



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Oct 29, 2019 – 01:34 PM EDT

PDB ID : 6J2N
EMDB ID: : EMD-9770
Title : yeast proteasome in substrate-processing state (C3-b)
Authors : Cong, Y.
Deposited on : 2019-01-02
Resolution : 7.50 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) : 2.4

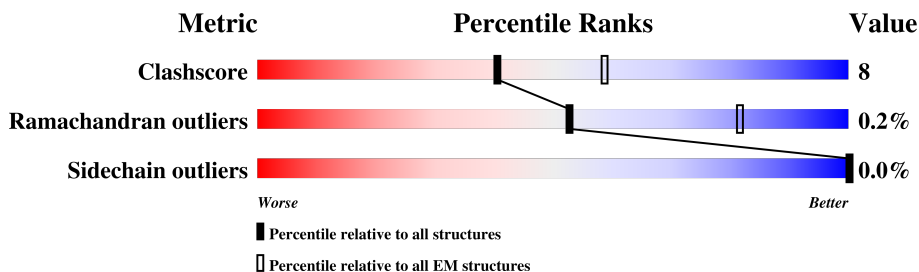
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY










The reported resolution of this entry is 7.50 Å.

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









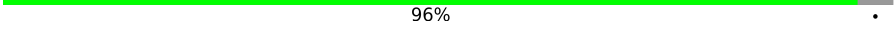

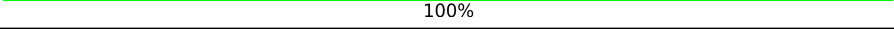

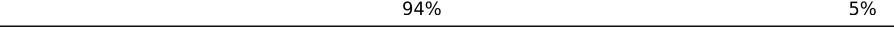
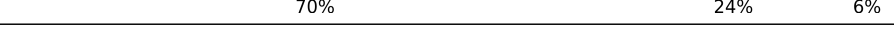
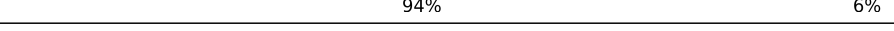

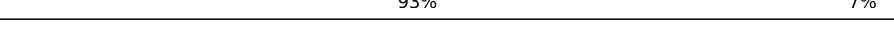

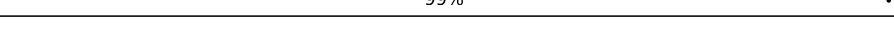


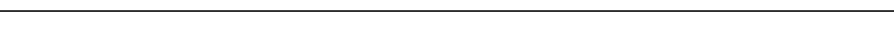

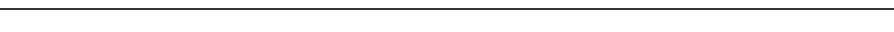
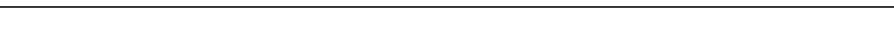


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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	
1	b	215	
2	2	261	
2	i	261	
3	3	205	
3	h	205	
4	4	198	
4	g	198	
5	5	287	










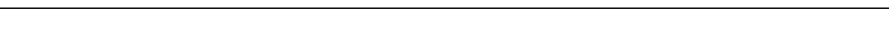
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Mol	Chain	Length	Quality of chain
5	f	287	 74%26%
6	6	241	 78%15%8%
6	e	241	 92%8%
7	7	266	 67%20%14%
7	a	266	 87%13%
8	A	252	 73%23%.
8	c	252	 96%.
9	B	250	 72%28%
9	j	250	 100%
10	C	258	 73%21%5%
10	d	258	 94%5%
11	D	254	 70%24%6%
11	n	254	 94%6%
12	E	260	 74%19%7%
12	m	260	 93%7%
13	F	234	 74%26%
13	l	234	 99%.
14	G	288	 66%18%16%
14	k	288	 84%16%
15	H	467	 57%20%23%
16	I	437	 61%22%17%
17	J	405	 70%22%8%
18	K	428	 64%25%11%
19	L	437	 64%19%17%
20	M	434	 62%22%15%

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Mol	Chain	Length	Quality of chain
21	N	945	 73%16%10%
22	O	393	 82%16%.
23	P	445	 83%14%.
24	Q	434	 81%18%.
25	R	429	 74%19%7%
26	S	523	 76%15%9%
27	T	274	 81%18%.
28	U	338	 59%17%25%
29	V	306	 68%25%7%
30	W	268	 59%13%.26%
31	X	156	 61%10%29%
32	Y	89	 24%6%.70%
33	Z	993	 69%13%18%

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 106100 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	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		
1	b	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	226	Total	C	N	O	S	0	0
			1719	1082	298	332	7		
2	i	226	Total	C	N	O	S	0	0
			1719	1082	298	332	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	195	Total	C	N	O	S	0	0
			1561	992	264	299	6		
4	g	195	Total	C	N	O	S	0	0
			1561	992	264	299	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	229	Total	C	N	O	S	0	0
			1790	1133	306	344	7		
7	a	232	Total	C	N	O	S	0	0
			1815	1148	311	349	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	241	Total	C	N	O	S	0	0
			1907	1214	320	365	8		
8	c	241	Total	C	N	O	S	0	0
			1907	1214	320	365	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	240	Total	C	N	O	S	0	0
			1881	1176	329	372	4		
11	n	240	Total	C	N	O	S	0	0
			1881	1176	329	372	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	231	Total	C	N	O	S	0	0
			1773	1114	307	348	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
			1892	1203	329	356	4		
14	k	243	Total	C	N	O	S	0	0
			1892	1203	329	356	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	359	Total	C	N	O	S	0	0
			2792	1755	499	523	15		

- 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	361	Total	C	N	O	S	0	0
			2853	1798	507	536	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	284	Total	C	N	O	S	0	0
			2236	1405	381	436	14		

- 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	111	Total	C	N	O	S	0	0
			906	586	148	169	3		

- 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.

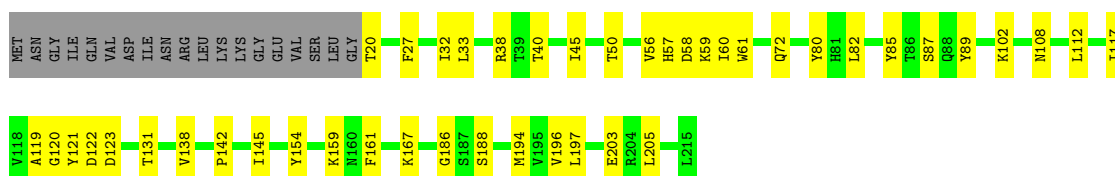
Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	813	Total	C	N	O	S	0	0
			6290	3995	1029	1237	29		

3 Residue-property plots [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. 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.

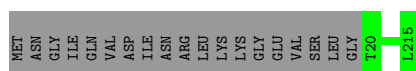
- Molecule 1: Proteasome subunit beta type-1

Chain 1: 



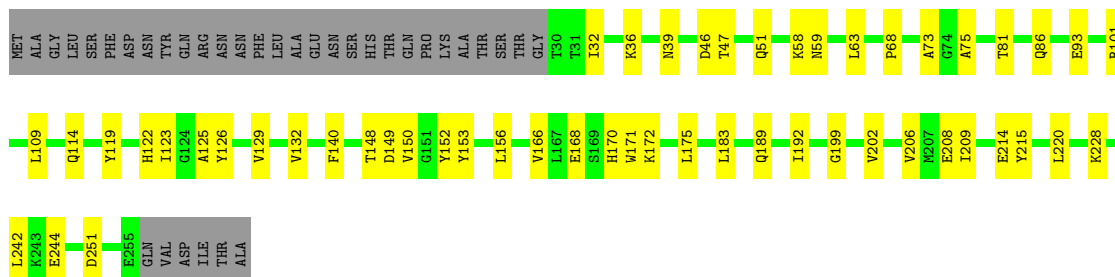
- Molecule 1: Proteasome subunit beta type-1

Chain b: 




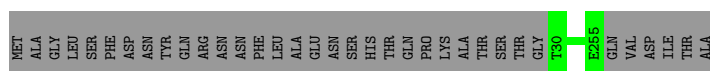
- Molecule 2: Proteasome subunit beta type-2

Chain 2: 



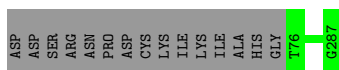
- Molecule 2: Proteasome subunit beta type-2

Chain i: 

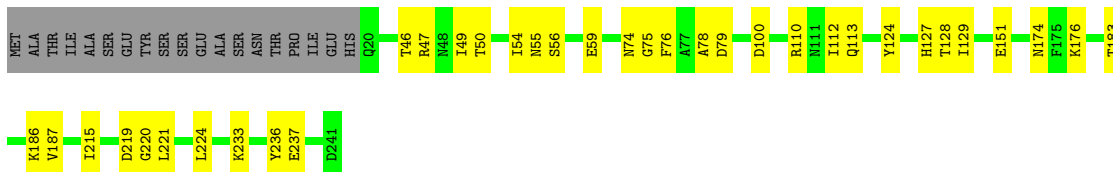
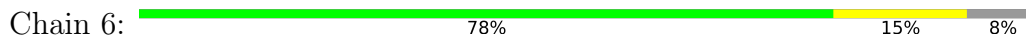


- Molecule 3: Proteasome subunit beta type-3

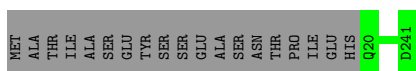
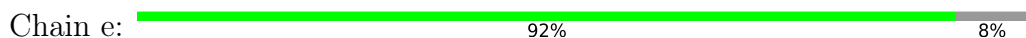
Chain 3: 



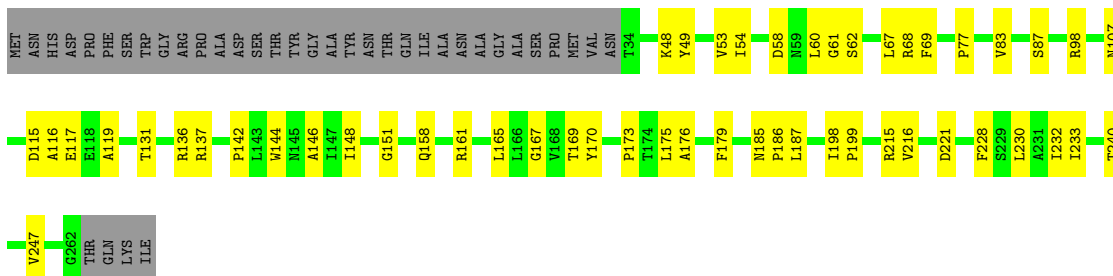
- Molecule 6: Proteasome subunit beta type-6



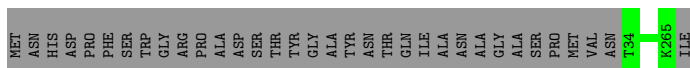
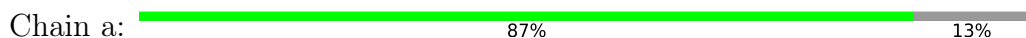
- Molecule 6: Proteasome subunit beta type-6



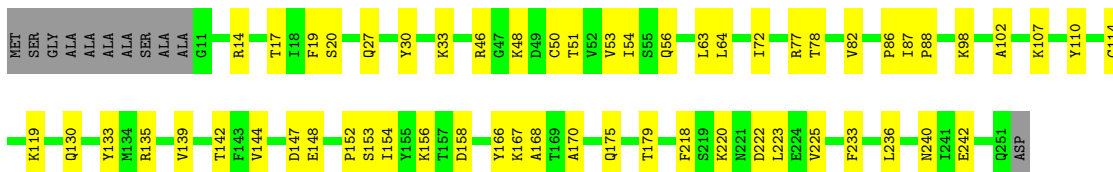
- Molecule 7: Proteasome subunit beta type-7



- Molecule 7: Proteasome subunit beta type-7

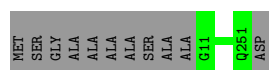


- Molecule 8: Proteasome subunit alpha type-1



- Molecule 8: Proteasome subunit alpha type-1

Chain c:  96%



- Molecule 9: Proteasome subunit alpha type-2

Chain B:  72% 28%



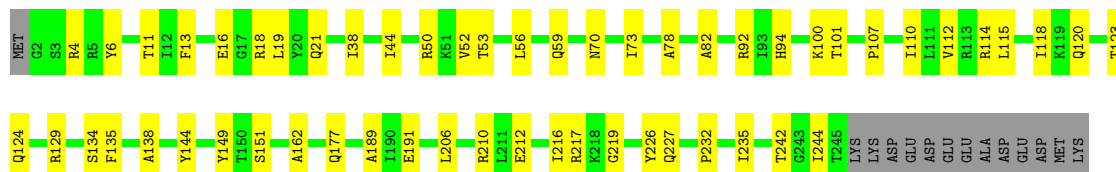
- Molecule 9: Proteasome subunit alpha type-2

Chain j:  100%

There are no outlier residues recorded for this chain.

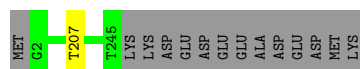
- Molecule 10: Proteasome subunit alpha type-3

Chain C:  73% 21% 5%



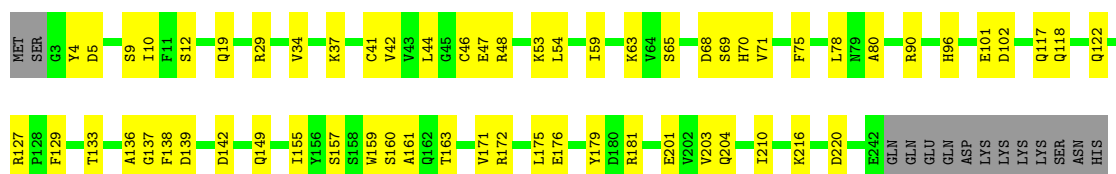
- Molecule 10: Proteasome subunit alpha type-3

Chain d:  94% 5%



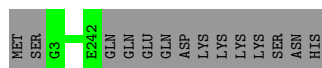
- Molecule 11: Proteasome subunit alpha type-4

Chain D:  70% 24% 6%



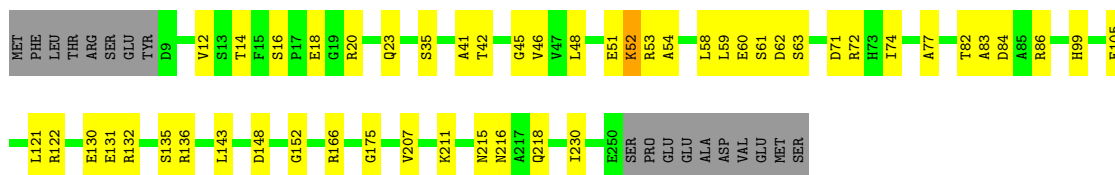
- Molecule 11: Proteasome subunit alpha type-4

Chain n:  94% 6%



- Molecule 12: Proteasome subunit alpha type-5

Chain E:  74% 19% 7%



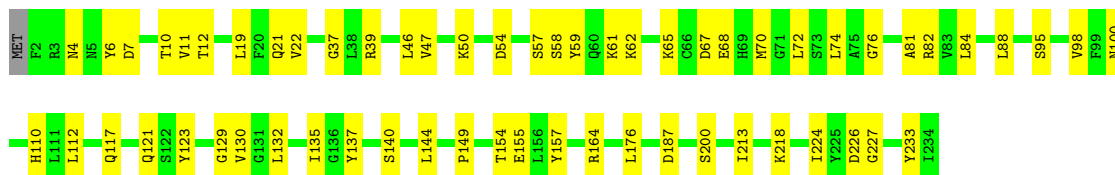
- Molecule 12: Proteasome subunit alpha type-5

Chain m:  93% 7%



- Molecule 13: Proteasome subunit alpha type-6

Chain F:  74% 26%



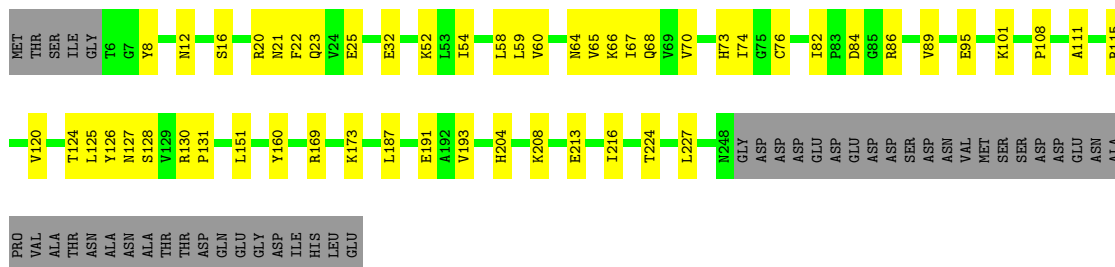
- Molecule 13: Proteasome subunit alpha type-6

Chain l:  99% .



- Molecule 14: Probable proteasome subunit alpha type-7

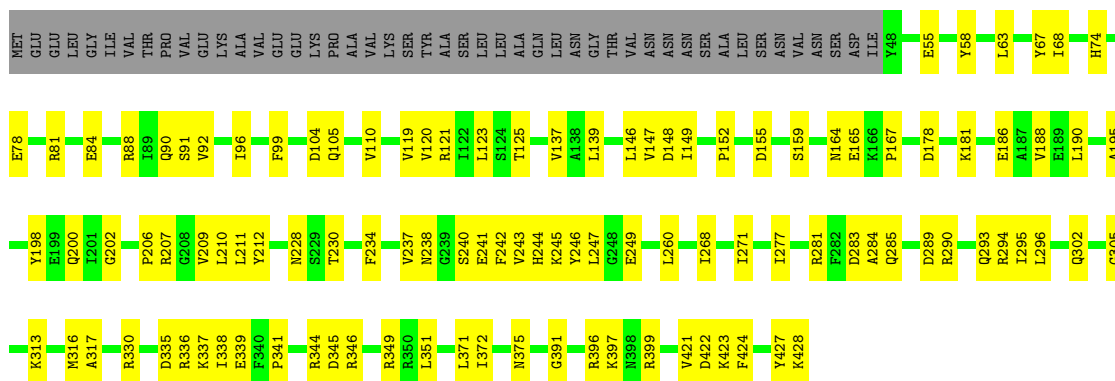
Chain G:  66% 18% 16%



- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|
| Met | Thr | Ala | Val | Thr | Ser | Ser | Asn | Ile | Leu | Glu | Thr | His | Glu | Ser | Ser | Gly | Ile | Lys | Pro | Trp | Phe | E24 | I34 | R35 | T38 | R42 | R43 | L44 | E61 | S70 | V79 | S90 | D81 | L85 | K93 | V96 | D97 | Q111 | R116 | S117 | D118 | M121 | N128 | V134 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|

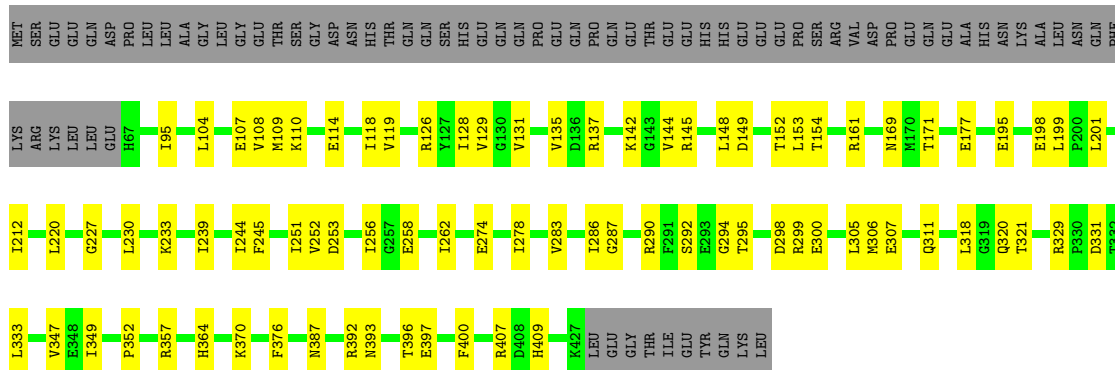
- Molecule 18: 26S protease regulatory subunit 6B homolog

Chain K:



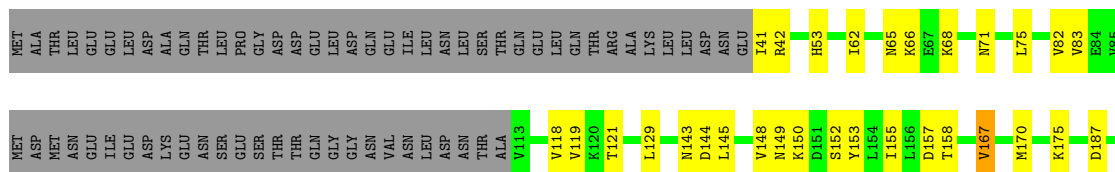
- Molecule 19: 26S protease subunit RPT4

Chain L:



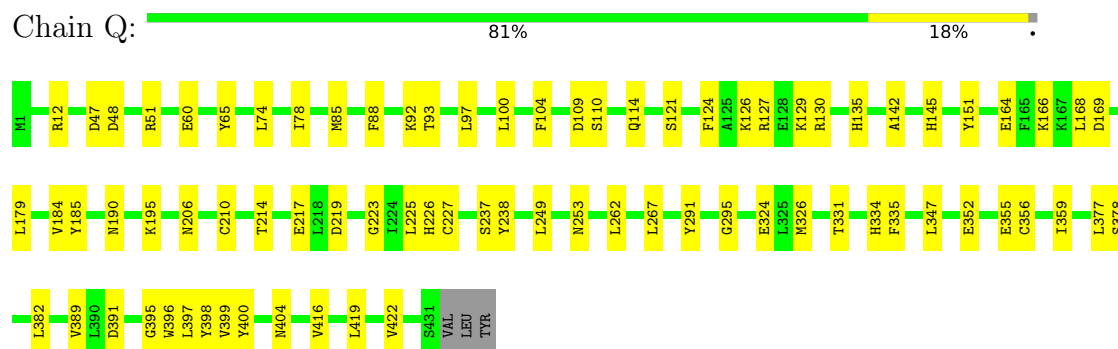
- Molecule 20: 26S protease regulatory subunit 6A

Chain M:

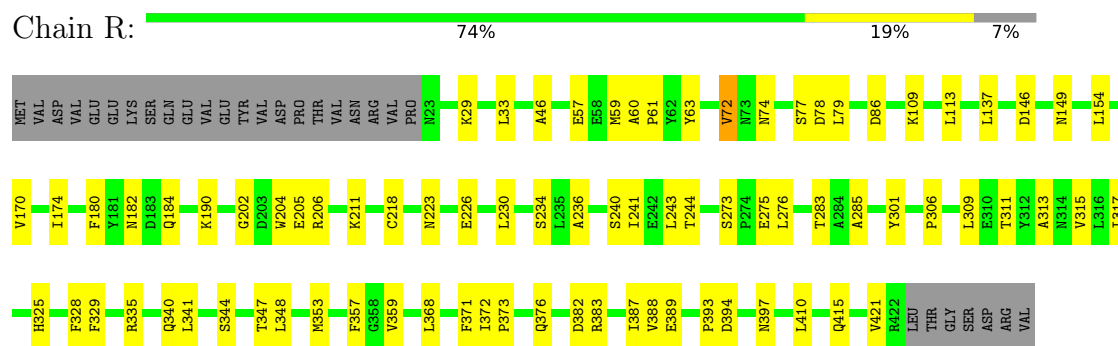




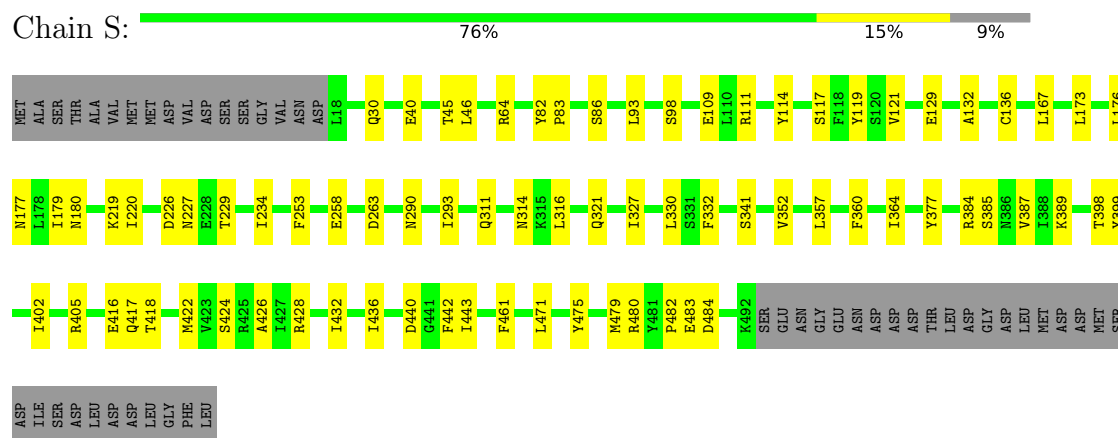
- Molecule 24: 26S proteasome regulatory subunit RPN6



- Molecule 25: 26S proteasome regulatory subunit RPN7

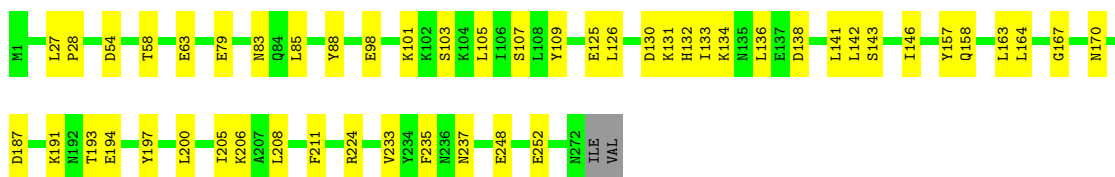


- Molecule 26: 26S proteasome regulatory subunit RPN3



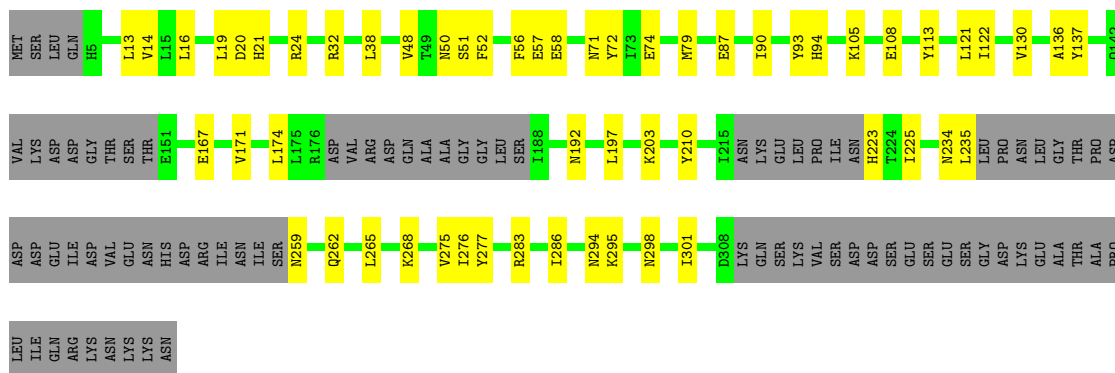
- Molecule 27: 26S proteasome regulatory subunit RPN12





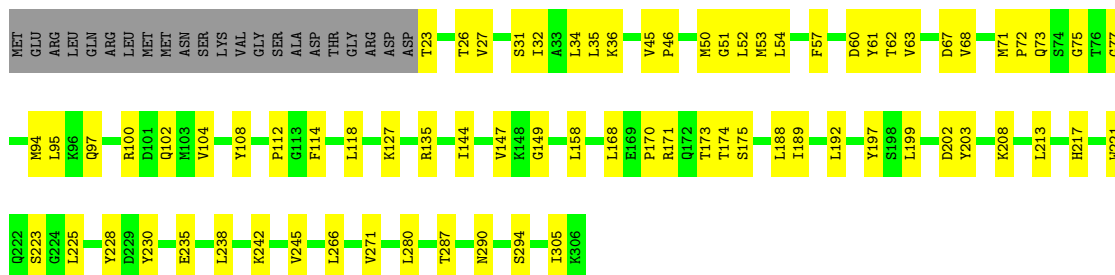
- Molecule 28: 26S proteasome regulatory subunit RPN8

Chain U:  59% 17% 25%



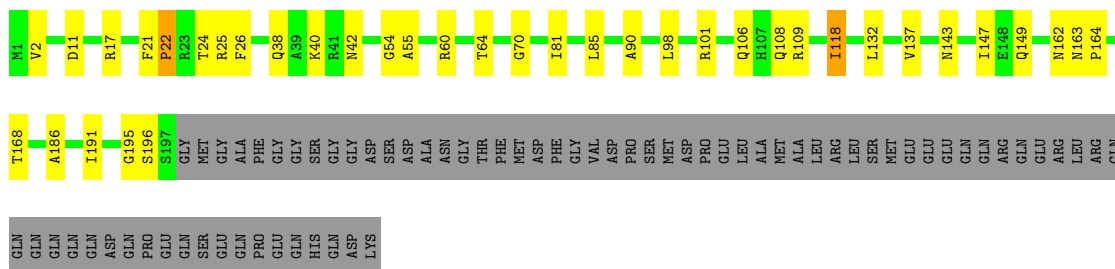
- Molecule 29: Ubiquitin carboxyl-terminal hydrolase RPN11

Chain V:  68% 25% 7%



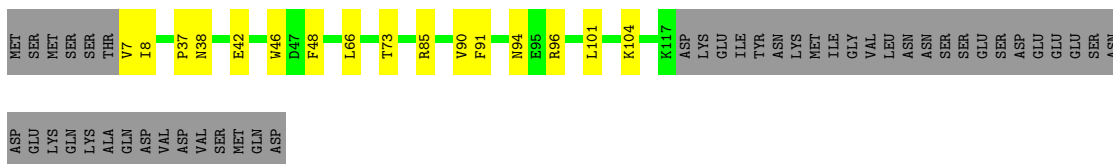
- Molecule 30: 26S proteasome regulatory subunit RPN10

Chain W: 59% 13% . 26%

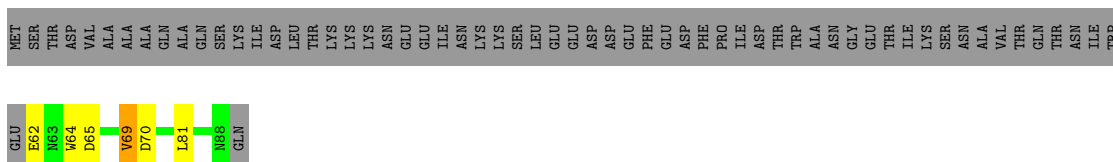


- Molecule 31: 26S proteasome regulatory subunit RPN13

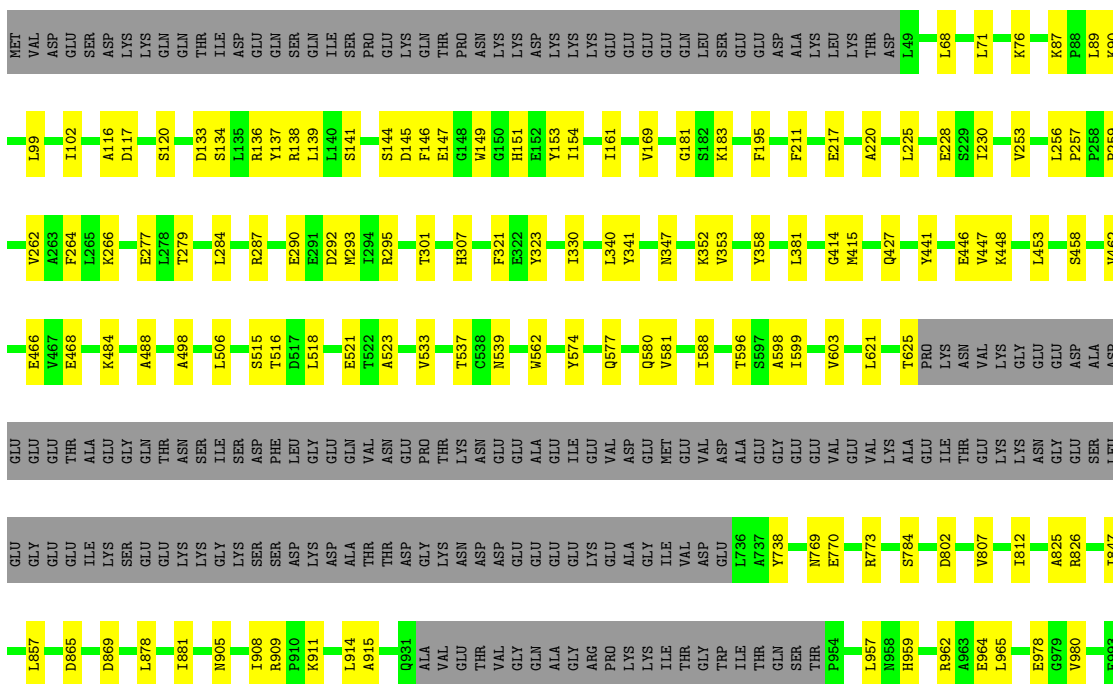
Chain X:  61% 10% 29%



- Molecule 32: 26S proteasome complex subunit SEM1



- Molecule 33: 26S proteasome regulatory subunit RPN1



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	6171	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	0/1541	0.41	0/2087
1	b	0.23	0/1541	0.41	0/2087
10	C	0.23	0/1934	0.39	0/2618
10	d	0.23	0/1934	0.41	0/2618
11	D	0.23	0/1910	0.39	0/2586
11	n	0.23	0/1910	0.40	0/2586
12	E	0.23	0/1886	0.41	0/2541
12	m	0.25	0/1886	0.40	0/2541
13	F	0.23	0/1823	0.41	0/2463
13	l	0.23	0/1800	0.41	0/2433
14	G	0.24	0/1932	0.38	0/2609
14	k	0.24	0/1932	0.39	0/2609
15	H	0.27	1/2831 (0.0%)	0.40	0/3808
16	I	0.25	0/2869	0.42	0/3867
17	J	0.23	0/2964	0.39	0/3981
18	K	0.23	0/3062	0.40	0/4132
19	L	0.24	0/2896	0.39	0/3895
2	2	0.23	0/1750	0.40	0/2373
2	i	0.23	0/1750	0.41	0/2373
20	M	0.23	0/2903	0.40	0/3909
21	N	0.24	1/6670 (0.0%)	0.39	0/9023
22	O	0.23	0/3243	0.39	0/4374
23	P	0.22	0/3599	0.37	0/4854
24	Q	0.23	0/3527	0.38	0/4748
25	R	0.23	0/3272	0.38	0/4412
26	S	0.23	0/3966	0.37	0/5355
27	T	0.24	0/2279	0.40	0/3077
28	U	0.23	0/2087	0.37	0/2811
29	V	0.23	0/2271	0.43	0/3064
3	3	0.24	0/1611	0.40	0/2174
3	h	0.24	0/1611	0.40	0/2174
30	W	0.26	0/1557	0.43	0/2111
31	X	0.23	0/931	0.41	0/1262
32	Y	0.23	0/239	0.39	0/322

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
33	Z	0.26	1/6404 (0.0%)	0.40	0/8686
4	4	0.23	0/1589	0.39	0/2142
4	g	0.23	0/1589	0.39	0/2142
5	5	0.23	0/1681	0.39	0/2274
5	f	0.23	0/1681	0.39	0/2274
6	6	0.24	0/1795	0.39	0/2420
6	e	0.24	0/1795	0.40	0/2420
7	7	0.24	0/1821	0.41	0/2470
7	a	0.24	0/1846	0.42	0/2503
8	A	0.24	0/1945	0.39	0/2634
8	c	0.24	0/1945	0.38	0/2634
9	B	0.24	0/1952	0.40	0/2642
9	j	0.24	0/1952	0.39	0/2642
All	All	0.24	3/107912 (0.0%)	0.40	0/145760

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	Z	468	GLU	C-N	8.44	1.50	1.34
15	H	192	ASP	C-N	6.36	1.46	1.34
21	N	217	MET	C-N	6.12	1.45	1.34

There are no bond angle outliers.

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	1	1512	0	1478	33	0
1	b	1512	0	1478	0	0
2	2	1719	0	1716	39	0
2	i	1719	0	1716	0	0
3	3	1581	0	1571	41	0
3	h	1581	0	1571	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	4	1561	0	1569	28	0
4	g	1561	0	1569	0	0
5	5	1644	0	1592	28	0
5	f	1644	0	1592	0	0
6	6	1757	0	1708	25	0
6	e	1757	0	1708	0	0
7	7	1790	0	1790	33	0
7	a	1815	0	1818	0	0
8	A	1907	0	1901	43	0
8	c	1907	0	1901	0	0
9	B	1915	0	1929	52	0
9	j	1915	0	1929	0	0
10	C	1904	0	1901	46	0
10	d	1904	0	1901	0	0
11	D	1881	0	1892	54	0
11	n	1881	0	1892	0	0
12	E	1861	0	1836	43	0
12	m	1861	0	1836	0	0
13	F	1795	0	1797	45	0
13	l	1773	0	1775	0	0
14	G	1892	0	1883	44	0
14	k	1892	0	1883	0	0
15	H	2792	0	2879	66	0
16	I	2831	0	2881	70	0
17	J	2928	0	3057	63	0
18	K	3019	0	3084	84	0
19	L	2853	0	2926	58	0
20	M	2866	0	2938	73	0
21	N	6562	0	6625	101	0
22	O	3182	0	3207	42	0
23	P	3545	0	3629	36	0
24	Q	3471	0	3495	48	0
25	R	3218	0	3216	53	0
26	S	3894	0	3938	56	0
27	T	2235	0	2207	35	0
28	U	2061	0	2116	54	0
29	V	2236	0	2242	64	0
30	W	1534	0	1542	28	0
31	X	906	0	888	10	0
32	Y	236	0	203	9	0
33	Z	6290	0	6236	81	0
All	All	106100	0	106441	1348	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 1348 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)
28:U:210:TYR:HH	28:U:223:HIS:N	1.59	0.99
21:N:510:HIS:HB3	21:N:513:ILE:HB	1.48	0.93
27:T:103:SER:HB2	27:T:142:LEU:HD23	1.53	0.89
21:N:742:TRP:HD1	29:V:61:TYR:HH	1.27	0.82
27:T:107:SER:HB3	27:T:142:LEU:HD13	1.62	0.81

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	194/215 (90%)	187 (96%)	7 (4%)	0	100	100
1	b	194/215 (90%)	187 (96%)	7 (4%)	0	100	100
2	2	224/261 (86%)	215 (96%)	9 (4%)	0	100	100
2	i	224/261 (86%)	217 (97%)	7 (3%)	0	100	100
3	3	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
3	h	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
4	4	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
4	g	193/198 (98%)	186 (96%)	7 (4%)	0	100	100
5	5	210/287 (73%)	205 (98%)	5 (2%)	0	100	100
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	7	227/266 (85%)	218 (96%)	9 (4%)	0	100	100
7	a	230/266 (86%)	221 (96%)	9 (4%)	0	100	100
8	A	239/252 (95%)	229 (96%)	10 (4%)	0	100	100
8	c	239/252 (95%)	234 (98%)	5 (2%)	0	100	100
9	B	248/250 (99%)	239 (96%)	9 (4%)	0	100	100
9	j	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
10	C	242/258 (94%)	235 (97%)	7 (3%)	0	100	100
10	d	242/258 (94%)	231 (96%)	10 (4%)	1 (0%)	36	77
11	D	238/254 (94%)	226 (95%)	12 (5%)	0	100	100
11	n	238/254 (94%)	228 (96%)	10 (4%)	0	100	100
12	E	240/260 (92%)	226 (94%)	13 (5%)	1 (0%)	36	77
12	m	240/260 (92%)	230 (96%)	9 (4%)	1 (0%)	36	77
13	F	231/234 (99%)	218 (94%)	13 (6%)	0	100	100
13	l	229/234 (98%)	225 (98%)	4 (2%)	0	100	100
14	G	241/288 (84%)	233 (97%)	8 (3%)	0	100	100
14	k	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
15	H	353/467 (76%)	316 (90%)	37 (10%)	0	100	100
16	I	361/437 (83%)	333 (92%)	28 (8%)	0	100	100
17	J	371/405 (92%)	351 (95%)	20 (5%)	0	100	100
18	K	379/428 (89%)	347 (92%)	32 (8%)	0	100	100
19	L	359/437 (82%)	334 (93%)	25 (7%)	0	100	100
20	M	363/434 (84%)	332 (92%)	29 (8%)	2 (1%)	27	70
21	N	843/945 (89%)	793 (94%)	46 (6%)	4 (0%)	31	74
22	O	385/393 (98%)	342 (89%)	42 (11%)	1 (0%)	43	81
23	P	430/445 (97%)	391 (91%)	39 (9%)	0	100	100
24	Q	429/434 (99%)	397 (92%)	32 (8%)	0	100	100
25	R	398/429 (93%)	357 (90%)	38 (10%)	3 (1%)	21	65
26	S	473/523 (90%)	451 (95%)	21 (4%)	1 (0%)	49	85
27	T	270/274 (98%)	238 (88%)	32 (12%)	0	100	100
28	U	245/338 (72%)	242 (99%)	2 (1%)	1 (0%)	36	77
29	V	282/306 (92%)	242 (86%)	37 (13%)	3 (1%)	16	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	W	195/268 (73%)	176 (90%)	16 (8%)	3 (2%)	11	51
31	X	109/156 (70%)	96 (88%)	13 (12%)	0	100	100
32	Y	25/89 (28%)	18 (72%)	6 (24%)	1 (4%)	3	29
33	Z	807/993 (81%)	740 (92%)	67 (8%)	0	100	100
All	All	13376/15139 (88%)	12565 (94%)	789 (6%)	22 (0%)	53	85

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	N	180	SER
21	N	874	ILE
28	U	130	VAL
30	W	22	PRO
10	d	207	THR

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	162/178 (91%)	162 (100%)	0	100	100
1	b	162/178 (91%)	162 (100%)	0	100	100
2	2	185/214 (86%)	185 (100%)	0	100	100
2	i	185/214 (86%)	185 (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	173/175 (99%)	173 (100%)	0	100	100
4	g	173/175 (99%)	173 (100%)	0	100	100
5	5	169/235 (72%)	169 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	7	195/224 (87%)	195 (100%)	0	100	100
7	a	198/224 (88%)	198 (100%)	0	100	100
8	A	206/210 (98%)	206 (100%)	0	100	100
8	c	206/210 (98%)	206 (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	212/226 (94%)	212 (100%)	0	100	100
11	n	212/226 (94%)	212 (100%)	0	100	100
12	E	198/215 (92%)	197 (100%)	1 (0%)	90	95
12	m	198/215 (92%)	198 (100%)	0	100	100
13	F	192/193 (100%)	192 (100%)	0	100	100
13	l	190/193 (98%)	190 (100%)	0	100	100
14	G	201/239 (84%)	201 (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	308/377 (82%)	308 (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
27	T	254/256 (99%)	254 (100%)	0	100	100
28	U	234/308 (76%)	234 (100%)	0	100	100
29	V	249/268 (93%)	249 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	W	171/230 (74%)	171 (100%)	0	100	100
31	X	101/144 (70%)	101 (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	11624/13054 (89%)	11623 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	E	52	LYS

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

Mol	Chain	Res	Type
14	G	23	GLN
15	H	217	GLN
27	T	236	ASN
14	G	64	ASN
11	n	118	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.