



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 22, 2017 – 05:48 AM EDT

PDB ID : 5A5B
EMDB ID: : EMD-3034
Title : Structure of the 26S proteasome-Ubp6 complex
Authors : Aufderheide, A.; Beck, F.; Stengel, F.; Hartwig, M.; Schweitzer, A.; Pfeifer, G.; Goldberg, A.L.; Sakata, E.; Baumeister, W.; Foerster, F.
Deposited on : unknown
Resolution : 9.50 Å(reported)
Based on PDB ID : 4C43, 1VJV

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
Mogul : 1.7.2 (RC1), CSD as538be (2017)
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

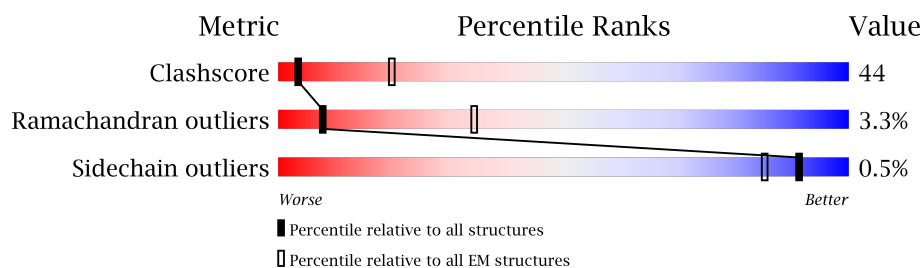
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.50 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.



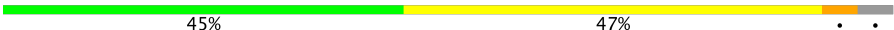










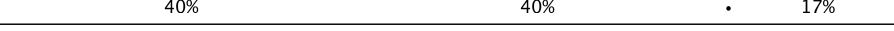






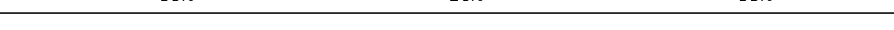
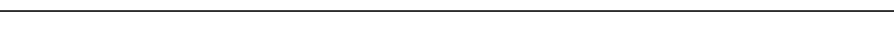

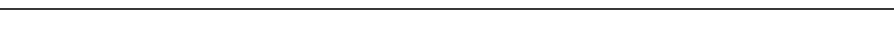
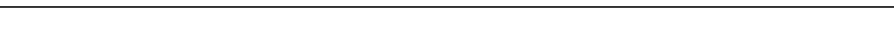


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	<div> <div>47%</div> <div>44%</div> <div>• 5%</div> </div>
2	2	261	<div> <div>55%</div> <div>26%</div> <div>5%</div> <div>15%</div> </div>
3	3	205	<div> <div>65%</div> <div>33%</div> <div>•</div> </div>
4	4	198	<div> <div>63%</div> <div>35%</div> <div>•</div> </div>
5	5	287	<div> <div>40%</div> <div>31%</div> <div>•</div> <div>26%</div> </div>
6	6	241	<div> <div>57%</div> <div>33%</div> <div>•</div> <div>8%</div> </div>
7	7	266	<div> <div>48%</div> <div>37%</div> <div>•</div> <div>12%</div> </div>
8	8	416	<div> <div>75%</div> <div>13%</div> <div>12%</div> </div>
9	9	76	<div> <div>62%</div> <div>37%</div> <div>•</div> </div>


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Mol	Chain	Length	Quality of chain
10	A	252	
11	B	250	
12	C	258	
13	D	254	
14	E	260	
15	F	234	
16	G	288	
17	H	467	
18	I	437	
19	J	405	
20	K	428	
21	L	437	
22	M	434	
23	N	945	
24	O	393	
25	P	445	
26	Q	434	
27	R	429	
28	S	523	
29	T	274	
30	U	338	
31	V	306	
32	W	268	
33	X	156	
34	Y	89	

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Mol	Chain	Length	Quality of chain
35	Z	993	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	GLZ	9	76	-	-	X	-

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 83748 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	conflict	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 UBIQUITIN CARBOXYL-TERMINAL HYDROLASE 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	8	368	Total	C	N	O	S	Se	10	1
			3008	1922	500	571	5	10		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
8	85	MSE	-	expression tag	UNP P43593
8	86	GLY	-	expression tag	UNP P43593
8	87	SER	-	expression tag	UNP P43593
8	88	ASP	-	expression tag	UNP P43593
8	89	LYS	-	expression tag	UNP P43593
8	90	ILE	-	expression tag	UNP P43593
8	91	HIS	-	expression tag	UNP P43593
8	92	HIS	-	expression tag	UNP P43593
8	93	HIS	-	expression tag	UNP P43593
8	94	HIS	-	expression tag	UNP P43593
8	95	HIS	-	expression tag	UNP P43593
8	96	HIS	-	expression tag	UNP P43593
8	500	MSE	-	expression tag	UNP P43593
8	182	VAL	ILE	conflict	UNP P43593

- Molecule 9 is a protein called UBIQUITIN ALDEHYDE.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	76	Total	C	N	O	S	0	0
			601	378	105	117	1		

- Molecule 10 is a protein called PROTEASOME COMPONENT C7-ALPHA.

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

- Molecule 11 is a protein called PROTEASOME COMPONENT Y7.

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

- Molecule 12 is a protein called PROTEASOME COMPONENT Y13.

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

- Molecule 13 is a protein called PROTEASOME COMPONENT PRE6.

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

- Molecule 14 is a protein called PROTEASOME COMPONENT PUP2.

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

- Molecule 15 is a protein called PROTEASOME COMPONENT PRE5.

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

- Molecule 16 is a protein called PROTEASOME COMPONENT C1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	245	Total	C	N	O	S	0	0
			1900	1207	331	358	4		

- Molecule 17 is a protein called 26S PROTEASE REGULATORY SUBUNIT 7 HOMOLOG.

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

- Molecule 18 is a protein called 26S PROTEASE REGULATORY SUBUNIT 4 HOMOLOG.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	I	362	Total	C	N	O	S	0	0
			2822	1773	471	563	15		

- Molecule 19 is a protein called 26S PROTEASE REGULATORY SUBUNIT 8 HOMOLOG.

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

- Molecule 20 is a protein called 26S PROTEASE REGULATORY SUBUNIT 6B HOMOLOG.

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

- Molecule 21 is a protein called 26S PROTEASE SUBUNIT RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	L	361	Total	C	N	O	S	0	0
			2853	1798	507	536	12		

- Molecule 22 is a protein called 26S PROTEASE REGULATORY SUBUNIT 6A.

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

- Molecule 23 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN2.

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

- Molecule 24 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN9.

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

- Molecule 25 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	P	415	Total	C	N	O	S	0	0
			3401	2166	571	655	9		

- Molecule 26 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN6.

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

- Molecule 27 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN7.

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

- Molecule 28 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S	353	Total	C	N	O	S	0	0
			2893	1857	482	541	13		

- Molecule 29 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN12.

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

- Molecule 30 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN8.

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

- Molecule 31 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	V	247	Total	C	N	O	S	0	0
			1942	1225	328	376	13		

- Molecule 32 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN10.

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

- Molecule 33 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN13.

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

- Molecule 34 is a protein called 26S PROTEASOME COMPLEX SUBUNIT SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	Y	19	Total	C	N	O	0	0
			168	101	30	37		

- Molecule 35 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Z	813	Total	C	N	O	S	0	0
			6289	3995	1029	1236	29		

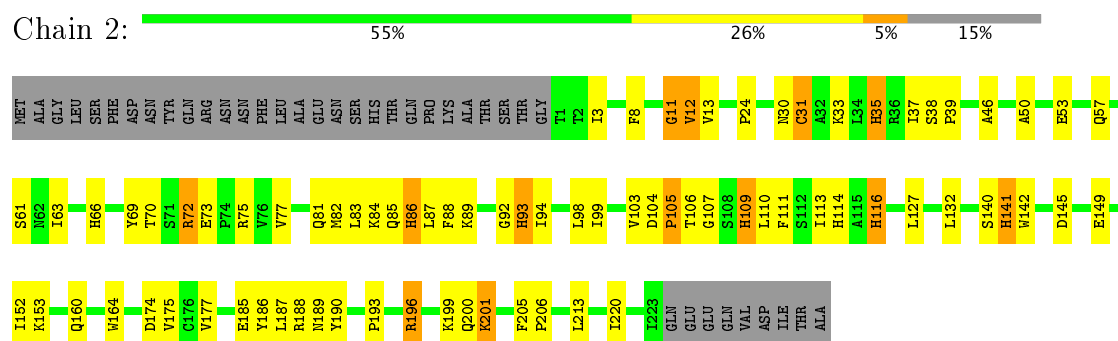
3 Residue-property plots

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.

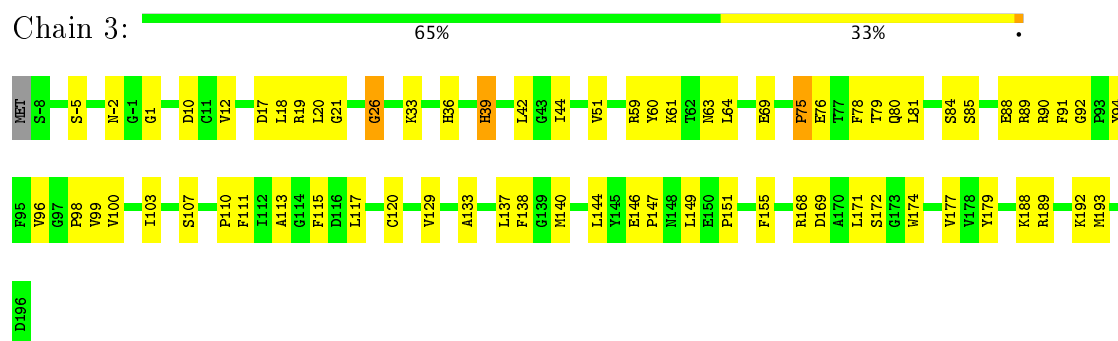
- Molecule 1: PROTEASOME COMPONENT PRE3



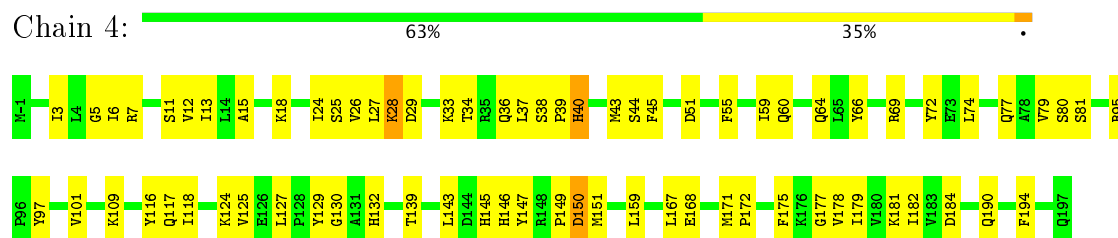
- Molecule 2: PROTEASOME COMPONENT PUP1



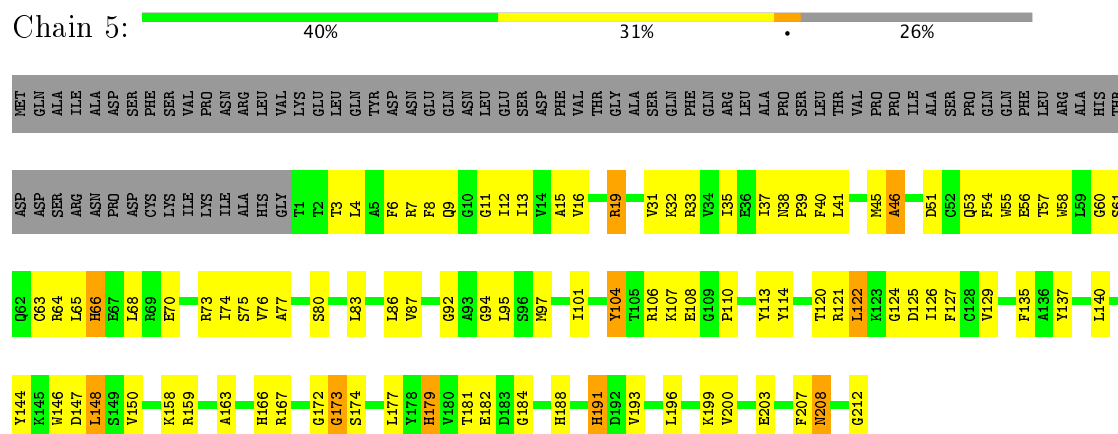
- Molecule 3: PROTEASOME COMPONENT PUP3



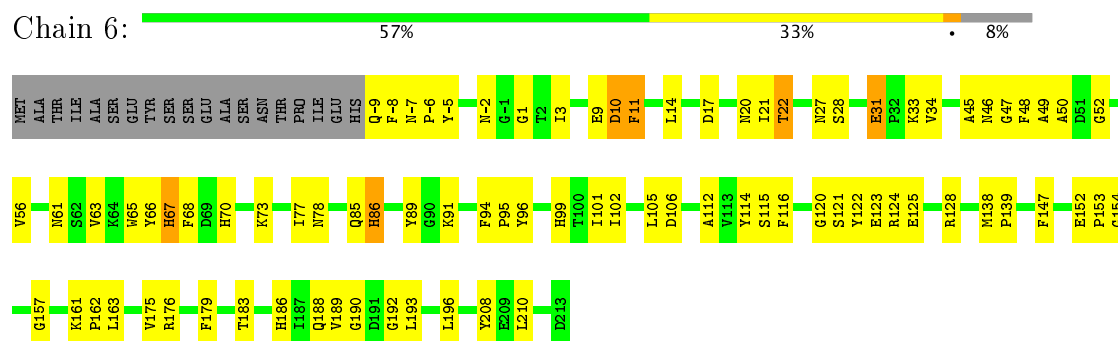
- Molecule 4: PROTEASOME COMPONENT C11



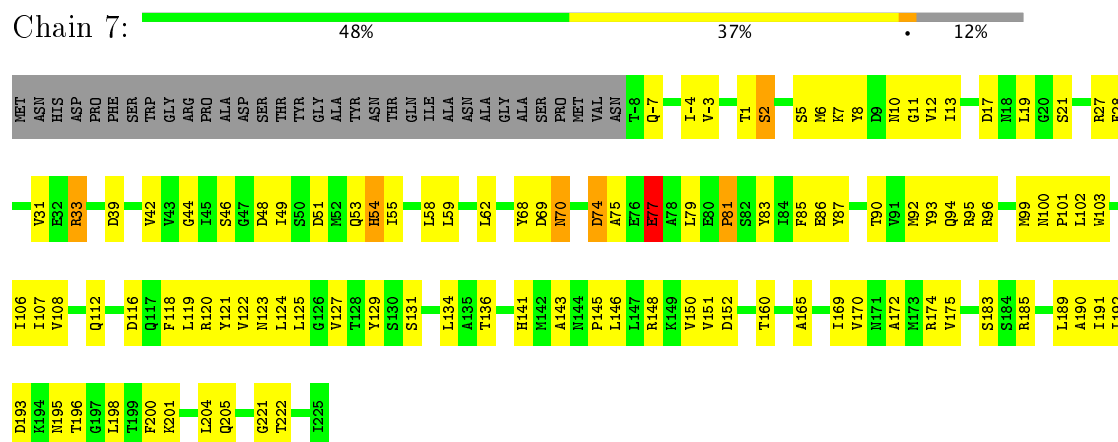
• Molecule 5: PROTEASOME COMPONENT PRE2



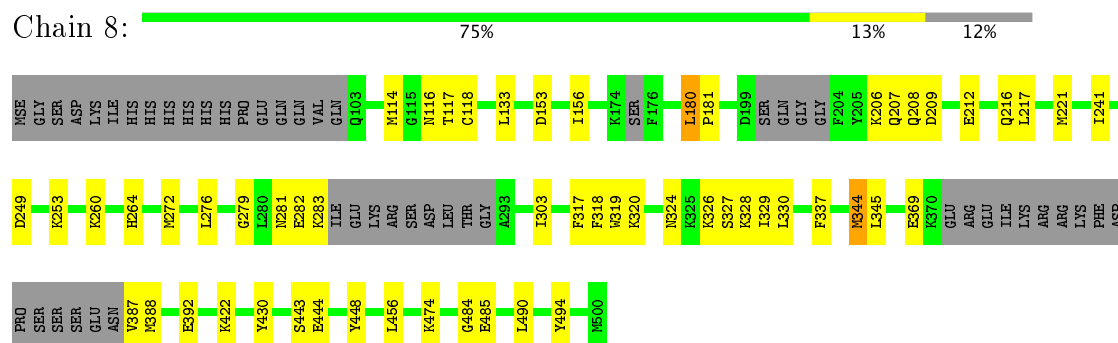
• Molecule 6: PROTEASOME COMPONENT C5



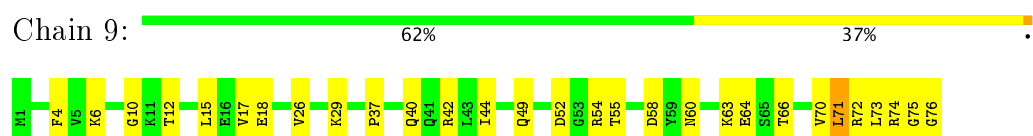
• Molecule 7: PROTEASOME COMPONENT PRE4



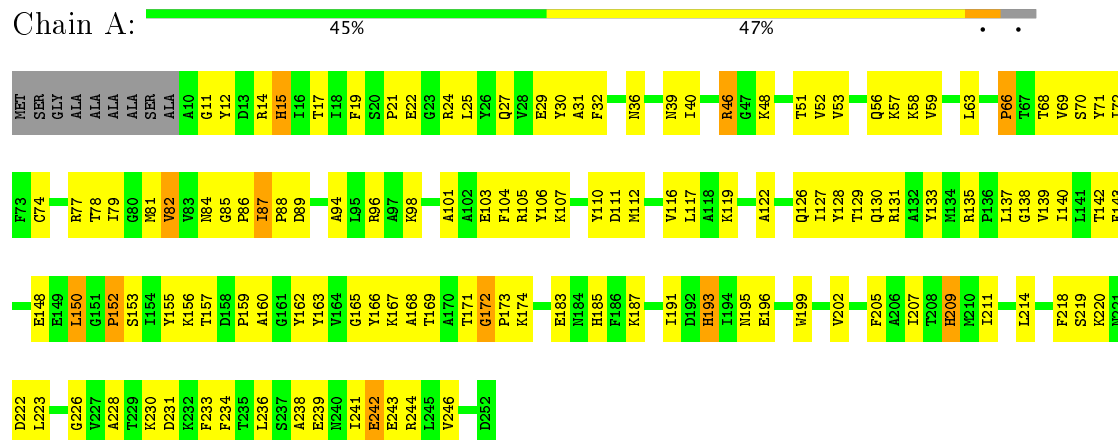
• Molecule 8: UBIQUITIN CARBOXYL-TERMINAL HYDROLASE 6



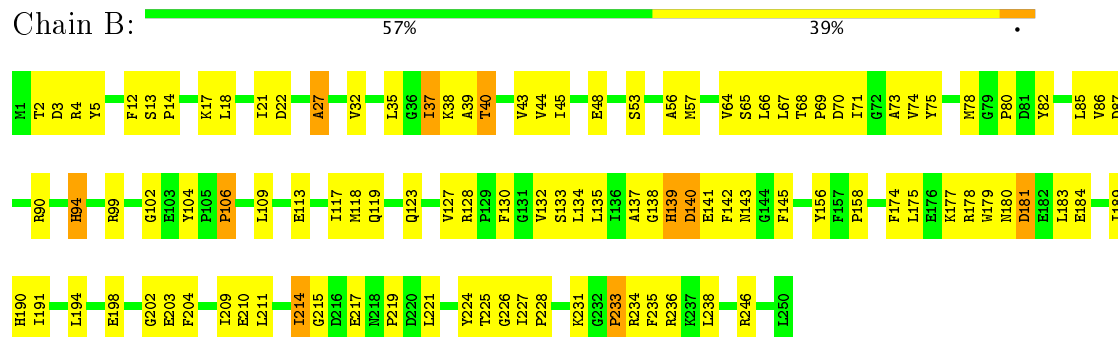
• Molecule 9: UBIQUITIN ALDEHYDE



• Molecule 10: PROTEASOME COMPONENT C7-ALPHA

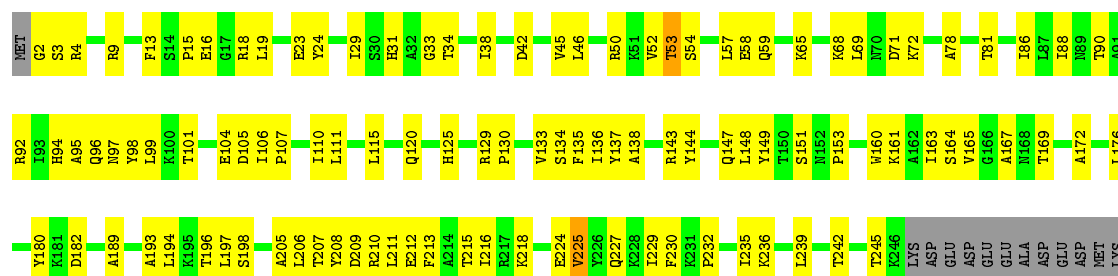


• Molecule 11: PROTEASOME COMPONENT Y7



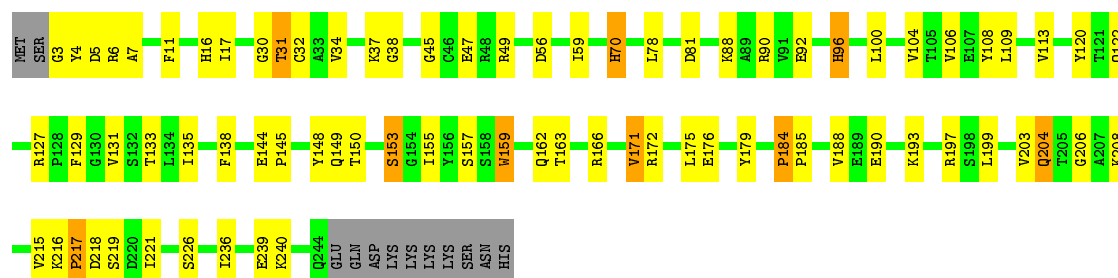
• Molecule 12: PROTEASOME COMPONENT Y13





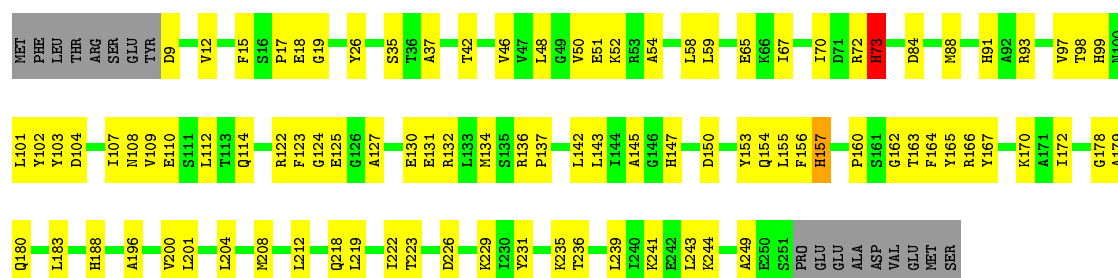
• Molecule 13: PROTEASOME COMPONENT PRE6

Chain D: 65% 27% 5%



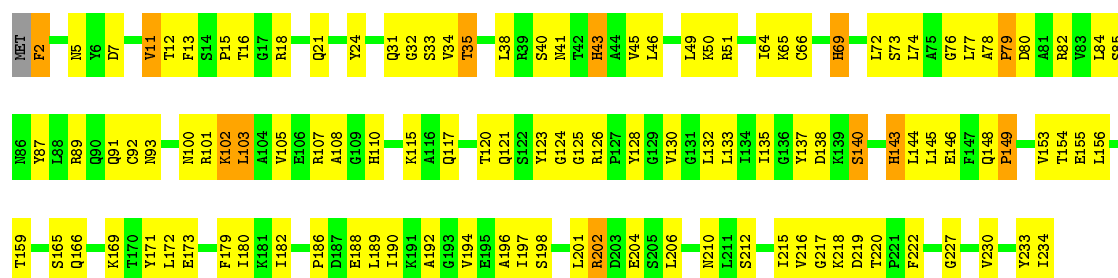
• Molecule 14: PROTEASOME COMPONENT PUP2

Chain E: 57% 36% 7%



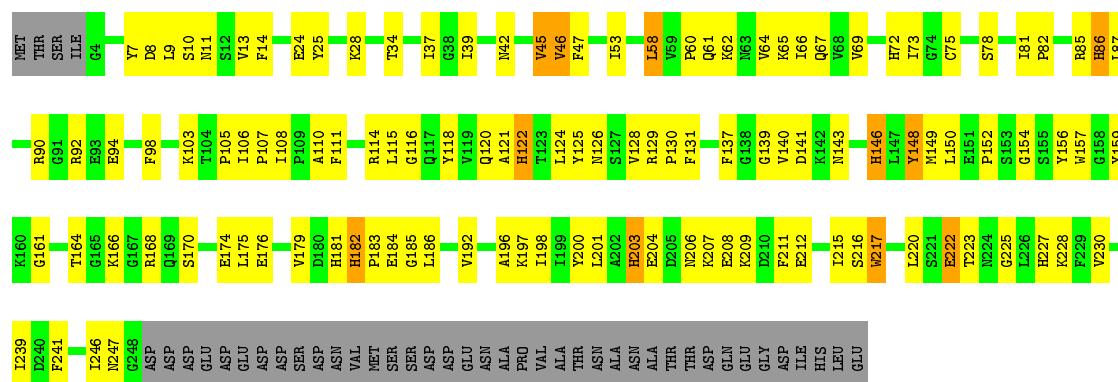
• Molecule 15: PROTEASOME COMPONENT PRE5

Chain F: 50% 44% 5%



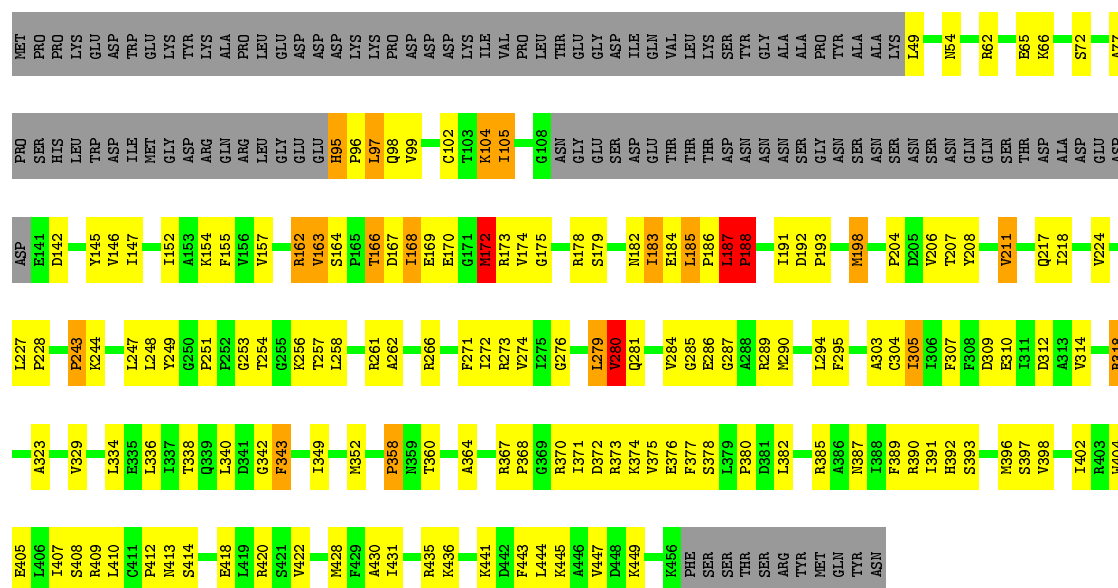
• Molecule 16: PROTEASOME COMPONENT C1

Chain G: 44% 37% 15%



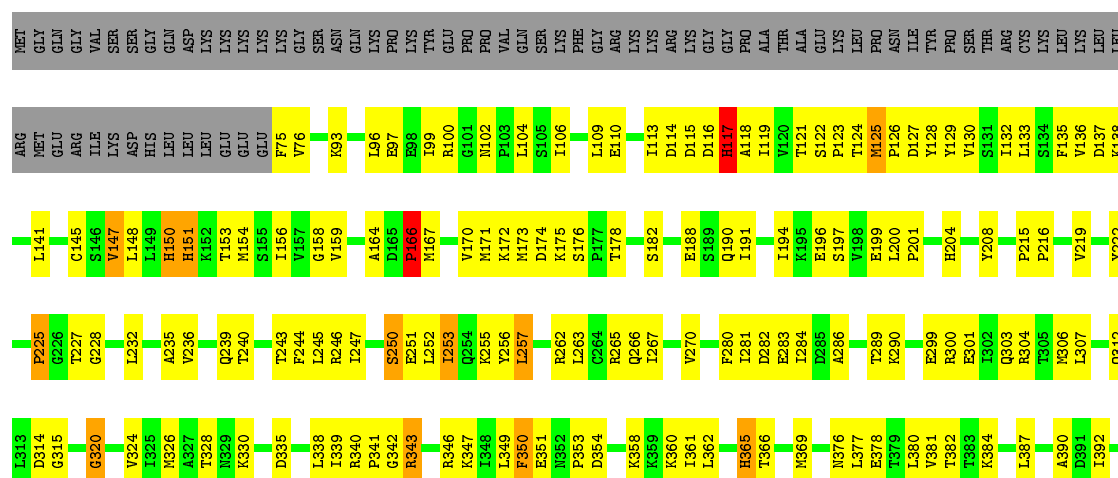
• Molecule 17: 26S PROTEASE REGULATORY SUBUNIT 7 HOMOLOG

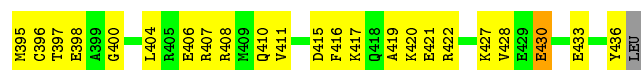
Chain H: 43% 29% 23%



• Molecule 18: 26S PROTEASE REGULATORY SUBUNIT 4 HOMOLOG

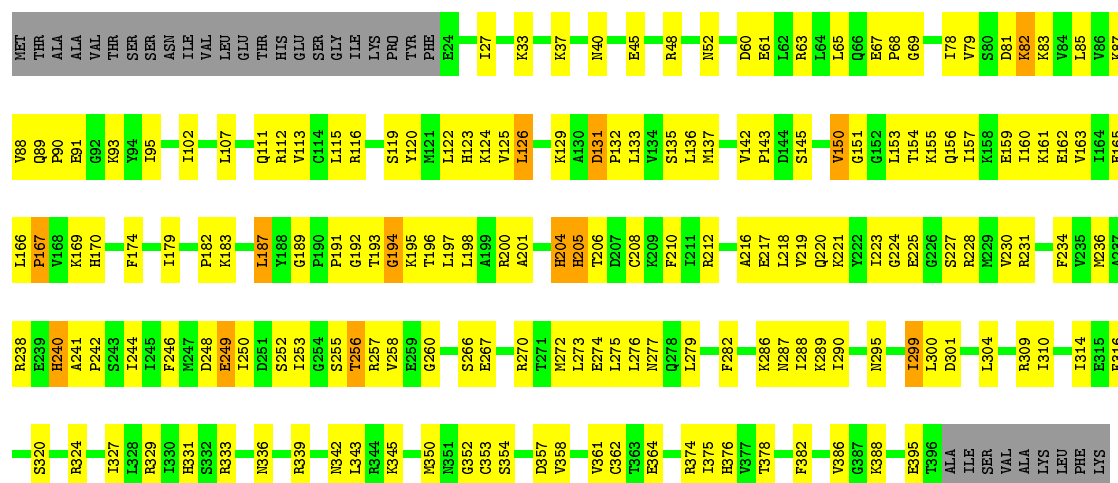
Chain I: 43% 37% 17%





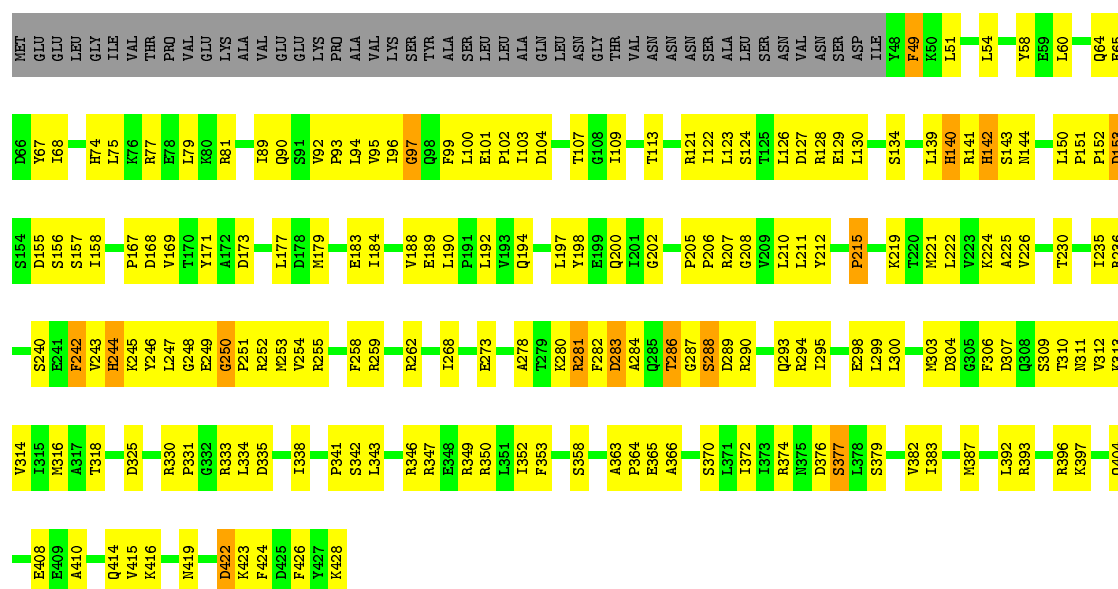
• Molecule 19: 26S PROTEASE REGULATORY SUBUNIT 8 HOMOLOG

Chain J: 49% 40% 8%



• Molecule 20: 26S PROTEASE REGULATORY SUBUNIT 6B HOMOLOG

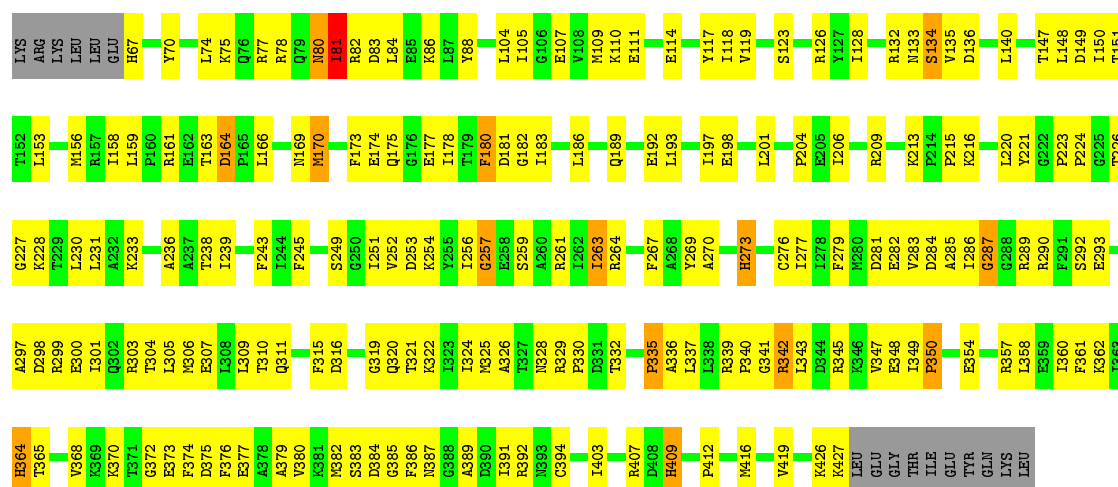
Chain K: 46% 40% 11%



• Molecule 21: 26S PROTEASE SUBUNIT RPT4

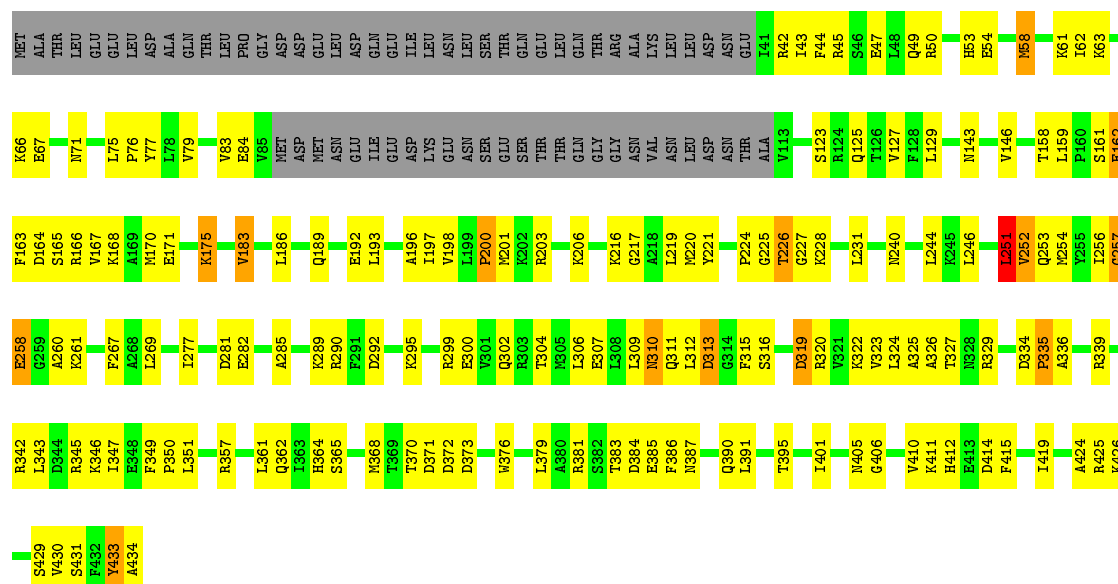
Chain L: 40% 40% 17%





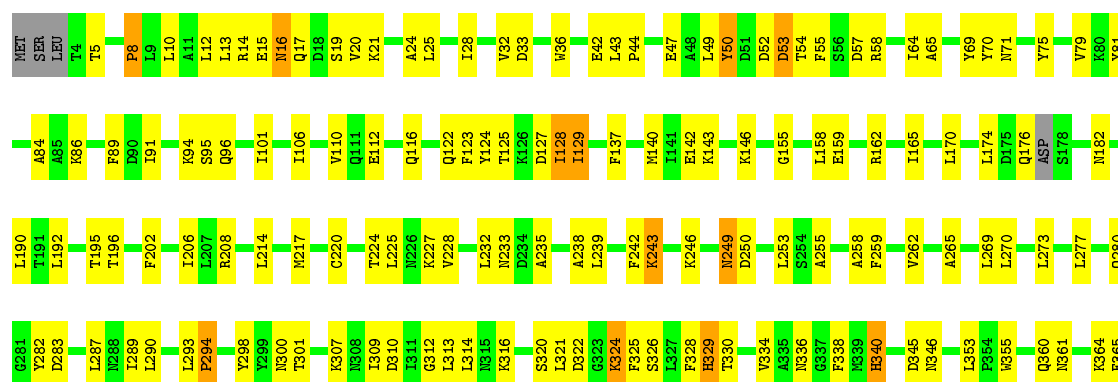
• Molecule 22: 26S PROTEASE REGULATORY SUBUNIT 6A

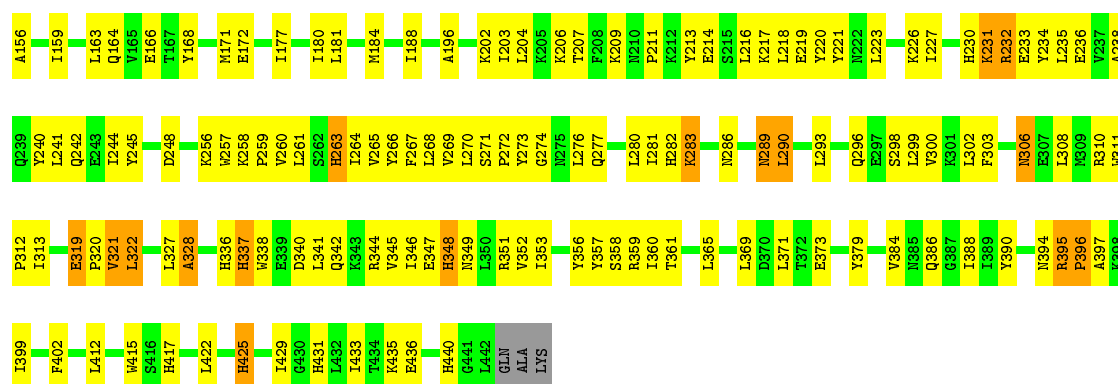
Chain M: 48% 33% 15%



• Molecule 23: 26S PROTEASOME REGULATORY SUBUNIT RPN2

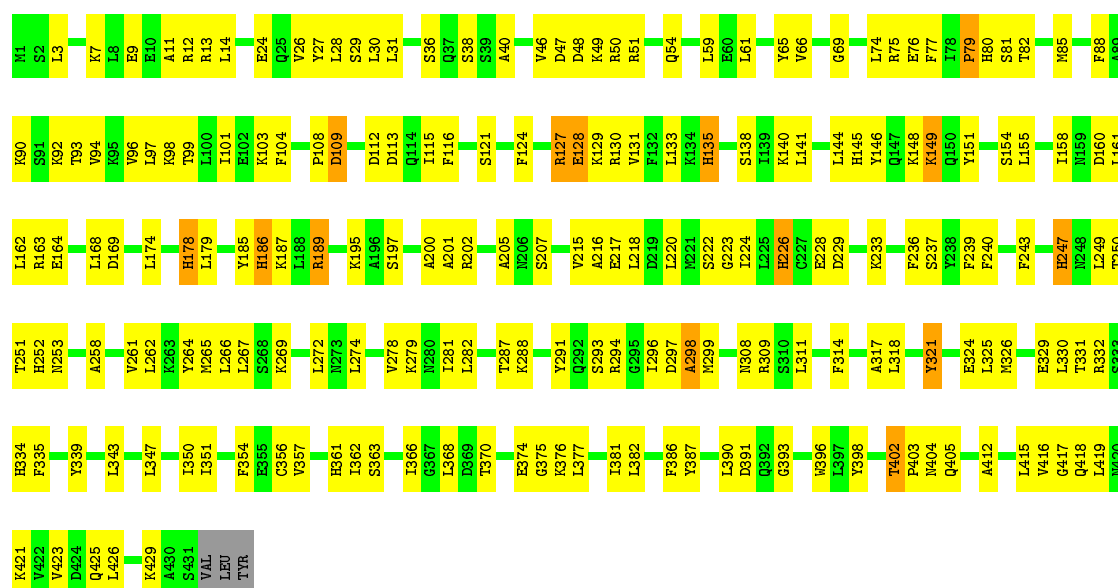
Chain N: 53% 33% 10%

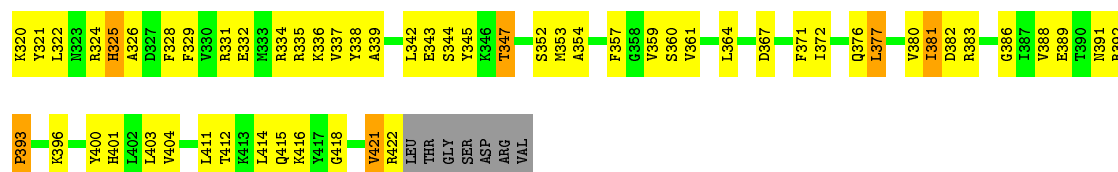




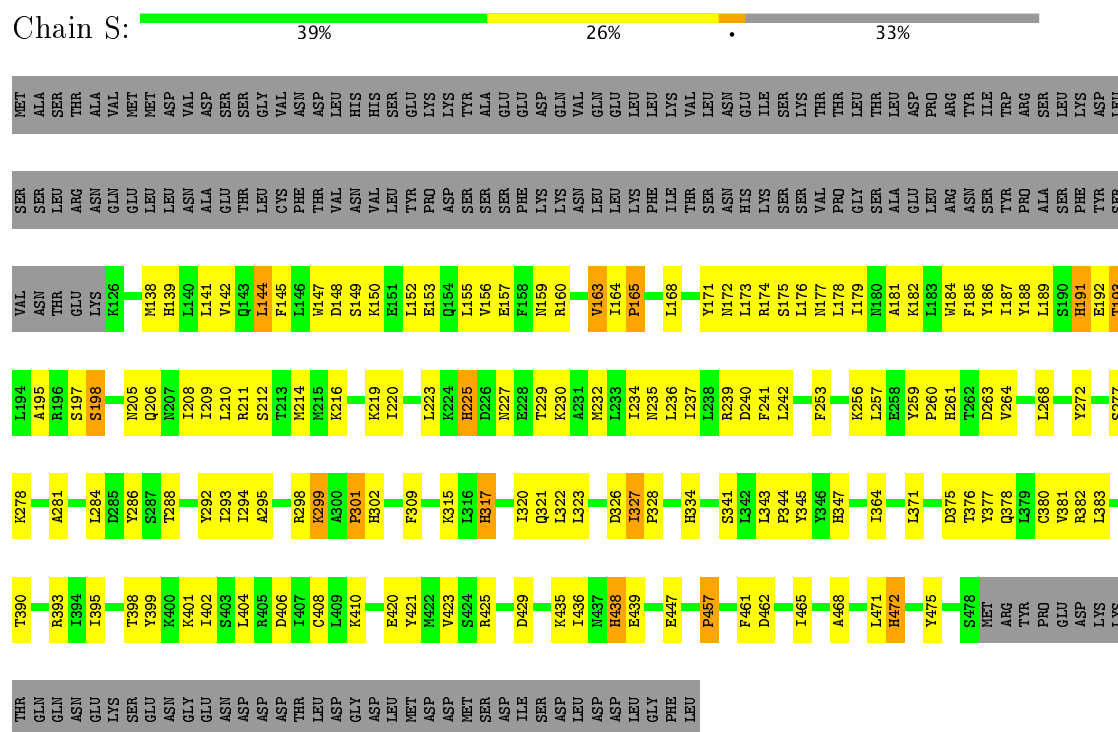
• Molecule 26: 26S PROTEASOME REGULATORY SUBUNIT RPN6

Chain Q: 53% 43%

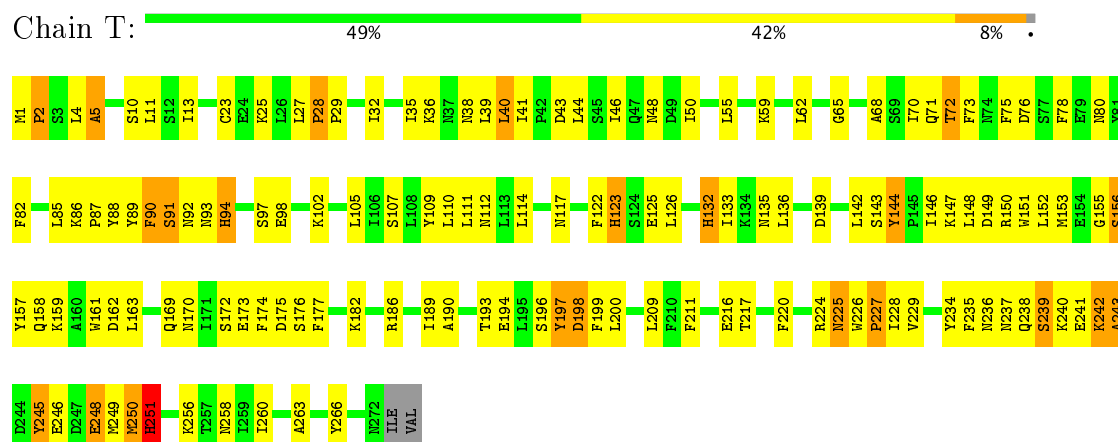




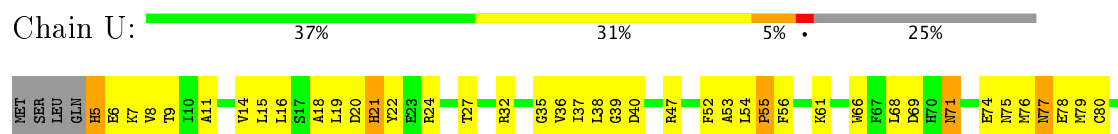
• Molecule 28: 26S PROTEASOME REGULATORY SUBUNIT RPN3

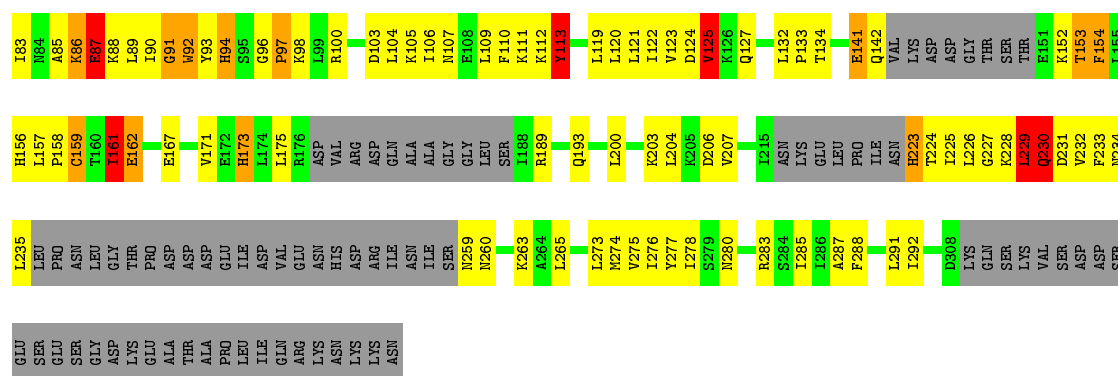


• Molecule 29: 26S PROTEASOME REGULATORY SUBUNIT RPN12



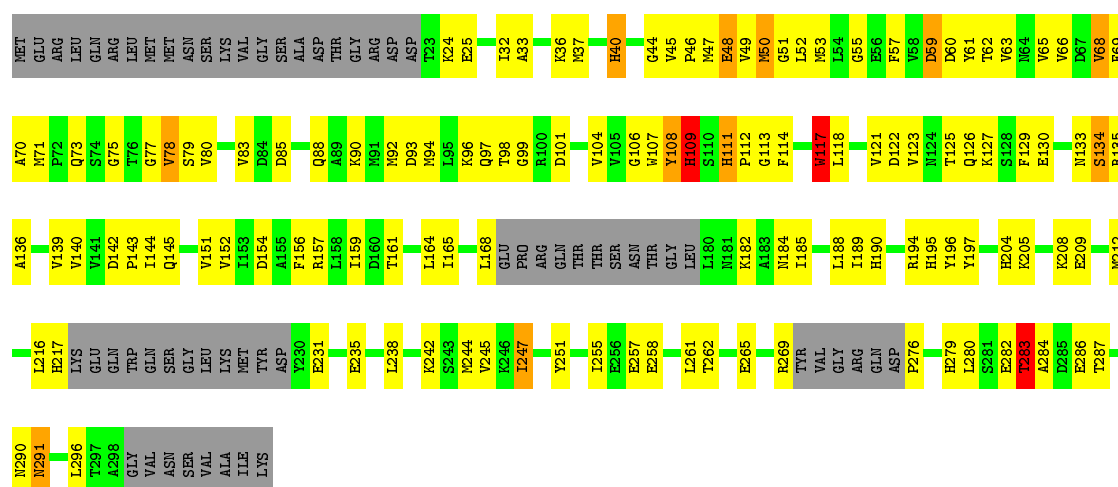
• Molecule 30: 26S PROTEASOME REGULATORY SUBUNIT RPN8





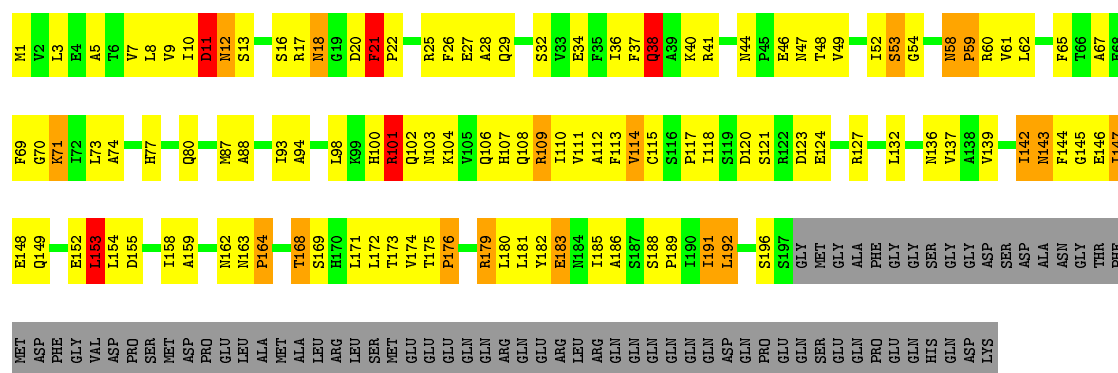
- Molecule 31: 26S PROTEASOME REGULATORY SUBUNIT RPN11

Chain V:  38% 38% .. 19%



- Molecule 32: 26S PROTEASOME REGULATORY SUBUNIT RPN10

Chain W: 29% 35% 7% 1% 26%



- Molecule 33: 26S PROTEASOME REGULATORY SUBUNIT RPN13

Chain X:  35% 40% 6% 19%



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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53000	Depositor
Resolution determination method	FSC	Depositor
CTF correction method	MICROGRAPH	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GLZ

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	A	1.23	10/1959 (0.5%)	1.21	10/2652 (0.4%)
11	B	1.21	8/1952 (0.4%)	1.21	5/2642 (0.2%)
12	C	1.16	11/1943 (0.6%)	1.19	2/2629 (0.1%)
13	D	1.12	7/1928 (0.4%)	1.13	2/2610 (0.1%)
14	E	1.19	8/1892 (0.4%)	1.14	2/2549 (0.1%)
15	F	1.23	13/1823 (0.7%)	1.16	4/2463 (0.2%)
16	G	1.24	15/1940 (0.8%)	1.22	4/2619 (0.2%)
17	H	1.08	7/2831 (0.2%)	1.28	11/3808 (0.3%)
18	I	1.17	14/2859 (0.5%)	1.20	8/3853 (0.2%)
19	J	1.17	13/2962 (0.4%)	1.15	4/3975 (0.1%)
2	2	1.24	14/1723 (0.8%)	1.25	4/2337 (0.2%)
20	K	1.21	10/3061 (0.3%)	1.37	11/4129 (0.3%)
21	L	1.16	11/2895 (0.4%)	1.14	3/3892 (0.1%)
22	M	1.17	10/2903 (0.3%)	1.24	14/3909 (0.4%)
23	N	1.15	31/6670 (0.5%)	1.21	26/9023 (0.3%)
24	O	0.73	10/3243 (0.3%)	0.95	4/4374 (0.1%)
25	P	1.17	12/3452 (0.3%)	1.20	12/4657 (0.3%)
26	Q	1.11	16/3527 (0.5%)	1.09	7/4748 (0.1%)
27	R	1.05	12/3272 (0.4%)	1.08	4/4412 (0.1%)
28	S	1.08	13/2945 (0.4%)	1.11	2/3976 (0.1%)
29	T	1.04	9/2279 (0.4%)	1.07	3/3077 (0.1%)
3	3	1.18	7/1611 (0.4%)	1.17	2/2174 (0.1%)
30	U	1.82	12/2087 (0.6%)	1.16	11/2811 (0.4%)
31	V	1.20	12/1969 (0.6%)	1.26	16/2652 (0.6%)
32	W	1.40	12/1556 (0.8%)	1.73	16/2108 (0.8%)
33	X	1.20	4/1058 (0.4%)	1.33	5/1432 (0.3%)
34	Y	0.97	0/169	0.94	0/223
35	Z	1.03	31/6403 (0.5%)	1.12	15/8686 (0.2%)
4	4	1.16	8/1613 (0.5%)	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%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
7	7	1.14	6/1855 (0.3%)	1.14	2/2514 (0.1%)
8	8	0.64	2/3093 (0.1%)	0.75	1/4141 (0.0%)
9	9	0.47	0/603	0.75	1/811 (0.1%)
All	All	1.14	375/85159 (0.4%)	1.17	225/114927 (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
10	A	0	3
13	D	0	1
15	F	0	1
17	H	0	6
19	J	0	1
21	L	0	4
22	M	0	2
23	N	0	7
24	O	0	2
25	P	0	3
26	Q	0	1
27	R	0	2
28	S	0	1
29	T	0	2
30	U	0	6
31	V	0	6
32	W	0	11
33	X	0	3
35	Z	0	7
6	6	0	1
7	7	0	2
All	All	0	73

The worst 5 of 375 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	U	230	GLN	N-CA	70.24	2.86	1.46
32	W	38	GLN	C-N	-38.10	0.46	1.34
20	K	242	PHE	C-N	21.53	1.83	1.34
22	M	257	GLY	C-N	20.41	1.80	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	Z	134	SER	N-CA	16.22	1.78	1.46

The worst 5 of 225 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	W	154	LEU	O-C-N	34.34	177.64	122.70
20	K	242	PHE	O-C-N	27.34	166.44	122.70
20	K	242	PHE	C-N-CA	-26.79	54.71	121.70
32	W	154	LEU	CA-C-N	-25.06	62.07	117.20
23	N	889	ARG	NE-CZ-NH1	23.10	131.85	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
10	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	199	0
2	2	1692	0	1699	93	0
3	3	1581	0	1574	102	0
4	4	1585	0	1590	91	0
5	5	1646	0	1595	122	0
6	6	1757	0	1711	86	0
7	7	1824	0	1832	150	0
8	8	3008	0	2929	210	0
9	9	601	0	624	148	0
10	A	1921	0	1909	159	0
11	B	1915	0	1929	144	0
12	C	1913	0	1914	146	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	D	1899	0	1908	108	0
14	E	1867	0	1841	161	0
15	F	1795	0	1797	178	0
16	G	1900	0	1888	192	0
17	H	2792	0	2878	342	0
18	I	2822	0	2869	288	0
19	J	2928	0	3054	358	0
20	K	3019	0	3079	411	0
21	L	2853	0	2925	284	0
22	M	2866	0	2936	288	0
23	N	6562	0	6625	481	0
24	O	3182	0	3207	604	0
25	P	3401	0	3483	321	0
26	Q	3471	0	3494	359	0
27	R	3218	0	3216	408	0
28	S	2893	0	2937	244	0
29	T	2235	0	2206	305	0
30	U	2061	0	2116	376	0
31	V	1942	0	1954	250	0
32	W	1534	0	1538	204	0
33	X	1032	0	1017	182	0
34	Y	168	0	153	17	0
35	Z	6289	0	6233	619	0
All	All	83748	0	84215	7435	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 44.

The worst 5 of 7435 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)
35:Z:321:PHE:CZ	35:Z:350:GLY:HA2	1.23	1.67
8:8:320:LYS:HE3	17:H:164:SER:CB	1.22	1.66
24:O:373:TRP:CD1	30:U:200:LEU:HD21	1.29	1.65
26:Q:243:PHE:HZ	26:Q:287:THR:CA	1.07	1.64
24:O:373:TRP:HD1	30:U:200:LEU:CD2	1.02	1.61

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	8	368/416 (88%)	364 (99%)	4 (1%)	0	100	100
9	9	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
10	A	241/252 (96%)	217 (90%)	20 (8%)	4 (2%)	11	50
11	B	248/250 (99%)	227 (92%)	15 (6%)	6 (2%)	7	42
12	C	243/258 (94%)	224 (92%)	16 (7%)	3 (1%)	15	57
13	D	240/254 (94%)	221 (92%)	16 (7%)	3 (1%)	14	56
14	E	241/260 (93%)	225 (93%)	13 (5%)	3 (1%)	15	57
15	F	231/234 (99%)	209 (90%)	19 (8%)	3 (1%)	14	56
16	G	243/288 (84%)	224 (92%)	16 (7%)	3 (1%)	15	57
17	H	353/467 (76%)	298 (84%)	36 (10%)	19 (5%)	2	25
18	I	358/437 (82%)	326 (91%)	25 (7%)	7 (2%)	9	46
19	J	367/405 (91%)	337 (92%)	21 (6%)	9 (2%)	6	41
20	K	377/428 (88%)	336 (89%)	29 (8%)	12 (3%)	5	36
21	L	357/437 (82%)	326 (91%)	18 (5%)	13 (4%)	4	33
22	M	363/434 (84%)	322 (89%)	29 (8%)	12 (3%)	4	35
23	N	843/945 (89%)	786 (93%)	37 (4%)	20 (2%)	7	42
24	O	385/393 (98%)	309 (80%)	44 (11%)	32 (8%)	1	16
25	P	413/445 (93%)	374 (91%)	22 (5%)	17 (4%)	3	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Q	429/434 (99%)	390 (91%)	28 (6%)	11 (3%)	6	40
27	R	398/429 (93%)	345 (87%)	36 (9%)	17 (4%)	3	29
28	S	351/523 (67%)	308 (88%)	31 (9%)	12 (3%)	4	35
29	T	270/274 (98%)	235 (87%)	16 (6%)	19 (7%)	1	19
30	U	245/338 (72%)	226 (92%)	9 (4%)	10 (4%)	3	30
31	V	239/306 (78%)	212 (89%)	18 (8%)	9 (4%)	4	32
32	W	193/268 (72%)	156 (81%)	17 (9%)	20 (10%)	0	10
33	X	125/156 (80%)	101 (81%)	19 (15%)	5 (4%)	3	31
34	Y	17/89 (19%)	17 (100%)	0	0	100	100
35	Z	807/993 (81%)	690 (86%)	68 (8%)	49 (6%)	2	22
All	All	10502/12162 (86%)	9449 (90%)	711 (7%)	342 (3%)	8	35

5 of 342 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	4	150	ASP
11	B	203	GLU
13	D	31	THR
13	D	204	GLN
17	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	7	199/224 (89%)	199 (100%)	0	100	100
8	8	331/369 (90%)	325 (98%)	6 (2%)	64	84
9	9	68/68 (100%)	64 (94%)	4 (6%)	23	55
10	A	207/210 (99%)	207 (100%)	0	100	100
11	B	209/209 (100%)	209 (100%)	0	100	100
12	C	204/216 (94%)	204 (100%)	0	100	100
13	D	214/226 (95%)	214 (100%)	0	100	100
14	E	199/215 (93%)	199 (100%)	0	100	100
15	F	192/193 (100%)	192 (100%)	0	100	100
16	G	201/239 (84%)	200 (100%)	1 (0%)	91	95
17	H	303/399 (76%)	302 (100%)	1 (0%)	94	96
18	I	319/385 (83%)	318 (100%)	1 (0%)	94	96
19	J	325/352 (92%)	324 (100%)	1 (0%)	94	96
20	K	334/374 (89%)	333 (100%)	1 (0%)	94	96
21	L	308/377 (82%)	308 (100%)	0	100	100
22	M	315/375 (84%)	315 (100%)	0	100	100
23	N	713/797 (90%)	710 (100%)	3 (0%)	93	95
24	O	363/368 (99%)	361 (99%)	2 (1%)	89	94
25	P	388/415 (94%)	380 (98%)	8 (2%)	59	80
26	Q	388/391 (99%)	388 (100%)	0	100	100
27	R	351/379 (93%)	351 (100%)	0	100	100
28	S	330/489 (68%)	330 (100%)	0	100	100
29	T	254/256 (99%)	254 (100%)	0	100	100
30	U	234/308 (76%)	228 (97%)	6 (3%)	51	75
31	V	217/268 (81%)	214 (99%)	3 (1%)	71	86
32	W	171/230 (74%)	169 (99%)	2 (1%)	75	88
33	X	116/144 (81%)	114 (98%)	2 (2%)	66	84
34	Y	18/81 (22%)	18 (100%)	0	100	100
35	Z	692/850 (81%)	692 (100%)	0	100	100
All	All	9215/10583 (87%)	9172 (100%)	43 (0%)	91	95

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	N	905	LEU
25	P	43	GLU
32	W	8	LEU
24	O	20	PRO
24	O	58	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 173 such sidechains are listed below:

Mol	Chain	Res	Type
21	L	67	HIS
23	N	707	ASN
32	W	103	ASN
21	L	80	ASN
23	N	71	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GLZ	9	76	-	3,3,3	2.25	1 (33%)	1,2,2	3.28	1 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GLZ	9	76	-	-	0/0/1/1	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	9	76	GLZ	O-C	3.84	1.43	1.19

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	9	76	GLZ	O-C-CA	-3.28	109.89	125.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	9	76	GLZ	18	0

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
32	W	3
19	J	2
20	K	2
31	V	2
21	L	2

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Mol	Chain	Number of breaks
22	M	2
18	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