



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:15 PM BST

PDB ID : 4CR3
EMDB ID: : EMD-2595
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 : 9.30 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

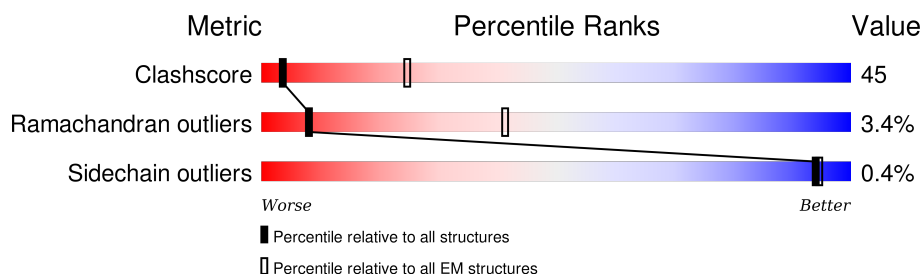
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.30 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.







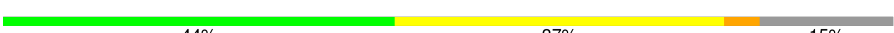








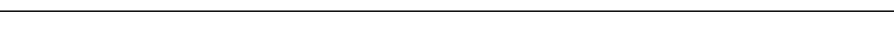


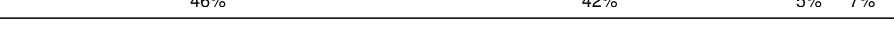
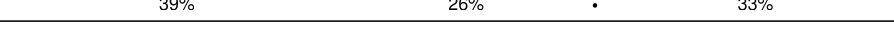

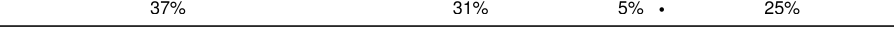




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	47% 44% 5%
2	2	261	55% 26% 5% 15%
3	3	205	65% 33% .
4	4	198	64% 35% .
5	5	287	40% 31% . 26%
6	6	241	56% 34% . 8%
7	7	266	48% 37% . 12%
8	A	252	45% 47% . .
9	B	250	57% 39% .

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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		

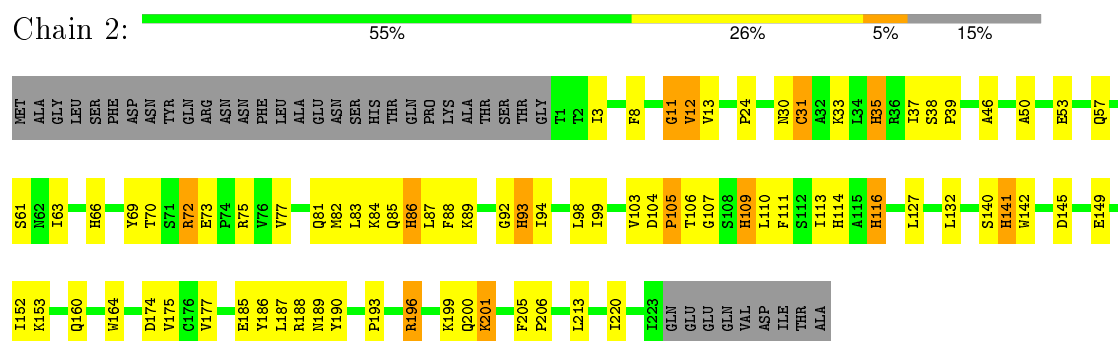
3 Residue-property plots

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.

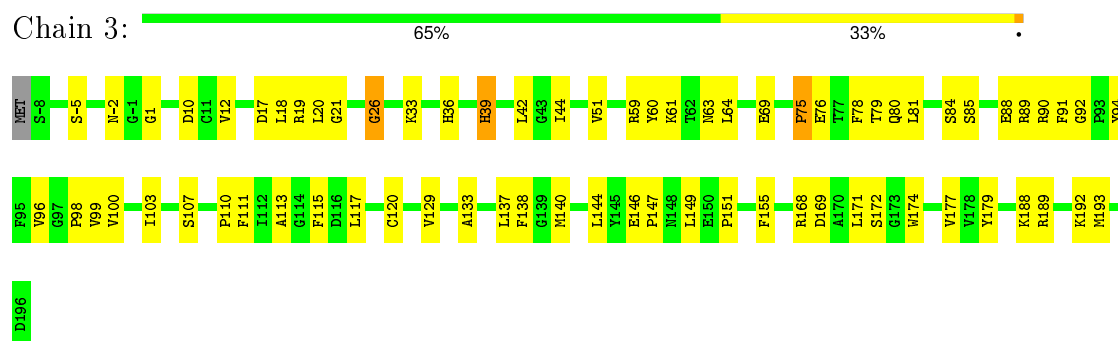
- Molecule 1: PROTEASOME COMPONENT PRE3



- Molecule 2: PROTEASOME COMPONENT PUP1

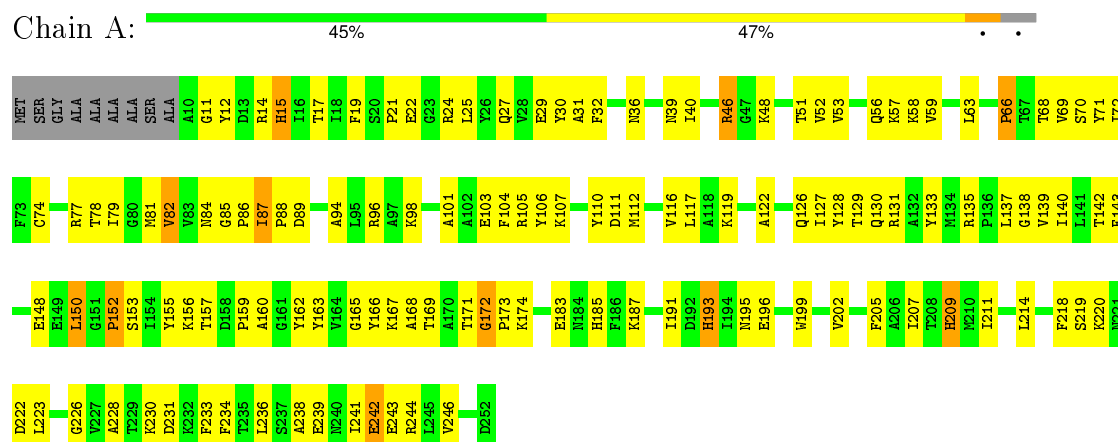


- Molecule 3: PROTEASOME COMPONENT PUP3

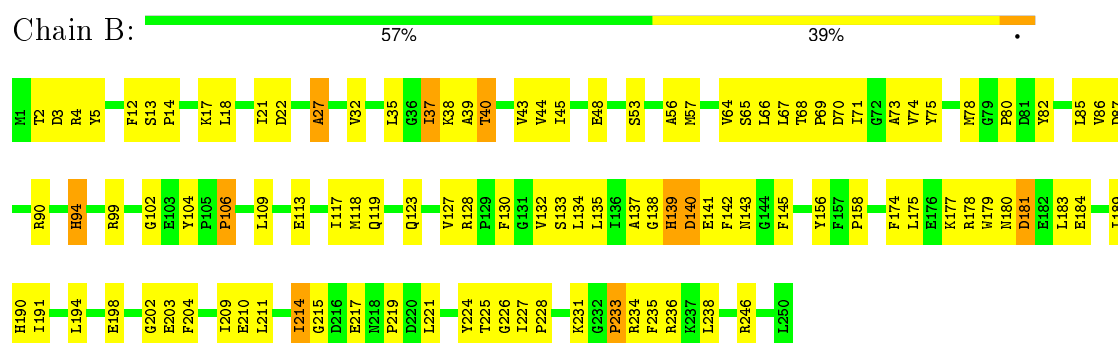


- Molecule 4: PROTEASOME COMPONENT C11

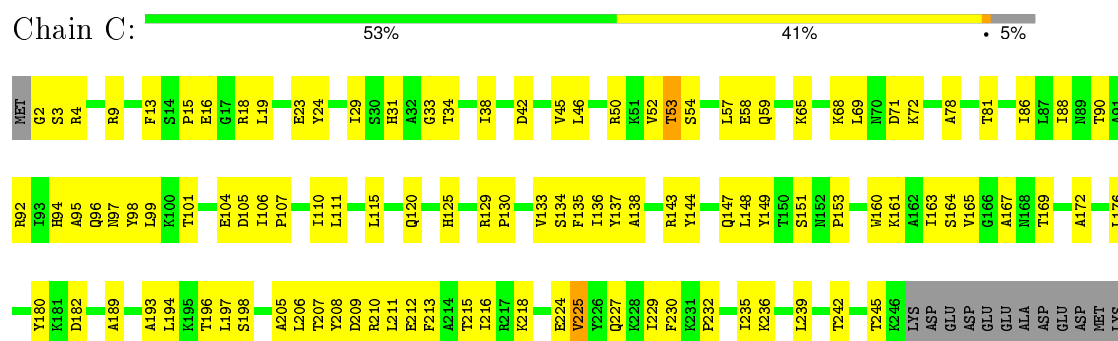
- Molecule 8: PROTEASOME COMPONENT C7-ALPHA



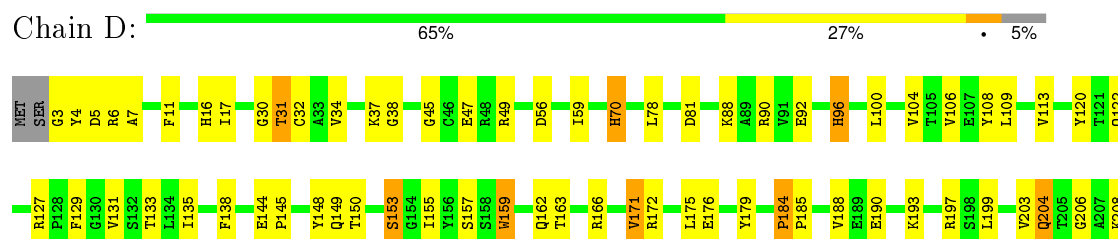
- Molecule 9: PROTEASOME COMPONENT Y7



- Molecule 10: PROTEASOME COMPONENT Y13

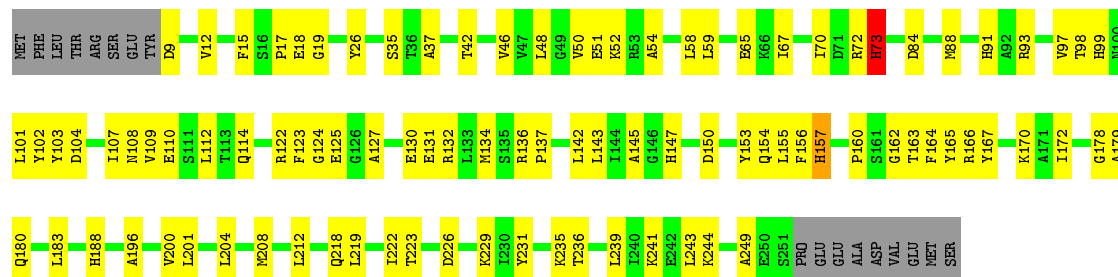


- Molecule 11: PROTEASOME COMPONENT PRE6



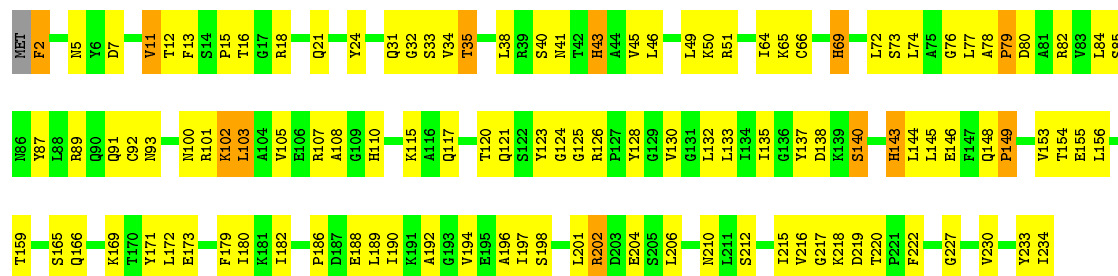
- Molecule 12: PROTEASOME COMPONENT PUP2

Chain E:  57% 36% 7%



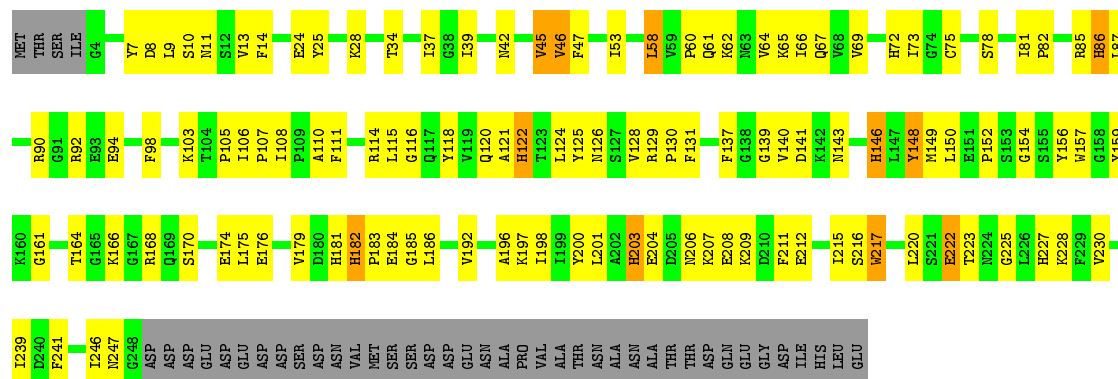
- Molecule 13: PROTEASOME COMPONENT PRE5

Chain F:  50% 44% 5%



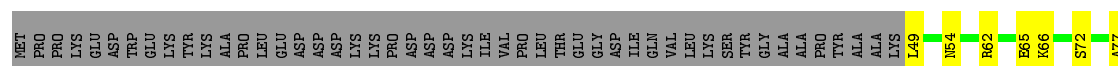
- Molecule 14: PROTEASOME COMPONENT C1

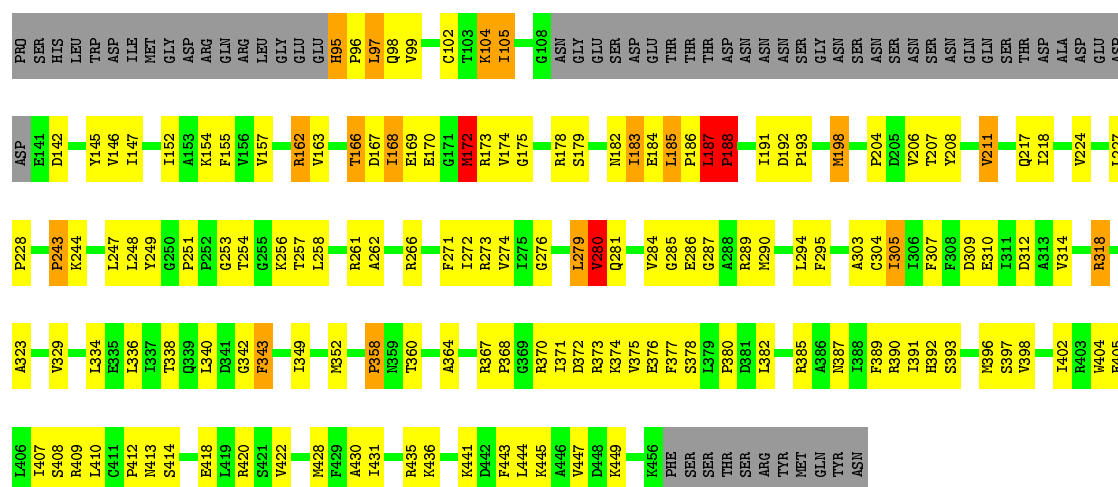
Chain G: 44% 37% 15%



- Molecule 15: 26S PROTEASE REGULATORY SUBUNIT 7 HOMOLOG

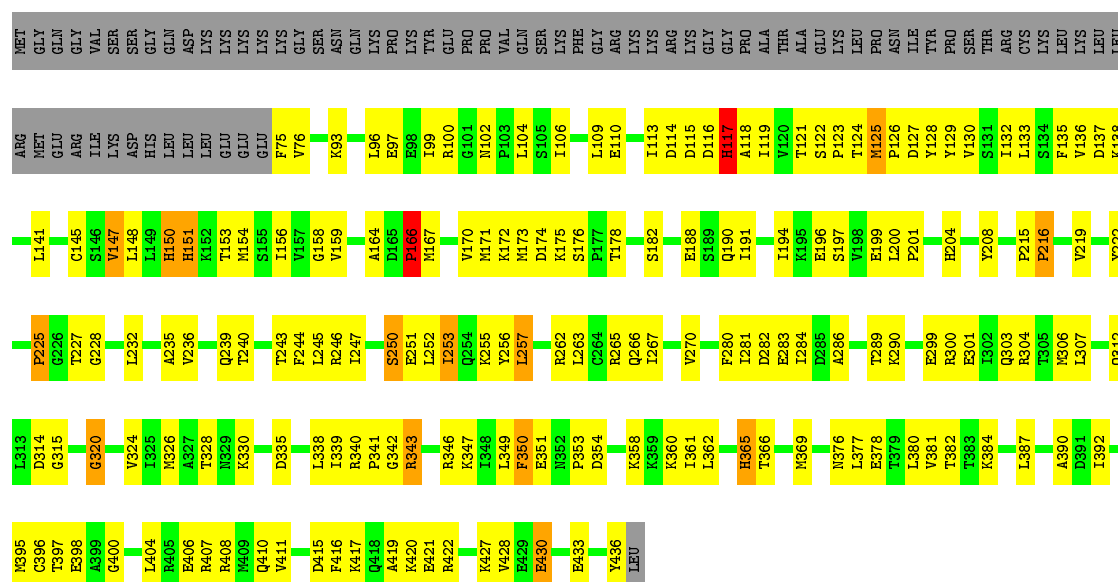
Chain H:  43% 29% . . 23%





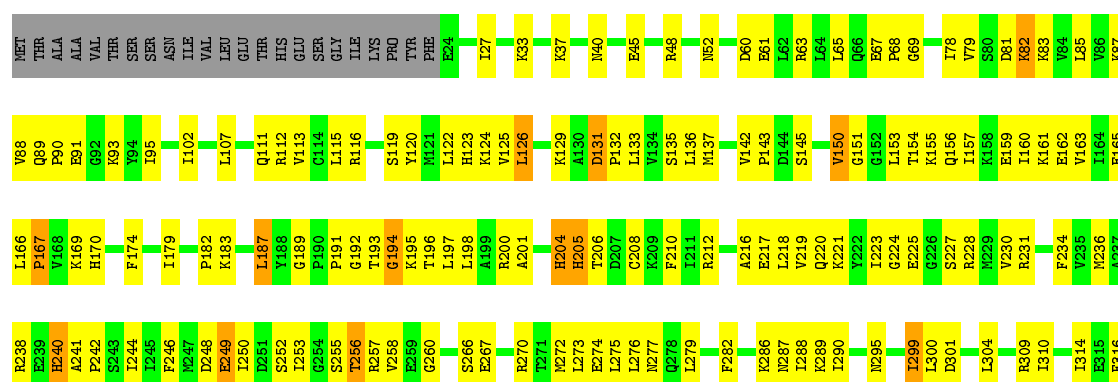
• Molecule 16: 26S PROTEASE REGULATORY SUBUNIT 4 HOMOLOG

Chain I: 43% 37% 17%



• Molecule 17: 26S PROTEASE REGULATORY SUBUNIT 8 HOMOLOG

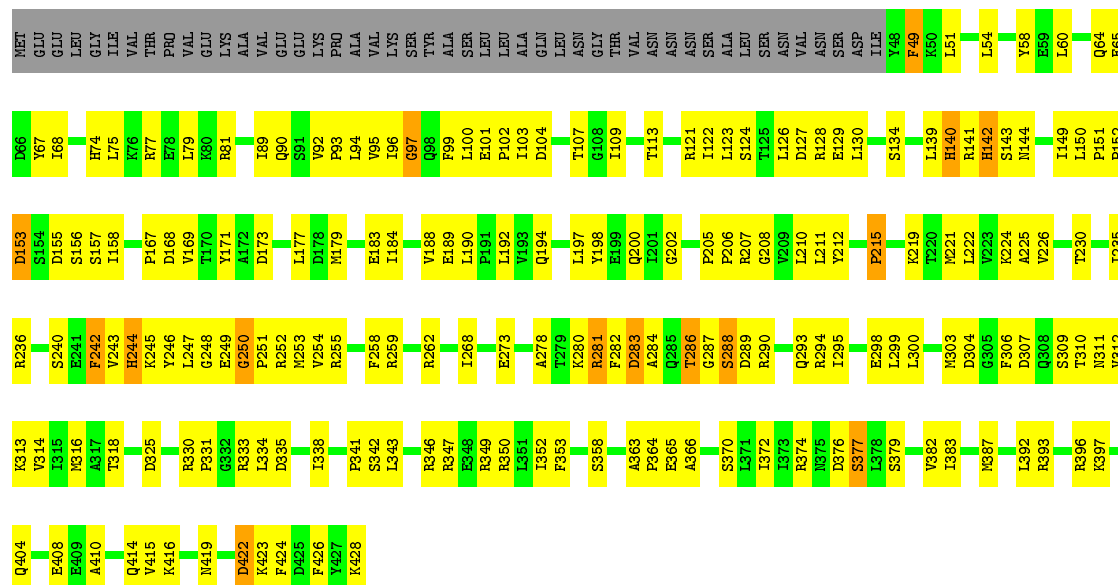
Chain J: 49% 40% 8%





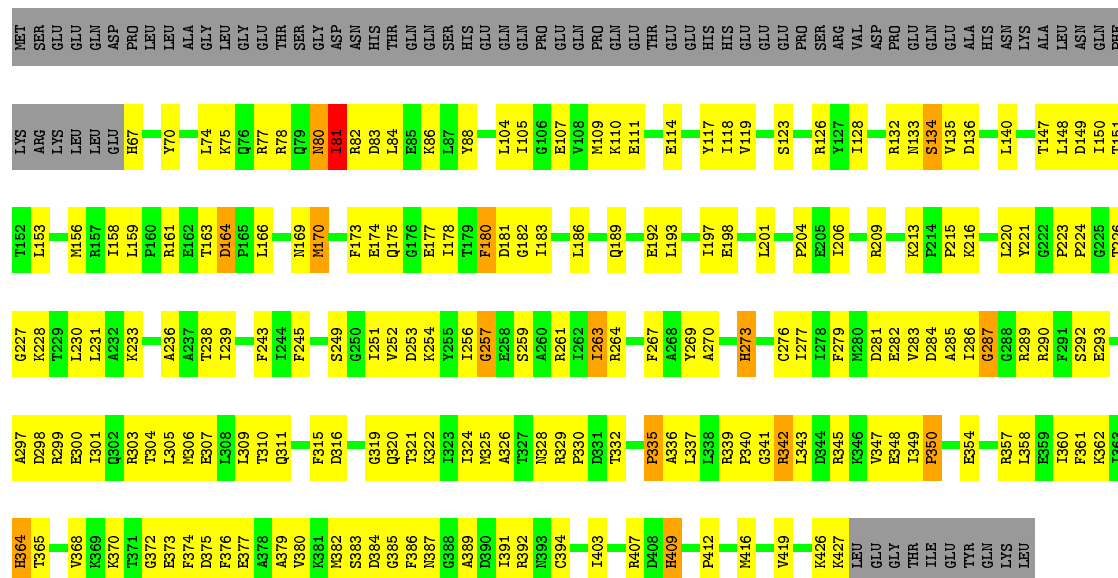
• Molecule 18: 26S PROTEASE REGULATORY SUBUNIT 6B HOMOLOG

Chain K: 46% 40% 11%



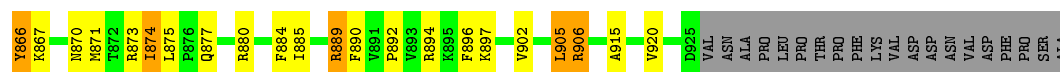
• Molecule 19: 26S PROTEASE SUBUNIT RPT4

Chain L: 40% 40% 17%



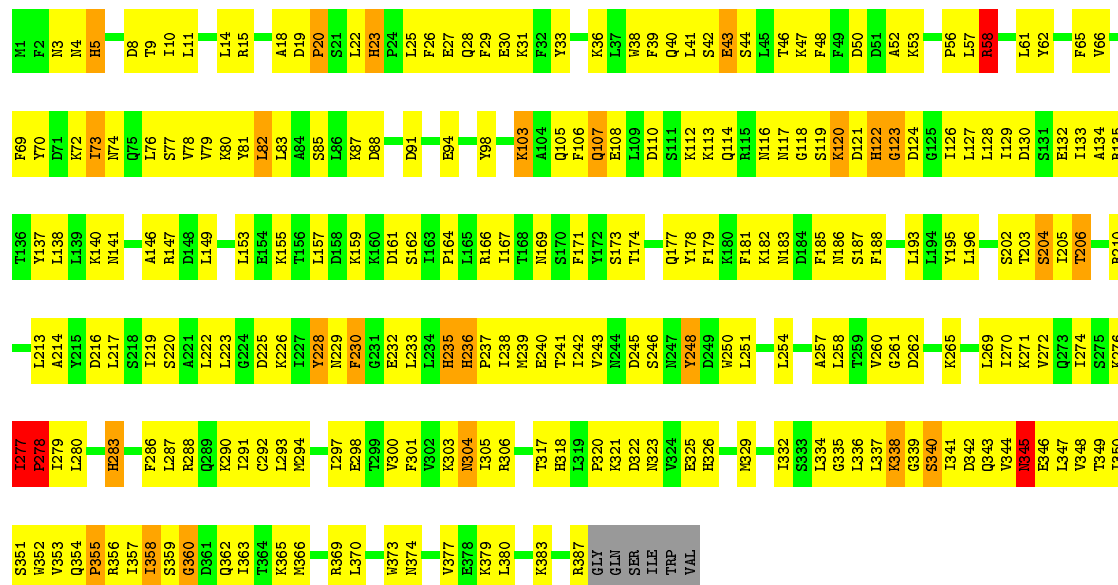
• Molecule 20: 26S PROTEASE REGULATORY SUBUNIT 6A

Chain M: 48% 33% 15%



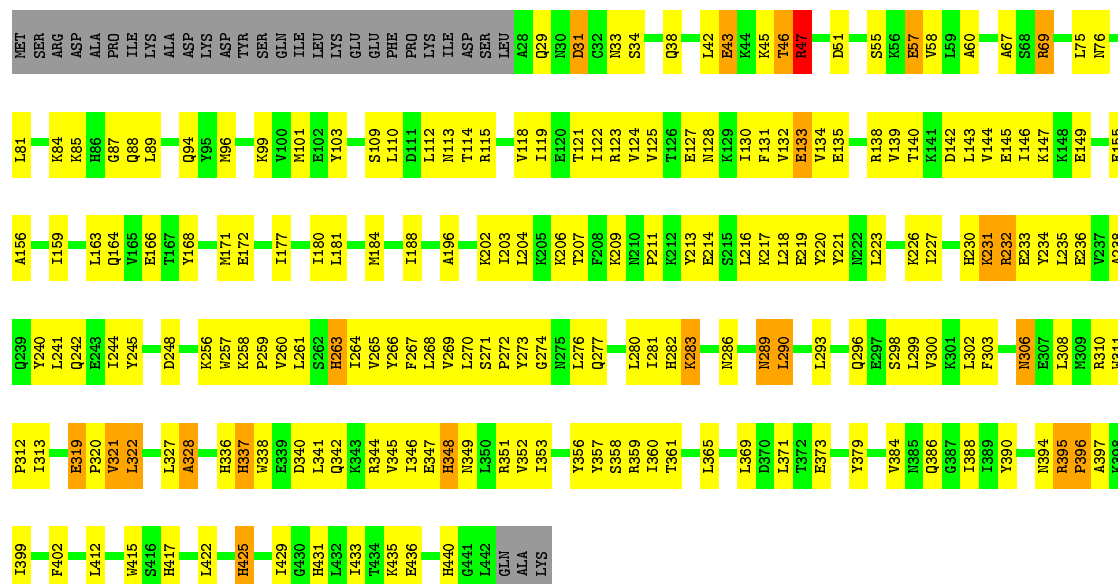
• Molecule 22: 26S PROTEASOME REGULATORY SUBUNIT RPN9

Chain O: 37% 54% 6% ..



• Molecule 23: 26S PROTEASOME REGULATORY SUBUNIT RPN5

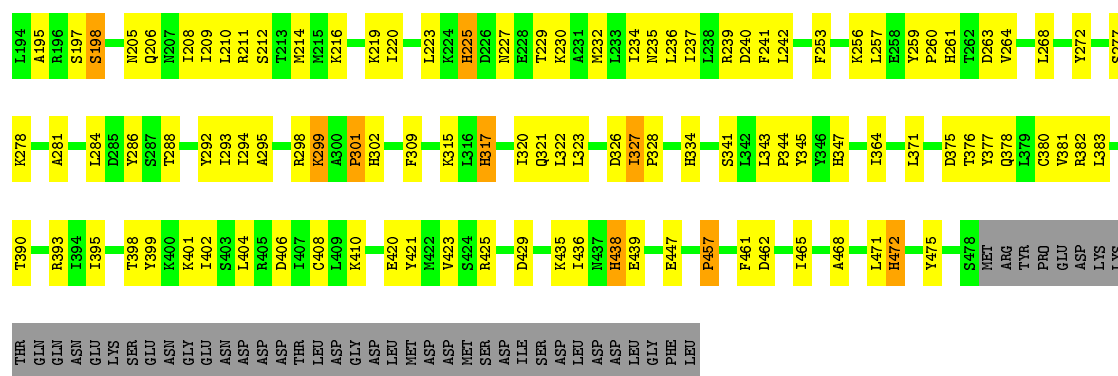
Chain P: 48% 40% 5% 7%



• Molecule 24: 26S PROTEASOME REGULATORY SUBUNIT RPN6

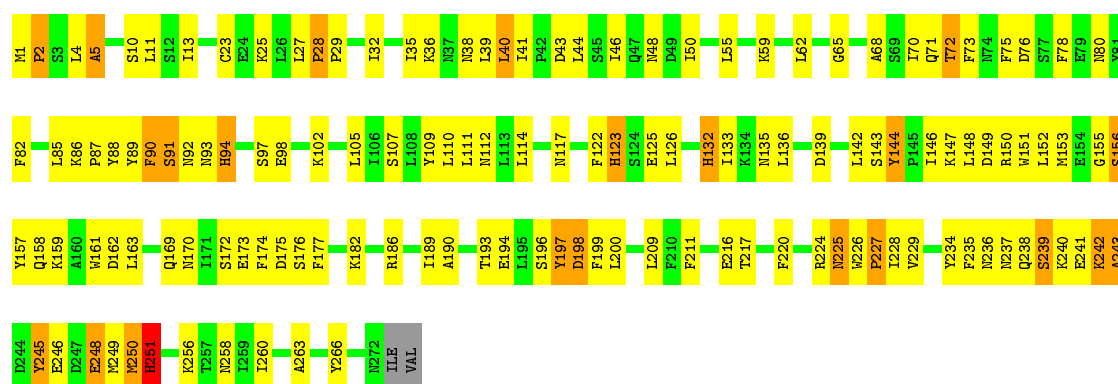
Chain Q: 53% 43% ..





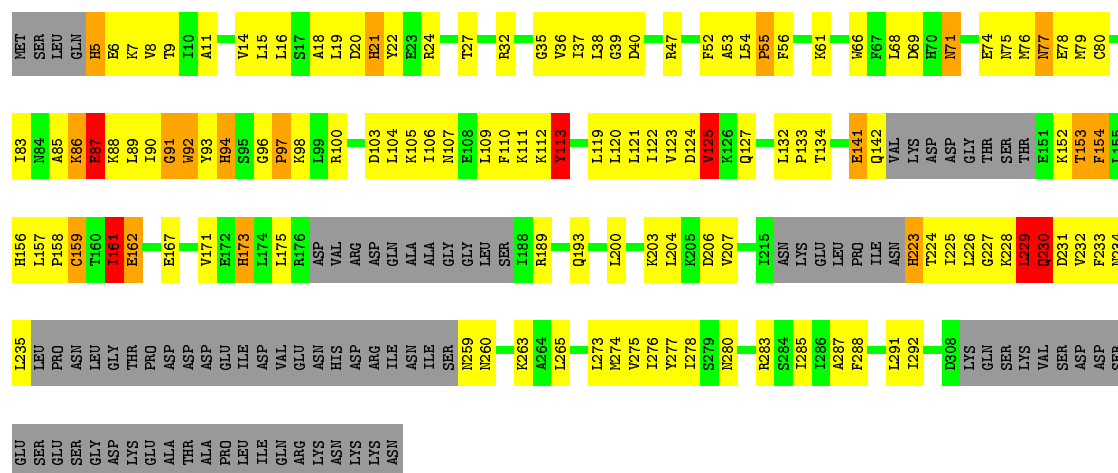
• Molecule 27: 26S PROTEASOME REGULATORY SUBUNIT RPN12

Chain T: 49% 42% 8%



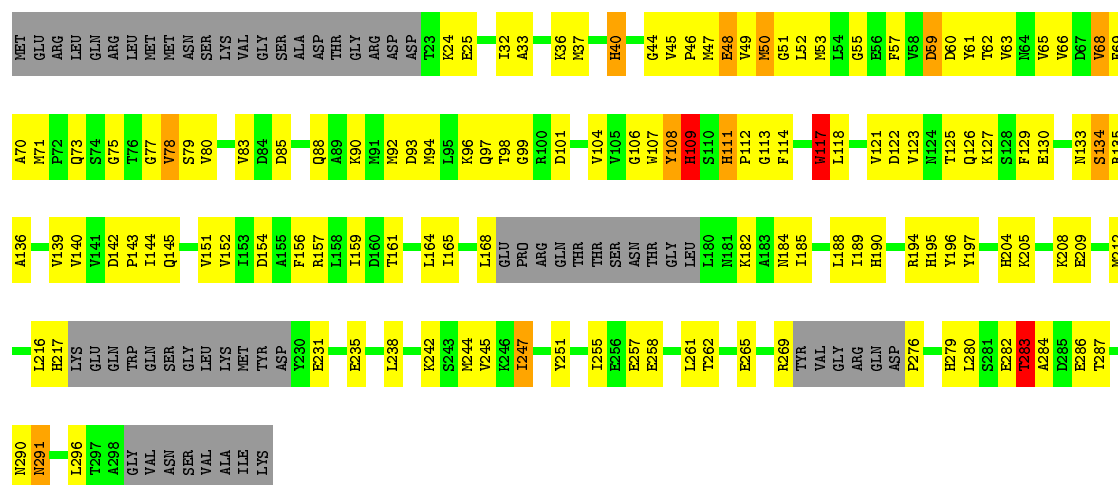
• Molecule 28: 26S PROTEASOME REGULATORY SUBUNIT RPN8

Chain U: 37% 31% 5% 25%



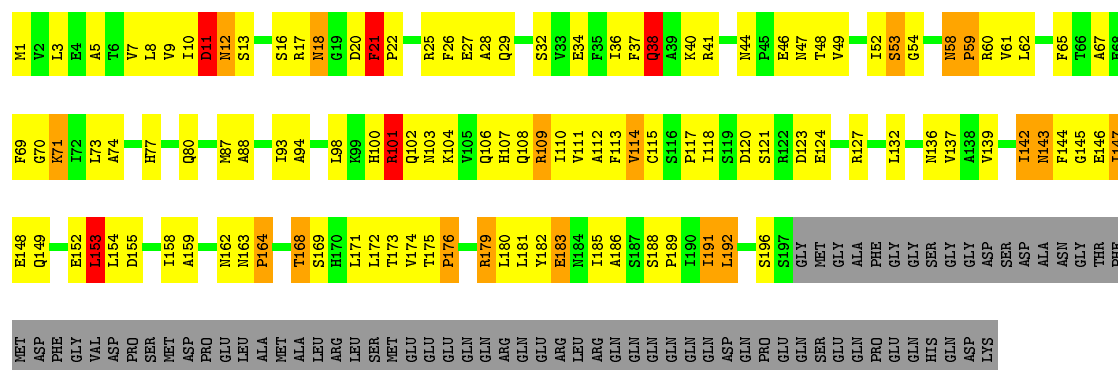
• Molecule 29: 26S PROTEASOME REGULATORY SUBUNIT RPN11

Chain V: 38% 38% 19%



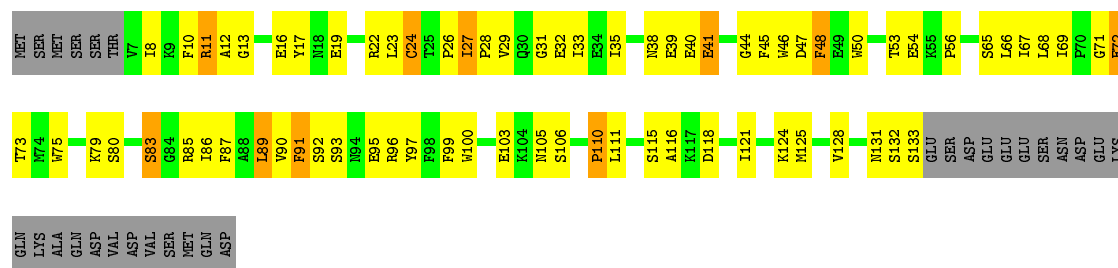
• Molecule 30: 26S PROTEASOME REGULATORY SUBUNIT RPN10

Chain W: 29% 35% 7% 26%



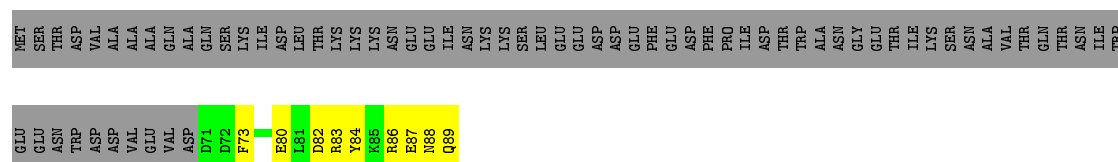
• Molecule 31: 26S PROTEASOME REGULATORY SUBUNIT RPN13

Chain X: 35% 40% 6% 19%



• Molecule 32: 26S PROTEASOME COMPLEX SUBUNIT SEM1

Chain Y: 11% 10% 79%



● Molecule 33: 26S PROTEASOME REGULATORY SUBUNIT RPN1

Chain Z: 

VAL	ASP	GLU	SER	ASP	LYS	LYS	GLN	THR	ILE	ASP	GLU	GLN	LYS	THR	PRO	ASN	LYS	LYS	ASP	LYS	LYS	GLU	GLU	GLU	GLU	GLU	LEU	SER	GLU	GLU	GLU	ASP	ALA	LYS	LEU	LYS	THR	ASP	L49	L52	V53	E54	R55	L56	K57	D60	S61	S62																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
L63	Y64	S67	L68	K72	S81	M82	K87	P88	L89	R90	F91	L92	R93	P94	T95	Y96	P97	D98	L99	I102	Y103	T107	D108	P109	N110	L111	K112	S113	S114	L115	L116	D117	V118	L119	S120	I121	M124	T125	Y126	S127	E128	N129	H132	D133	R134	L135	L136	Y137	R138	L139																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
D142	V143	F146	E147	H151	E152	Y153	H156	L157	I161	Y165	V169	E176	T177	K183	S184	D185	G186	S187	A188	T189	S191	G192	F193	E194	F195	S196	K197	T200	L201	R202	L203	C204	L205	D206	Y210	F211	L212	V213	E214	N215	G216	E217	E218	D219	A220	L224																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
I227	E228	S229	I230	D231	K232	Q235	F236	V237	R244	V245	Y248	V253	P254	P258	P259	E260	K183	S184	D185	G186	S187	A188	T189	S191	G192	F193	E194	F195	S196	K197	T200	L201	R202	L203	C204	L205	D206	Y210	F211	L212	V213	E214	N215	G216	E217	E218	D219	A220	L224																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
D228	I229	L230	G231	N232	K233	L234	H235	L236	L237	L238	L239	L240	L241	L242	L243	L244	L245	L246	L247	L248	L249	L250	L251	L252	L253	L254	L255	L256	L257	L258	L259	L260	L261	L262	L263	L264	L265	L266	L267	L268	L269	L270	L271	L272	L273	L274	L275	L276	L277	L278	L279	L280	L281	L282	L283	L284	L285	L286	L287	L288	L289	L290	L291	L292	L293	L294	L295	L296	L297	L298	L299	L300	L301	L302	L303	L304	L305	L306	L307	L308	L309	L310	L311	L312	L313	L314	L315	L316	L317	L318	L319	L320	L321	L322	L323	L324	L325	L326	L327	L328	L329	L330	L331	L332	L333	L334	L335	L336	L337	L338	L339	L340	L341	L342	L343	L344	L345	L346	L347	L348	L349	L350	L351	L352	L353	L354	L355	L356	L357	L358	L359	L360	L361	L362	L363	L364	L365	L366	L367	L368	L369	L370	L371	L372	L373	L374	L375	L376	L377	L378	L379	L380	L381	L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000	L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	L1029	L1030	L1031	L1032	L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1047	L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060	L1061	L1062	L1063	L1064	L1065	L1066	L1067	L1068	L1069	L1070	L1071	L1072	L1073	L1074	L1075	L1076	L1077	L1078	L1079	L1080	L1081	L1082	L1083	L1084	L1085	L1086	L1087	L1088	L1089	L1090	L1091	L1092	L1093	L1094	L1095	L1096	L1097	L1098	L1099	L1100	L1101	L1102	L1103	L1104	L1105	L1106	L1107	L1108	L1109	L1110	L1111	L1112	L1113	L1114	L1115	L1116	L1117	L1118	L1119	L1120	L1121	L1122	L1123	L1124	L1125	L1126	L1127	L1128	L1129	L1130	L1131	L1132	L1133	L1134	L1135	L1136	L1137	L1138	L1139	L1140	L1141	L1142	L1143	L1144	L1145	L1146	L1147	L1148	L1149	L1150	L1151	L1152	L1153	L1154	L1155	L1156	L1157	L1158	L1159	L1160	L1161	L1162	L1163	L1164	L1165	L1166	L1167	L1168	L1169	L1170	L1171	L1172	L1173	L1174	L1175	L1176	L1177	L1178	L1179	L1180	L1181	L1182	L1183	L1184	L1185	L1186	L1187	L1188	L1189	L1190	L1191	L1192	L1193	L1194	L1195	L1196	L1197	L1198	L1199	L1200	L1201	L1202	L1203	L1204	L1205	L1206	L1207	L1208	L1209	L1210	L1211	L1212	L1213	L1214	L1215	L1216	L1217	L1218	L1219	L1220	L1221	L1222	L1223	L1224	L1225	L1226	L1227	L1228	L1229	L1230	L1231	L1232	L1233	L1234	L1235	L1236	L1237	L1238	L1239	L1240	L1241	L1242	L1243	L1244	L1245	L1246	L1247	L1248	L1249	L1250	L1251	L1252	L1253	L1254	L1255	L1256	L1257	L1258	L1259	L1260	L1261	L1262	L1263	L1264	L1265	L1266	L1267	L1268	L1269	L1270	L1271	L1272	L1273	L1274	L1275	L1276	L1277	L1278	L1279	L1280	L1281	L1282	L1283	L1284	L1285	L1286	L1287	L1288	L1289	L1290	L1291	L1292	L1293	L1294	L1295	L1296	L1297	L1298	L1299	L1300	L1301	L1302	L1303	L1304	L1305	L1306	L1307	L1308	L1309	L1310	L1311	L1312	L1313	L1314	L1315	L1316	L1317	L1318	L1319	L1320	L1321	L1322	L1323	L1324	L1325	L1326	L1327	L1328	L1329	L1330	L1331	L1332	L1333	L1334	L1335	L1336	L1337	L1338	L1339	L1340	L1341	L1342	L1343	L1344	L1345	L1346	L1347	L1348	L1349	L1350	L1351	L1352	L1353	L1354	L1355	L1356	L1357	L1358	L1359	L1360	L1361	L1362	L1363	L1364	L1365	L1366	L1367	L1368	L1369	L1370	L1371	L1372	L1373	L1374	L1375	L1376	L1377	L1378	L1379	L1380	L1381	L1382	L1383	L1384	L1385	L1386	L1387	L1388	L1389	L1390	L1391	L1392	L1393	L1394	L1395	L1396	L1397	L1398	L1399	L1400	L1401	L1402	L1403	L1404	L1405	L1406	L1407	L1408	L1409	L1410	L1411	L1412	L1413	L1414	L1415	L1416	L1417	L1418	L1419	L1420	L1421	L1422	L1423	L1424	L1425	L1426	L1427	L1428	L1429	L1430	L1431	L1432	L1433	L1434	L1435	L1436	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447	L1448	L1449	L1450	L1451	L1452	L1453	L1454	L1455	L1456	L1457	L1458	L1459	L1460	L1461	L1462	L1463	L1464	L1465	L1466	L1467	L1468	L1469	L1470	L1471	L1472	L1473	L1474	L1475	L1476	L1477	L1478	L1479	L1480	L1481	L1482	L1483	L1484	L1485	L1486	L1487

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 (8KX 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	1.21	8/1605 (0.5%)	1.20	5/2171 (0.2%)
10	C	1.16	11/1943 (0.6%)	1.18	2/2629 (0.1%)
11	D	1.12	7/1928 (0.4%)	1.13	2/2610 (0.1%)
12	E	1.19	8/1892 (0.4%)	1.14	2/2549 (0.1%)
13	F	1.23	13/1823 (0.7%)	1.16	4/2463 (0.2%)
14	G	1.24	15/1940 (0.8%)	1.22	4/2619 (0.2%)
15	H	1.08	7/2831 (0.2%)	1.28	11/3808 (0.3%)
16	I	1.17	15/2859 (0.5%)	1.20	8/3853 (0.2%)
17	J	1.17	13/2962 (0.4%)	1.15	4/3975 (0.1%)
18	K	1.21	11/3061 (0.4%)	1.37	11/4129 (0.3%)
19	L	1.16	11/2895 (0.4%)	1.14	3/3892 (0.1%)
2	2	1.24	14/1723 (0.8%)	1.25	4/2337 (0.2%)
20	M	1.17	10/2903 (0.3%)	1.24	14/3909 (0.4%)
21	N	1.15	31/6670 (0.5%)	1.21	26/9023 (0.3%)
22	O	0.73	10/3243 (0.3%)	0.95	4/4374 (0.1%)
23	P	1.17	12/3452 (0.3%)	1.20	12/4657 (0.3%)
24	Q	1.11	16/3527 (0.5%)	1.09	7/4748 (0.1%)
25	R	1.05	11/3272 (0.3%)	1.08	4/4412 (0.1%)
26	S	1.08	13/2945 (0.4%)	1.11	2/3976 (0.1%)
27	T	1.04	9/2279 (0.4%)	1.07	3/3077 (0.1%)
28	U	1.83	12/2087 (0.6%)	1.16	11/2811 (0.4%)
29	V	1.20	12/1969 (0.6%)	1.26	16/2652 (0.6%)
3	3	1.18	7/1611 (0.4%)	1.17	2/2174 (0.1%)
30	W	1.40	12/1556 (0.8%)	1.73	16/2108 (0.8%)
31	X	1.20	4/1058 (0.4%)	1.33	5/1432 (0.3%)
32	Y	0.97	0/169	0.95	0/223
33	Z	1.03	31/6403 (0.5%)	1.12	15/8686 (0.2%)
4	4	1.16	7/1613 (0.4%)	1.22	2/2173 (0.1%)
5	5	1.19	8/1683 (0.5%)	1.22	3/2277 (0.1%)
6	6	1.22	11/1795 (0.6%)	1.18	4/2420 (0.2%)
7	7	1.14	6/1855 (0.3%)	1.14	2/2514 (0.1%)
8	A	1.23	10/1959 (0.5%)	1.21	10/2652 (0.4%)
9	B	1.21	8/1952 (0.4%)	1.21	5/2642 (0.2%)
All	All	1.16	373/81463 (0.5%)	1.19	223/109975 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	1
11	D	0	1
13	F	0	1
15	H	0	6
17	J	0	1
19	L	0	4
20	M	0	2
21	N	0	7
22	O	0	2
23	P	0	3
24	Q	0	1
25	R	0	2
26	S	0	1
27	T	0	2
28	U	0	6
29	V	0	6
30	W	0	11
31	X	0	3
33	Z	0	7
6	6	0	1
7	7	0	2
8	A	0	3
All	All	0	73

The worst 5 of 373 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	U	230	GLN	N-CA	70.25	2.86	1.46
30	W	38	GLN	C-N	-38.06	0.46	1.34
18	K	242	PHE	C-N	21.55	1.83	1.34
20	M	257	GLY	C-N	20.38	1.80	1.34
33	Z	134	SER	N-CA	16.20	1.78	1.46

The worst 5 of 223 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	W	154	LEU	O-C-N	34.31	177.59	122.70
18	K	242	PHE	O-C-N	27.36	166.48	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	242	PHE	C-N-CA	-26.80	54.71	121.70
30	W	154	LEU	CA-C-N	-25.04	62.10	117.20
21	N	889	ARG	NE-CZ-NH1	23.00	131.80	120.30

There are no chirality outliers.

5 of 73 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	-2	LEU	Peptide
6	6	-9	GLN	Peptide
7	7	100	ASN	Peptide
7	7	33	ARG	Peptide
8	A	46	ARG	Mainchain

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	200	0
2	2	1692	0	1699	93	0
3	3	1581	0	1574	101	0
4	4	1585	0	1590	91	0
5	5	1646	0	1595	122	0
6	6	1757	0	1711	87	0
7	7	1824	0	1832	150	0
8	A	1921	0	1909	159	0
9	B	1915	0	1929	144	0
10	C	1913	0	1914	146	0
11	D	1899	0	1908	109	0
12	E	1867	0	1841	163	0
13	F	1795	0	1797	178	0
14	G	1900	0	1888	192	0
15	H	2792	0	2878	283	0
16	I	2822	0	2869	288	0
17	J	2928	0	3054	357	0
18	K	3019	0	3079	411	0
19	L	2853	0	2925	285	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	M	2866	0	2936	287	0
21	N	6562	0	6625	482	0
22	O	3182	0	3207	604	0
23	P	3401	0	3483	320	0
24	Q	3471	0	3494	359	0
25	R	3218	0	3216	408	0
26	S	2893	0	2937	245	0
27	T	2235	0	2206	305	0
28	U	2061	0	2116	375	0
29	V	1942	0	1954	251	0
30	W	1534	0	1538	204	0
31	X	1032	0	1017	181	0
32	Y	168	0	153	17	0
33	Z	6289	0	6233	619	0
All	All	80139	0	80662	7214	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 45.

The worst 5 of 7214 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:321:PHE:CZ	33:Z:350:GLY:HA2	1.23	1.67
22:O:373:TRP:CD1	28:U:200:LEU:HD21	1.29	1.65
24:Q:243:PHE:HZ	24:Q:287:THR:CA	1.07	1.64
22:O:373:TRP:HD1	28:U:200:LEU:CD2	1.01	1.62
33:Z:321:PHE:CE1	33:Z:350:GLY:HA2	1.26	1.60

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	203/215 (94%)	189 (93%)	13 (6%)	1 (0%)	34	77
2	2	221/261 (85%)	207 (94%)	10 (4%)	4 (2%)	11	53
3	3	202/205 (98%)	188 (93%)	12 (6%)	2 (1%)	19	65
4	4	196/198 (99%)	181 (92%)	13 (7%)	2 (1%)	19	65
5	5	210/287 (73%)	194 (92%)	11 (5%)	5 (2%)	7	47
6	6	220/241 (91%)	206 (94%)	11 (5%)	3 (1%)	14	58
7	7	231/266 (87%)	208 (90%)	16 (7%)	7 (3%)	5	42
8	A	241/252 (96%)	217 (90%)	20 (8%)	4 (2%)	11	55
9	B	248/250 (99%)	227 (92%)	15 (6%)	6 (2%)	7	47
10	C	243/258 (94%)	224 (92%)	16 (7%)	3 (1%)	16	61
11	D	240/254 (94%)	221 (92%)	16 (7%)	3 (1%)	15	60
12	E	241/260 (93%)	225 (93%)	13 (5%)	3 (1%)	16	61
13	F	231/234 (99%)	209 (90%)	19 (8%)	3 (1%)	15	60
14	G	243/288 (84%)	224 (92%)	16 (7%)	3 (1%)	16	61
15	H	353/467 (76%)	298 (84%)	36 (10%)	19 (5%)	2	29
16	I	358/437 (82%)	326 (91%)	25 (7%)	7 (2%)	9	51
17	J	367/405 (91%)	337 (92%)	21 (6%)	9 (2%)	7	46
18	K	377/428 (88%)	336 (89%)	29 (8%)	12 (3%)	5	41
19	L	357/437 (82%)	326 (91%)	18 (5%)	13 (4%)	4	38
20	M	363/434 (84%)	322 (89%)	29 (8%)	12 (3%)	5	40
21	N	843/945 (89%)	786 (93%)	37 (4%)	20 (2%)	7	47
22	O	385/393 (98%)	309 (80%)	44 (11%)	32 (8%)	1	18
23	P	413/445 (93%)	374 (91%)	22 (5%)	17 (4%)	3	35
24	Q	429/434 (99%)	390 (91%)	28 (6%)	11 (3%)	7	45
25	R	398/429 (93%)	345 (87%)	36 (9%)	17 (4%)	3	34
26	S	351/523 (67%)	308 (88%)	31 (9%)	12 (3%)	5	40
27	T	270/274 (98%)	235 (87%)	16 (6%)	19 (7%)	1	22
28	U	245/338 (72%)	226 (92%)	9 (4%)	10 (4%)	3	35
29	V	239/306 (78%)	212 (89%)	18 (8%)	9 (4%)	4	37
30	W	193/268 (72%)	156 (81%)	17 (9%)	20 (10%)	1	12
31	X	125/156 (80%)	101 (81%)	19 (15%)	5 (4%)	4	35
32	Y	17/89 (19%)	17 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	Z	807/993 (81%)	690 (86%)	68 (8%)	49 (6%)	2	26
All	All	10060/11670 (86%)	9014 (90%)	704 (7%)	342 (3%)	8	40

5 of 342 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	4	150	ASP
9	B	203	GLU
11	D	31	THR
11	D	204	GLN
15	H	183	ILE

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%)	181 (100%)	1 (0%)	92	96
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%)	168 (99%)	1 (1%)	90	95
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	I	319/385 (83%)	318 (100%)	1 (0%)	94	96
17	J	325/352 (92%)	324 (100%)	1 (0%)	94	96
18	K	334/374 (89%)	333 (100%)	1 (0%)	94	96
19	L	308/377 (82%)	308 (100%)	0	100	100
20	M	315/375 (84%)	315 (100%)	0	100	100
21	N	713/797 (90%)	710 (100%)	3 (0%)	93	96
22	O	363/368 (99%)	361 (99%)	2 (1%)	90	95
23	P	388/415 (94%)	380 (98%)	8 (2%)	61	84
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%)	228 (97%)	6 (3%)	54	80
29	V	217/268 (81%)	214 (99%)	3 (1%)	74	89
30	W	171/230 (74%)	169 (99%)	2 (1%)	78	90
31	X	116/144 (81%)	114 (98%)	2 (2%)	68	87
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%)	8783 (100%)	33 (0%)	94	96

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	P	43	GLU
23	P	85	LYS
30	W	101	ARG
23	P	57	GLU
23	P	58	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 171 such sidechains are listed below:

Mol	Chain	Res	Type
19	L	80	ASN
21	N	738	GLN
30	W	136	ASN

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Mol	Chain	Res	Type
19	L	320	GLN
21	N	182	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.