



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:20 PM BST

PDB ID : 4CR2
EMDB ID: : EMD-2594
Title : Deep classification of a large cryo-EM dataset defines the conformational landscape of the 26S proteasome
Authors : Unverdorben, P.; Beck, F.; Sledz, P.; Schweitzer, A.; Pfeifer, G.; Plitzko, J.M.; Baumeister, W.; Foerster, F.
Deposited on : 2014-02-25
Resolution : 7.70 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

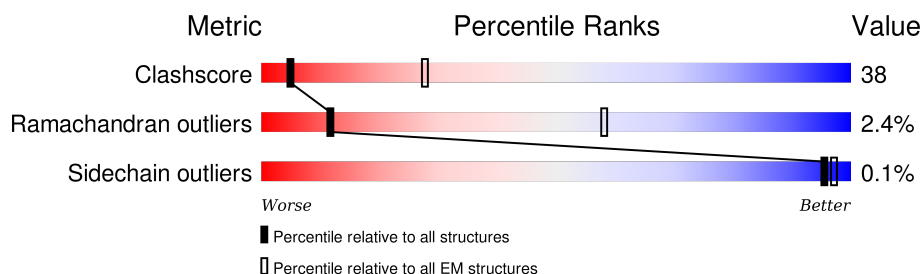
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.70 Å.

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












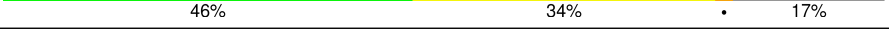



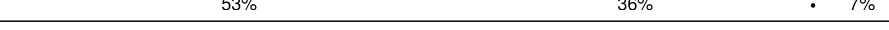


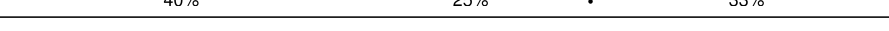




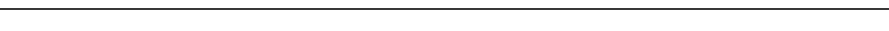


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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

Mol	Chain	Length	Quality of chain
1	1	215	
2	2	261	
3	3	205	
4	4	198	
5	5	287	
6	6	241	
7	7	266	
8	A	252	
9	B	250	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	C	258	
11	D	254	
12	E	260	
13	F	234	
14	G	288	
15	H	467	
16	I	437	
17	J	405	
18	K	428	
19	L	437	
20	M	434	
21	N	945	
22	O	393	
23	P	445	
24	Q	434	
25	R	429	
26	S	523	
27	T	274	
28	U	338	
29	V	306	
30	W	268	
31	X	156	
32	Y	89	
33	Z	993	

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 80139 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PROTEASOME COMPONENT PRE3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	205	Total	C	N	O	S	0	0
			1576	996	261	312	7		

- Molecule 2 is a protein called PROTEASOME COMPONENT PUP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	223	Total	C	N	O	S	0	0
			1692	1067	294	324	7		

- Molecule 3 is a protein called PROTEASOME COMPONENT PUP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

- Molecule 4 is a protein called PROTEASOME COMPONENT C11.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	198	Total	C	N	O	S	0	0
			1585	1005	269	305	6		

- Molecule 5 is a protein called PROTEASOME COMPONENT PRE2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	212	Total	C	N	O	S	0	0
			1646	1045	282	312	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	33	ARG	LYS	SEE REMARK 999	UNP P30656

- Molecule 6 is a protein called PROTEASOME COMPONENT C5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		

- Molecule 7 is a protein called PROTEASOME COMPONENT PRE4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	233	Total	C	N	O	S	0	0
			1824	1154	312	351	7		

- Molecule 8 is a protein called PROTEASOME COMPONENT C7-ALPHA.

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

- Molecule 9 is a protein called PROTEASOME COMPONENT Y7.

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

- Molecule 10 is a protein called PROTEASOME COMPONENT Y13.

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

- Molecule 11 is a protein called PROTEASOME COMPONENT PRE6.

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

- Molecule 12 is a protein called PROTEASOME COMPONENT PUP2.

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

- Molecule 13 is a protein called PROTEASOME COMPONENT PRE5.

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

- Molecule 14 is a protein called PROTEASOME COMPONENT C1.

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

- Molecule 15 is a protein called 26S PROTEASE REGULATORY SUBUNIT 7 HOMOLOG.

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

- Molecule 16 is a protein called 26S PROTEASE REGULATORY SUBUNIT 4 HOMOLOG.

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

- Molecule 17 is a protein called 26S PROTEASE REGULATORY SUBUNIT 8 HOMOLOG.

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

- Molecule 18 is a protein called 26S PROTEASE REGULATORY SUBUNIT 6B HOMOLOG.

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

- Molecule 19 is a protein called 26S PROTEASE SUBUNIT RPT4.

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

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

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

- Molecule 21 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN2.

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

- Molecule 22 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN9.

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

- Molecule 23 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN5.

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

- Molecule 24 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN6.

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

- Molecule 25 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN7.

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

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

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

- Molecule 27 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN12.

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

- Molecule 28 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN8.

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

- Molecule 29 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN11.

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

- Molecule 30 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN10.

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

- Molecule 31 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN13.

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

- Molecule 32 is a protein called 26S PROTEASOME COMPLEX SUBUNIT SEM1.

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

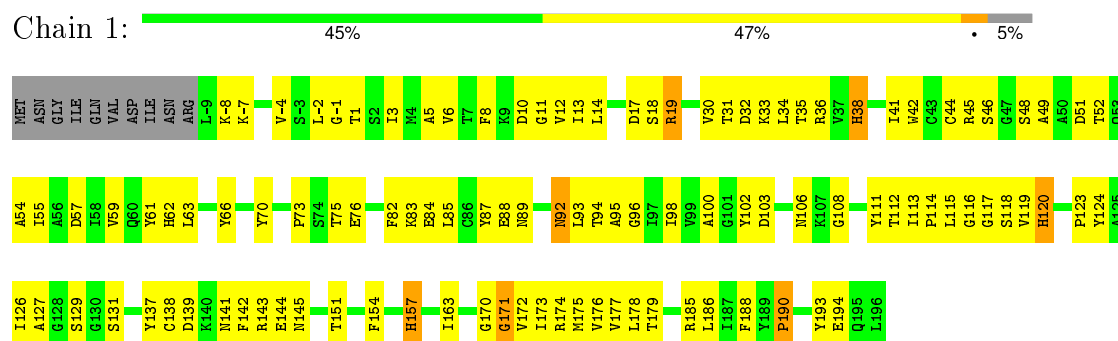
- Molecule 33 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN1.

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

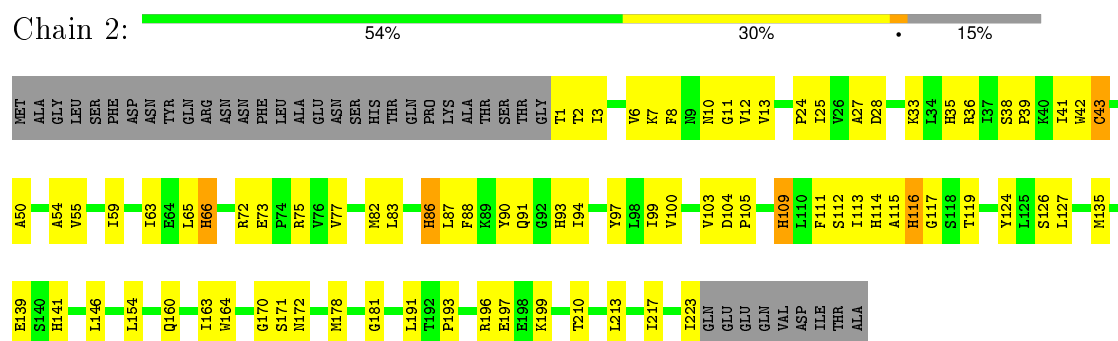
3 Residue-property plots

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

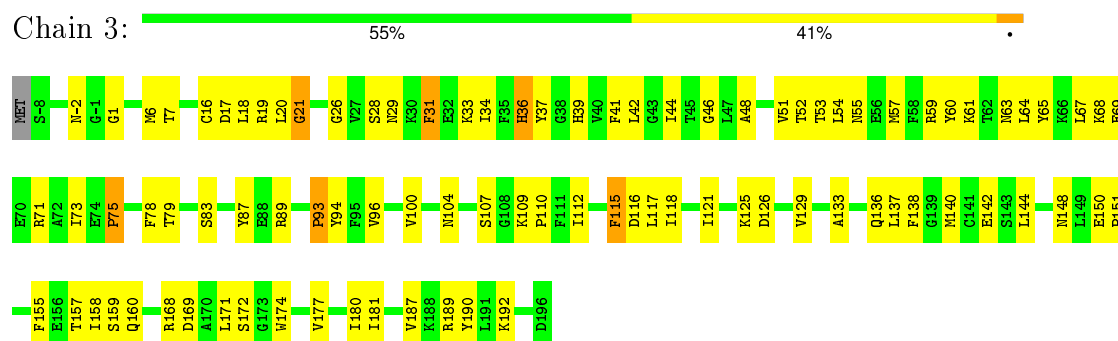
• Molecule 1: PROTEASOME COMPONENT PRE3



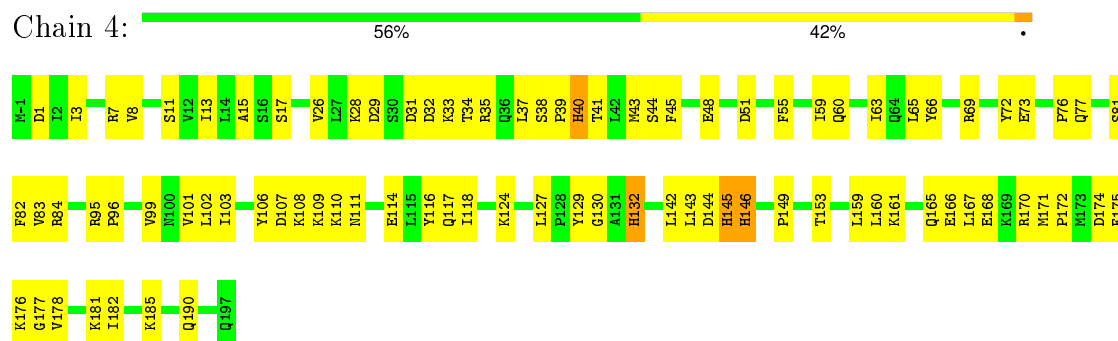
• Molecule 2: PROTEASOME COMPONENT PUP1



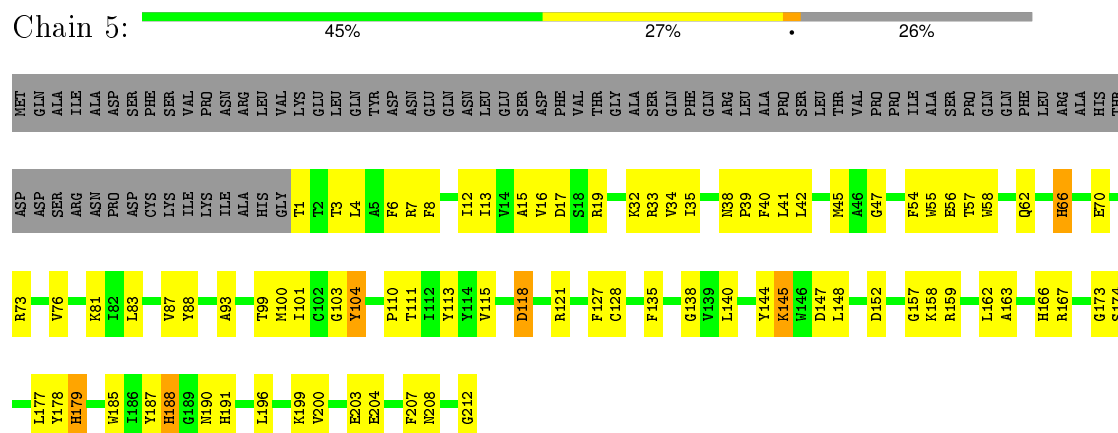
• Molecule 3: PROTEASOME COMPONENT PUP3



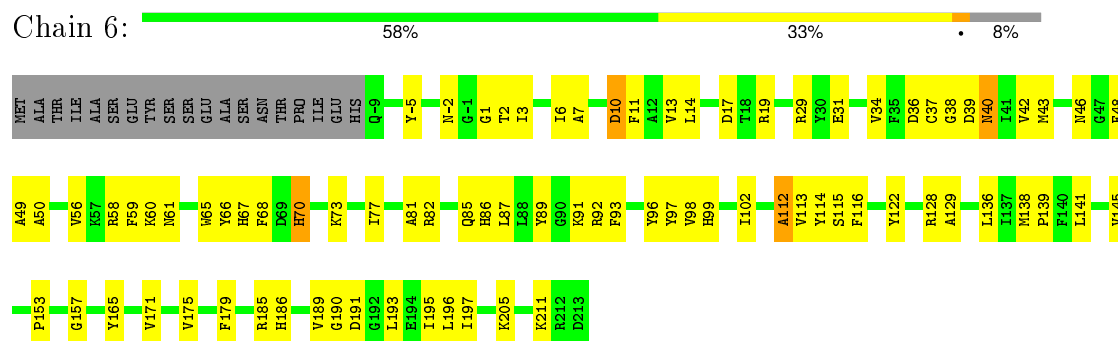
• Molecule 4: PROTEASOME COMPONENT C11



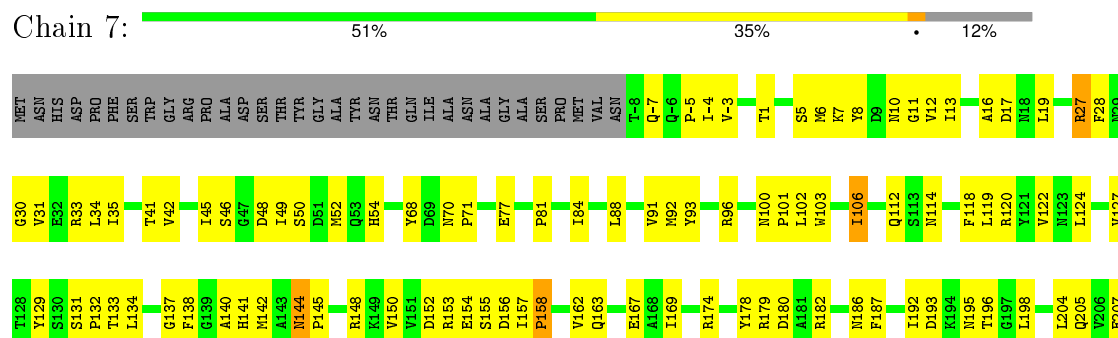
• Molecule 5: PROTEASOME COMPONENT PRE2



• Molecule 6: PROTEASOME COMPONENT C5



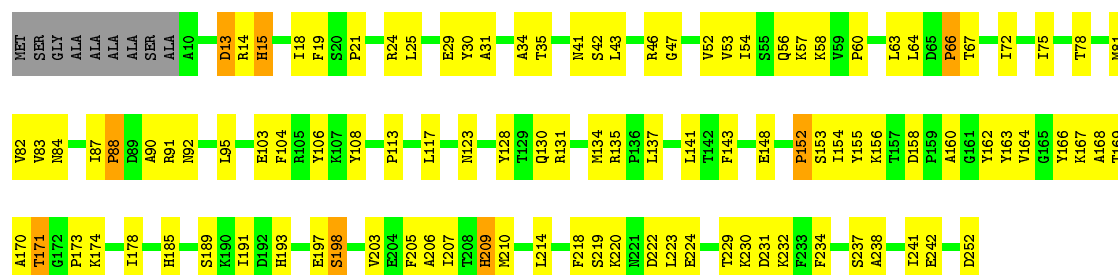
• Molecule 7: PROTEASOME COMPONENT PRE4





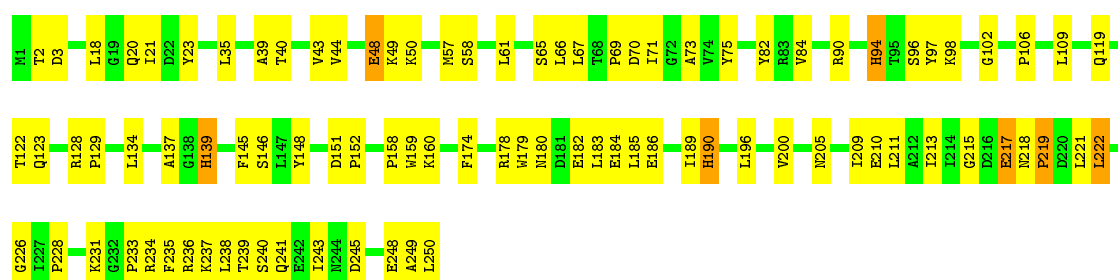
• Molecule 8: PROTEASOME COMPONENT C7-ALPHA

Chain A: 54% 39%



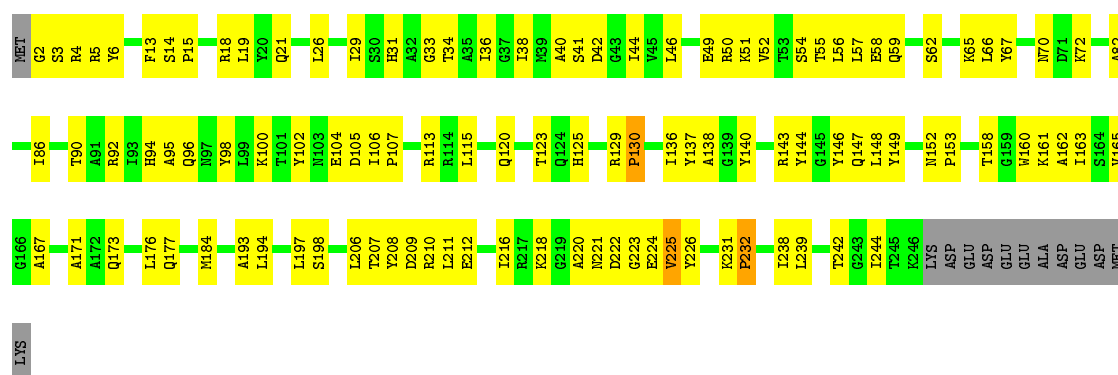
• Molecule 9: PROTEASOME COMPONENT Y7

Chain B: 63% 34%



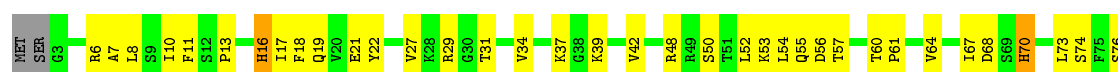
• Molecule 10: PROTEASOME COMPONENT Y13

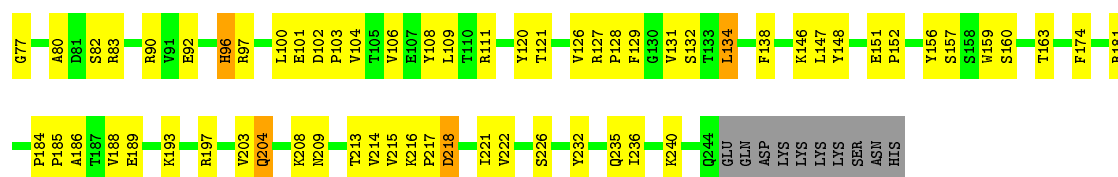
Chain C: 52% 41% 5%



• Molecule 11: PROTEASOME COMPONENT PRE6

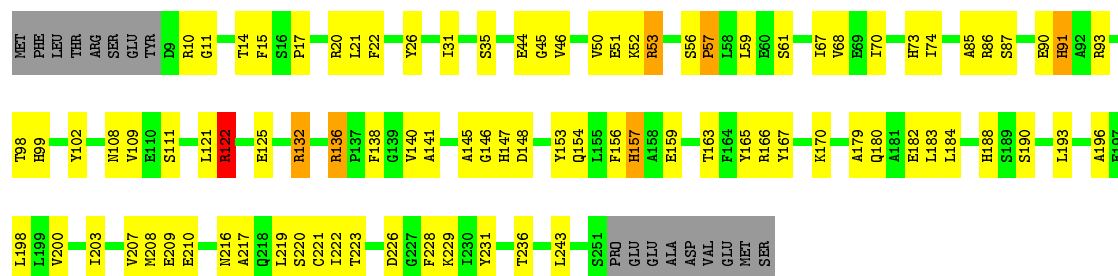
Chain D: 56% 37% 5%





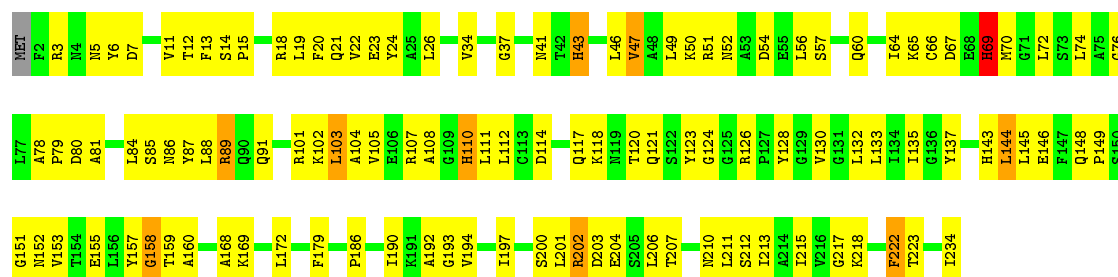
• Molecule 12: PROTEASOME COMPONENT PUP2

Chain E: 59% 32% 7%



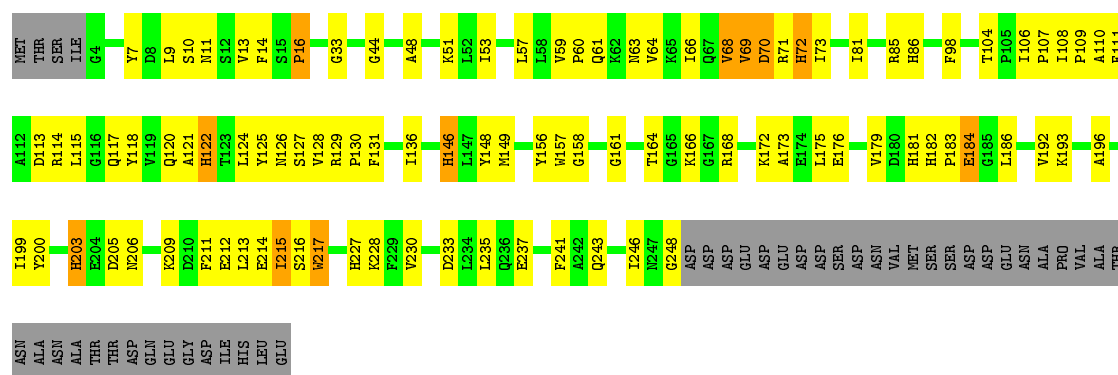
• Molecule 13: PROTEASOME COMPONENT PRE5

Chain F: 50% 45%



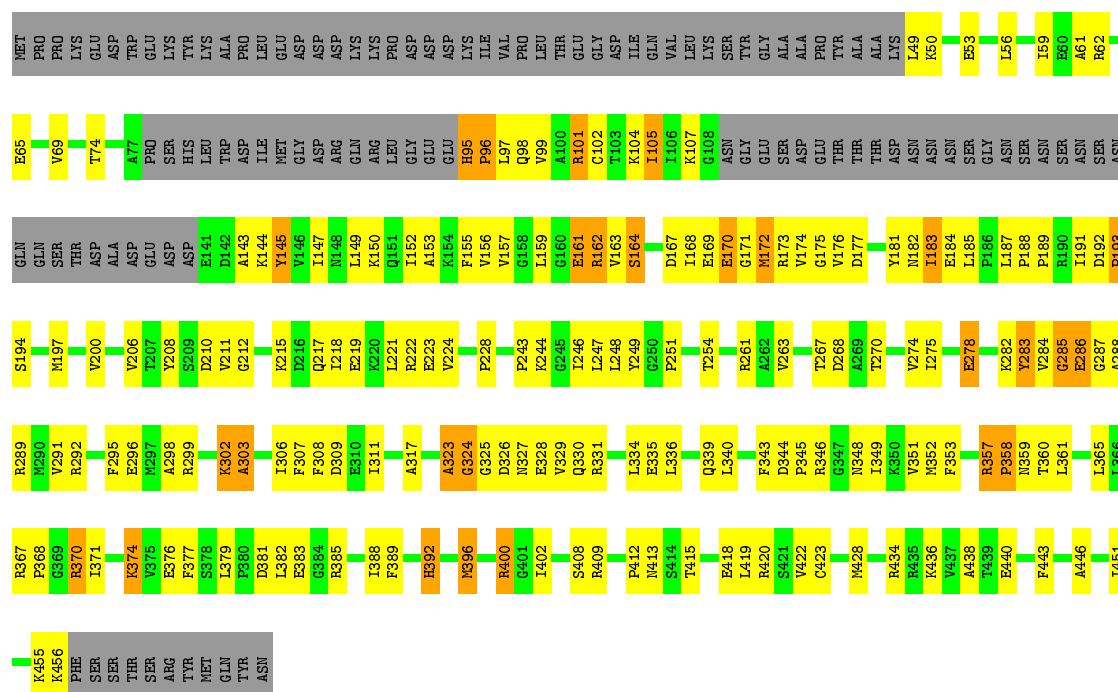
• Molecule 14: PROTEASOME COMPONENT C1

Chain G: 51% 31% 15%



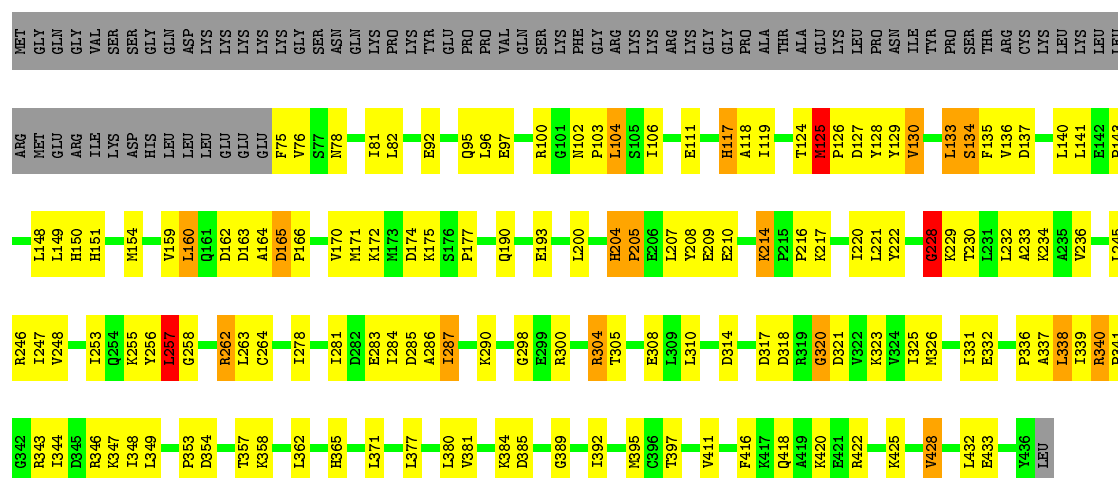
• Molecule 15: 26S PROTEASE REGULATORY SUBUNIT 7 HOMOLOG

Chain H: 38% 33% 6% 23%



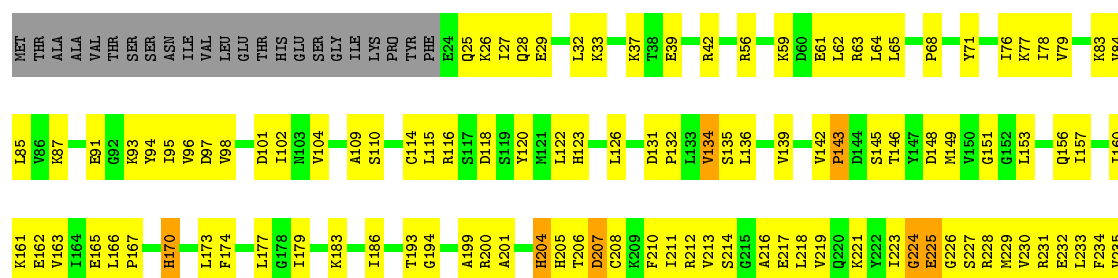
• Molecule 16: 26S PROTEASE REGULATORY SUBUNIT 4 HOMOLOG

Chain I: 49% 29% 17%

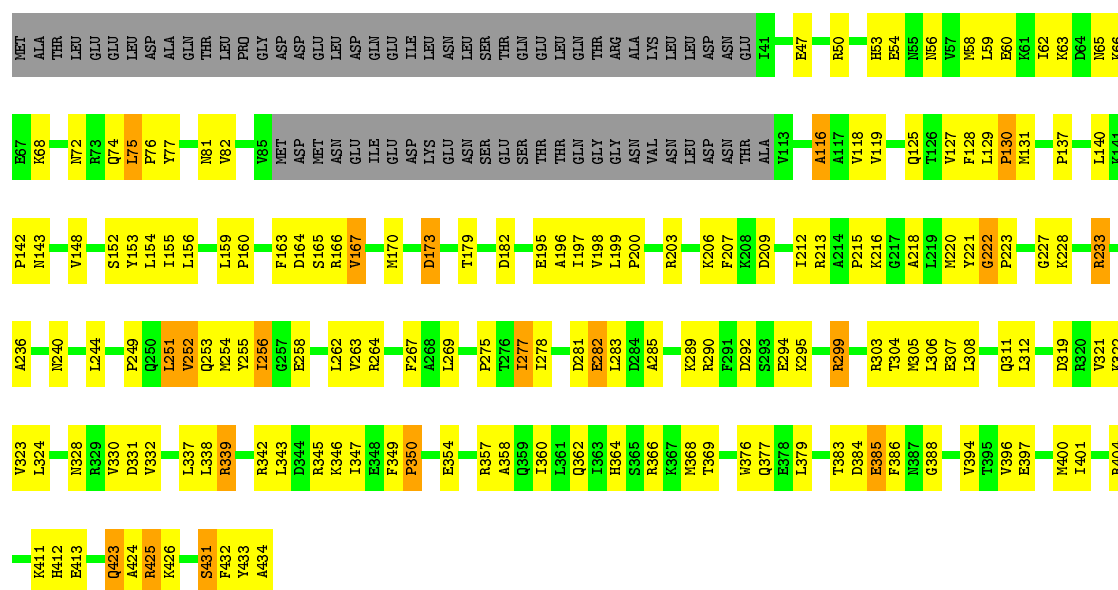


• Molecule 17: 26S PROTEASE REGULATORY SUBUNIT 8 HOMOLOG

Chain J: 48% 41% 8%

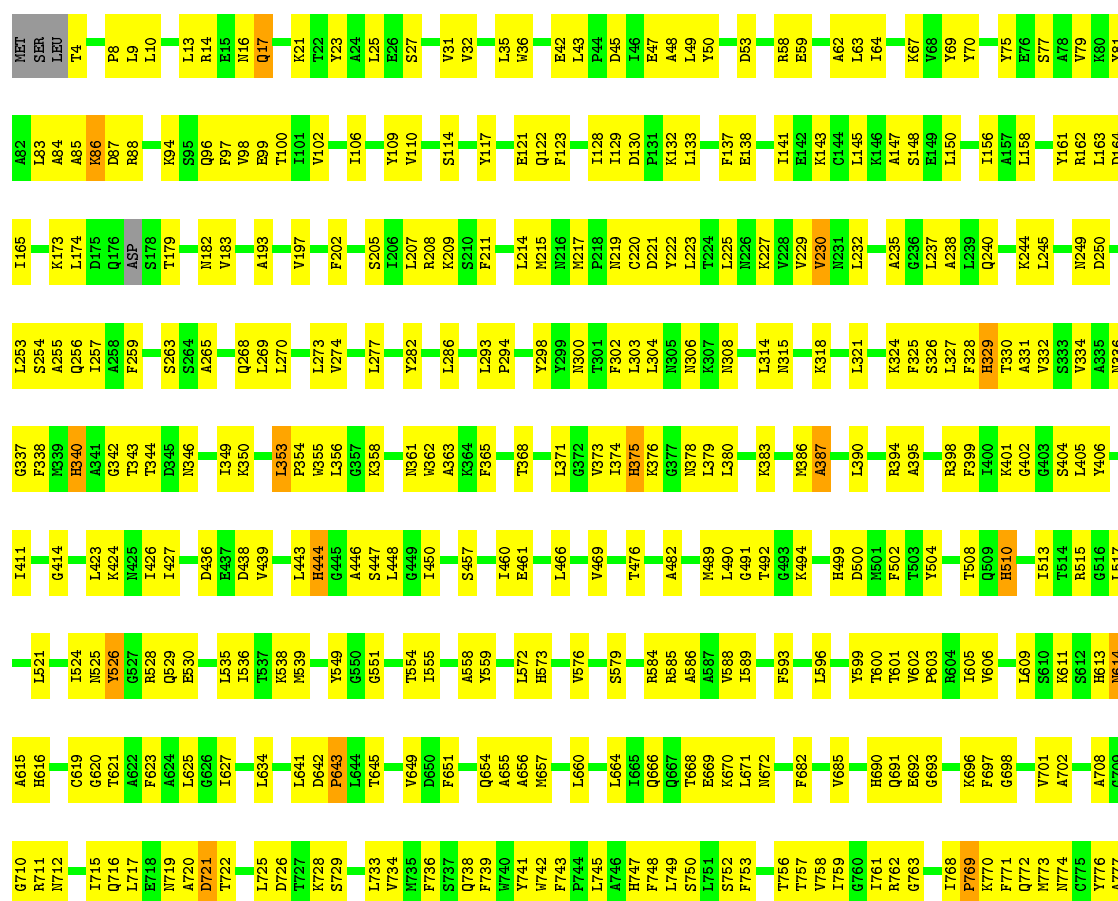


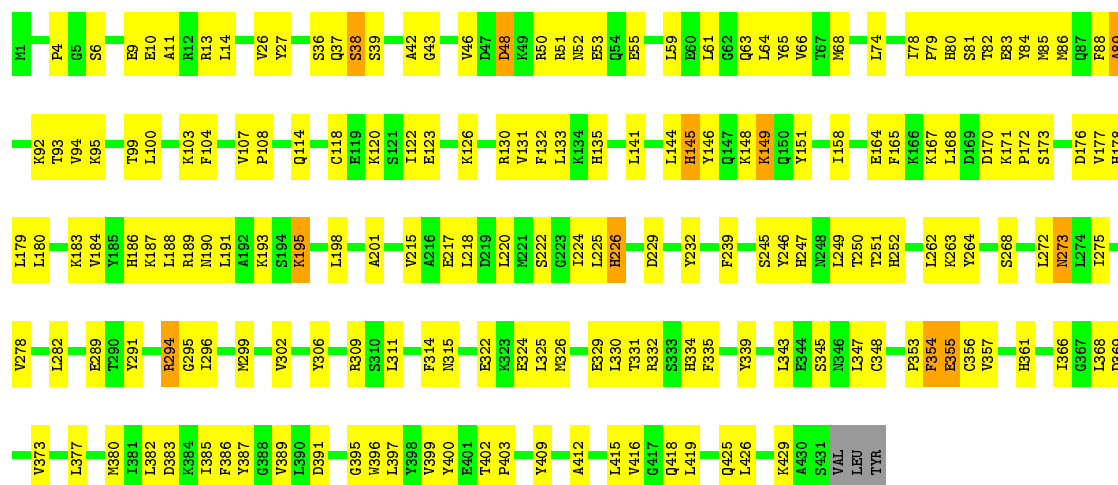
Chain M: 



• Molecule 21: 26S PROTEASOME REGULATORY SUBUNIT RPN2

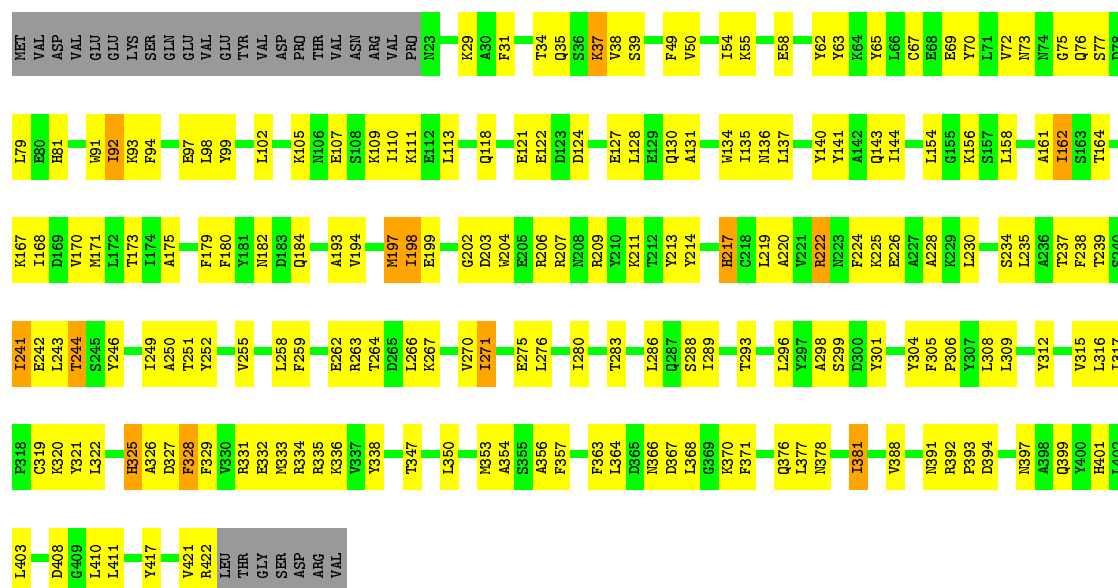
Chain N: 





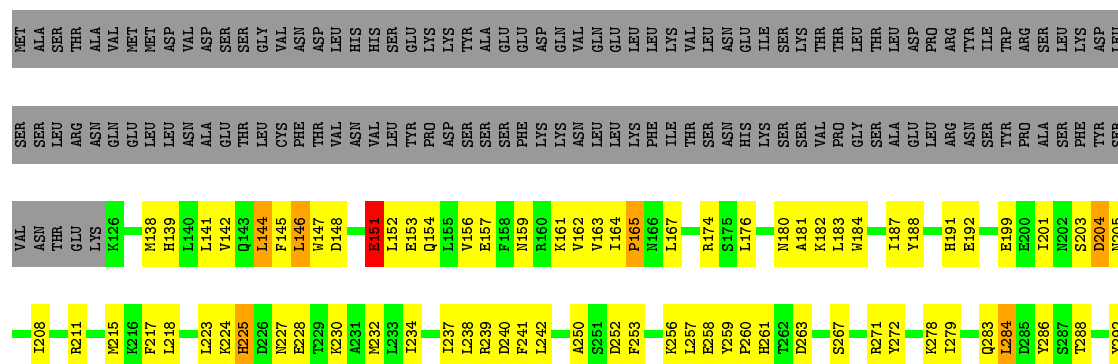
• Molecule 25: 26S PROTEASOME REGULATORY SUBUNIT RPN7

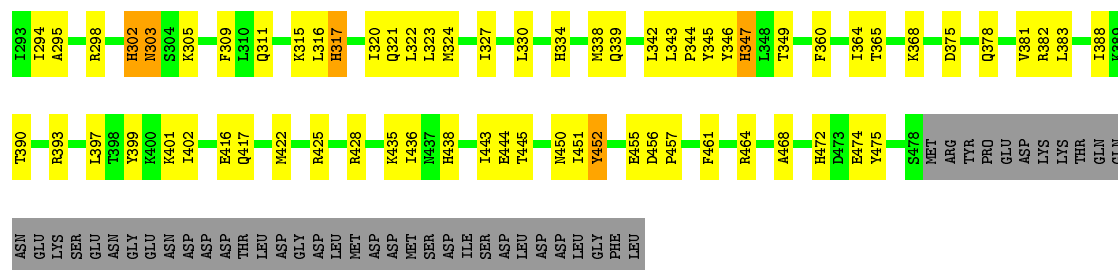
Chain R: 50% 41% 7%



• Molecule 26: 26S PROTEASOME REGULATORY SUBUNIT RPN3

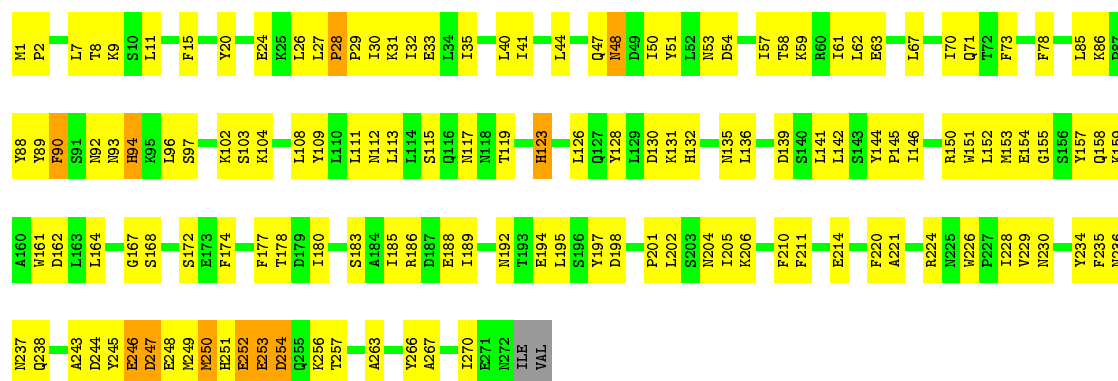
Chain S: 40% 25% 33%





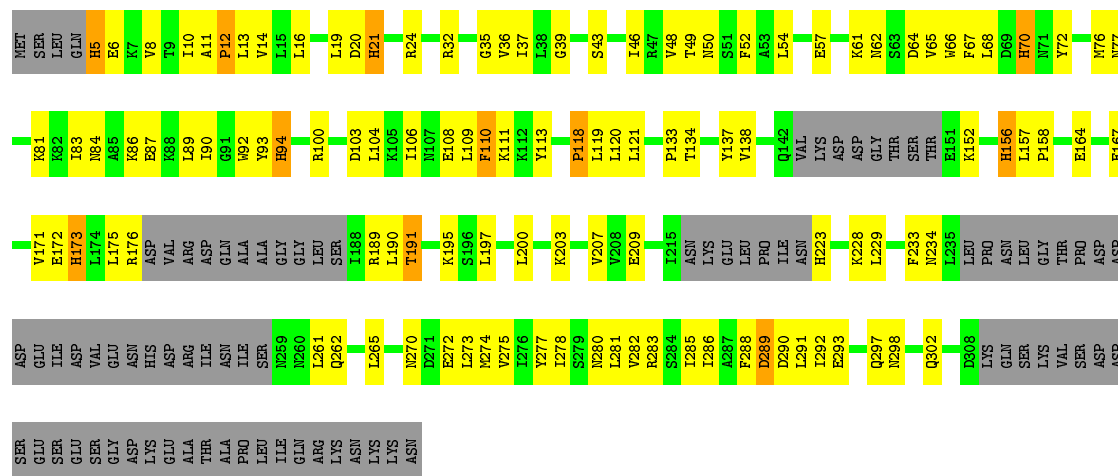
• Molecule 27: 26S PROTEASOME REGULATORY SUBUNIT RPN12

Chain T: 48% 47%



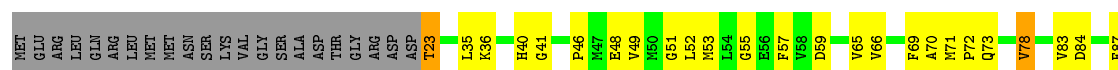
• Molecule 28: 26S PROTEASOME REGULATORY SUBUNIT RPN8

Chain U: 42% 30% 25%



• Molecule 29: 26S PROTEASOME REGULATORY SUBUNIT RPN11

Chain V: 47% 31% 19%



TRP	L878	T795	ASP	ASN	P594	L440	K366	I294	P211	G130	S61	VAL	MET
ILE	A879	F799	ASP	GLU	M595	Y441	S567	R295	L212	K131	Y64	ASP	ASP
THR	S880	S800	GLU	ALA	A598	V442	V368	S296	H214	H132	E65	GLU	GLU
GLN	T884	H801	GLU	ILE	I599	D443	F369	F297	E217	L135	L68	SER	SER
SER	A885	L805	GLU	GLU	E600	E446	S370	D299	E217	R136	L71	LYS	LYS
THR	V886	E806	LYS	VAL	V601	V447	A372	A300	V221	Y137	L71	LYS	LYS
P354	G887	M809	GLU	ASP	G604	K448	S376	S302	D222	R138	S74	GLN	GLN
V955	L888	M809	ALA	ASP	G604	A449	S376	D303	L223	L139	I75	THR	THR
L956	V889	I812	ILE	ILE	Y608	L452	Q379	P304	L224	S141	K76	ILE	ILE
L957	S890	V813	VAL	GLU	T609	L455	A382	V305	L227	D142	K77	ASP	ASP
N958	P891	F813	ASP	VAL	G610	G456	S383	M306	E228	W149	N77	GLU	GLU
G960	S892	C818	GLU	ASP	T611	I457	S384	H307	E229	H150	S78	GLN	GLN
F893	F893	G821	ALA	ALA	G612	H532	P385	Q309	S229	H151	T79	SER	SER
R962	M894	G821	GLU	GLU	L616	V533	V386	Q309	K232	G150	S81	GLN	GLN
E961	H897	T822	GLY	GLY	L620	V535	N387	A311	L233	Y153	N82	ILE	ILE
A963	V740	N823	GLU	GLU	L621	G536	G388	Y312	P234	L154	P86	SER	SER
E964	A739	A744	VAL	VAL	H622	T537	F389	I313	Q236	R155	K87	PRO	PRO
L965	V740	L745	GLU	GLU	H623	I542	L392	A315	F236	H156	K87	GLU	GLU
D968	A744	L746	VAL	VAL	L624	I546	G393	A316	N240	L157	P88	LYS	LYS
I971	A747	L748	LYS	LYS	L625	I546	X394	Q317	T241	A158	L89	GLN	GLN
S972	L748	G749	ALA	ALA	PRD	I546	E468	K318	F242	E159	F91	THR	THR
Y973	G749	E750	GLU	GLU	LYS	I546	P469	G395	Q243	E160	L92	ASN	ASN
T974	E750	D751	ILE	ILE	LYS	N549	L472	S320	R244	V164	T95	LYS	LYS
S975	E751	L752	THR	THR	ASN	F550	L473	S320	R244	Y165	T95	LYS	LYS
H976	L752	G753	GLU	GLU	VAL	E557	L474	F321	V245	G100	Y96	ASP	ASP
I977	G753	H756	LYS	LYS	LYS	E552	L474	E322	C246	Q168	P97	LYS	LYS
V980	L756	M756	LYS	LYS	GLY	R553	Y477	G325	Q247	V169	D98	LYS	LYS
L983	S757	L758	GLY	GLY	GLU	T554	V478	V326	N249	D172	L99	LYS	LYS
K984	L758	R759	ASP	ASP	ASP	A555	P481	Q327	N249	T177	S101	GLU	GLU
K985	R759	H760	SER	SER	ALA	I556	E557	D328	P258	S178	Y103	GLU	GLU
E991	H760	F761	LEU	LEU	LEU	L558	D482	D404	P259	G100	W106	LEU	LEU
E992	F761	G762	GLU	GLU	GLU	K359	T483	N405	P259	S178	Y103	LEU	LEU
E993	G762	H763	GLY	GLY	GLU	K494	K494	N406	P259	G100	W106	LEU	LEU
	H763	L764	GLU	GLU	GLU	I485	I485	Y403	A263	S182	T107	SER	SER
	L764	M765	GLU	GLU	GLU	S486	K409	K409	T267	R183	D108	GLU	GLU
	M765	H766	ILE	ILE	ALA	L566	L410	L340	A268	S194	P109	GLU	GLU
	H766	Y767	LYS	LYS	LYS	L566	K411	L342	Y269	S187	N110	ASP	ASP
	Y767	G768	GLY	GLY	GLY	I572	G414	L342	T270	A188	L111	ALA	ALA
	G768	N769	GLU	GLU	THR	Y574	N415	L346	T271	A189	K112	LYS	LYS
	N769	E770	LYS	LYS	ASN	Q577	N419	R357	Y272	T190	L115	LEU	LEU
	E770	H771	LYS	LYS	SER	Q577	Y419	L348	Q275	E194	L115	LYS	LYS
	H771	I772	LYS	LYS	ILE	G494	I422	T349	Q275	A116	D117	THR	THR
	I772	R773	LYS	LYS	SER	E579	G423	G350	L278	F195	V118	ASP	ASP
	R773	R774	LYS	LYS	SER	A496	G423	P351	T279	S196	L119	LYS	LYS
	R774	M775	SER	SER	PHE	F497	S424	K352	L279	K197	L119	LYS	LYS
	M775	V776	LEU	LEU	GLY	K501	I425	V353	L284	E198	S120	LEU	LEU
	V776	P777	GLY	GLY	LYS	N502	Y426	P354	L284	L201	S120	LEU	LEU
	P777	M780	ASP	ASP	GLY	D582	Q427	P354	L284	L201	S120	LEU	LEU
	M780	G781	ASP	ASP	GLY	D583	V584	P354	L284	L201	S120	LEU	LEU
	G781	N868	ALA	ALA	GLN	V505	N428	P354	L284	L201	S120	LEU	LEU
	N868	H871	VAL	VAL	VAL	L506	N428	P354	L284	L201	S120	LEU	LEU
	H871	I782	THR	THR	THR	L506	N428	P354	L284	L201	S120	LEU	LEU
	I782	V783	THR	THR	THR	L506	N428	P354	L284	L201	S120	LEU	LEU
	V783	K791	ASP	ASP	GLY	L509	L433	H361	L284	L201	S120	LEU	LEU
	K791	N874	GLY	GLY	PRO	L510	L436	L362	L284	L201	S120	LEU	LEU
	N874		THR	THR	THR	P511	L436	L362	L284	L201	S120	LEU	LEU
			LYS	LYS	LYS	H593	L436	L362	L284	L201	S120	LEU	LEU
			ASN	ASN	LYS	H593	L436	L362	L284	L201	S120	LEU	LEU

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	MICROGRAPH	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	Depositor
Image detector	TVIPS TEMCAM-F816 (8K X 8K)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	1	1.19	7/1605 (0.4%)	1.18	2/2171 (0.1%)
10	C	1.14	6/1943 (0.3%)	1.20	0/2629
11	D	1.16	6/1928 (0.3%)	1.21	2/2610 (0.1%)
12	E	1.23	11/1892 (0.6%)	1.23	4/2549 (0.2%)
13	F	1.17	8/1823 (0.4%)	1.21	4/2463 (0.2%)
14	G	1.24	12/1940 (0.6%)	1.20	3/2619 (0.1%)
15	H	1.12	8/2831 (0.3%)	1.23	13/3808 (0.3%)
16	I	1.14	11/2859 (0.4%)	1.16	10/3853 (0.3%)
17	J	1.19	13/2963 (0.4%)	1.17	4/3978 (0.1%)
18	K	1.15	12/3061 (0.4%)	1.19	7/4129 (0.2%)
19	L	1.18	11/2896 (0.4%)	1.27	9/3895 (0.2%)
2	2	1.20	10/1723 (0.6%)	1.23	3/2337 (0.1%)
20	M	1.18	12/2903 (0.4%)	1.26	15/3909 (0.4%)
21	N	1.12	19/6670 (0.3%)	1.13	12/9023 (0.1%)
22	O	1.09	13/3243 (0.4%)	1.10	1/4374 (0.0%)
23	P	1.04	12/3452 (0.3%)	1.11	1/4657 (0.0%)
24	Q	1.09	14/3527 (0.4%)	1.09	4/4748 (0.1%)
25	R	1.06	6/3272 (0.2%)	1.07	1/4412 (0.0%)
26	S	1.08	13/2945 (0.4%)	1.07	2/3976 (0.1%)
27	T	1.03	5/2279 (0.2%)	1.11	5/3077 (0.2%)
28	U	1.16	11/2087 (0.5%)	1.10	3/2811 (0.1%)
29	V	1.19	14/1969 (0.7%)	1.17	1/2652 (0.0%)
3	3	1.17	7/1611 (0.4%)	1.16	0/2174
30	W	1.19	9/1557 (0.6%)	1.24	7/2111 (0.3%)
31	X	1.16	5/1058 (0.5%)	1.18	3/1432 (0.2%)
32	Y	1.04	0/169	1.14	0/223
33	Z	1.11	31/6403 (0.5%)	1.11	10/8686 (0.1%)
4	4	1.17	7/1613 (0.4%)	1.17	1/2173 (0.0%)
5	5	1.18	9/1683 (0.5%)	1.13	2/2277 (0.1%)
6	6	1.16	7/1795 (0.4%)	1.17	2/2420 (0.1%)
7	7	1.16	7/1855 (0.4%)	1.17	3/2514 (0.1%)
8	A	1.20	10/1959 (0.5%)	1.16	1/2652 (0.0%)
9	B	1.23	9/1952 (0.5%)	1.17	3/2642 (0.1%)
All	All	1.14	335/81466 (0.4%)	1.16	138/109984 (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
11	D	0	1
12	E	0	3
13	F	0	1
15	H	0	8
16	I	0	4
18	K	0	2
19	L	0	4
20	M	0	2
21	N	0	1
22	O	0	4
23	P	0	2
24	Q	0	1
25	R	0	2
27	T	0	4
29	V	0	1
30	W	0	1
33	Z	0	2
7	7	0	1
All	All	0	44

The worst 5 of 335 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	M	251	LEU	C-N	-21.72	0.84	1.34
17	J	224	GLY	C-N	17.02	1.73	1.34
19	L	257	GLY	C-N	-8.59	1.14	1.34
25	R	306	PRO	N-CD	8.54	1.59	1.47
22	O	201	PRO	N-CD	8.22	1.59	1.47

The worst 5 of 138 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	257	GLY	O-C-N	-21.29	88.64	122.70
20	M	299	ARG	NE-CZ-NH1	14.99	127.79	120.30
19	L	257	GLY	CA-C-N	13.23	146.30	117.20
19	L	257	GLY	C-N-CA	12.51	152.97	121.70
18	K	252	ARG	NE-CZ-NH2	-11.18	114.71	120.30

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	7	100	ASN	Peptide
11	D	104	VAL	Peptide
12	E	122	ARG	Sidechain
12	E	132	ARG	Sidechain
12	E	136	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1576	0	1555	171	0
2	2	1692	0	1699	108	0
3	3	1581	0	1574	135	0
4	4	1585	0	1590	109	0
5	5	1646	0	1595	95	0
6	6	1757	0	1708	104	0
7	7	1824	0	1832	109	0
8	A	1921	0	1910	162	0
9	B	1915	0	1929	115	0
10	C	1913	0	1914	145	0
11	D	1899	0	1908	141	0
12	E	1867	0	1840	134	0
13	F	1795	0	1797	190	0
14	G	1900	0	1888	161	0
15	H	2792	0	2879	337	0
16	I	2822	0	2868	285	0
17	J	2928	0	3054	250	0
18	K	3019	0	3082	222	0
19	L	2853	0	2925	248	0
20	M	2866	0	2936	262	0
21	N	6562	0	6625	493	0
22	O	3182	0	3207	254	0
23	P	3401	0	3482	280	0
24	Q	3471	0	3494	277	0
25	R	3218	0	3216	296	0
26	S	2893	0	2937	218	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	T	2235	0	2207	174	0
28	U	2061	0	2115	247	0
29	V	1942	0	1954	186	0
30	W	1534	0	1542	145	0
31	X	1032	0	1017	103	0
32	Y	168	0	153	12	0
33	Z	6289	0	6235	798	0
All	All	80139	0	80667	6086	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 38.

The worst 5 of 6086 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)
33:Z:574:TYR:CE2	33:Z:584:VAL:HG11	1.29	1.68
23:P:131:PHE:CZ	23:P:167:THR:HG22	1.24	1.65
15:H:172:MET:HB2	16:I:129:TYR:CD2	1.26	1.62
15:H:396:MET:CE	15:H:438:ALA:CB	1.78	1.57
15:H:172:MET:CB	16:I:129:TYR:CE2	1.82	1.57

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	1	203/215 (94%)	188 (93%)	11 (5%)	4 (2%)	9 51
2	2	221/261 (85%)	211 (96%)	10 (4%)	0	100 100
3	3	202/205 (98%)	184 (91%)	15 (7%)	3 (2%)	13 57
4	4	196/198 (99%)	180 (92%)	13 (7%)	3 (2%)	13 57

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	5	210/287 (73%)	197 (94%)	10 (5%)	3 (1%)	14	58
6	6	220/241 (91%)	205 (93%)	11 (5%)	4 (2%)	11	53
7	7	231/266 (87%)	212 (92%)	17 (7%)	2 (1%)	21	67
8	A	241/252 (96%)	226 (94%)	12 (5%)	3 (1%)	16	61
9	B	248/250 (99%)	233 (94%)	12 (5%)	3 (1%)	16	61
10	C	243/258 (94%)	229 (94%)	11 (4%)	3 (1%)	16	61
11	D	240/254 (94%)	224 (93%)	14 (6%)	2 (1%)	24	69
12	E	241/260 (93%)	223 (92%)	14 (6%)	4 (2%)	11	55
13	F	231/234 (99%)	214 (93%)	12 (5%)	5 (2%)	8	49
14	G	243/288 (84%)	226 (93%)	13 (5%)	4 (2%)	12	56
15	H	353/467 (76%)	305 (86%)	27 (8%)	21 (6%)	2	27
16	I	358/437 (82%)	318 (89%)	29 (8%)	11 (3%)	5	42
17	J	369/405 (91%)	334 (90%)	26 (7%)	9 (2%)	7	47
18	K	377/428 (88%)	338 (90%)	32 (8%)	7 (2%)	10	52
19	L	359/437 (82%)	318 (89%)	36 (10%)	5 (1%)	14	58
20	M	363/434 (84%)	323 (89%)	29 (8%)	11 (3%)	5	42
21	N	843/945 (89%)	786 (93%)	49 (6%)	8 (1%)	21	67
22	O	385/393 (98%)	340 (88%)	31 (8%)	14 (4%)	4	38
23	P	413/445 (93%)	382 (92%)	19 (5%)	12 (3%)	6	43
24	Q	429/434 (99%)	395 (92%)	23 (5%)	11 (3%)	7	45
25	R	398/429 (93%)	354 (89%)	32 (8%)	12 (3%)	5	42
26	S	351/523 (67%)	312 (89%)	29 (8%)	10 (3%)	6	44
27	T	270/274 (98%)	240 (89%)	18 (7%)	12 (4%)	3	33
28	U	245/338 (72%)	237 (97%)	7 (3%)	1 (0%)	39	80
29	V	239/306 (78%)	222 (93%)	10 (4%)	7 (3%)	6	43
30	W	195/268 (73%)	171 (88%)	14 (7%)	10 (5%)	2	30
31	X	125/156 (80%)	106 (85%)	14 (11%)	5 (4%)	4	35
32	Y	17/89 (19%)	17 (100%)	0	0	100	100
33	Z	807/993 (81%)	722 (90%)	52 (6%)	33 (4%)	3	35
All	All	10066/11670 (86%)	9172 (91%)	652 (6%)	242 (2%)	12	47

5 of 242 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	A	168	ALA
11	D	204	GLN
13	F	41	ASN
15	H	183	ILE
15	H	185	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	169/178 (95%)	169 (100%)	0	100	100
2	2	182/214 (85%)	182 (100%)	0	100	100
3	3	172/173 (99%)	172 (100%)	0	100	100
4	4	175/175 (100%)	175 (100%)	0	100	100
5	5	169/235 (72%)	167 (99%)	2 (1%)	78	90
6	6	185/201 (92%)	185 (100%)	0	100	100
7	7	199/224 (89%)	199 (100%)	0	100	100
8	A	207/210 (99%)	207 (100%)	0	100	100
9	B	209/209 (100%)	209 (100%)	0	100	100
10	C	204/216 (94%)	204 (100%)	0	100	100
11	D	214/226 (95%)	214 (100%)	0	100	100
12	E	199/215 (93%)	199 (100%)	0	100	100
13	F	192/193 (100%)	192 (100%)	0	100	100
14	G	201/239 (84%)	200 (100%)	1 (0%)	92	96
15	H	303/399 (76%)	302 (100%)	1 (0%)	94	96
16	I	319/385 (83%)	318 (100%)	1 (0%)	94	96
17	J	325/352 (92%)	325 (100%)	0	100	100
18	K	334/374 (89%)	333 (100%)	1 (0%)	94	96
19	L	308/377 (82%)	307 (100%)	1 (0%)	94	96
20	M	315/375 (84%)	315 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	N	713/797 (90%)	713 (100%)	0	100	100
22	O	363/368 (99%)	363 (100%)	0	100	100
23	P	388/415 (94%)	387 (100%)	1 (0%)	94	96
24	Q	388/391 (99%)	388 (100%)	0	100	100
25	R	351/379 (93%)	351 (100%)	0	100	100
26	S	330/489 (68%)	330 (100%)	0	100	100
27	T	254/256 (99%)	254 (100%)	0	100	100
28	U	234/308 (76%)	233 (100%)	1 (0%)	93	96
29	V	217/268 (81%)	217 (100%)	0	100	100
30	W	171/230 (74%)	171 (100%)	0	100	100
31	X	116/144 (81%)	116 (100%)	0	100	100
32	Y	18/81 (22%)	18 (100%)	0	100	100
33	Z	692/850 (81%)	692 (100%)	0	100	100
All	All	8816/10146 (87%)	8807 (100%)	9 (0%)	95	97

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	I	257	LEU
28	U	61	LYS
19	L	253	ASP
14	G	217	TRP
18	K	246	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 154 such sidechains are listed below:

Mol	Chain	Res	Type
20	M	423	GLN
22	O	235	HIS
33	Z	327	GLN
21	N	176	GLN
21	N	679	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.