wwPDB/EMDataBank EM Map/Model Validation Summary Report (i)

Nov 21, 2016 – 04:32 PM EST

PDB ID	:	5T0J
EMDB ID:	:	EMD-8337
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	:	2016-08-16
Resolution	:	8.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

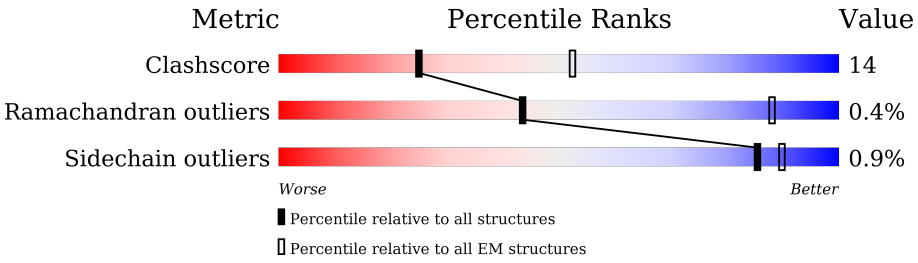
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
EM map analysis	:	NOT EXECUTED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

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 8.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	f	749	91% · 7%
2	G	245	62% 33% · ·
3	H	233	69% 29% ·
4	I	260	63% 32% · ·
5	J	247	68% 28% · ·
6	K	240	65% 30% · 5%
7	L	268	62% 26% 11%
8	M	254	69% 26% 6%
9	N	238	63% 17% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	O	276	64% 16% 20%
11	P	204	80% 20%
12	Q	201	72% 27%
13	R	262	58% 19% 23%
14	S	240	74% 15% 11%
15	T	263	62% 20% 18%
16	A	433	52% 30% 17%
17	B	440	47% 32% 21%
18	D	418	54% 36% 9%
19	E	403	61% 26% 12%
20	F	439	54% 28% 17%
21	C	398	59% 38%
22	U	953	60% 25% 15%
23	V	533	56% 33% 10%
24	W	456	71% 27%
25	X	422	43% 14% 43%
26	Y	389	63% 32%
27	Z	324	65% 23% 12%
28	a	376	98%
29	b	377	51% 49%
30	c	309	87% 10%
31	d	349	72% 26%
32	e	70	54% 43%

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 76674 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 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	f	694	5331	3364	899	1027	41	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	G	240	1826	1160	305	348	13	0	0

- Molecule 3 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	232	1708	1081	289	333	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	I	250	1912	1204	329	371	8	0	0

- Molecule 5 is a protein called Proteasome subunit alpha type-7.

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

- Molecule 6 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	K	228	1722	1080	284	348	10	0	0

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

- Molecule 8 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		

- Molecule 9 is a protein called Proteasome subunit beta type-6.

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

- Molecule 10 is a protein called Proteasome subunit beta type-7.

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

- Molecule 11 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		

- Molecule 12 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

- Molecule 13 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

- Molecule 14 is a protein called Proteasome subunit beta type-1.

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

- Molecule 15 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		

- Molecule 16 is a protein called 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A	361	Total	C	N	O	S	0	0
			2835	1788	501	528	18		

- Molecule 17 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	B	348	Total	C	N	O	S	0	0
			2717	1708	460	537	12		

- Molecule 18 is a protein called 26S protease regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	D	380	Total	C	N	O	S	0	0
			3040	1923	524	580	13		

- Molecule 19 is a protein called 26S protease regulatory subunit 10B.

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

- Molecule 20 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	F	366	Total	C	N	O	S	0	0
			2863	1802	496	549	16		

- Molecule 21 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	C	392	Total	C	N	O	S	0	0
			3078	1932	551	577	18		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	806	Total	C	N	O	S	0	0
			6287	3990	1075	1178	44		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	480	Total	C	N	O	S	0	0
			3852	2444	684	710	14		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	456	Total	C	N	O	S	0	0
			3703	2339	635	704	25		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	241	Total	C	N	O	S	0	0
			1905	1212	320	365	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	378	Total	C	N	O	S	0	0
			3115	1987	533	578	17		

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	286	Total	C	N	O	S	0	0
			2281	1457	392	427	5		

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	373	Total	C	N	O	S	0	0
			2995	1911	510	559	15		

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	278	Total	C	N	O	S	0	0
			2187	1389	374	406	18		

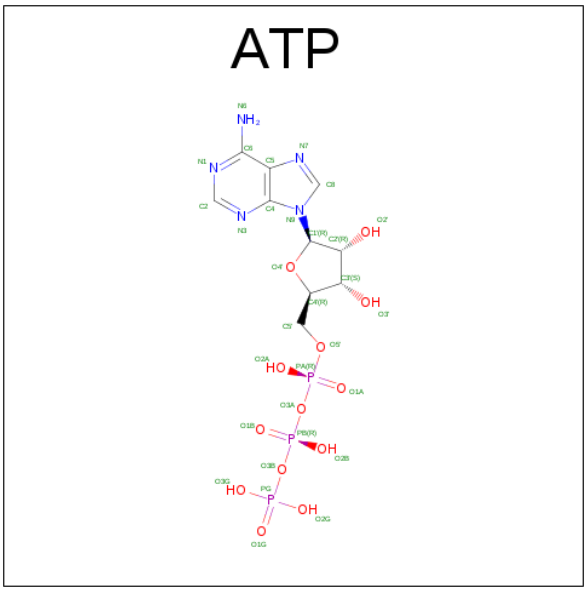
- Molecule 31 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

- Molecule 32 is a protein called 26S proteasome complex subunit DSS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	40	Total	C	N	O	S	0	0
			334	200	55	77	2		

- Molecule 33 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
33	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
33	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
33	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
33	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

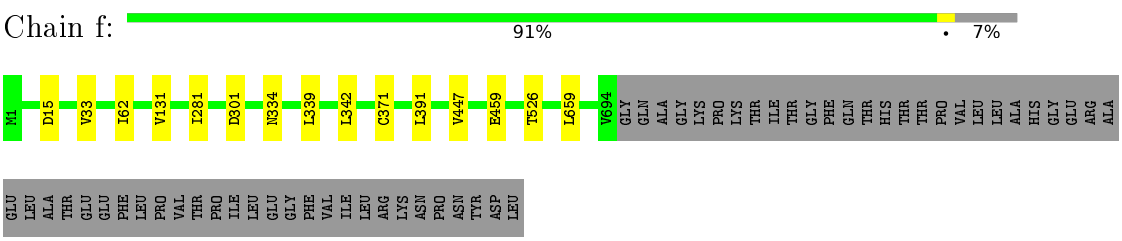
Mol	Chain	Residues	Atoms		AltConf
34	c	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

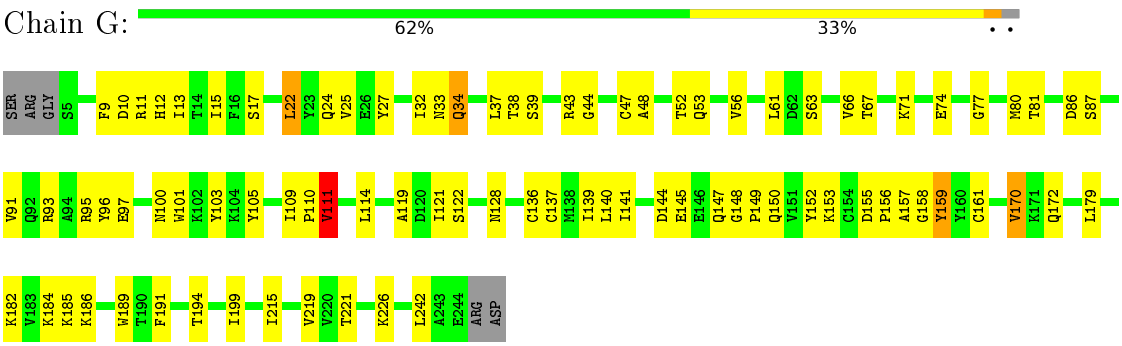
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 2

Chain f:



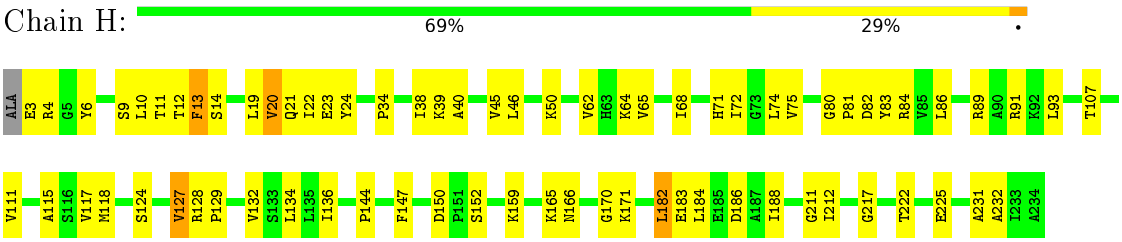
- Molecule 2: Proteasome subunit alpha type-6

Chain G:



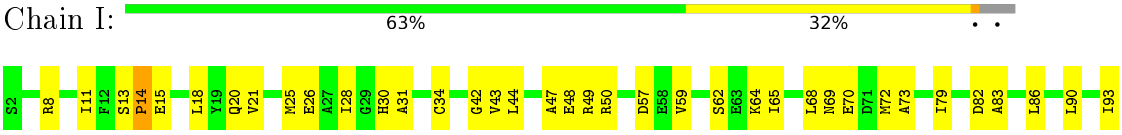
- Molecule 3: Proteasome subunit alpha type-2

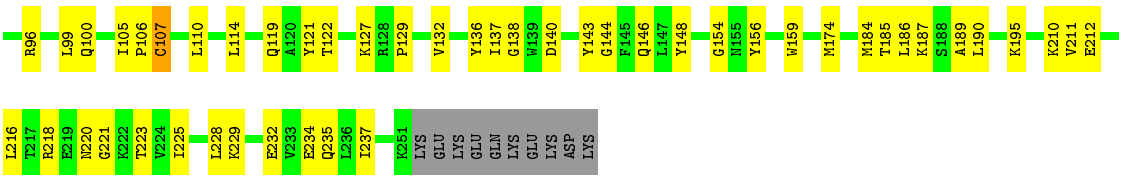
Chain H:



- Molecule 4: Proteasome subunit alpha type-4

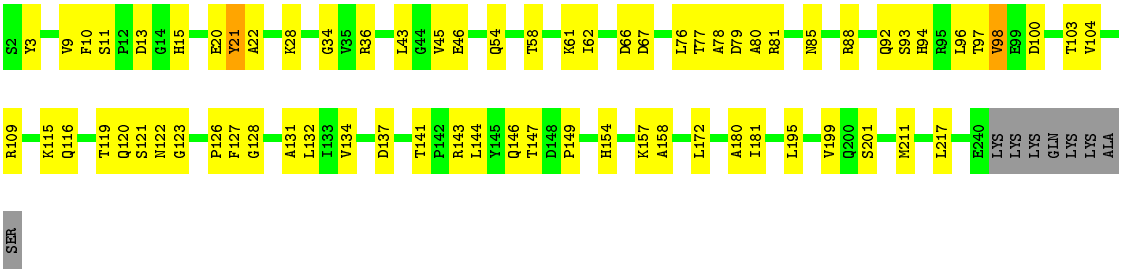
Chain I:





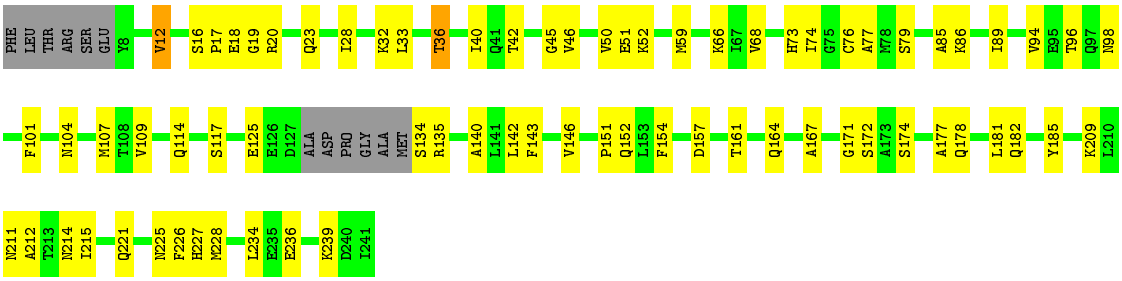
• Molecule 5: Proteasome subunit alpha type-7

Chain J:



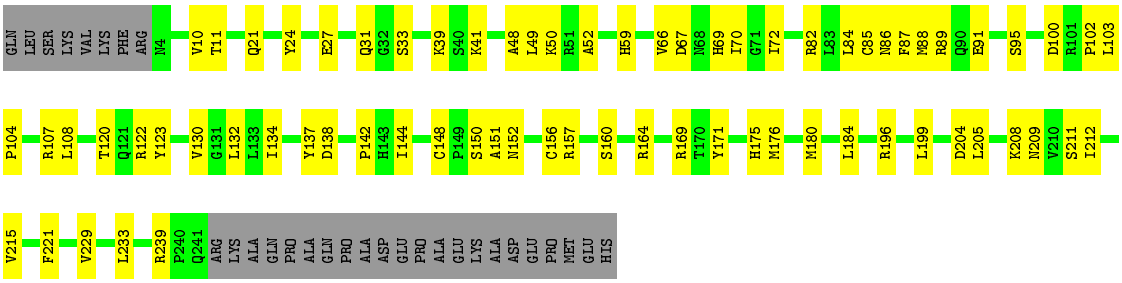
• Molecule 6: Proteasome subunit alpha type-5

Chain K:



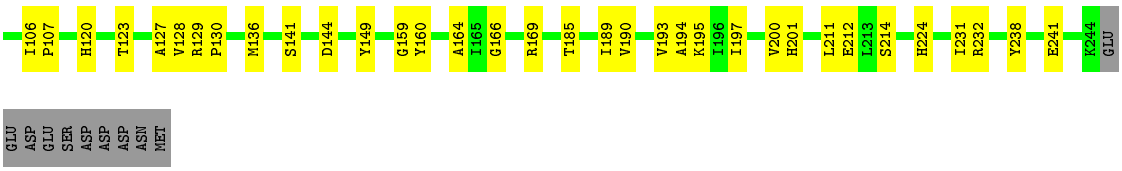
• Molecule 7: Proteasome subunit alpha type-1

Chain L:



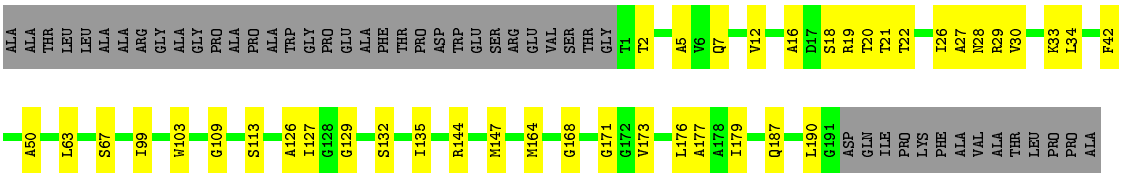
• Molecule 8: Proteasome subunit alpha type-3

Chain M:



• Molecule 9: Proteasome subunit beta type-6

Chain N:

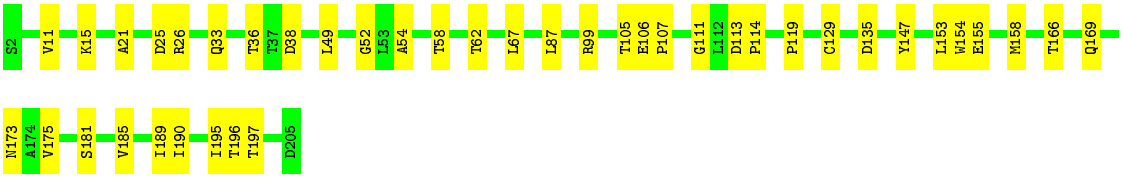


• Molecule 10: Proteasome subunit beta type-7

Chain O:

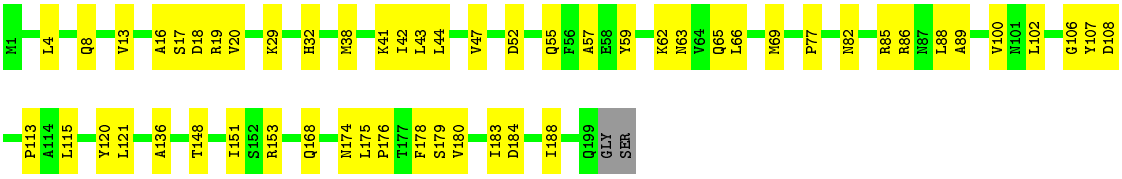
• Molecule 11: Proteasome subunit beta type-3

Chain P:



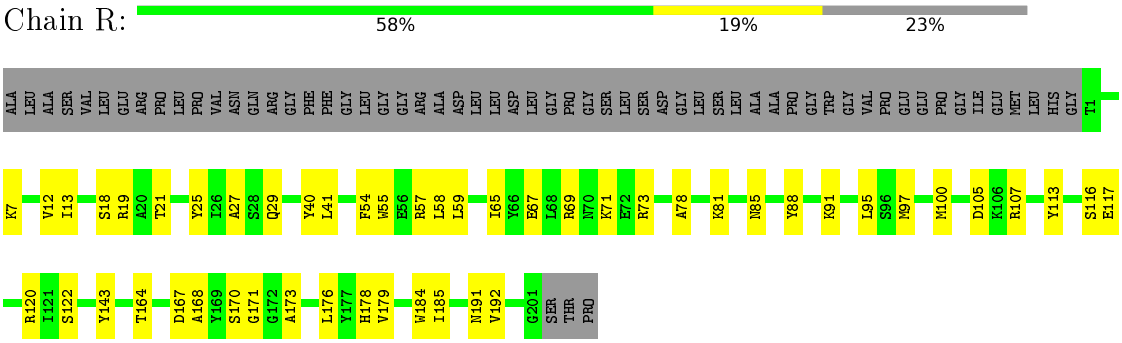
• Molecule 12: Proteasome subunit beta type-2

Chain Q:



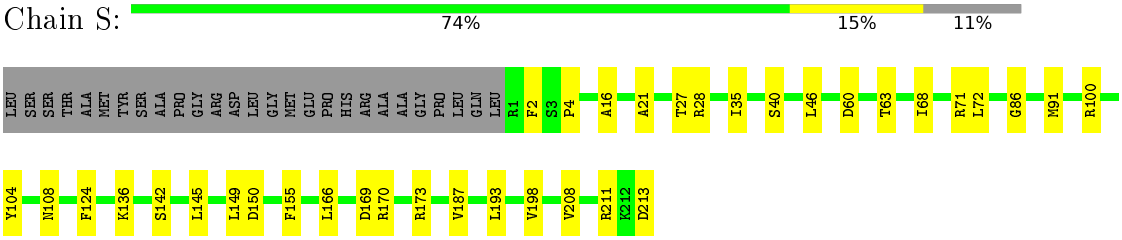
• Molecule 13: Proteasome subunit beta type-5

Chain R:



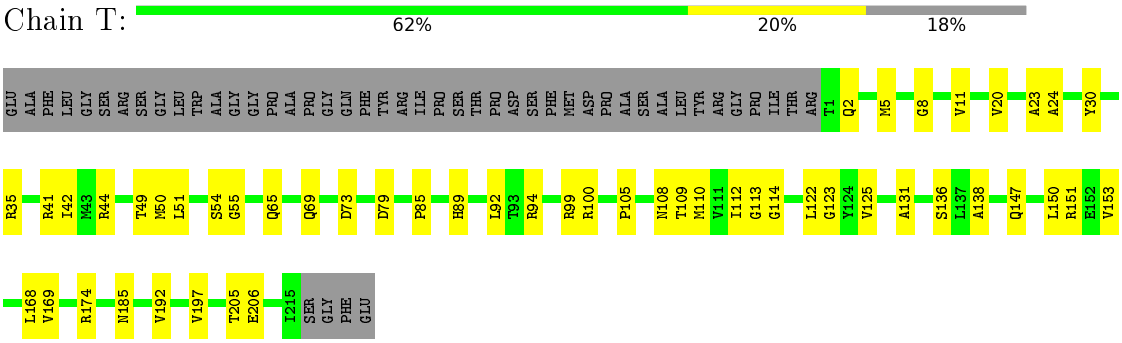
• Molecule 14: Proteasome subunit beta type-1

Chain S:



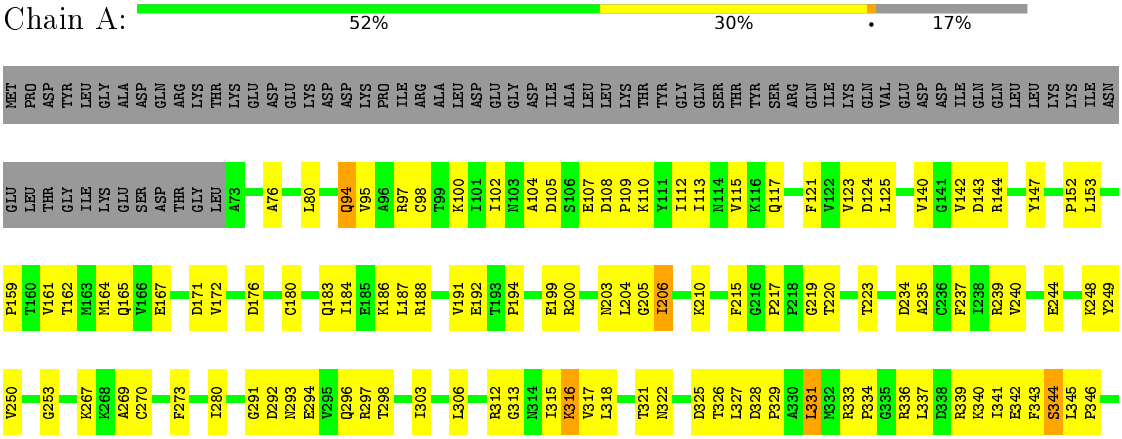
• Molecule 15: Proteasome subunit beta type-4

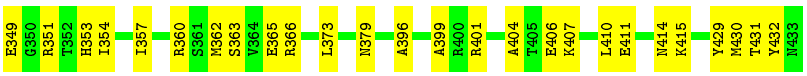
Chain T:



• Molecule 16: 26S protease regulatory subunit 7

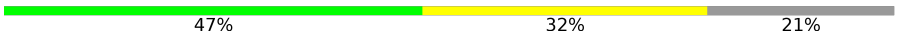
Chain A:

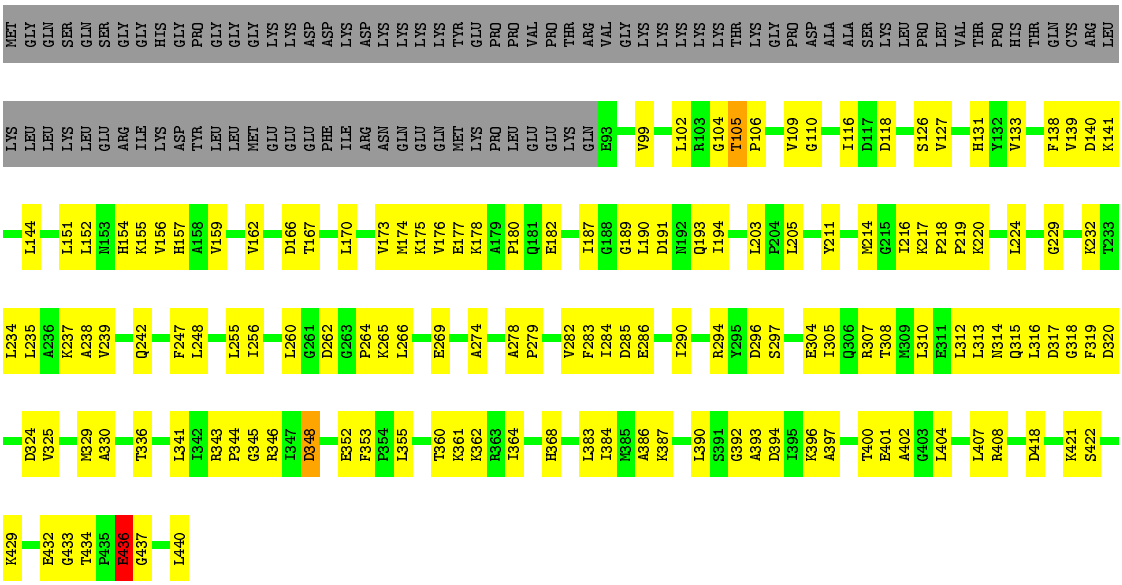




• Molecule 17: 26S protease regulatory subunit 4

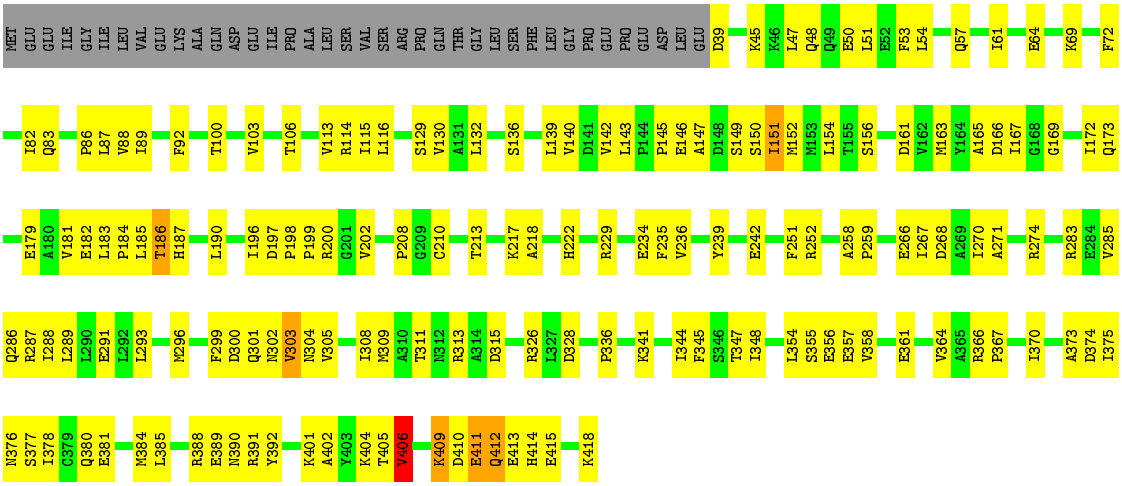
Chain B:





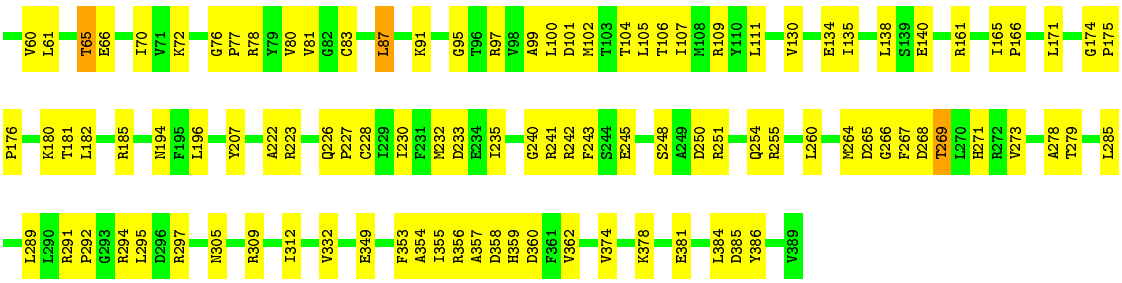
• Molecule 18: 26S protease regulatory subunit 6B

Chain D:



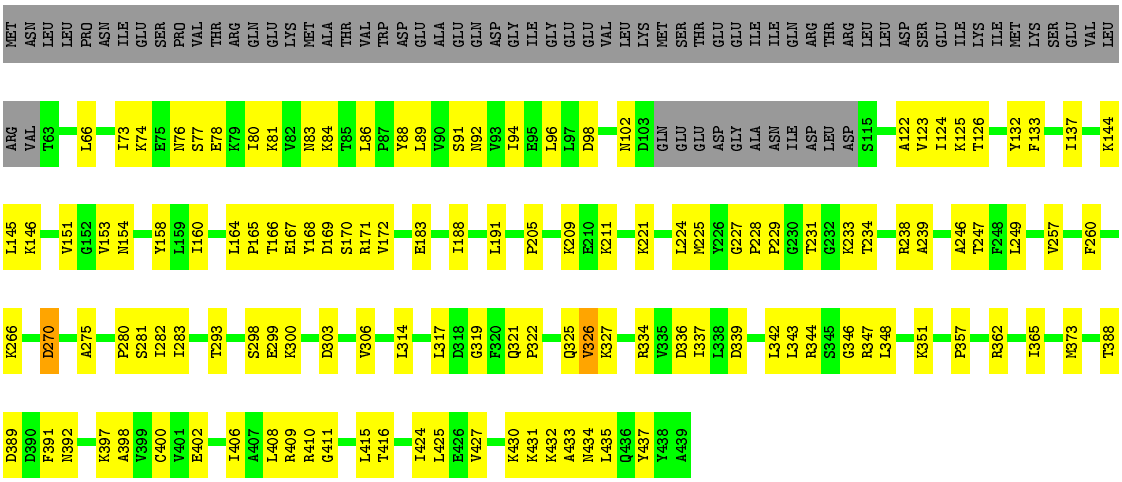
• Molecule 19: 26S protease regulatory subunit 10B

Chain E:



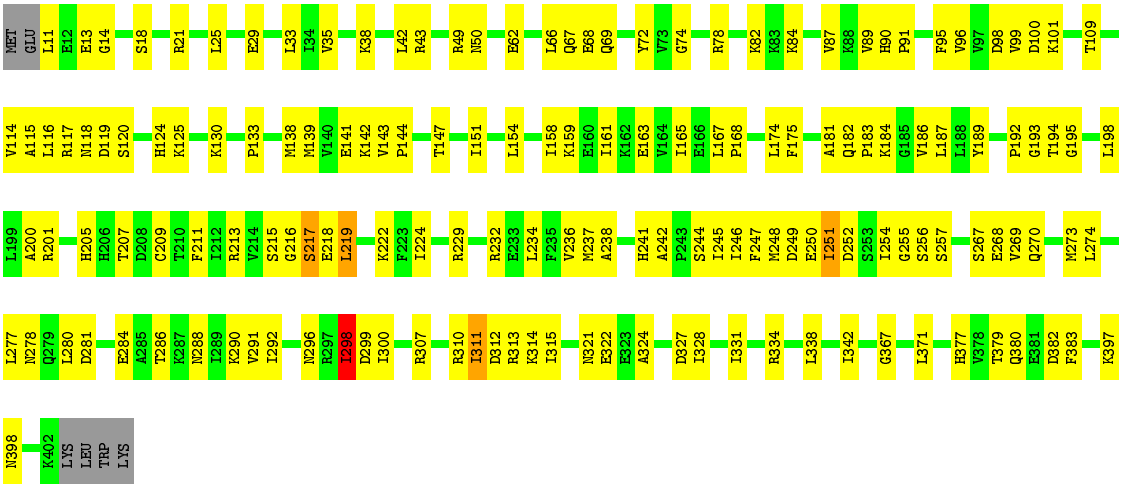
• Molecule 20: 26S protease regulatory subunit 6A

Chain F:



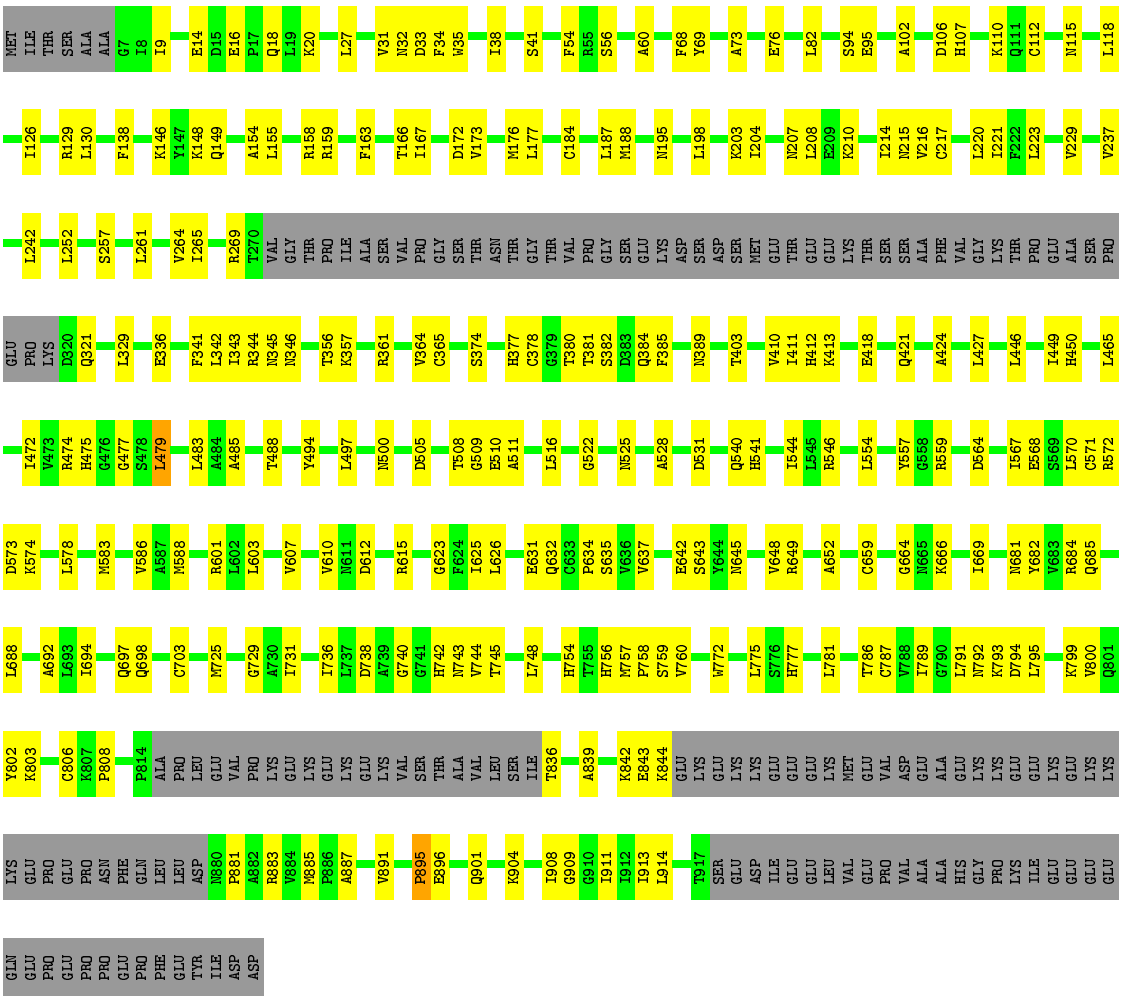
• Molecule 21: 26S protease regulatory subunit 8

Chain C:



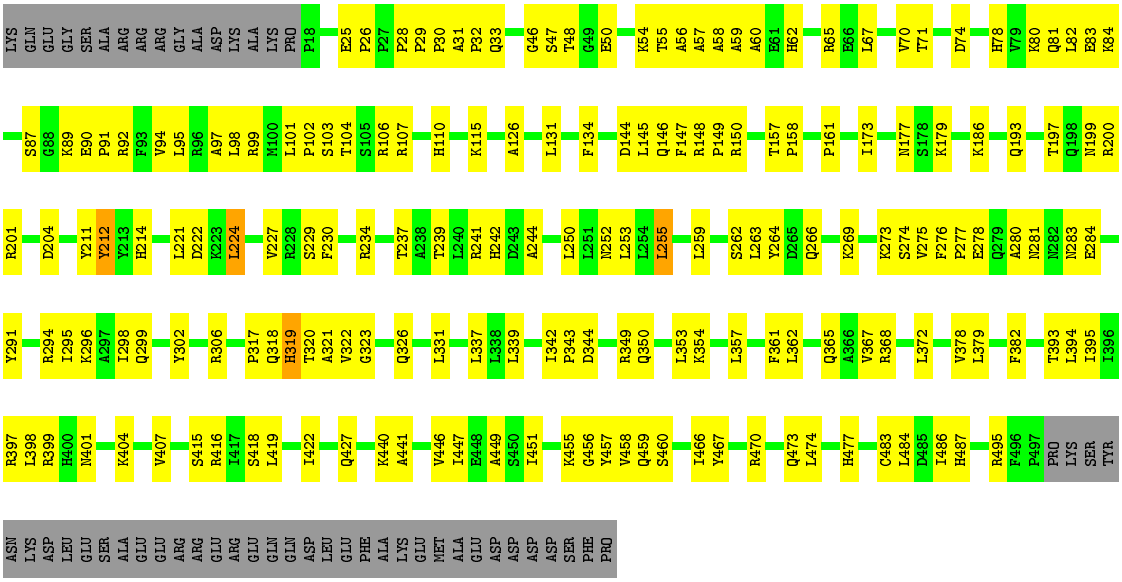
• Molecule 22: 26S proteasome non-ATPase regulatory subunit 1

Chain U:



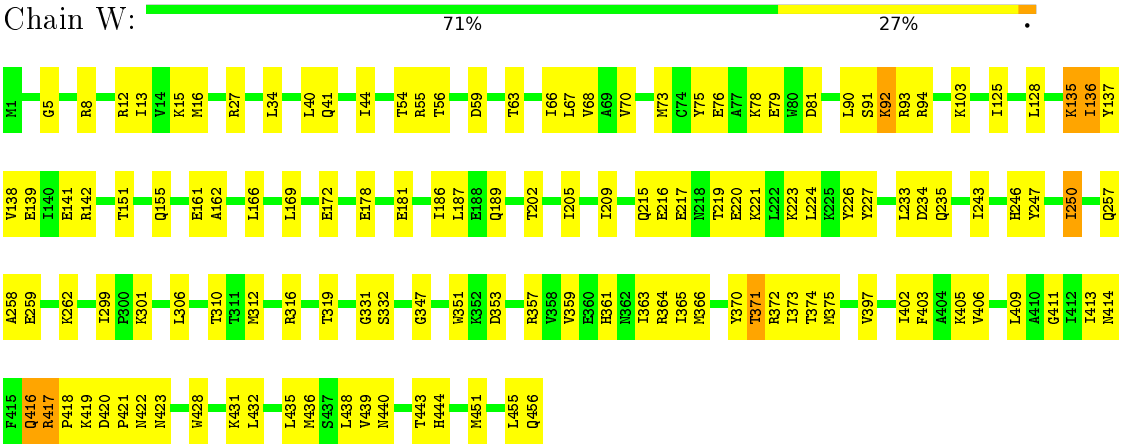
• Molecule 23: 26S proteasome non-ATPase regulatory subunit 3

Chain V:



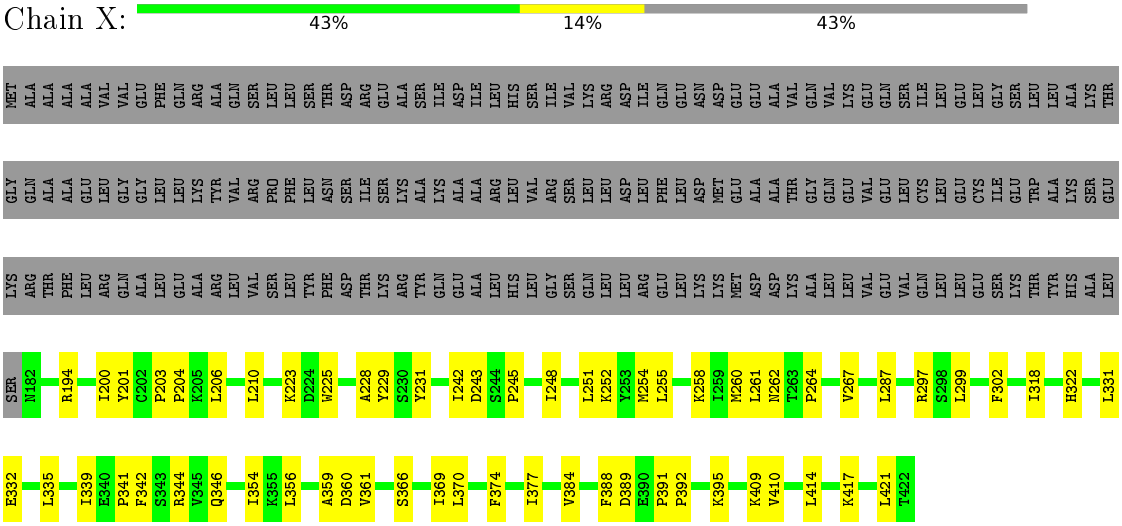
- Molecule 24: 26S proteasome non-ATPase regulatory subunit 12

Chain W:



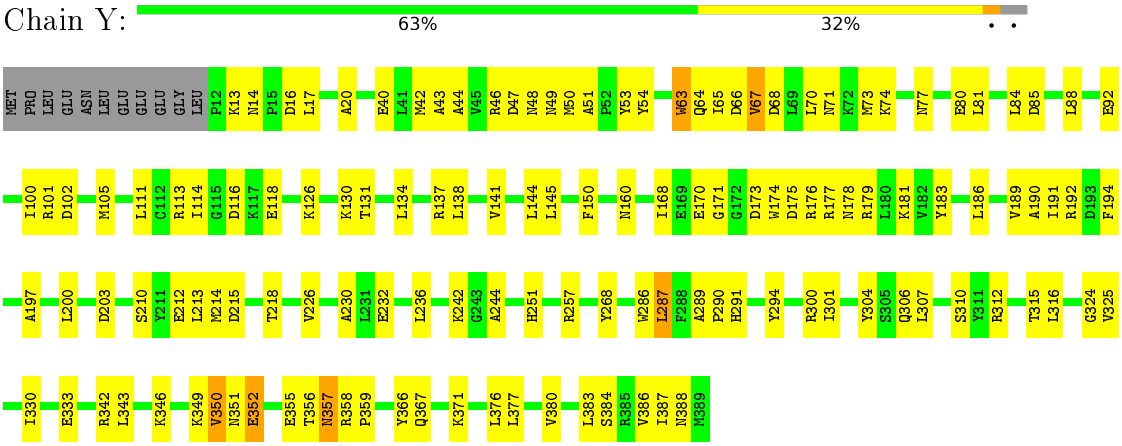
- Molecule 25: 26S proteasome non-ATPase regulatory subunit 11

Chain X:



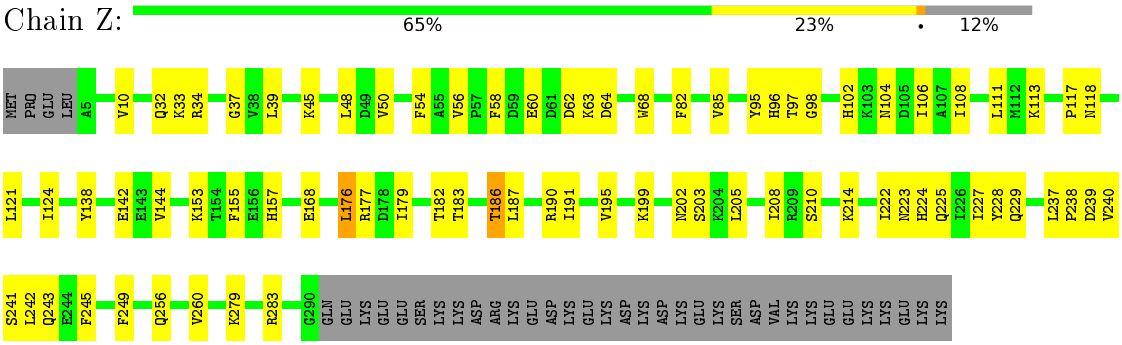
- Molecule 26: 26S proteasome non-ATPase regulatory subunit 6

Chain Y:



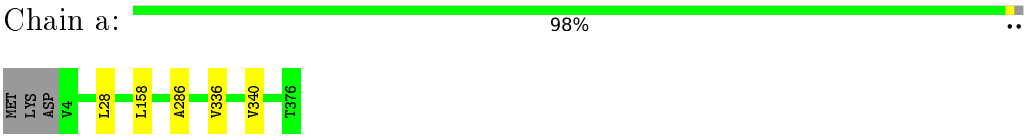
- Molecule 27: 26S proteasome non-ATPase regulatory subunit 7

Chain Z:



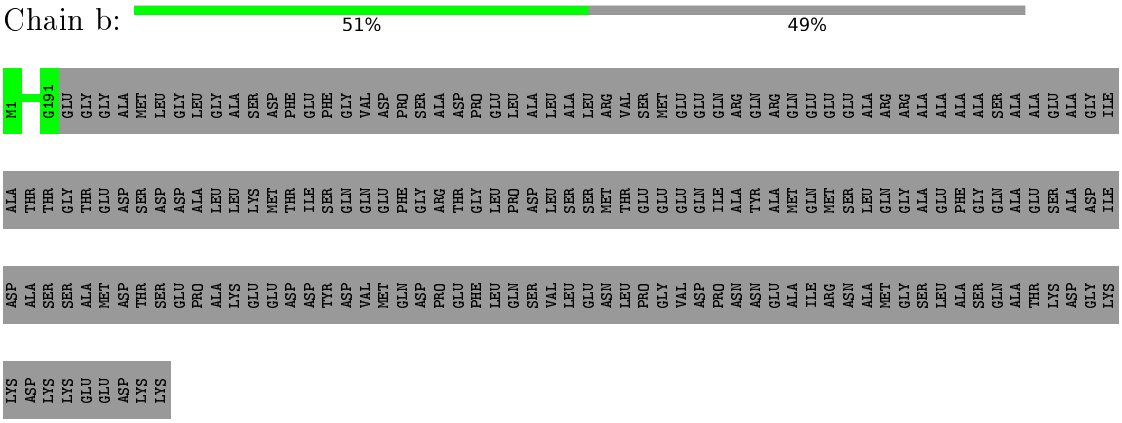
• Molecule 28: 26S proteasome non-ATPase regulatory subunit 13

Chain a:



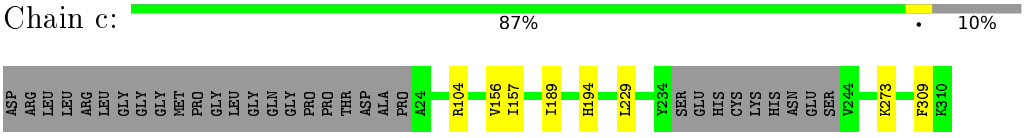
• Molecule 29: 26S proteasome non-ATPase regulatory subunit 4

Chain b:



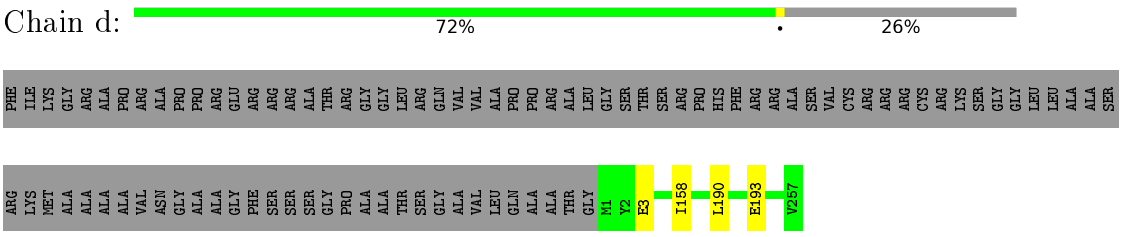
• Molecule 30: 26S proteasome non-ATPase regulatory subunit 14

Chain c:



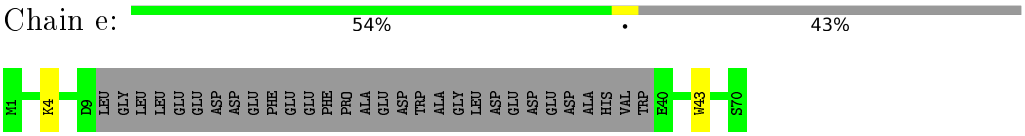
• Molecule 31: 26S proteasome non-ATPase regulatory subunit 8

Chain d:



• Molecule 32: 26S proteasome complex subunit DSS1

Chain e:


54%
43%
M1
K4
D9
LEU
GLY
LEU
LEU
GLU
GLU
ASP
ASP
GLU
PHE
GLU
GLU
PHE
PRO
ALA
GLU
ASP
TRP
ALA
GLY
LEU
ASP
GLU
ASP
GLU
ASP
ALA
HIS
VAL
TRP
E40
W43
S70

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	14382	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

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

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	f	0.24	0/5413	0.50	1/7317 (0.0%)
10	O	0.23	0/1670	0.43	0/2265
11	P	0.23	0/1614	0.40	0/2177
12	Q	0.24	0/1603	0.41	0/2174
13	R	0.23	0/1579	0.39	0/2134
14	S	0.24	0/1671	0.41	0/2253
15	T	0.24	0/1700	0.41	0/2305
16	A	0.25	0/2886	0.50	0/3899
17	B	0.25	0/2756	0.50	0/3721
18	D	0.25	0/3090	0.51	1/4168 (0.0%)
19	E	0.39	1/2835 (0.0%)	0.45	0/3821
2	G	0.24	0/1859	0.45	0/2523
20	F	0.26	0/2903	0.50	0/3912
21	C	0.27	1/3117 (0.0%)	0.50	2/4189 (0.0%)
22	U	0.23	0/6396	0.40	0/8646
23	V	1.26	6/3929 (0.2%)	0.50	0/5309
24	W	0.24	0/3751	0.47	2/5042 (0.0%)
25	X	0.23	0/1936	0.41	0/2614
26	Y	0.24	0/3173	0.47	2/4273 (0.0%)
27	Z	0.24	0/2324	0.48	0/3150
28	a	0.23	0/3053	0.42	0/4133
29	b	0.26	0/1478	0.44	0/2001
3	H	0.25	0/1743	0.49	0/2372
30	c	0.26	1/2226 (0.0%)	0.46	0/3007
31	d	0.25	0/2162	0.48	0/2919
32	e	3.67	1/338 (0.3%)	0.75	2/450 (0.4%)
4	I	0.60	1/1942 (0.1%)	0.59	4/2628 (0.2%)
5	J	3.05	6/1728 (0.3%)	0.48	0/2358
6	K	0.24	0/1747	0.43	0/2364
7	L	0.23	0/1885	0.43	0/2552
8	M	0.23	0/1891	0.40	0/2552
9	N	0.23	0/1454	0.41	0/1967

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
All	All	0.64	17/77852 (0.0%)	0.46	14/105195 (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
17	B	0	1
18	D	0	3
23	V	0	1
24	W	0	1
26	Y	0	1
28	a	0	1
31	d	0	1
All	All	0	9

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	e	4	LYS	CD-CE	67.17	3.19	1.51
5	J	21	TYR	CD2-CE2	67.11	2.40	1.39
5	J	21	TYR	CD1-CE1	65.88	2.38	1.39
5	J	21	TYR	CE1-CZ	49.34	2.02	1.38
5	J	21	TYR	CE2-CZ	45.57	1.97	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	14	PRO	O-C-N	-15.43	98.01	122.70
32	e	4	LYS	CD-CE-NZ	8.24	130.65	111.70
4	I	14	PRO	CA-C-N	7.71	134.15	117.20
32	e	4	LYS	CG-CD-CE	7.23	133.60	111.90
4	I	14	PRO	N-CA-CB	-7.13	94.75	103.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	B	436	GLU	Peptide
18	D	258	ALA	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
18	D	406	VAL	Peptide
18	D	412	GLN	Peptide
23	V	319	HIS	Peptide

5.2 Too-close contacts (i)

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	f	5331	0	5344	0	0
2	G	1826	0	1796	71	0
3	H	1708	0	1594	58	0
4	I	1912	0	1851	86	0
5	J	1704	0	1517	90	0
6	K	1722	0	1673	51	0
7	L	1850	0	1822	51	0
8	M	1856	0	1814	47	0
9	N	1430	0	1398	23	0
10	O	1643	0	1644	30	0
11	P	1585	0	1598	29	0
12	Q	1570	0	1547	41	0
13	R	1548	0	1499	35	0
14	S	1641	0	1618	25	0
15	T	1667	0	1628	37	0
16	A	2835	0	2879	114	0
17	B	2717	0	2755	119	0
18	D	3040	0	3076	129	0
19	E	2790	0	2846	85	0
20	F	2863	0	2931	100	0
21	C	3078	0	3193	132	0
22	U	6287	0	6338	144	0
23	V	3852	0	3893	130	0
24	W	3703	0	3822	94	0
25	X	1905	0	1951	46	0
26	Y	3115	0	3120	102	0
27	Z	2281	0	2312	57	0
28	a	2995	0	3012	0	0
29	b	1458	0	1505	0	0
30	c	2187	0	2215	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	d	2116	0	2146	0	0
32	e	334	0	294	0	0
33	A	31	0	12	1	0
33	D	31	0	12	2	0
33	E	31	0	12	3	0
33	F	31	0	12	1	0
34	c	1	0	0	0	0
All	All	76674	0	76679	1703	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 14.

The worst 5 of 1703 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)
23:V:212:TYR:CE1	23:V:212:TYR:CZ	1.76	1.73
5:J:21:TYR:CD1	5:J:21:TYR:CG	1.85	1.64
5:J:21:TYR:CG	5:J:21:TYR:CD2	1.86	1.64
23:V:212:TYR:CZ	23:V:212:TYR:CE2	1.76	1.63
5:J:21:TYR:CE2	5:J:21:TYR:CZ	1.97	1.51

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	f	686/749 (92%)	575 (84%)	107 (16%)	4 (1%)	30 74
2	G	238/245 (97%)	221 (93%)	15 (6%)	2 (1%)	24 69
3	H	230/233 (99%)	200 (87%)	28 (12%)	2 (1%)	21 67
4	I	248/260 (95%)	223 (90%)	25 (10%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	J	237/247 (96%)	214 (90%)	21 (9%)	2 (1%)	24	69
6	K	224/240 (93%)	196 (88%)	27 (12%)	1 (0%)	39	80
7	L	236/268 (88%)	221 (94%)	15 (6%)	0	100	100
8	M	238/254 (94%)	221 (93%)	17 (7%)	0	100	100
9	N	189/238 (79%)	179 (95%)	10 (5%)	0	100	100
10	O	218/276 (79%)	207 (95%)	11 (5%)	0	100	100
11	P	202/204 (99%)	187 (93%)	15 (7%)	0	100	100
12	Q	197/201 (98%)	183 (93%)	14 (7%)	0	100	100
13	R	199/262 (76%)	185 (93%)	14 (7%)	0	100	100
14	S	211/240 (88%)	199 (94%)	12 (6%)	0	100	100
15	T	213/263 (81%)	202 (95%)	11 (5%)	0	100	100
16	A	359/433 (83%)	307 (86%)	51 (14%)	1 (0%)	46	83
17	B	344/440 (78%)	304 (88%)	38 (11%)	2 (1%)	30	74
18	D	378/418 (90%)	323 (85%)	51 (14%)	4 (1%)	17	63
19	E	351/403 (87%)	317 (90%)	34 (10%)	0	100	100
20	F	362/439 (82%)	327 (90%)	34 (9%)	1 (0%)	46	83
21	C	390/398 (98%)	344 (88%)	42 (11%)	4 (1%)	19	65
22	U	798/953 (84%)	738 (92%)	59 (7%)	1 (0%)	56	90
23	V	478/533 (90%)	421 (88%)	57 (12%)	0	100	100
24	W	454/456 (100%)	407 (90%)	44 (10%)	3 (1%)	26	71
25	X	239/422 (57%)	213 (89%)	26 (11%)	0	100	100
26	Y	376/389 (97%)	332 (88%)	42 (11%)	2 (0%)	34	77
27	Z	284/324 (88%)	253 (89%)	30 (11%)	1 (0%)	39	80
28	a	371/376 (99%)	331 (89%)	38 (10%)	2 (0%)	34	77
29	b	189/377 (50%)	175 (93%)	14 (7%)	0	100	100
30	c	274/309 (89%)	246 (90%)	25 (9%)	3 (1%)	17	63
31	d	255/349 (73%)	229 (90%)	26 (10%)	0	100	100
32	e	36/70 (51%)	31 (86%)	5 (14%)	0	100	100
All	All	9704/11269 (86%)	8711 (90%)	958 (10%)	35 (0%)	43	80

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	f	62	ILE
1	f	447	VAL
2	G	111	VAL
22	U	364	VAL
24	W	68	VAL

5.3.2 Protein sidechains (i)

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	f	582/628 (93%)	572 (98%)	10 (2%)	68	87
2	G	193/209 (92%)	189 (98%)	4 (2%)	61	84
3	H	164/190 (86%)	162 (99%)	2 (1%)	78	90
4	I	193/220 (88%)	191 (99%)	2 (1%)	82	92
5	J	152/210 (72%)	151 (99%)	1 (1%)	88	94
6	K	186/202 (92%)	184 (99%)	2 (1%)	80	91
7	L	198/229 (86%)	198 (100%)	0	100	100
8	M	192/211 (91%)	192 (100%)	0	100	100
9	N	148/180 (82%)	148 (100%)	0	100	100
10	O	177/227 (78%)	177 (100%)	0	100	100
11	P	172/173 (99%)	172 (100%)	0	100	100
12	Q	164/171 (96%)	164 (100%)	0	100	100
13	R	153/201 (76%)	153 (100%)	0	100	100
14	S	174/198 (88%)	174 (100%)	0	100	100
15	T	175/214 (82%)	175 (100%)	0	100	100
16	A	308/372 (83%)	302 (98%)	6 (2%)	65	86
17	B	304/385 (79%)	297 (98%)	7 (2%)	58	83
18	D	333/366 (91%)	330 (99%)	3 (1%)	84	93
19	E	308/353 (87%)	302 (98%)	6 (2%)	65	86
20	F	312/379 (82%)	309 (99%)	3 (1%)	82	92

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	C	340/346 (98%)	336 (99%)	4 (1%)	78 90
22	U	685/816 (84%)	681 (99%)	4 (1%)	90 95
23	V	414/459 (90%)	412 (100%)	2 (0%)	92 96
24	W	416/416 (100%)	412 (99%)	4 (1%)	82 92
25	X	208/362 (58%)	207 (100%)	1 (0%)	92 96
26	Y	334/344 (97%)	332 (99%)	2 (1%)	90 95
27	Z	257/295 (87%)	255 (99%)	2 (1%)	86 94
28	a	333/336 (99%)	331 (99%)	2 (1%)	90 95
29	b	167/312 (54%)	167 (100%)	0	100 100
30	c	243/267 (91%)	239 (98%)	4 (2%)	70 88
31	d	231/293 (79%)	228 (99%)	3 (1%)	76 89
32	e	38/63 (60%)	37 (97%)	1 (3%)	54 80
All	All	8254/9627 (86%)	8179 (99%)	75 (1%)	85 93

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	B	436	GLU
19	E	269	THR
30	c	273	LYS
18	D	186	THR
19	E	87	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
19	E	190	GLN
21	C	288	ASN
28	a	257	GLN
19	E	316	HIS
21	C	129	ASN

5.3.3 RNA

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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\#\|Z\| > 2$
33	ATP	A	501	-	26,33,33	0.95	1 (3%)	26,52,52	1.65	1 (3%)
33	ATP	D	501	-	26,33,33	0.95	1 (3%)	26,52,52	1.68	2 (7%)
33	ATP	E	401	-	26,33,33	0.96	1 (3%)	26,52,52	1.65	1 (3%)
33	ATP	F	501	-	26,33,33	0.96	1 (3%)	26,52,52	1.66	1 (3%)

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
33	ATP	A	501	-	-	0/18/38/38	0/3/3/3
33	ATP	D	501	-	-	0/18/38/38	0/3/3/3
33	ATP	E	401	-	-	0/18/38/38	0/3/3/3
33	ATP	F	501	-	-	0/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	501	ATP	C5-C4	3.07	1.47	1.40
33	A	501	ATP	C5-C4	3.09	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	E	401	ATP	C5-C4	3.12	1.47	1.40
33	F	501	ATP	C5-C4	3.13	1.47	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	D	501	ATP	N3-C2-N1	-6.76	123.56	128.87
33	F	501	ATP	N3-C2-N1	-6.65	123.65	128.87
33	A	501	ATP	N3-C2-N1	-6.57	123.71	128.87
33	E	401	ATP	N3-C2-N1	-6.49	123.77	128.87
33	D	501	ATP	O4'-C1'-N9	2.36	112.57	108.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	A	501	ATP	1	0
33	D	501	ATP	2	0
33	E	401	ATP	3	0
33	F	501	ATP	1	0

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
1	f	3
17	B	1
19	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	f	110:ALA	C	111:LEU	N	8.87
1	f	79:ASN	C	80:TYR	N	7.82
1	f	348:ASP	C	349:SER	N	6.24
1	B	216:ILE	C	217:LYS	N	4.90
1	E	175:PRO	C	176:PRO	N	1.65