



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jul 11, 2018 – 10:01 PM EDT

PDB ID : 5T0C  
EMDB ID: : EMD-8332  
Title : Structural basis for dynamic regulation of the human 26S proteasome  
Authors : Chen, S.; Wu, J.; Lu, Y.; Ma, Y.B.; Lee, B.H.; Yu, Z.; Ouyang, Q.; Finley, D.;  
Kirschner, M.W.; Mao, Y.  
Deposited on : 2016-08-15  
Resolution : 3.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031172

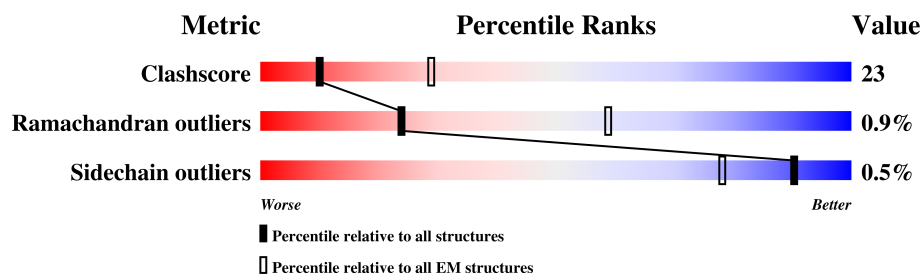
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 Å.

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






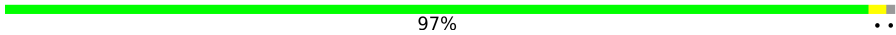
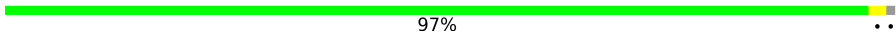




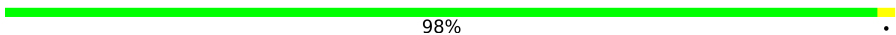
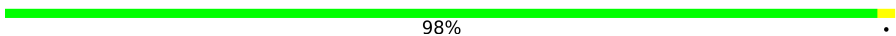














Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	AU	953	
1	BU	953	
2	AV	533	
2	BV	533	
3	AW	456	
3	BW	456	
4	AX	422	
4	BX	422	
5	AY	389	

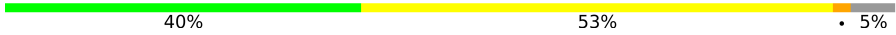
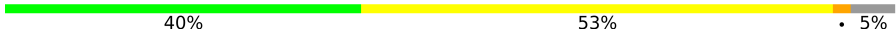























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Mol	Chain	Length	Quality of chain
5	BY	389	
6	AZ	324	
6	BZ	324	
7	Aa	376	
7	Ba	376	
8	Ab	377	
8	Bb	377	
9	Ac	310	
9	Bc	310	
10	Ad	257	
10	Bd	257	
11	Ae	70	
11	Be	70	
12	Af	908	
12	Bf	908	
13	AA	433	
13	BA	433	
14	AB	440	
14	BB	440	
15	AD	418	
15	BD	418	
16	AE	389	
16	BE	389	
17	AF	439	
17	BF	439	





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Mol	Chain	Length	Quality of chain
18	AC	406	
18	BC	406	
19	AG	245	
19	BG	245	
20	AH	233	
20	BH	233	
21	AI	260	
21	BI	260	
22	AJ	247	
22	BJ	247	
23	AK	240	
23	BK	240	
24	AL	268	
24	BL	268	
25	AM	254	
25	BM	254	
26	AN	238	
26	BN	238	
27	AO	276	
27	BO	276	
28	AP	204	
28	BP	204	
29	AQ	201	
29	BQ	201	
30	AR	262	

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Mol	Chain	Length	Quality of chain
30	BR	262	
31	AS	240	
31	BS	240	
32	AT	263	
32	BT	263	

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
34	ATP	AE	401	-	-	X	-
34	ATP	BE	401	-	-	X	-

## 2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 155574 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 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AU	806	Total	C	N	O	S	0	0
			6287	3990	1075	1178	44		
1	BU	806	Total	C	N	O	S	0	0
			6287	3990	1075	1178	44		

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AV	480	Total	C	N	O	S	0	0
			3852	2444	684	710	14		
2	BV	480	Total	C	N	O	S	0	0
			3852	2444	684	710	14		

- Molecule 3 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AW	456	Total	C	N	O	S	0	0
			3703	2339	635	704	25		
3	BW	456	Total	C	N	O	S	0	0
			3703	2339	635	704	25		

- Molecule 4 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AX	380	Total	C	N	O	S	0	0
			3009	1918	509	570	12		
4	BX	380	Total	C	N	O	S	0	0
			3009	1918	509	570	12		

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AY	378	Total	C	N	O	S	0	0
			3115	1987	533	578	17		
5	BY	378	Total	C	N	O	S	0	0
			3115	1987	533	578	17		

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AZ	286	Total	C	N	O	S	0	0
			2281	1457	392	427	5		
6	BZ	286	Total	C	N	O	S	0	0
			2281	1457	392	427	5		

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Aa	373	Total	C	N	O	S	0	0
			2995	1911	510	559	15		
7	Ba	373	Total	C	N	O	S	0	0
			2995	1911	510	559	15		

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Ab	191	Total	C	N	O	S	0	0
			1458	910	261	279	8		
8	Bb	191	Total	C	N	O	S	0	0
			1458	910	261	279	8		

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Ac	287	Total	C	N	O	S	0	0
			2260	1430	389	422	19		
9	Bc	287	Total	C	N	O	S	0	0
			2260	1430	389	422	19		

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Ad	257	Total	C	N	O	S	0	0
			2116	1371	346	390	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	Bd	257	Total	C	N	O	S	0	0
			2116	1371	346	390	9		

- Molecule 11 is a protein called 26S proteasome complex subunit DSS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Ae	40	Total	C	N	O	S	0	0
			334	200	55	77	2		
11	Be	40	Total	C	N	O	S	0	0
			334	200	55	77	2		

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Af	694	Total	C	N	O	S	0	0
			5331	3364	899	1027	41		
12	Bf	694	Total	C	N	O	S	0	0
			5331	3364	899	1027	41		

- Molecule 13 is a protein called 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AA	361	Total	C	N	O	S	0	0
			2835	1788	501	528	18		
13	BA	361	Total	C	N	O	S	0	0
			2835	1788	501	528	18		

- Molecule 14 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AB	341	Total	C	N	O	S	0	0
			2662	1671	453	526	12		
14	BB	341	Total	C	N	O	S	0	0
			2662	1671	453	526	12		

- Molecule 15 is a protein called 26S protease regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AD	380	Total	C	N	O	S	0	0
			3040	1923	524	580	13		
15	BD	380	Total	C	N	O	S	0	0
			3040	1923	524	580	13		



- Molecule 16 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AE	353	Total	C	N	O	S	0	0
			2790	1755	494	525	16		
16	BE	353	Total	C	N	O	S	0	0
			2790	1755	494	525	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AF	366	Total	C	N	O	S	0	0
			2863	1802	496	549	16		
17	BF	366	Total	C	N	O	S	0	0
			2863	1802	496	549	16		

- Molecule 18 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AC	384	Total	C	N	O	S	0	0
			3015	1894	540	564	17		
18	BC	384	Total	C	N	O	S	0	0
			3015	1894	540	564	17		

- Molecule 19 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AG	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		
19	BG	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

- Molecule 20 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AH	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		
20	BH	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

- Molecule 21 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AI	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		
21	BI	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 22 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AJ	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		
22	BJ	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		

- Molecule 23 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AK	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		
23	BK	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		

- Molecule 24 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AL	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		
24	BL	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

- Molecule 25 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AM	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		
25	BM	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		

- Molecule 26 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AN	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	BN	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		

- Molecule 27 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AO	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		
27	BO	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		

- Molecule 28 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AP	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		
28	BP	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		

- Molecule 29 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AQ	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		
29	BQ	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

- Molecule 30 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AR	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		
30	BR	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

- Molecule 31 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AS	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		
31	BS	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		

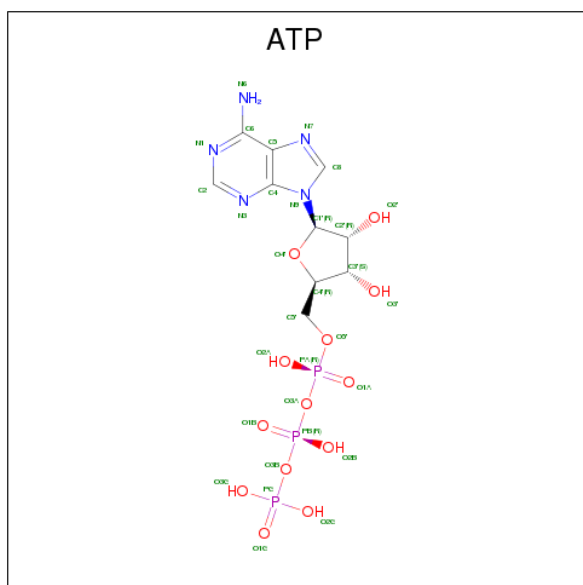
- Molecule 32 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AT	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		
32	BT	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
33	Ac	1	Total	Zn	0
			1	1	
33	Bc	1	Total	Zn	0
			1	1	

- Molecule 34 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



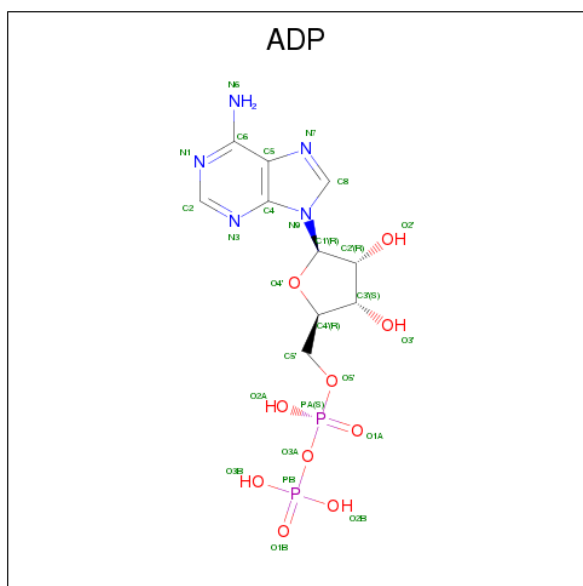
Mol	Chain	Residues	Atoms					AltConf
34	AA	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	AD	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	AE	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	AF	1	Total	C	N	O	P	0
			31	10	5	13	3	

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Mol	Chain	Residues	Atoms					AltConf
34	BA	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	BD	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	BE	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	BF	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 35 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

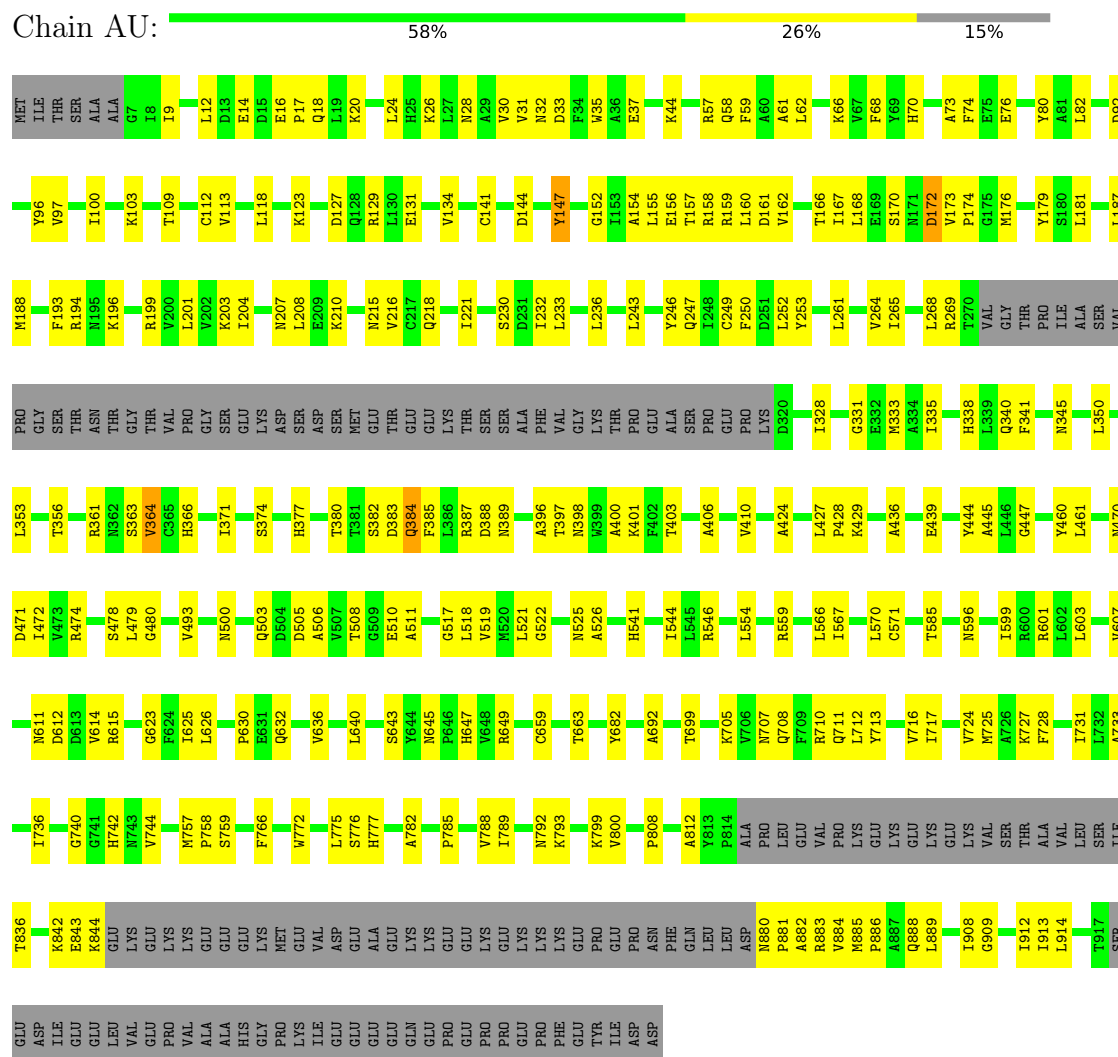


Mol	Chain	Residues	Atoms					AltConf
35	AB	1	Total	C	N	O	P	0
			27	10	5	10	2	
35	AC	1	Total	C	N	O	P	0
			27	10	5	10	2	
35	BB	1	Total	C	N	O	P	0
			27	10	5	10	2	
35	BC	1	Total	C	N	O	P	0
			27	10	5	10	2	

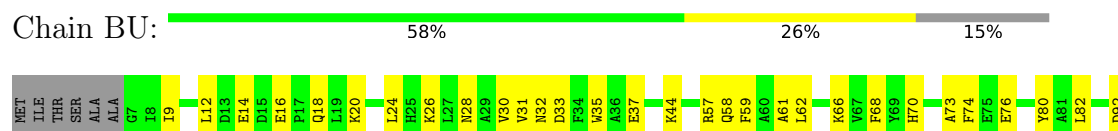
### 3 Residue-property plots

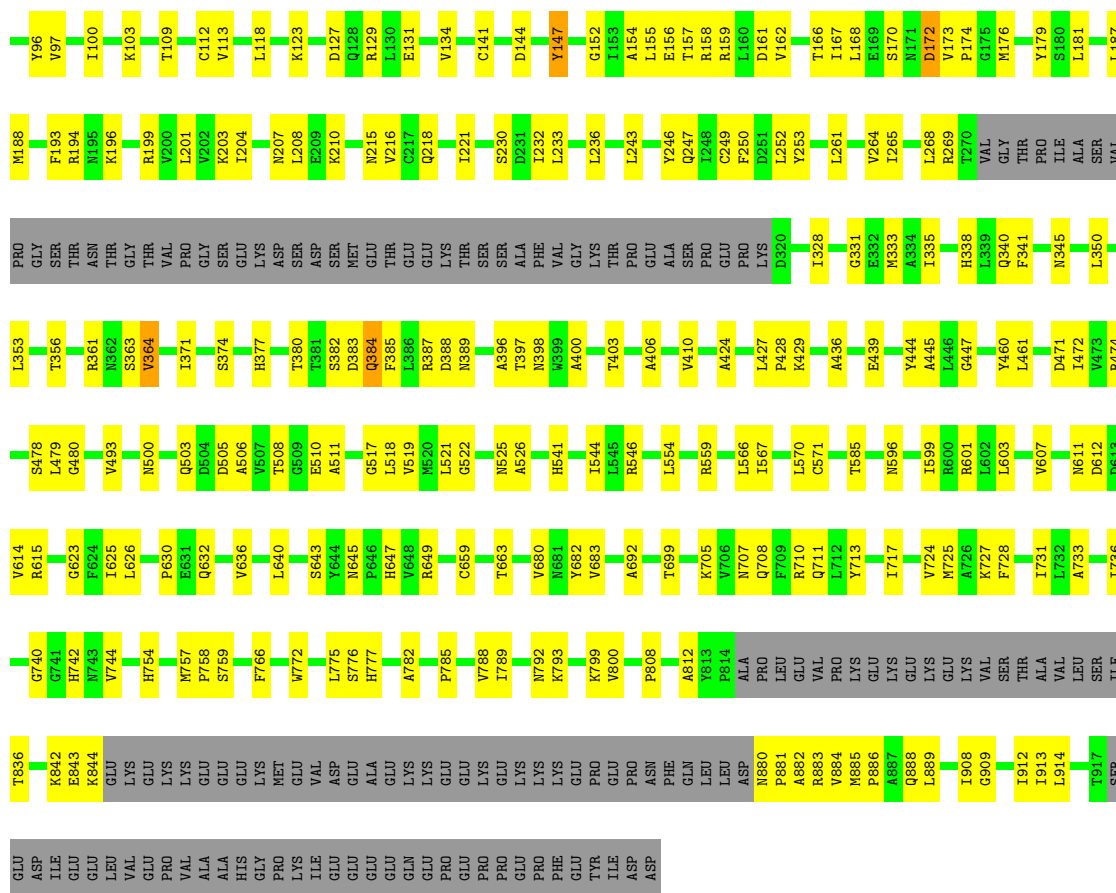
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: 26S proteasome non-ATPase regulatory subunit 1



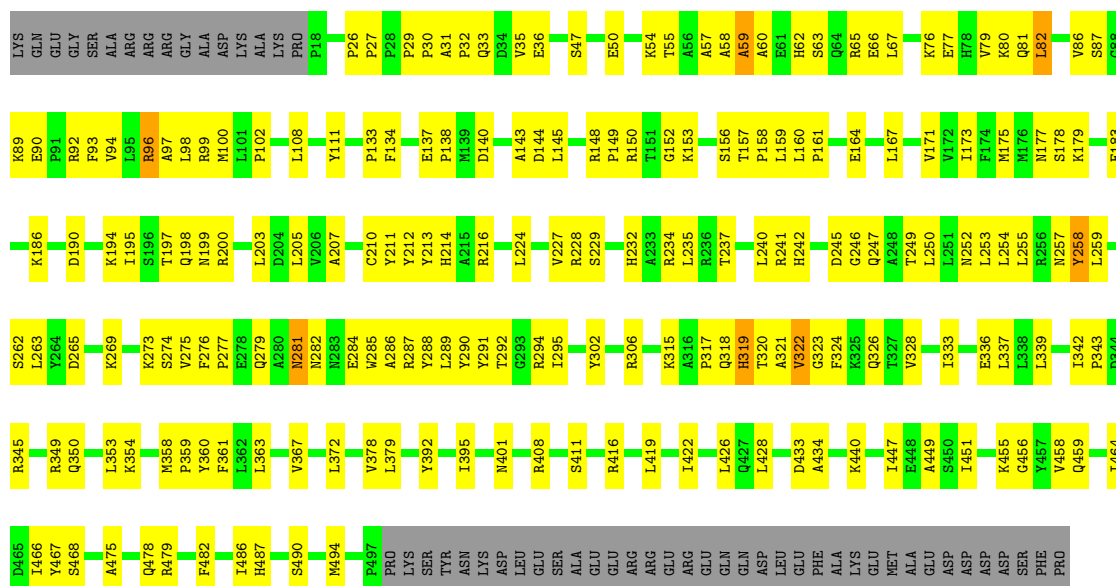
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 1





• Molecule 2: 26S proteasome non-ATPase regulatory subunit 3

Chain AV: 53% 36% 10%



• Molecule 2: 26S proteasome non-ATPase regulatory subunit 3

10%



35%



34%

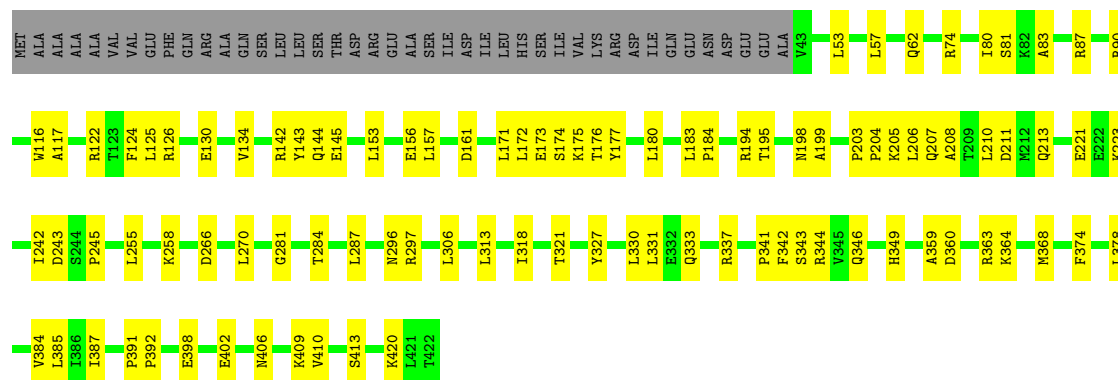






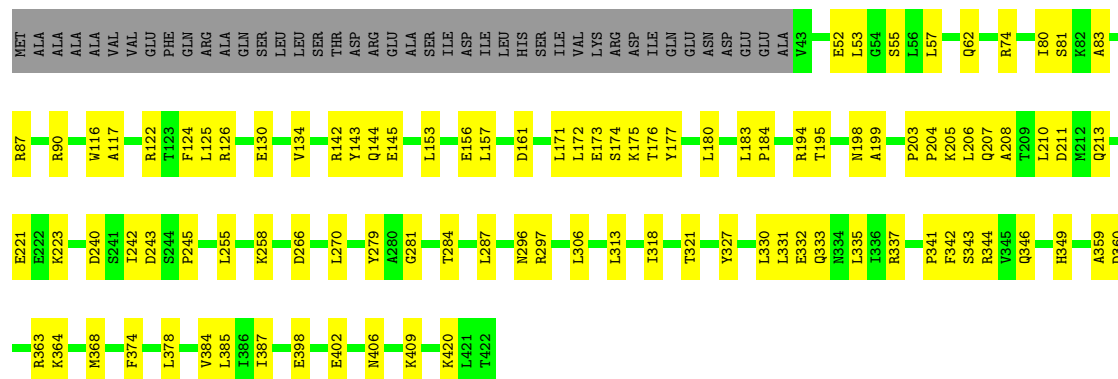
• Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

Chain AX:  67%  23%  10%



• Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

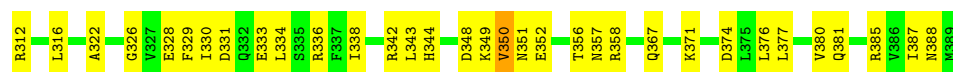
Chain BX:  67%  23%  10%



• Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

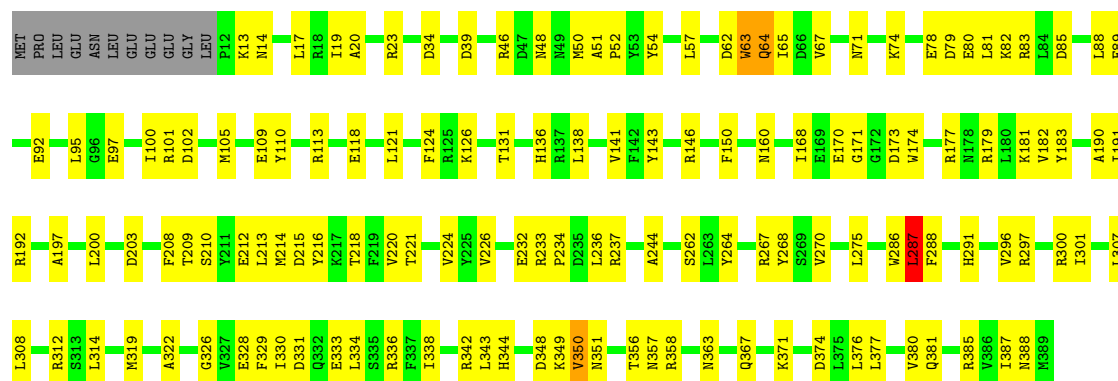
Chain AY:  62%  34%  ..





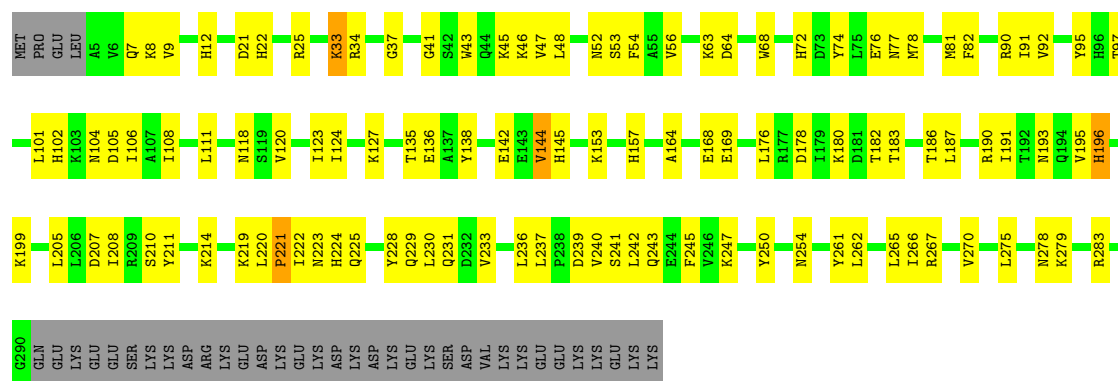
• Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

Chain BY: 62% 34% ..



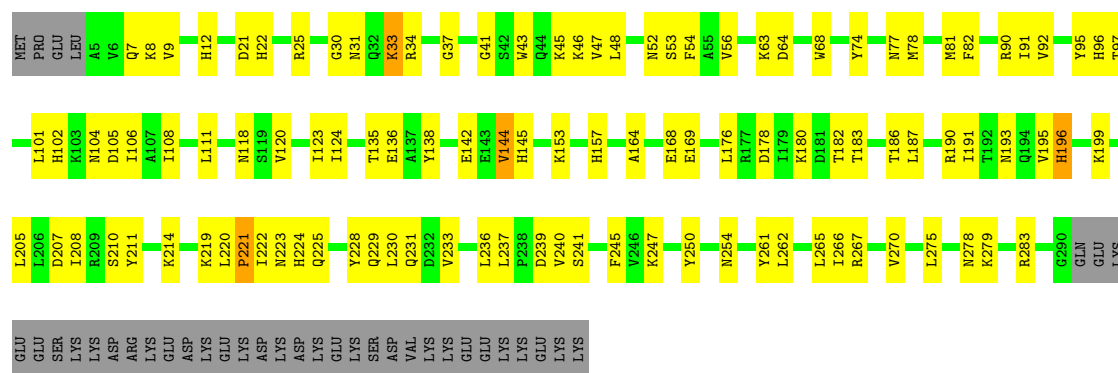
• Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

Chain AZ: 54% 33% 12%



• Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

Chain BZ: 55% 32% 12%



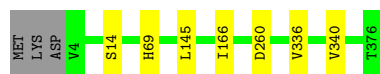
• Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

Chain Aa:  97%



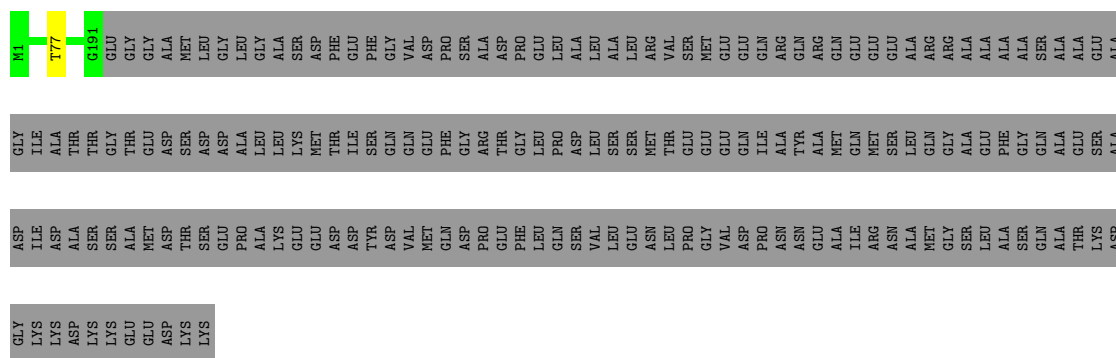
- Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

Chain Ba:  97%



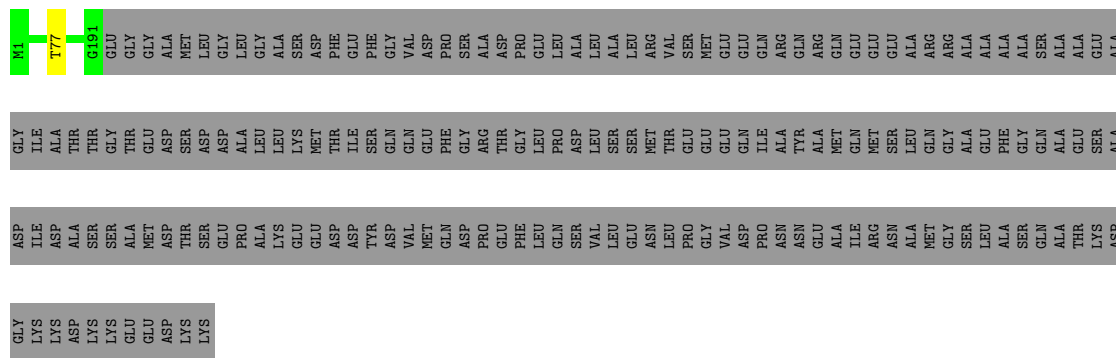
- Molecule 8: 26S proteasome non-ATPase regulatory subunit 4

Chain Ab:  50% 49%



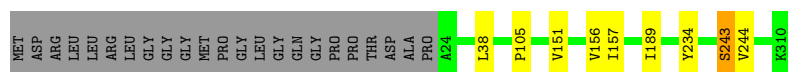
- Molecule 8: 26S proteasome non-ATPase regulatory subunit 4

Chain Bb:  50% 49%



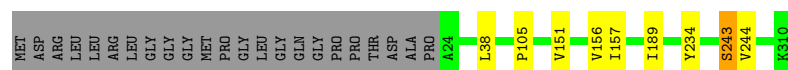
- Molecule 9: 26S proteasome non-ATPase regulatory subunit 14

Chain Ac:  90% 7%



- Molecule 9: 26S proteasome non-ATPase regulatory subunit 14

Chain Bc:  90% • 7%



- Molecule 10: 26S proteasome non-ATPase regulatory subunit 8

Chain Ad:  98%



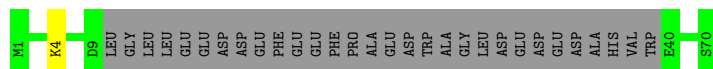
- Molecule 10: 26S proteasome non-ATPase regulatory subunit 8

Chain Bd: 98%



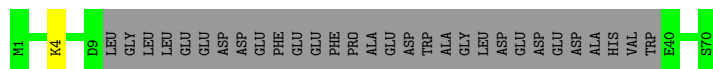
- Molecule 11: 26S proteasome complex subunit DSS1

Chain Ae:  56% 43%

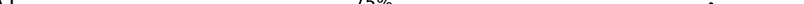


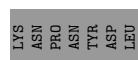
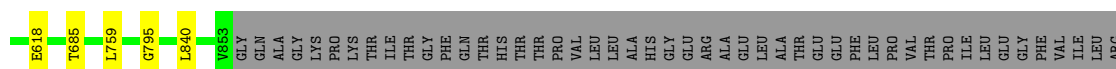
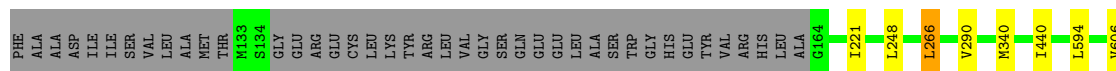
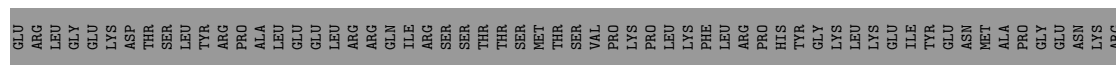
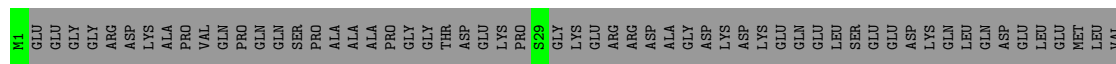
- Molecule 11: 26S proteasome complex subunit DSS1

Chain Be:  56% 0% 43%



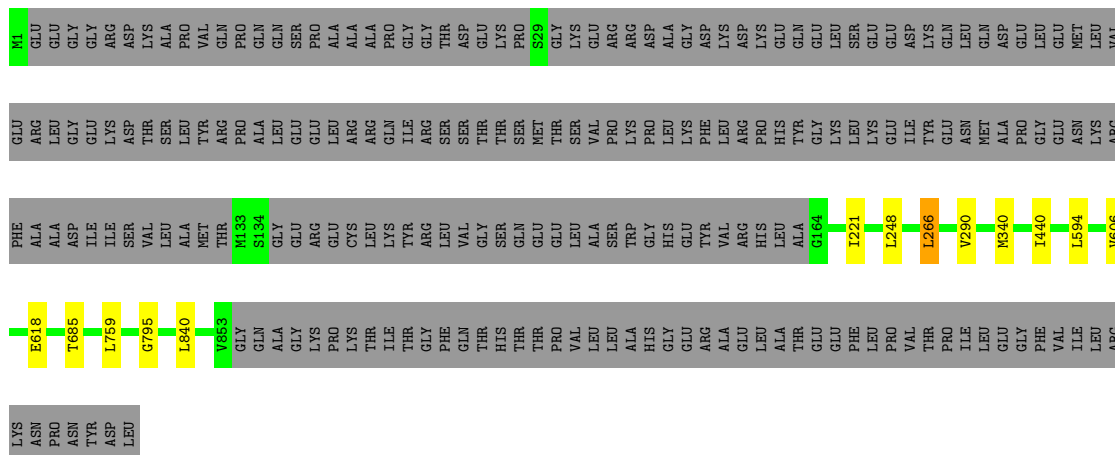
- Molecule 12: 26S proteasome non-ATPase regulatory subunit 2

Chain Af:  75% 24%



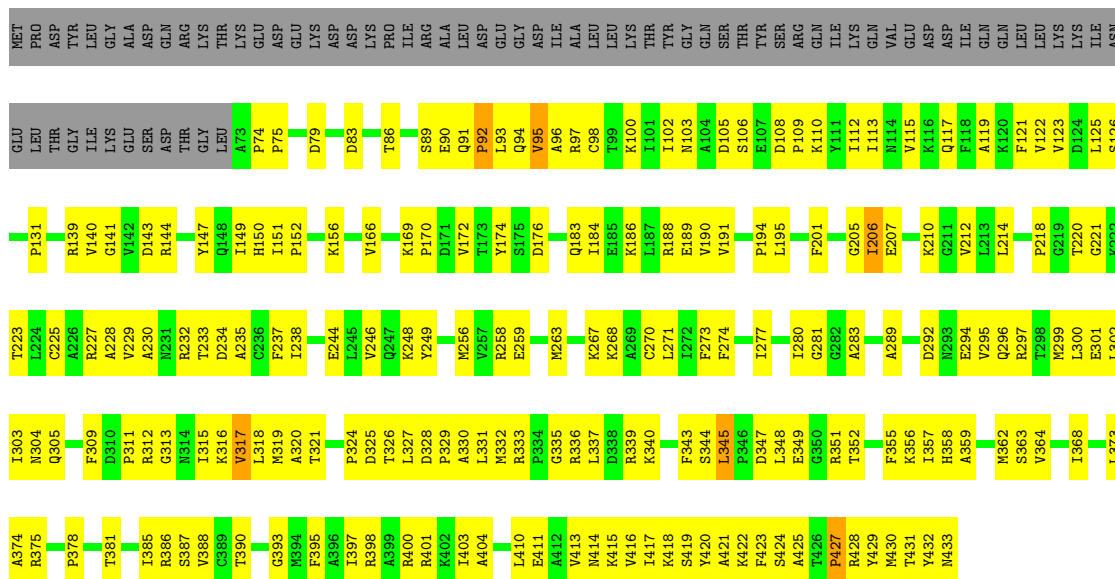
- Molecule 12: 26S proteasome non-ATPase regulatory subunit 2

Chain Bf:



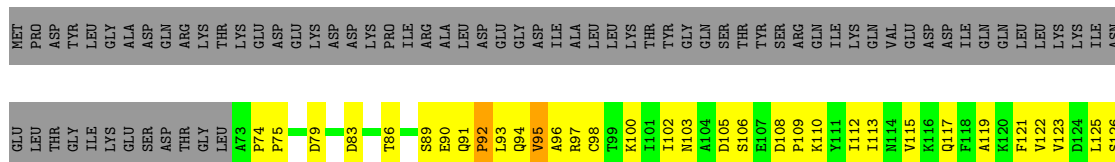
- Molecule 13: 26S protease regulatory subunit 7

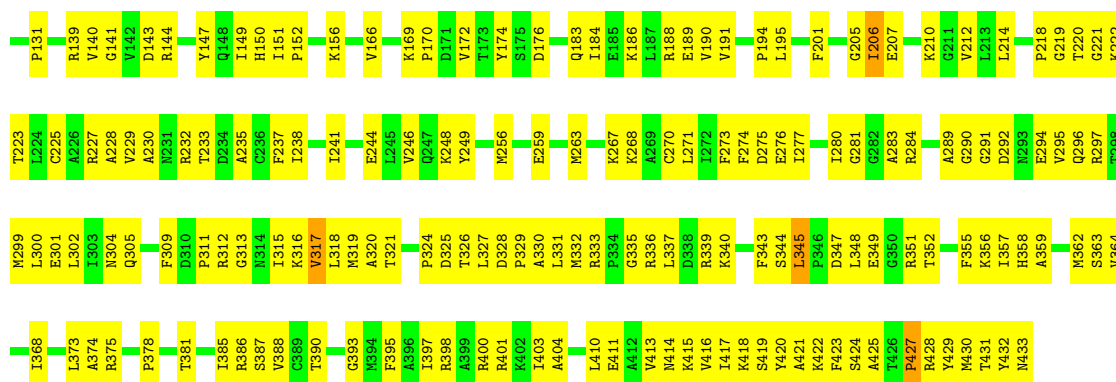
Chain AA:



- Molecule 13: 26S protease regulatory subunit 7

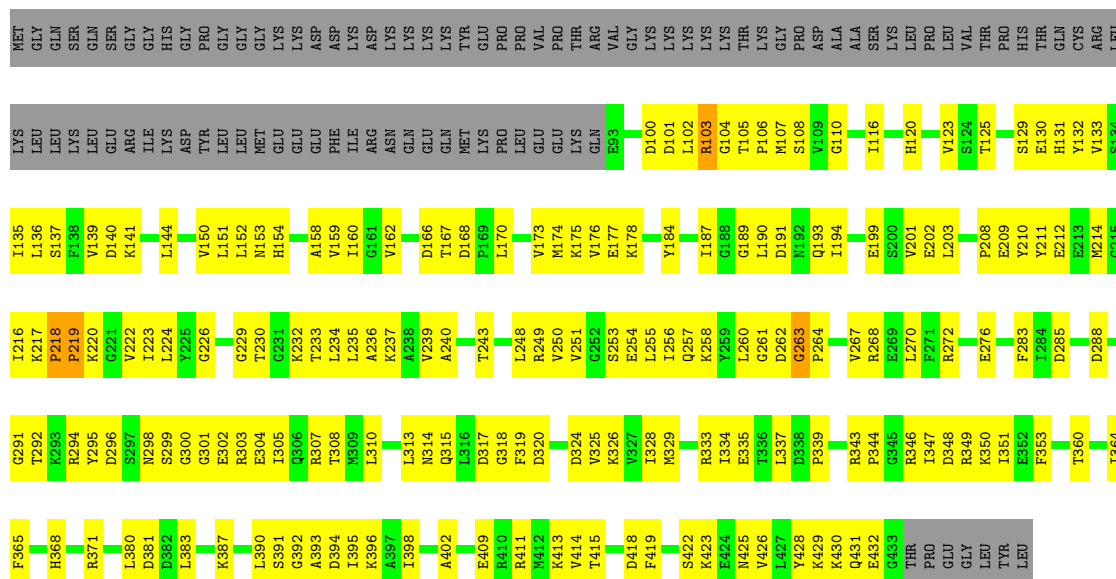
Chain BA:





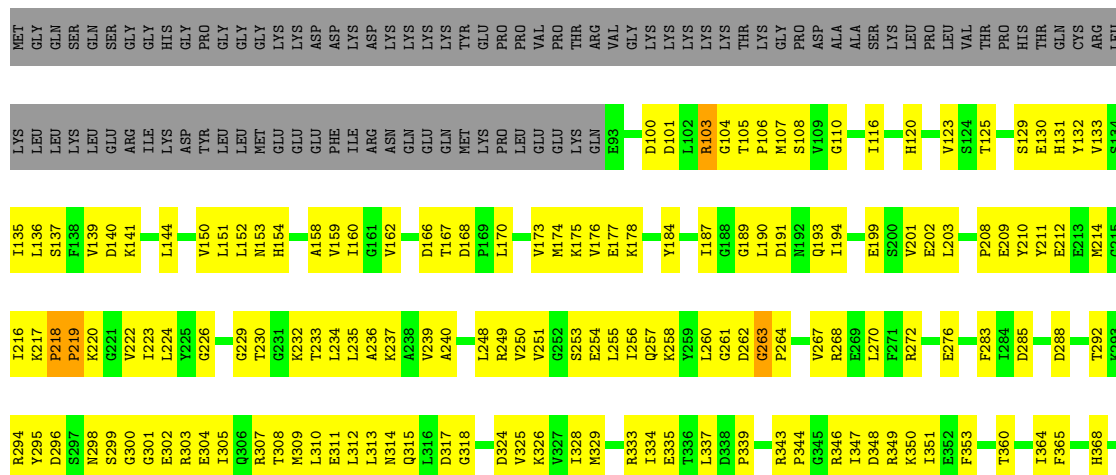
• Molecule 14: 26S protease regulatory subunit 4

Chain AB: 36% 40% 23%



• Molecule 14: 26S protease regulatory subunit 4

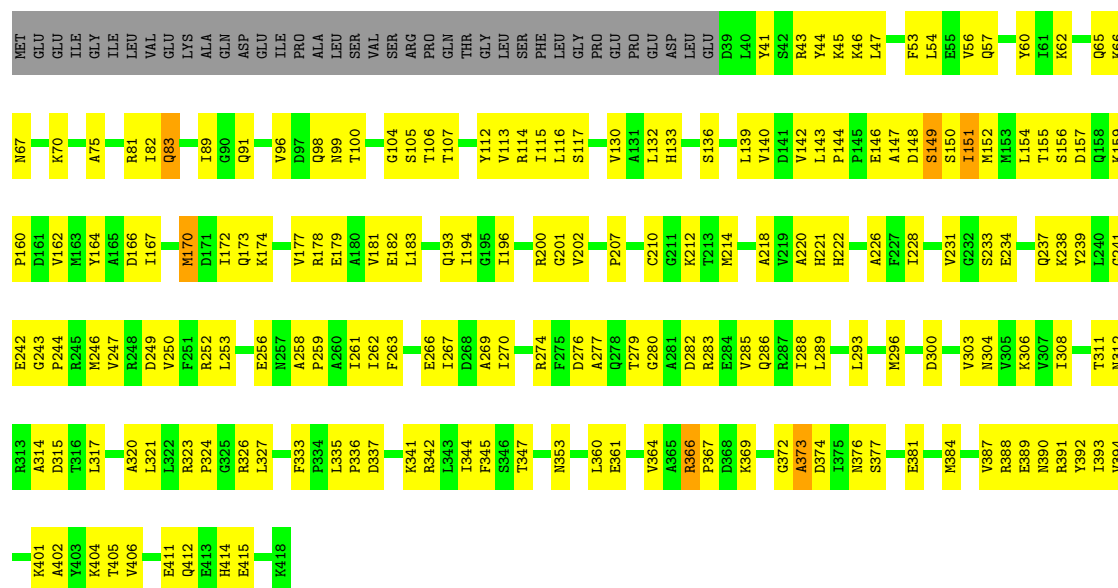
Chain BB: 37% 40% 23%





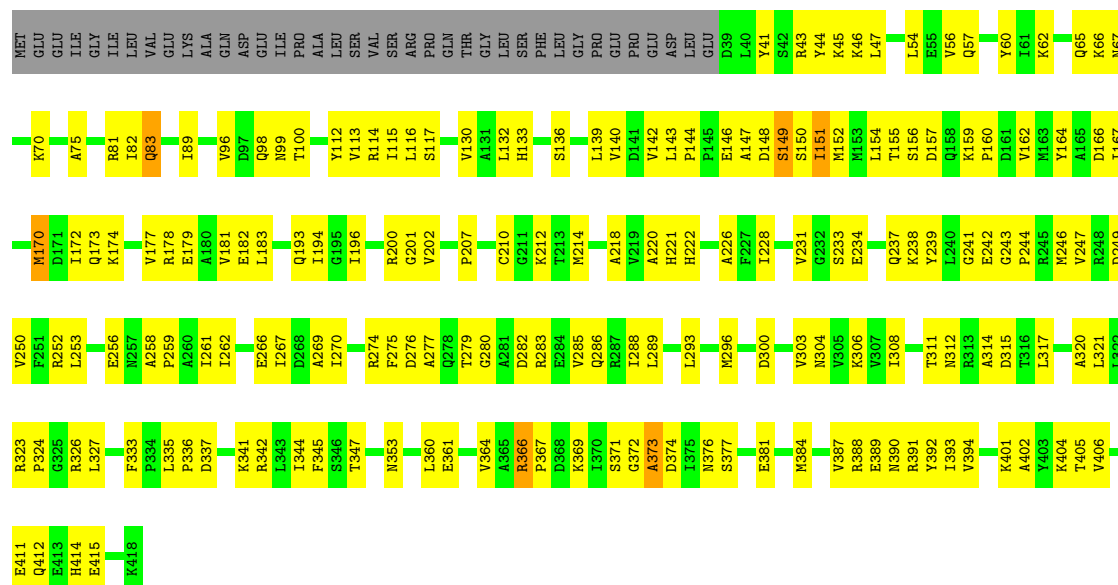
• Molecule 15: 26S protease regulatory subunit 6B

Chain AD: 47% 42% 9%



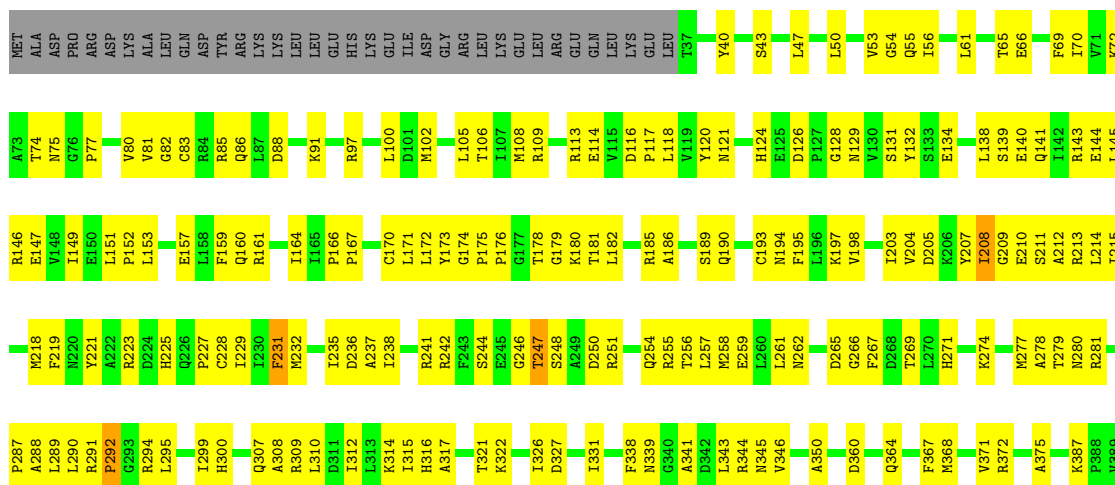
• Molecule 15: 26S protease regulatory subunit 6B

Chain BD: 48% 41% 9%

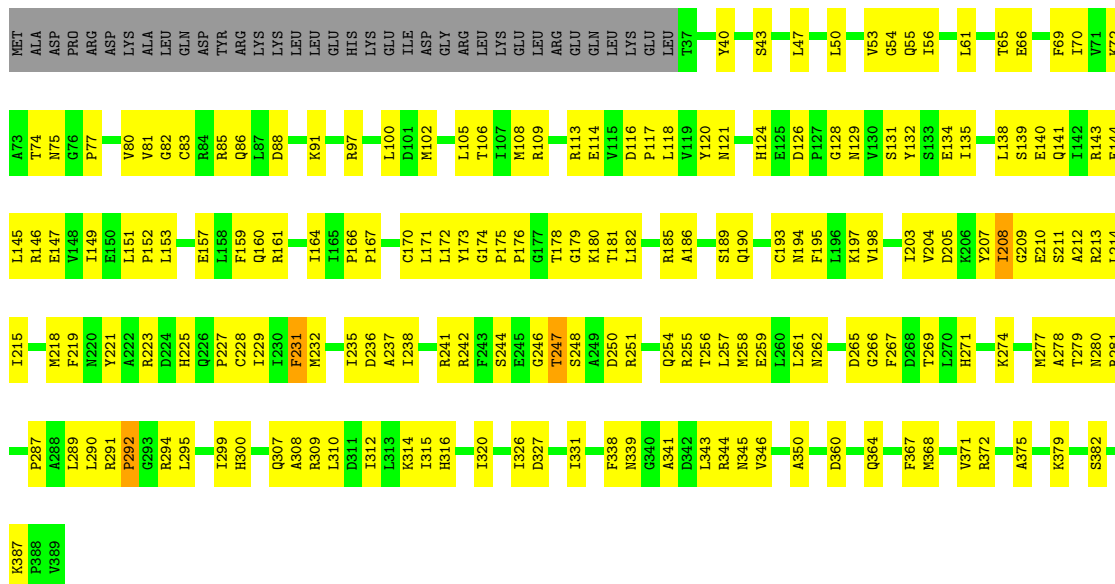


• Molecule 16: 26S protease regulatory subunit 10B

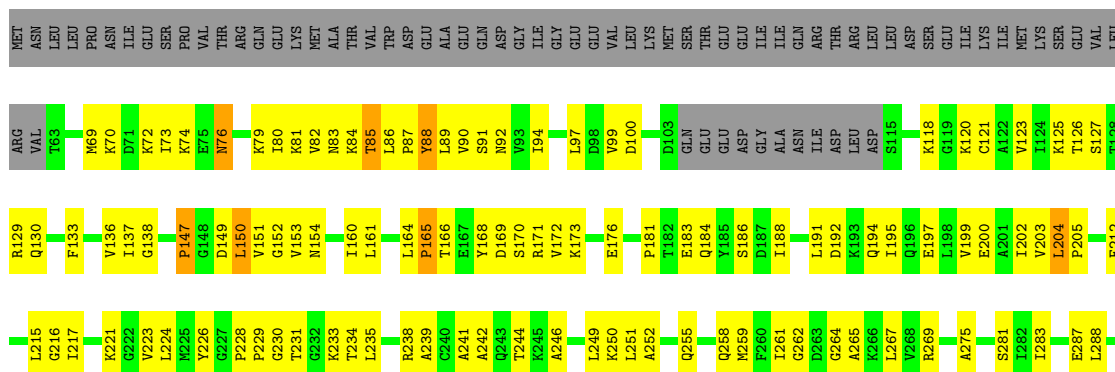
Chain AE: 44% 45% 9%



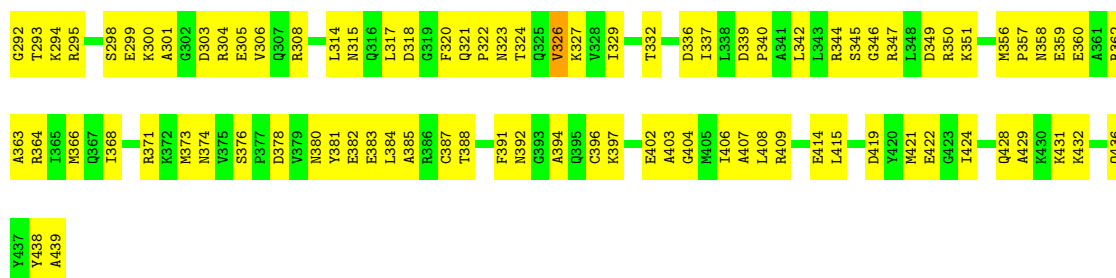
- Molecule 16: 26S protease regulatory subunit 10B



- Molecule 17: 26S protease regulatory subunit 6A

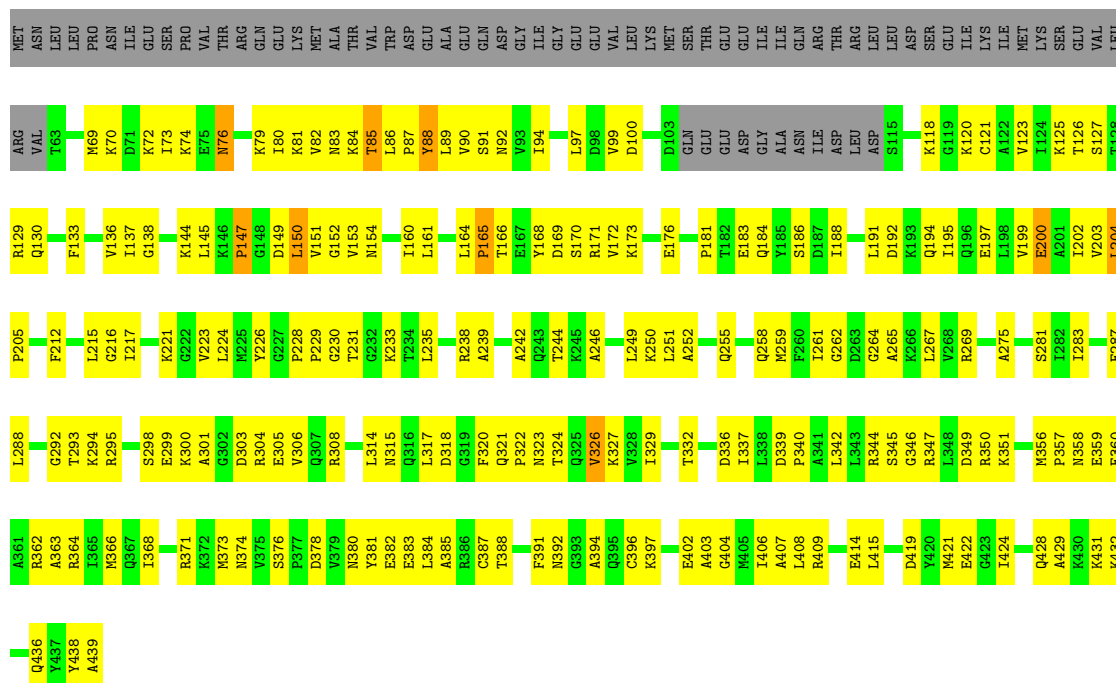






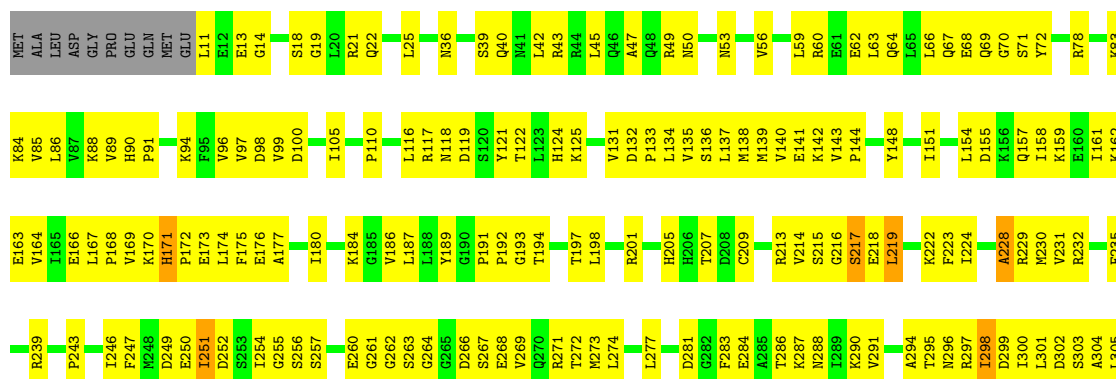
- Molecule 17: 26S protease regulatory subunit 6A

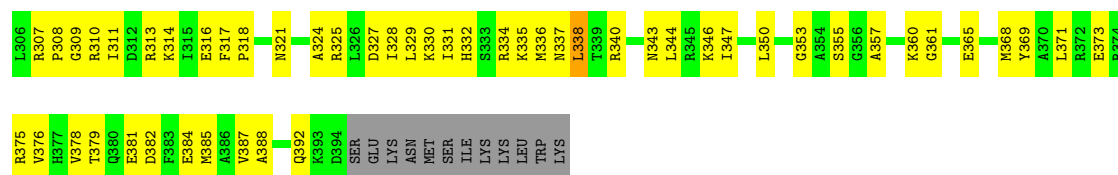
Chain BF: 38% 43% 17%



- Molecule 18: 26S protease regulatory subunit 8

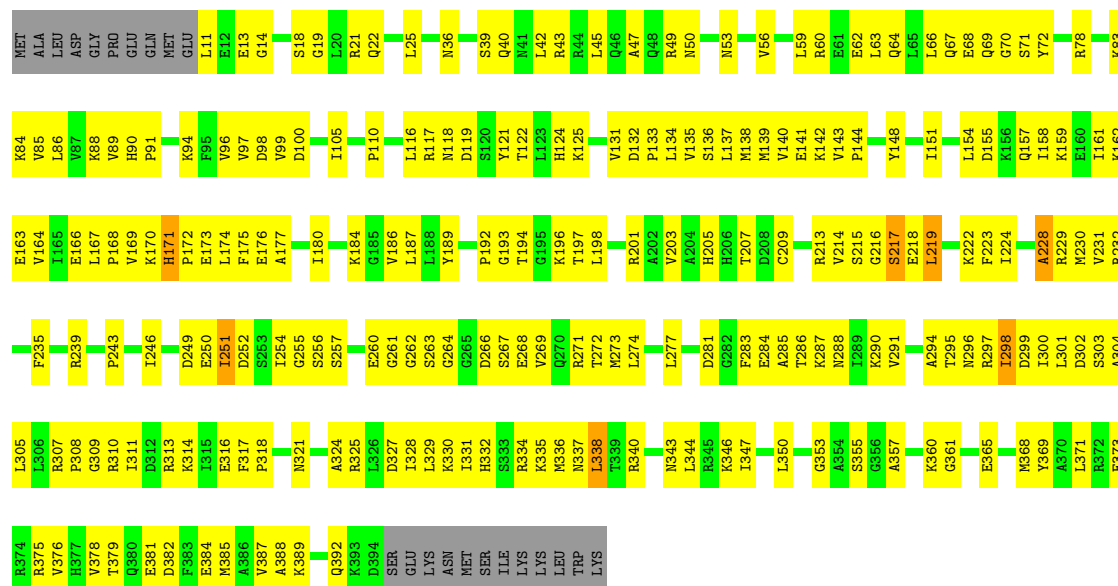
Chain AC: 40% 53% 5%





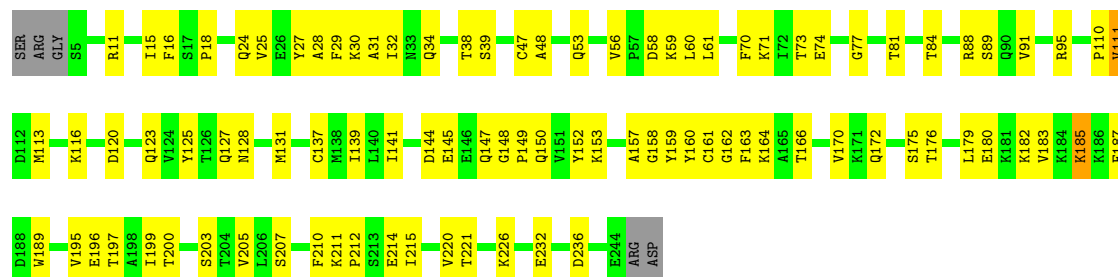
• Molecule 18: 26S protease regulatory subunit 8

Chain BC: 40% 53% 5%



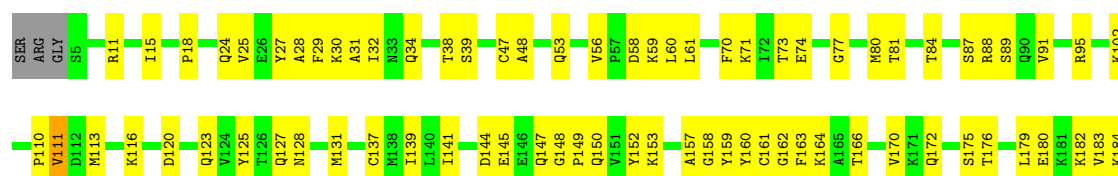
• Molecule 19: Proteasome subunit alpha type-6

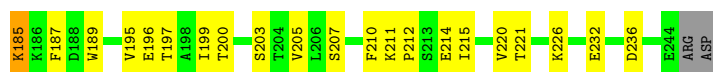
Chain AG: 60% 37% 2%



• Molecule 19: Proteasome subunit alpha type-6

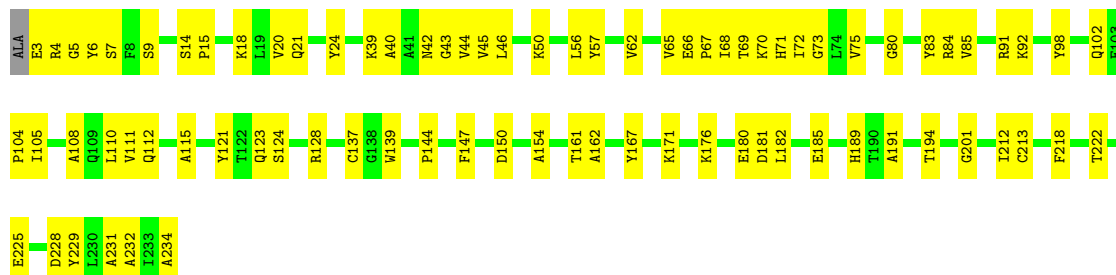
Chain BG: 59% 38% 2%





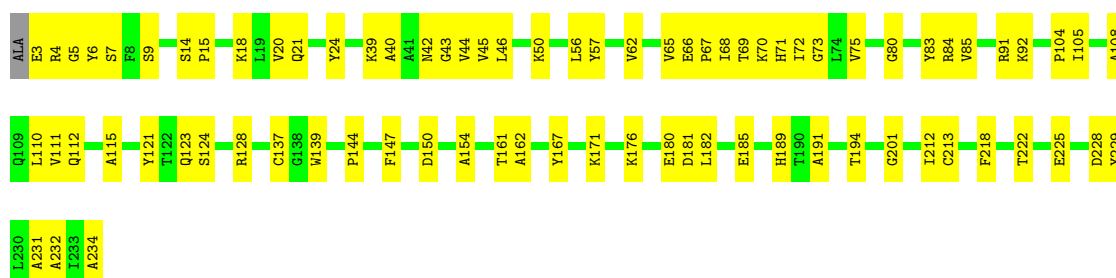
• Molecule 20: Proteasome subunit alpha type-2

Chain AH: 65% 35%



• Molecule 20: Proteasome subunit alpha type-2

Chain BH: 66% 34%



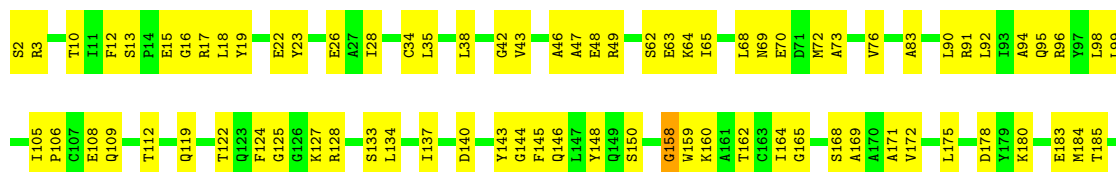
• Molecule 21: Proteasome subunit alpha type-4

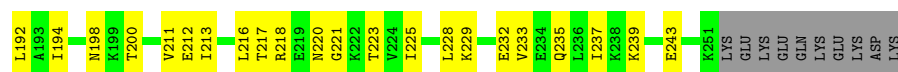
Chain AI: 59% 37%



• Molecule 21: Proteasome subunit alpha type-4

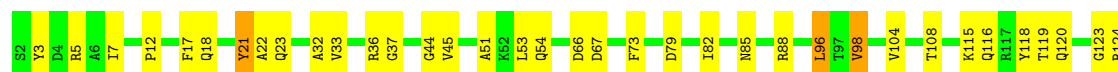
Chain BI: 57% 38%





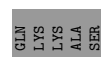
• Molecule 22: Proteasome subunit alpha type-7

Chain AJ: 68% 27%



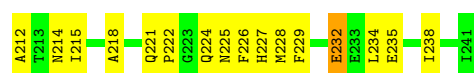
• Molecule 22: Proteasome subunit alpha type-7

Chain BJ: 67% 28%



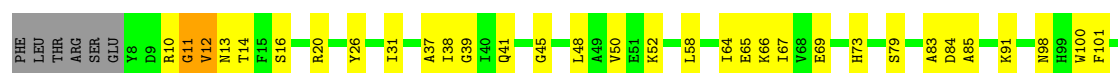
• Molecule 23: Proteasome subunit alpha type-5

Chain AK: 62% 32% 5%

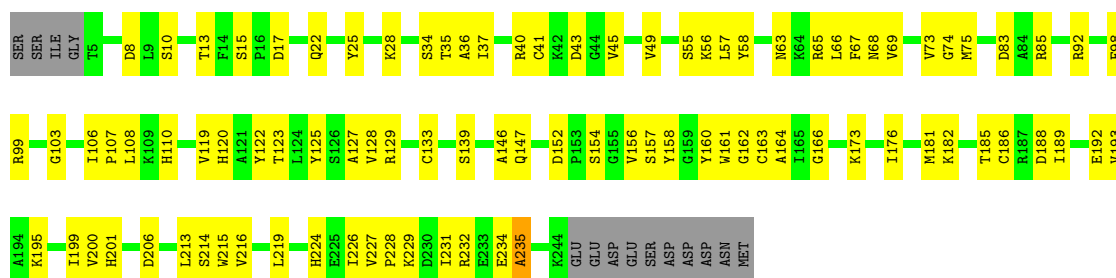


• Molecule 23: Proteasome subunit alpha type-5

Chain BK: 63% 31% 5%

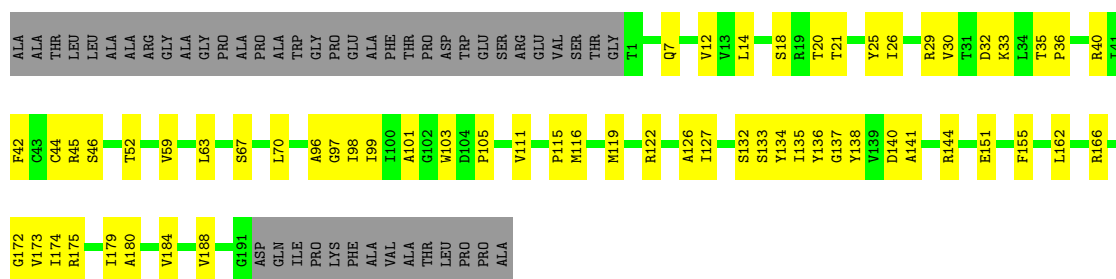






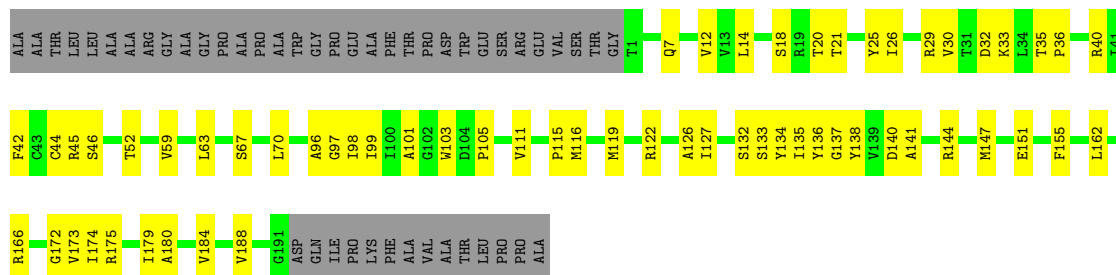
• Molecule 26: Proteasome subunit beta type-6

Chain AN: 55% 25% 20%



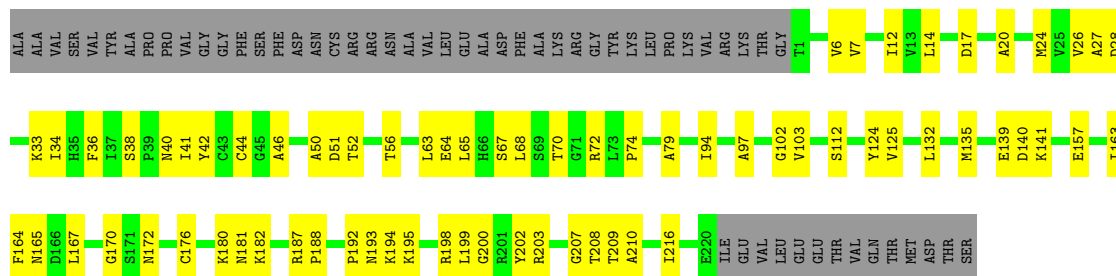
• Molecule 26: Proteasome subunit beta type-6

Chain BN: 55% 26% 20%



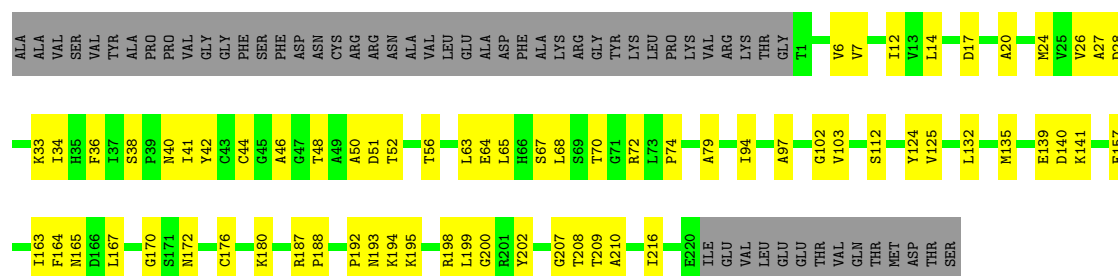
• Molecule 27: Proteasome subunit beta type-7

Chain AO: 54% 26% 20%



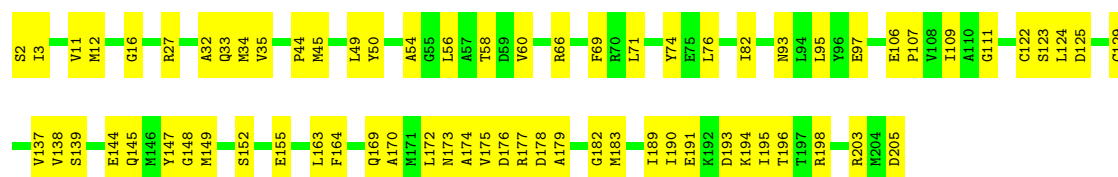
• Molecule 27: Proteasome subunit beta type-7

Chain BO: 55% 25% 20%



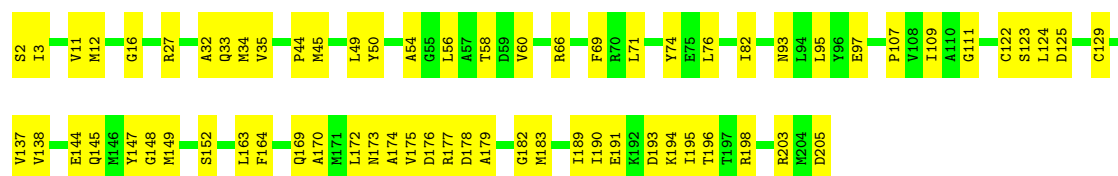
• Molecule 28: Proteasome subunit beta type-3

Chain AP: 66% 34%



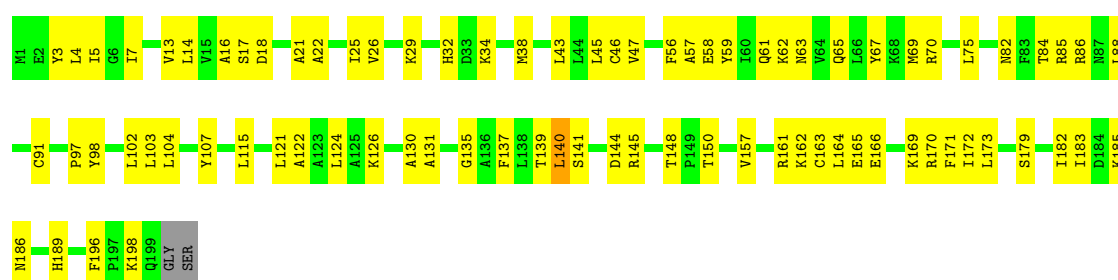
• Molecule 28: Proteasome subunit beta type-3

Chain BP: 67% 33%



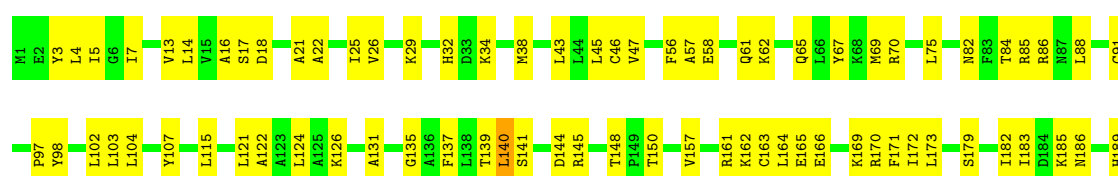
• Molecule 29: Proteasome subunit beta type-2

Chain AQ: 59% 40%



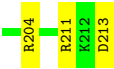
• Molecule 29: Proteasome subunit beta type-2

Chain BQ: 60% 38%

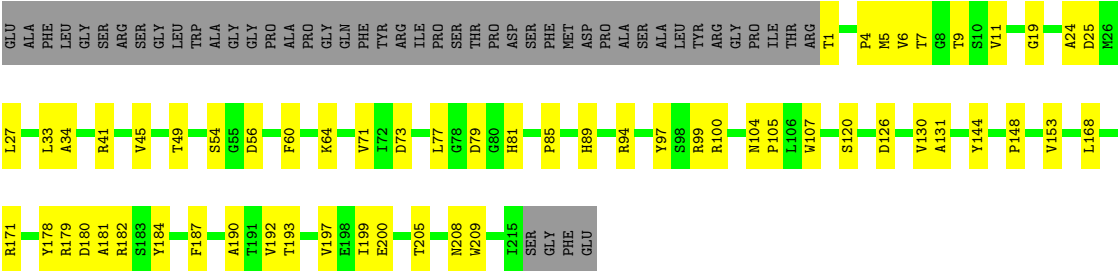




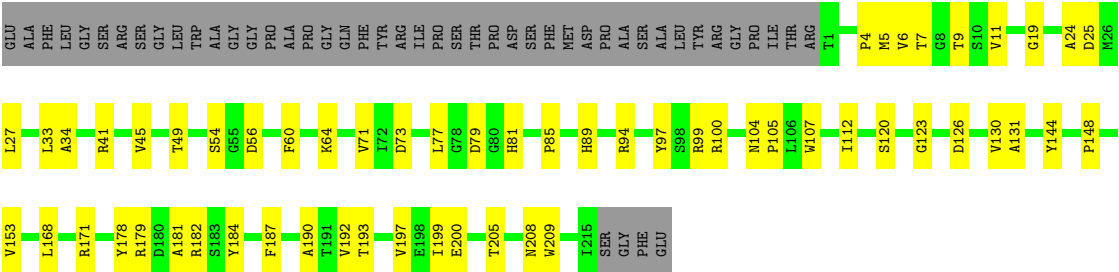




● Molecule 32: Proteasome subunit beta type-4



● Molecule 32: Proteasome subunit beta type-4



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	86420	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	-3000	Depositor
Magnification	28736	Depositor
Image detector	GATAN K2 SUMMIT (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: ZN, ATP, 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	AU	0.29	0/6396	0.49	0/8646
1	BU	0.29	0/6396	0.49	0/8646
10	Ad	0.30	0/2162	0.57	0/2919
10	Bd	0.30	0/2162	0.57	0/2919
11	Ae	0.28	0/338	0.56	0/450
11	Be	0.28	0/338	0.56	0/450
12	Af	0.33	2/5413 (0.0%)	0.63	3/7317 (0.0%)
12	Bf	0.33	2/5413 (0.0%)	0.63	3/7317 (0.0%)
13	AA	0.31	0/2886	0.56	1/3899 (0.0%)
13	BA	0.31	0/2886	0.56	1/3899 (0.0%)
14	AB	0.29	0/2700	0.54	0/3645
14	BB	0.29	0/2700	0.54	0/3645
15	AD	0.29	0/3090	0.58	1/4168 (0.0%)
15	BD	0.29	0/3090	0.58	1/4168 (0.0%)
16	AE	0.29	0/2835	0.54	0/3821
16	BE	0.29	0/2835	0.54	0/3821
17	AF	0.32	0/2903	0.59	2/3912 (0.1%)
17	BF	0.32	0/2903	0.59	2/3912 (0.1%)
18	AC	0.29	0/3054	0.57	2/4107 (0.0%)
18	BC	0.29	0/3054	0.57	2/4107 (0.0%)
19	AG	0.30	0/1859	0.51	0/2523
19	BG	0.30	0/1859	0.51	0/2523
2	AV	0.31	0/3929	0.57	0/5309
2	BV	0.31	0/3929	0.57	0/5309
20	AH	0.30	0/1743	0.50	0/2372
20	BH	0.30	0/1743	0.50	0/2372
21	AI	0.31	0/1942	0.53	0/2628
21	BI	0.31	0/1942	0.53	0/2628
22	AJ	0.30	0/1728	0.48	0/2358
22	BJ	0.30	0/1728	0.48	0/2358
23	AK	0.30	0/1747	0.53	0/2364
23	BK	0.30	0/1747	0.53	0/2364

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
24	AL	0.28	0/1885	0.49	0/2552
24	BL	0.28	0/1885	0.49	0/2552
25	AM	0.31	0/1891	0.49	0/2552
25	BM	0.31	0/1891	0.49	0/2552
26	AN	0.29	0/1454	0.48	0/1967
26	BN	0.29	0/1454	0.48	0/1967
27	AO	0.28	0/1670	0.48	0/2265
27	BO	0.28	0/1670	0.48	0/2265
28	AP	0.31	0/1614	0.49	0/2177
28	BP	0.31	0/1614	0.49	0/2177
29	AQ	0.31	0/1603	0.51	1/2174 (0.0%)
29	BQ	0.31	0/1603	0.51	1/2174 (0.0%)
3	AW	0.29	0/3751	0.54	3/5042 (0.1%)
3	BW	0.29	0/3751	0.54	3/5042 (0.1%)
30	AR	0.30	0/1579	0.46	0/2134
30	BR	0.30	0/1579	0.46	0/2134
31	AS	0.29	0/1671	0.48	0/2253
31	BS	0.29	0/1671	0.48	0/2253
32	AT	0.30	0/1700	0.49	0/2305
32	BT	0.30	0/1700	0.49	0/2305
4	AX	0.27	0/3053	0.45	0/4115
4	BX	0.27	0/3053	0.45	0/4115
5	AY	0.30	0/3173	0.53	2/4273 (0.0%)
5	BY	0.30	0/3173	0.53	2/4273 (0.0%)
6	AZ	0.28	0/2324	0.55	0/3150
6	BZ	0.28	0/2324	0.55	0/3150
7	Aa	0.36	1/3053 (0.0%)	0.52	0/4133
7	Ba	0.36	1/3053 (0.0%)	0.52	0/4133
8	Ab	0.27	0/1478	0.48	0/2001
8	Bb	0.27	0/1478	0.48	0/2001
9	Ac	0.33	0/2302	0.60	1/3110 (0.0%)
9	Bc	0.33	0/2302	0.60	1/3110 (0.0%)
All	All	0.30	6/157852 (0.0%)	0.54	32/213282 (0.0%)

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
16	AE	0	1
16	BE	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
18	AC	0	1
18	BC	0	1
23	AK	0	1
23	BK	0	1
9	Ac	0	1
9	Bc	0	1
All	All	0	8

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Aa	145	LEU	C-N	11.88	1.56	1.34
7	Ba	145	LEU	C-N	11.88	1.56	1.34
12	Af	840	LEU	C-N	6.42	1.46	1.34
12	Bf	840	LEU	C-N	6.42	1.46	1.34
12	Af	340	MET	C-N	-5.33	1.21	1.34

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	BF	150	LEU	CB-CG-CD2	8.79	125.95	111.00
17	AF	150	LEU	CB-CG-CD2	8.76	125.90	111.00
17	BF	204	LEU	CA-CB-CG	6.02	129.15	115.30
17	AF	204	LEU	CA-CB-CG	6.02	129.15	115.30
12	Af	618	GLU	N-CA-C	6.00	127.21	111.00

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	AC	171	HIS	Peptide
16	AE	175	PRO	Peptide
23	AK	232	GLU	Peptide
9	Ac	243	SER	Peptide
9	Bc	243	SER	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	AU	6287	0	6338	172	0
1	BU	6287	0	6338	171	0
2	AV	3852	0	3893	161	0
2	BV	3852	0	3893	158	0
3	AW	3703	0	3822	150	0
3	BW	3703	0	3822	150	0
4	AX	3009	0	3113	87	0
4	BX	3009	0	3113	87	0
5	AY	3115	0	3120	107	0
5	BY	3115	0	3120	112	0
6	AZ	2281	0	2312	97	0
6	BZ	2281	0	2312	94	0
7	Aa	2995	0	3012	0	0
7	Ba	2995	0	3012	0	0
8	Ab	1458	0	1505	0	0
8	Bb	1458	0	1505	0	0
9	Ac	2260	0	2276	0	0
9	Bc	2260	0	2276	0	0
10	Ad	2116	0	2146	0	0
10	Bd	2116	0	2146	0	0
11	Ae	334	0	294	0	0
11	Be	334	0	294	0	0
12	Af	5331	0	5343	0	0
12	Bf	5331	0	5343	0	0
13	AA	2835	0	2879	187	0
13	BA	2835	0	2879	192	0
14	AB	2662	0	2702	212	0
14	BB	2662	0	2702	211	0
15	AD	3040	0	3074	217	0
15	BD	3040	0	3074	212	0
16	AE	2790	0	2846	187	0
16	BE	2790	0	2846	186	0
17	AF	2863	0	2931	213	0
17	BF	2863	0	2931	220	0
18	AC	3015	0	3125	262	0
18	BC	3015	0	3125	261	0
19	AG	1826	0	1796	69	0
19	BG	1826	0	1796	70	0
20	AH	1708	0	1594	81	0
20	BH	1708	0	1594	80	0
21	AI	1912	0	1851	81	0
21	BI	1912	0	1851	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	AJ	1704	0	1517	64	0
22	BJ	1704	0	1517	65	0
23	AK	1722	0	1673	79	0
23	BK	1722	0	1673	78	0
24	AL	1850	0	1822	80	0
24	BL	1850	0	1822	80	0
25	AM	1856	0	1814	82	0
25	BM	1856	0	1814	80	0
26	AN	1430	0	1391	99	0
26	BN	1430	0	1392	107	0
27	AO	1643	0	1643	178	0
27	BO	1643	0	1643	179	0
28	AP	1585	0	1594	146	0
28	BP	1585	0	1594	143	0
29	AQ	1570	0	1540	141	0
29	BQ	1570	0	1540	135	0
30	AR	1548	0	1490	127	0
30	BR	1548	0	1490	130	0
31	AS	1641	0	1613	219	0
31	BS	1641	0	1613	222	0
32	AT	1667	0	1626	85	0
32	BT	1667	0	1626	78	0
33	Ac	1	0	0	0	0
33	Bc	1	0	0	0	0
34	AA	31	0	12	2	0
34	AD	31	0	12	2	0
34	AE	31	0	12	9	0
34	AF	31	0	12	2	0
34	BA	31	0	12	2	0
34	BD	31	0	12	2	0
34	BE	31	0	12	9	0
34	BF	31	0	12	2	0
35	AB	27	0	12	7	0
35	AC	27	0	12	3	0
35	BB	27	0	12	7	0
35	BC	27	0	12	4	0
All	All	155574	0	155535	5748	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 23.

The worst 5 of 5748 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)
31:AS:185:ARG:HA	27:BO:26:VAL:CG2	1.29	1.61
26:AN:138:TYR:CA	26:BN:138:TYR:HB2	1.23	1.59
27:AO:26:VAL:CG2	31:BS:185:ARG:HA	1.33	1.58
31:AS:180:ILE:CG2	27:BO:195:LYS:CE	1.75	1.58
26:AN:138:TYR:HB2	26:BN:138:TYR:CA	1.22	1.58

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	AU	798/953 (84%)	762 (96%)	34 (4%)	2 (0%)	43	79
1	BU	798/953 (84%)	762 (96%)	34 (4%)	2 (0%)	43	79
2	AV	478/533 (90%)	431 (90%)	40 (8%)	7 (2%)	11	51
2	BV	478/533 (90%)	431 (90%)	39 (8%)	8 (2%)	10	49
3	AW	454/456 (100%)	412 (91%)	38 (8%)	4 (1%)	19	60
3	BW	454/456 (100%)	412 (91%)	38 (8%)	4 (1%)	19	60
4	AX	378/422 (90%)	363 (96%)	15 (4%)	0	100	100
4	BX	378/422 (90%)	363 (96%)	15 (4%)	0	100	100
5	AY	376/389 (97%)	342 (91%)	30 (8%)	4 (1%)	16	57
5	BY	376/389 (97%)	342 (91%)	30 (8%)	4 (1%)	16	57
6	AZ	284/324 (88%)	257 (90%)	23 (8%)	4 (1%)	12	52
6	BZ	284/324 (88%)	257 (90%)	23 (8%)	4 (1%)	12	52
7	Aa	371/376 (99%)	343 (92%)	23 (6%)	5 (1%)	13	54
7	Ba	371/376 (99%)	343 (92%)	23 (6%)	5 (1%)	13	54
8	Ab	189/377 (50%)	180 (95%)	8 (4%)	1 (0%)	31	71
8	Bb	189/377 (50%)	180 (95%)	8 (4%)	1 (0%)	31	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	Ac	285/310 (92%)	252 (88%)	27 (10%)	6 (2%)	8	46
9	Bc	285/310 (92%)	252 (88%)	27 (10%)	6 (2%)	8	46
10	Ad	255/257 (99%)	227 (89%)	25 (10%)	3 (1%)	14	56
10	Bd	255/257 (99%)	227 (89%)	25 (10%)	3 (1%)	14	56
11	Ae	36/70 (51%)	32 (89%)	3 (8%)	1 (3%)	5	40
11	Be	36/70 (51%)	32 (89%)	3 (8%)	1 (3%)	5	40
12	Af	686/908 (76%)	571 (83%)	110 (16%)	5 (1%)	24	65
12	Bf	686/908 (76%)	571 (83%)	110 (16%)	5 (1%)	24	65
13	AA	359/433 (83%)	317 (88%)	33 (9%)	9 (2%)	6	42
13	BA	359/433 (83%)	317 (88%)	33 (9%)	9 (2%)	6	42
14	AB	339/440 (77%)	303 (89%)	32 (9%)	4 (1%)	14	56
14	BB	339/440 (77%)	303 (89%)	32 (9%)	4 (1%)	14	56
15	AD	378/418 (90%)	330 (87%)	44 (12%)	4 (1%)	16	57
15	BD	378/418 (90%)	330 (87%)	44 (12%)	4 (1%)	16	57
16	AE	351/389 (90%)	307 (88%)	40 (11%)	4 (1%)	16	57
16	BE	351/389 (90%)	307 (88%)	40 (11%)	4 (1%)	16	57
17	AF	362/439 (82%)	326 (90%)	32 (9%)	4 (1%)	16	57
17	BF	362/439 (82%)	326 (90%)	31 (9%)	5 (1%)	12	52
18	AC	382/406 (94%)	341 (89%)	37 (10%)	4 (1%)	17	58
18	BC	382/406 (94%)	341 (89%)	37 (10%)	4 (1%)	17	58
19	AG	238/245 (97%)	221 (93%)	14 (6%)	3 (1%)	13	54
19	BG	238/245 (97%)	221 (93%)	14 (6%)	3 (1%)	13	54
20	AH	230/233 (99%)	216 (94%)	14 (6%)	0	100	100
20	BH	230/233 (99%)	216 (94%)	14 (6%)	0	100	100
21	AI	248/260 (95%)	226 (91%)	21 (8%)	1 (0%)	36	75
21	BI	248/260 (95%)	226 (91%)	21 (8%)	1 (0%)	36	75
22	AJ	237/247 (96%)	226 (95%)	7 (3%)	4 (2%)	10	49
22	BJ	237/247 (96%)	226 (95%)	7 (3%)	4 (2%)	10	49
23	AK	224/240 (93%)	201 (90%)	21 (9%)	2 (1%)	19	60
23	BK	224/240 (93%)	202 (90%)	20 (9%)	2 (1%)	19	60
24	AL	236/268 (88%)	214 (91%)	22 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	BL	236/268 (88%)	214 (91%)	22 (9%)	0	100	100
25	AM	238/254 (94%)	219 (92%)	17 (7%)	2 (1%)	21	62
25	BM	238/254 (94%)	219 (92%)	17 (7%)	2 (1%)	21	62
26	AN	189/238 (79%)	184 (97%)	5 (3%)	0	100	100
26	BN	189/238 (79%)	184 (97%)	5 (3%)	0	100	100
27	AO	218/276 (79%)	211 (97%)	7 (3%)	0	100	100
27	BO	218/276 (79%)	211 (97%)	7 (3%)	0	100	100
28	AP	202/204 (99%)	181 (90%)	21 (10%)	0	100	100
28	BP	202/204 (99%)	181 (90%)	21 (10%)	0	100	100
29	AQ	197/201 (98%)	181 (92%)	16 (8%)	0	100	100
29	BQ	197/201 (98%)	181 (92%)	16 (8%)	0	100	100
30	AR	199/262 (76%)	192 (96%)	7 (4%)	0	100	100
30	BR	199/262 (76%)	192 (96%)	7 (4%)	0	100	100
31	AS	211/240 (88%)	201 (95%)	10 (5%)	0	100	100
31	BS	211/240 (88%)	201 (95%)	10 (5%)	0	100	100
32	AT	213/263 (81%)	204 (96%)	9 (4%)	0	100	100
32	BT	213/263 (81%)	204 (96%)	9 (4%)	0	100	100
All	All	19682/22662 (87%)	17947 (91%)	1567 (8%)	168 (1%)	24	60

5 of 168 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AU	364	VAL
3	AW	136	ILE
5	AY	350	VAL
9	Ac	157	ILE
9	Ac	244	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AU	685/816 (84%)	681 (99%)	4 (1%)	87	94
1	BU	685/816 (84%)	681 (99%)	4 (1%)	87	94
2	AV	414/459 (90%)	409 (99%)	5 (1%)	74	88
2	BV	414/459 (90%)	409 (99%)	5 (1%)	74	88
3	AW	416/416 (100%)	413 (99%)	3 (1%)	85	93
3	BW	416/416 (100%)	413 (99%)	3 (1%)	85	93
4	AX	327/362 (90%)	325 (99%)	2 (1%)	87	94
4	BX	327/362 (90%)	325 (99%)	2 (1%)	87	94
5	AY	334/344 (97%)	334 (100%)	0	100	100
5	BY	334/344 (97%)	334 (100%)	0	100	100
6	AZ	257/295 (87%)	256 (100%)	1 (0%)	92	96
6	BZ	257/295 (87%)	256 (100%)	1 (0%)	92	96
7	Aa	333/336 (99%)	332 (100%)	1 (0%)	93	97
7	Ba	333/336 (99%)	332 (100%)	1 (0%)	93	97
8	Ab	167/312 (54%)	167 (100%)	0	100	100
8	Bb	167/312 (54%)	167 (100%)	0	100	100
9	Ac	252/268 (94%)	250 (99%)	2 (1%)	83	92
9	Bc	252/268 (94%)	250 (99%)	2 (1%)	83	92
10	Ad	231/231 (100%)	230 (100%)	1 (0%)	92	96
10	Bd	231/231 (100%)	230 (100%)	1 (0%)	92	96
11	Ae	38/63 (60%)	38 (100%)	0	100	100
11	Be	38/63 (60%)	38 (100%)	0	100	100
12	Af	582/763 (76%)	578 (99%)	4 (1%)	85	93
12	Bf	582/763 (76%)	578 (99%)	4 (1%)	85	93
13	AA	308/372 (83%)	307 (100%)	1 (0%)	93	97
13	BA	308/372 (83%)	307 (100%)	1 (0%)	93	97
14	AB	298/385 (77%)	296 (99%)	2 (1%)	85	93
14	BB	298/385 (77%)	296 (99%)	2 (1%)	85	93
15	AD	333/366 (91%)	331 (99%)	2 (1%)	87	94
15	BD	333/366 (91%)	331 (99%)	2 (1%)	87	94
16	AE	308/341 (90%)	306 (99%)	2 (1%)	87	94
16	BE	308/341 (90%)	306 (99%)	2 (1%)	87	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	AF	312/379 (82%)	309 (99%)	3 (1%)	78	89
17	BF	312/379 (82%)	309 (99%)	3 (1%)	78	89
18	AC	332/352 (94%)	329 (99%)	3 (1%)	81	91
18	BC	332/352 (94%)	329 (99%)	3 (1%)	81	91
19	AG	193/209 (92%)	193 (100%)	0	100	100
19	BG	193/209 (92%)	193 (100%)	0	100	100
20	AH	164/190 (86%)	163 (99%)	1 (1%)	87	94
20	BH	164/190 (86%)	163 (99%)	1 (1%)	87	94
21	AI	193/220 (88%)	193 (100%)	0	100	100
21	BI	193/220 (88%)	193 (100%)	0	100	100
22	AJ	152/210 (72%)	150 (99%)	2 (1%)	71	87
22	BJ	152/210 (72%)	150 (99%)	2 (1%)	71	87
23	AK	186/202 (92%)	186 (100%)	0	100	100
23	BK	186/202 (92%)	186 (100%)	0	100	100
24	AL	198/229 (86%)	198 (100%)	0	100	100
24	BL	198/229 (86%)	198 (100%)	0	100	100
25	AM	192/211 (91%)	191 (100%)	1 (0%)	90	96
25	BM	192/211 (91%)	191 (100%)	1 (0%)	90	96
26	AN	148/180 (82%)	148 (100%)	0	100	100
26	BN	148/180 (82%)	148 (100%)	0	100	100
27	AO	177/227 (78%)	177 (100%)	0	100	100
27	BO	177/227 (78%)	177 (100%)	0	100	100
28	AP	172/173 (99%)	172 (100%)	0	100	100
28	BP	172/173 (99%)	172 (100%)	0	100	100
29	AQ	164/171 (96%)	163 (99%)	1 (1%)	87	94
29	BQ	164/171 (96%)	163 (99%)	1 (1%)	87	94
30	AR	153/201 (76%)	153 (100%)	0	100	100
30	BR	153/201 (76%)	153 (100%)	0	100	100
31	AS	174/198 (88%)	174 (100%)	0	100	100
31	BS	174/198 (88%)	174 (100%)	0	100	100
32	AT	175/214 (82%)	175 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	BT	175/214 (82%)	175 (100%)	0	100	100
All	All	16736/19390 (86%)	16654 (100%)	82 (0%)	90	96

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	AJ	21	TYR
2	BV	36	GLU
18	BC	53	ASN
22	AJ	176	TYR
1	BU	147	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 105 such sidechains are listed below:

Mol	Chain	Res	Type
31	AS	146	GLN
9	Bc	172	HIS
26	BN	123	GLN
31	AS	151	ASN
2	BV	33	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

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	ATP	AA	501	-	27,33,33	0.96	1 (3%)	27,52,52	2.00	4 (14%)
35	ADP	AB	501	-	25,29,29	1.06	1 (4%)	25,45,45	1.65	5 (20%)
35	ADP	AC	501	-	25,29,29	1.06	1 (4%)	25,45,45	1.60	3 (12%)
34	ATP	AD	501	-	27,33,33	0.95	1 (3%)	27,52,52	1.78	5 (18%)
34	ATP	AE	401	-	27,33,33	1.00	2 (7%)	27,52,52	1.78	4 (14%)
34	ATP	AF	501	-	27,33,33	0.99	1 (3%)	27,52,52	1.87	4 (14%)
34	ATP	BA	501	-	27,33,33	0.96	1 (3%)	27,52,52	2.01	4 (14%)
35	ADP	BB	501	-	25,29,29	1.06	1 (4%)	25,45,45	1.65	5 (20%)
35	ADP	BC	501	-	25,29,29	1.07	1 (4%)	25,45,45	1.61	3 (12%)
34	ATP	BD	501	-	27,33,33	0.95	1 (3%)	27,52,52	1.78	5 (18%)
34	ATP	BE	401	-	27,33,33	1.00	2 (7%)	27,52,52	1.78	4 (14%)
34	ATP	BF	501	-	27,33,33	0.99	1 (3%)	27,52,52	1.86	4 (14%)

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	ATP	AA	501	-	-	0/18/38/38	0/3/3/3
35	ADP	AB	501	-	-	0/12/32/32	0/3/3/3
35	ADP	AC	501	-	-	0/12/32/32	0/3/3/3
34	ATP	AD	501	-	-	0/18/38/38	0/3/3/3
34	ATP	AE	401	-	-	0/18/38/38	0/3/3/3
34	ATP	AF	501	-	-	0/18/38/38	0/3/3/3
34	ATP	BA	501	-	-	0/18/38/38	0/3/3/3
35	ADP	BB	501	-	-	0/12/32/32	0/3/3/3
35	ADP	BC	501	-	-	0/12/32/32	0/3/3/3
34	ATP	BD	501	-	-	0/18/38/38	0/3/3/3
34	ATP	BE	401	-	-	0/18/38/38	0/3/3/3
34	ATP	BF	501	-	-	0/18/38/38	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	AE	401	ATP	C8-N9	-2.02	1.34	1.36
34	BE	401	ATP	C8-N9	-2.02	1.34	1.36
34	AA	501	ATP	C5-C4	2.91	1.47	1.40
34	BA	501	ATP	C5-C4	2.91	1.47	1.40
34	BD	501	ATP	C5-C4	3.00	1.47	1.40

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	AD	501	ATP	N3-C2-N1	-6.21	123.55	128.86
34	BD	501	ATP	N3-C2-N1	-6.19	123.57	128.86
34	BA	501	ATP	N3-C2-N1	-5.77	123.92	128.86
34	AA	501	ATP	N3-C2-N1	-5.75	123.94	128.86
35	BC	501	ADP	N3-C2-N1	-5.28	124.34	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	AA	501	ATP	2	0
35	AB	501	ADP	7	0
35	AC	501	ADP	3	0
34	AD	501	ATP	2	0
34	AE	401	ATP	9	0
34	AF	501	ATP	2	0
34	BA	501	ATP	2	0
35	BB	501	ADP	7	0
35	BC	501	ADP	4	0
34	BD	501	ATP	2	0
34	BE	401	ATP	9	0
34	BF	501	ATP	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
12	Bf	3
12	Af	3

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Bf	269:ALA	C	270:LEU	N	9.72
1	Af	269:ALA	C	270:LEU	N	9.71
1	Af	238:ASN	C	239:TYR	N	7.22
1	Bf	238:ASN	C	239:TYR	N	7.22
1	Af	507:ASP	C	508:SER	N	5.88