



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 07:18 am GMT

PDB ID : 1RYP
Title : CRYSTAL STRUCTURE OF THE 20S PROTEASOME FROM YEAST AT 2.4 ANGSTROMS RESOLUTION
Authors : Groll, M.; Ditzel, L.; Loewe, J.; Stock, D.; Bochtler, M.; Bartunik, H.D.; Huber, R.
Deposited on : 1997-02-26
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

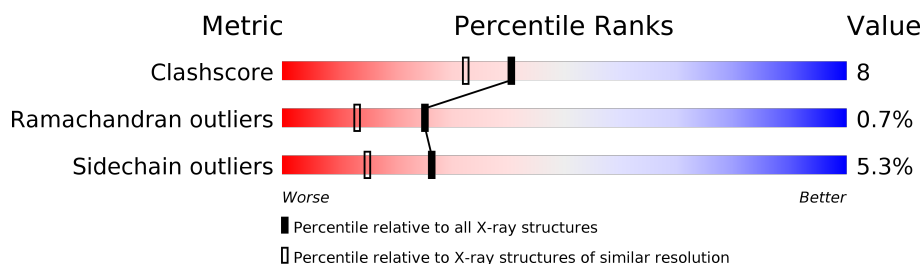
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)






















The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	243	
1	O	243	
2	B	250	
2	P	250	
3	C	244	
3	Q	244	
4	D	241	

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Mol	Chain	Length	Quality of chain
4	R	241	 68% 27% 5%
5	E	242	 79% 18% .
5	S	242	 75% 24% .
6	F	233	 70% 27% .
6	T	233	 70% 27% .
7	G	244	 80% 16% .
7	U	244	 75% 20% 5%
8	H	205	 76% 23% .
8	V	205	 78% 21%
9	I	222	 82% 16% .
9	W	222	 81% 18% .
10	J	204	 85% 14%
10	X	204	 83% 17%
11	K	198	 79% 21% .
11	Y	198	 77% 23% .
12	L	212	 85% 13% .
12	Z	212	 89% 9% .
13	1	222	 84% 15% .
13	M	222	 81% 18% .
14	2	233	 80% 19% .
14	N	233	 83% 16% .

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 52604 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 20S PROTEASOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
1	O	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			

- Molecule 2 is a protein called 20S PROTEASOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
2	P	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 3 is a protein called 20S PROTEASOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	3			
3	Q	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	3			

- Molecule 4 is a protein called 20S PROTEASOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			
4	R	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			

- Molecule 5 is a protein called 20S PROTEASOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			
5	S	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			

- Molecule 6 is a protein called 20S PROTEASOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
6	T	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

- Molecule 7 is a protein called 20S PROTEASOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			
7	U	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			

- Molecule 8 is a protein called 20S PROTEASOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	205	Total	C	N	O	S	0	0	0
			1574	995	261	311	7			
8	V	205	Total	C	N	O	S	0	0	0
			1574	995	261	311	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	ALA	THR	CONFLICT	UNP P38624
V	1	ALA	THR	CONFLICT	UNP P38624

- Molecule 9 is a protein called 20S PROTEASOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			
9	W	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			

- Molecule 10 is a protein called 20S PROTEASOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
10	X	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 11 is a protein called 20S PROTEASOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			
11	Y	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

- Molecule 12 is a protein called 20S PROTEASOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	212	Total	C	N	O	S	0	0	0
			1646	1045	282	312	7			
12	Z	212	Total	C	N	O	S	0	0	0
			1646	1045	282	312	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	33	ARG	LYS	CONFLICT	UNP P30656
Z	33	ARG	LYS	CONFLICT	UNP P30656

- Molecule 13 is a protein called 20S PROTEASOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
13	1	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 14 is a protein called 20S PROTEASOME.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	2	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	J	2	Total	Mg	0	0
			2	2		
15	1	1	Total	Mg	0	0
			1	1		
15	E	1	Total	Mg	0	0
			1	1		
15	H	1	Total	Mg	0	0
			1	1		
15	I	1	Total	Mg	0	0
			1	1		
15	V	1	Total	Mg	0	0
			1	1		
15	W	1	Total	Mg	0	0
			1	1		
15	Z	1	Total	Mg	0	0
			1	1		
15	A	2	Total	Mg	0	0
			2	2		
15	U	1	Total	Mg	0	0
			1	1		
15	X	2	Total	Mg	0	0
			2	2		
15	O	2	Total	Mg	0	0
			2	2		
15	L	1	Total	Mg	0	0
			1	1		
15	S	1	Total	Mg	0	0
			1	1		
15	M	1	Total	Mg	0	0
			1	1		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	1	139	Total O 139 139	0	0
16	2	153	Total O 153 153	0	0
16	A	113	Total O 113 113	0	0
16	B	109	Total O 109 109	0	0
16	C	73	Total O 73 73	0	0
16	D	66	Total O 66 66	0	0
16	E	88	Total O 88 88	0	0
16	F	58	Total O 58 58	0	0
16	G	91	Total O 91 91	0	0
16	H	114	Total O 114 114	0	0
16	I	122	Total O 122 122	0	0
16	J	113	Total O 113 113	0	0
16	K	117	Total O 117 117	0	0
16	L	100	Total O 100 100	0	0
16	M	135	Total O 135 135	0	0
16	N	158	Total O 158 158	0	0
16	O	108	Total O 108 108	0	0
16	P	105	Total O 105 105	0	0
16	Q	78	Total O 78 78	0	0
16	R	63	Total O 63 63	0	0
16	S	88	Total O 88 88	0	0
16	T	55	Total O 55 55	0	0

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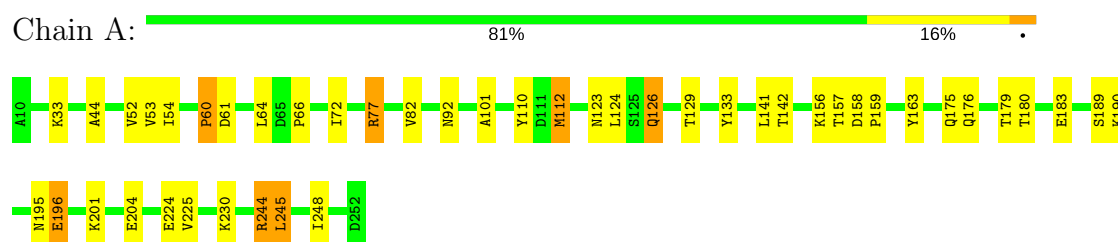
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	U	92	Total 92	O 92	0	0
16	V	121	Total 121	O 121	0	0
16	W	124	Total 124	O 124	0	0
16	X	110	Total 110	O 110	0	0
16	Y	115	Total 115	O 115	0	0
16	Z	100	Total 100	O 100	0	0

3 Residue-property plots [i](#)

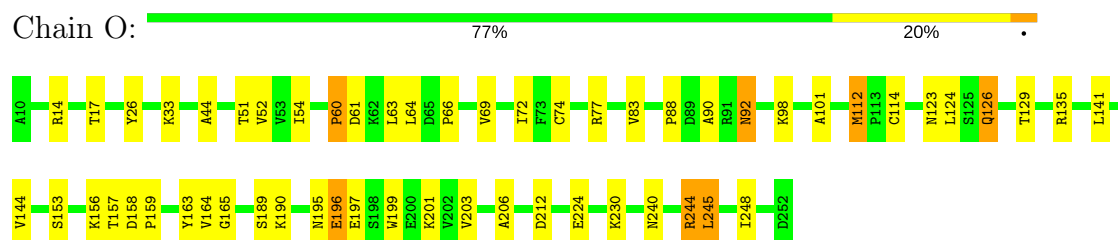
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

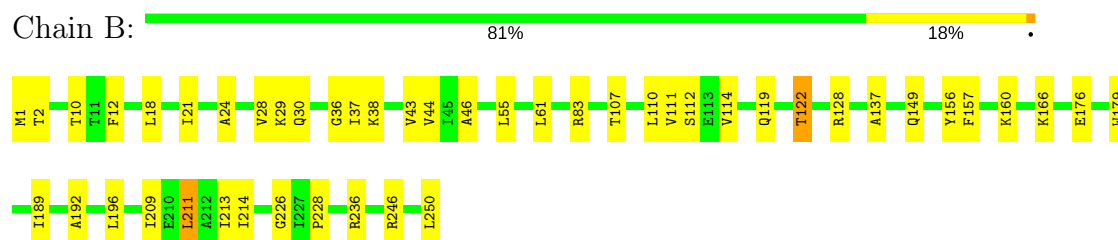
• Molecule 1: 20S PROTEASOME



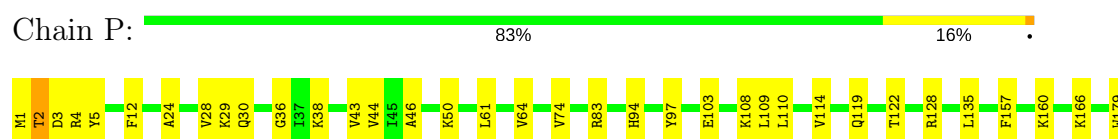
• Molecule 1: 20S PROTEASOME



• Molecule 2: 20S PROTEASOME



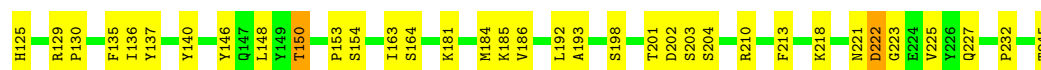
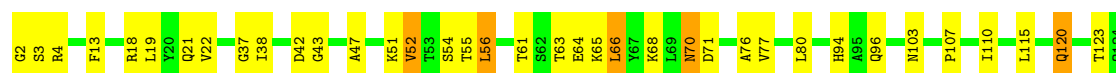
• Molecule 2: 20S PROTEASOME





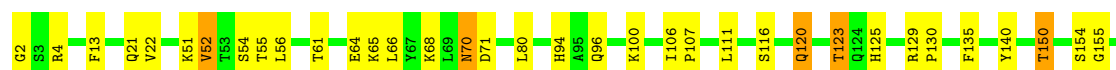
• Molecule 3: 20S PROTEASOME

Chain C: 70% 27%



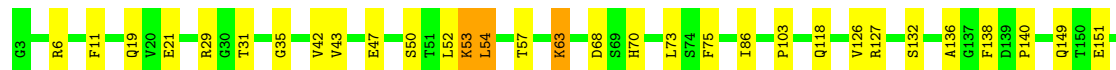
• Molecule 3: 20S PROTEASOME

Chain Q: 77% 20%



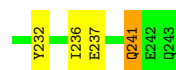
• Molecule 4: 20S PROTEASOME

Chain D: 72% 24%



• Molecule 4: 20S PROTEASOME

Chain R: 68% 27% 5%



• Molecule 5: 20S PROTEASOME

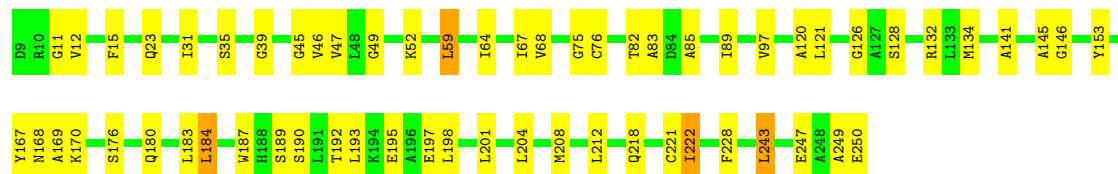
Chain E: 79% 18%





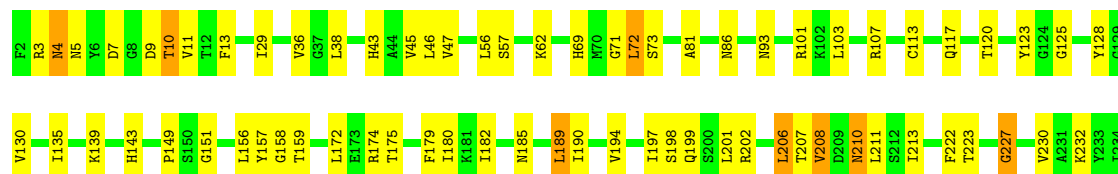
• Molecule 5: 20S PROTEASOME

Chain S: 75% 24%



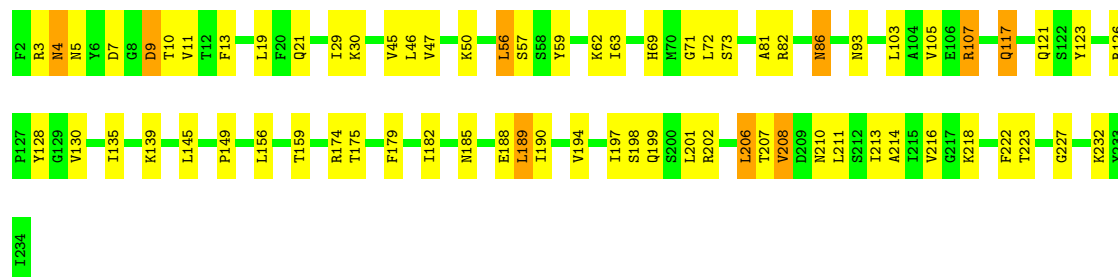
• Molecule 6: 20S PROTEASOME

Chain F: 70% 27%



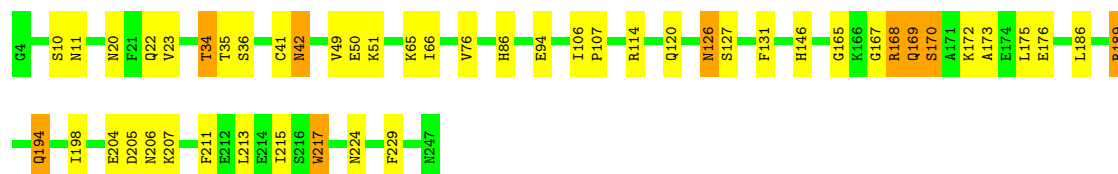
• Molecule 6: 20S PROTEASOME

Chain T: 70% 27%



• Molecule 7: 20S PROTEASOME

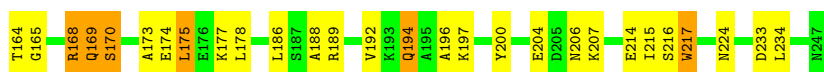
Chain G: 80% 16%



• Molecule 7: 20S PROTEASOME

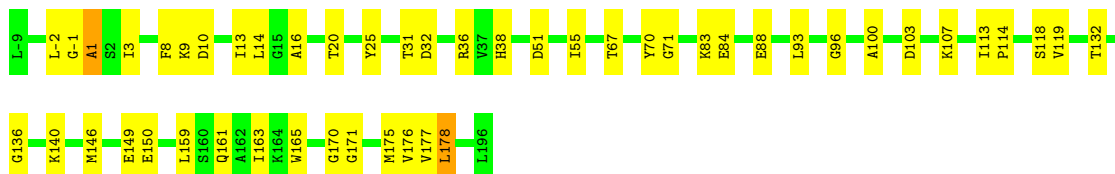
Chain U: 75% 20% 5%





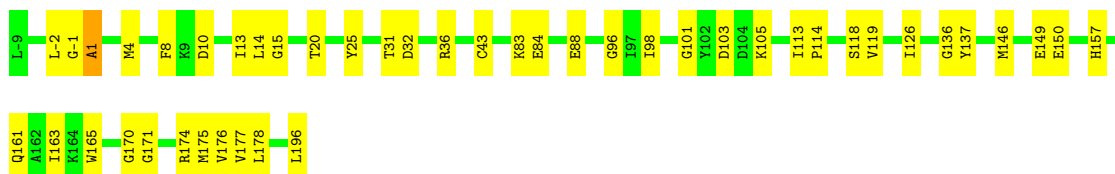
• Molecule 8: 20S PROTEASOME

Chain H: 76% 23%



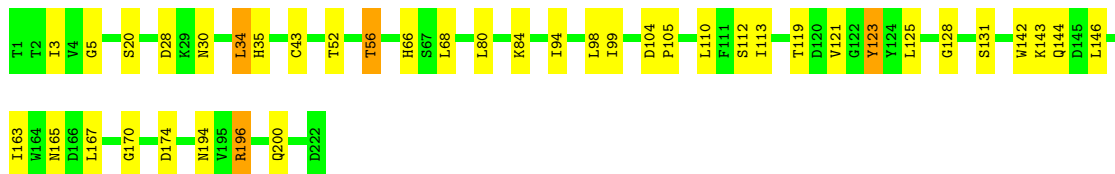
• Molecule 8: 20S PROTEASOME

Chain V: 78% 21%



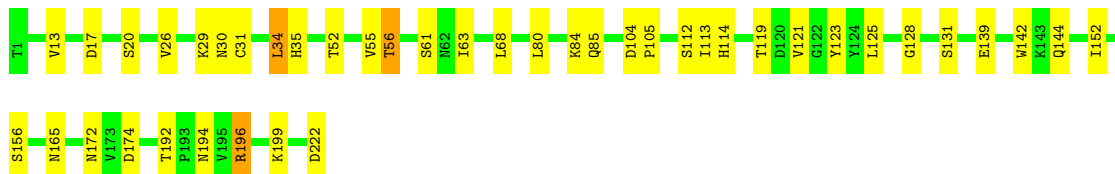
• Molecule 9: 20S PROTEASOME

Chain I: 82% 16%



• Molecule 9: 20S PROTEASOME

Chain W: 81% 18%

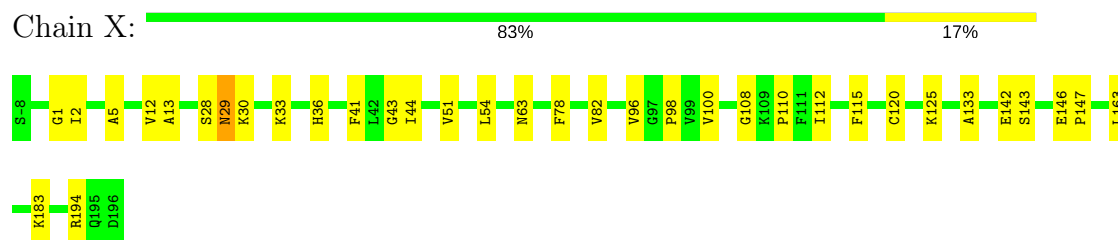


• Molecule 10: 20S PROTEASOME

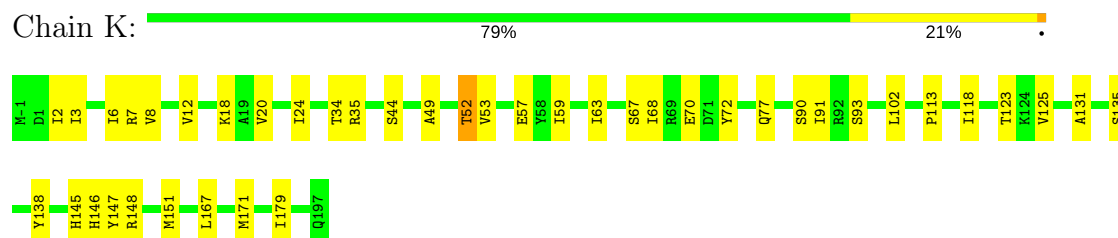
Chain J: 85% 14%



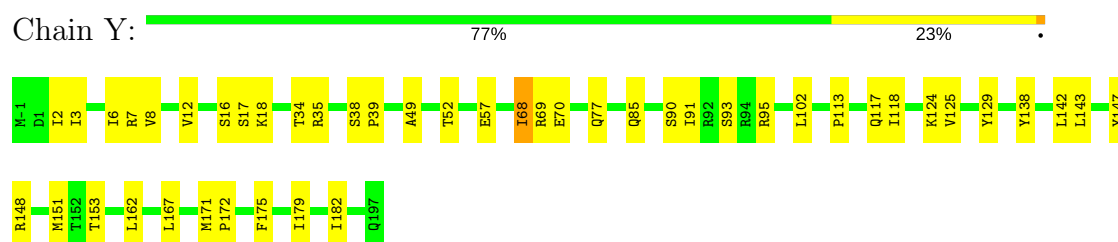
• Molecule 10: 20S PROTEASOME



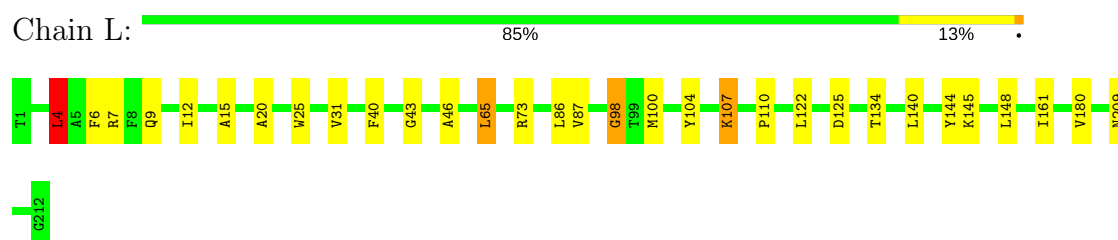
• Molecule 11: 20S PROTEASOME



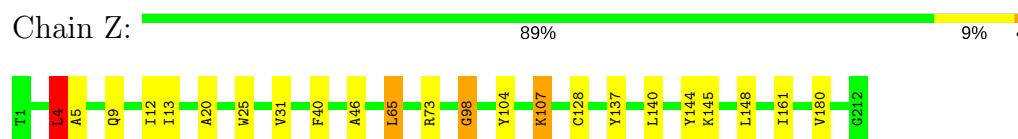
• Molecule 11: 20S PROTEASOME



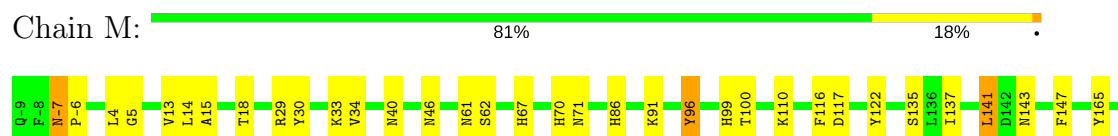
• Molecule 12: 20S PROTEASOME



• Molecule 12: 20S PROTEASOME



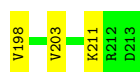
• Molecule 13: 20S PROTEASOME





• Molecule 13: 20S PROTEASOME

Chain 1: 84% 15%



• Molecule 14: 20S PROTEASOME

Chain N: 83% 16%



• Molecule 14: 20S PROTEASOME

Chain 2: 80% 19%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.49Å 300.70Å 144.42Å 90.00° 112.89° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90	Depositor
% Data completeness (in resolution range)	90.5 (50.00-1.90)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.286 , 0.330	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	52604	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.56	1/1959 (0.1%)	0.72	0/2652
1	O	0.58	1/1959 (0.1%)	0.73	0/2652
2	B	0.54	0/1952	0.75	1/2642 (0.0%)
2	P	0.52	0/1952	0.74	1/2642 (0.0%)
3	C	0.52	0/1935	0.74	1/2618 (0.0%)
3	Q	0.52	0/1935	0.75	0/2618
4	D	0.53	0/1920	0.74	1/2598 (0.0%)
4	R	0.53	0/1920	0.74	1/2598 (0.0%)
5	E	0.52	0/1887	0.76	2/2541 (0.1%)
5	S	0.52	0/1887	0.73	2/2541 (0.1%)
6	F	0.50	0/1823	0.72	1/2463 (0.0%)
6	T	0.49	0/1823	0.70	0/2463
7	G	0.54	0/1937	0.73	0/2614
7	U	0.53	0/1937	0.76	0/2614
8	H	0.58	0/1603	0.77	2/2168 (0.1%)
8	V	0.58	0/1603	0.76	2/2168 (0.1%)
9	I	0.55	0/1716	0.76	0/2326
9	W	0.54	0/1716	0.77	1/2326 (0.0%)
10	J	0.56	0/1611	0.77	0/2174
10	X	0.55	0/1611	0.76	0/2174
11	K	0.56	0/1613	0.78	0/2173
11	Y	0.57	0/1613	0.79	0/2173
12	L	0.55	0/1683	0.76	2/2277 (0.1%)
12	Z	0.53	0/1683	0.76	2/2277 (0.1%)
13	1	0.56	0/1795	0.77	0/2420
13	M	0.55	0/1795	0.77	1/2420 (0.0%)
14	2	0.57	0/1855	0.81	2/2514 (0.1%)
14	N	0.55	0/1855	0.77	3/2514 (0.1%)
All	All	0.54	2/50578 (0.0%)	0.75	25/68360 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
9	I	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	112	MET	SD-CE	-5.62	1.46	1.77
1	O	112	MET	SD-CE	-5.05	1.49	1.77

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	52	LEU	CA-CB-CG	6.80	130.93	115.30
5	S	134	MET	N-CA-C	-6.60	93.17	111.00
5	E	134	MET	N-CA-C	-6.44	93.61	111.00
12	L	4	LEU	CA-CB-CG	6.42	130.07	115.30
4	R	52	LEU	CA-CB-CG	6.03	129.17	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	I	123	TYR	Sidechain

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	1921	0	1910	35	0
1	O	1921	0	1910	42	0
2	B	1915	0	1929	30	0
2	P	1915	0	1929	28	0
3	C	1905	0	1901	46	0
3	Q	1905	0	1901	38	0
4	D	1891	0	1900	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	R	1891	0	1900	57	0
5	E	1862	0	1836	33	0
5	S	1862	0	1836	34	0
6	F	1795	0	1797	47	0
6	T	1795	0	1797	46	0
7	G	1897	0	1886	30	0
7	U	1897	0	1886	40	0
8	H	1574	0	1553	31	0
8	V	1574	0	1553	31	0
9	I	1685	0	1688	27	0
9	W	1685	0	1688	30	0
10	J	1581	0	1574	18	0
10	X	1581	0	1574	24	0
11	K	1585	0	1590	29	0
11	Y	1585	0	1590	31	0
12	L	1646	0	1595	27	0
12	Z	1646	0	1595	16	0
13	1	1757	0	1711	26	0
13	M	1757	0	1711	31	0
14	2	1824	0	1832	29	0
14	N	1824	0	1832	22	0
15	1	1	0	0	0	0
15	A	2	0	0	0	0
15	E	1	0	0	0	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0
15	J	2	0	0	0	0
15	L	1	0	0	0	0
15	M	1	0	0	0	0
15	O	2	0	0	0	0
15	S	1	0	0	0	0
15	U	1	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	X	2	0	0	0	0
15	Z	1	0	0	0	0
16	1	139	0	0	3	0
16	2	153	0	0	1	0
16	A	113	0	0	0	0
16	B	109	0	0	1	0
16	C	73	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	D	66	0	0	0	0
16	E	88	0	0	2	0
16	F	58	0	0	1	0
16	G	91	0	0	1	0
16	H	114	0	0	2	0
16	I	122	0	0	0	0
16	J	113	0	0	0	0
16	K	117	0	0	1	0
16	L	100	0	0	0	0
16	M	135	0	0	2	0
16	N	158	0	0	0	0
16	O	108	0	0	3	0
16	P	105	0	0	1	0
16	Q	78	0	0	3	0
16	R	63	0	0	0	0
16	S	88	0	0	1	0
16	T	55	0	0	0	0
16	U	92	0	0	1	0
16	V	121	0	0	1	0
16	W	124	0	0	1	0
16	X	110	0	0	0	0
16	Y	115	0	0	2	0
16	Z	100	0	0	0	0
All	All	52604	0	49404	812	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 8.

The worst 5 of 812 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)
1:O:101:ALA:HA	1:O:112:MET:HE2	1.37	1.06
1:A:101:ALA:HA	1:A:112:MET:HE2	1.46	0.96
3:C:125:HIS:HB3	4:D:126:VAL:HG12	1.50	0.94
13:1:18:THR:CG2	13:1:30:TYR:HA	1.98	0.93
12:Z:107:LYS:HD2	12:Z:107:LYS:H	1.34	0.92

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	241/243 (99%)	233 (97%)	7 (3%)	1 (0%)	38	26
1	O	241/243 (99%)	231 (96%)	9 (4%)	1 (0%)	38	26
2	B	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	38	26
2	P	248/250 (99%)	235 (95%)	10 (4%)	3 (1%)	15	5
3	C	242/244 (99%)	225 (93%)	13 (5%)	4 (2%)	11	2
3	Q	242/244 (99%)	224 (93%)	14 (6%)	4 (2%)	11	2
4	D	239/241 (99%)	223 (93%)	12 (5%)	4 (2%)	11	2
4	R	239/241 (99%)	222 (93%)	13 (5%)	4 (2%)	11	2
5	E	240/242 (99%)	231 (96%)	7 (3%)	2 (1%)	22	11
5	S	240/242 (99%)	228 (95%)	9 (4%)	3 (1%)	14	4
6	F	231/233 (99%)	214 (93%)	14 (6%)	3 (1%)	14	4
6	T	231/233 (99%)	209 (90%)	19 (8%)	3 (1%)	14	4
7	G	242/244 (99%)	230 (95%)	10 (4%)	2 (1%)	22	11
7	U	242/244 (99%)	222 (92%)	17 (7%)	3 (1%)	15	5
8	H	203/205 (99%)	193 (95%)	9 (4%)	1 (0%)	32	20
8	V	203/205 (99%)	192 (95%)	10 (5%)	1 (0%)	32	20
9	I	220/222 (99%)	212 (96%)	8 (4%)	0	100	100
9	W	220/222 (99%)	212 (96%)	8 (4%)	0	100	100
10	J	202/204 (99%)	197 (98%)	5 (2%)	0	100	100
10	X	202/204 (99%)	198 (98%)	4 (2%)	0	100	100
11	K	196/198 (99%)	191 (97%)	3 (2%)	2 (1%)	18	7
11	Y	196/198 (99%)	188 (96%)	6 (3%)	2 (1%)	18	7
12	L	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
12	Z	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
13	1	220/222 (99%)	212 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	220/222 (99%)	211 (96%)	9 (4%)	0	100	100
14	2	231/233 (99%)	219 (95%)	12 (5%)	0	100	100
14	N	231/233 (99%)	217 (94%)	14 (6%)	0	100	100
All	All	6330/6386 (99%)	6017 (95%)	269 (4%)	44 (1%)	25	13

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	222	ASP
4	D	54	LEU
4	D	185	PRO
1	O	60	PRO
3	Q	222	ASP

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	207/207 (100%)	196 (95%)	11 (5%)	26	15
1	O	207/207 (100%)	196 (95%)	11 (5%)	26	15
2	B	209/209 (100%)	200 (96%)	9 (4%)	33	22
2	P	209/209 (100%)	203 (97%)	6 (3%)	48	39
3	C	203/203 (100%)	187 (92%)	16 (8%)	14	6
3	Q	203/203 (100%)	188 (93%)	15 (7%)	16	7
4	D	213/213 (100%)	195 (92%)	18 (8%)	12	5
4	R	213/213 (100%)	196 (92%)	17 (8%)	14	5
5	E	198/198 (100%)	186 (94%)	12 (6%)	22	11
5	S	198/198 (100%)	187 (94%)	11 (6%)	25	13
6	F	192/192 (100%)	176 (92%)	16 (8%)	13	5
6	T	192/192 (100%)	176 (92%)	16 (8%)	13	5
7	G	201/201 (100%)	184 (92%)	17 (8%)	12	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	U	201/201 (100%)	183 (91%)	18 (9%)	11	4
8	H	168/168 (100%)	162 (96%)	6 (4%)	40	29
8	V	168/168 (100%)	165 (98%)	3 (2%)	64	60
9	I	181/181 (100%)	174 (96%)	7 (4%)	37	26
9	W	181/181 (100%)	171 (94%)	10 (6%)	25	14
10	J	172/172 (100%)	169 (98%)	3 (2%)	66	62
10	X	172/172 (100%)	168 (98%)	4 (2%)	56	49
11	K	175/175 (100%)	171 (98%)	4 (2%)	56	49
11	Y	175/175 (100%)	170 (97%)	5 (3%)	48	39
12	L	169/169 (100%)	163 (96%)	6 (4%)	40	29
12	Z	169/169 (100%)	164 (97%)	5 (3%)	46	37
13	1	185/185 (100%)	174 (94%)	11 (6%)	23	12
13	M	185/185 (100%)	175 (95%)	10 (5%)	26	14
14	2	199/199 (100%)	190 (96%)	9 (4%)	32	21
14	N	199/199 (100%)	191 (96%)	8 (4%)	36	25
All	All	5344/5344 (100%)	5060 (95%)	284 (5%)	26	15

5 of 284 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	62	SER
2	P	211	LEU
12	Z	104	TYR
13	M	117	ASP
1	O	77	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 172 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	10	ASN
3	Q	94	HIS
13	1	99	HIS
14	N	100	ASN
1	O	123	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 20 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](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.