



wwPDB EM Map/Model Validation Report

Aug 8, 2016 – 02:51 PM EDT

PDB ID : 5GJQ
EMDB ID: : EMD-9511
Title : Structure of the human 26S proteasome bound to USP14-UbA1
Authors : Huang, X.L.; Luan, B.; Wu, J.P.; Shi, Y.G.
Deposited on : 2016-07-01
Resolution : 4.50 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

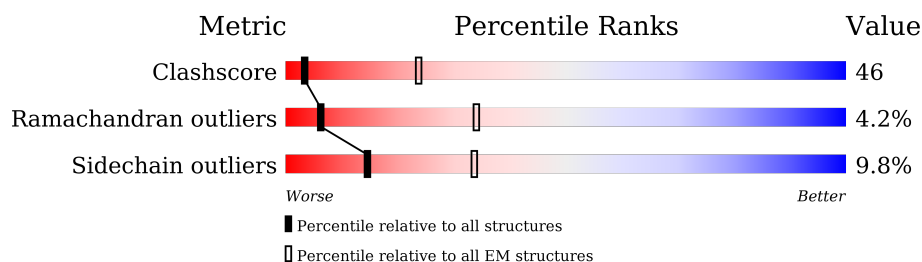
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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.






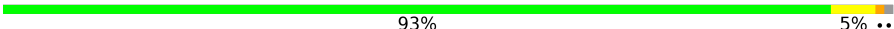













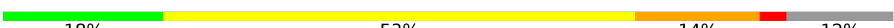

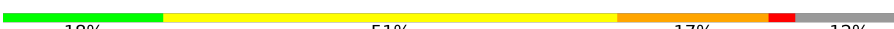
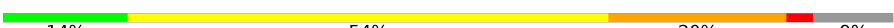
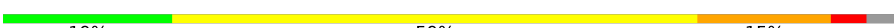
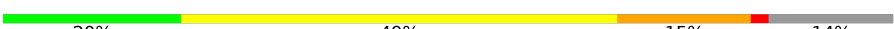


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	a	239	78% 6% 15%
1	o	239	75% 10% 15%
2	B	246	68% 29% ..
2	h	246	93% 6% .
3	b	277	76% . 21%
3	p	277	73% 6% . 21%
4	C	234	79% 18% .
4	i	234	87% 12% .
5	c	205	92% 8%

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Mol	Chain	Length	Quality of chain
5	q	205	
6	D	261	
6	j	261	
7	d	201	
7	r	201	
8	E	248	
8	k	248	
9	e	263	
9	s	263	
10	F	241	
10	l	241	
11	f	241	
11	t	241	
12	G	263	
12	m	263	
13	g	264	
13	u	264	
14	H	433	
15	I	440	
16	J	406	
17	K	418	
18	L	389	
19	M	439	
20	N	953	
21	X	255	

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Mol	Chain	Length	Quality of chain
21	n	255	 89% 5% 5%
22	O	376	 54% 38% 7% .
23	P	456	 42% 43% 5% . 9%
24	Q	422	 30% 57% 12% .
25	R	389	 37% 50% 9% . .
26	S	534	 43% 27% . 26%
27	T	350	 33% 35% 5% . 26%
28	U	324	 33% 44% 10% 13%
29	V	310	 30% 43% 8% . 17%
30	W	377	 18% 29% . . 49%
31	Y	70	 43% 37% . 16%
32	Z	908	 50% 27% . 19%
33	x	494	 55% 15% . 28%
34	y	76	 93% 7%

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
35	ADP	H	501	-	-	X	-
35	ADP	K	501	-	-	X	-

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 98461 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-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	202	Total	C	N	O	S	0	0
			1509	945	258	294	12		
1	o	202	Total	C	N	O	S	0	0
			1509	945	258	294	12		

- Molecule 2 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	244	Total	C	N	O	S	0	0
			1845	1171	309	352	13		
2	h	244	Total	C	N	O	S	0	0
			1853	1177	311	352	13		

- Molecule 3 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	b	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		
3	p	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		

- Molecule 4 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	233	Total	C	N	O	S	0	0
			1707	1081	287	334	5		
4	i	231	Total	C	N	O	S	0	0
			1744	1112	290	336	6		

- Molecule 5 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	c	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		
5	q	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		

- Molecule 6 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		
6	j	250	Total	C	N	O	S	0	0
			1913	1203	330	372	8		

- Molecule 7 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	d	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		
7	r	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

- Molecule 8 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	243	Total	C	N	O	S	0	0
			1724	1068	312	339	5		
8	k	243	Total	C	N	O	S	0	0
			1691	1051	309	327	4		

- Molecule 9 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	e	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		
9	s	201	Total	C	N	O	S	0	0
			1551	977	273	292	9		

- Molecule 10 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	234	Total	C	N	O	S	0	0
			1766	1108	290	357	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	l	234	Total	C	N	O	S	0	0
			1726	1107	291	317	11		

- Molecule 11 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	f	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		
11	t	213	Total	C	N	O	S	0	0
			1644	1039	282	313	10		

- Molecule 12 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		
12	m	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	g	216	Total	C	N	O	S	0	0
			1672	1055	286	319	12		
13	u	217	Total	C	N	O	S	0	0
			1678	1058	290	318	12		

- Molecule 14 is a protein called 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	380	Total	C	N	O	S	0	0
			2879	1809	513	539	18		

- Molecule 15 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	359	Total	C	N	O	S	0	0
			2720	1708	465	535	12		

- Molecule 16 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	358	Total	C	N	O	S	0	0
			2820	1780	506	518	16		

- Molecule 17 is a protein called 26S protease regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	380	Total	C	N	O	S	0	0
			3039	1923	524	579	13		

- Molecule 18 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	375	Total	C	N	O	S	0	0
			2860	1796	512	536	16		

- Molecule 19 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	376	Total	C	N	O	S	0	0
			2858	1802	496	545	15		

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	823	Total	C	N	O	S	0	0
			5462	3499	933	1012	18		

- Molecule 21 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	n	243	Total	C	N	O	S	0	0
			1873	1189	317	356	11		
21	X	243	Total	C	N	O	S	0	0
			1873	1189	317	356	11		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	372	Total	C	N	O	S	0	0
			2372	1518	405	438	11		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	413	Total	C	N	O	S	0	0
			2828	1819	489	514	6		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	421	Total	C	N	O	S	0	0
			2948	1864	509	567	8		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	376	Total	C	N	O	S	0	0
			2767	1794	461	503	9		

- Molecule 26 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S	395	Total	C	N	O	S	0	0
			2600	1662	463	472	3		

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	258	Total	C	N	O	S	0	0
			1702	1102	280	315	5		

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U	283	Total	C	N	O	S	0	0
			2131	1370	369	388	4		

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	257	Total	C	N	O	S	0	0
			2011	1276	341	377	17		

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	193	Total	C	N	O	S	0	0
			1300	818	228	250	4		

- Molecule 31 is a protein called 26S proteasome complex subunit DSS1.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	Y	59	Total	C	N	O	0	0
			308	184	60	64		

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Z	732	Total	C	N	O	0	0
			3608	2144	732	732		

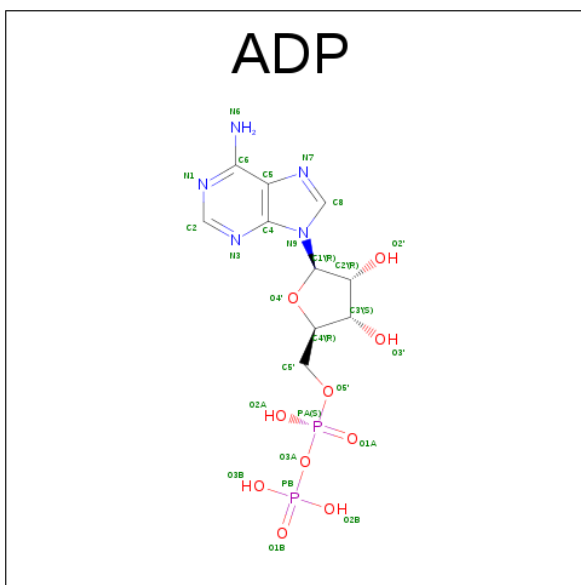
- Molecule 33 is a protein called Ubiquitin carboxyl-terminal hydrolase 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	x	355	Total	C	N	O	S	0	0
			2810	1782	470	538	20		

- Molecule 34 is a protein called Polyubiquitin-B.

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

- Molecule 35 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

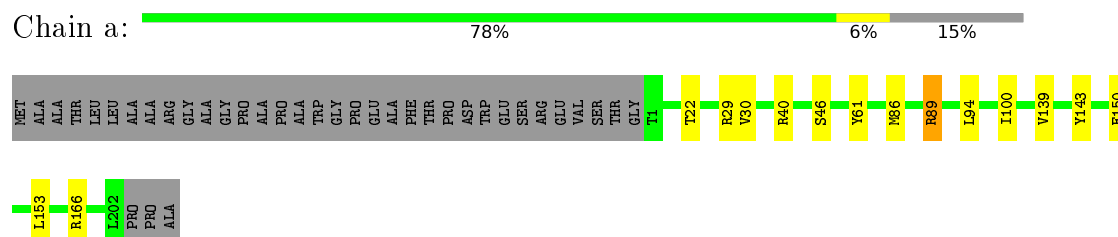


Mol	Chain	Residues	Atoms					AltConf
35	H	1	Total 27	C 10	N 5	O 10	P 2	0
35	I	1	Total 27	C 10	N 5	O 10	P 2	0
35	J	1	Total 27	C 10	N 5	O 10	P 2	0
35	K	1	Total 27	C 10	N 5	O 10	P 2	0
35	L	1	Total 27	C 10	N 5	O 10	P 2	0
35	M	1	Total 27	C 10	N 5	O 10	P 2	0

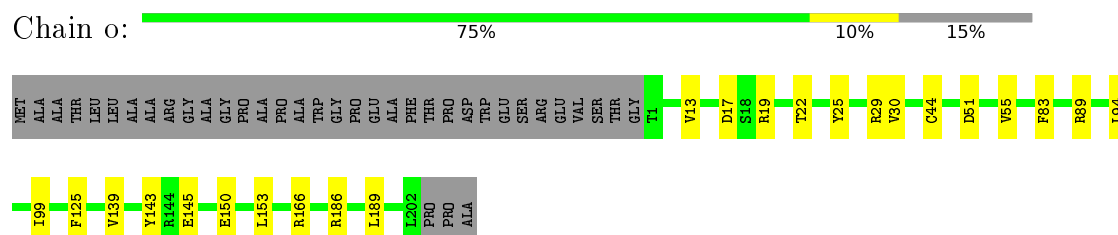
3 Residue-property plots [i](#)

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

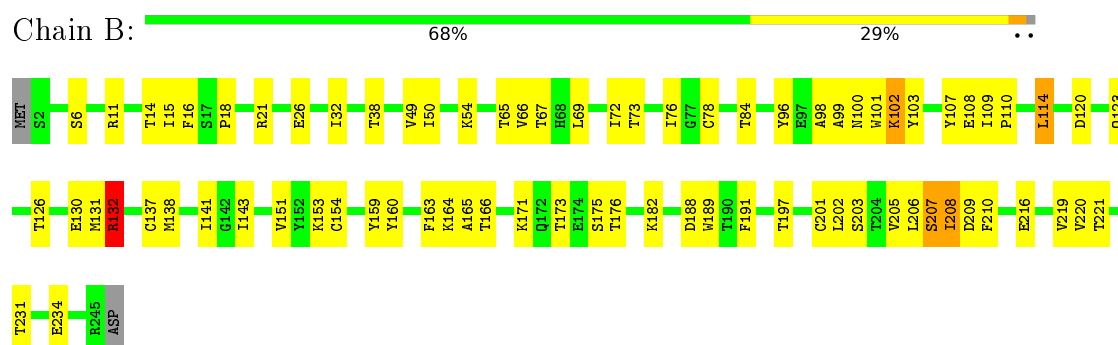
- Molecule 1: Proteasome subunit beta type-6



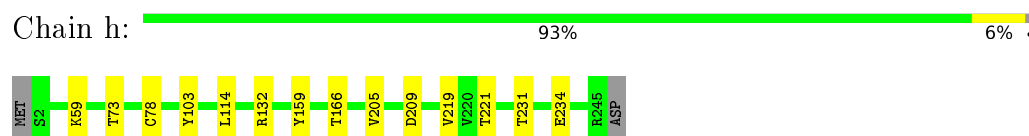
- Molecule 1: Proteasome subunit beta type-6




- Molecule 2: Proteasome subunit alpha type-6

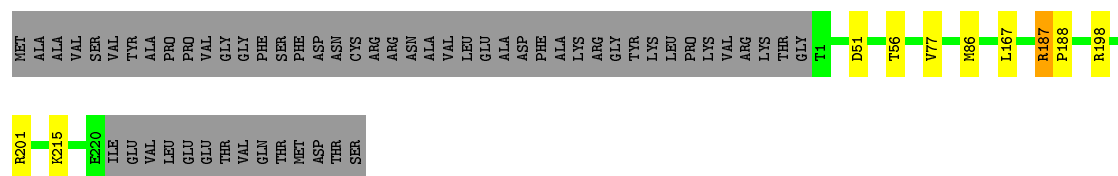


- Molecule 2: Proteasome subunit alpha type-6



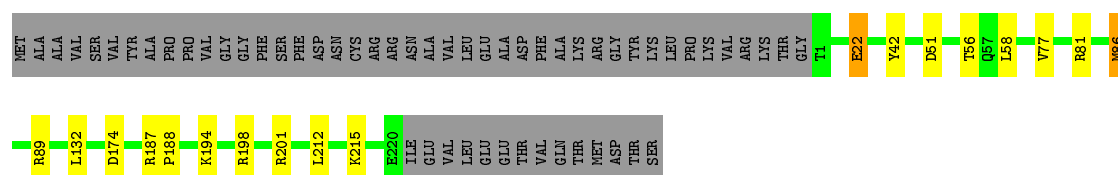
- Molecule 3: Proteasome subunit beta type-7

Chain b:  76% 21%




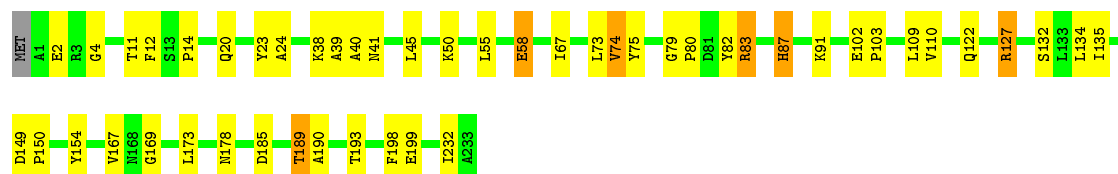
- Molecule 3: Proteasome subunit beta type-7

Chain p:  73% 6% 21%




- Molecule 4: Proteasome subunit alpha type-2

Chain C:  79% 18%



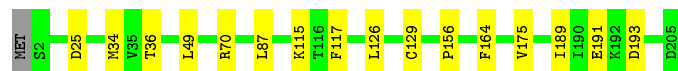
- Molecule 4: Proteasome subunit alpha type-2

Chain i:  87% 12%




- Molecule 5: Proteasome subunit beta type-3

Chain c:  92% 8%




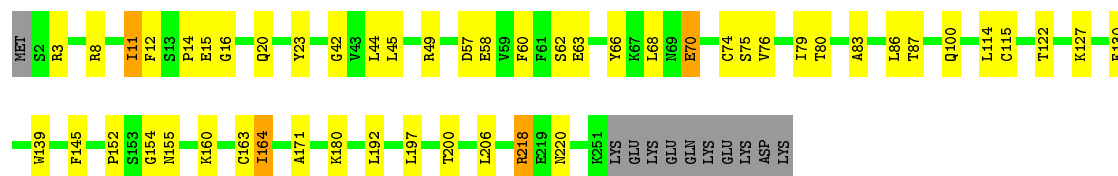
- Molecule 5: Proteasome subunit beta type-3

Chain q:  90% 10%



- Molecule 6: Proteasome subunit alpha type-4

Chain D:  76% 18% . .



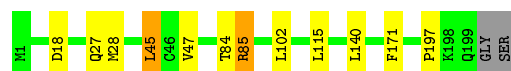
- Molecule 6: Proteasome subunit alpha type-4

Chain j:  89% 7% .




- Molecule 7: Proteasome subunit beta type-2

Chain d:  93% 5% ..




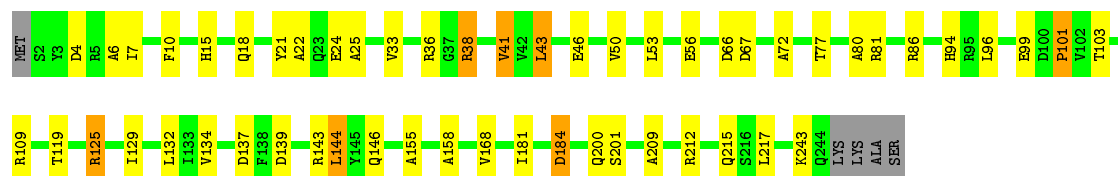
- Molecule 7: Proteasome subunit beta type-2

Chain r:  89% 9% .




- Molecule 8: Proteasome subunit alpha type-7

Chain E:  76% 19% . .



- Molecule 8: Proteasome subunit alpha type-7

Chain k:  90% 8% .

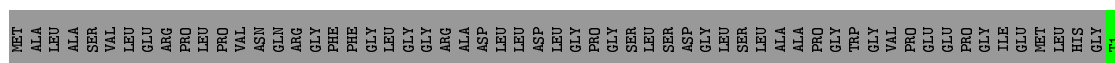


- Molecule 9: Proteasome subunit beta type-5

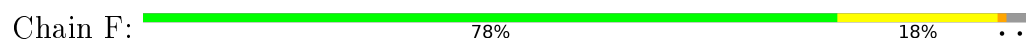
Chain e:  72% 5% 24%



• Molecule 9: Proteasome subunit beta type-5



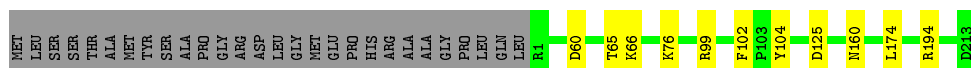
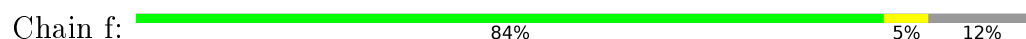
• Molecule 10: Proteasome subunit alpha type-5



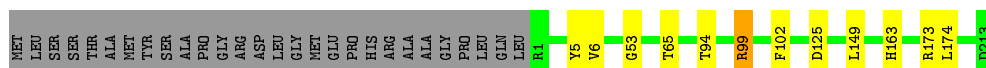
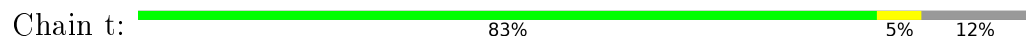
• Molecule 10: Proteasome subunit alpha type-5



• Molecule 11: Proteasome subunit beta type-1

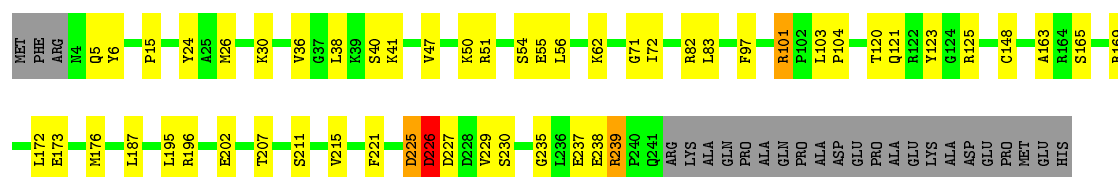


• Molecule 11: Proteasome subunit beta type-1



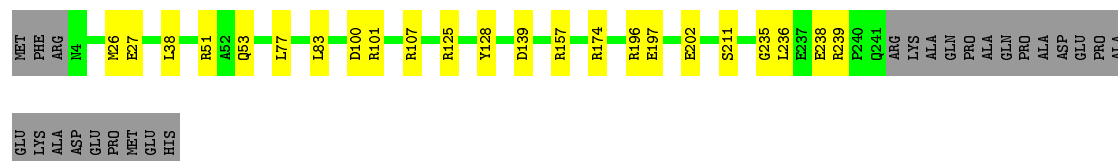
• Molecule 12: Proteasome subunit alpha type-1





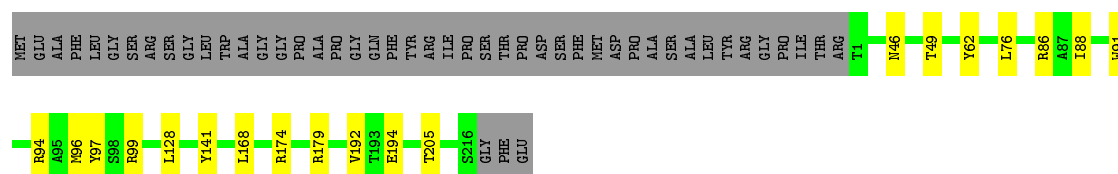
• Molecule 12: Proteasome subunit alpha type-1

Chain m: 82% 9% 10%



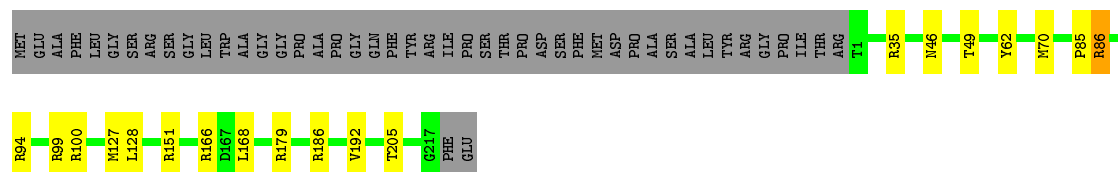
• Molecule 13: Proteasome subunit beta type-4

Chain g: 75% 7% 18%



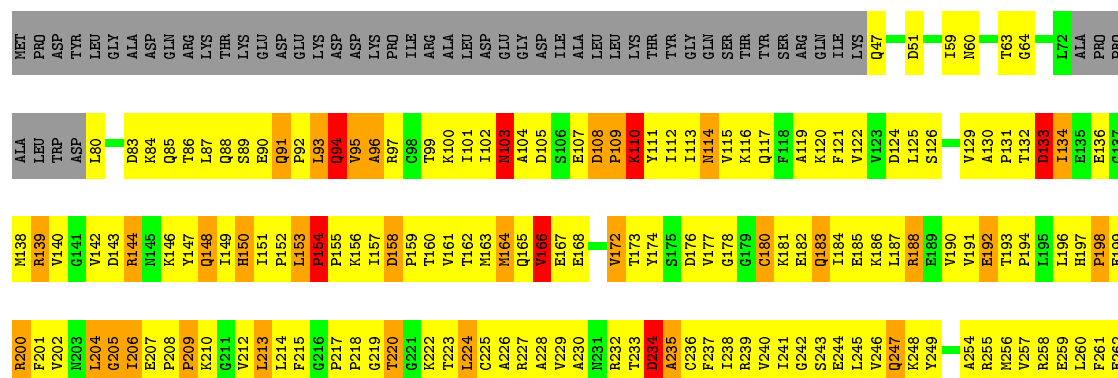
• Molecule 13: Proteasome subunit beta type-4

Chain u: 75% 7% 18%

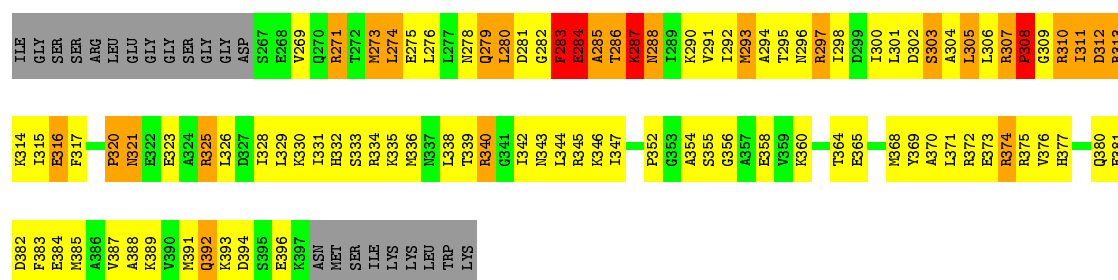


• Molecule 14: 26S protease regulatory subunit 7

Chain H: 18% 53% 14% 12%

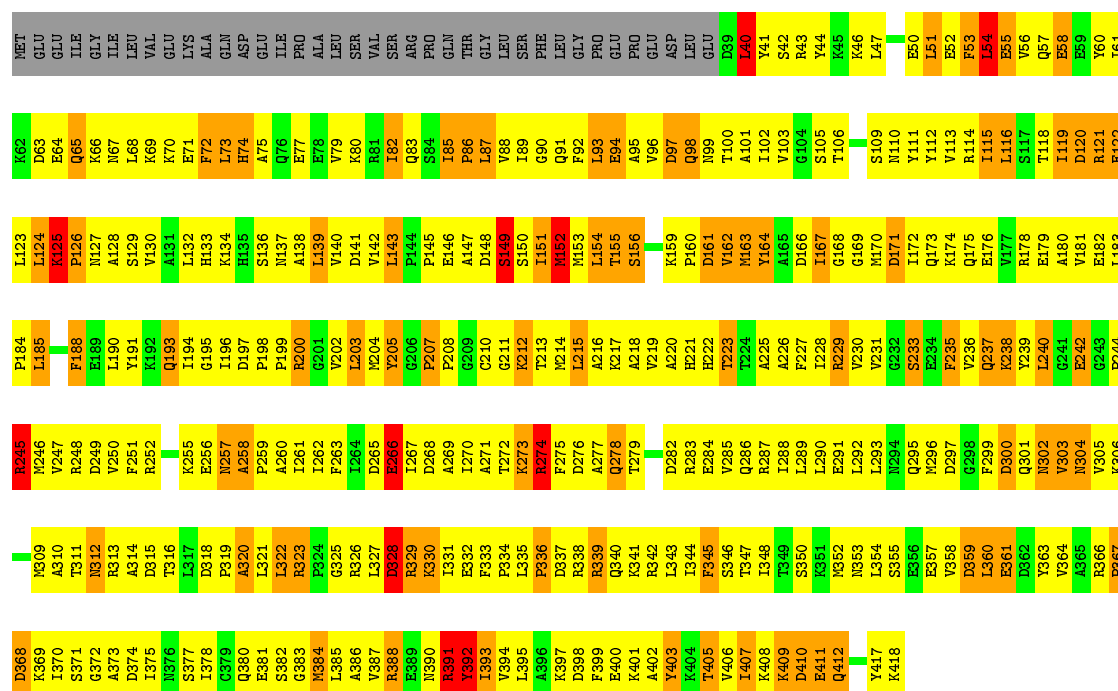






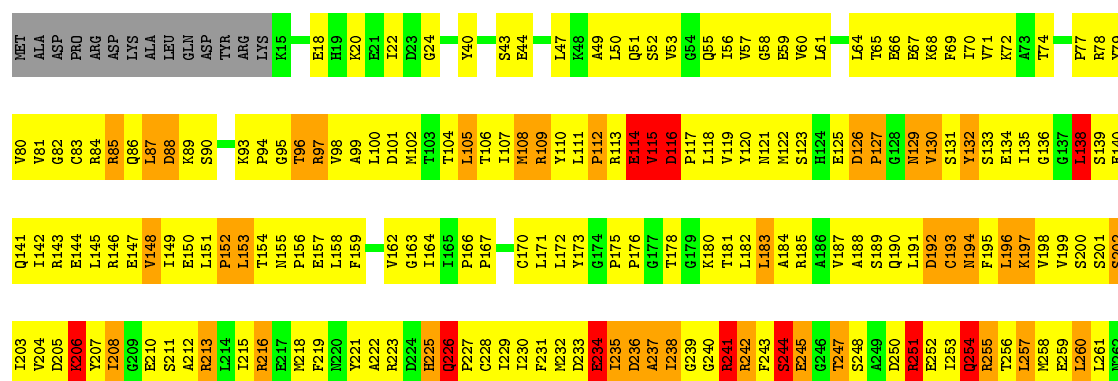
• Molecule 17: 26S protease regulatory subunit 6B

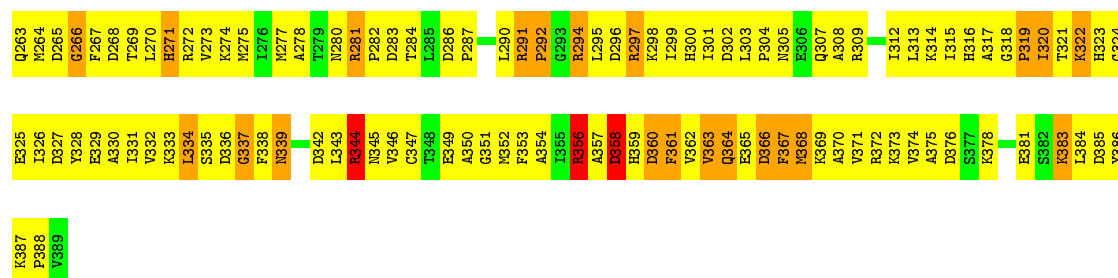
Chain K: 14% 54% 20% 9%



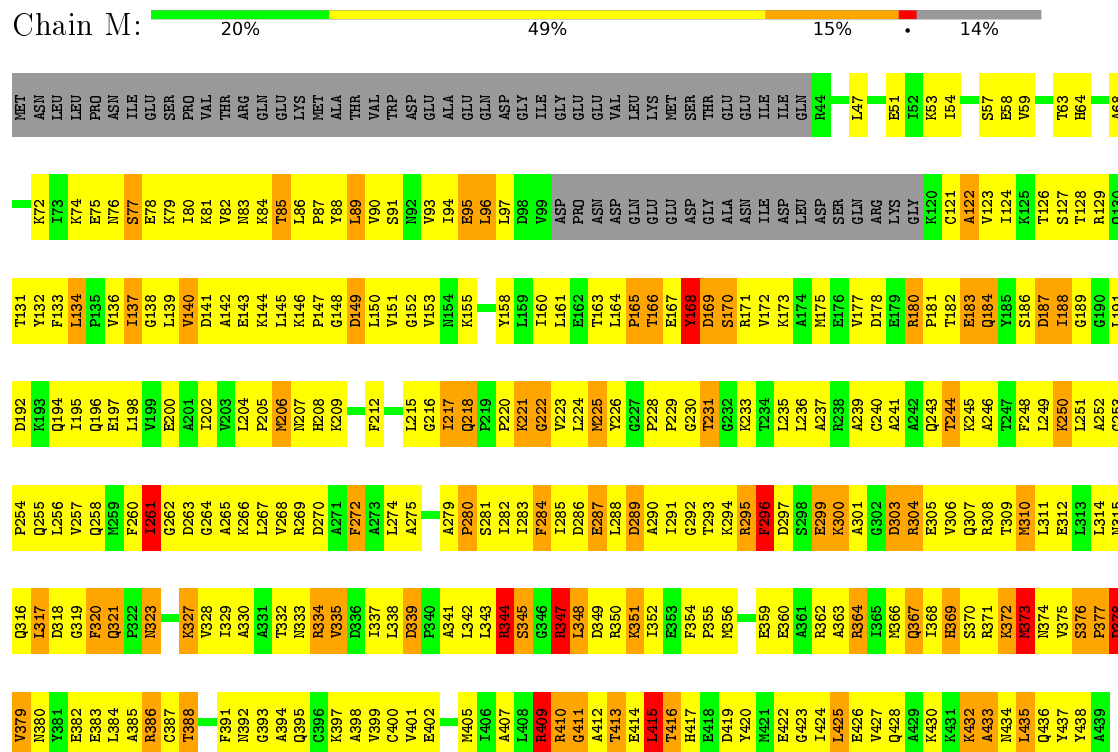
• Molecule 18: 26S protease regulatory subunit 10B

Chain L: 19% 59% 15%

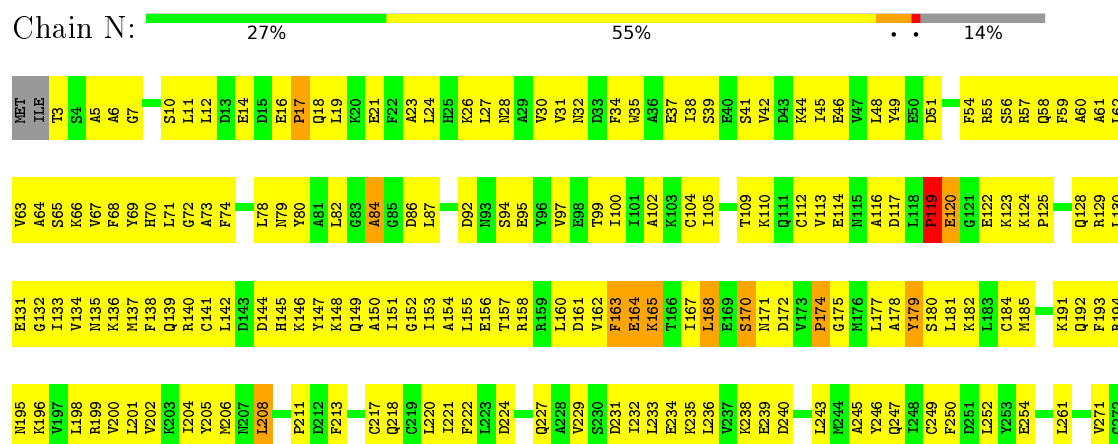


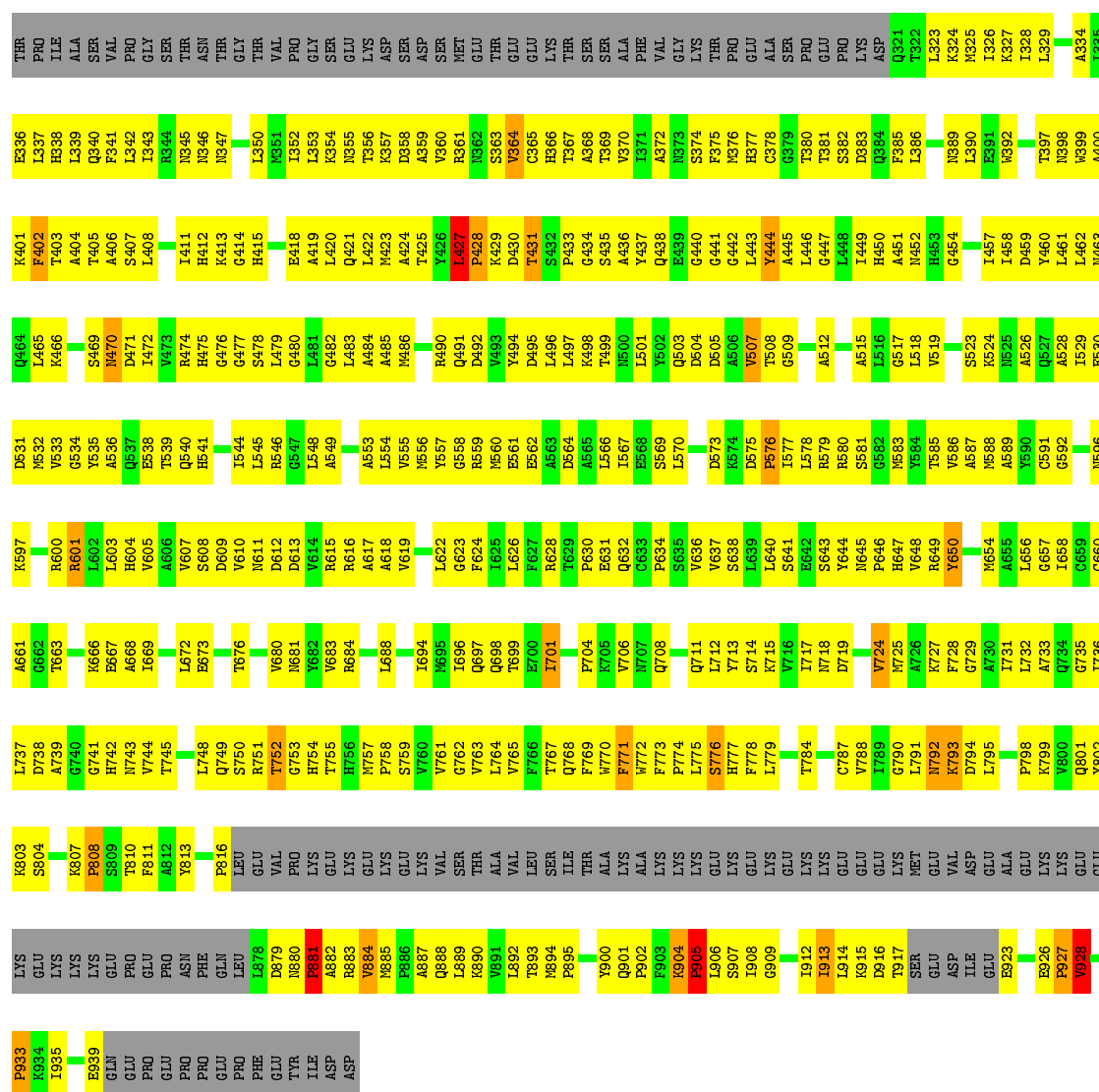


• Molecule 19: 26S protease regulatory subunit 6A



• Molecule 20: 26S proteasome non-ATPase regulatory subunit 1





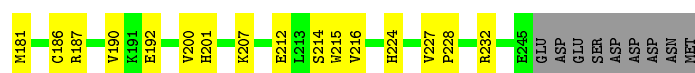
- Molecule 21: Proteasome subunit alpha type-3

Chain n: 89% 5% 5%

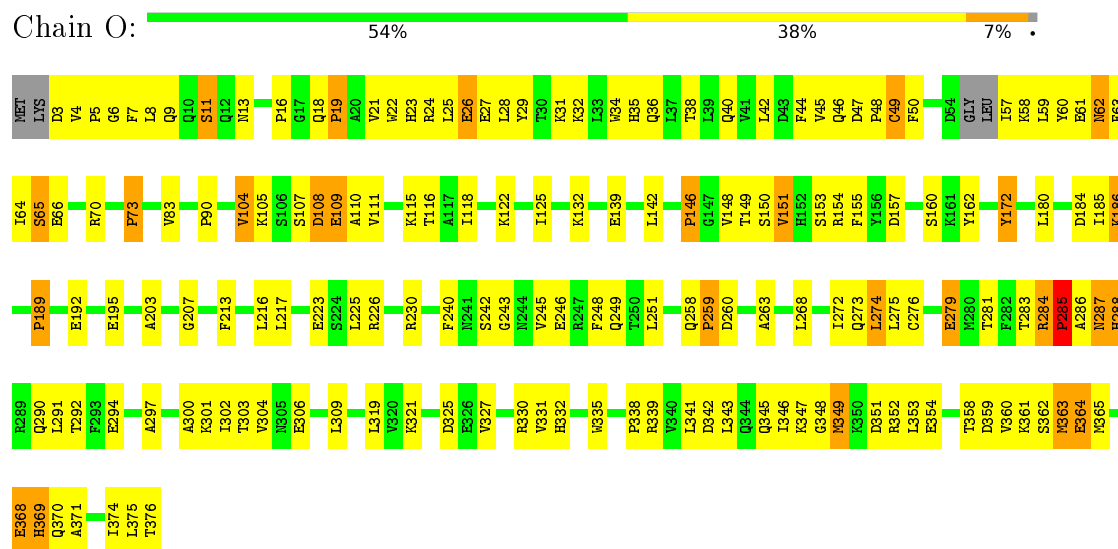


- Molecule 21: Proteasome subunit alpha type-3

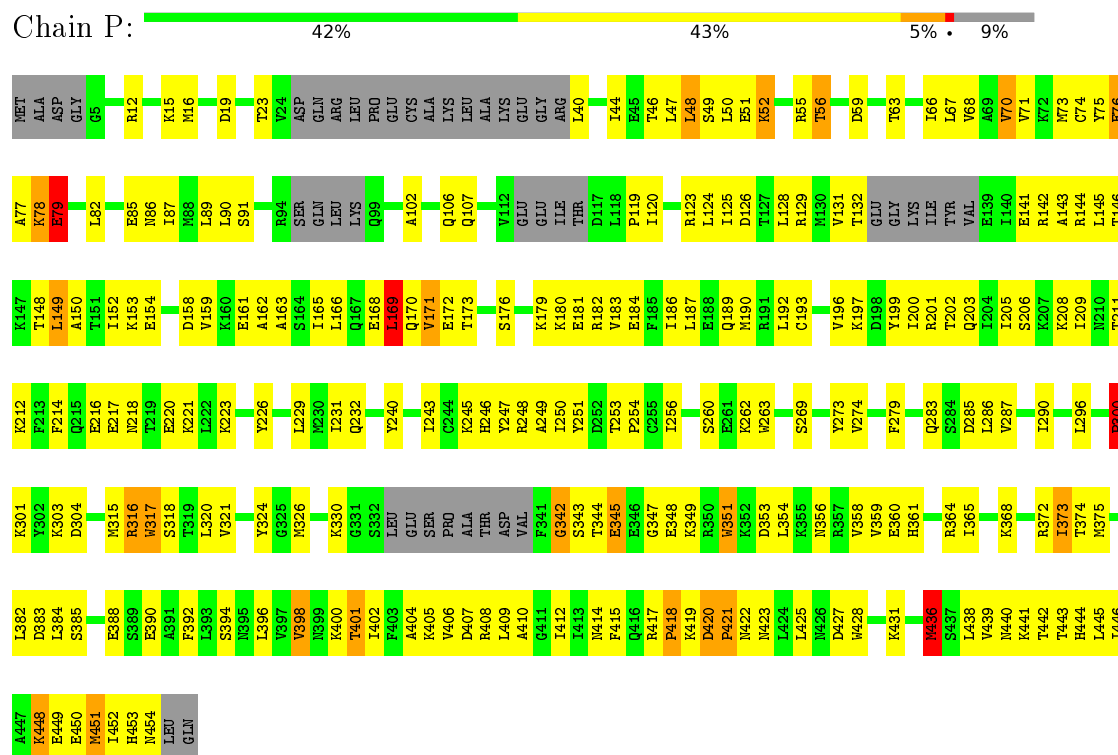
Chain X: 76% 18% 5%



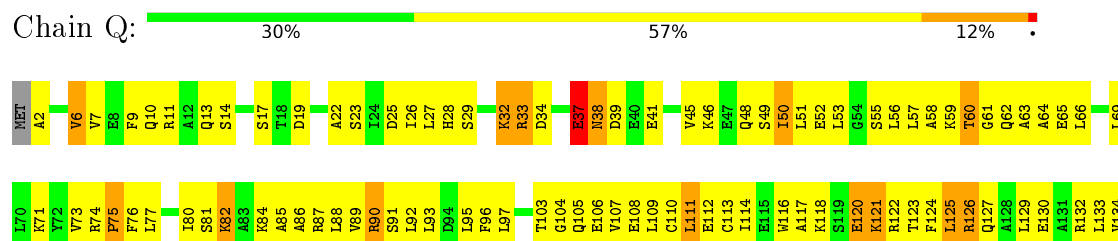
- Molecule 22: 26S proteasome non-ATPase regulatory subunit 13

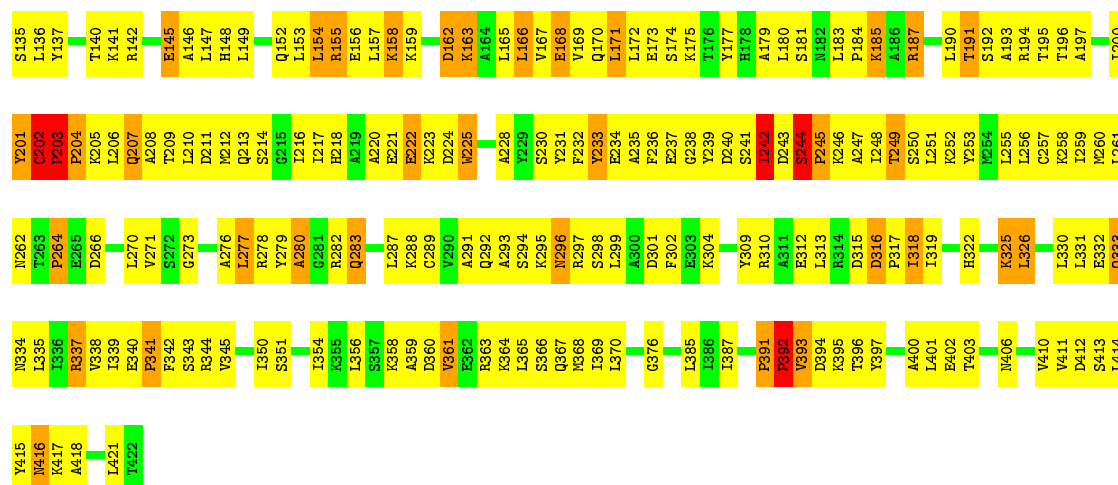


- Molecule 23: 26S proteasome non-ATPase regulatory subunit 12

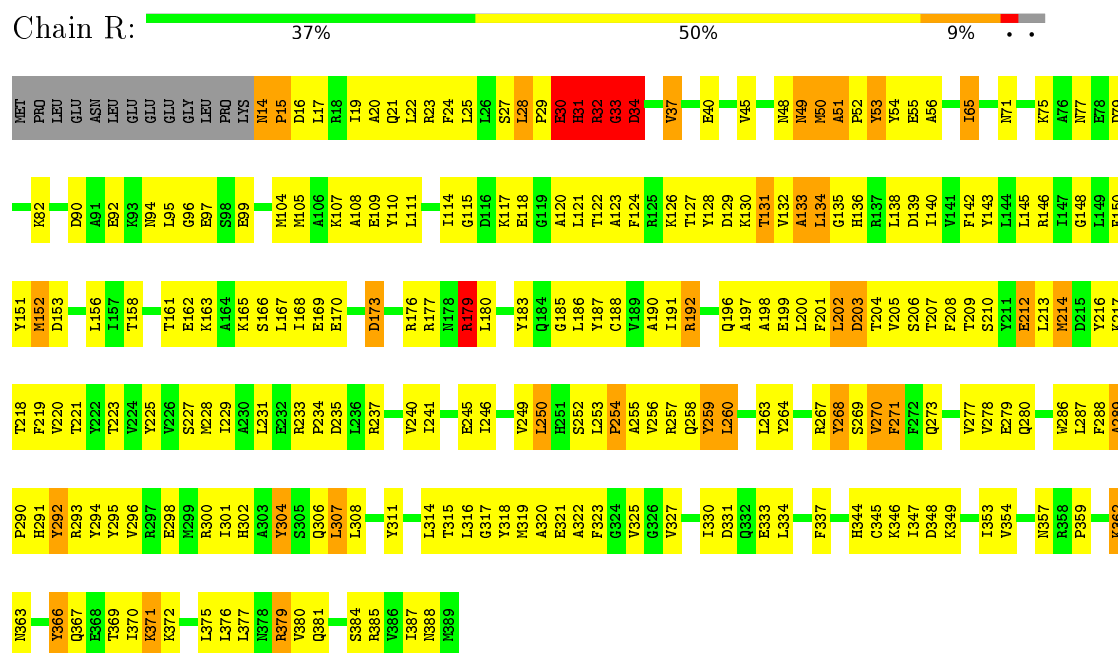


- Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

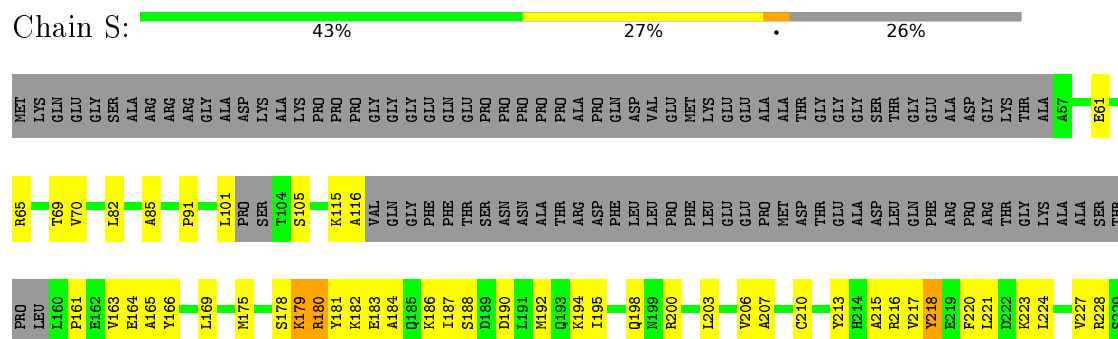


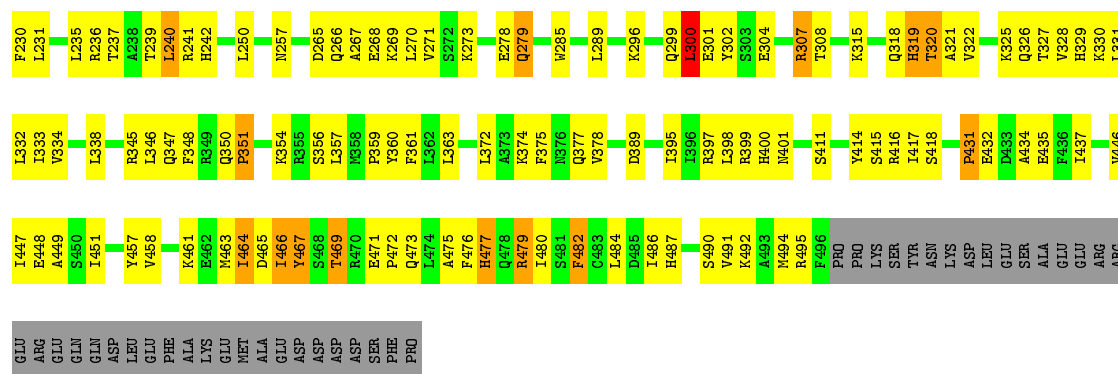


- Molecule 25: 26S proteasome non-ATPase regulatory subunit 6

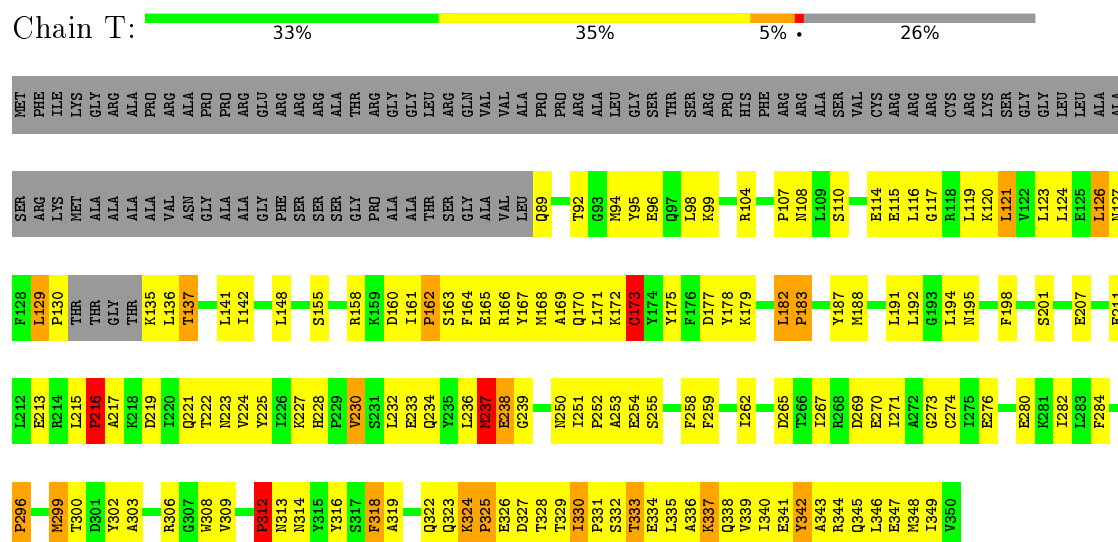


- Molecule 26: 26S proteasome non-ATPase regulatory subunit 3

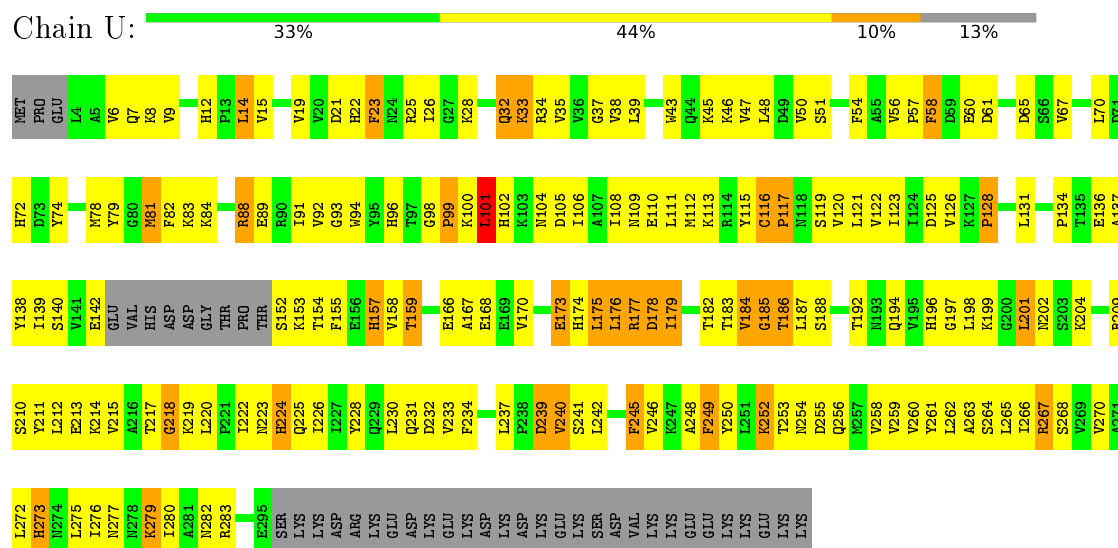




- Molecule 27: 26S proteasome non-ATPase regulatory subunit 8

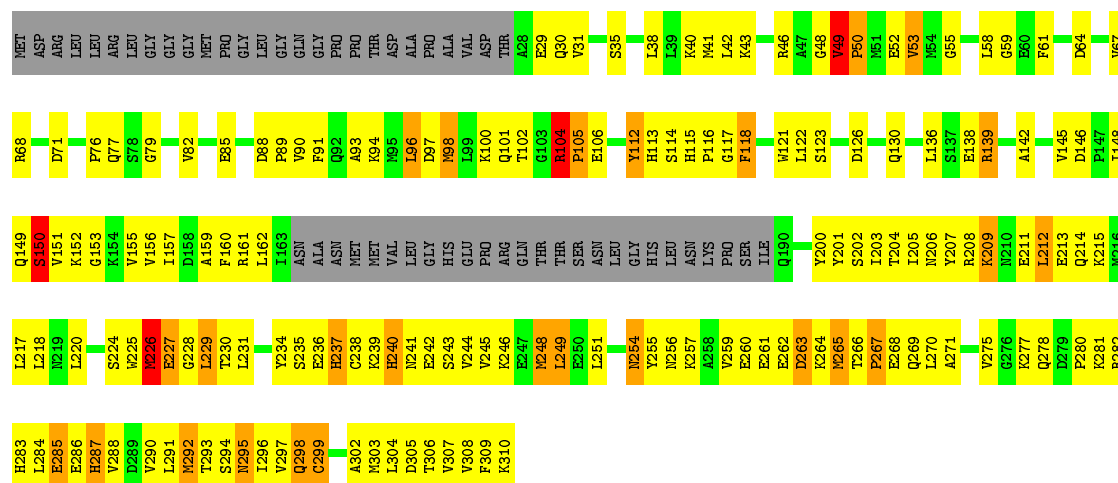


- Molecule 28: 26S proteasome non-ATPase regulatory subunit 7



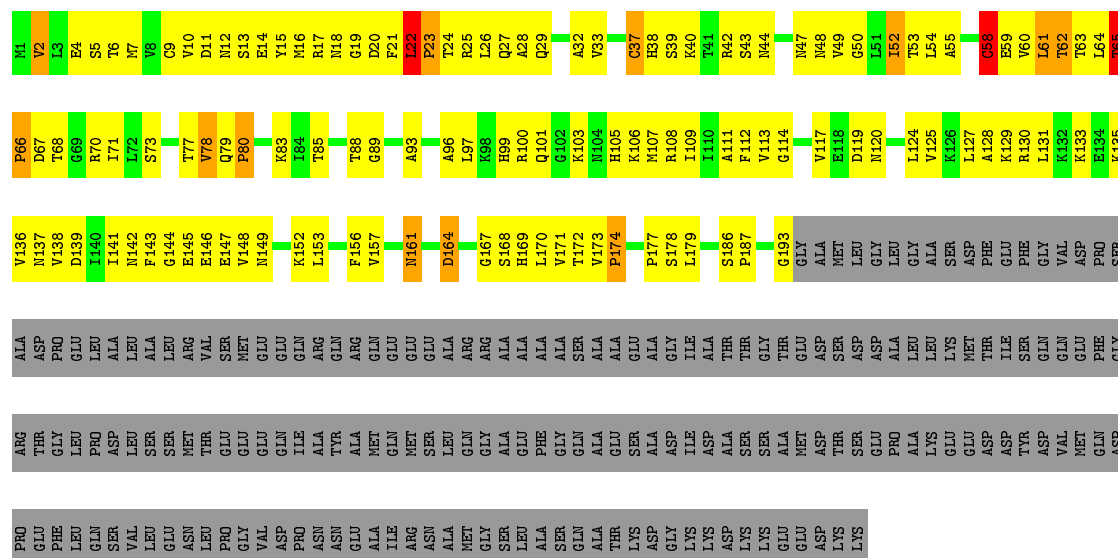
- Molecule 29: 26S proteasome non-ATPase regulatory subunit 14

Chain V:  30% 43% 8% • 17%



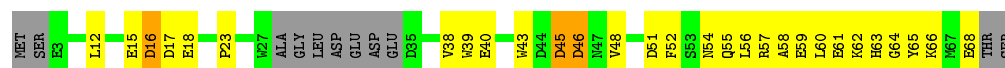
- Molecule 30: 26S proteasome non-ATPase regulatory subunit 4

Chain W:  18% 29% .. 49%



- Molecule 31: 26S proteasome complex subunit DSS1

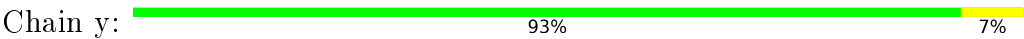
Chain Y:  43% 37% . 16%



- Molecule 32: 26S proteasome non-ATPase regulatory subunit 2

Chain Z: 50% 27% • 19%





4 Experimental information ⓘ

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	141293	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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, ADP

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	a	1.10	3/1535 (0.2%)	1.10	6/2078 (0.3%)
1	o	1.13	4/1535 (0.3%)	1.18	13/2078 (0.6%)
10	F	0.76	0/1794	0.84	0/2430
10	l	0.95	1/1753 (0.1%)	1.01	4/2346 (0.2%)
11	f	1.03	1/1671 (0.1%)	1.05	2/2253 (0.1%)
11	t	1.08	2/1674 (0.1%)	1.14	4/2257 (0.2%)
12	G	0.77	0/1885	0.88	3/2552 (0.1%)
12	m	0.95	1/1885 (0.1%)	1.01	4/2552 (0.2%)
13	g	1.01	3/1705 (0.2%)	1.06	7/2312 (0.3%)
13	u	1.04	1/1711 (0.1%)	1.10	9/2319 (0.4%)
14	H	0.82	1/2925 (0.0%)	1.09	8/3952 (0.2%)
15	I	0.80	1/2756 (0.0%)	1.01	8/3727 (0.2%)
16	J	0.77	0/2857	0.95	4/3844 (0.1%)
17	K	0.81	1/3089 (0.0%)	0.99	7/4168 (0.2%)
18	L	0.79	4/2904 (0.1%)	1.09	12/3924 (0.3%)
19	M	0.75	0/2896	0.91	3/3912 (0.1%)
2	B	0.83	1/1878 (0.1%)	0.88	2/2549 (0.1%)
2	h	1.01	0/1886	1.00	2/2557 (0.1%)
20	N	0.41	1/5520 (0.0%)	0.60	1/7446 (0.0%)
21	X	0.83	0/1908	0.87	1/2575 (0.0%)
21	n	0.93	2/1908 (0.1%)	0.98	4/2575 (0.2%)
22	O	0.56	0/2387	0.74	3/3211 (0.1%)
23	P	0.54	0/2857	0.72	4/3855 (0.1%)
24	Q	0.62	1/2981 (0.0%)	0.76	4/4045 (0.1%)
25	R	0.65	1/2817 (0.0%)	0.80	6/3811 (0.2%)
26	S	0.57	0/2623	0.70	2/3545 (0.1%)
27	T	0.56	0/1716	0.68	3/2310 (0.1%)
28	U	0.58	0/2167	0.75	2/2936 (0.1%)
29	V	0.60	0/2047	0.83	4/2763 (0.1%)
3	b	0.98	0/1670	1.06	2/2265 (0.1%)
3	p	1.06	2/1670 (0.1%)	1.15	8/2265 (0.4%)
30	W	0.52	0/1312	0.76	3/1769 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
31	Y	0.58	0/307	0.84	1/424 (0.2%)
32	Z	0.32	0/3603	0.53	1/5005 (0.0%)
33	x	0.67	0/2860	0.90	2/3852 (0.1%)
34	y	0.60	0/603	0.75	0/811
4	C	0.82	0/1742	0.89	4/2372 (0.2%)
4	i	1.11	5/1780 (0.3%)	1.10	7/2417 (0.3%)
5	c	1.08	2/1614 (0.1%)	1.11	6/2177 (0.3%)
5	q	1.21	5/1614 (0.3%)	1.19	4/2177 (0.2%)
6	D	0.81	2/1942 (0.1%)	0.89	1/2628 (0.0%)
6	j	0.99	1/1943 (0.1%)	1.04	7/2629 (0.3%)
7	d	0.99	0/1603	1.09	6/2174 (0.3%)
7	r	1.12	2/1603 (0.1%)	1.17	10/2174 (0.5%)
8	E	0.78	0/1748	0.88	5/2386 (0.2%)
8	k	0.95	2/1716 (0.1%)	1.04	5/2347 (0.2%)
9	e	1.08	2/1579 (0.1%)	1.11	7/2134 (0.3%)
9	s	1.13	4/1582 (0.3%)	1.10	6/2138 (0.3%)
All	All	0.83	56/99761 (0.1%)	0.94	217/135026 (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
14	H	0	1
15	I	0	4
16	J	0	1
17	K	0	1
18	L	0	4
19	M	0	2
20	N	0	3
22	O	0	2
23	P	0	2
24	Q	0	6
25	R	0	5
27	T	0	1
28	U	0	1
29	V	0	3
3	b	0	2
30	W	0	7
31	Y	0	2
32	Z	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
34	y	0	2
4	i	0	1
6	j	0	1
7	r	0	1
All	All	0	59

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	q	155	GLU	CD-OE2	13.15	1.40	1.25
18	L	116	ASP	N-CA	-10.28	1.25	1.46
4	i	22	GLU	CG-CD	8.89	1.65	1.51
3	p	81	ARG	CZ-NH2	8.66	1.44	1.33
5	c	164	PHE	CG-CD1	-8.04	1.26	1.38

The worst 5 of 217 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	115	VAL	CA-C-N	-22.22	68.32	117.20
14	H	336	ARG	NE-CZ-NH1	-21.51	109.54	120.30
18	L	115	VAL	C-N-CA	-18.03	76.64	121.70
14	H	336	ARG	NE-CZ-NH2	16.39	128.50	120.30
17	K	200	ARG	NE-CZ-NH1	14.57	127.59	120.30

There are no chirality outliers.

5 of 59 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	H	154	PRO	Peptide
15	I	105	THR	Peptide
15	I	137	SER	Peptide
15	I	299	SER	Mainchain
3	b	187	ARG	Mainchain,Peptide

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	a	1509	0	1473	0	0
1	o	1509	0	1473	0	0
2	B	1845	0	1805	84	0
2	h	1853	0	1827	0	0
3	b	1643	0	1644	0	0
3	p	1643	0	1644	0	0
4	C	1707	0	1591	50	0
4	i	1744	0	1693	0	0
5	c	1585	0	1598	0	0
5	q	1585	0	1598	0	0
6	D	1912	0	1851	46	0
6	j	1913	0	1848	0	0
7	d	1570	0	1547	0	0
7	r	1570	0	1547	0	0
8	E	1724	0	1525	41	0
8	k	1691	0	1468	0	0
9	e	1548	0	1499	0	0
9	s	1551	0	1508	0	0
10	F	1766	0	1714	32	0
10	l	1726	0	1722	0	0
11	f	1641	0	1618	0	0
11	t	1644	0	1627	0	0
12	G	1850	0	1822	51	0
12	m	1850	0	1822	0	0
13	g	1672	0	1630	0	0
13	u	1678	0	1640	0	0
14	H	2879	0	2812	649	0
15	I	2720	0	2685	780	0
16	J	2820	0	2927	735	0
17	K	3039	0	3072	927	0
18	L	2860	0	2827	739	0
19	M	2858	0	2852	607	0
20	N	5462	0	4587	714	0
21	X	1873	0	1832	47	0
21	n	1873	0	1832	0	0
22	O	2372	0	1859	173	0
23	P	2828	0	2378	332	0
24	Q	2948	0	2659	493	0
25	R	2767	0	2471	427	0
26	S	2600	0	2160	278	0
27	T	1702	0	1373	183	0
28	U	2131	0	2038	351	0
29	V	2011	0	1980	292	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	W	1300	0	1134	204	0
31	Y	308	0	140	17	0
32	Z	3608	0	1688	206	0
33	x	2810	0	2763	0	0
34	y	601	0	630	0	0
35	H	27	0	12	9	0
35	I	27	0	12	6	0
35	J	27	0	12	8	0
35	K	27	0	12	20	0
35	L	27	0	12	5	0
35	M	27	0	12	4	0
All	All	98461	0	91505	7657	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 46.

The worst 5 of 7657 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:23:PHE:CE2	28:U:126:VAL:HG11	1.18	1.67
20:N:35:TRP:CH2	26:S:273:LYS:HE2	1.19	1.67
17:K:41:TYR:CE2	20:N:155:LEU:HD23	1.21	1.63
14:H:111:TYR:CE2	14:H:125:LEU:CD2	1.77	1.62
14:H:111:TYR:CE2	14:H:125:LEU:HD22	1.31	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	a	200/239 (84%)	195 (98%)	4 (2%)	1 (0%)	34 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	o	200/239 (84%)	195 (98%)	4 (2%)	1 (0%)	34	77
2	B	242/246 (98%)	228 (94%)	9 (4%)	5 (2%)	9	52
2	h	242/246 (98%)	230 (95%)	12 (5%)	0	100	100
3	b	218/277 (79%)	210 (96%)	7 (3%)	1 (0%)	34	77
3	p	218/277 (79%)	207 (95%)	9 (4%)	2 (1%)	21	67
4	C	231/234 (99%)	204 (88%)	24 (10%)	3 (1%)	15	60
4	i	229/234 (98%)	202 (88%)	24 (10%)	3 (1%)	15	60
5	c	202/205 (98%)	189 (94%)	11 (5%)	2 (1%)	19	65
5	q	202/205 (98%)	188 (93%)	11 (5%)	3 (2%)	13	58
6	D	248/261 (95%)	236 (95%)	11 (4%)	1 (0%)	39	80
6	j	248/261 (95%)	233 (94%)	12 (5%)	3 (1%)	16	62
7	d	197/201 (98%)	186 (94%)	10 (5%)	1 (0%)	34	77
7	r	197/201 (98%)	186 (94%)	9 (5%)	2 (1%)	19	65
8	E	241/248 (97%)	223 (92%)	12 (5%)	6 (2%)	7	48
8	k	241/248 (97%)	224 (93%)	11 (5%)	6 (2%)	7	48
9	e	199/263 (76%)	195 (98%)	4 (2%)	0	100	100
9	s	199/263 (76%)	191 (96%)	8 (4%)	0	100	100
10	F	232/241 (96%)	216 (93%)	14 (6%)	2 (1%)	21	67
10	l	232/241 (96%)	215 (93%)	15 (6%)	2 (1%)	21	67
11	f	211/241 (88%)	205 (97%)	6 (3%)	0	100	100
11	t	211/241 (88%)	202 (96%)	9 (4%)	0	100	100
12	G	236/263 (90%)	223 (94%)	10 (4%)	3 (1%)	15	60
12	m	236/263 (90%)	222 (94%)	10 (4%)	4 (2%)	11	56
13	g	214/264 (81%)	203 (95%)	10 (5%)	1 (0%)	34	77
13	u	215/264 (81%)	205 (95%)	9 (4%)	1 (0%)	34	77
14	H	376/433 (87%)	254 (68%)	81 (22%)	41 (11%)	0	11
15	I	355/440 (81%)	264 (74%)	63 (18%)	28 (8%)	1	19
16	J	354/406 (87%)	253 (72%)	68 (19%)	33 (9%)	1	16
17	K	378/418 (90%)	260 (69%)	73 (19%)	45 (12%)	0	9
18	L	373/389 (96%)	268 (72%)	69 (18%)	36 (10%)	1	14
19	M	372/439 (85%)	257 (69%)	72 (19%)	43 (12%)	0	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	N	815/953 (86%)	610 (75%)	176 (22%)	29 (4%)	4	40
21	X	241/255 (94%)	233 (97%)	5 (2%)	3 (1%)	16	62
21	n	241/255 (94%)	232 (96%)	7 (3%)	2 (1%)	24	70
22	O	368/376 (98%)	292 (79%)	55 (15%)	21 (6%)	2	28
23	P	401/456 (88%)	333 (83%)	55 (14%)	13 (3%)	5	43
24	Q	419/422 (99%)	324 (77%)	67 (16%)	28 (7%)	1	24
25	R	374/389 (96%)	292 (78%)	60 (16%)	22 (6%)	2	27
26	S	389/534 (73%)	332 (85%)	42 (11%)	15 (4%)	4	37
27	T	254/350 (73%)	191 (75%)	44 (17%)	19 (8%)	1	21
28	U	279/324 (86%)	224 (80%)	42 (15%)	13 (5%)	3	32
29	V	253/310 (82%)	210 (83%)	32 (13%)	11 (4%)	3	35
30	W	191/377 (51%)	143 (75%)	38 (20%)	10 (5%)	2	30
31	Y	55/70 (79%)	36 (66%)	12 (22%)	7 (13%)	0	8
32	Z	722/908 (80%)	560 (78%)	113 (16%)	49 (7%)	1	24
33	x	349/494 (71%)	245 (70%)	62 (18%)	42 (12%)	0	9
34	y	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
All	All	13374/15440 (87%)	11297 (84%)	1514 (11%)	563 (4%)	6	35

5 of 563 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	F	120	ALA
12	G	238	GLU
14	H	95	VAL
14	H	108	ASP
14	H	109	PRO

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	a	155/181 (86%)	148 (96%)	7 (4%)	34	70
1	o	155/181 (86%)	148 (96%)	7 (4%)	34	70
2	B	193/210 (92%)	182 (94%)	11 (6%)	25	65
2	h	195/210 (93%)	183 (94%)	12 (6%)	23	62
3	b	177/228 (78%)	170 (96%)	7 (4%)	38	73
3	p	177/228 (78%)	168 (95%)	9 (5%)	29	67
4	C	163/191 (85%)	155 (95%)	8 (5%)	31	68
4	i	177/191 (93%)	163 (92%)	14 (8%)	15	53
5	c	172/174 (99%)	163 (95%)	9 (5%)	29	67
5	q	172/174 (99%)	163 (95%)	9 (5%)	29	67
6	D	193/221 (87%)	182 (94%)	11 (6%)	25	65
6	j	193/221 (87%)	183 (95%)	10 (5%)	29	67
7	d	164/171 (96%)	156 (95%)	8 (5%)	31	68
7	r	164/171 (96%)	157 (96%)	7 (4%)	35	71
8	E	152/211 (72%)	142 (93%)	10 (7%)	21	60
8	k	142/211 (67%)	134 (94%)	8 (6%)	26	65
9	e	153/202 (76%)	149 (97%)	4 (3%)	54	81
9	s	154/202 (76%)	148 (96%)	6 (4%)	39	73
10	F	190/203 (94%)	185 (97%)	5 (3%)	54	81
10	l	191/203 (94%)	185 (97%)	6 (3%)	47	78
11	f	174/199 (87%)	166 (95%)	8 (5%)	33	70
11	t	175/199 (88%)	168 (96%)	7 (4%)	38	73
12	G	198/224 (88%)	191 (96%)	7 (4%)	43	76
12	m	198/224 (88%)	183 (92%)	15 (8%)	16	55
13	g	175/215 (81%)	166 (95%)	9 (5%)	29	67
13	u	175/215 (81%)	164 (94%)	11 (6%)	22	61
14	H	292/372 (78%)	238 (82%)	54 (18%)	2	15
15	I	291/385 (76%)	231 (79%)	60 (21%)	1	11
16	J	310/352 (88%)	246 (79%)	64 (21%)	1	11
17	K	333/366 (91%)	268 (80%)	65 (20%)	2	14
18	L	298/341 (87%)	239 (80%)	59 (20%)	1	13
19	M	296/379 (78%)	240 (81%)	56 (19%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	N	377/816 (46%)	345 (92%)	32 (8%)	13	50
21	X	193/212 (91%)	186 (96%)	7 (4%)	42	75
21	n	193/212 (91%)	184 (95%)	9 (5%)	32	69
22	O	144/336 (43%)	119 (83%)	25 (17%)	2	18
23	P	202/416 (49%)	182 (90%)	20 (10%)	10	42
24	Q	249/362 (69%)	207 (83%)	42 (17%)	2	20
25	R	226/344 (66%)	196 (87%)	30 (13%)	5	30
26	S	163/460 (35%)	153 (94%)	10 (6%)	23	62
27	T	109/294 (37%)	92 (84%)	17 (16%)	3	23
28	U	212/295 (72%)	184 (87%)	28 (13%)	5	30
29	V	219/268 (82%)	188 (86%)	31 (14%)	4	28
30	W	109/312 (35%)	102 (94%)	7 (6%)	22	61
31	Y	4/63 (6%)	4 (100%)	0	100	100
33	x	305/439 (70%)	254 (83%)	51 (17%)	3	20
34	y	68/68 (100%)	64 (94%)	4 (6%)	24	63
All	All	9120/12352 (74%)	8224 (90%)	896 (10%)	14	42

5 of 896 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	L	134	GLU
19	M	372	LYS
30	W	37	CYS
18	L	226	GLN
10	l	208	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 134 such sidechains are listed below:

Mol	Chain	Res	Type
20	N	347	ASN
24	Q	127	GLN
33	x	307	ASN
20	N	645	ASN
1	o	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	$\# Z > 2$
34	GLZ	y	76	34	3,3,3	0.83	0	0,2,2	0.00	-

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
34	GLZ	y	76	34	-	0/0/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

6 ligands are 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$
35	ADP	H	501	-	24,29,29	1.51	4 (16%)	23,45,45	2.93	7 (30%)
35	ADP	I	501	-	24,29,29	1.54	3 (12%)	23,45,45	2.20	7 (30%)
35	ADP	J	501	-	24,29,29	1.29	4 (16%)	23,45,45	2.59	6 (26%)
35	ADP	K	501	-	24,29,29	1.33	3 (12%)	23,45,45	2.44	9 (39%)
35	ADP	L	401	-	24,29,29	1.06	1 (4%)	23,45,45	2.60	5 (21%)
35	ADP	M	501	-	24,29,29	1.17	1 (4%)	23,45,45	2.06	6 (26%)

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
35	ADP	H	501	-	-	0/12/32/32	0/3/3/3
35	ADP	I	501	-	-	0/12/32/32	0/3/3/3
35	ADP	J	501	-	-	0/12/32/32	0/3/3/3
35	ADP	K	501	-	-	0/12/32/32	0/3/3/3
35	ADP	L	401	-	-	0/12/32/32	0/3/3/3
35	ADP	M	501	-	-	0/12/32/32	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	J	501	ADP	C2'-C1'	-2.70	1.49	1.53
35	J	501	ADP	O4'-C4'	-2.35	1.39	1.45
35	K	501	ADP	C2-N3	2.09	1.35	1.32
35	I	501	ADP	C8-N7	2.14	1.38	1.34
35	H	501	ADP	C2-N1	2.15	1.38	1.33

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
35	J	501	ADP	N3-C2-N1	-9.38	121.50	128.87
35	L	401	ADP	N3-C2-N1	-9.24	121.62	128.87
35	H	501	ADP	N3-C2-N1	-7.23	123.19	128.87
35	M	501	ADP	N3-C2-N1	-6.92	123.43	128.87
35	I	501	ADP	N3-C2-N1	-6.84	123.50	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	H	501	ADP	9	0
35	I	501	ADP	6	0
35	J	501	ADP	8	0
35	K	501	ADP	20	0
35	L	401	ADP	5	0
35	M	501	ADP	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.