



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Apr 1, 2019 – 09:32 AM EDT

PDB ID : 6J2Q
EMDB ID: : EMD-9771
Title : Yeast proteasome in Ub-accepted state (C1-b)
Authors : Cong, Y.
Deposited on : 2019-01-02
Resolution : 3.80 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

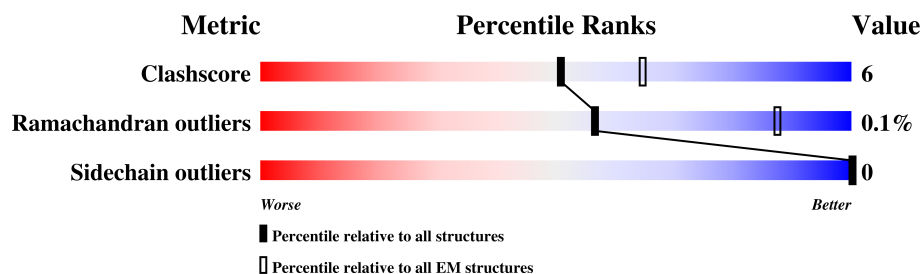
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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.









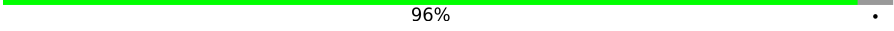

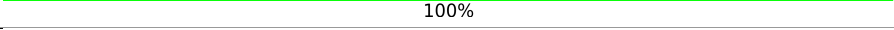

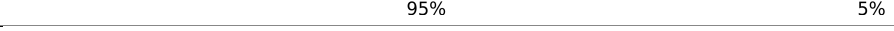

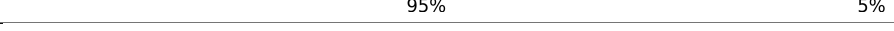

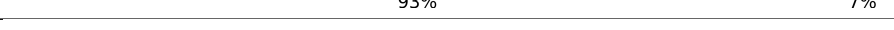

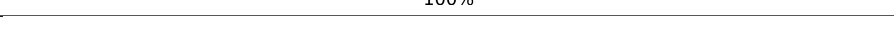
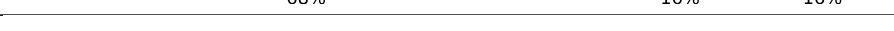
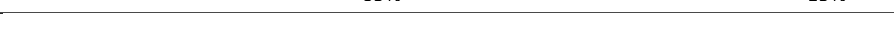
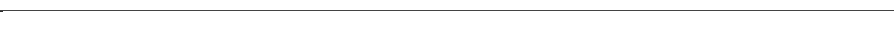
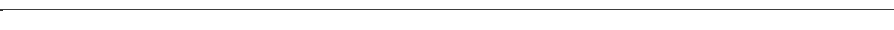




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1	215	75% 20% 5%
1	b	215	95% 5%
2	2	261	72% 13% 15%
2	i	261	85% 15%
3	3	205	79% 20%
3	h	205	99%
4	4	198	80% 20%
4	g	198	100%
5	5	287	62% 12% 26%














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Mol	Chain	Length	Quality of chain
5	f	287	 74% 26%
6	6	241	 79% 13% 8%
6	e	241	 92% 8%
7	7	266	 72% 15% 12%
7	a	266	 88% 12%
8	A	252	 78% 19% .
8	c	252	 96% .
9	B	250	 80% 20%
9	j	250	 100%
10	C	258	 77% 18% 5%
10	d	258	 95% 5%
11	D	254	 79% 16% 5%
11	n	254	 95% 5%
12	E	260	 76% 17% 7%
12	m	260	 93% 7%
13	F	234	 76% 23%
13	l	234	 100%
14	G	288	 68% 16% 16%
14	k	288	 85% 15%
15	H	467	 58% 18% 24%
16	I	437	 69% 14% 17%
17	J	405	 73% 20% 8%
18	K	428	 71% 18% 11%
19	L	437	 68% 17% 15%
20	M	434	 67% 18% 15%

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Mol	Chain	Length	Quality of chain
21	N	945	 77%13%10%
22	O	393	 82%16%2%
23	P	445	 81%16%3%
24	Q	434	 91%9%0%
25	R	429	 77%17%7%
26	S	523	 81%10%9%
27	T	274	 89%11%0%
28	U	338	 64%12%25%
29	V	306	 64%20%16%
30	W	268	 56%17%26%
31	X	156	 68%13%19%
32	Y	89	 24%7%70%
33	Z	993	 70%12%18%

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 106311 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	205	Total	C	N	O	S	0	0
			1576	996	261	312	7		
1	b	205	Total	C	N	O	S	0	0
			1576	996	261	312	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	222	Total	C	N	O	S	0	0
			1684	1061	293	323	7		
2	i	222	Total	C	N	O	S	0	0
			1684	1061	293	323	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		
3	h	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	198	Total	C	N	O	S	0	0
			1585	1005	269	305	6		
4	g	198	Total	C	N	O	S	0	0
			1585	1005	269	305	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		
5	f	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		
6	e	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		

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

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

- Molecule 8 is a protein called Proteasome subunit alpha type-1.

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

- Molecule 9 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	250	Total	C	N	O	S	0	0
			1915	1219	315	377	4		
9	j	250	Total	C	N	O	S	0	0
			1915	1219	315	377	4		

- Molecule 10 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	d	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		

- Molecule 11 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	241	Total	C	N	O	S	0	0
			1890	1181	331	374	4		
11	n	241	Total	C	N	O	S	0	0
			1890	1181	331	374	4		

- Molecule 12 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	242	Total	C	N	O	S	0	0
			1861	1162	314	378	7		
12	m	242	Total	C	N	O	S	0	0
			1861	1162	314	378	7		

- Molecule 13 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	233	Total	C	N	O	S	0	0
			1795	1129	312	350	4		
13	l	233	Total	C	N	O	S	0	0
			1795	1129	312	350	4		

- Molecule 14 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	243	Total	C	N	O	S	0	0
			1888	1201	328	355	4		
14	k	244	Total	C	N	O	S	0	0
			1896	1205	330	357	4		

- Molecule 15 is a protein called 26S protease regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	355	Total	C	N	O	S	0	0
			2787	1755	500	515	17		

- Molecule 16 is a protein called 26S protease regulatory subunit 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	363	Total	C	N	O	S	0	0
			2831	1779	472	565	15		

- Molecule 17 is a protein called 26S protease regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	373	Total	C	N	O	S	0	0
			2928	1837	527	547	17		

- Molecule 18 is a protein called 26S protease regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	381	Total	C	N	O	S	0	0
			3019	1898	530	581	10		

- Molecule 19 is a protein called 26S protease subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	371	Total	C	N	O	S	0	0
			2937	1852	519	554	12		

- Molecule 20 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	367	Total	C	N	O	S	0	0
			2866	1799	503	553	11		

- Molecule 21 is a protein called 26S proteasome regulatory subunit RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	849	Total	C	N	O	S	0	0
			6562	4174	1099	1261	28		

- Molecule 22 is a protein called 26S proteasome regulatory subunit RPN9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	387	Total	C	N	O	S	0	0
			3182	2047	520	606	9		

- Molecule 23 is a protein called 26S proteasome regulatory subunit RPN5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	432	Total	C	N	O	S	0	0
			3545	2260	592	684	9		

- Molecule 24 is a protein called 26S proteasome regulatory subunit RPN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	431	Total	C	N	O	S	0	0
			3471	2205	574	676	16		

- Molecule 25 is a protein called 26S proteasome regulatory subunit RPN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	400	Total	C	N	O	S	0	0
			3218	2051	527	630	10		

- Molecule 26 is a protein called 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S	475	Total	C	N	O	S	0	0
			3894	2488	653	738	15		

- Molecule 27 is a protein called 26S proteasome regulatory subunit RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	272	Total	C	N	O	S	0	0
			2235	1432	355	441	7		

- Molecule 28 is a protein called 26S proteasome regulatory subunit RPN8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U	255	Total	C	N	O	S	0	0
			2061	1312	352	391	6		

- Molecule 29 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	258	Total	C	N	O	S	0	0
			2025	1273	344	395	13		

- Molecule 30 is a protein called 26S proteasome regulatory subunit RPN10.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	197	Total	C	N	O	S	0	0
			1534	962	269	300	3		

- Molecule 31 is a protein called 26S proteasome regulatory subunit RPN13.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	X	127	Total	C	N	O	S	0	0
			1032	664	169	195	4		

- Molecule 32 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Y	27	Total	C	N	O	0	0
			236	143	39	54		

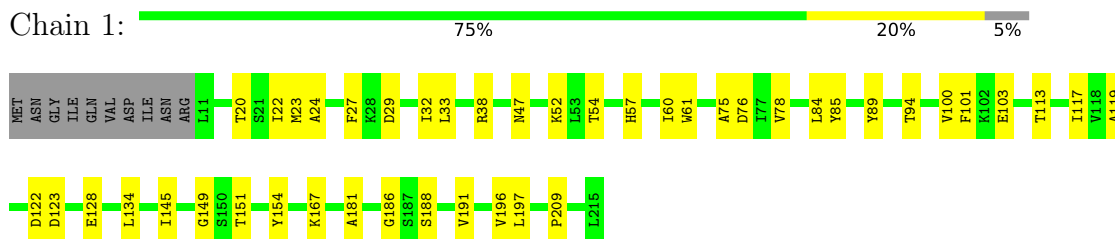
- Molecule 33 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	813	Total	C	N	O	S	0	0
			6290	3995	1029	1237	29		

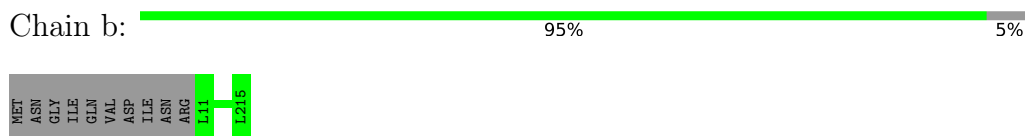
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

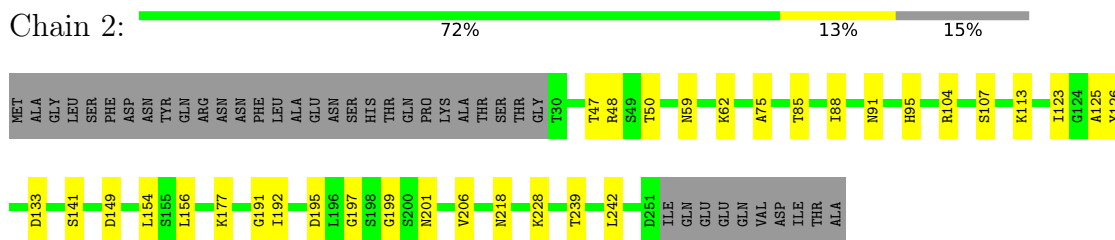
- Molecule 1: Proteasome subunit beta type-1



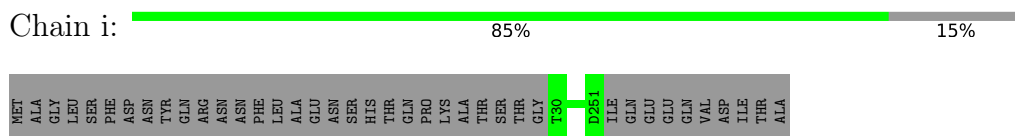
- Molecule 1: Proteasome subunit beta type-1



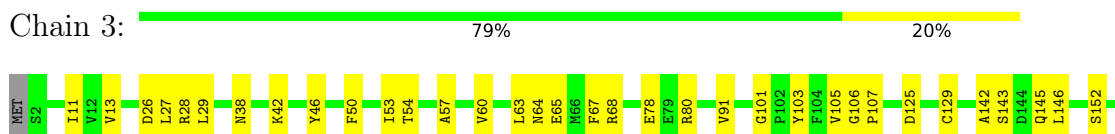
- Molecule 2: Proteasome subunit beta type-2



- Molecule 2: Proteasome subunit beta type-2



- Molecule 3: Proteasome subunit beta type-3





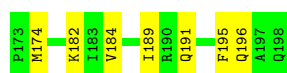
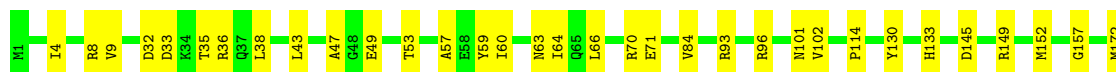
• Molecule 3: Proteasome subunit beta type-3

Chain h: 99%



• Molecule 4: Proteasome subunit beta type-4

Chain 4: 80% 20%



• Molecule 4: Proteasome subunit beta type-4

Chain g: 100%

There are no outlier residues recorded for this chain.

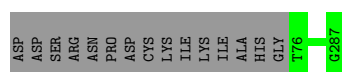
• Molecule 5: Proteasome subunit beta type-5

Chain 5: 62% 12% 26%



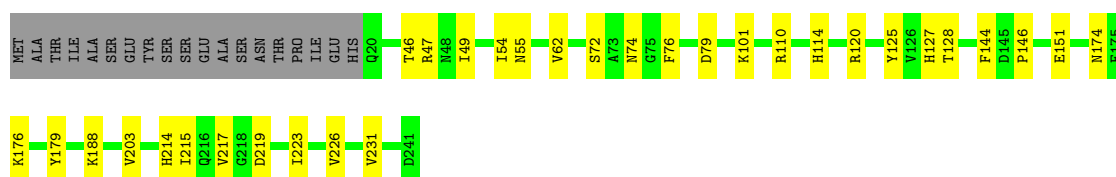
• Molecule 5: Proteasome subunit beta type-5

Chain f: 74% 26%



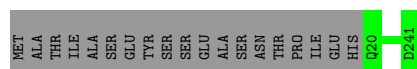
• Molecule 6: Proteasome subunit beta type-6

Chain 6: 79% 13% 8%



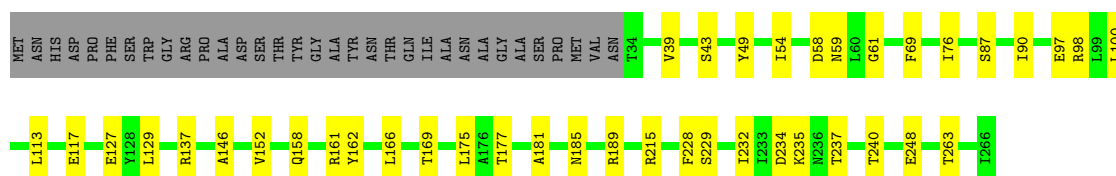
- Molecule 6: Proteasome subunit beta type-6

Chain e: 92% 8%



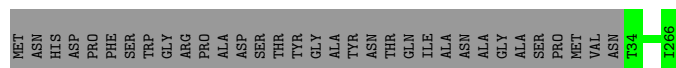
- Molecule 7: Proteasome subunit beta type-7

Chain 7: 72% 15% 12%



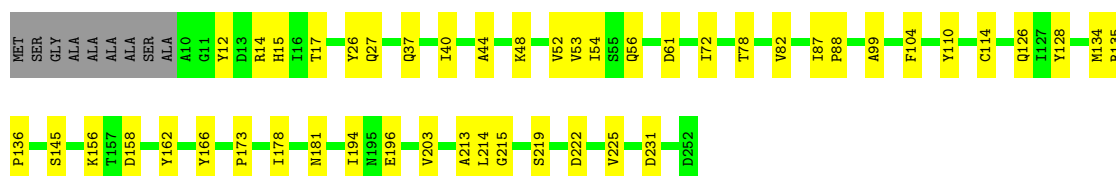
- Molecule 7: Proteasome subunit beta type-7

Chain a: 88% 12%



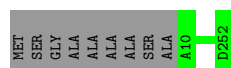
- Molecule 8: Proteasome subunit alpha type-1

Chain A: 78% 19% .



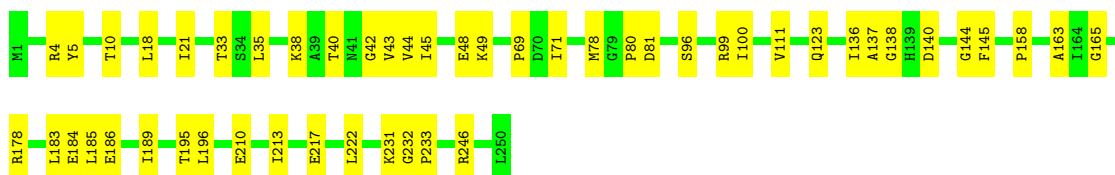
- Molecule 8: Proteasome subunit alpha type-1

Chain c: 96% .



- Molecule 9: Proteasome subunit alpha type-2

Chain B: 80% 20%



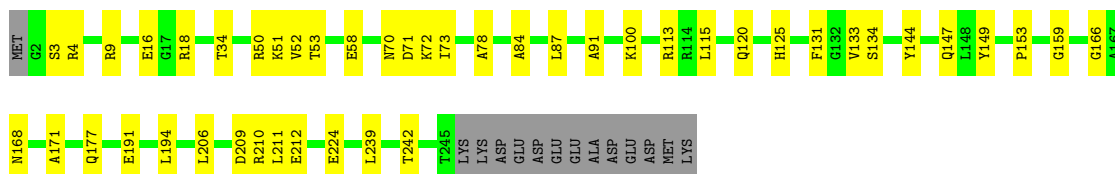
- Molecule 9: Proteasome subunit alpha type-2

Chain j: 100%

There are no outlier residues recorded for this chain.

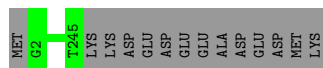
- Molecule 10: Proteasome subunit alpha type-3

Chain C: 77% 18% 5%

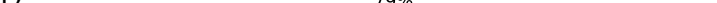


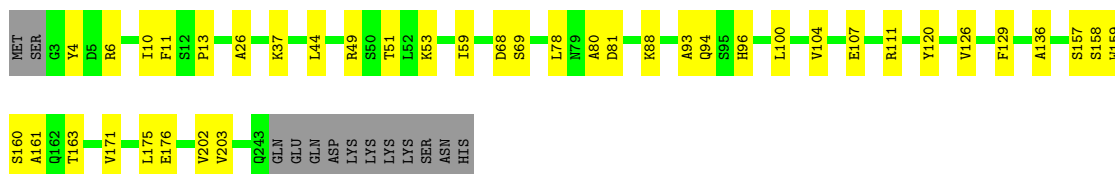
- Molecule 10: Proteasome subunit alpha type-3

Chain d: 95% 5%



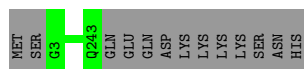
- Molecule 11: Proteasome subunit alpha type-4

Chain D:  79% 16% 5%



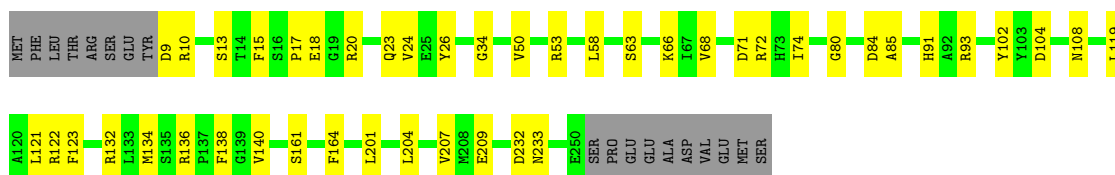
- Molecule 11: Proteasome subunit alpha type-4

Chain n: 95% 5%

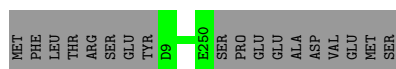


- Molecule 12: Proteasome subunit alpha type-5

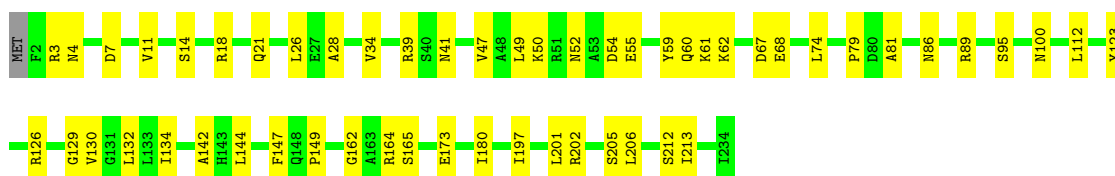
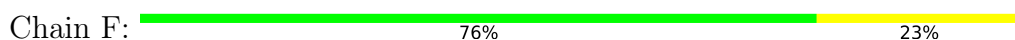
Chain E:  76% 17% 7%



- Molecule 12: Proteasome subunit alpha type-5



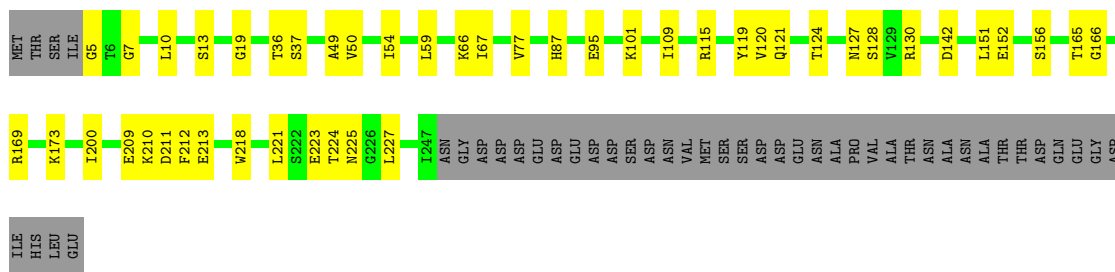
- Molecule 13: Proteasome subunit alpha type-6



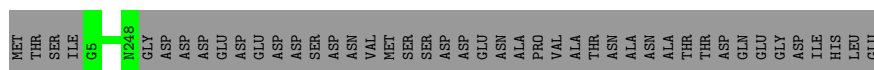
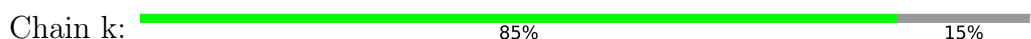
- Molecule 13: Proteasome subunit alpha type-6



- Molecule 14: Probable proteasome subunit alpha type-7

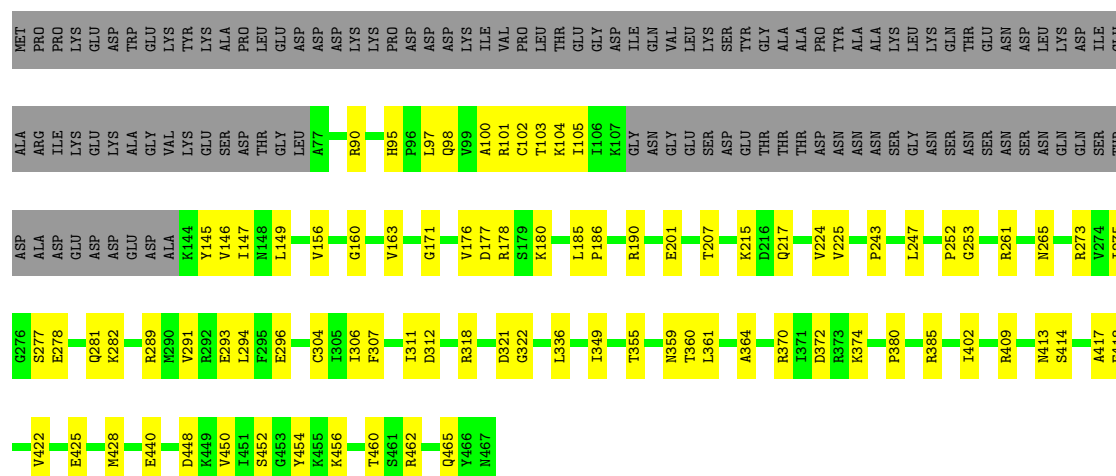


- Molecule 14: Probable proteasome subunit alpha type-7



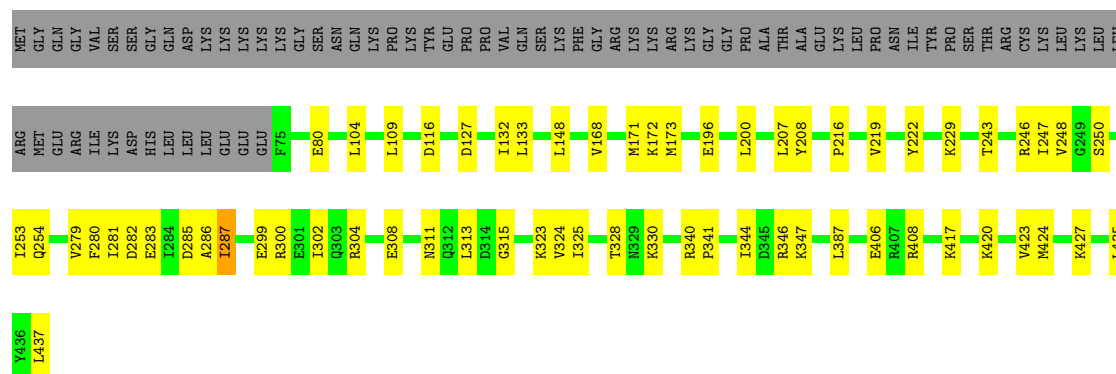
- Molecule 15: 26S protease regulatory subunit 7 homolog

Chain H:  58% 18% 24%



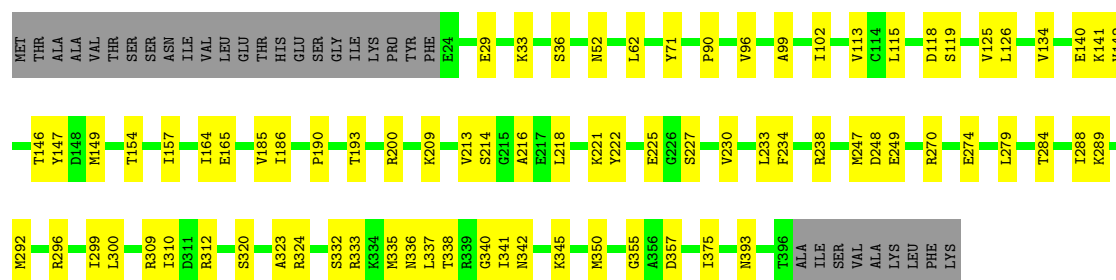
- Molecule 16: 26S protease regulatory subunit 4 homolog

Chain I:  69% 14% 17%



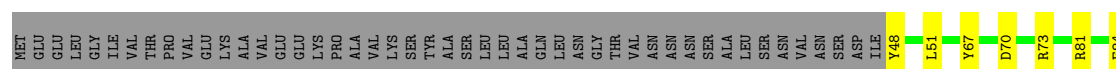
- Molecule 17: 26S protease regulatory subunit 8 homolog

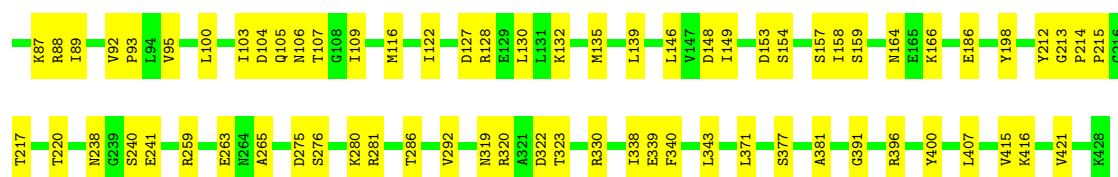
Chain J:  73% 20% 8%



- Molecule 18: 26S protease regulatory subunit 6B homolog

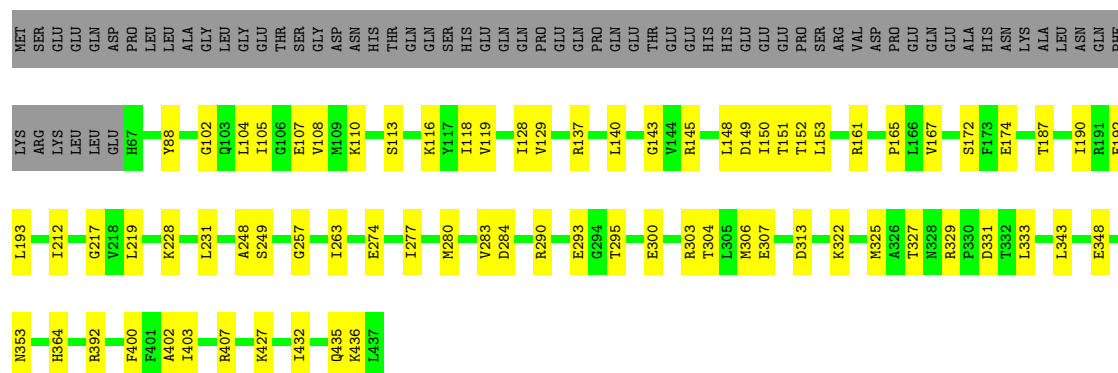
Chain K:  71% 18% 11%





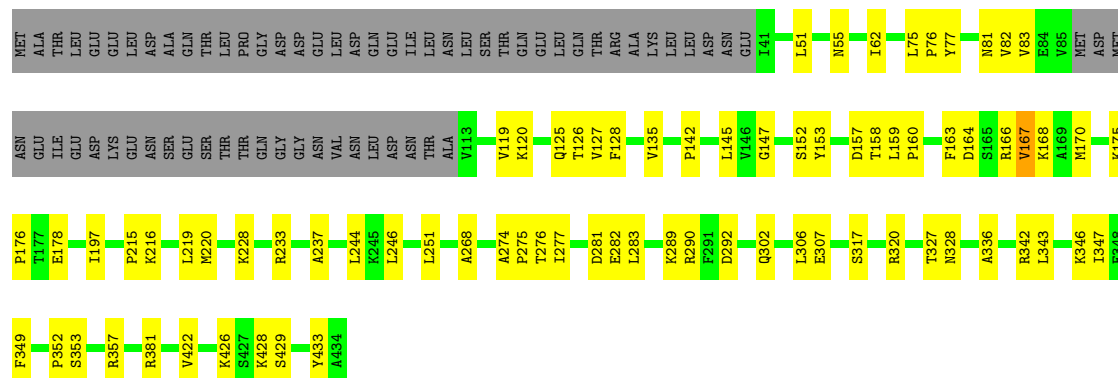
• Molecule 19: 26S protease subunit RPT4

Chain L: 68% 17% 15%



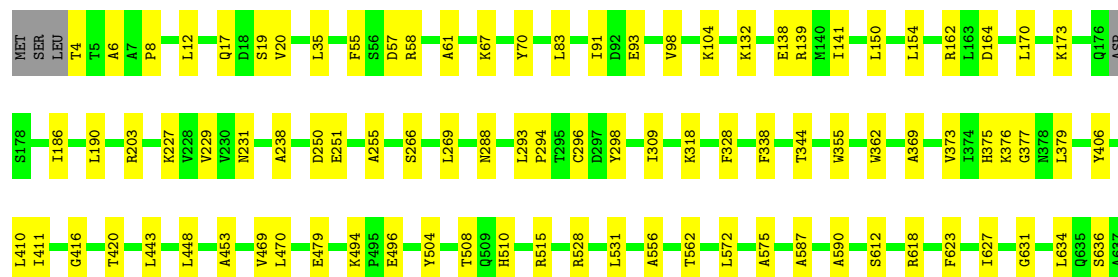
• Molecule 20: 26S protease regulatory subunit 6A

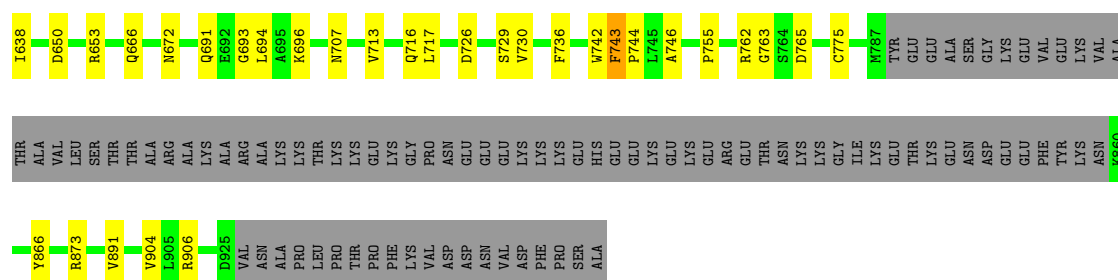
Chain M: 67% 18% 15%



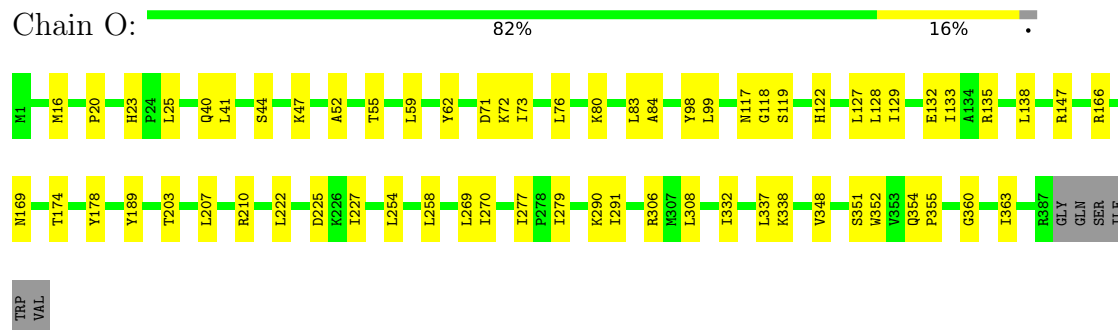
• Molecule 21: 26S proteasome regulatory subunit RPN2

Chain N: 77% 13% 10%

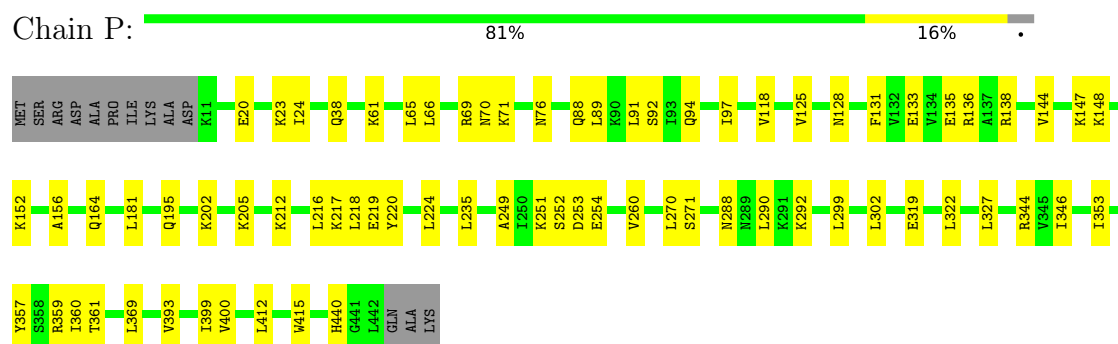




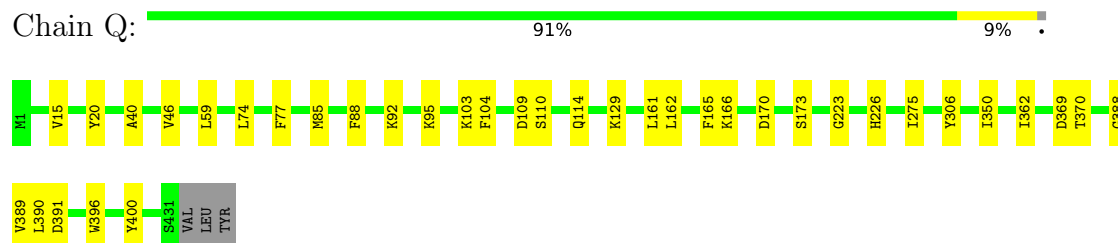
• Molecule 22: 26S proteasome regulatory subunit RPN9



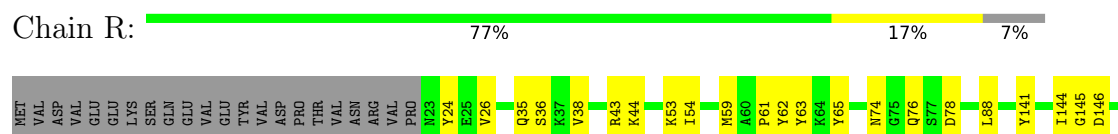
• Molecule 23: 26S proteasome regulatory subunit RPN5



• Molecule 24: 26S proteasome regulatory subunit RPN6

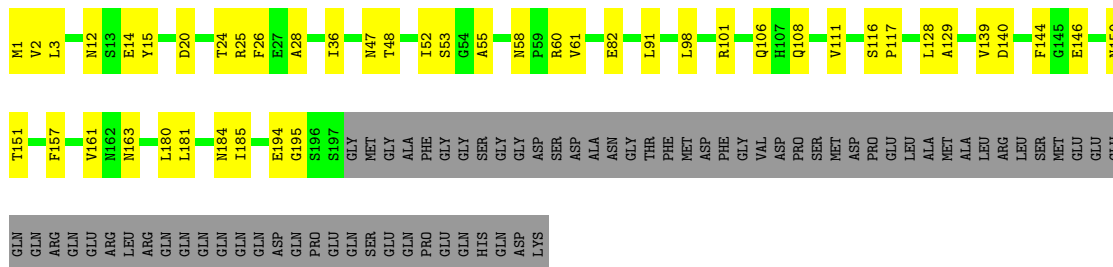


• Molecule 25: 26S proteasome regulatory subunit RPN7



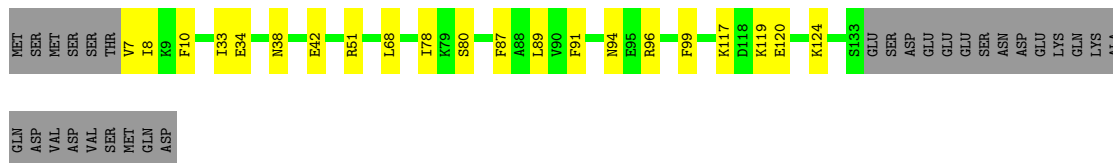
- Molecule 30: 26S proteasome regulatory subunit RPN10

Chain W:



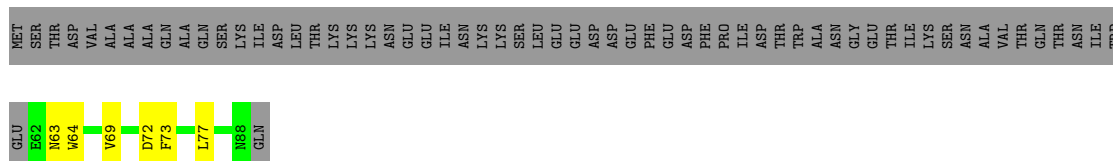
- Molecule 31: 26S proteasome regulatory subunit RPN13

Chain X:



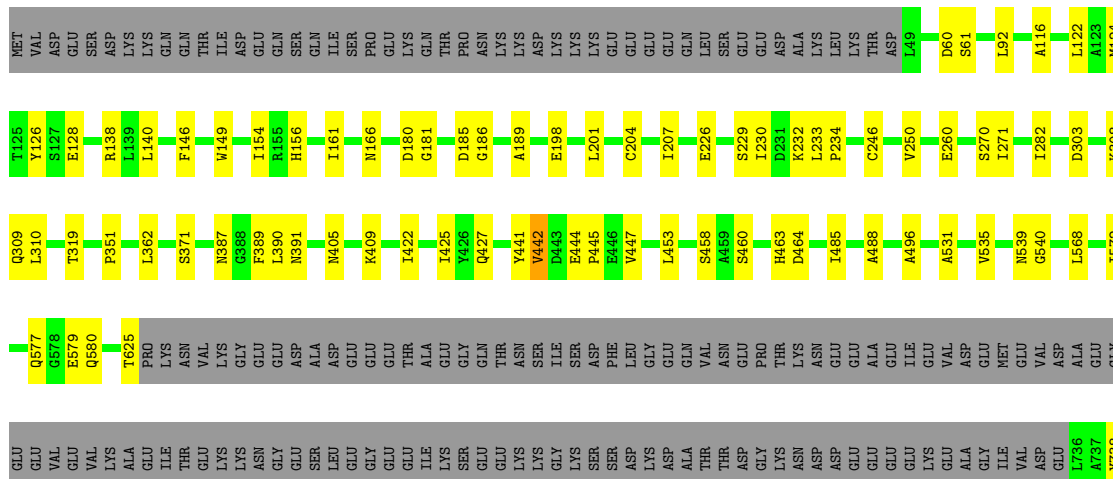
- Molecule 32: 26S proteasome complex subunit SEM1

Chain Y:



- Molecule 33: 26S proteasome regulatory subunit RPN1

Chain Z:



PRO	LVS	LVS	ILE	THR	GLY	TRP	ILE	THR	GLN	THR	SER	THR	P964	P955	L956	L957	E961	S972	Y973	T974	S975	H976	I977	V980	L983	E983	K754	L758	V783	T795	H801	D802	A803	I812	L827	L830	L831	Y837	T848	H856	L857	G858	K859	M862	S880	T884	F901	L904	P910	L914	D918	V925	R928	Q931	ALA	VAL	GLU	THR	VAL	GLY	GLN	ALA	GLY	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	77729	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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 > 2$	RMSZ	# $ Z > 2$
1	1	0.23	0/1605	0.41	0/2171
1	b	0.23	0/1605	0.42	0/2171
10	C	0.23	0/1934	0.41	0/2618
10	d	0.23	0/1934	0.40	0/2618
11	D	0.22	0/1919	0.39	0/2598
11	n	0.23	0/1919	0.39	0/2598
12	E	0.23	0/1886	0.40	0/2541
12	m	0.23	0/1886	0.39	0/2541
13	F	0.24	0/1823	0.42	0/2463
13	l	0.23	0/1823	0.41	0/2463
14	G	0.24	0/1928	0.40	0/2603
14	k	0.24	0/1936	0.40	0/2614
15	H	0.24	0/2834	0.41	0/3816
16	I	0.23	0/2869	0.41	0/3867
17	J	0.23	0/2964	0.39	0/3981
18	K	0.31	1/3062 (0.0%)	0.40	0/4132
19	L	0.33	1/2981 (0.0%)	0.39	0/4008
2	2	0.23	0/1715	0.41	0/2326
2	i	0.23	0/1715	0.41	0/2326
20	M	0.24	0/2903	0.42	0/3909
21	N	0.25	1/6670 (0.0%)	0.38	0/9023
22	O	0.25	1/3243 (0.0%)	0.39	0/4374
23	P	0.22	0/3599	0.37	0/4854
24	Q	0.23	0/3527	0.36	0/4748
25	R	0.23	0/3272	0.37	0/4412
26	S	0.23	0/3966	0.36	0/5355
27	T	0.23	0/2279	0.38	0/3077
28	U	0.22	0/2087	0.37	0/2811
29	V	0.23	0/2054	0.42	0/2770
3	3	0.24	0/1611	0.40	0/2174
3	h	0.24	0/1611	0.41	0/2174
30	W	0.23	0/1557	0.40	0/2111
31	X	0.23	0/1058	0.40	0/1432
32	Y	0.24	0/239	0.43	0/322

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
33	Z	0.23	0/6404	0.39	0/8686
4	4	0.23	0/1613	0.40	0/2173
4	g	0.23	0/1613	0.39	0/2173
5	5	0.23	0/1681	0.40	0/2274
5	f	0.23	0/1681	0.40	0/2274
6	6	0.24	0/1795	0.40	0/2420
6	e	0.24	0/1795	0.40	0/2420
7	7	0.24	0/1855	0.41	0/2514
7	a	0.23	0/1855	0.41	0/2514
8	A	0.23	0/1959	0.39	0/2652
8	c	0.24	0/1959	0.39	0/2652
9	B	0.24	0/1952	0.40	0/2642
9	j	0.24	0/1952	0.40	0/2642
All	All	0.24	4/108128 (0.0%)	0.39	0/146037

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	274	GLU	C-N	12.44	1.57	1.34
18	K	265	ALA	C-N	11.26	1.55	1.34
21	N	743	PHE	C-N	6.50	1.46	1.34
22	O	55	THR	C-N	5.11	1.44	1.34

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	1	1576	0	1552	27	0
1	b	1576	0	1552	0	0
2	2	1684	0	1685	21	0
2	i	1684	0	1685	0	0
3	3	1581	0	1571	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	h	1581	0	1571	0	0
4	4	1585	0	1590	26	0
4	g	1585	0	1590	0	0
5	5	1644	0	1592	26	0
5	f	1644	0	1592	0	0
6	6	1757	0	1708	23	0
6	e	1757	0	1708	0	0
7	7	1824	0	1829	28	0
7	a	1824	0	1829	0	0
8	A	1921	0	1910	33	0
8	c	1921	0	1910	0	0
9	B	1915	0	1929	32	0
9	j	1915	0	1929	0	0
10	C	1904	0	1901	32	0
10	d	1904	0	1901	0	0
11	D	1890	0	1900	29	0
11	n	1890	0	1900	0	0
12	E	1861	0	1836	35	0
12	m	1861	0	1836	0	0
13	F	1795	0	1797	37	0
13	l	1795	0	1797	0	0
14	G	1888	0	1880	33	0
14	k	1896	0	1886	0	0
15	H	2787	0	2851	57	0
16	I	2831	0	2881	50	0
17	J	2928	0	3057	52	0
18	K	3019	0	3084	51	0
19	L	2937	0	3011	55	0
20	M	2866	0	2938	53	0
21	N	6562	0	6625	72	0
22	O	3182	0	3207	36	0
23	P	3545	0	3629	45	0
24	Q	3471	0	3495	20	0
25	R	3218	0	3216	44	0
26	S	3894	0	3938	33	0
27	T	2235	0	2207	19	0
28	U	2061	0	2116	31	0
29	V	2025	0	2035	44	0
30	W	1534	0	1542	28	0
31	X	1032	0	1015	12	0
32	Y	236	0	203	5	0
33	Z	6290	0	6236	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	106311	0	106652	1029	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 6.

The worst 5 of 1029 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)
22:O:147:ARG:HD3	23:P:288:ASN:HD21	1.47	0.78
29:V:24:LYS:H	29:V:174:THR:HG22	1.50	0.77
19:L:165:PRO:HD2	20:M:83:VAL:HB	1.67	0.75
9:B:78:MET:HG2	9:B:80:PRO:HD2	1.69	0.73
30:W:12:ASN:ND2	30:W:53:SER:OG	2.23	0.72

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 PDB entries followed by that with respect to all EM entries.

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	1	203/215 (94%)	191 (94%)	12 (6%)	0	100	100
1	b	203/215 (94%)	193 (95%)	10 (5%)	0	100	100
2	2	220/261 (84%)	213 (97%)	7 (3%)	0	100	100
2	i	220/261 (84%)	214 (97%)	6 (3%)	0	100	100
3	3	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
3	h	202/205 (98%)	192 (95%)	9 (4%)	1 (0%)	31	71
4	4	196/198 (99%)	190 (97%)	6 (3%)	0	100	100
4	g	196/198 (99%)	188 (96%)	8 (4%)	0	100	100
5	5	210/287 (73%)	204 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	f	210/287 (73%)	203 (97%)	7 (3%)	0	100	100
6	6	220/241 (91%)	212 (96%)	8 (4%)	0	100	100
6	e	220/241 (91%)	211 (96%)	9 (4%)	0	100	100
7	7	231/266 (87%)	220 (95%)	11 (5%)	0	100	100
7	a	231/266 (87%)	221 (96%)	10 (4%)	0	100	100
8	A	241/252 (96%)	234 (97%)	7 (3%)	0	100	100
8	c	241/252 (96%)	234 (97%)	7 (3%)	0	100	100
9	B	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
9	j	248/250 (99%)	238 (96%)	10 (4%)	0	100	100
10	C	242/258 (94%)	232 (96%)	10 (4%)	0	100	100
10	d	242/258 (94%)	233 (96%)	9 (4%)	0	100	100
11	D	239/254 (94%)	229 (96%)	10 (4%)	0	100	100
11	n	239/254 (94%)	230 (96%)	9 (4%)	0	100	100
12	E	240/260 (92%)	227 (95%)	13 (5%)	0	100	100
12	m	240/260 (92%)	234 (98%)	6 (2%)	0	100	100
13	F	231/234 (99%)	222 (96%)	9 (4%)	0	100	100
13	l	231/234 (99%)	222 (96%)	9 (4%)	0	100	100
14	G	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
14	k	242/288 (84%)	235 (97%)	7 (3%)	0	100	100
15	H	351/467 (75%)	319 (91%)	32 (9%)	0	100	100
16	I	361/437 (83%)	331 (92%)	29 (8%)	1 (0%)	43	79
17	J	371/405 (92%)	338 (91%)	32 (9%)	1 (0%)	43	79
18	K	379/428 (89%)	340 (90%)	37 (10%)	2 (0%)	31	71
19	L	369/437 (84%)	336 (91%)	33 (9%)	0	100	100
20	M	363/434 (84%)	326 (90%)	36 (10%)	1 (0%)	43	79
21	N	843/945 (89%)	814 (97%)	29 (3%)	0	100	100
22	O	385/393 (98%)	352 (91%)	33 (9%)	0	100	100
23	P	430/445 (97%)	398 (93%)	32 (7%)	0	100	100
24	Q	429/434 (99%)	407 (95%)	22 (5%)	0	100	100
25	R	398/429 (93%)	360 (90%)	37 (9%)	1 (0%)	43	79
26	S	473/523 (90%)	453 (96%)	19 (4%)	1 (0%)	49	83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	T	270/274 (98%)	246 (91%)	24 (9%)	0	100	100
28	U	245/338 (72%)	241 (98%)	4 (2%)	0	100	100
29	V	252/306 (82%)	227 (90%)	23 (9%)	2 (1%)	21	62
30	W	195/268 (73%)	181 (93%)	14 (7%)	0	100	100
31	X	125/156 (80%)	113 (90%)	12 (10%)	0	100	100
32	Y	25/89 (28%)	19 (76%)	5 (20%)	1 (4%)	3	32
33	Z	807/993 (81%)	757 (94%)	49 (6%)	1 (0%)	53	87
All	All	13400/15139 (88%)	12648 (94%)	740 (6%)	12 (0%)	56	87

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	I	287	ILE
18	K	158	ILE
18	K	292	VAL
25	R	241	ILE
3	h	105	VAL

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 PDB entries followed by that with respect to all EM entries.

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	1	169/178 (95%)	169 (100%)	0	100	100
1	b	169/178 (95%)	169 (100%)	0	100	100
2	2	181/214 (85%)	181 (100%)	0	100	100
2	i	181/214 (85%)	181 (100%)	0	100	100
3	3	172/173 (99%)	172 (100%)	0	100	100
3	h	172/173 (99%)	172 (100%)	0	100	100
4	4	175/175 (100%)	175 (100%)	0	100	100
4	g	175/175 (100%)	175 (100%)	0	100	100
5	5	169/235 (72%)	169 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	f	169/235 (72%)	169 (100%)	0	100	100
6	6	185/201 (92%)	185 (100%)	0	100	100
6	e	185/201 (92%)	185 (100%)	0	100	100
7	7	199/224 (89%)	199 (100%)	0	100	100
7	a	199/224 (89%)	199 (100%)	0	100	100
8	A	207/210 (99%)	207 (100%)	0	100	100
8	c	207/210 (99%)	207 (100%)	0	100	100
9	B	209/209 (100%)	209 (100%)	0	100	100
9	j	209/209 (100%)	209 (100%)	0	100	100
10	C	203/216 (94%)	203 (100%)	0	100	100
10	d	203/216 (94%)	203 (100%)	0	100	100
11	D	213/226 (94%)	213 (100%)	0	100	100
11	n	213/226 (94%)	213 (100%)	0	100	100
12	E	198/215 (92%)	198 (100%)	0	100	100
12	m	198/215 (92%)	198 (100%)	0	100	100
13	F	192/193 (100%)	192 (100%)	0	100	100
13	l	192/193 (100%)	192 (100%)	0	100	100
14	G	200/239 (84%)	200 (100%)	0	100	100
14	k	201/239 (84%)	201 (100%)	0	100	100
15	H	303/399 (76%)	303 (100%)	0	100	100
16	I	320/385 (83%)	320 (100%)	0	100	100
17	J	325/352 (92%)	325 (100%)	0	100	100
18	K	334/374 (89%)	334 (100%)	0	100	100
19	L	317/377 (84%)	317 (100%)	0	100	100
20	M	315/375 (84%)	315 (100%)	0	100	100
21	N	713/797 (90%)	713 (100%)	0	100	100
22	O	363/368 (99%)	363 (100%)	0	100	100
23	P	405/415 (98%)	405 (100%)	0	100	100
24	Q	388/391 (99%)	388 (100%)	0	100	100
25	R	351/379 (93%)	351 (100%)	0	100	100
26	S	447/489 (91%)	447 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	T	254/256 (99%)	254 (100%)	0	100	100
28	U	234/308 (76%)	234 (100%)	0	100	100
29	V	227/268 (85%)	227 (100%)	0	100	100
30	W	171/230 (74%)	171 (100%)	0	100	100
31	X	116/144 (81%)	116 (100%)	0	100	100
32	Y	26/81 (32%)	26 (100%)	0	100	100
33	Z	692/850 (81%)	692 (100%)	0	100	100
All	All	11646/13054 (89%)	11646 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
17	J	52	ASN
21	N	34	GLN
28	U	127	GLN
17	J	205	HIS
18	K	182	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 carbohydrates 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.