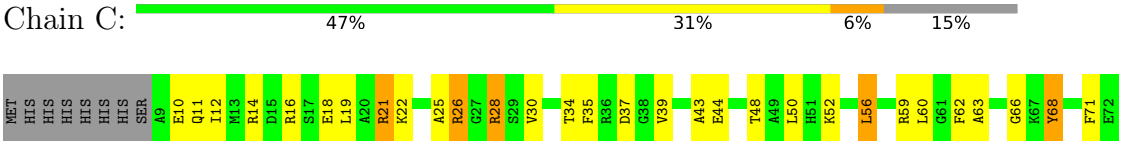
• Molecule 1: proteasome alpha-type subunit 1

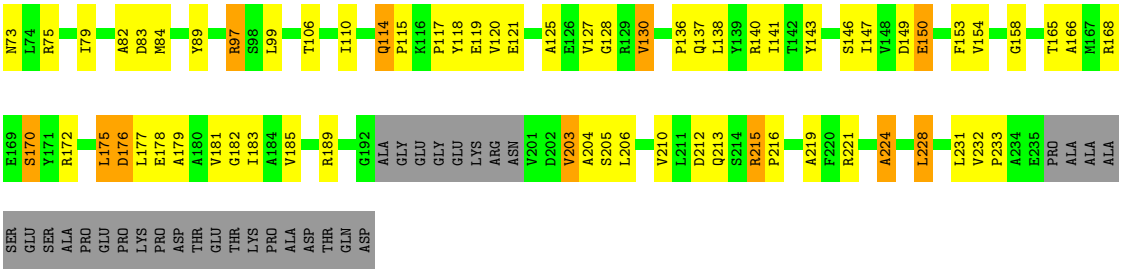
Chain B:



• Molecule 1: proteasome alpha-type subunit 1

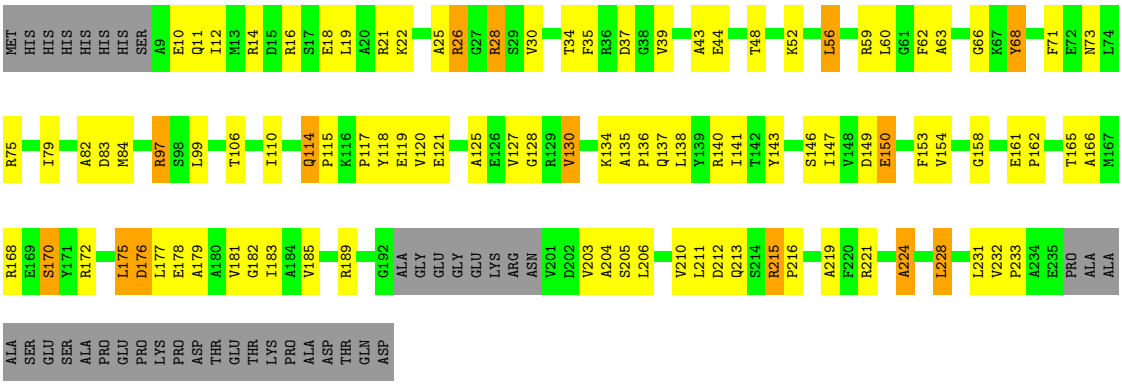
Chain C:





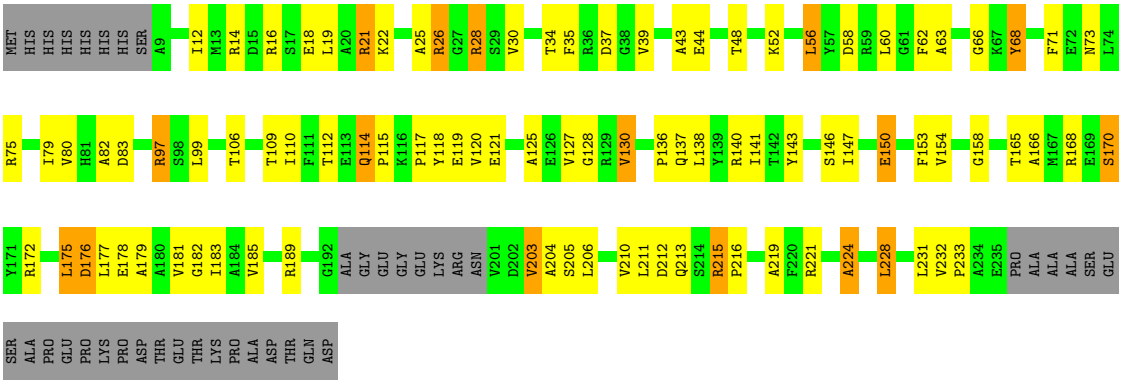
• Molecule 1: proteasome alpha-type subunit 1

Chain D:



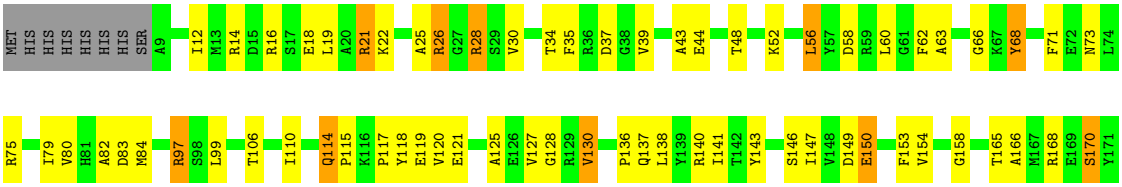
• Molecule 1: proteasome alpha-type subunit 1

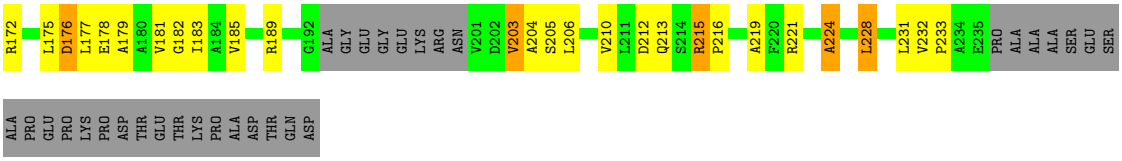
Chain E:



• Molecule 1: proteasome alpha-type subunit 1

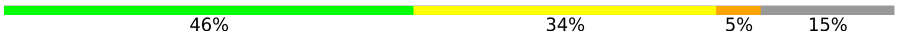
Chain F:

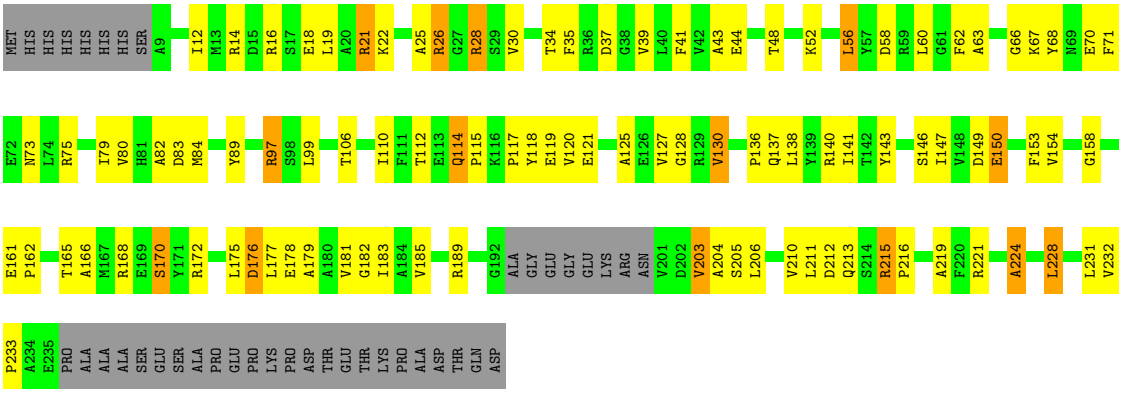




• Molecule 1: proteasome alpha-type subunit 1

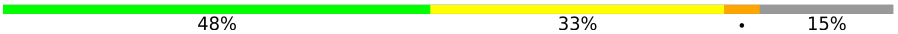
Chain G:

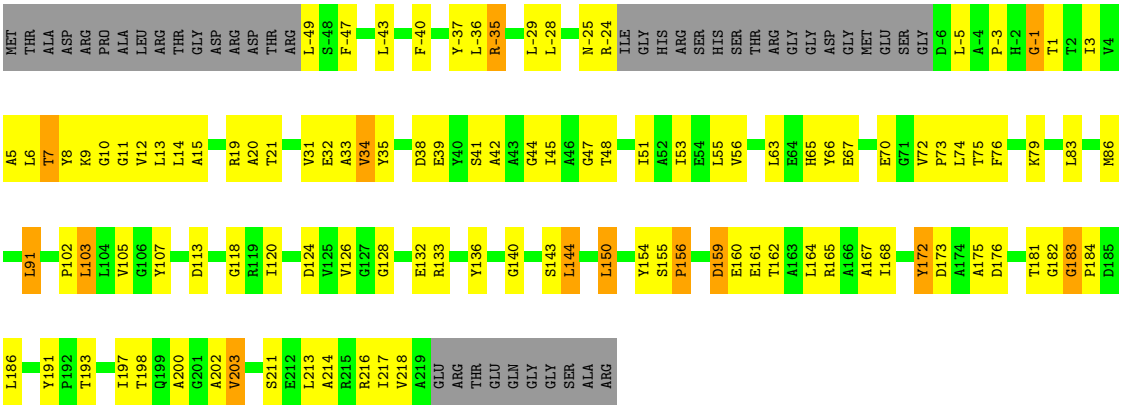




• Molecule 2: proteasome beta-type subunit 1

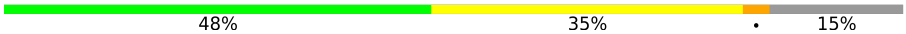
Chain H:

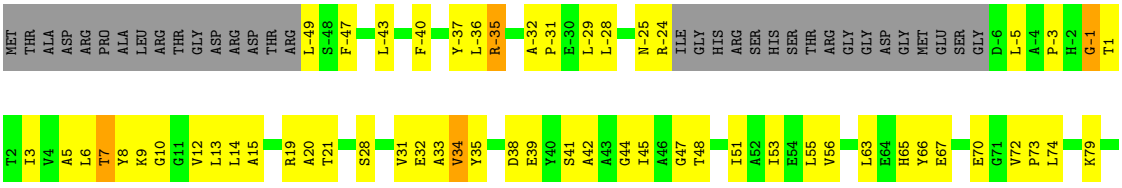


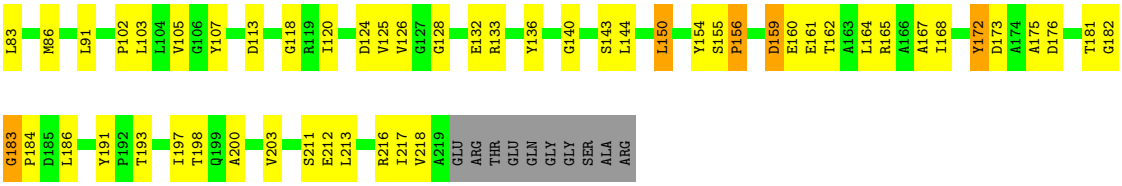


• Molecule 2: proteasome beta-type subunit 1

Chain I:

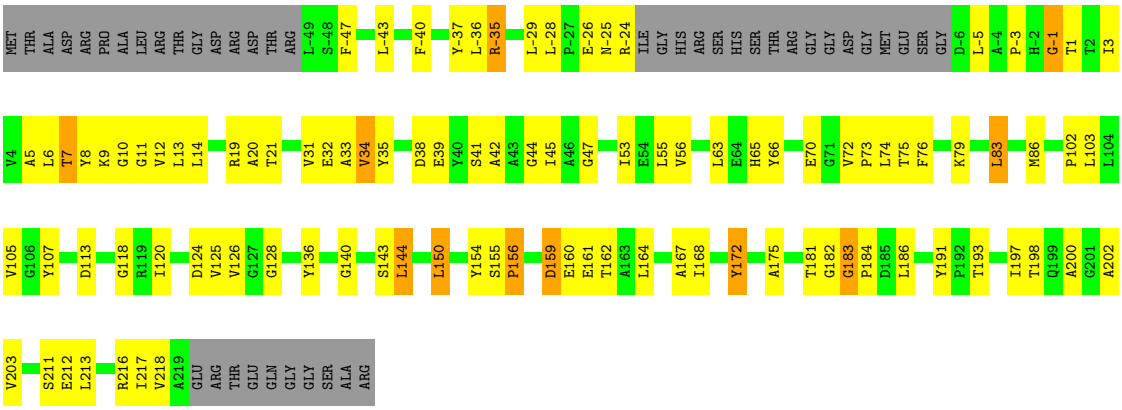






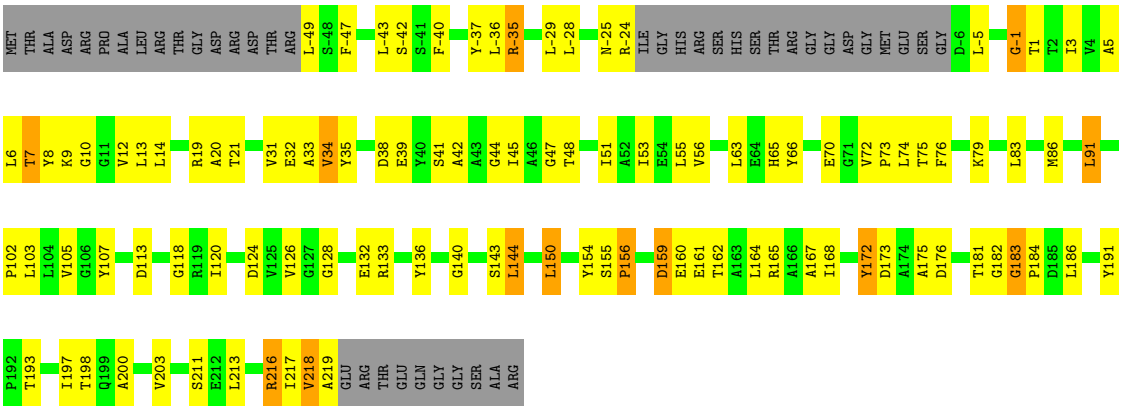
• Molecule 2: proteasome beta-type subunit 1

Chain J:



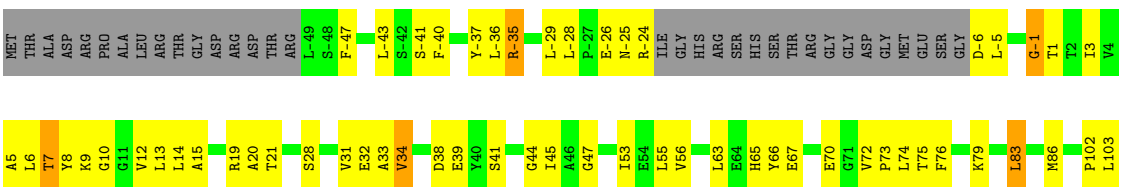
• Molecule 2: proteasome beta-type subunit 1

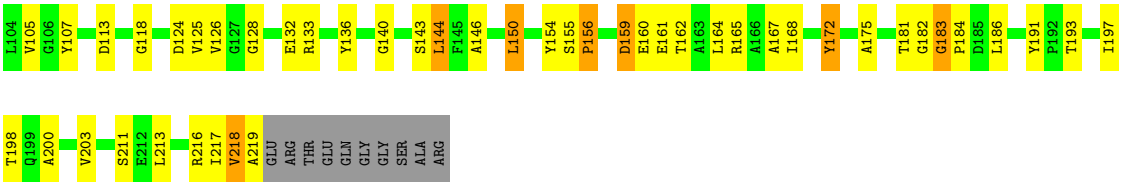
Chain K:



• Molecule 2: proteasome beta-type subunit 1

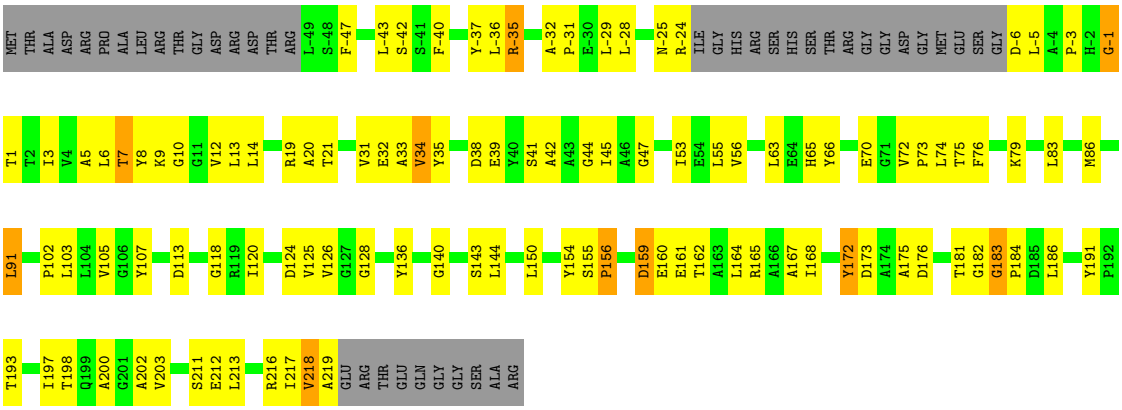
Chain L:





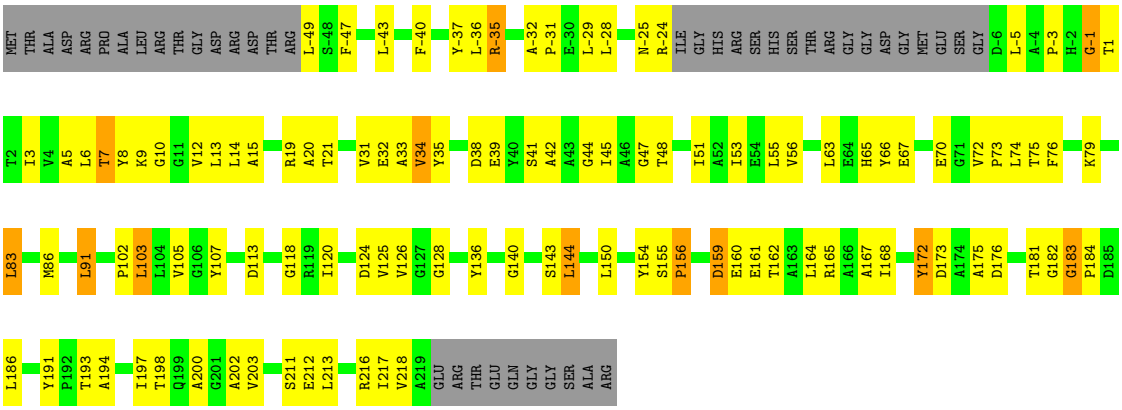
• Molecule 2: proteasome beta-type subunit 1

Chain M:



• Molecule 2: proteasome beta-type subunit 1

Chain N:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	152.09Å 212.37Å 250.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 3.10	Depositor
% Data completeness (in resolution range)	88.7 (19.96-3.10)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	25013	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

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	0.45	0/1720	0.64	0/2325
1	B	0.44	0/1720	0.64	0/2325
1	C	0.45	0/1720	0.64	0/2325
1	D	0.44	0/1720	0.63	0/2325
1	E	0.44	0/1720	0.63	0/2325
1	F	0.45	0/1720	0.64	0/2325
1	G	0.46	0/1720	0.64	0/2325
2	H	0.53	0/1892	0.72	0/2569
2	I	0.52	0/1892	0.72	0/2569
2	J	0.52	0/1892	0.72	0/2569
2	K	0.52	0/1892	0.72	0/2569
2	L	0.51	0/1892	0.72	0/2569
2	M	0.52	0/1892	0.71	0/2569
2	N	0.52	0/1892	0.72	0/2569
All	All	0.49	0/25284	0.68	0/34258

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

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	1695	0	1693	110	0
1	B	1695	0	1693	105	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1695	0	1693	104	1
1	D	1695	0	1693	103	0
1	E	1695	0	1693	93	0
1	F	1695	0	1693	99	0
1	G	1695	0	1693	103	0
2	H	1864	0	1837	88	0
2	I	1864	0	1837	79	0
2	J	1864	0	1837	75	0
2	K	1864	0	1837	78	0
2	L	1864	0	1837	78	0
2	M	1864	0	1837	76	0
2	N	1864	0	1837	84	0
3	A	4	0	0	0	0
3	B	5	0	0	1	0
3	C	3	0	0	3	0
3	D	6	0	0	4	0
3	E	5	0	0	1	0
3	F	2	0	0	1	0
3	G	1	0	0	0	0
3	H	13	0	0	3	0
3	I	14	0	0	3	0
3	J	13	0	0	0	0
3	K	8	0	0	2	0
3	L	12	0	0	3	0
3	M	6	0	0	2	0
3	N	8	0	0	1	0
All	All	25013	0	24710	1216	1

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 24.

The worst 5 of 1216 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:219:ALA:HA	3:M:231:HOH:O	1.59	1.02
2:I:-35:ARG:HH11	2:I:-35:ARG:HB2	1.26	0.97
2:L:-35:ARG:HH11	2:L:-35:ARG:HB2	1.29	0.97
2:N:-35:ARG:HB2	2:N:-35:ARG:HH11	1.28	0.97
2:H:-35:ARG:HH11	2:H:-35:ARG:HB2	1.27	0.96

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:ARG:NH1	1:C:172:ARG:NH1[4_576]	1.55	0.65

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	215/259 (83%)	178 (83%)	30 (14%)	7 (3%)	4	21
1	B	215/259 (83%)	179 (83%)	29 (14%)	7 (3%)	4	21
1	C	215/259 (83%)	181 (84%)	25 (12%)	9 (4%)	3	16
1	D	215/259 (83%)	179 (83%)	28 (13%)	8 (4%)	3	19
1	E	215/259 (83%)	180 (84%)	26 (12%)	9 (4%)	3	16
1	F	215/259 (83%)	178 (83%)	28 (13%)	9 (4%)	3	16
1	G	215/259 (83%)	178 (83%)	29 (14%)	8 (4%)	3	19
2	H	247/294 (84%)	224 (91%)	17 (7%)	6 (2%)	6	27
2	I	247/294 (84%)	221 (90%)	20 (8%)	6 (2%)	6	27
2	J	247/294 (84%)	222 (90%)	19 (8%)	6 (2%)	6	27
2	K	247/294 (84%)	222 (90%)	18 (7%)	7 (3%)	5	25
2	L	247/294 (84%)	223 (90%)	17 (7%)	7 (3%)	5	25
2	M	247/294 (84%)	224 (91%)	16 (6%)	7 (3%)	5	25
2	N	247/294 (84%)	224 (91%)	17 (7%)	6 (2%)	6	27
All	All	3234/3871 (84%)	2813 (87%)	319 (10%)	102 (3%)	4	22

5 of 102 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	224	ALA

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Mol	Chain	Res	Type
1	B	28	ARG
1	B	224	ALA
1	C	28	ARG

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	174/206 (84%)	162 (93%)	12 (7%)	15	45
1	B	174/206 (84%)	162 (93%)	12 (7%)	15	45
1	C	174/206 (84%)	162 (93%)	12 (7%)	15	45
1	D	174/206 (84%)	163 (94%)	11 (6%)	18	48
1	E	174/206 (84%)	162 (93%)	12 (7%)	15	45
1	F	174/206 (84%)	163 (94%)	11 (6%)	18	48
1	G	174/206 (84%)	163 (94%)	11 (6%)	18	48
2	H	189/222 (85%)	173 (92%)	16 (8%)	10	37
2	I	189/222 (85%)	172 (91%)	17 (9%)	9	34
2	J	189/222 (85%)	172 (91%)	17 (9%)	9	34
2	K	189/222 (85%)	172 (91%)	17 (9%)	9	34
2	L	189/222 (85%)	173 (92%)	16 (8%)	10	37
2	M	189/222 (85%)	172 (91%)	17 (9%)	9	34
2	N	189/222 (85%)	171 (90%)	18 (10%)	8	31
All	All	2541/2996 (85%)	2342 (92%)	199 (8%)	12	40

5 of 199 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	7	THR
2	K	159	ASP
2	J	38	ASP
2	J	212	GLU

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Mol	Chain	Res	Type
2	L	21	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	-44	ASN
2	N	-44	ASN
2	L	-2	HIS
2	M	-44	ASN
2	N	96	GLN

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.