



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

Jul 24, 2017 – 03:49 AM EDT

PDB ID : 5M32  
EMDB ID: : EMD-4146  
Title : Human 26S proteasome in complex with Oprozomib  
Authors : Haselbach, D.; Schrader, J.; Lambrecht, F.; Henneberg, F.; Chari, A.; Stark, H.  
Deposited on : unknown  
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

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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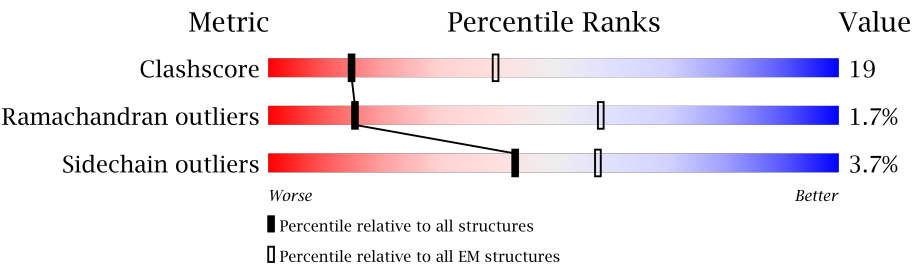
MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

# 1 Overall quality at a glance i

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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	234	<div><div>73%</div><div>24%</div><div>..</div></div>
1	O	234	<div><div>74%</div><div>23%</div><div>..</div></div>
2	B	261	<div><div>68%</div><div>18%</div><div>•</div><div>10%</div></div>
2	P	261	<div><div>70%</div><div>19%</div><div>•</div><div>•</div><div>7%</div></div>
3	C	234	<div><div>74%</div><div>23%</div><div>..</div></div>
4	D	241	<div><div>78%</div><div>17%</div><div>•</div><div>•</div></div>
4	R	241	<div><div>78%</div><div>17%</div><div>•</div><div>•</div></div>
5	E	234	<div><div>78%</div><div>19%</div><div>•</div></div>
6	F	255	<div><div>68%</div><div>21%</div><div>•</div><div>9%</div></div>



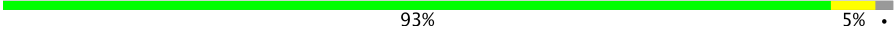



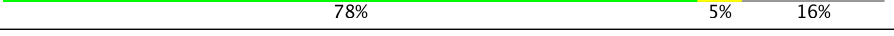
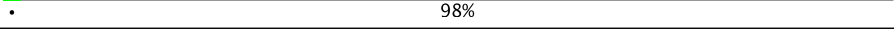
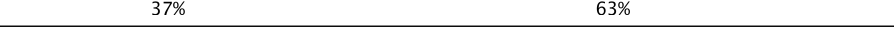
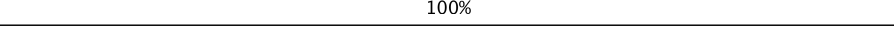
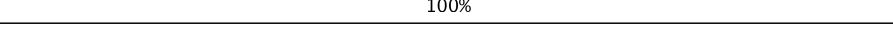
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Mol	Chain	Length	Quality of chain
6	T	255	
7	G	246	
7	U	246	
8	H	277	
8	V	277	
9	I	205	
9	W	205	
10	J	196	
10	X	196	
11	K	204	
11	Y	204	
12	L	241	
12	Z	241	
13	M	264	
13	a	264	
14	N	239	
14	b	239	
15	Q	235	
16	S	238	
17	c	433	
18	d	428	
19	e	418	
20	f	379	
21	g	439	
22	h	355	

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Mol	Chain	Length	Quality of chain
23	i	953	
24	j	534	
25	k	456	
26	l	422	
27	m	389	
28	n	324	
29	o	376	
30	p	377	
31	q	310	
32	r	350	
33	s	70	
34	t	4	
34	u	4	

## 2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 76085 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 alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	230	Total	C	N	O	S	0	0
			1763	1132	297	328	6		
1	O	230	Total	C	N	O	S	0	0
			1764	1126	301	331	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	234	Total	C	N	O	S	0	0
			1836	1164	315	348	9		
2	P	244	Total	C	N	O	S	0	0
			1875	1187	323	355	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	234	Total	C	N	O	S	0	0
			1771	1107	315	344	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	48	ALA	LYS	conflict	UNP O14818
C	179	ASP	GLU	conflict	UNP O14818
C	200	GLU	GLN	conflict	UNP O14818

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	233	Total	C	N	O	S	0	0
			1757	1103	290	353	11		
4	R	233	Total	C	N	O	S	0	0
			1768	1112	294	351	11		

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	234	Total	C	N	O	S	0	0
			1805	1133	321	340	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	185	ASP	ASN	conflict	UNP P25786
E	234	ASP	GLU	conflict	UNP P25786

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	232	Total	C	N	O	S	0	0
			1818	1153	310	344	11		
6	T	240	Total	C	N	O	S	0	0
			1877	1190	320	356	11		

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	233	Total	C	N	O	S	0	0
			1806	1147	301	345	13		
7	U	241	Total	C	N	O	S	0	0
			1841	1168	308	352	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	221	Total	C	N	O	S	0	0
			1663	1047	283	321	12		
8	V	220	Total	C	N	O	S	1	0
			1627	1025	273	318	11		

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	204	Total	C	N	O	S	0	0
			1590	1013	265	293	19		
9	W	204	Total	C	N	O	S	0	0
			1586	1010	263	294	19		

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	196	Total	C	N	O	S	0	0
			1560	1001	266	284	9		
10	X	196	Total	C	N	O	S	0	0
			1563	1002	267	285	9		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	182	VAL	ILE	conflict	UNP P49721
J	186	ASP	ASN	conflict	UNP P49721
J	190	ASN	ASP	conflict	UNP P49721
J	192	GLU	ASP	conflict	UNP P49721
J	195	ALA	SER	conflict	UNP P49721
X	182	VAL	ILE	conflict	UNP P49721
X	186	ASP	ASN	conflict	UNP P49721
X	190	ASN	ASP	conflict	UNP P49721
X	192	GLU	ASP	conflict	UNP P49721
X	195	ALA	SER	conflict	UNP P49721

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	200	Total	C	N	O	S	0	0
			1545	974	269	293	9		
11	Y	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	213	Total	C	N	O	S	1	0
			1637	1038	277	312	10		
12	Z	213	Total	C	N	O	S	0	0
			1642	1040	281	311	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	216	Total	C	N	O	S	0	0
			1687	1064	291	320	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	216	Total	C	N	O	S	0	0
			1679	1059	290	318	12		

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	202	Total	C	N	O	S	0	0
			1513	948	258	295	12		
14	b	203	Total	C	N	O	S	0	0
			1519	952	259	296	12		

- Molecule 15 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	235	Total	C	N	O	S	0	0
			1785	1118	318	344	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	179	ASP	GLU	conflict	UNP O14818

- Molecule 16 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	238	Total	C	N	O	S	0	0
			1834	1147	329	347	11		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	2	ALA	PHE	conflict	UNP P25786
S	3	ALA	ARG	conflict	UNP P25786
S	185	ASP	ASN	conflict	UNP P25786
S	234	ASP	GLU	conflict	UNP P25786

- Molecule 17 is a protein called 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	c	347	Total	C	N	O	S	0	0
			2728	1722	485	503	18		



- Molecule 18 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	d	333	Total	C	N	O	S	0	0
			2560	1614	433	501	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	e	361	Total	C	N	O	S	0	0
			2776	1752	488	525	11		

- Molecule 20 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	f	348	Total	C	N	O	S	0	0
			2692	1692	483	501	16		

- Molecule 21 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	g	363	Total	C	N	O	S	0	0
			2777	1753	480	529	15		

- Molecule 22 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	h	332	Total	C	N	O	S	0	0
			2518	1589	447	466	16		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	i	230	Total	C	N	O	0	0
			1145	685	230	230		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	j	155	Total	C	N	O	0	0
			779	470	155	154		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	k	364	Total	C	N	O	0	0
			1819	1092	364	363		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	l	415	Total	C	N	O	S	0	0
			2572	1598	474	494	6		

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	m	375	Total	C	N	O	S	0	0
			2421	1513	434	468	6		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
28	n	206	Total	C	N	O	0	0
			1030	618	206	206		

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	o	75	Total	C	N	O	0	0
			377	227	75	75		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
30	p	101	Total	C	N	O	0	0
			504	303	101	100		

- Molecule 31 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	q	259	Total	C	N	O	0	0
			1311	789	261	261		

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	r	8	Total	C	N	O	0	0
			40	25	8	7		

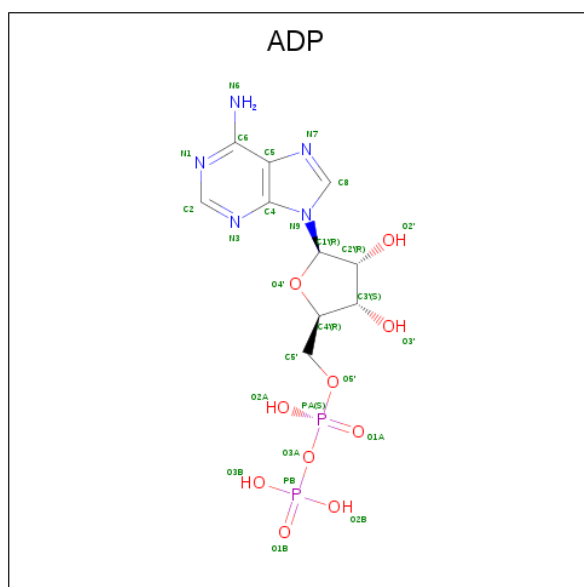
- Molecule 33 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	s	26	Total	C	N	O	0	0
			130	79	26	25		

- Molecule 34 is a protein called bound Oprozomib.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	t	4	Total	C	N	O	S	0	0
			37	25	4	7	1		
34	u	4	Total	C	N	O	S	0	0
			37	25	4	7	1		

- 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	c	1	Total	C	N	O	P	0
			27	10	5	10	2	
35	d	1	Total	C	N	O	P	0
			27	10	5	10	2	
35	e	1	Total	C	N	O	P	0
			27	10	5	10	2	

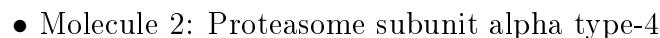
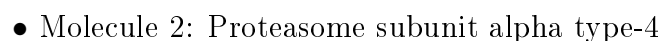
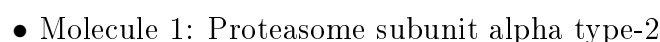
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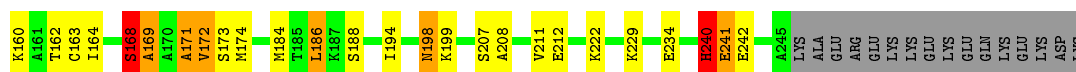
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Mol	Chain	Residues	Atoms					AltConf
35	g	1	Total	C	N	O	P	0
			54	20	10	20	4	
35	g	1	Total	C	N	O	P	0
			54	20	10	20	4	
35	h	1	Total	C	N	O	P	0
			27	10	5	10	2	



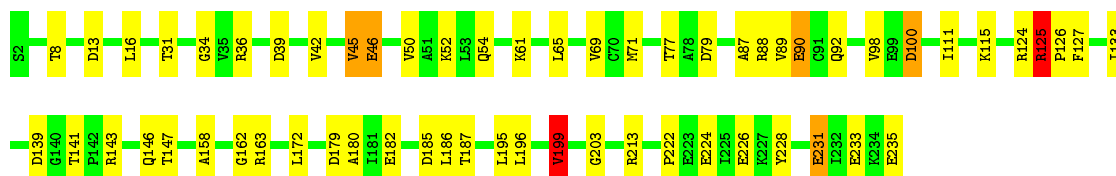
- Molecule 1: Proteasome subunit alpha type-2





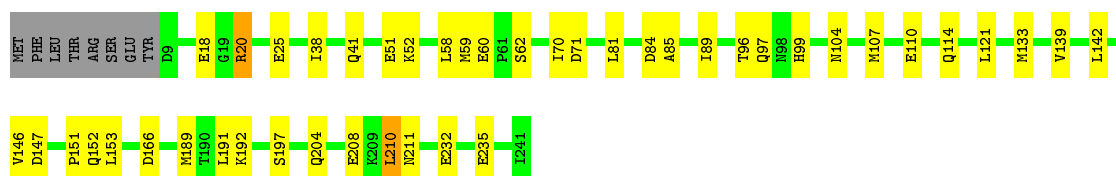
• Molecule 3: Proteasome subunit alpha type-7

Chain C: 74% 23%



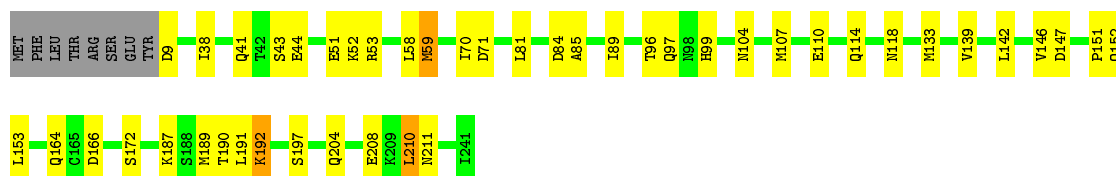
• Molecule 4: Proteasome subunit alpha type-5

Chain D: 78% 17%



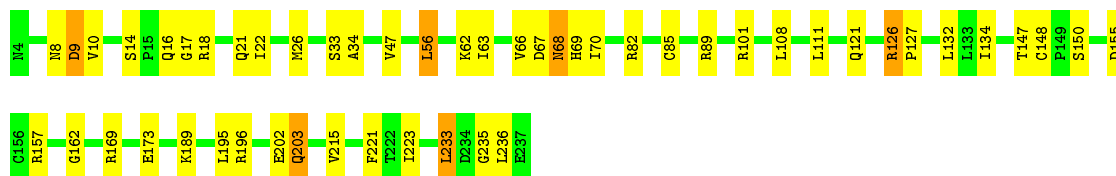
• Molecule 4: Proteasome subunit alpha type-5

Chain R: 78% 17%



• Molecule 5: Proteasome subunit alpha type-1

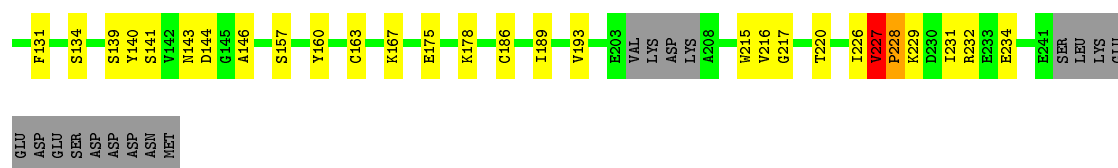
Chain E: 78% 19%



• Molecule 6: Proteasome subunit alpha type-3

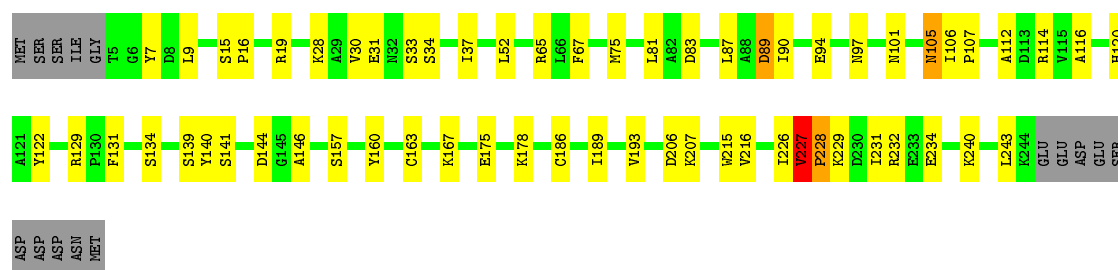
Chain F: 68% 21% 9%





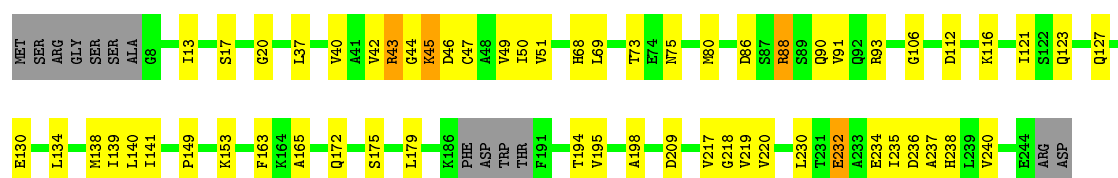
• Molecule 6: Proteasome subunit alpha type-3

Chain T: 70% 22% 6%



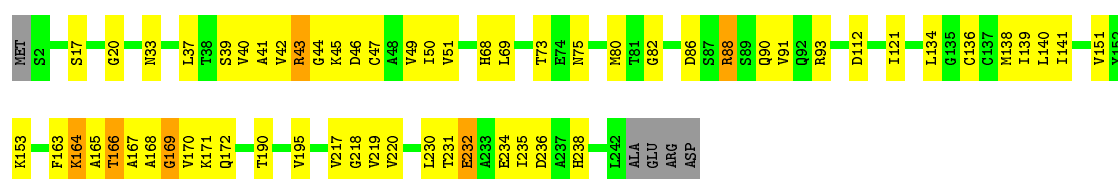
• Molecule 7: Proteasome subunit alpha type-6

Chain G: 71% 22% 5%



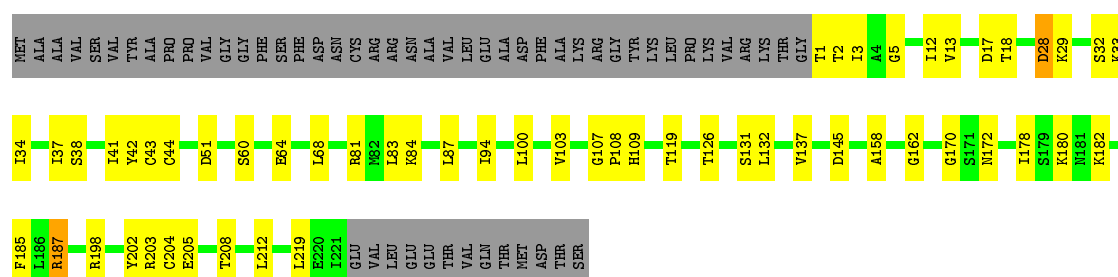
• Molecule 7: Proteasome subunit alpha type-6

Chain U: 74% 22% . .

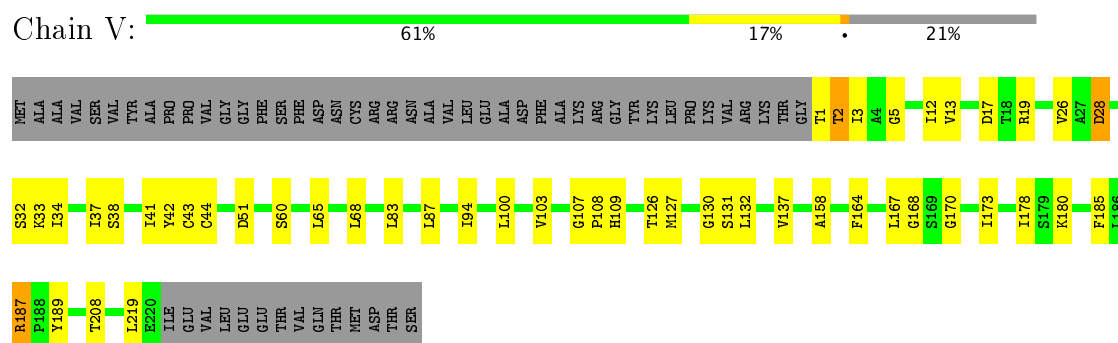


• Molecule 8: Proteasome subunit beta type-7

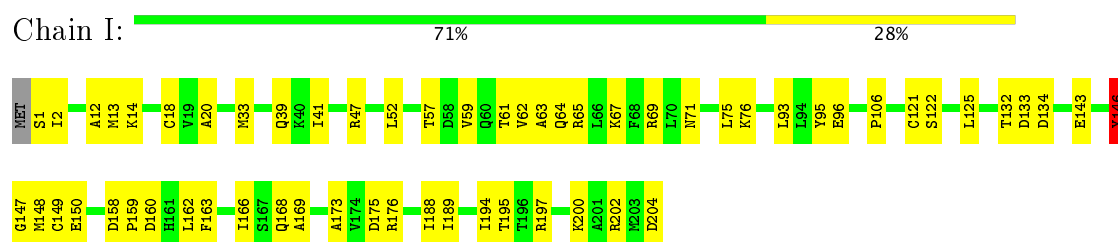
Chain H: 60% 19% 20%



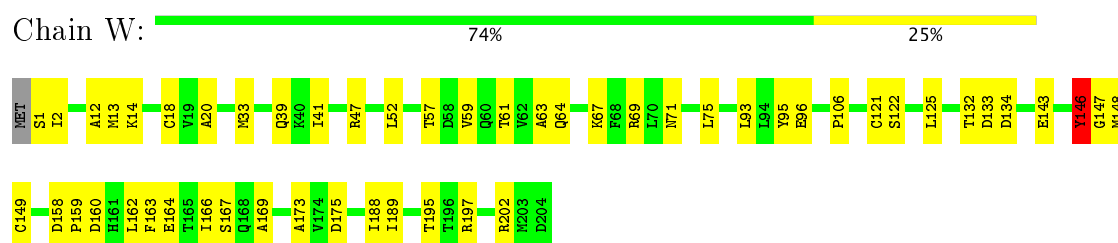
- Molecule 8: Proteasome subunit beta type-7



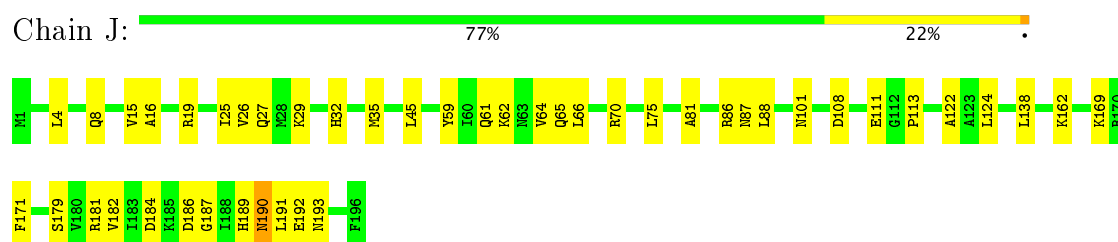
- Molecule 9: Proteasome subunit beta type-3



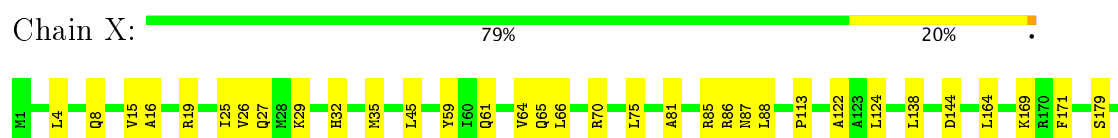
- Molecule 9: Proteasome subunit beta type-3



- Molecule 10: Proteasome subunit beta type-2



- Molecule 10: Proteasome subunit beta type-2

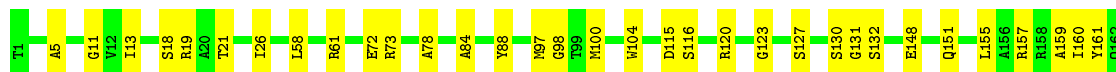






• Molecule 11: Proteasome subunit beta type-5

Chain K: 76% 22%



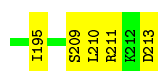
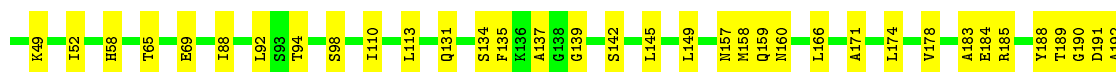
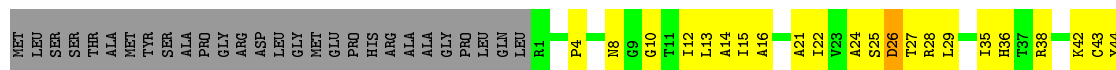
• Molecule 11: Proteasome subunit beta type-5

Chain Y: 74% 25%



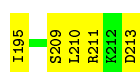
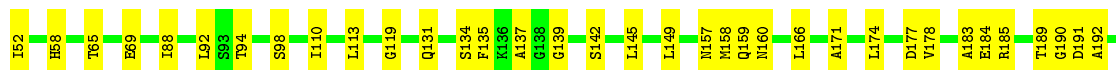
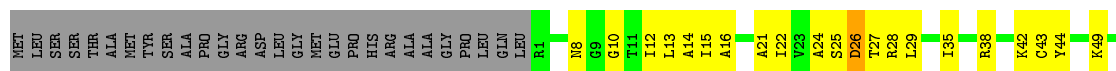
• Molecule 12: Proteasome subunit beta type-1

Chain L: 63% 25% 12%

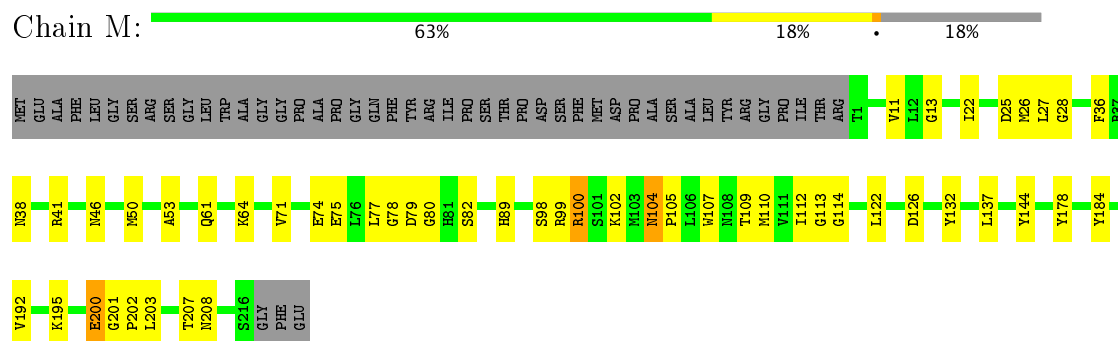


• Molecule 12: Proteasome subunit beta type-1

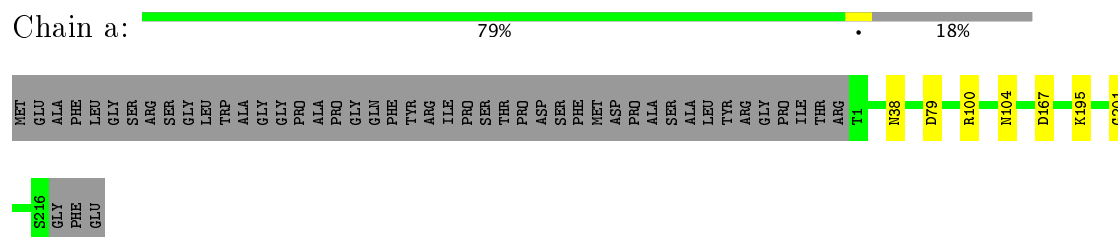
Chain Z: 63% 25% 12%



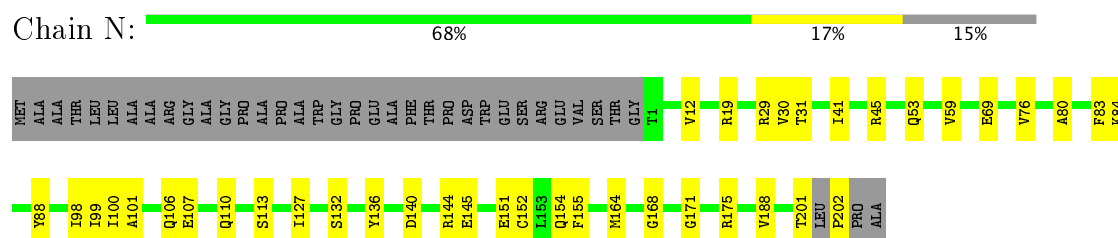
• Molecule 13: Proteasome subunit beta type-4



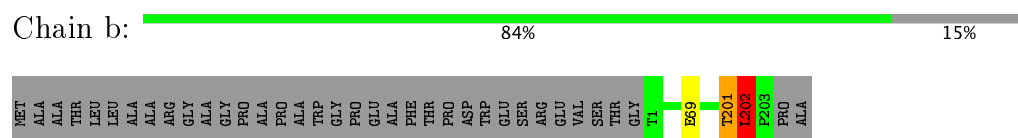
- Molecule 13: Proteasome subunit beta type-4



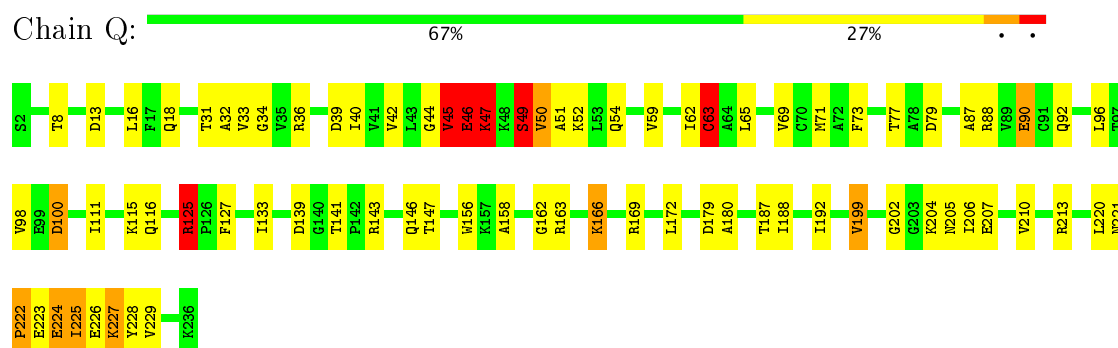
- Molecule 14: Proteasome subunit beta type-6



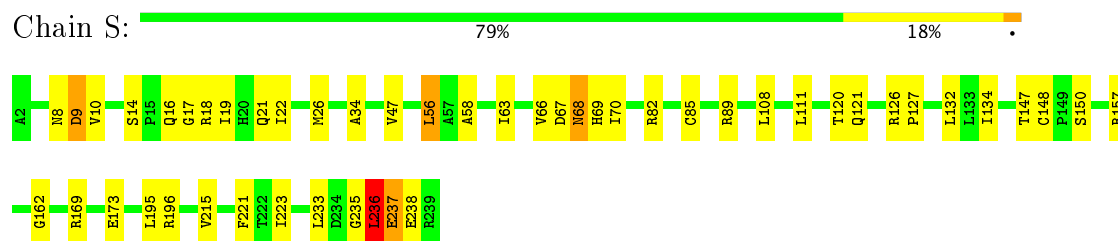
- Molecule 14: Proteasome subunit beta type-6



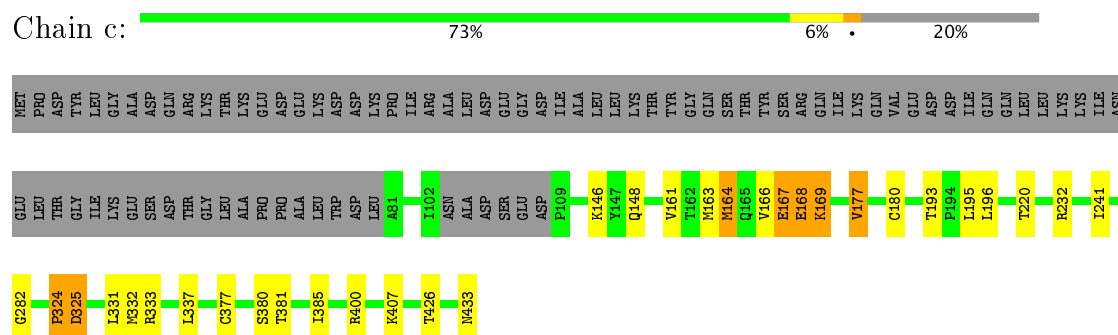
- Molecule 15: Proteasome subunit alpha type-7



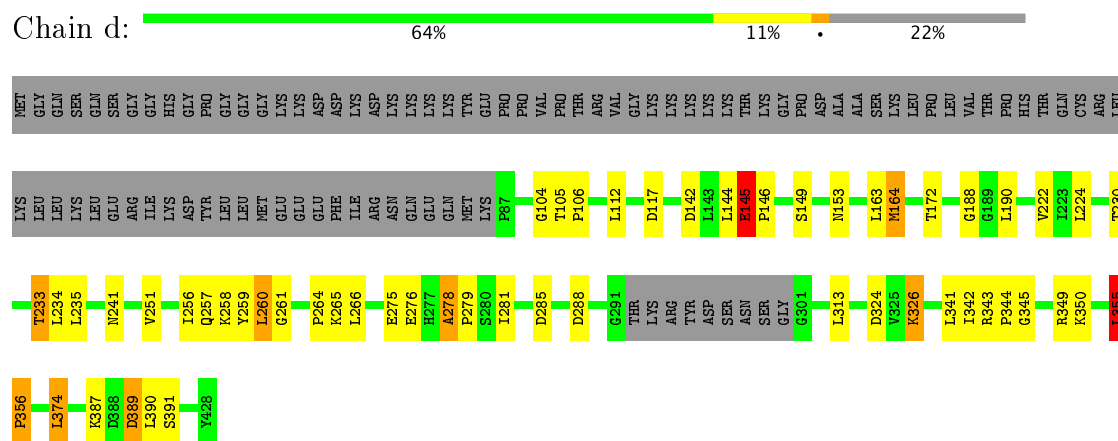
- Molecule 16: Proteasome subunit alpha type-1



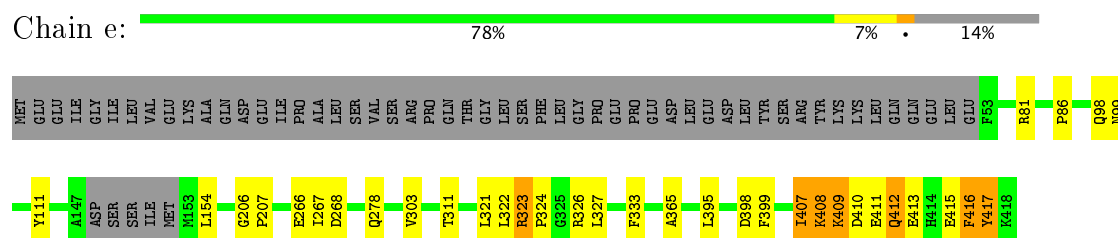
- Molecule 17: 26S protease regulatory subunit 7



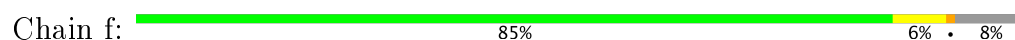
- Molecule 18: 26S protease regulatory subunit 4



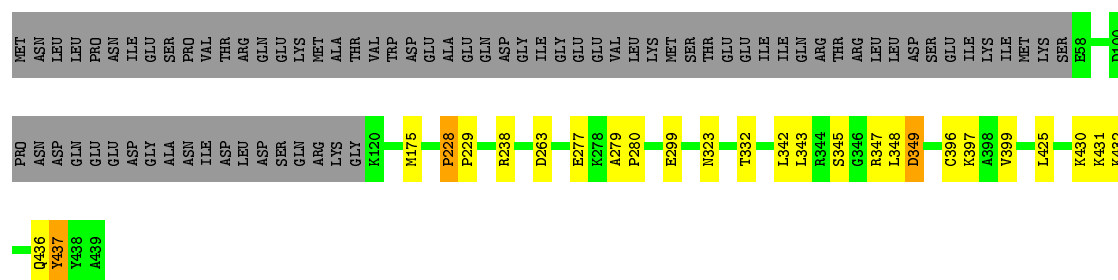
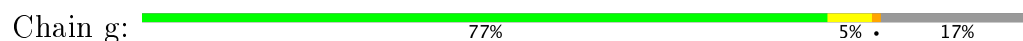
- Molecule 19: 26S protease regulatory subunit 6B



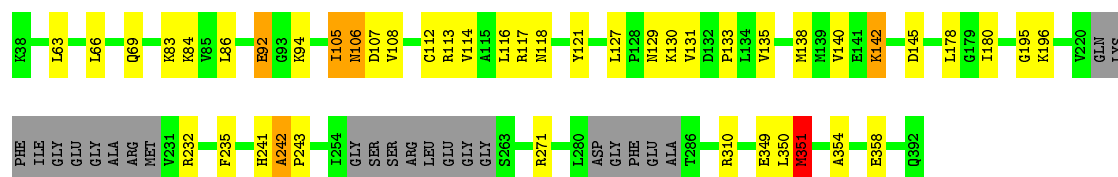
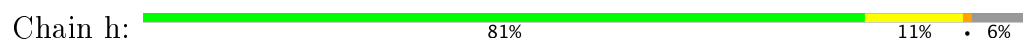
- Molecule 20: 26S protease regulatory subunit 10B



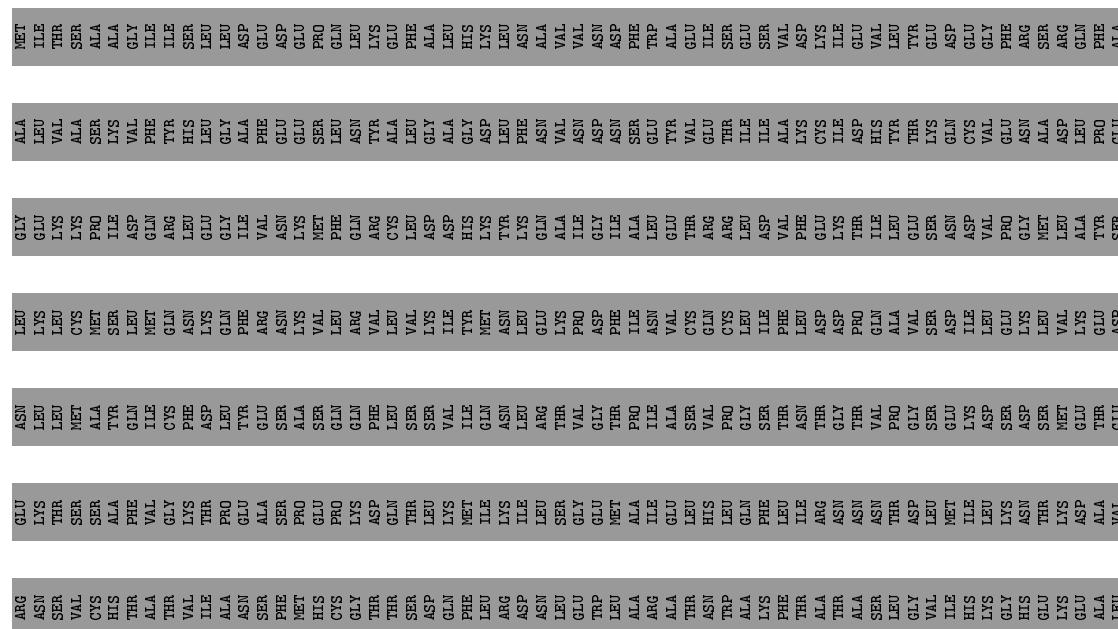
- Molecule 21: 26S protease regulatory subunit 6A

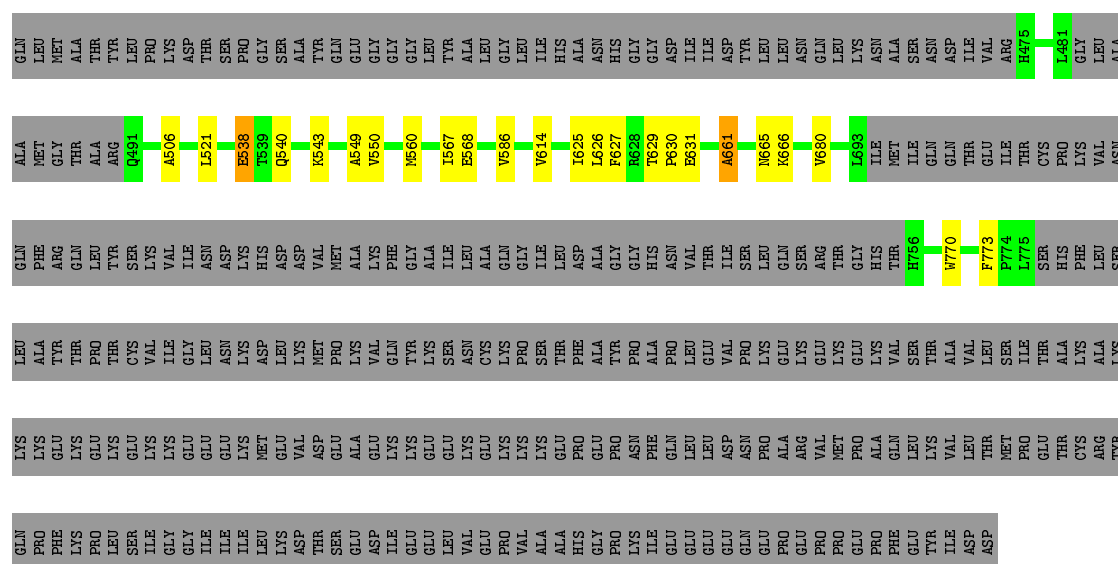


- Molecule 22: 26S protease regulatory subunit 8



- Molecule 23: 26S proteasome non-ATPase regulatory subunit 1





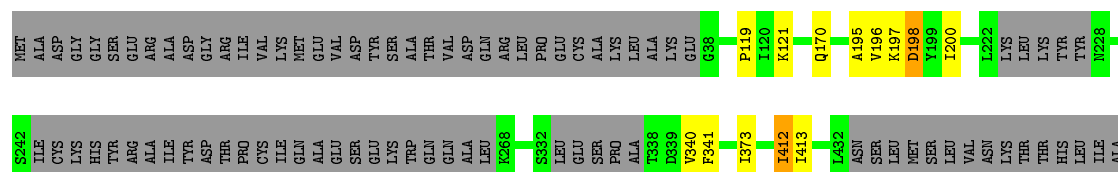
- Molecule 24: 26S proteasome non-ATPase regulatory subunit 3

Chain j:  28% . 71%



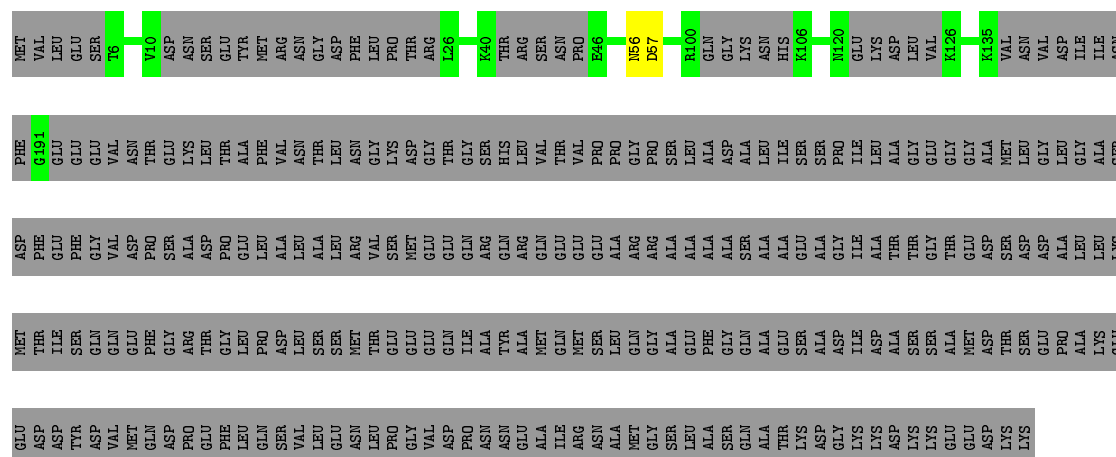
- Molecule 25: 26S proteasome non-ATPase regulatory subunit 12

Chain k:  77% 20%

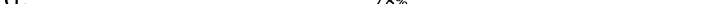


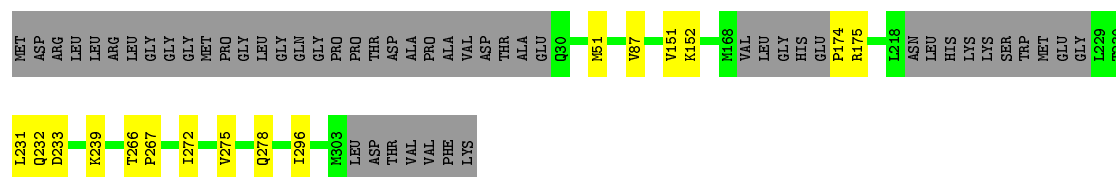


Chain p:  26% . 73%



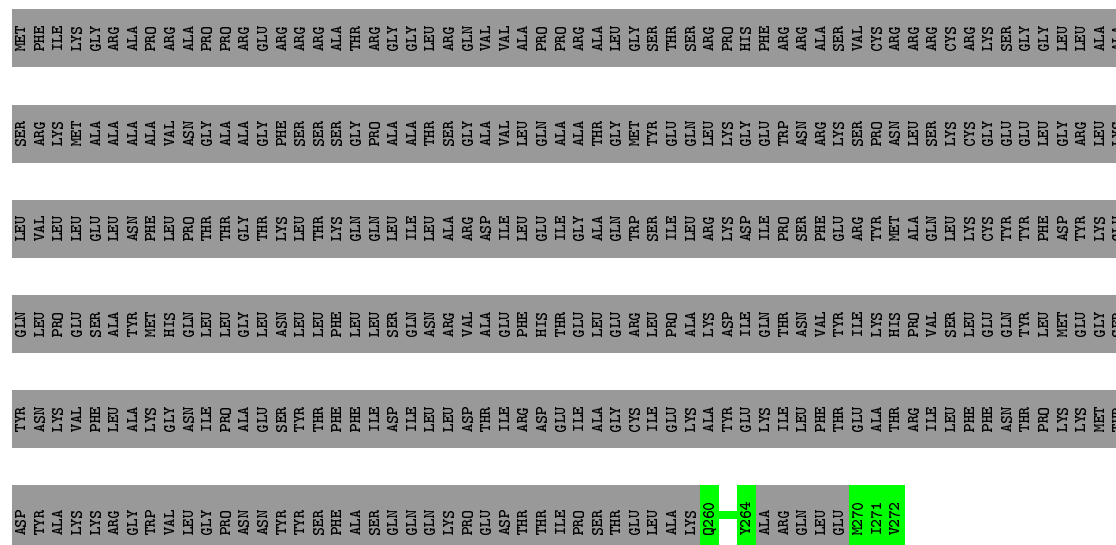
- Molecule 31: 26S proteasome non-ATPase regulatory subunit 14

Chain q:  78% 5% 16%



- Molecule 32: 26S proteasome non-ATPase regulatory subunit 8

Chain r:  98%



- Molecule 33: 26S proteasome complex subunit SEM1

Chain s:  37% 63%

MET	SER	GLU	LYS	LYS	GLN	PRO	VAL	ASP	LEU	GLY	LEU	LEU	GLU	GLU	ASP	ASP	GLU	PHE	GLU	PHE	GLU	PRO	ALA	GLU	ASP	TRP	ALA	GLY	LEU	ASP	GLU	ASP	GLU	ASP	ALA	HIS	VAL	HE3	GLY	TYR	LYS	MET	GLU	THR	SER
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 34: bound Oprozomib

Chain t:  100%

There are no outlier residues recorded for this chain.

- Molecule 34: bound Oprozomib

Chain u:  100%

There are no outlier residues recorded for this chain.



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	233000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	2	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	8400	Depositor
Magnification	110236	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 7C9, 6VA, 6V9, 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	0.40	0/1802	0.69	4/2446 (0.2%)
1	O	0.41	0/1802	0.70	5/2446 (0.2%)
10	J	0.39	0/1592	0.62	0/2153
10	X	0.39	0/1595	0.62	0/2157
11	K	0.44	0/1576	0.65	0/2131
11	Y	0.44	0/1590	0.65	0/2147
12	L	0.40	0/1670	0.73	4/2254 (0.2%)
12	Z	0.40	0/1672	0.73	4/2253 (0.2%)
13	M	0.42	0/1720	0.70	1/2328 (0.0%)
13	a	0.43	0/1712	0.68	0/2319
14	N	0.43	0/1539	0.62	0/2082
14	b	0.43	0/1546	0.69	2/2094 (0.1%)
15	Q	0.85	2/1810 (0.1%)	0.85	8/2456 (0.3%)
16	S	0.43	0/1868	0.85	8/2531 (0.3%)
17	c	0.37	0/2774	0.72	1/3739 (0.0%)
18	d	0.40	0/2597	1.00	14/3514 (0.4%)
19	e	0.36	0/2818	0.83	4/3812 (0.1%)
2	B	0.37	0/1864	0.77	4/2513 (0.2%)
2	P	0.38	0/1904	0.83	7/2573 (0.3%)
20	f	0.36	0/2734	0.70	4/3690 (0.1%)
21	g	0.37	0/2815	0.79	2/3804 (0.1%)
22	h	0.35	0/2550	0.75	2/3442 (0.1%)
23	i	0.30	0/1150	0.74	2/1599 (0.1%)
24	j	0.32	0/780	0.72	0/1086
25	k	0.28	0/1819	0.66	2/2536 (0.1%)
26	l	0.33	0/2601	0.68	2/3569 (0.1%)
27	m	0.34	0/2450	0.74	4/3356 (0.1%)
28	n	0.30	0/1032	0.74	1/1438 (0.1%)
29	o	0.30	0/378	0.62	0/528
3	C	0.41	0/1796	0.69	2/2438 (0.1%)
30	p	0.26	0/501	0.52	0/691
31	q	0.31	0/1318	0.78	2/1836 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
32	r	0.26	0/38	0.60	0/50
33	s	0.33	0/129	0.69	0/179
4	D	0.36	0/1784	0.68	1/2416 (0.0%)
4	R	0.36	0/1795	0.68	1/2424 (0.0%)
5	E	0.42	0/1839	0.84	8/2492 (0.3%)
6	F	0.44	0/1852	0.73	2/2494 (0.1%)
6	T	0.43	0/1912	0.74	3/2576 (0.1%)
7	G	0.39	0/1836	0.70	1/2481 (0.0%)
7	U	0.39	0/1875	0.67	1/2542 (0.0%)
8	H	0.42	0/1690	0.74	2/2289 (0.1%)
8	V	0.42	0/1657	0.73	2/2252 (0.1%)
9	I	0.40	0/1619	0.68	2/2184 (0.1%)
9	W	0.40	0/1614	0.68	2/2176 (0.1%)
All	All	0.40	2/77015 (0.0%)	0.73	114/104516 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	O	0	1
10	J	0	1
10	X	0	1
13	a	0	1
14	b	0	2
15	Q	0	4
16	S	0	5
17	c	0	7
18	d	0	12
19	e	0	4
2	B	0	4
2	P	0	10
20	f	0	3
21	g	0	3
22	h	0	4
23	i	0	4
24	j	0	4
25	k	0	8
26	l	0	7
27	m	0	8

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Mol	Chain	#Chirality outliers	#Planarity outliers
28	n	0	9
29	o	0	1
3	C	0	1
30	p	0	1
31	q	0	6
4	D	0	1
4	R	0	1
5	E	0	4
6	F	0	3
6	T	0	3
7	G	0	3
7	U	0	2
8	H	0	1
8	V	0	1
9	I	0	2
9	W	0	2
All	All	0	136

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Q	45	VAL	C-N	-30.59	0.63	1.34
15	Q	63	CYS	C-N	9.29	1.55	1.34

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	e	323	ARG	C-N-CD	-26.33	62.68	120.60
18	d	145	GLU	C-N-CD	-25.89	63.65	120.60
21	g	228	PRO	C-N-CD	-22.40	71.32	120.60
15	Q	63	CYS	O-C-N	-14.91	98.84	122.70
31	q	266	THR	C-N-CD	-14.89	87.84	120.60

There are no chirality outliers.

5 of 136 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	TRP	Peptide
1	A	139	ASN	Peptide
2	B	229	LYS	Peptide
2	B	54	LYS	Peptide

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Mol	Chain	Res	Type	Group
2	B	60	PHE	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	1763	0	1741	42	0
1	O	1764	0	1732	33	0
2	B	1836	0	1838	40	0
2	P	1875	0	1865	35	0
3	C	1771	0	1712	56	0
4	D	1757	0	1713	33	0
4	R	1768	0	1756	27	0
5	E	1805	0	1765	28	0
6	F	1818	0	1792	37	0
6	T	1877	0	1857	35	0
7	G	1806	0	1816	44	0
7	U	1841	0	1809	69	0
8	H	1663	0	1681	55	0
8	V	1627	0	1608	46	0
9	I	1590	0	1612	41	0
9	W	1586	0	1607	32	0
10	J	1560	0	1561	40	0
10	X	1563	0	1565	33	0
11	K	1545	0	1495	29	0
11	Y	1559	0	1520	35	0
12	L	1637	0	1620	39	0
12	Z	1642	0	1630	40	0
13	M	1687	0	1666	35	0
13	a	1679	0	1651	0	0
14	N	1513	0	1483	23	0
14	b	1519	0	1487	0	0
15	Q	1785	0	1734	142	0
16	S	1834	0	1788	29	0
17	c	2728	0	2775	0	0
18	d	2560	0	2556	0	0
19	e	2776	0	2740	0	0
20	f	2692	0	2696	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	g	2777	0	2782	0	0
22	h	2518	0	2530	0	0
23	i	1145	0	592	0	0
24	j	779	0	366	0	0
25	k	1819	0	809	0	0
26	l	2572	0	1980	0	0
27	m	2421	0	1885	0	0
28	n	1030	0	474	0	0
29	o	377	0	173	0	0
30	p	504	0	238	0	0
31	q	1311	0	656	0	0
32	r	40	0	17	0	0
33	s	130	0	56	0	0
34	t	37	0	0	0	0
34	u	37	0	0	0	0
35	c	27	0	11	0	0
35	d	27	0	11	0	0
35	e	27	0	12	0	0
35	g	54	0	24	0	0
35	h	27	0	12	0	0
All	All	76085	0	70499	1007	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 19.

The worst 5 of 1007 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)
15:Q:192:ILE:CD1	15:Q:228:TYR:HB3	1.27	1.61
7:U:163:PHE:CD2	7:U:166:THR:HG21	1.37	1.57
15:Q:188:ILE:CG2	15:Q:228:TYR:CZ	1.79	1.56
3:C:50:VAL:HA	3:C:54:GLN:CG	1.29	1.56
15:Q:192:ILE:HD13	15:Q:228:TYR:CB	1.17	1.54

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	228/234 (97%)	197 (86%)	31 (14%)	0	100	100
1	O	228/234 (97%)	197 (86%)	31 (14%)	0	100	100
2	B	228/261 (87%)	195 (86%)	30 (13%)	3 (1%)	14	56
2	P	242/261 (93%)	203 (84%)	35 (14%)	4 (2%)	11	51
3	C	232/234 (99%)	191 (82%)	38 (16%)	3 (1%)	14	56
4	D	231/241 (96%)	199 (86%)	32 (14%)	0	100	100
4	R	231/241 (96%)	199 (86%)	32 (14%)	0	100	100
5	E	232/234 (99%)	190 (82%)	41 (18%)	1 (0%)	38	77
6	F	228/255 (89%)	195 (86%)	31 (14%)	2 (1%)	20	62
6	T	238/255 (93%)	202 (85%)	34 (14%)	2 (1%)	22	65
7	G	229/246 (93%)	206 (90%)	21 (9%)	2 (1%)	20	62
7	U	239/246 (97%)	213 (89%)	25 (10%)	1 (0%)	38	77
8	H	219/277 (79%)	208 (95%)	11 (5%)	0	100	100
8	V	219/277 (79%)	208 (95%)	11 (5%)	0	100	100
9	I	202/205 (98%)	182 (90%)	18 (9%)	2 (1%)	18	61
9	W	202/205 (98%)	182 (90%)	18 (9%)	2 (1%)	18	61
10	J	194/196 (99%)	175 (90%)	19 (10%)	0	100	100
10	X	194/196 (99%)	175 (90%)	19 (10%)	0	100	100
11	K	198/204 (97%)	174 (88%)	24 (12%)	0	100	100
11	Y	199/204 (98%)	175 (88%)	24 (12%)	0	100	100
12	L	212/241 (88%)	184 (87%)	28 (13%)	0	100	100
12	Z	211/241 (88%)	184 (87%)	27 (13%)	0	100	100
13	M	214/264 (81%)	192 (90%)	21 (10%)	1 (0%)	32	73
13	a	214/264 (81%)	192 (90%)	21 (10%)	1 (0%)	32	73
14	N	199/239 (83%)	179 (90%)	20 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	b	201/239 (84%)	179 (89%)	21 (10%)	1 (0%)	32	73
15	Q	233/235 (99%)	186 (80%)	38 (16%)	9 (4%)	3	35
16	S	236/238 (99%)	195 (83%)	39 (16%)	2 (1%)	22	65
17	c	343/433 (79%)	256 (75%)	74 (22%)	13 (4%)	4	36
18	d	329/428 (77%)	251 (76%)	59 (18%)	19 (6%)	2	27
19	e	355/418 (85%)	279 (79%)	63 (18%)	13 (4%)	4	36
20	f	346/379 (91%)	285 (82%)	51 (15%)	10 (3%)	5	41
21	g	359/439 (82%)	292 (81%)	60 (17%)	7 (2%)	9	50
22	h	324/355 (91%)	248 (76%)	59 (18%)	17 (5%)	2	29
23	i	224/953 (24%)	173 (77%)	31 (14%)	20 (9%)	1	15
24	j	147/534 (28%)	111 (76%)	32 (22%)	4 (3%)	6	43
25	k	354/456 (78%)	272 (77%)	77 (22%)	5 (1%)	13	54
26	l	411/422 (97%)	341 (83%)	62 (15%)	8 (2%)	9	50
27	m	373/389 (96%)	318 (85%)	51 (14%)	4 (1%)	17	60
28	n	200/324 (62%)	147 (74%)	46 (23%)	7 (4%)	4	38
29	o	73/376 (19%)	56 (77%)	12 (16%)	5 (7%)	1	23
30	p	90/377 (24%)	78 (87%)	11 (12%)	1 (1%)	17	60
31	q	253/310 (82%)	191 (76%)	54 (21%)	8 (3%)	5	39
32	r	4/350 (1%)	4 (100%)	0	0	100	100
33	s	24/70 (34%)	19 (79%)	5 (21%)	0	100	100
All	All	10342/13680 (76%)	8678 (84%)	1487 (14%)	177 (2%)	15	51

5 of 177 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	69	HIS
6	F	227	VAL
6	F	228	PRO
7	G	69	LEU
13	M	79	ASP

### 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	181/191 (95%)	178 (98%)	3 (2%)	66	85
1	O	181/191 (95%)	178 (98%)	3 (2%)	66	85
2	B	195/221 (88%)	183 (94%)	12 (6%)	21	59
2	P	194/221 (88%)	184 (95%)	10 (5%)	27	64
3	C	179/197 (91%)	169 (94%)	10 (6%)	25	62
4	D	189/203 (93%)	182 (96%)	7 (4%)	39	71
4	R	192/203 (95%)	186 (97%)	6 (3%)	45	75
5	E	192/200 (96%)	188 (98%)	4 (2%)	59	82
6	F	190/212 (90%)	188 (99%)	2 (1%)	78	89
6	T	197/212 (93%)	195 (99%)	2 (1%)	80	90
7	G	197/210 (94%)	194 (98%)	3 (2%)	70	87
7	U	196/210 (93%)	191 (97%)	5 (3%)	51	78
8	H	181/228 (79%)	178 (98%)	3 (2%)	66	85
8	V	173/228 (76%)	171 (99%)	2 (1%)	75	88
9	I	173/174 (99%)	172 (99%)	1 (1%)	89	95
9	W	172/174 (99%)	171 (99%)	1 (1%)	89	95
10	J	163/166 (98%)	161 (99%)	2 (1%)	75	88
10	X	164/166 (99%)	162 (99%)	2 (1%)	75	88
11	K	154/159 (97%)	150 (97%)	4 (3%)	51	78
11	Y	156/159 (98%)	152 (97%)	4 (3%)	51	78
12	L	175/199 (88%)	173 (99%)	2 (1%)	78	89
12	Z	175/199 (88%)	173 (99%)	2 (1%)	78	89
13	M	179/215 (83%)	174 (97%)	5 (3%)	49	76
13	a	177/215 (82%)	172 (97%)	5 (3%)	49	76
14	N	157/181 (87%)	156 (99%)	1 (1%)	89	95
14	b	157/181 (87%)	156 (99%)	1 (1%)	89	95
15	Q	182/199 (92%)	169 (93%)	13 (7%)	17	55
16	S	194/202 (96%)	190 (98%)	4 (2%)	59	82
17	c	297/372 (80%)	279 (94%)	18 (6%)	22	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	d	281/375 (75%)	256 (91%)	25 (9%)	11	45
19	e	289/366 (79%)	268 (93%)	21 (7%)	16	54
20	f	287/331 (87%)	273 (95%)	14 (5%)	29	65
21	g	291/379 (77%)	274 (94%)	17 (6%)	23	61
22	h	266/307 (87%)	237 (89%)	29 (11%)	7	36
23	i	8/816 (1%)	8 (100%)	0	100	100
24	j	5/460 (1%)	5 (100%)	0	100	100
25	k	5/416 (1%)	5 (100%)	0	100	100
26	l	148/362 (41%)	142 (96%)	6 (4%)	35	69
27	m	154/344 (45%)	143 (93%)	11 (7%)	17	55
28	n	5/295 (2%)	5 (100%)	0	100	100
29	o	2/336 (1%)	2 (100%)	0	100	100
30	p	3/312 (1%)	3 (100%)	0	100	100
31	q	14/268 (5%)	14 (100%)	0	100	100
32	r	1/294 (0%)	1 (100%)	0	100	100
All	All	7071/11549 (61%)	6811 (96%)	260 (4%)	43	71

5 of 260 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	a	195	LYS
18	d	256	ILE
22	h	349	GLU
17	c	161	VAL
17	c	333	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	108	GLN
4	R	99	HIS
22	h	332	HIS
1	O	111	GLN
2	P	84	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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
34	6V9	t	1	34	6,8,9	0.76	0	3,10,12	4.93	3 (100%)
34	7C9	t	2	34	6,6,7	0.43	0	2,6,8	1.36	0
34	7C9	t	3	34	6,6,7	0.51	0	2,6,8	1.54	1 (50%)
34	6V9	u	1	34	6,8,9	0.66	0	3,10,12	4.78	3 (100%)
34	7C9	u	2	34	6,6,7	0.51	0	2,6,8	1.32	0
34	7C9	u	3	34	6,6,7	0.55	0	2,6,8	1.74	1 (50%)

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	6V9	t	1	34	-	0/0/2/4	0/1/1/1
34	7C9	t	2	34	-	0/3/5/7	0/0/0/0
34	7C9	t	3	34	-	0/3/5/7	0/0/0/0
34	6V9	u	1	34	-	0/0/2/4	0/1/1/1
34	7C9	u	2	34	-	0/3/5/7	0/0/0/0
34	7C9	u	3	34	-	0/3/5/7	0/0/0/0

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	t	1	6V9	O1-C4-C3	-6.45	118.73	124.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	u	1	6V9	O1-C4-C3	-6.13	119.02	124.32
34	u	1	6V9	C2-C1-S	-3.30	115.67	120.12
34	t	1	6V9	C2-C1-S	-3.28	115.70	120.12
34	u	3	7C9	O18-C05-C04	-2.42	118.33	125.02

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	c	501	18,17	25,29,29	0.94	1 (4%)	24,45,45	1.63	2 (8%)
35	ADP	d	501	18	25,29,29	0.96	1 (4%)	24,45,45	1.62	2 (8%)
35	ADP	e	501	19,20	25,29,29	0.98	1 (4%)	24,45,45	1.68	2 (8%)
35	ADP	g	501	21	25,29,29	0.92	1 (4%)	24,45,45	1.67	2 (8%)
35	ADP	g	502	-	25,29,29	0.91	1 (4%)	24,45,45	1.61	2 (8%)
35	ADP	h	401	22	25,29,29	0.91	1 (4%)	24,45,45	1.64	2 (8%)

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	c	501	18,17	-	0/12/32/32	0/3/3/3
35	ADP	d	501	18	-	0/12/32/32	0/3/3/3
35	ADP	e	501	19,20	-	0/12/32/32	0/3/3/3
35	ADP	g	501	21	-	0/12/32/32	0/3/3/3
35	ADP	g	502	-	-	0/12/32/32	0/3/3/3
35	ADP	h	401	22	-	0/12/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	g	502	ADP	C5-C4	2.71	1.46	1.40
35	c	501	ADP	C5-C4	2.74	1.46	1.40
35	h	401	ADP	C5-C4	2.82	1.46	1.40
35	g	501	ADP	C5-C4	2.86	1.47	1.40
35	d	501	ADP	C5-C4	2.90	1.47	1.40

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	g	501	ADP	N3-C2-N1	-5.98	123.65	128.86
35	e	501	ADP	N3-C2-N1	-5.90	123.72	128.86
35	h	401	ADP	N3-C2-N1	-5.83	123.78	128.86
35	g	502	ADP	N3-C2-N1	-5.78	123.82	128.86
35	d	501	ADP	N3-C2-N1	-5.71	123.89	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
15	Q	1

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Mol	Chain	Number of breaks
19	e	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	e	414:HIS	C	415:GLU	N	4.11
1	Q	45:VAL	C	46:GLU	N	0.63