



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:55 PM UTC

PDB ID : 1FNT / pdb_00001fnt
Title : CRYSTAL STRUCTURE OF THE 20S PROTEASOME FROM YEAST IN
COMPLEX WITH THE PROTEASOME ACTIVATOR PA26 FROM TRY-
PANOSOME BRUCEI AT 3.2 ANGSTROMS RESOLUTION
Authors : Whitby, F.G.; Masters, E.; Kramer, L.; Knowlton, J.R.; Yao, Y.; Wang, C.C.;
Hill, C.P.
Deposited on : 2000-08-23
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

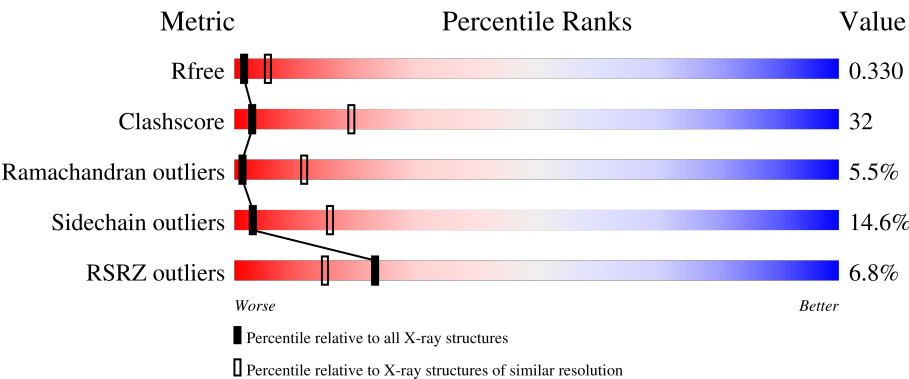
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	252	8% 29% 46% 19% 6%
1	O	252	4% 26% 48% 20% 6%
2	B	250	5% 38% 43% 17% ..
2	P	250	3% 39% 43% 16% ..
3	C	245	4% 40% 39% 17% ..

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Mol	Chain	Length	Quality of chain
3	Q	245	
4	D	254	
4	R	254	
5	E	260	
5	S	260	
6	F	234	
6	T	234	
7	G	287	
7	U	287	
8	H	196	
8	V	196	
9	I	232	
9	W	232	
10	J	205	
10	X	205	
11	K	198	
11	Y	198	
12	L	212	
12	Z	212	
13	M	222	
13	a	222	
14	N	233	
14	b	233	
15	c	231	
15	d	231	

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Mol	Chain	Length	Quality of chain
15	e	231	
15	f	231	
15	g	231	
15	h	231	
15	i	231	
15	j	231	
15	k	231	
15	l	231	
15	m	231	
15	n	231	
15	o	231	
15	p	231	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 70622 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 C7-ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	0	0
			1881	1197	314	362	8			
1	O	238	Total	C	N	O	S	0	0	0
			1881	1197	314	362	8			

- Molecule 2 is a protein called PROTEASOME COMPONENT Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	247	Total	C	N	O	S	0	0	0
			1868	1188	309	368	3			
2	P	247	Total	C	N	O	S	0	0	0
			1868	1188	309	368	3			

- Molecule 3 is a protein called PROTEASOME COMPONENT Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	S	0	0	0
			1868	1180	312	373	3			
3	Q	241	Total	C	N	O	S	0	0	0
			1868	1180	312	373	3			

- Molecule 4 is a protein called PROTEASOME COMPONENT PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	239	Total	C	N	O	S	0	0	0
			1862	1163	326	369	4			
4	R	239	Total	C	N	O	S	0	0	0
			1862	1163	326	369	4			

- Molecule 5 is a protein called PROTEASOME COMPONENT PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	244	Total	C	N	O	S	0	0	0
			1871	1168	316	380	7			
5	S	244	Total	C	N	O	S	0	0	0
			1871	1168	316	380	7			

- Molecule 6 is a protein called PROTEASOME COMPONENT PRE5.

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

- Molecule 7 is a protein called PROTEASOME COMPONENT C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	240	Total	C	N	O	S	0	0	0
			1869	1188	326	351	4			
7	U	240	Total	C	N	O	S	0	0	0
			1869	1188	326	351	4			

- Molecule 8 is a protein called PROTEASOME COMPONENT PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	196	Total	C	N	O	S	0	0	0
			1510	954	250	299	7			
8	V	196	Total	C	N	O	S	0	0	0
			1510	954	250	299	7			

- Molecule 9 is a protein called PROTEASOME COMPONENT PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
9	W	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			

- Molecule 10 is a protein called PROTEASOME COMPONENT PUP3.

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

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

- Molecule 11 is a protein called PROTEASOME COMPONENT C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			
11	Y	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

- Molecule 12 is a protein called PROTEASOME COMPONENT PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	212	Total	C	N	O	S	0	0	0
			1646	1045	282	312	7			
12	Z	212	Total	C	N	O	S	0	0	0
			1646	1045	282	312	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	33	ARG	LYS	engineered mutation	UNP P30656
Z	33	ARG	LYS	engineered mutation	UNP P30656

- Molecule 13 is a protein called PROTEASOME COMPONENT C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
13	a	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 14 is a protein called PROTEASOME COMPONENT PRE4.

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

- Molecule 15 is a protein called PROTEASOME ACTIVATOR PROTEIN PA26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	c	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	d	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	e	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	f	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	g	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	h	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	i	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	j	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	k	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	l	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	m	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	n	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	o	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	p	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	49	VAL	THR	see remark 999	UNP Q9U8G2
c	226	THR	SER	see remark 999	UNP Q9U8G2
d	49	VAL	THR	see remark 999	UNP Q9U8G2
d	226	THR	SER	see remark 999	UNP Q9U8G2
e	49	VAL	THR	see remark 999	UNP Q9U8G2
e	226	THR	SER	see remark 999	UNP Q9U8G2
f	49	VAL	THR	see remark 999	UNP Q9U8G2
f	226	THR	SER	see remark 999	UNP Q9U8G2
g	49	VAL	THR	see remark 999	UNP Q9U8G2
g	226	THR	SER	see remark 999	UNP Q9U8G2
h	49	VAL	THR	see remark 999	UNP Q9U8G2
h	226	THR	SER	see remark 999	UNP Q9U8G2

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Chain	Residue	Modelled	Actual	Comment	Reference
i	49	VAL	THR	see remark 999	UNP Q9U8G2
i	226	THR	SER	see remark 999	UNP Q9U8G2
j	49	VAL	THR	see remark 999	UNP Q9U8G2
j	226	THR	SER	see remark 999	UNP Q9U8G2
k	49	VAL	THR	see remark 999	UNP Q9U8G2
k	226	THR	SER	see remark 999	UNP Q9U8G2
l	49	VAL	THR	see remark 999	UNP Q9U8G2
l	226	THR	SER	see remark 999	UNP Q9U8G2
m	49	VAL	THR	see remark 999	UNP Q9U8G2
m	226	THR	SER	see remark 999	UNP Q9U8G2
n	49	VAL	THR	see remark 999	UNP Q9U8G2
n	226	THR	SER	see remark 999	UNP Q9U8G2
o	49	VAL	THR	see remark 999	UNP Q9U8G2
o	226	THR	SER	see remark 999	UNP Q9U8G2
p	49	VAL	THR	see remark 999	UNP Q9U8G2
p	226	THR	SER	see remark 999	UNP Q9U8G2

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Mg 1 1	0	0
16	H	1	Total Mg 1 1	0	0
16	I	1	Total Mg 1 1	0	0
16	J	2	Total Mg 2 2	0	0
16	L	1	Total Mg 1 1	0	0
16	M	1	Total Mg 1 1	0	0
16	U	1	Total Mg 1 1	0	0
16	V	1	Total Mg 1 1	0	0
16	W	1	Total Mg 1 1	0	0
16	X	2	Total Mg 2 2	0	0
16	Z	1	Total Mg 1 1	0	0

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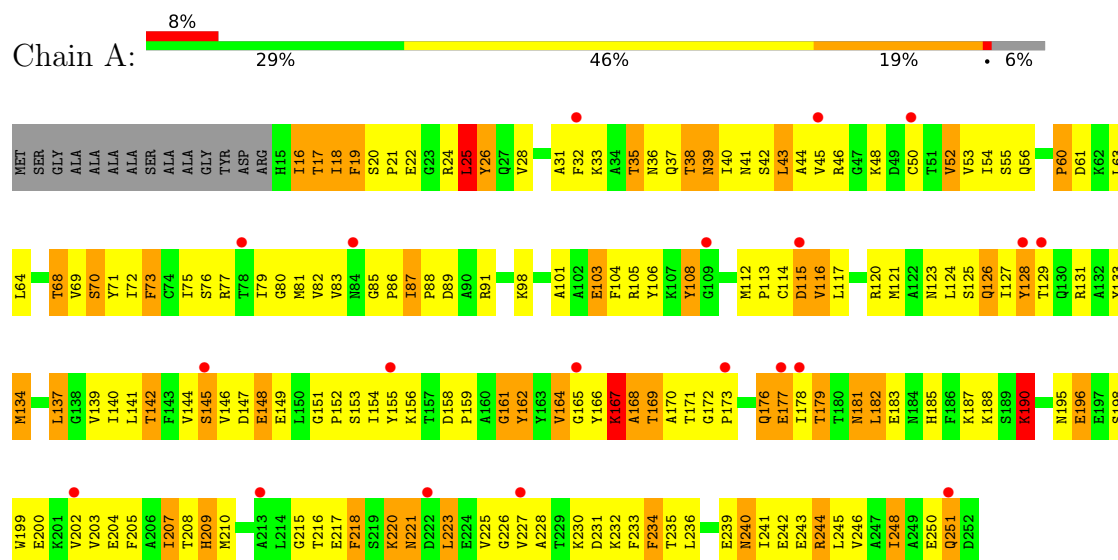
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	a	1	Total	Mg	0	0
			1	1		

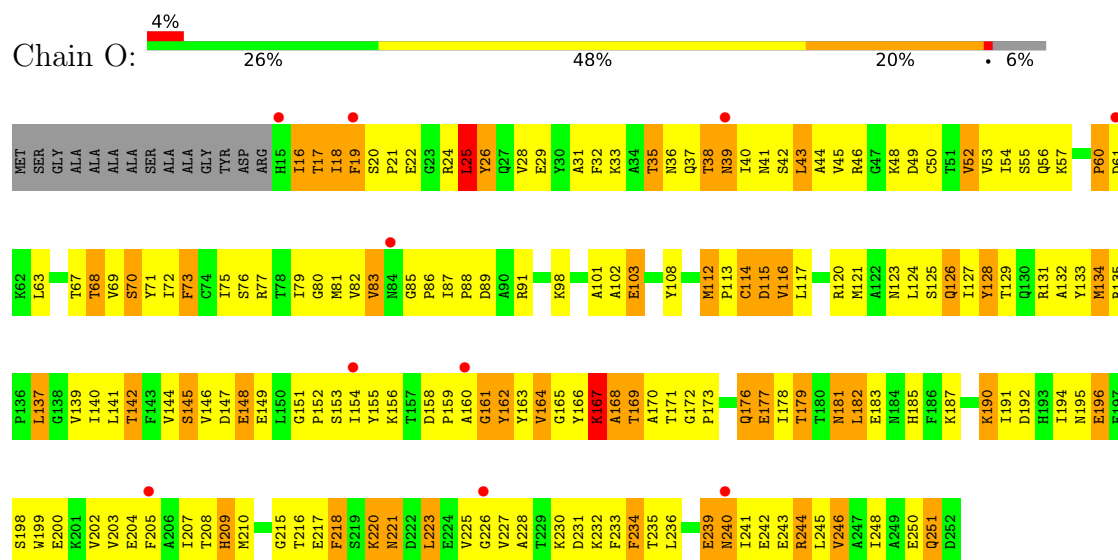
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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 C7-ALPHA

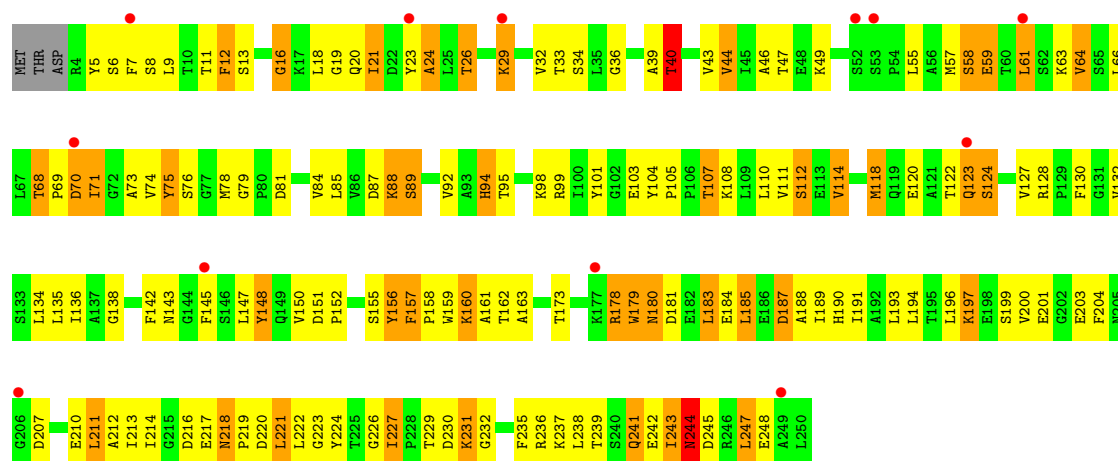


• Molecule 1: PROTEASOME COMPONENT C7-ALPHA

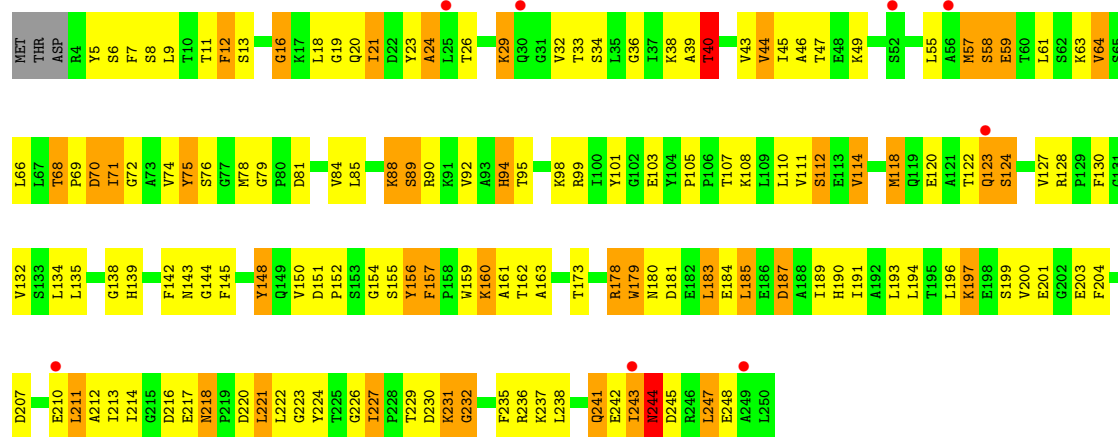


• Molecule 2: PROTEASOME COMPONENT Y7

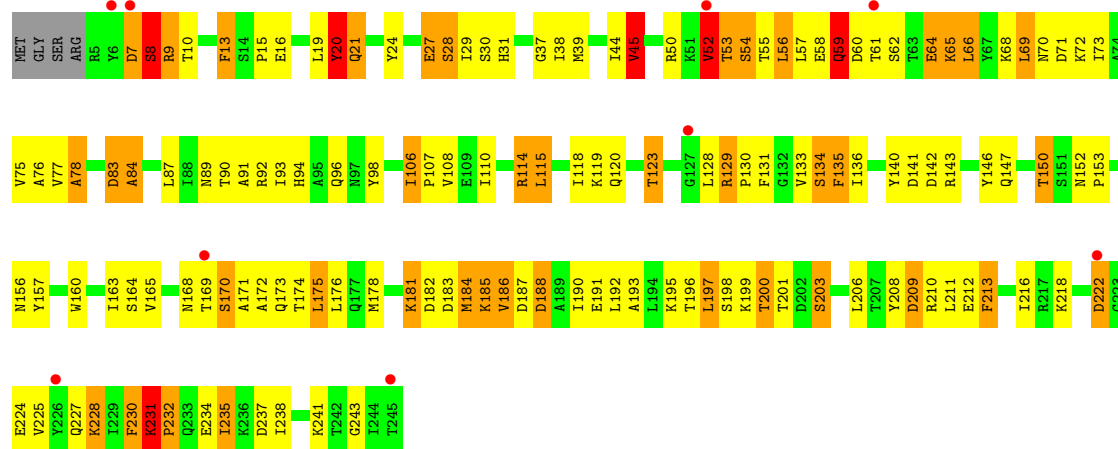




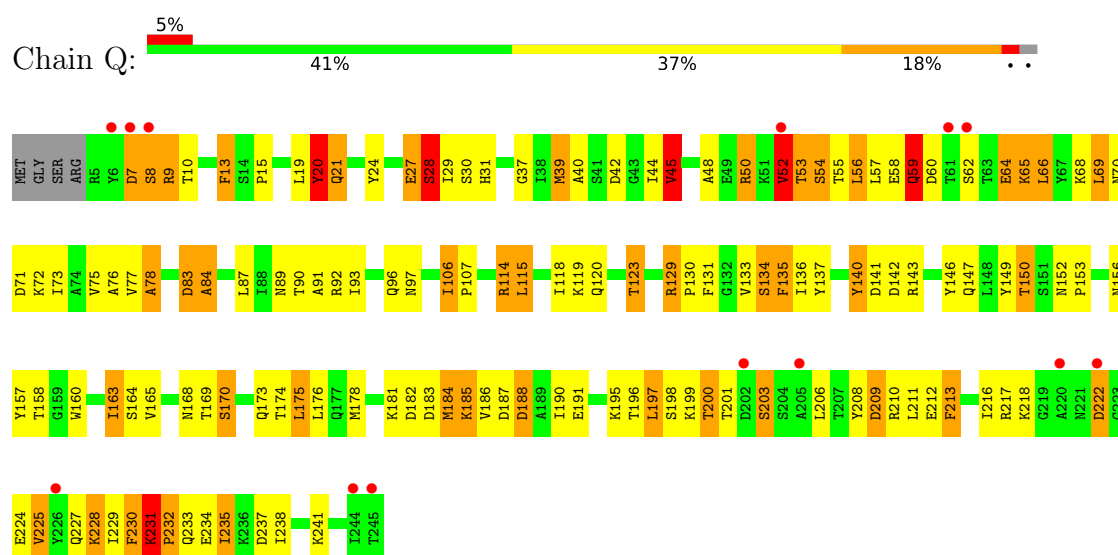
• Molecule 2: PROTEASOME COMPONENT Y7



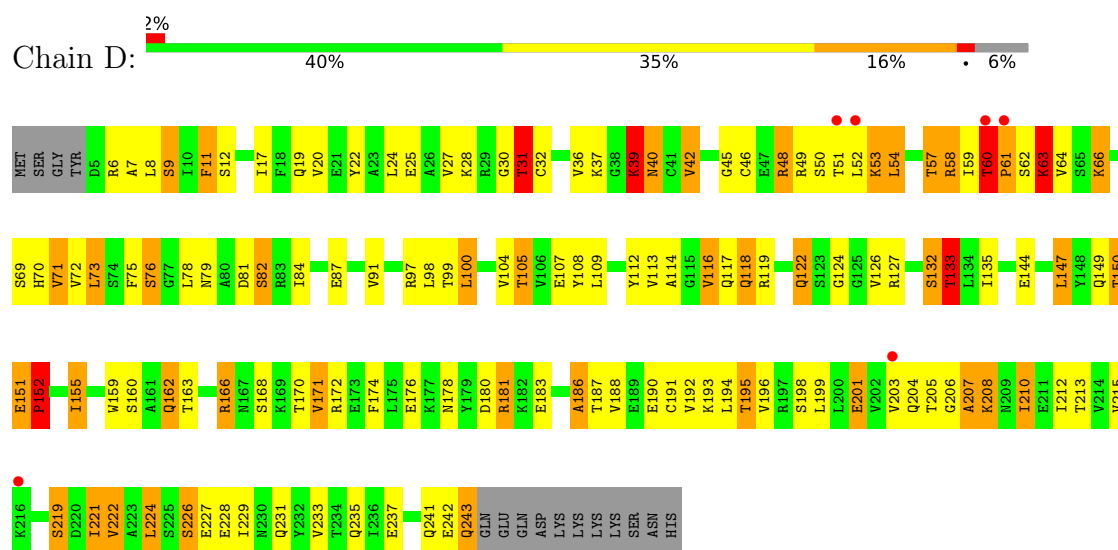
• Molecule 3: PROTEASOME COMPONENT Y13



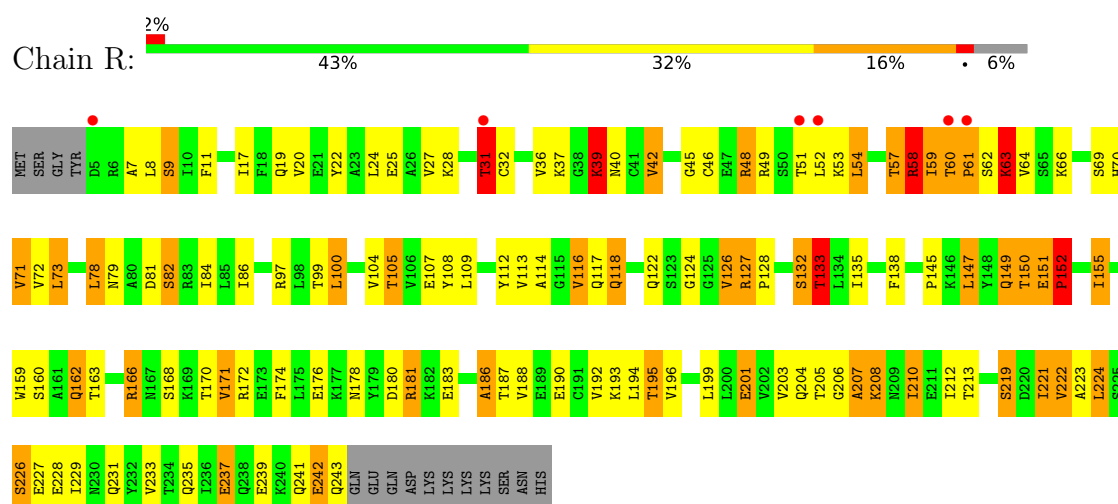
• Molecule 3: PROTEASOME COMPONENT Y13



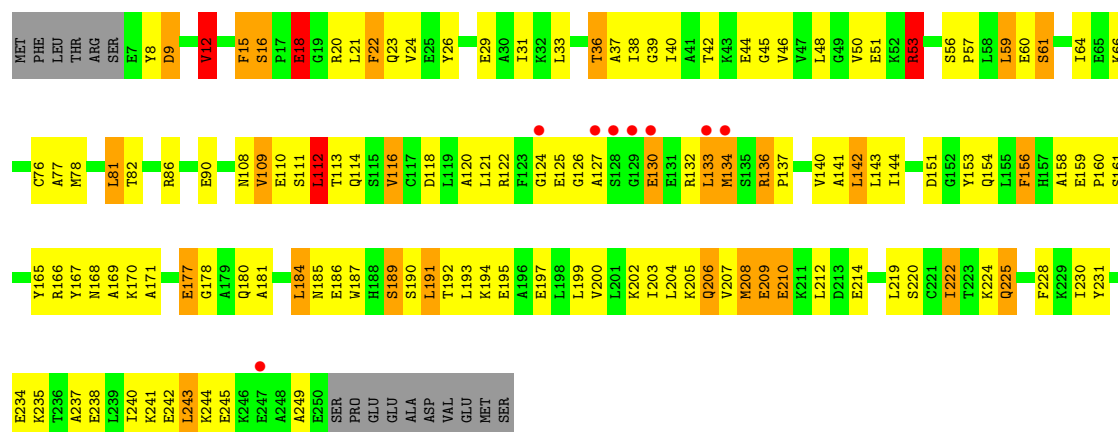
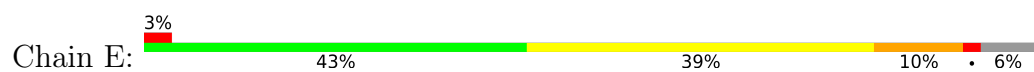
• Molecule 4: PROTEASOME COMPONENT PRE6



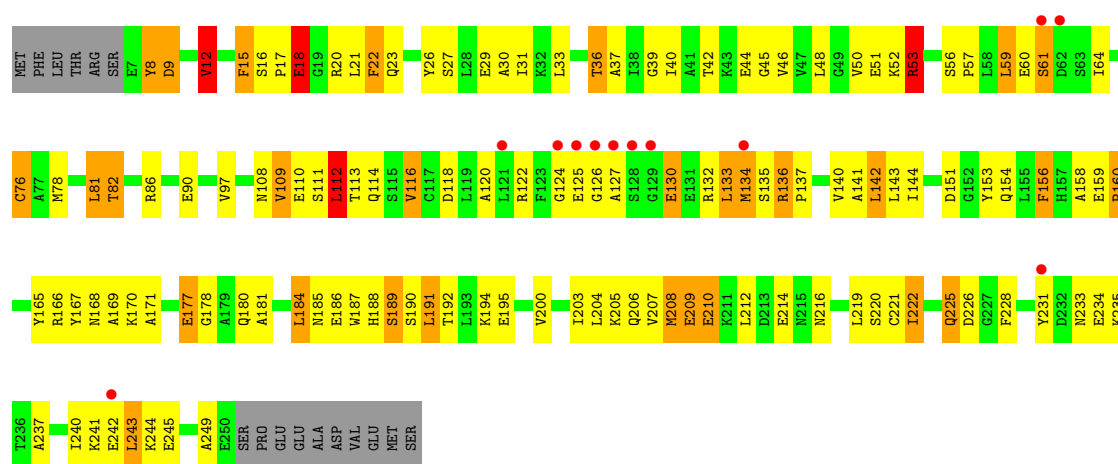
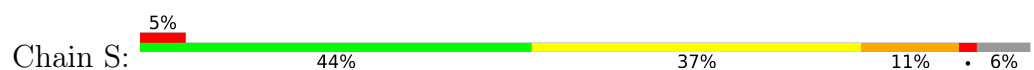
• Molecule 4: PROTEASOME COMPONENT PRE6



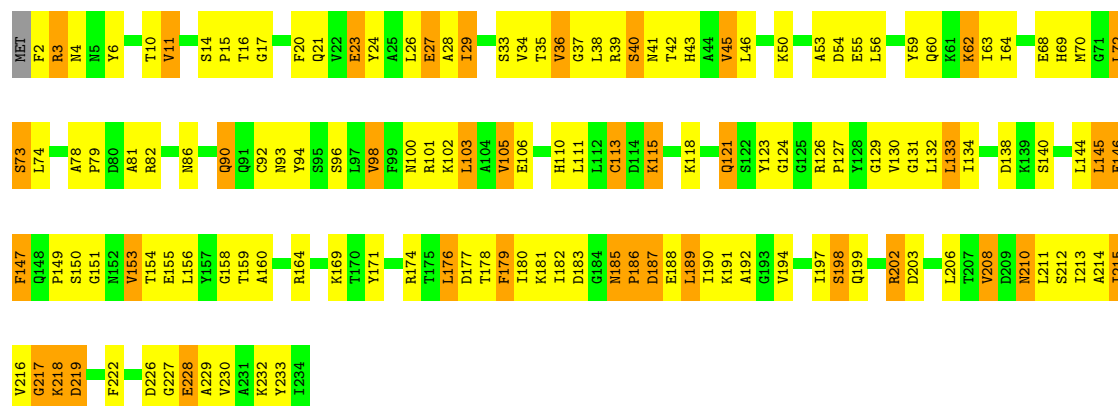
• Molecule 5: PROTEASOME COMPONENT PUP2



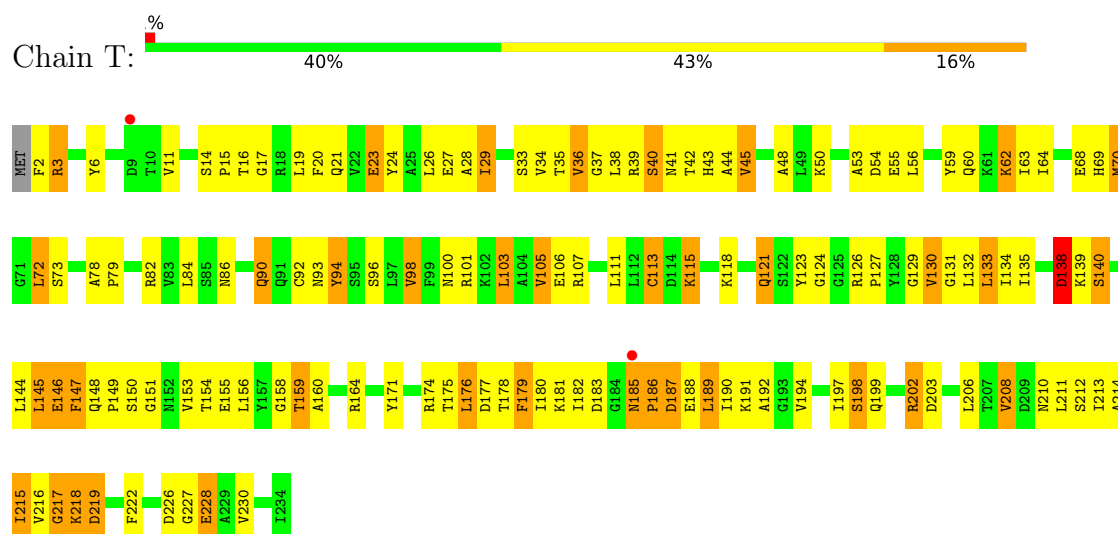
• Molecule 5: PROTEASOME COMPONENT PUP2



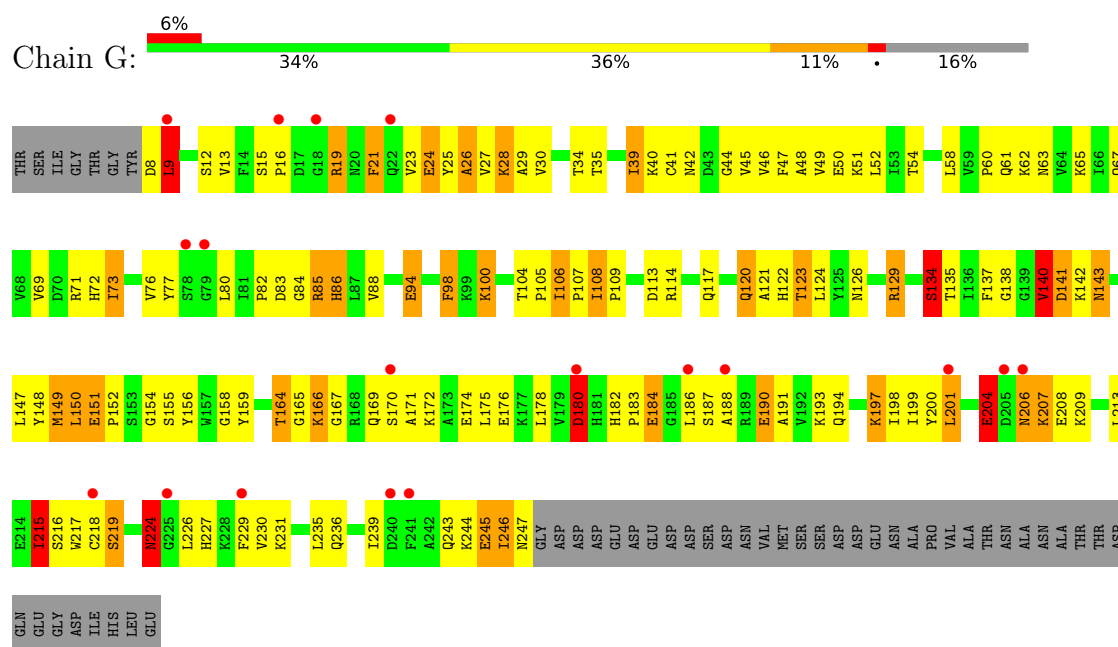
• Molecule 6: PROTEASOME COMPONENT PRE5



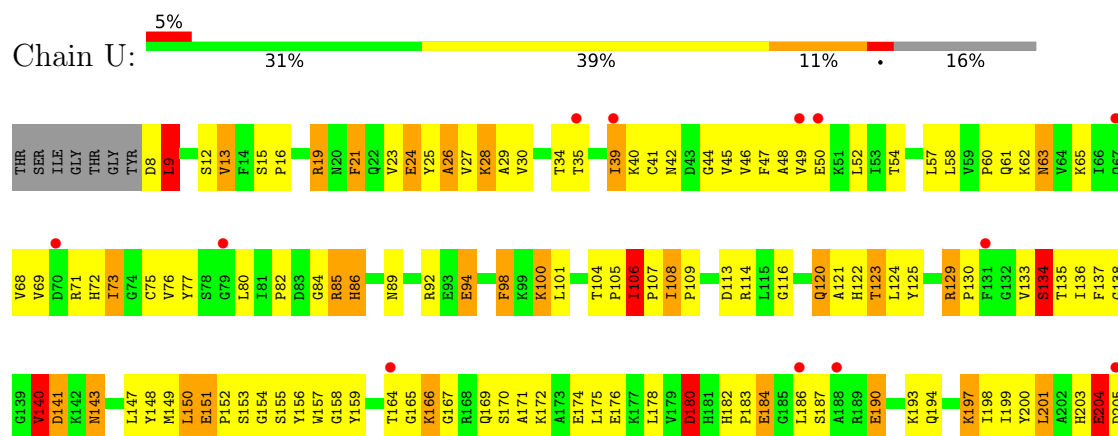
• Molecule 6: PROTEASOME COMPONENT PRE5



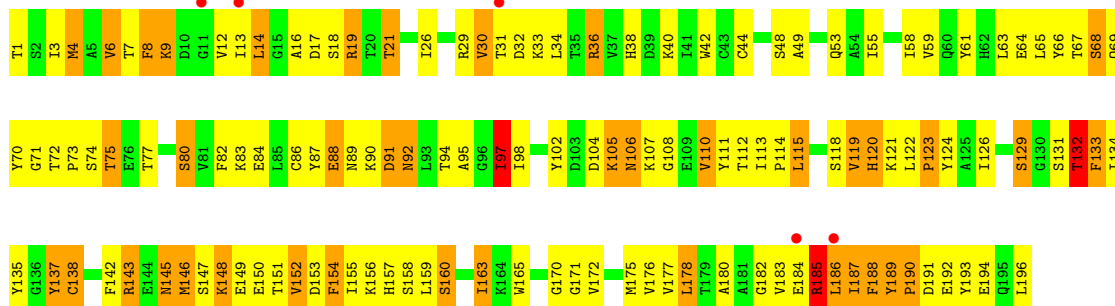
• Molecule 7: PROTEASOME COMPONENT C1



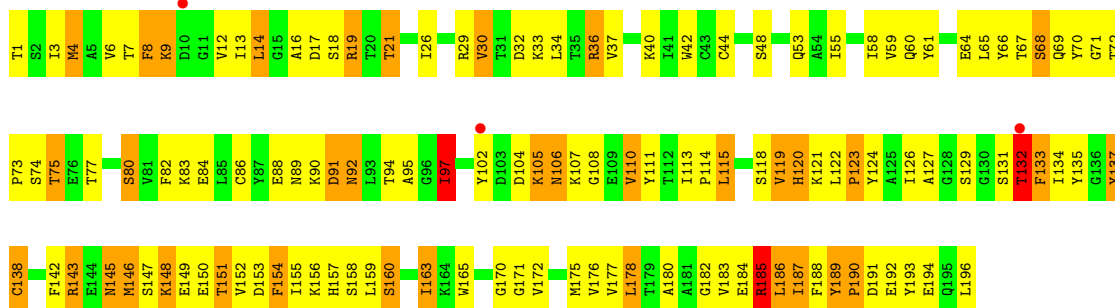
• Molecule 7: PROTEASOME COMPONENT C1



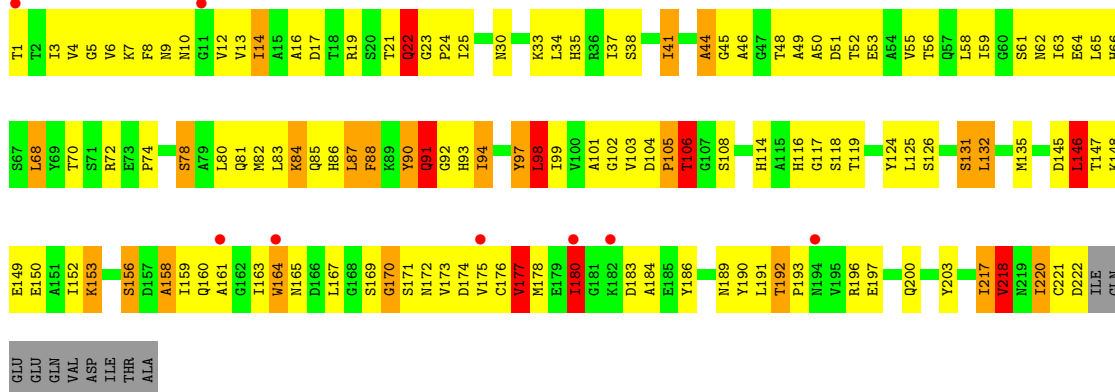
- Molecule 8: PROTEASOME COMPONENT PRE3



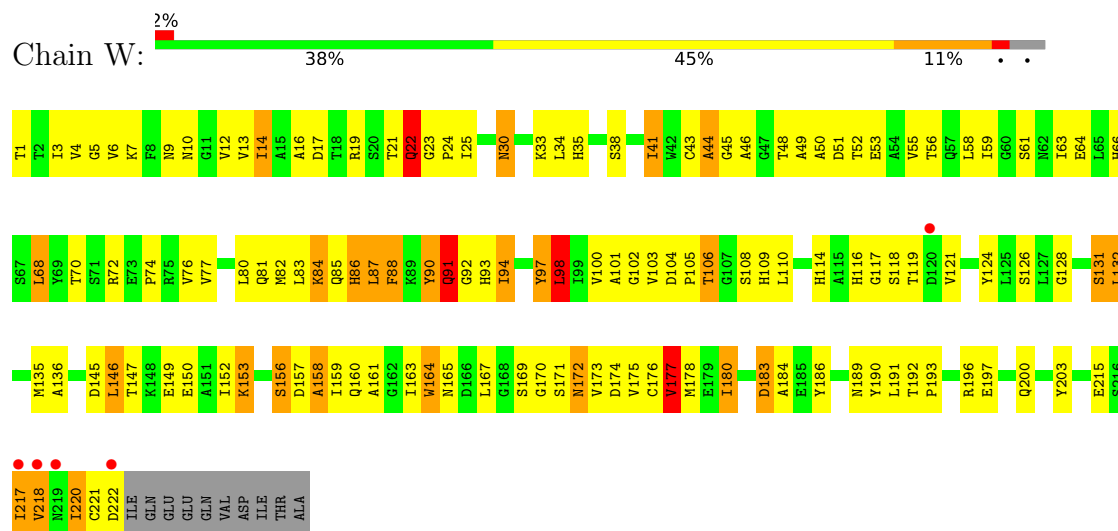
- Molecule 8: PROTEASOME COMPONENT PRE3



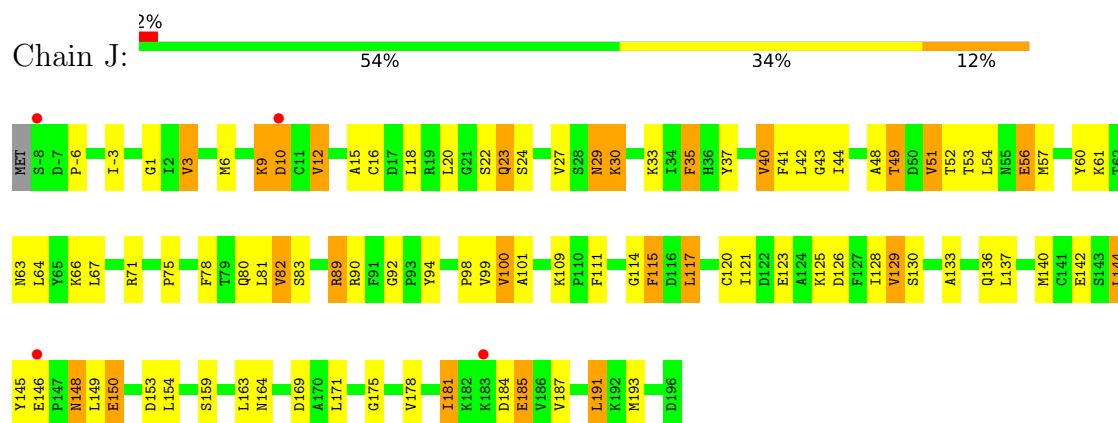
- Molecule 9: PROTEASOME COMPONENT PUP1



- Molecule 9: PROTEASOME COMPONENT PUP1



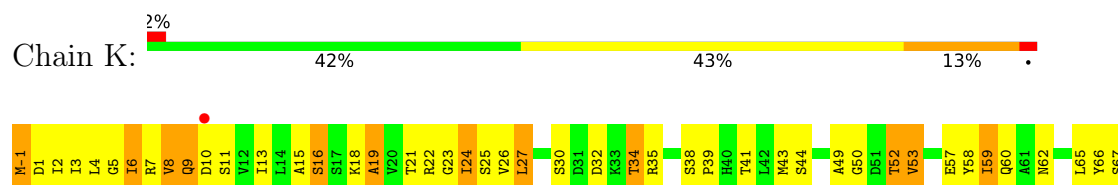
- Molecule 10: PROTEASOME COMPONENT PUP3

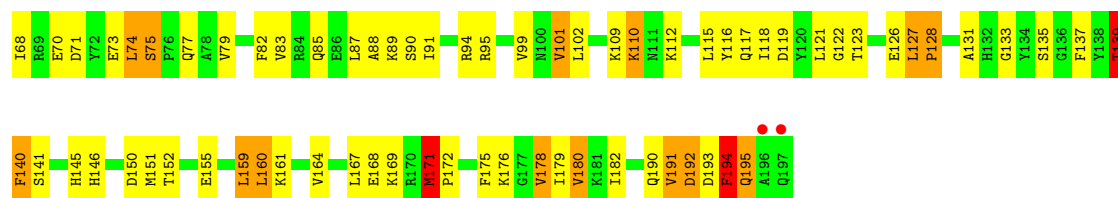


- Molecule 10: PROTEASOME COMPONENT PUP3

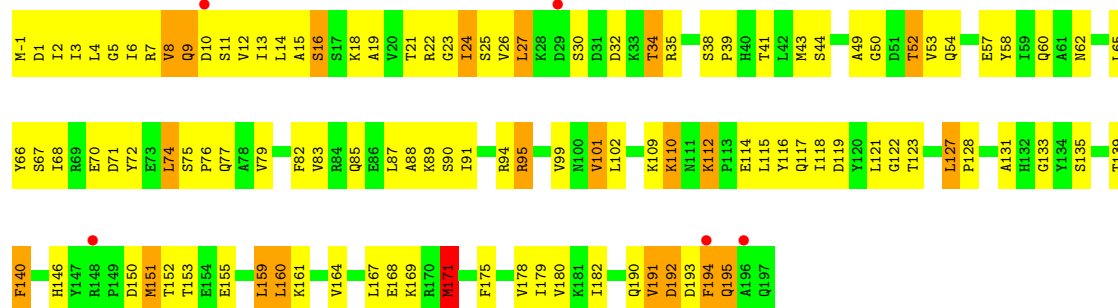
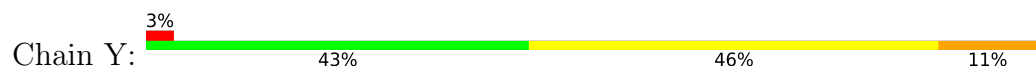


- Molecule 11: PROTEASOME COMPONENT C11

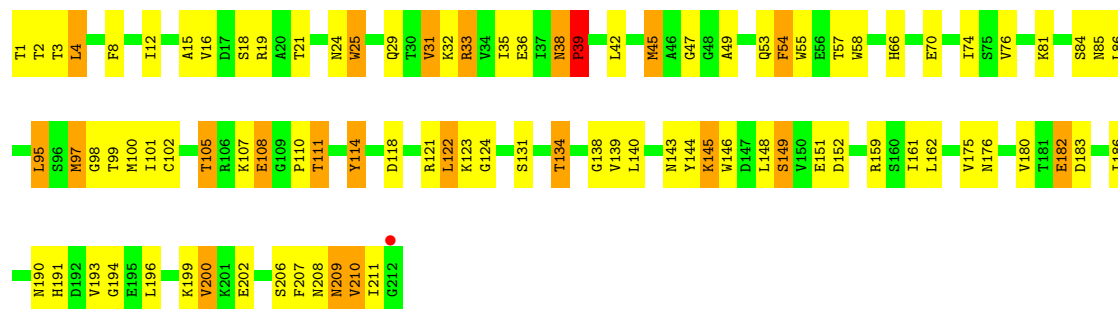




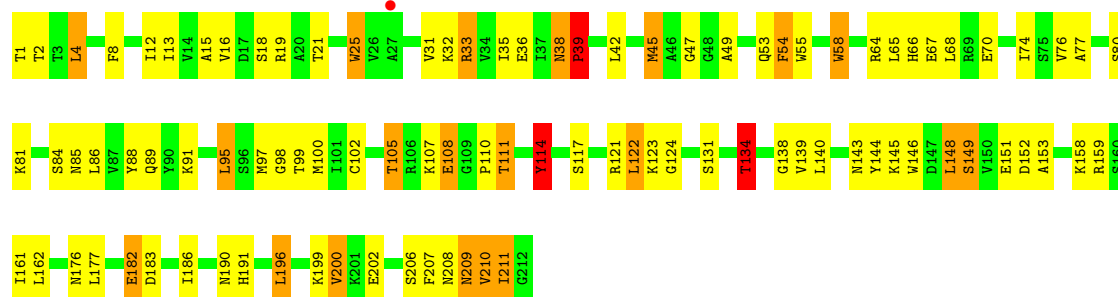
• Molecule 11: PROTEASOME COMPONENT C11



• Molecule 12: PROTEASOME COMPONENT PRE2

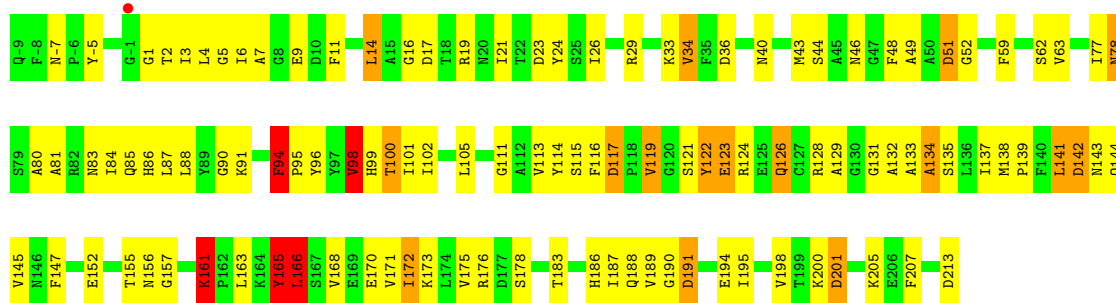


• Molecule 12: PROTEASOME COMPONENT PRE2



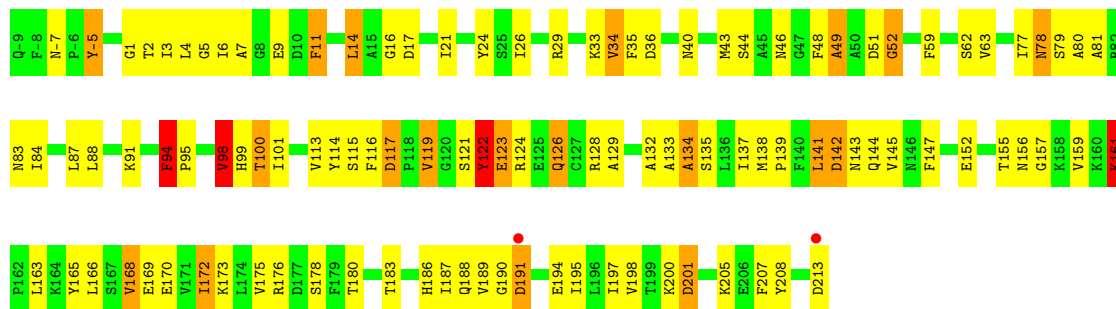
• Molecule 13: PROTEASOME COMPONENT C5

Chain M: 



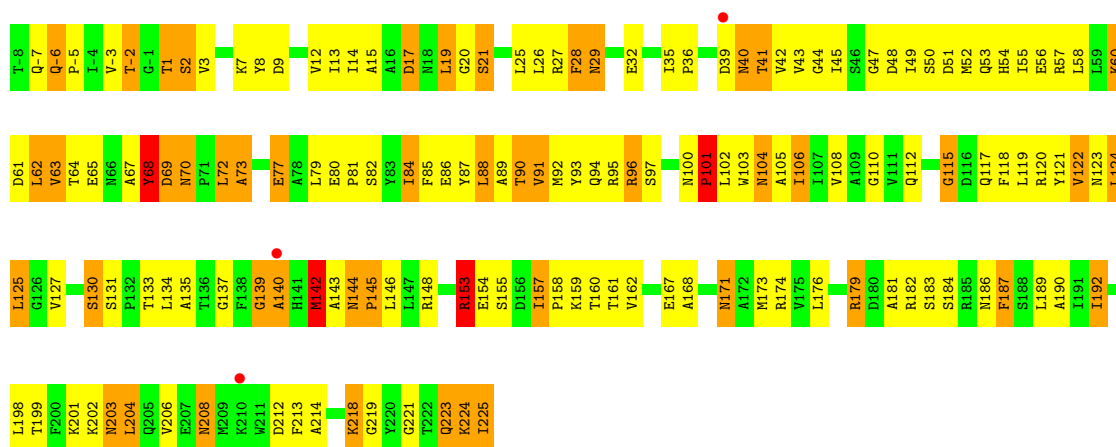
• Molecule 13: PROTEASOME COMPONENT C5

Chain a: 



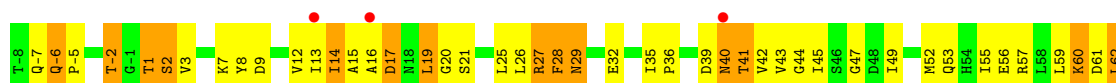
• Molecule 14: PROTEASOME COMPONENT PRE4

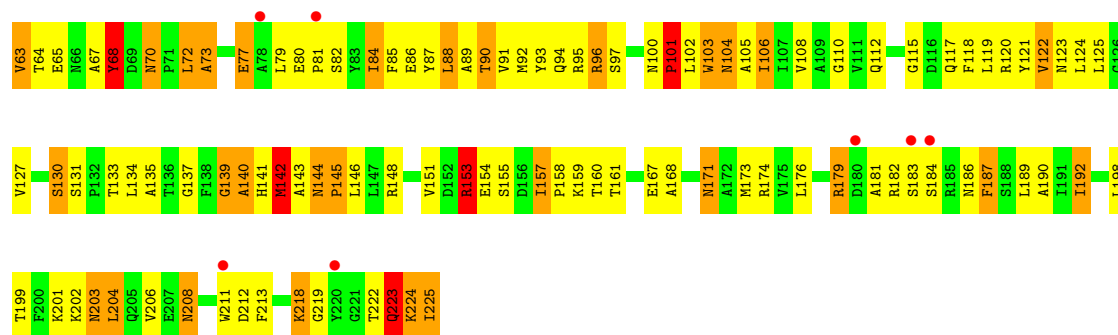
Chain N: 



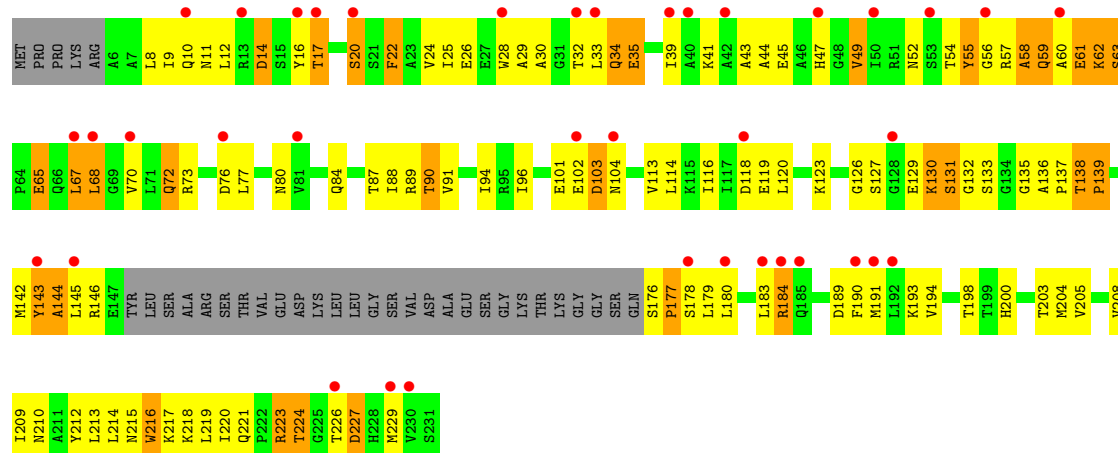
• Molecule 14: PROTEASOME COMPONENT PRE4

Chain b: 

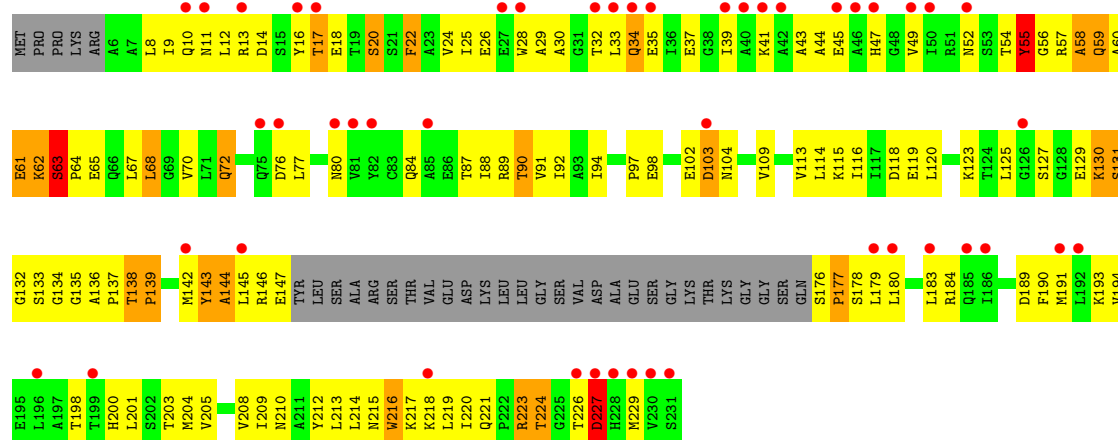




• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

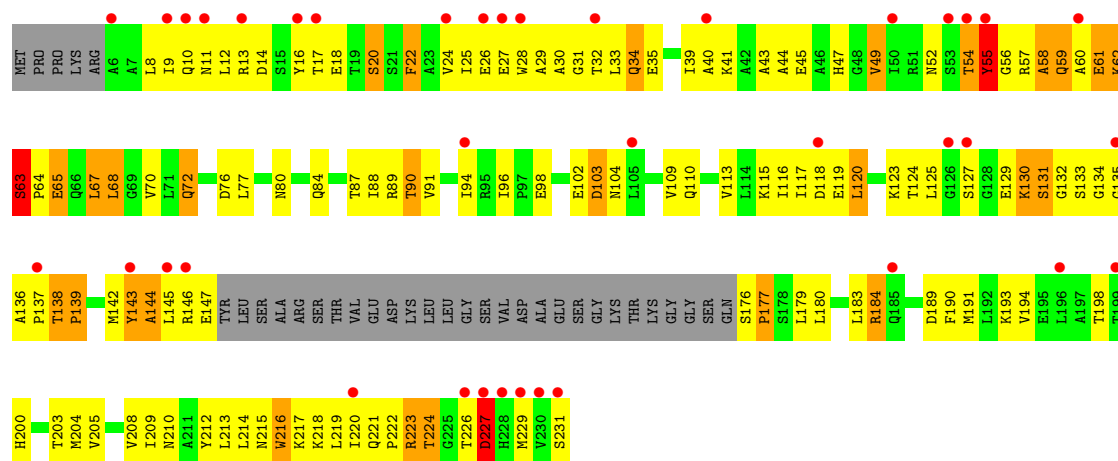


• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

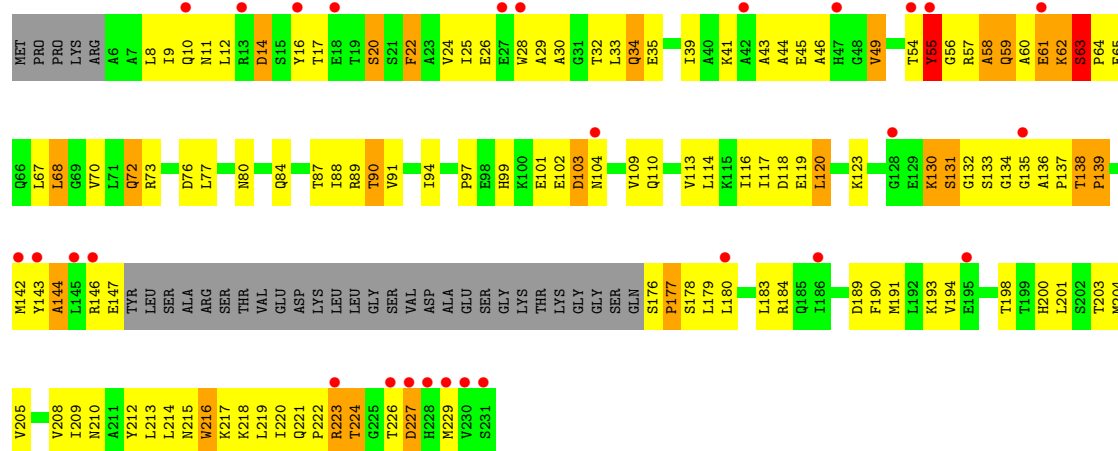


• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

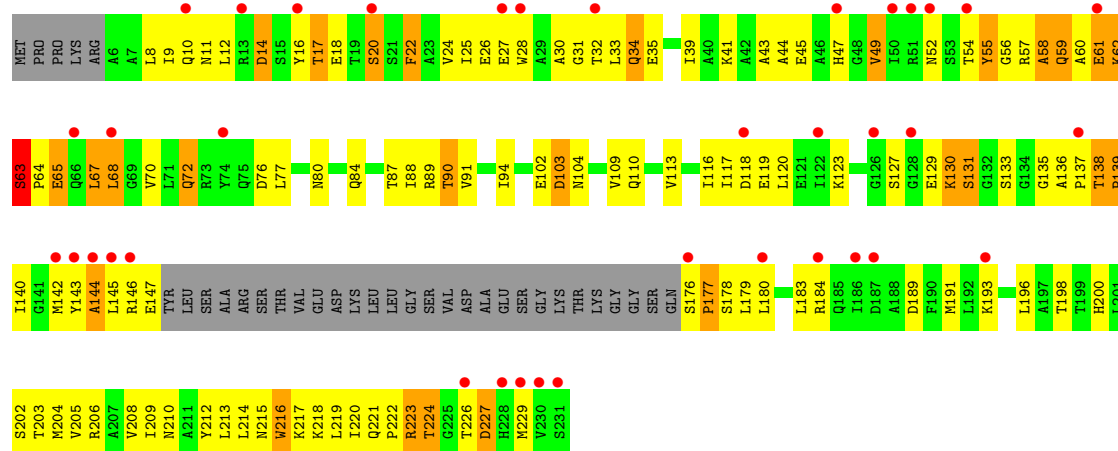




• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26



• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26



[illegible][illegible]

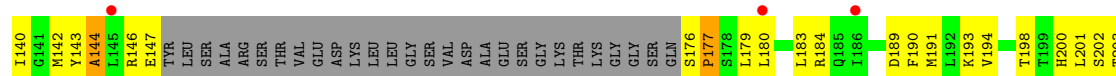
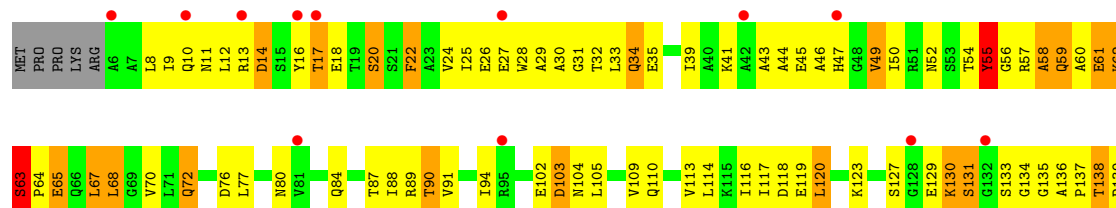
Chain j:

10% 32% 43% 10% 14%

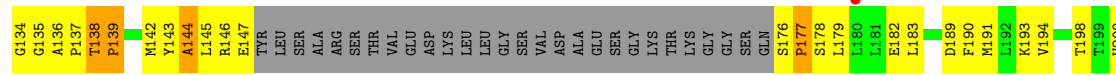
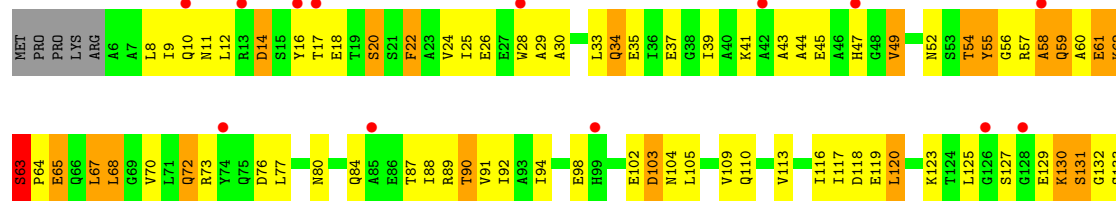
State	Value
NET	10%
PRO	32%
PRO	32%
ARG	32%
ARG	32%
A6	43%
A7	43%
L8	43%
L9	43%
Q10	43%
N11	43%
L12	43%
R13	43%
D14	43%
S15	43%
Y16	43%
T17	43%
E18	43%
T19	43%
S20	43%
S21	43%
F22	43%
A23	43%
V24	43%
I25	43%
E26	43%
E27	43%
W28	43%
A29	43%
A30	43%
G31	43%
T32	43%
L33	43%
Q34	43%
E35	43%
I39	10%
A40	10%
K41	10%
A42	10%
A43	10%
A44	10%
E45	10%
A46	10%
H47	10%
G48	10%
V49	10%
I50	14%
R51	14%
N52	14%
S53	14%
T54	14%
Y55	14%
G56	14%
R57	14%
A58	14%
Q59	14%
A60	14%
E61	14%
V62	14%
S63	10%
P64	10%
E65	10%
Q66	10%
L67	10%
L68	10%
G69	10%
V70	10%
L71	10%
R72	10%
R73	10%
D76	10%
L77	10%
N80	10%
Q84	10%
T87	10%
I88	10%
R89	10%
T90	10%
V91	10%
T94	10%
H99	10%
E102	10%
D103	10%
N104	10%
L105	10%
V109	10%
V113	10%
L114	10%
K115	10%
L116	10%
I117	10%
D118	10%
E119	10%
L120	10%
K123	10%
T124	10%
S127	10%
G128	10%
E129	10%
L130	10%
S131	10%
G132	10%
S133	10%
G134	10%
G135	10%
A136	10%
P137	10%
T138	10%
P139	10%
I140	10%
G141	10%
M142	10%
Y143	10%
A144	10%
L145	10%
R146	10%
E147	10%
T148	10%
LEU	10%
SER	10%
ALA	10%
ARG	10%
SER	10%
THR	10%
VAL	10%
GLU	10%
ASP	10%
LYS	10%
LEU	10%
LEU	10%
R89	10%
GLY	10%
SER	10%
VAL	10%
ASP	10%
ALA	10%
GLU	10%
SER	10%
GLY	10%
LYS	10%
THR	10%
LYS	10%
GLY	10%
SER	10%
GLN	10%
S176	10%
P177	10%
L178	10%
L179	10%
L180	10%
L183	10%
R184	10%
Q185	10%
L186	10%
D189	10%
F190	10%
M191	10%
L192	10%
K193	10%
V194	10%
E195	10%
T198	10%
L199	10%
H200	10%
T201	10%



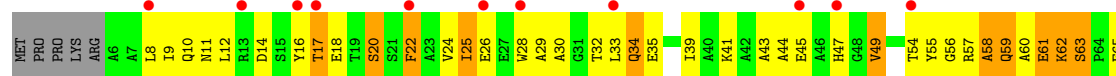
● Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

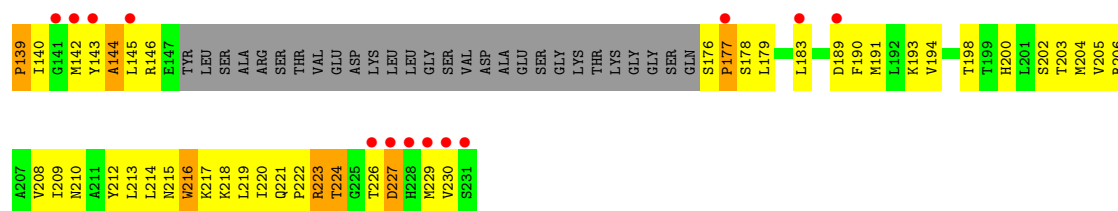


● Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

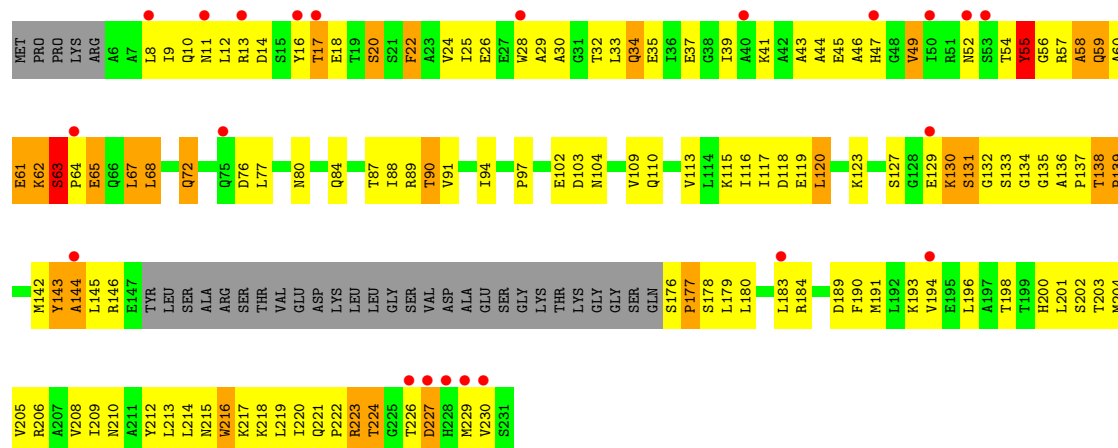


● Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

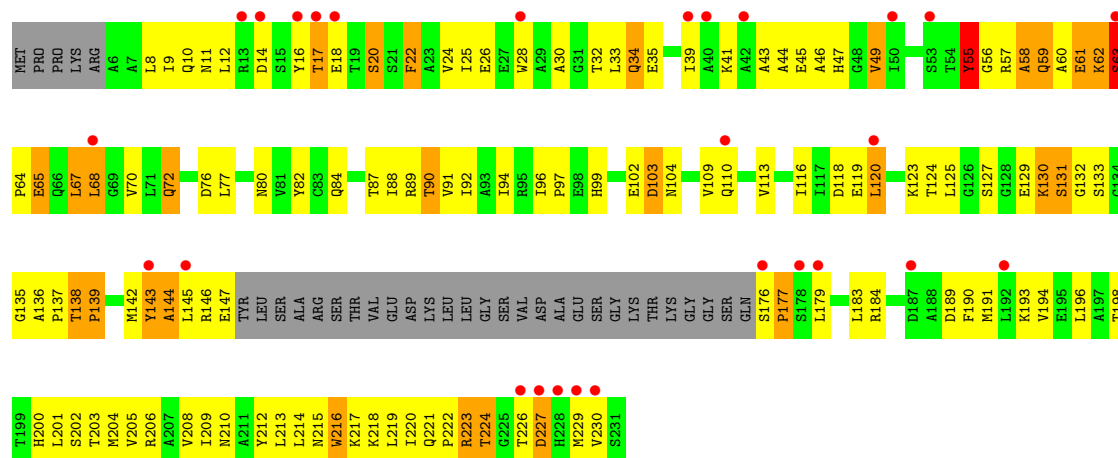




• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

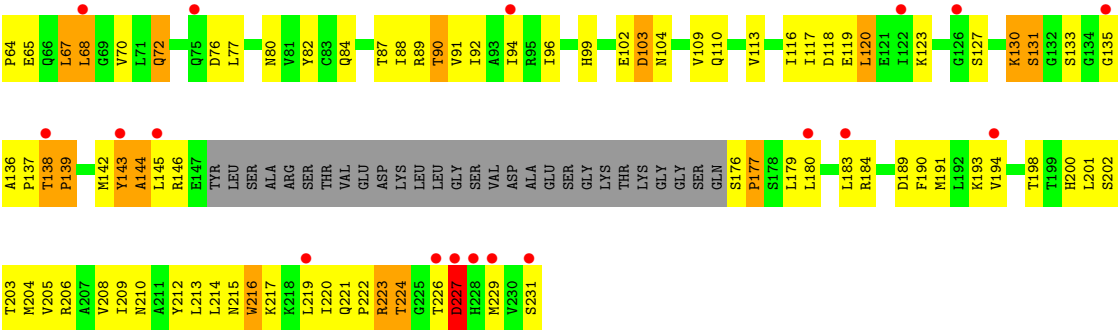


• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26



• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	192.96Å 232.13Å 296.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 50.00 – 3.22	Depositor EDS
% Data completeness (in resolution range)	86.6 (50.00-3.20) 88.1 (50.00-3.22)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.25Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.255 , 0.325 0.267 , 0.330	Depositor DCC
R_{free} test set	1028 reflections (0.54%)	wwPDB-VP
Wilson B-factor (Å ²)	71.3	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 85.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	70622	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.82	0/1918	1.36	28/2597 (1.1%)
1	O	0.76	1/1918 (0.1%)	1.34	31/2597 (1.2%)
2	B	0.80	0/1903	1.39	39/2578 (1.5%)
2	P	0.78	0/1903	1.38	38/2578 (1.5%)
3	C	0.82	1/1897 (0.1%)	1.29	25/2569 (1.0%)
3	Q	0.85	3/1897 (0.2%)	1.28	22/2569 (0.9%)
4	D	0.80	3/1890 (0.2%)	1.37	36/2560 (1.4%)
4	R	0.79	2/1890 (0.1%)	1.39	32/2560 (1.2%)
5	E	0.85	1/1896 (0.1%)	1.26	18/2555 (0.7%)
5	S	0.82	0/1896	1.25	20/2555 (0.8%)
6	F	0.73	0/1823	1.21	18/2463 (0.7%)
6	T	0.73	0/1823	1.23	20/2463 (0.8%)
7	G	0.72	0/1908	1.22	21/2576 (0.8%)
7	U	0.71	0/1908	1.25	24/2576 (0.9%)
8	H	0.79	0/1539	1.28	21/2084 (1.0%)
8	V	0.75	0/1539	1.29	22/2084 (1.1%)
9	I	0.82	0/1715	1.18	16/2326 (0.7%)
9	W	0.79	0/1715	1.17	15/2326 (0.6%)
10	J	0.78	0/1611	1.27	21/2174 (1.0%)
10	X	0.79	0/1611	1.27	20/2174 (0.9%)
11	K	0.88	1/1613 (0.1%)	1.24	23/2173 (1.1%)
11	Y	0.81	0/1613	1.25	23/2173 (1.1%)
12	L	0.82	1/1683 (0.1%)	1.25	18/2277 (0.8%)
12	Z	0.79	0/1683	1.26	16/2277 (0.7%)
13	M	0.78	0/1795	1.28	24/2420 (1.0%)
13	a	0.78	1/1795 (0.1%)	1.26	21/2420 (0.9%)
14	N	0.79	0/1855	1.27	20/2514 (0.8%)
14	b	0.80	0/1855	1.26	18/2514 (0.7%)
15	c	0.79	1/1551 (0.1%)	1.28	18/2099 (0.9%)
15	d	0.79	1/1551 (0.1%)	1.27	15/2099 (0.7%)
15	e	0.78	1/1551 (0.1%)	1.28	21/2099 (1.0%)
15	f	0.78	1/1551 (0.1%)	1.27	17/2099 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	g	0.84	1/1551 (0.1%)	1.28	16/2099 (0.8%)
15	h	0.78	0/1551	1.27	18/2099 (0.9%)
15	i	0.78	1/1551 (0.1%)	1.28	15/2099 (0.7%)
15	j	0.75	1/1551 (0.1%)	1.30	12/2099 (0.6%)
15	k	0.75	1/1551 (0.1%)	1.30	18/2099 (0.9%)
15	l	0.73	0/1551	1.28	20/2099 (1.0%)
15	m	0.74	1/1551 (0.1%)	1.27	18/2099 (0.9%)
15	n	0.74	1/1551 (0.1%)	1.28	20/2099 (1.0%)
15	o	0.75	1/1551 (0.1%)	1.29	19/2099 (0.9%)
15	p	0.76	1/1551 (0.1%)	1.29	18/2099 (0.9%)
All	All	0.78	26/71806 (0.0%)	1.28	895/97118 (0.9%)

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
3	C	0	1
3	Q	0	1
9	I	0	1
9	W	0	1
13	M	0	1
13	a	0	2
14	N	0	1
14	b	0	1
All	All	0	9

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	g	32	THR	CA-CB	8.00	1.65	1.53
15	j	32	THR	CA-CB	7.50	1.64	1.53
15	c	32	THR	CA-CB	7.25	1.64	1.53
4	R	51	THR	CA-C	7.24	1.59	1.52
3	Q	52	VAL	CA-CB	7.15	1.64	1.54

The worst 5 of 895 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	8	LEU	N-CA-C	11.87	128.21	110.64
4	D	8	LEU	N-CA-C	11.82	128.14	110.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	j	144	ALA	N-CA-C	-11.02	98.14	112.24
15	g	144	ALA	N-CA-C	-10.87	98.32	112.24
15	e	144	ALA	N-CA-C	-10.65	98.61	112.24

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	20	TYR	Sidechain
9	I	190	TYR	Sidechain
13	M	165	TYR	Sidechain
14	N	68	TYR	Sidechain
3	Q	20	TYR	Sidechain

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	A	1881	0	1876	195	0
1	O	1881	0	1876	199	0
2	B	1868	0	1866	126	0
2	P	1868	0	1866	123	0
3	C	1868	0	1860	119	0
3	Q	1868	0	1860	120	0
4	D	1862	0	1866	89	0
4	R	1862	0	1866	86	0
5	E	1871	0	1840	100	0
5	S	1871	0	1840	93	0
6	F	1795	0	1797	119	0
6	T	1795	0	1797	116	0
7	G	1869	0	1864	143	0
7	U	1869	0	1864	148	0
8	H	1510	0	1476	138	0
8	V	1510	0	1476	128	0
9	I	1684	0	1688	98	0
9	W	1684	0	1688	111	0
10	J	1581	0	1574	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	X	1581	0	1574	76	0
11	K	1585	0	1590	85	0
11	Y	1585	0	1590	80	0
12	L	1646	0	1595	55	0
12	Z	1646	0	1595	74	0
13	M	1757	0	1711	78	0
13	a	1757	0	1710	76	0
14	N	1824	0	1832	136	0
14	b	1824	0	1832	135	0
15	c	1529	0	1545	129	0
15	d	1529	0	1545	133	0
15	e	1529	0	1545	136	0
15	f	1529	0	1545	126	0
15	g	1529	0	1545	134	0
15	h	1529	0	1545	135	0
15	i	1529	0	1545	135	0
15	j	1529	0	1545	130	0
15	k	1529	0	1545	136	0
15	l	1529	0	1545	138	0
15	m	1529	0	1545	133	0
15	n	1529	0	1545	138	0
15	o	1529	0	1545	134	0
15	p	1529	0	1545	132	0
16	G	1	0	0	0	0
16	H	1	0	0	0	0
16	I	1	0	0	0	0
16	J	2	0	0	0	0
16	L	1	0	0	0	0
16	M	1	0	0	0	0
16	U	1	0	0	0	0
16	V	1	0	0	0	0
16	W	1	0	0	0	0
16	X	2	0	0	0	0
16	Z	1	0	0	0	0
16	a	1	0	0	0	0
All	All	70622	0	70499	4544	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 32.

The worst 5 of 4544 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)
2:B:46:ALA:HB2	2:B:211:LEU:HD12	1.34	1.10
1:A:38:THR:HA	15:e:231:SER:HB3	1.34	1.06
15:p:25:ILE:HA	15:p:28:TRP:HD1	1.20	1.06
15:m:25:ILE:HA	15:m:28:TRP:HD1	1.20	1.05
15:k:176:SER:HB3	15:l:142:MET:HB2	1.36	1.05

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	236/252 (94%)	172 (73%)	44 (19%)	20 (8%)	0	3
1	O	236/252 (94%)	174 (74%)	42 (18%)	20 (8%)	0	3
2	B	245/250 (98%)	170 (69%)	56 (23%)	19 (8%)	1	5
2	P	245/250 (98%)	174 (71%)	53 (22%)	18 (7%)	1	6
3	C	239/245 (98%)	191 (80%)	29 (12%)	19 (8%)	1	5
3	Q	239/245 (98%)	187 (78%)	32 (13%)	20 (8%)	0	4
4	D	237/254 (93%)	186 (78%)	36 (15%)	15 (6%)	1	8
4	R	237/254 (93%)	186 (78%)	36 (15%)	15 (6%)	1	8
5	E	242/260 (93%)	192 (79%)	36 (15%)	14 (6%)	1	10
5	S	242/260 (93%)	192 (79%)	35 (14%)	15 (6%)	1	9
6	F	231/234 (99%)	189 (82%)	36 (16%)	6 (3%)	4	26
6	T	231/234 (99%)	190 (82%)	32 (14%)	9 (4%)	2	18
7	G	238/287 (83%)	193 (81%)	37 (16%)	8 (3%)	3	20
7	U	238/287 (83%)	194 (82%)	34 (14%)	10 (4%)	2	16
8	H	194/196 (99%)	148 (76%)	30 (16%)	16 (8%)	0	4
8	V	194/196 (99%)	147 (76%)	34 (18%)	13 (7%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	220/232 (95%)	178 (81%)	27 (12%)	15 (7%)	1	7
9	W	220/232 (95%)	176 (80%)	31 (14%)	13 (6%)	1	10
10	J	202/205 (98%)	165 (82%)	33 (16%)	4 (2%)	6	31
10	X	202/205 (98%)	168 (83%)	30 (15%)	4 (2%)	6	31
11	K	196/198 (99%)	163 (83%)	24 (12%)	9 (5%)	2	15
11	Y	196/198 (99%)	160 (82%)	28 (14%)	8 (4%)	2	17
12	L	210/212 (99%)	180 (86%)	27 (13%)	3 (1%)	9	39
12	Z	210/212 (99%)	178 (85%)	29 (14%)	3 (1%)	9	39
13	M	220/222 (99%)	188 (86%)	24 (11%)	8 (4%)	2	19
13	a	220/222 (99%)	186 (84%)	25 (11%)	9 (4%)	2	17
14	N	231/233 (99%)	169 (73%)	43 (19%)	19 (8%)	0	4
14	b	231/233 (99%)	170 (74%)	40 (17%)	21 (9%)	0	3
15	c	194/231 (84%)	162 (84%)	22 (11%)	10 (5%)	1	12
15	d	194/231 (84%)	162 (84%)	21 (11%)	11 (6%)	1	11
15	e	194/231 (84%)	161 (83%)	22 (11%)	11 (6%)	1	11
15	f	194/231 (84%)	161 (83%)	23 (12%)	10 (5%)	1	12
15	g	194/231 (84%)	161 (83%)	23 (12%)	10 (5%)	1	12
15	h	194/231 (84%)	162 (84%)	22 (11%)	10 (5%)	1	12
15	i	194/231 (84%)	162 (84%)	22 (11%)	10 (5%)	1	12
15	j	194/231 (84%)	162 (84%)	23 (12%)	9 (5%)	2	15
15	k	194/231 (84%)	160 (82%)	24 (12%)	10 (5%)	1	12
15	l	194/231 (84%)	159 (82%)	25 (13%)	10 (5%)	1	12
15	m	194/231 (84%)	160 (82%)	24 (12%)	10 (5%)	1	12
15	n	194/231 (84%)	161 (83%)	23 (12%)	10 (5%)	1	12
15	o	194/231 (84%)	159 (82%)	25 (13%)	10 (5%)	1	12
15	p	194/231 (84%)	163 (84%)	20 (10%)	11 (6%)	1	11
All	All	8998/9794 (92%)	7221 (80%)	1282 (14%)	495 (6%)	1	11

5 of 495 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	19	PHE

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Mol	Chain	Res	Type
1	A	60	PRO
1	A	115	ASP
1	A	221	ASN

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	204/210 (97%)	174 (85%)	30 (15%)	3	16
1	O	204/210 (97%)	174 (85%)	30 (15%)	3	16
2	B	200/209 (96%)	169 (84%)	31 (16%)	2	14
2	P	200/209 (96%)	168 (84%)	32 (16%)	2	13
3	C	198/204 (97%)	166 (84%)	32 (16%)	2	12
3	Q	198/204 (97%)	163 (82%)	35 (18%)	2	10
4	D	209/226 (92%)	167 (80%)	42 (20%)	1	7
4	R	209/226 (92%)	167 (80%)	42 (20%)	1	7
5	E	198/215 (92%)	166 (84%)	32 (16%)	2	12
5	S	198/215 (92%)	166 (84%)	32 (16%)	2	12
6	F	192/193 (100%)	161 (84%)	31 (16%)	2	13
6	T	192/193 (100%)	161 (84%)	31 (16%)	2	13
7	G	199/238 (84%)	164 (82%)	35 (18%)	2	10
7	U	199/238 (84%)	162 (81%)	37 (19%)	1	9
8	H	161/162 (99%)	129 (80%)	32 (20%)	1	7
8	V	161/162 (99%)	130 (81%)	31 (19%)	1	8
9	I	181/190 (95%)	151 (83%)	30 (17%)	2	11
9	W	181/190 (95%)	151 (83%)	30 (17%)	2	11
10	J	172/173 (99%)	147 (86%)	25 (14%)	3	16
10	X	172/173 (99%)	147 (86%)	25 (14%)	3	16
11	K	175/175 (100%)	151 (86%)	24 (14%)	3	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	Y	175/175 (100%)	152 (87%)	23 (13%)	4	19
12	L	169/169 (100%)	146 (86%)	23 (14%)	3	18
12	Z	169/169 (100%)	146 (86%)	23 (14%)	3	18
13	M	185/185 (100%)	164 (89%)	21 (11%)	5	24
13	a	185/185 (100%)	162 (88%)	23 (12%)	4	21
14	N	199/199 (100%)	165 (83%)	34 (17%)	2	11
14	b	199/199 (100%)	162 (81%)	37 (19%)	1	9
15	c	163/190 (86%)	143 (88%)	20 (12%)	4	22
15	d	163/190 (86%)	144 (88%)	19 (12%)	5	23
15	e	163/190 (86%)	144 (88%)	19 (12%)	5	23
15	f	163/190 (86%)	145 (89%)	18 (11%)	6	26
15	g	163/190 (86%)	144 (88%)	19 (12%)	5	23
15	h	163/190 (86%)	145 (89%)	18 (11%)	6	26
15	i	163/190 (86%)	147 (90%)	16 (10%)	7	31
15	j	163/190 (86%)	146 (90%)	17 (10%)	7	28
15	k	163/190 (86%)	144 (88%)	19 (12%)	5	23
15	l	163/190 (86%)	145 (89%)	18 (11%)	6	26
15	m	163/190 (86%)	146 (90%)	17 (10%)	7	28
15	n	163/190 (86%)	145 (89%)	18 (11%)	6	26
15	o	163/190 (86%)	147 (90%)	16 (10%)	7	31
15	p	163/190 (86%)	144 (88%)	19 (12%)	5	23
All	All	7566/8156 (93%)	6460 (85%)	1106 (15%)	3	16

5 of 1106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	f	183	LEU
15	h	55	TYR
15	f	180	LEU
15	m	54	THR
14	N	-6	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 299 such sidechains are listed below:

Mol	Chain	Res	Type
15	f	80	ASN
15	o	72	GLN
15	g	80	ASN
15	k	52	ASN
14	N	53	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 14 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	238/252 (94%)	0.95	20 (8%) 17 11	45, 88, 99, 100	0
1	O	238/252 (94%)	0.68	10 (4%) 40 25	51, 89, 99, 100	0
2	B	247/250 (98%)	0.64	12 (4%) 35 22	39, 78, 96, 100	0
2	P	247/250 (98%)	0.51	8 (3%) 50 31	46, 81, 98, 100	0
3	C	241/245 (98%)	0.38	9 (3%) 45 28	35, 71, 99, 100	0
3	Q	241/245 (98%)	0.48	13 (5%) 31 20	37, 77, 99, 100	0
4	D	239/254 (94%)	0.34	6 (2%) 58 39	34, 68, 98, 100	0
4	R	239/254 (94%)	0.30	6 (2%) 58 39	37, 74, 99, 100	0
5	E	244/260 (93%)	0.32	8 (3%) 49 30	29, 67, 98, 100	0
5	S	244/260 (93%)	0.42	12 (4%) 35 22	41, 72, 99, 100	0
6	F	233/234 (99%)	0.27	0 100 100	33, 69, 87, 98	0
6	T	233/234 (99%)	0.33	2 (0%) 81 64	45, 74, 92, 100	0
7	G	240/287 (83%)	0.76	18 (7%) 20 13	45, 82, 98, 100	0
7	U	240/287 (83%)	0.61	13 (5%) 31 20	52, 85, 99, 100	0
8	H	196/196 (100%)	0.66	5 (2%) 57 37	51, 79, 97, 100	0
8	V	196/196 (100%)	0.65	3 (1%) 72 52	56, 81, 98, 100	0
9	I	222/232 (95%)	0.54	8 (3%) 46 28	44, 74, 95, 100	0
9	W	222/232 (95%)	0.46	5 (2%) 61 41	44, 75, 93, 100	0
10	J	204/205 (99%)	0.09	4 (1%) 65 45	29, 60, 85, 100	0
10	X	204/205 (99%)	0.02	0 100 100	33, 60, 82, 95	0
11	K	198/198 (100%)	0.02	3 (1%) 72 52	23, 52, 80, 100	0
11	Y	198/198 (100%)	0.01	5 (2%) 58 39	30, 56, 84, 100	0
12	L	212/212 (100%)	-0.11	1 (0%) 87 76	30, 52, 72, 96	0
12	Z	212/212 (100%)	-0.14	1 (0%) 87 76	31, 52, 76, 92	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	222/222 (100%)	0.03	1 (0%) 87 76	28, 60, 79, 97	0
13	a	222/222 (100%)	0.06	2 (0%) 81 64	30, 61, 85, 99	0
14	N	233/233 (100%)	0.44	3 (1%) 75 55	37, 72, 95, 99	0
14	b	233/233 (100%)	0.57	10 (4%) 40 24	39, 74, 96, 100	0
15	c	198/231 (85%)	1.36	38 (19%) 3 2	58, 90, 99, 100	0
15	d	198/231 (85%)	1.46	47 (23%) 2 2	65, 92, 100, 100	0
15	e	198/231 (85%)	1.27	38 (19%) 3 2	58, 91, 100, 100	0
15	f	198/231 (85%)	1.17	28 (14%) 6 5	47, 89, 99, 100	0
15	g	198/231 (85%)	1.19	37 (18%) 3 2	48, 88, 99, 100	0
15	h	198/231 (85%)	1.14	30 (15%) 5 4	57, 86, 99, 100	0
15	i	198/231 (85%)	1.33	42 (21%) 2 2	56, 91, 100, 100	0
15	j	198/231 (85%)	1.08	22 (11%) 10 7	60, 94, 100, 100	0
15	k	198/231 (85%)	1.16	21 (10%) 11 8	65, 94, 100, 100	0
15	l	198/231 (85%)	1.02	23 (11%) 9 7	56, 93, 100, 100	0
15	m	198/231 (85%)	1.04	28 (14%) 6 5	56, 94, 100, 100	0
15	n	198/231 (85%)	1.00	22 (11%) 10 7	64, 94, 100, 100	0
15	o	198/231 (85%)	1.10	27 (13%) 7 5	70, 93, 100, 100	0
15	p	198/231 (85%)	1.11	28 (14%) 6 5	67, 95, 100, 100	0
All	All	9110/9794 (93%)	0.62	619 (6%) 23 15	23, 79, 99, 100	0

The worst 5 of 619 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	k	230	VAL	5.8
15	c	28	TRP	5.7
15	l	227	ASP	5.6
15	n	230	VAL	5.4
15	k	227	ASP	5.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	MG	H	1002	1/1	0.62	0.17	81,81,81,81	0
16	MG	X	1013	1/1	0.76	0.13	79,79,79,79	0
16	MG	V	1009	1/1	0.81	0.08	39,39,39,39	0
16	MG	U	1014	1/1	0.81	0.13	65,65,65,65	0
16	MG	L	1003	1/1	0.82	0.10	43,43,43,43	0
16	MG	X	1012	1/1	0.87	0.11	56,56,56,56	0
16	MG	I	1001	1/1	0.88	0.09	67,67,67,67	0
16	MG	J	1005	1/1	0.91	0.09	37,37,37,37	0
16	MG	W	1008	1/1	0.95	0.06	67,67,67,67	0
16	MG	J	1006	1/1	0.95	0.04	24,24,24,24	0
16	MG	M	1004	1/1	0.95	0.05	26,26,26,26	0
16	MG	G	1007	1/1	0.97	0.03	38,38,38,38	0
16	MG	a	1011	1/1	0.97	0.06	49,49,49,49	0
16	MG	Z	1010	1/1	0.98	0.04	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.