



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 20, 2017 – 07:01 PM EDT

PDB ID : 4CR3
EMDB ID: : EMD-2595
Title : Deep classification of a large cryo-EM dataset defines the conformational landscape of the 26S proteasome
Authors : Unverdorben, P.; Beck, F.; Sledz, P.; Schweitzer, A.; Pfeifer, G.; Plitzko, J.M.; Baumeister, W.; Foerster, F.
Deposited on : unknown
Resolution : 9.30 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
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
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) : rb-20029824

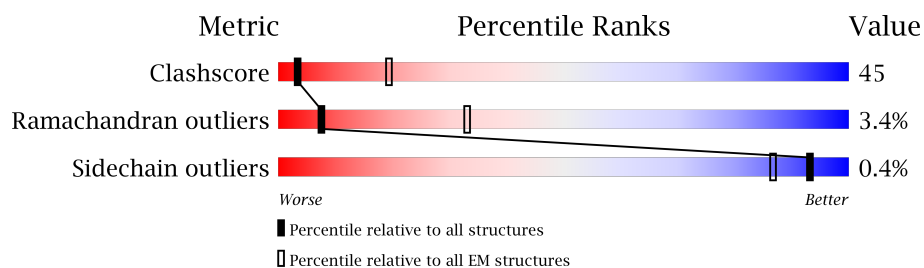
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.30 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.







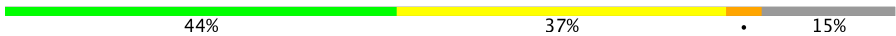
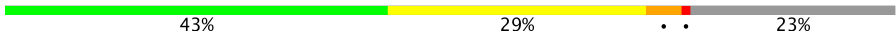
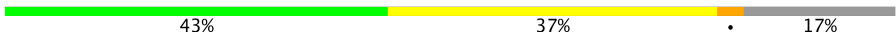

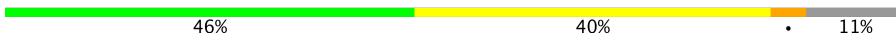
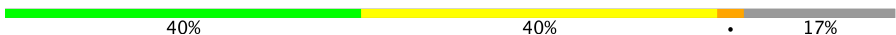






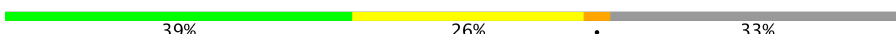

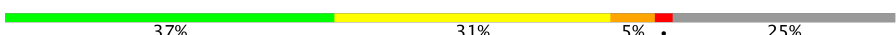

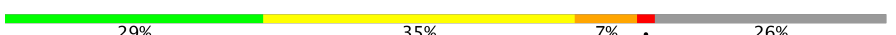



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	47% 44% 5%
2	2	261	55% 26% 5% 15%
3	3	205	65% 33% .
4	4	198	64% 35% .
5	5	287	40% 31% . 26%
6	6	241	56% 34% . 8%
7	7	266	48% 37% . 12%
8	A	252	45% 47% . .
9	B	250	57% 39% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	C	258	
11	D	254	
12	E	260	
13	F	234	
14	G	288	
15	H	467	
16	I	437	
17	J	405	
18	K	428	
19	L	437	
20	M	434	
21	N	945	
22	O	393	
23	P	445	
24	Q	434	
25	R	429	
26	S	523	
27	T	274	
28	U	338	
29	V	306	
30	W	268	
31	X	156	
32	Y	89	
33	Z	993	

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 80139 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 COMPONENT PRE3.

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

- Molecule 2 is a protein called PROTEASOME COMPONENT PUP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	223	Total	C	N	O	S	0	0
			1692	1067	294	324	7		

- Molecule 3 is a protein called PROTEASOME COMPONENT PUP3.

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

- Molecule 4 is a protein called PROTEASOME COMPONENT C11.

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

- Molecule 5 is a protein called PROTEASOME COMPONENT PRE2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	212	Total	C	N	O	S	0	0
			1646	1045	282	312	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	33	ARG	LYS	SEE REMARK 999	UNP P30656

- Molecule 6 is a protein called PROTEASOME COMPONENT C5.

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

- Molecule 7 is a protein called PROTEASOME COMPONENT PRE4.

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

- Molecule 8 is a protein called PROTEASOME COMPONENT C7-ALPHA.

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

- Molecule 9 is a protein called PROTEASOME COMPONENT Y7.

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

- Molecule 10 is a protein called PROTEASOME COMPONENT Y13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	245	Total	C	N	O	S	0	0
			1913	1207	323	380	3		

- Molecule 11 is a protein called PROTEASOME COMPONENT PRE6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	242	Total	C	N	O	S	0	0
			1899	1186	333	376	4		

- Molecule 12 is a protein called PROTEASOME COMPONENT PUP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	243	Total	C	N	O	S	0	0
			1867	1165	315	380	7		

- Molecule 13 is a protein called PROTEASOME COMPONENT PRE5.

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

- Molecule 14 is a protein called PROTEASOME COMPONENT C1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	245	Total	C	N	O	S	0	0
			1900	1207	331	358	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	362	Total	C	N	O	S	0	0
			2822	1773	471	563	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	415	Total	C	N	O	S	0	0
			3401	2166	571	655	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	353	Total	C	N	O	S	0	0
			2893	1857	482	541	13		

- 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 26S PROTEASOME REGULATORY SUBUNIT RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	247	Total	C	N	O	S	0	0
			1942	1225	328	376	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	19	Total	C	N	O	0	0
			168	101	30	37		

- 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
			6289	3995	1029	1236	29		

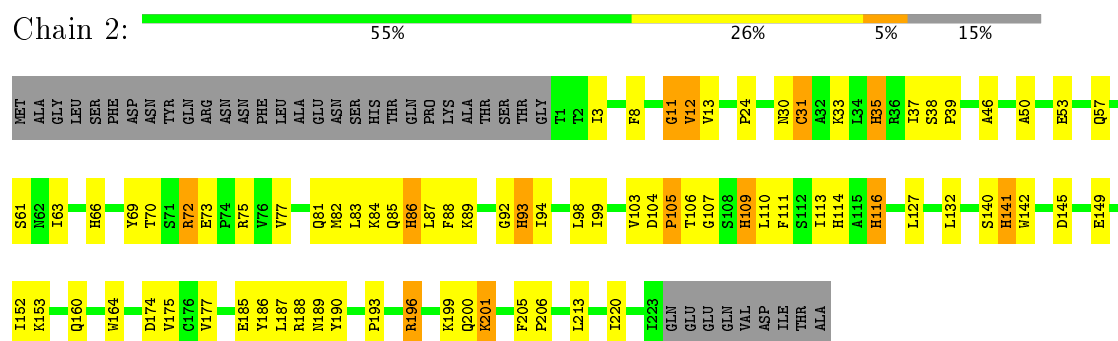
3 Residue-property plots

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.

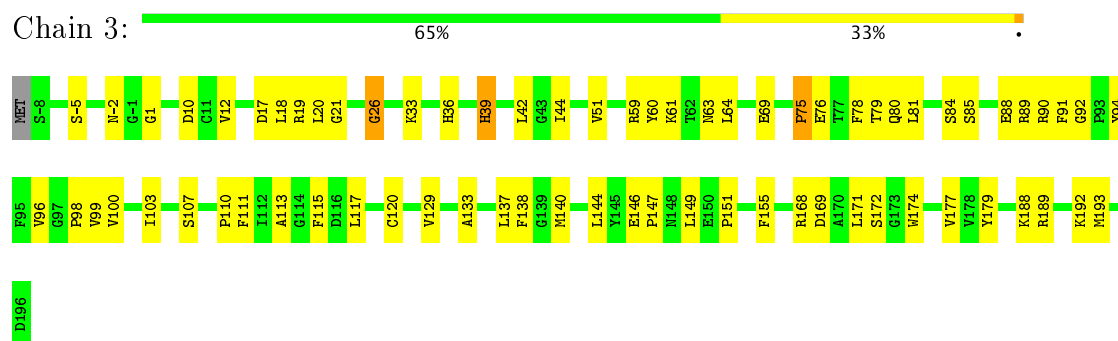
- Molecule 1: PROTEASOME COMPONENT PRE3



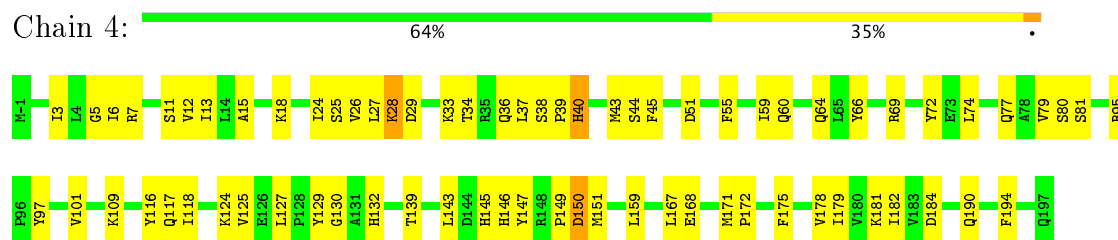
- Molecule 2: PROTEASOME COMPONENT PUP1



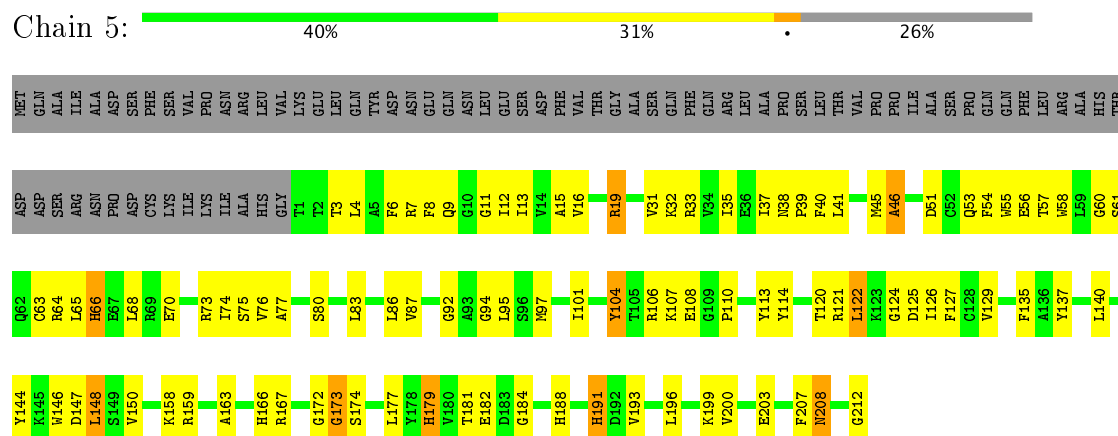
- Molecule 3: PROTEASOME COMPONENT PUP3



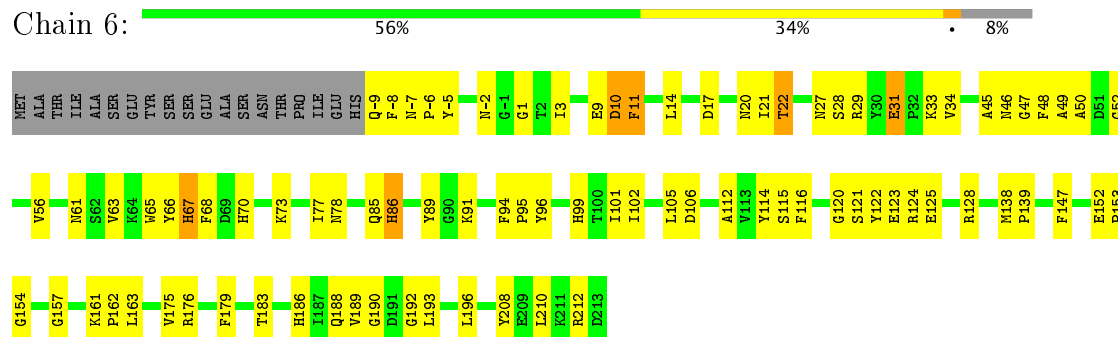
- Molecule 4: PROTEASOME COMPONENT C11



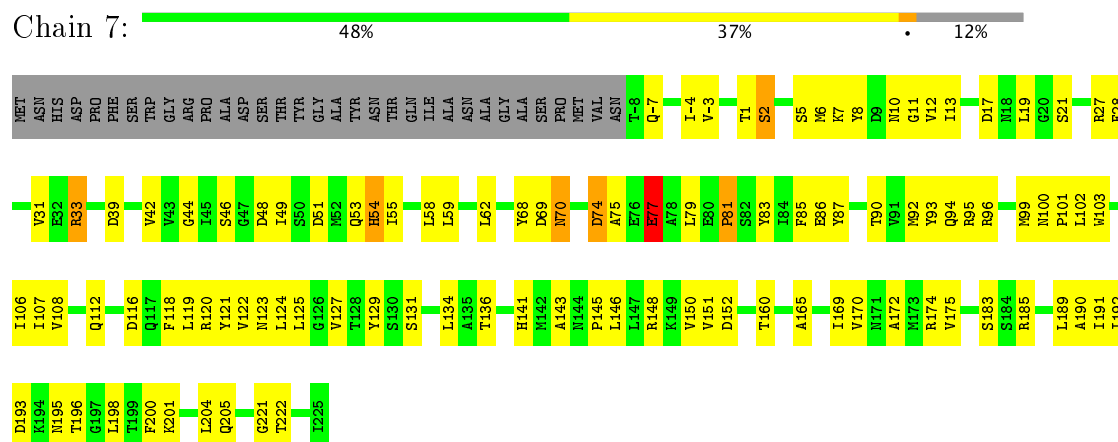
- Molecule 5: PROTEASOME COMPONENT PRE2



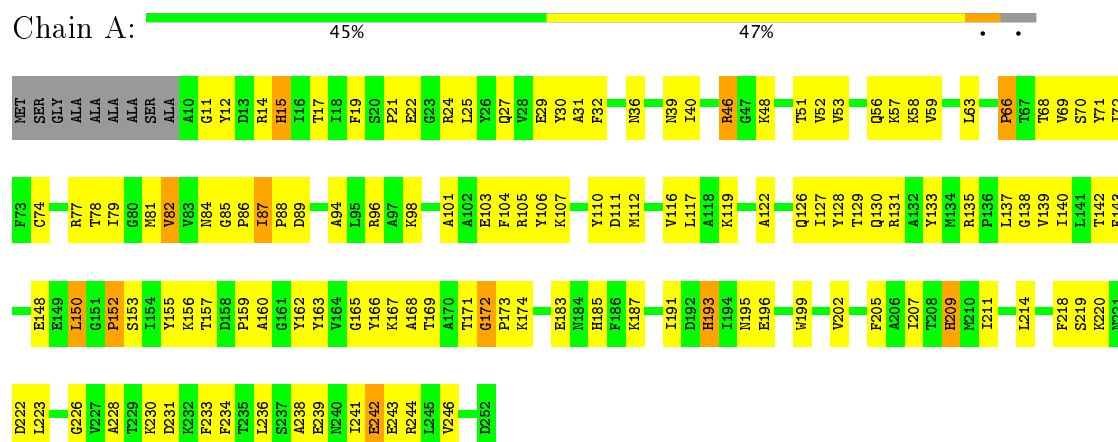
- Molecule 6: PROTEASOME COMPONENT C5



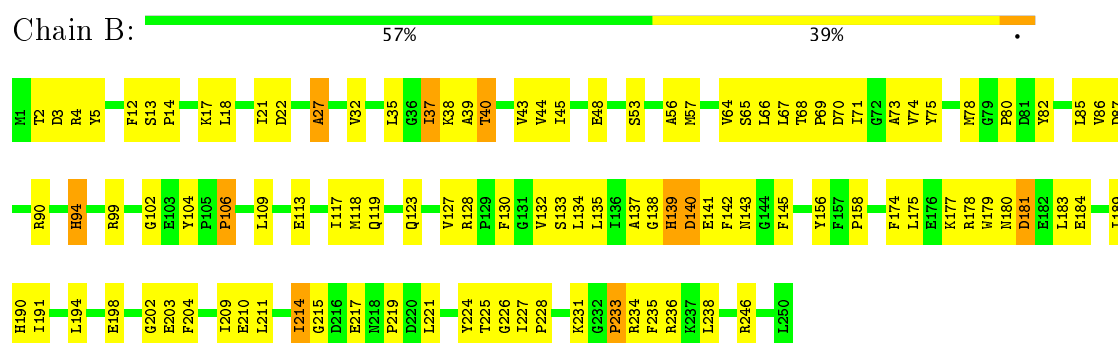
- Molecule 7: PROTEASOME COMPONENT PRE4



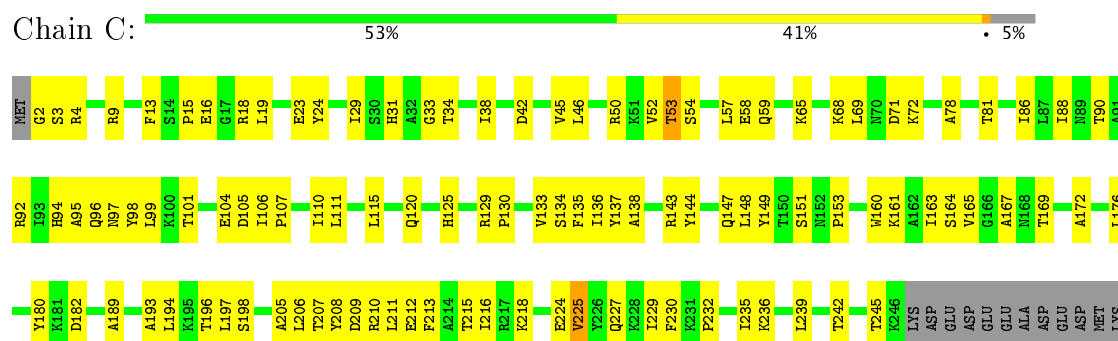
- Molecule 8: PROTEASOME COMPONENT C7-ALPHA



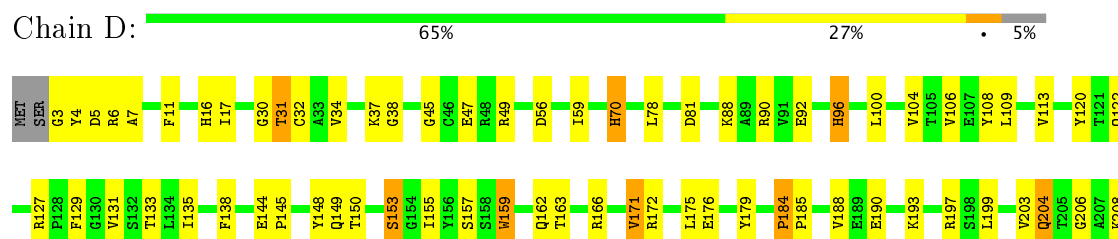
- Molecule 9: PROTEASOME COMPONENT Y7

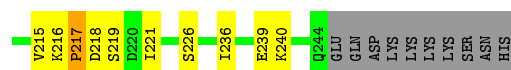


- Molecule 10: PROTEASOME COMPONENT Y13



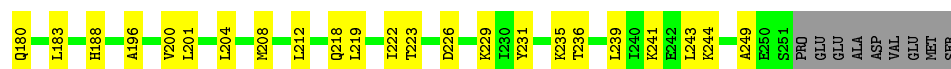
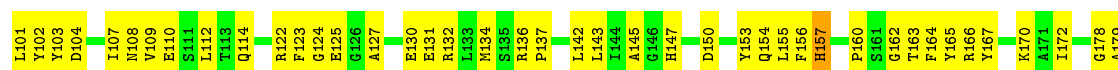
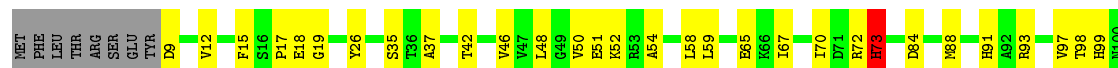
- Molecule 11: PROTEASOME COMPONENT PRE6





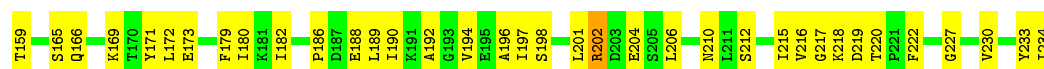
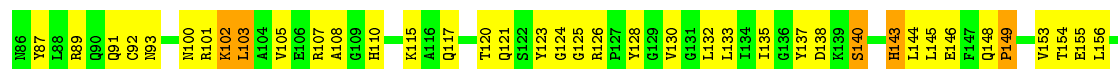
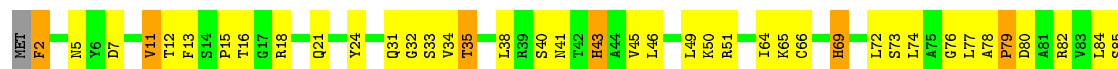
- Molecule 12: PROTEASOME COMPONENT PUP2

Chain E:  57% 36% 7%



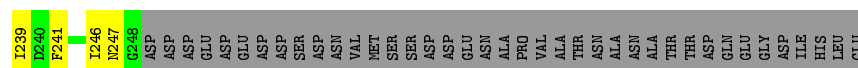
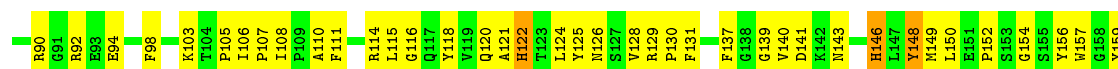
- Molecule 13: PROTEASOME COMPONENT PRE5

Chain F:  50% 44% 5%



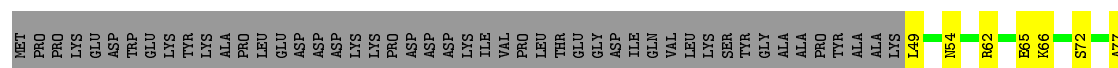
- Molecule 14: PROTEASOME COMPONENT C1

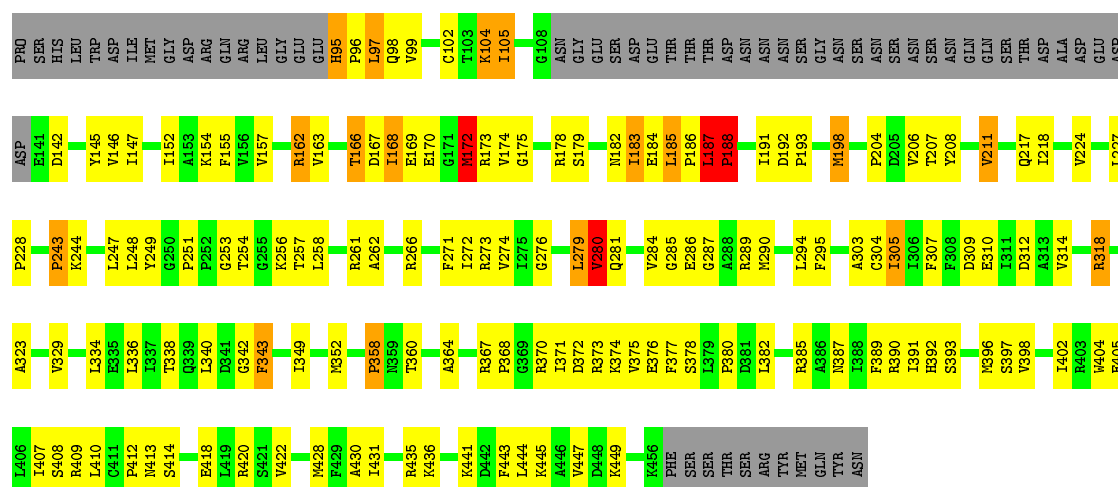
Chain G:  44% 37% 0 15%



- Molecule 15: 26S PROTEASE REGULATORY SUBUNIT 7 HOMOLOG

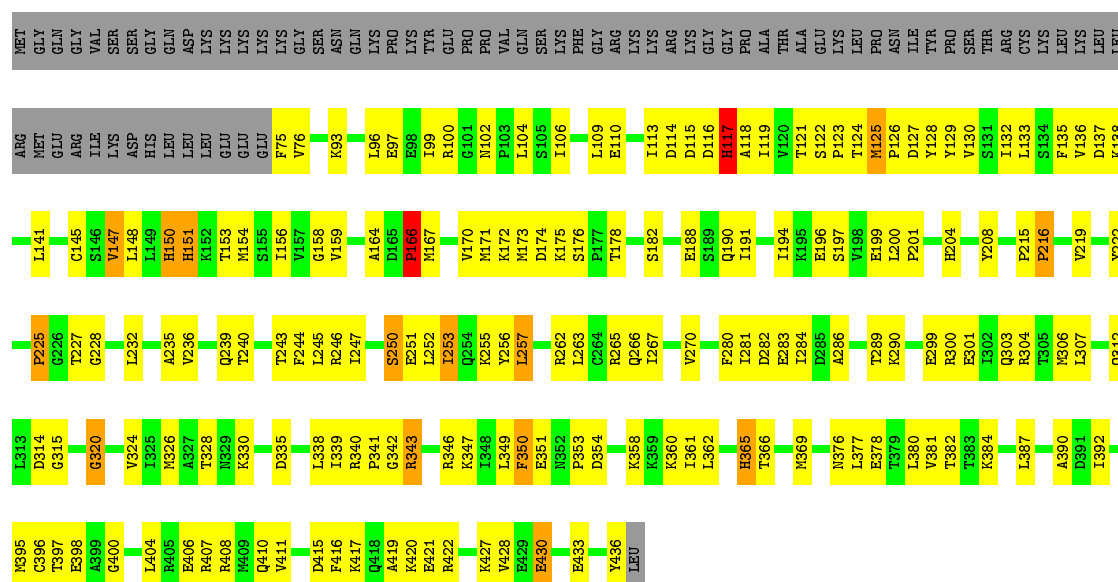
Chain H:  43% 29% 2% 1% 25%





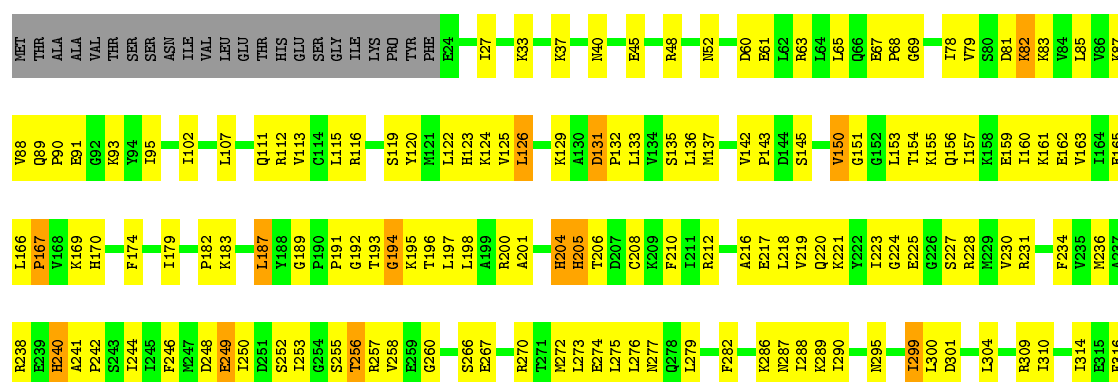
- Molecule 16: 26S PROTEASE REGULATORY SUBUNIT 4 HOMOLOG

Chain I:  43% 37% 2% 17%



- Molecule 17: 26S PROTEASE REGULATORY SUBUNIT 8 HOMOLOG

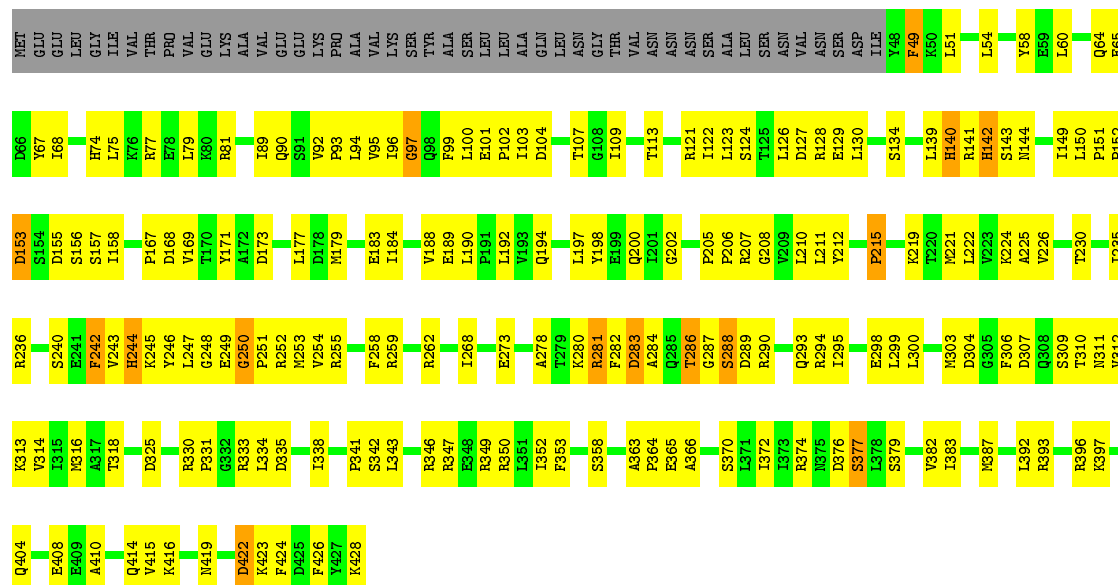
Chain J: 49% 40% 0% 8%





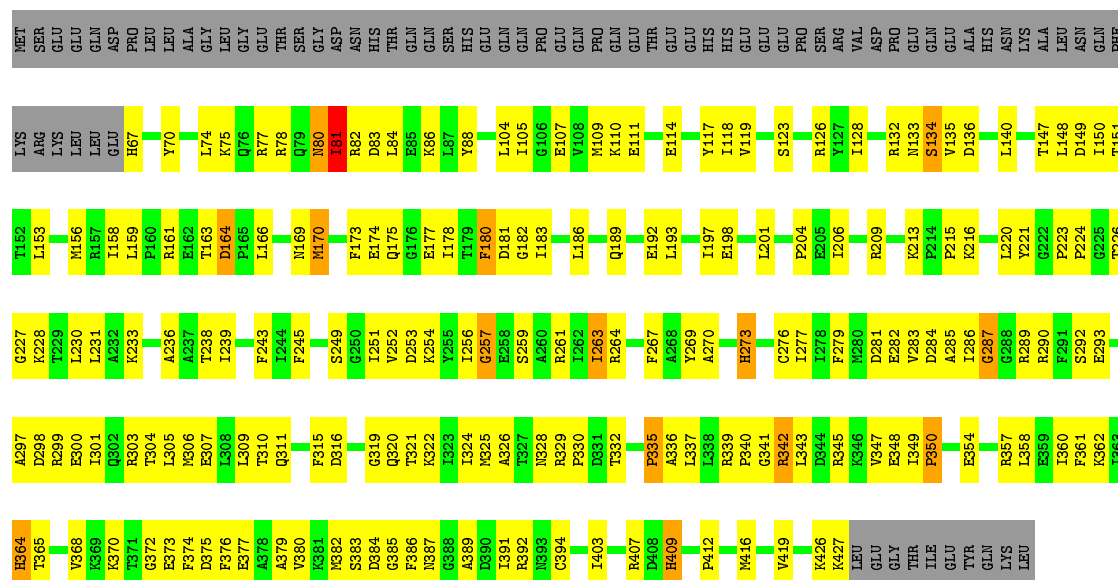
• Molecule 18: 26S PROTEASE REGULATORY SUBUNIT 6B HOMOLOG

Chain K: 46% 40% 11%



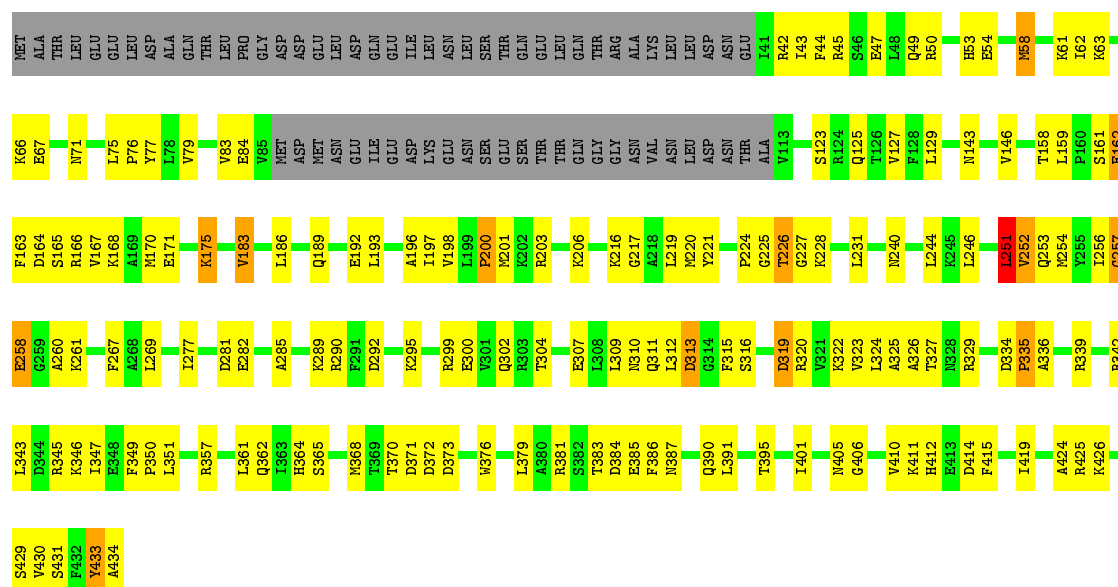
• Molecule 19: 26S PROTEASE SUBUNIT RPT4

Chain L: 40% 40% 17%



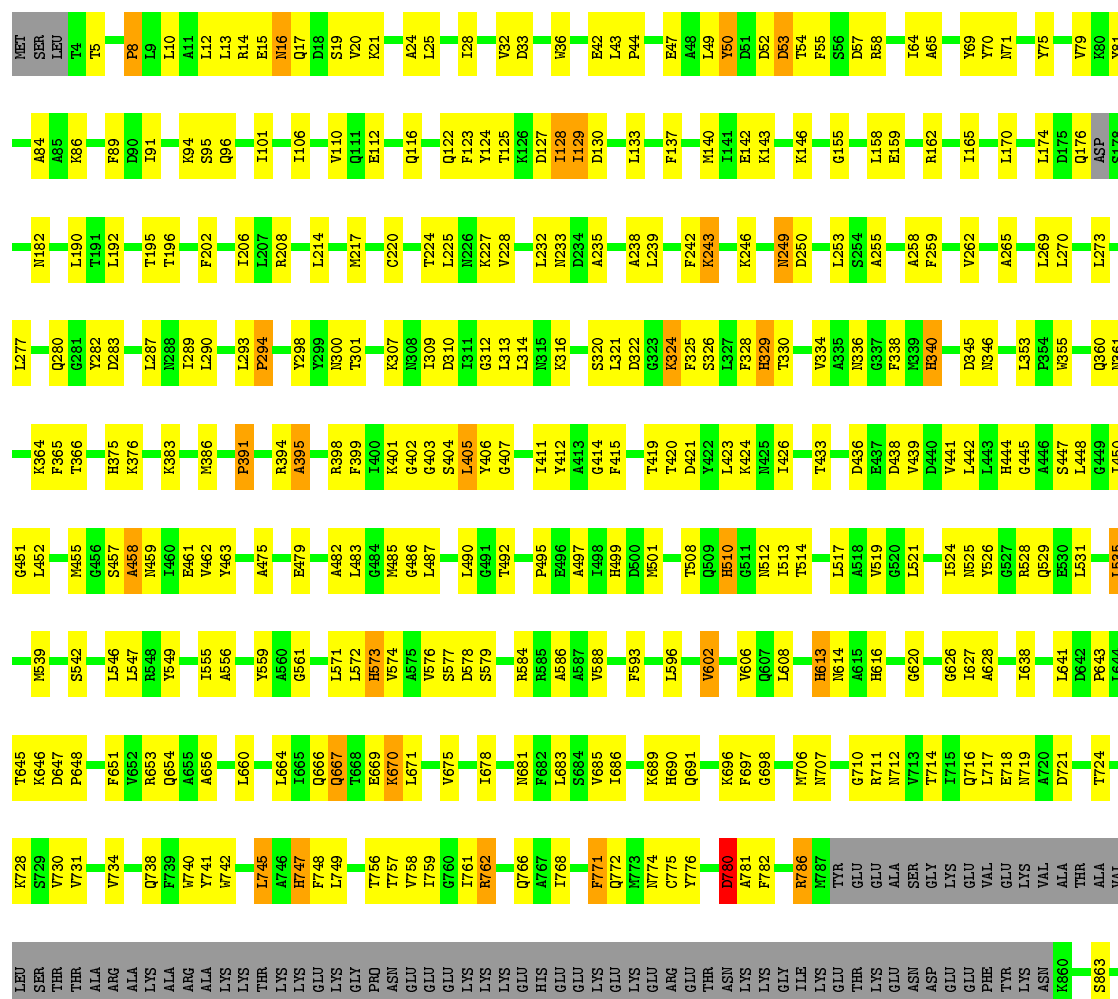
• Molecule 20: 26S PROTEASE REGULATORY SUBUNIT 6A

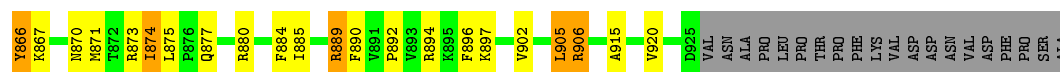
Chain M: 48% 33% 15%



- Molecule 21: 26S PROTEASOME REGULATORY SUBUNIT RPN2

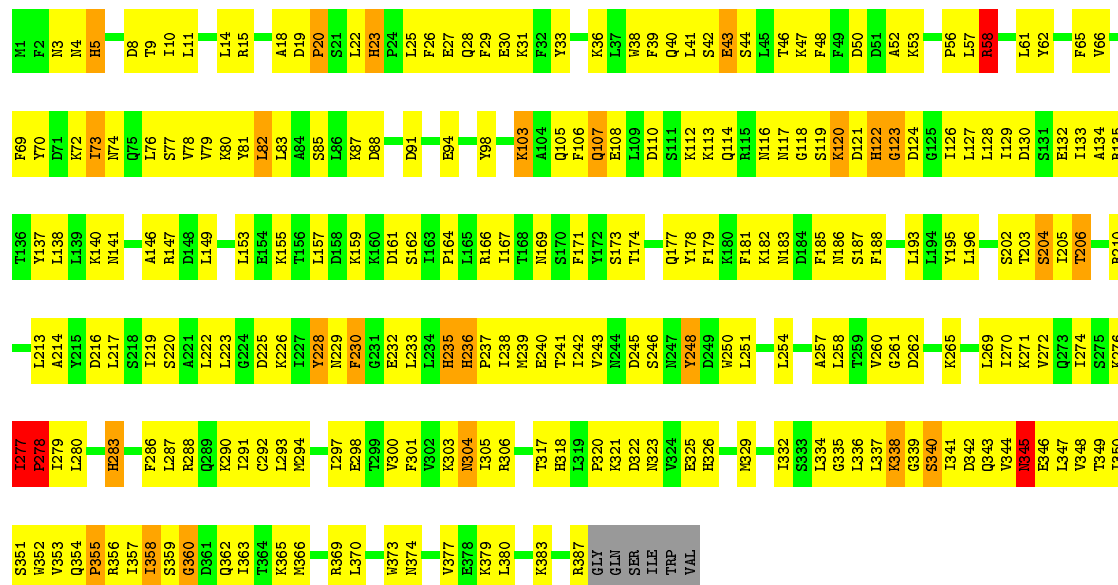
Chain N:  53% 33% 10%





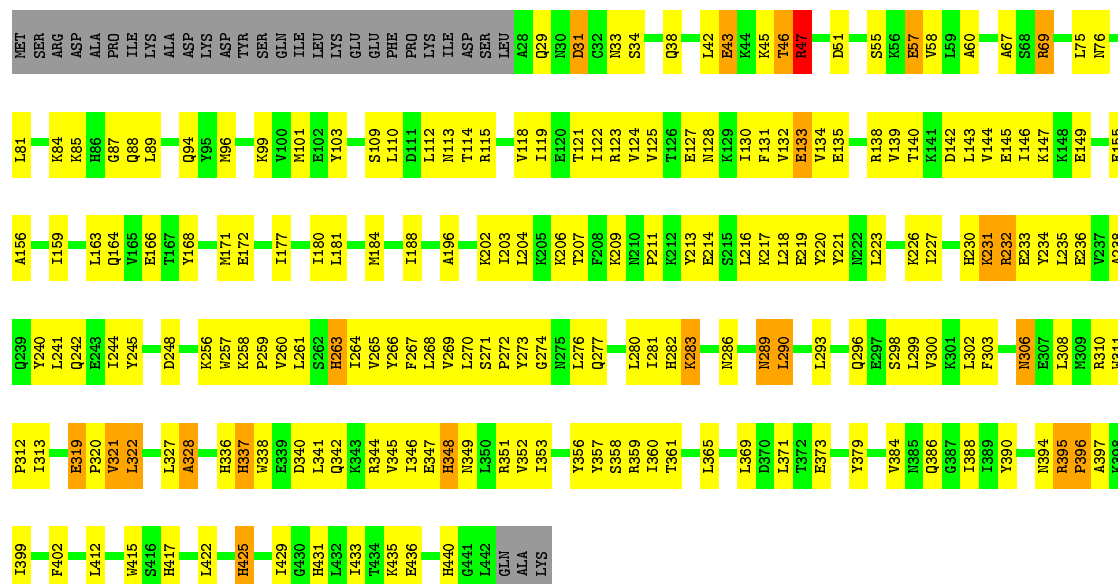
• Molecule 22: 26S PROTEASOME REGULATORY SUBUNIT RPN9

Chain O: 37% 54% 6% ..



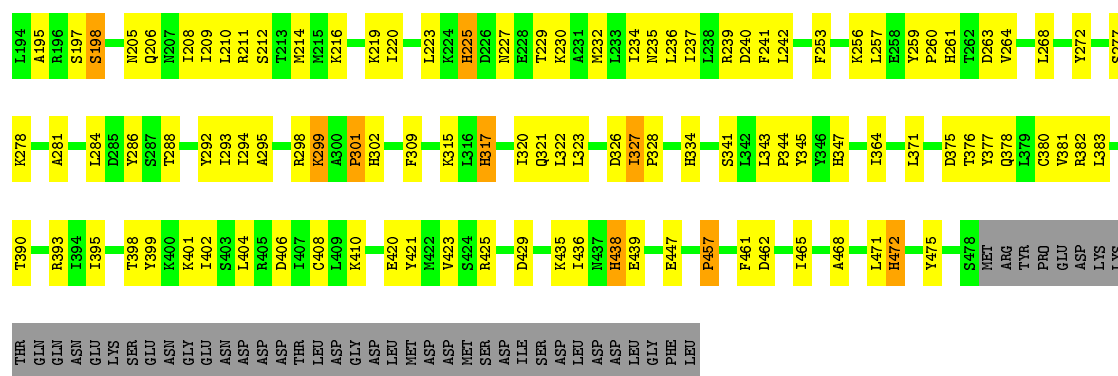
• Molecule 23: 26S PROTEASOME REGULATORY SUBUNIT RPN5

Chain P: 48% 40% 5% 7%



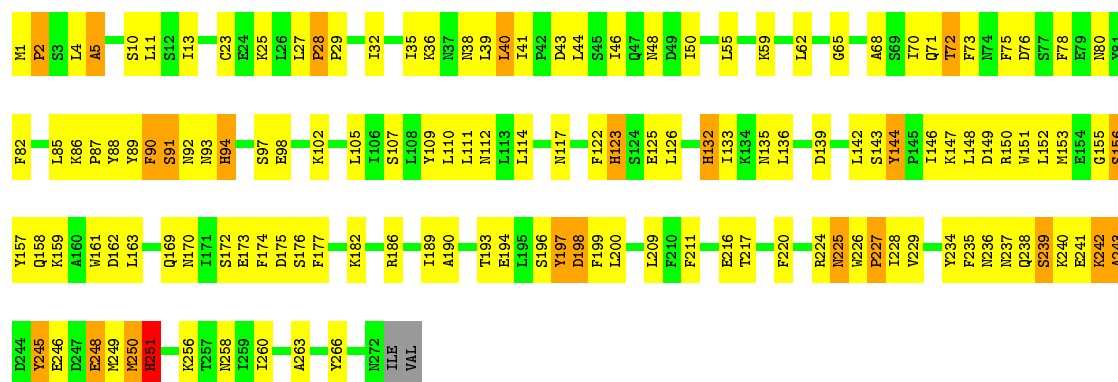
• Molecule 24: 26S PROTEASOME REGULATORY SUBUNIT RPN6

Chain Q: 53% 43% ..



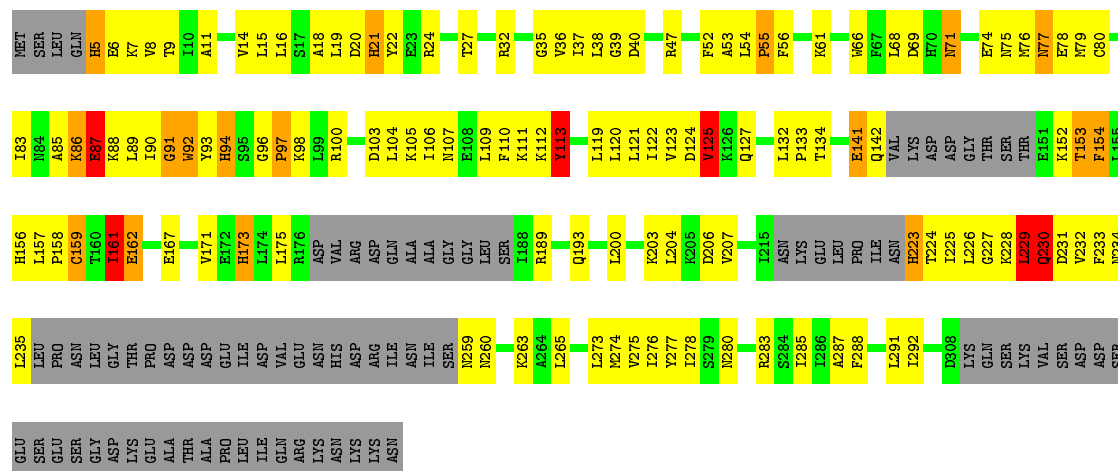
• Molecule 27: 26S PROTEASOME REGULATORY SUBUNIT RPN12

Chain T: 49% 42% 8%



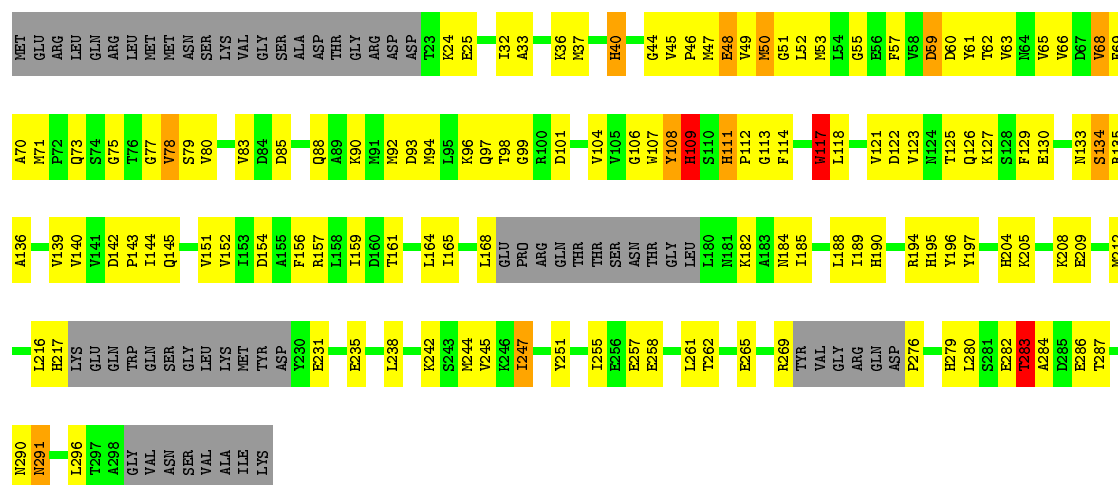
• Molecule 28: 26S PROTEASOME REGULATORY SUBUNIT RPN8

Chain U: 37% 31% 5% 25%

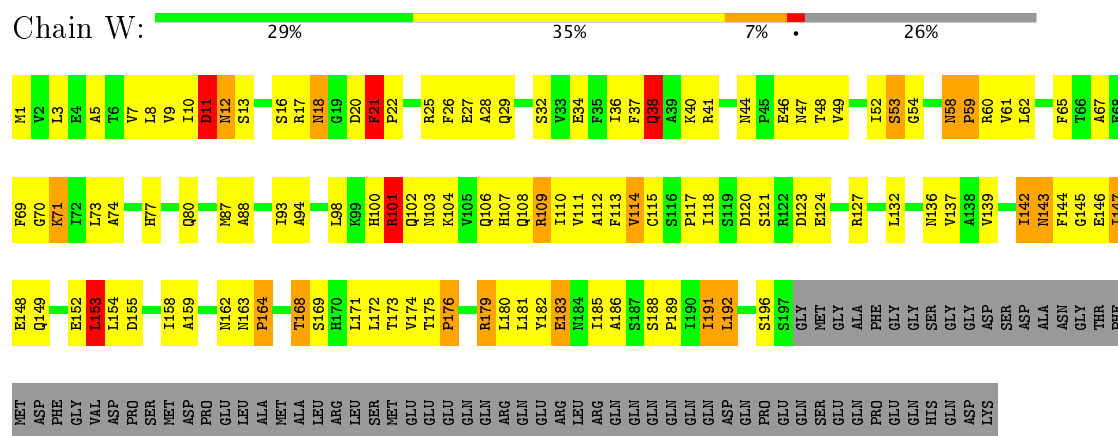


• Molecule 29: 26S PROTEASOME REGULATORY SUBUNIT RPN11

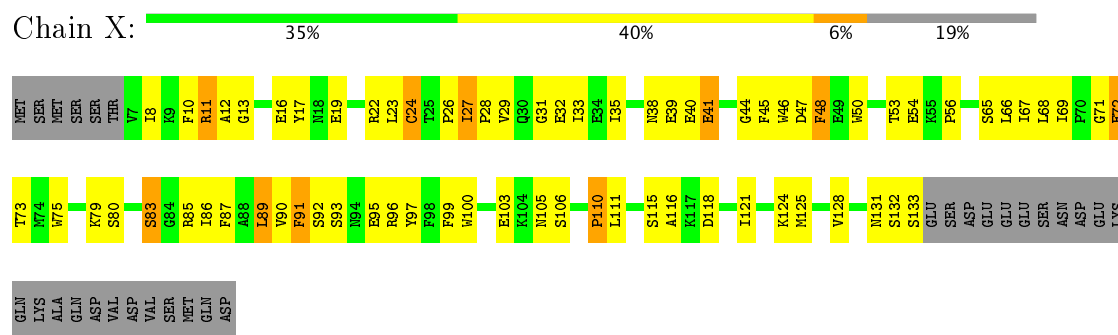
Chain V: 38% 38% 19%



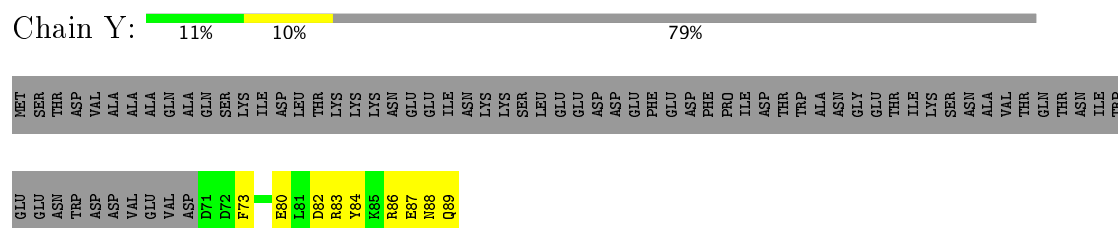
• Molecule 30: 26S PROTEASOME REGULATORY SUBUNIT RPN10



• Molecule 31: 26S PROTEASOME REGULATORY SUBUNIT RPN13

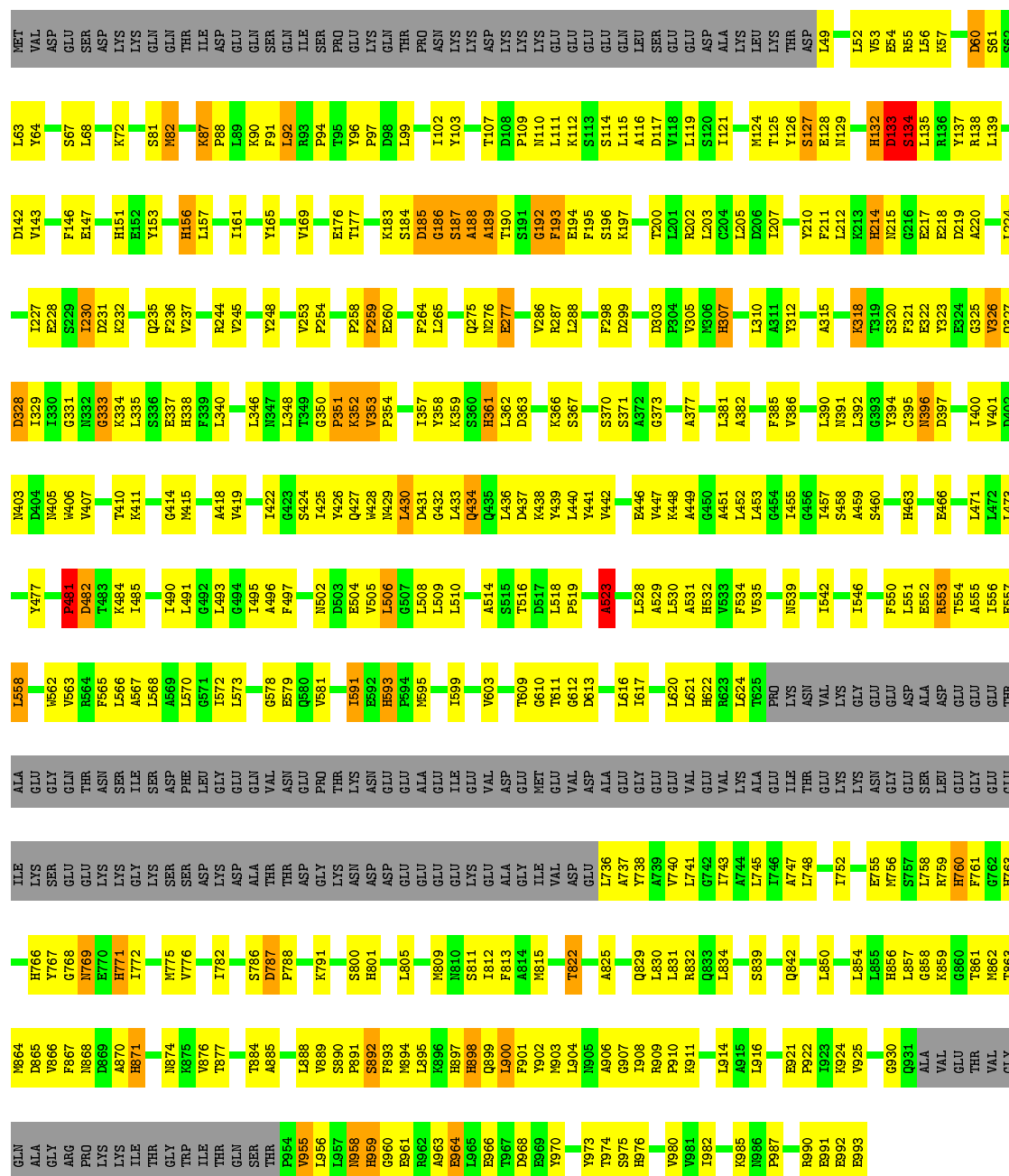


• Molecule 32: 26S PROTEASOME COMPLEX SUBUNIT SEM1



- Molecule 33: 26S PROTEASOME REGULATORY SUBUNIT RPN1

Chain Z: 41% 36% 5% 18%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	300000	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	MICROGRAPH	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	Depositor
Image detector	TVIPS TEMCAM-F816 (8k x 8k)	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	1.21	8/1605 (0.5%)	1.20	5/2171 (0.2%)
10	C	1.16	11/1943 (0.6%)	1.18	2/2629 (0.1%)
11	D	1.12	7/1928 (0.4%)	1.13	2/2610 (0.1%)
12	E	1.19	8/1892 (0.4%)	1.14	2/2549 (0.1%)
13	F	1.23	13/1823 (0.7%)	1.16	4/2463 (0.2%)
14	G	1.24	15/1940 (0.8%)	1.22	4/2619 (0.2%)
15	H	1.08	7/2831 (0.2%)	1.28	11/3808 (0.3%)
16	I	1.17	15/2859 (0.5%)	1.20	8/3853 (0.2%)
17	J	1.17	13/2962 (0.4%)	1.15	4/3975 (0.1%)
18	K	1.21	11/3061 (0.4%)	1.37	11/4129 (0.3%)
19	L	1.16	11/2895 (0.4%)	1.14	3/3892 (0.1%)
2	2	1.24	14/1723 (0.8%)	1.25	4/2337 (0.2%)
20	M	1.17	10/2903 (0.3%)	1.24	14/3909 (0.4%)
21	N	1.15	31/6670 (0.5%)	1.21	26/9023 (0.3%)
22	O	0.73	10/3243 (0.3%)	0.95	4/4374 (0.1%)
23	P	1.17	12/3452 (0.3%)	1.20	12/4657 (0.3%)
24	Q	1.11	16/3527 (0.5%)	1.09	7/4748 (0.1%)
25	R	1.05	11/3272 (0.3%)	1.08	4/4412 (0.1%)
26	S	1.08	13/2945 (0.4%)	1.11	2/3976 (0.1%)
27	T	1.04	9/2279 (0.4%)	1.07	3/3077 (0.1%)
28	U	1.83	12/2087 (0.6%)	1.16	11/2811 (0.4%)
29	V	1.20	12/1969 (0.6%)	1.26	16/2652 (0.6%)
3	3	1.18	7/1611 (0.4%)	1.17	2/2174 (0.1%)
30	W	1.40	12/1556 (0.8%)	1.73	16/2108 (0.8%)
31	X	1.20	4/1058 (0.4%)	1.33	5/1432 (0.3%)
32	Y	0.97	0/169	0.95	0/223
33	Z	1.03	31/6403 (0.5%)	1.12	15/8686 (0.2%)
4	4	1.16	7/1613 (0.4%)	1.22	2/2173 (0.1%)
5	5	1.19	8/1683 (0.5%)	1.22	3/2277 (0.1%)
6	6	1.22	11/1795 (0.6%)	1.18	4/2420 (0.2%)
7	7	1.14	6/1855 (0.3%)	1.14	2/2514 (0.1%)
8	A	1.23	10/1959 (0.5%)	1.21	10/2652 (0.4%)
9	B	1.21	8/1952 (0.4%)	1.21	5/2642 (0.2%)
All	All	1.16	373/81463 (0.5%)	1.19	223/109975 (0.2%)

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
1	1	0	1
11	D	0	1
13	F	0	1
15	H	0	6
17	J	0	1
19	L	0	4
20	M	0	2
21	N	0	7
22	O	0	2
23	P	0	3
24	Q	0	1
25	R	0	2
26	S	0	1
27	T	0	2
28	U	0	6
29	V	0	6
30	W	0	11
31	X	0	3
33	Z	0	7
6	6	0	1
7	7	0	2
8	A	0	3
All	All	0	73

The worst 5 of 373 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	U	230	GLN	N-CA	70.25	2.86	1.46
30	W	38	GLN	C-N	-38.06	0.46	1.34
18	K	242	PHE	C-N	21.55	1.83	1.34
20	M	257	GLY	C-N	20.38	1.80	1.34
33	Z	134	SER	N-CA	16.20	1.78	1.46

The worst 5 of 223 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	W	154	LEU	O-C-N	34.31	177.59	122.70
18	K	242	PHE	O-C-N	27.36	166.48	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	242	PHE	C-N-CA	-26.80	54.71	121.70
30	W	154	LEU	CA-C-N	-25.04	62.10	117.20
21	N	889	ARG	NE-CZ-NH1	23.00	131.80	120.30

There are no chirality outliers.

5 of 73 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	-2	LEU	Peptide
6	6	-9	GLN	Peptide
7	7	100	ASN	Peptide
7	7	33	ARG	Peptide
8	A	46	ARG	Mainchain

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	1555	200	0
2	2	1692	0	1699	93	0
3	3	1581	0	1574	101	0
4	4	1585	0	1590	91	0
5	5	1646	0	1595	122	0
6	6	1757	0	1711	87	0
7	7	1824	0	1832	150	0
8	A	1921	0	1909	159	0
9	B	1915	0	1929	144	0
10	C	1913	0	1914	146	0
11	D	1899	0	1908	109	0
12	E	1867	0	1841	163	0
13	F	1795	0	1797	178	0
14	G	1900	0	1888	192	0
15	H	2792	0	2878	283	0
16	I	2822	0	2869	288	0
17	J	2928	0	3054	357	0
18	K	3019	0	3079	411	0
19	L	2853	0	2925	285	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	M	2866	0	2936	287	0
21	N	6562	0	6625	482	0
22	O	3182	0	3207	604	0
23	P	3401	0	3483	320	0
24	Q	3471	0	3494	359	0
25	R	3218	0	3216	408	0
26	S	2893	0	2937	245	0
27	T	2235	0	2206	305	0
28	U	2061	0	2116	375	0
29	V	1942	0	1954	251	0
30	W	1534	0	1538	204	0
31	X	1032	0	1017	181	0
32	Y	168	0	153	17	0
33	Z	6289	0	6233	619	0
All	All	80139	0	80662	7214	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 45.

The worst 5 of 7214 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)
33:Z:321:PHE:CZ	33:Z:350:GLY:HA2	1.23	1.67
22:O:373:TRP:CD1	28:U:200:LEU:HD21	1.29	1.65
24:Q:243:PHE:HZ	24:Q:287:THR:CA	1.07	1.64
22:O:373:TRP:HD1	28:U:200:LEU:CD2	1.01	1.62
33:Z:321:PHE:CE1	33:Z:350:GLY:HA2	1.26	1.60

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%)	189 (93%)	13 (6%)	1 (0%)	32	74
2	2	221/261 (85%)	207 (94%)	10 (4%)	4 (2%)	10	49
3	3	202/205 (98%)	188 (93%)	12 (6%)	2 (1%)	18	61
4	4	196/198 (99%)	181 (92%)	13 (7%)	2 (1%)	18	61
5	5	210/287 (73%)	194 (92%)	11 (5%)	5 (2%)	7	42
6	6	220/241 (91%)	206 (94%)	11 (5%)	3 (1%)	13	54
7	7	231/266 (87%)	208 (90%)	16 (7%)	7 (3%)	5	37
8	A	241/252 (96%)	217 (90%)	20 (8%)	4 (2%)	11	50
9	B	248/250 (99%)	227 (92%)	15 (6%)	6 (2%)	7	42
10	C	243/258 (94%)	224 (92%)	16 (7%)	3 (1%)	15	57
11	D	240/254 (94%)	221 (92%)	16 (7%)	3 (1%)	14	56
12	E	241/260 (93%)	225 (93%)	13 (5%)	3 (1%)	15	57
13	F	231/234 (99%)	209 (90%)	19 (8%)	3 (1%)	14	56
14	G	243/288 (84%)	224 (92%)	16 (7%)	3 (1%)	15	57
15	H	353/467 (76%)	298 (84%)	36 (10%)	19 (5%)	2	25
16	I	358/437 (82%)	326 (91%)	25 (7%)	7 (2%)	9	46
17	J	367/405 (91%)	337 (92%)	21 (6%)	9 (2%)	6	41
18	K	377/428 (88%)	336 (89%)	29 (8%)	12 (3%)	5	36
19	L	357/437 (82%)	326 (91%)	18 (5%)	13 (4%)	4	33
20	M	363/434 (84%)	322 (89%)	29 (8%)	12 (3%)	4	35
21	N	843/945 (89%)	786 (93%)	37 (4%)	20 (2%)	7	42
22	O	385/393 (98%)	309 (80%)	44 (11%)	32 (8%)	1	16
23	P	413/445 (93%)	374 (91%)	22 (5%)	17 (4%)	3	30
24	Q	429/434 (99%)	390 (91%)	28 (6%)	11 (3%)	6	40
25	R	398/429 (93%)	345 (87%)	36 (9%)	17 (4%)	3	29
26	S	351/523 (67%)	308 (88%)	31 (9%)	12 (3%)	4	35
27	T	270/274 (98%)	235 (87%)	16 (6%)	19 (7%)	1	19
28	U	245/338 (72%)	226 (92%)	9 (4%)	10 (4%)	3	30
29	V	239/306 (78%)	212 (89%)	18 (8%)	9 (4%)	4	32
30	W	193/268 (72%)	156 (81%)	17 (9%)	20 (10%)	0	10
31	X	125/156 (80%)	101 (81%)	19 (15%)	5 (4%)	3	31
32	Y	17/89 (19%)	17 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	Z	807/993 (81%)	690 (86%)	68 (8%)	49 (6%)	2	22
All	All	10060/11670 (86%)	9014 (90%)	704 (7%)	342 (3%)	7	35

5 of 342 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	4	150	ASP
9	B	203	GLU
11	D	31	THR
11	D	204	GLN
15	H	183	ILE

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
2	2	182/214 (85%)	181 (100%)	1 (0%)	91	95
3	3	172/173 (99%)	172 (100%)	0	100	100
4	4	175/175 (100%)	175 (100%)	0	100	100
5	5	169/235 (72%)	168 (99%)	1 (1%)	89	94
6	6	185/201 (92%)	185 (100%)	0	100	100
7	7	199/224 (89%)	199 (100%)	0	100	100
8	A	207/210 (99%)	207 (100%)	0	100	100
9	B	209/209 (100%)	209 (100%)	0	100	100
10	C	204/216 (94%)	204 (100%)	0	100	100
11	D	214/226 (95%)	214 (100%)	0	100	100
12	E	199/215 (93%)	199 (100%)	0	100	100
13	F	192/193 (100%)	192 (100%)	0	100	100
14	G	201/239 (84%)	200 (100%)	1 (0%)	91	95
15	H	303/399 (76%)	302 (100%)	1 (0%)	94	96

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	I	319/385 (83%)	318 (100%)	1 (0%)	94	96
17	J	325/352 (92%)	324 (100%)	1 (0%)	94	96
18	K	334/374 (89%)	333 (100%)	1 (0%)	94	96
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%)	710 (100%)	3 (0%)	93	95
22	O	363/368 (99%)	361 (99%)	2 (1%)	89	94
23	P	388/415 (94%)	380 (98%)	8 (2%)	59	80
24	Q	388/391 (99%)	388 (100%)	0	100	100
25	R	351/379 (93%)	351 (100%)	0	100	100
26	S	330/489 (68%)	330 (100%)	0	100	100
27	T	254/256 (99%)	254 (100%)	0	100	100
28	U	234/308 (76%)	228 (97%)	6 (3%)	51	75
29	V	217/268 (81%)	214 (99%)	3 (1%)	71	86
30	W	171/230 (74%)	169 (99%)	2 (1%)	75	88
31	X	116/144 (81%)	114 (98%)	2 (2%)	66	84
32	Y	18/81 (22%)	18 (100%)	0	100	100
33	Z	692/850 (81%)	692 (100%)	0	100	100
All	All	8816/10146 (87%)	8783 (100%)	33 (0%)	93	95

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	P	43	GLU
23	P	85	LYS
30	W	101	ARG
23	P	57	GLU
23	P	58	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 171 such sidechains are listed below:

Mol	Chain	Res	Type
19	L	80	ASN
21	N	738	GLN
30	W	136	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	L	320	GLN
21	N	182	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](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
30	W	3
17	J	2
18	K	2
29	V	2
19	L	2
20	M	2
16	I	1

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	218:LEU	C	219:VAL	N	3.99
1	K	248:GLY	C	249:GLU	N	3.09
1	L	251:ILE	C	252:VAL	N	2.52
1	I	252:LEU	C	253:ILE	N	2.13
1	J	224:GLY	C	225:GLU	N	2.03