



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:26 AM UTC

PDB ID : 4V7O / pdb_00004v7o
Title : Proteasome Activator Complex
Authors : Hill, C.P.; Whitby, F.G.
Deposited on : 2009-12-22
Resolution : 3.00 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

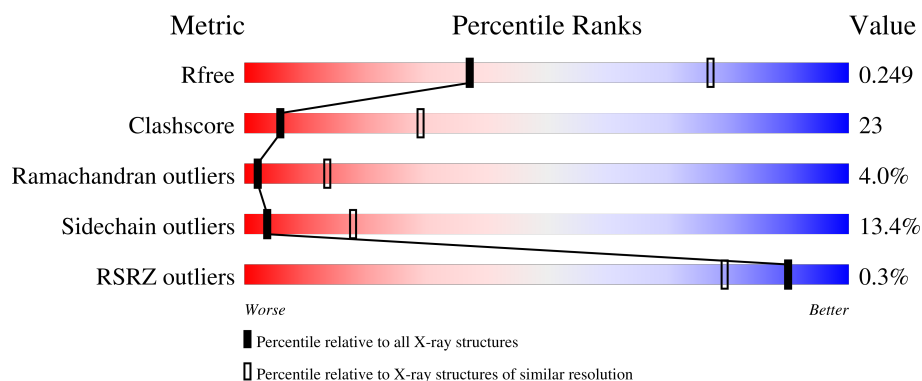
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



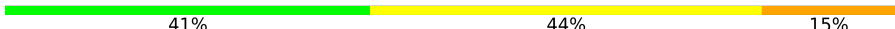
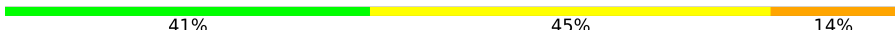
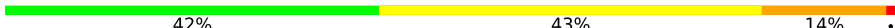
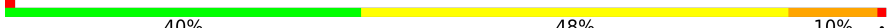
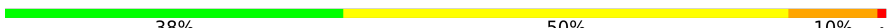
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	AA	243	63% 30% 6%
1	AC	243	64% 30% 6%
1	BA	243	66% 28% 5%
1	BO	243	65% 30% .
2	AG	231	65% 29% 6%

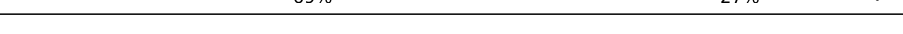
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Mol	Chain	Length	Quality of chain
2	AS	231	
2	BB	231	
2	BP	231	
3	AH	232	
3	AT	232	
3	BC	232	
3	BQ	232	
4	AI	227	
4	AU	227	
4	BD	227	
4	BR	227	
5	AJ	250	
5	AV	250	
5	BE	250	
5	BS	250	
6	AK	234	
6	AW	234	
6	BF	234	
6	BT	234	
7	AL	244	
7	AX	244	
7	BG	244	
7	BU	244	
8	AB	196	
8	AD	196	

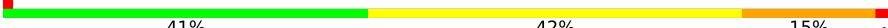
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Mol	Chain	Length	Quality of chain
8	BH	196	
8	BV	196	
9	AM	222	
9	AY	222	
9	BI	222	
9	BW	222	
10	AN	204	
10	AZ	204	
10	BJ	204	
10	BX	204	
11	A1	198	
11	AO	198	
11	BK	198	
11	BY	198	
12	A2	212	
12	AP	212	
12	BL	212	
12	BZ	212	
13	A3	222	
13	AQ	222	
13	B1	222	
13	BM	222	
14	A4	233	
14	AR	233	
14	B2	233	

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Mol	Chain	Length	Quality of chain
14	BN	233	 60% 33% 6%
15	AE	76	 66% 26% 8%
15	AF	76	 61% 34% 5%
15	B3	76	 64% 28% 8%
15	B6	76	 61% 33% 7%
16	A5	799	 49% 40% 10% .
16	A7	799	 48% 40% 10% .
16	B4	799	 50% 39% 10% .
16	B7	799	 49% 39% 10% .
17	A6	997	 40% 43% 15% .
17	A8	997	 41% 42% 15% .
17	B5	997	 42% 43% 14% .
17	B8	997	 41% 43% 15% .

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 158904 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	AA	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
1	AC	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
1	BA	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
1	BO	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			

- Molecule 2 is a protein called Proteasome component Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AG	231	Total	C	N	O	S	0	0	0
			1769	1126	292	348	3			
2	AS	231	Total	C	N	O	S	0	0	0
			1769	1126	292	348	3			
2	BB	231	Total	C	N	O	S	0	0	0
			1769	1126	292	348	3			
2	BP	231	Total	C	N	O	S	0	0	0
			1769	1126	292	348	3			

- Molecule 3 is a protein called Proteasome component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AH	232	Total	C	N	O	S	0	0	0
			1803	1139	300	361	3			
3	AT	232	Total	C	N	O	S	0	0	0
			1803	1139	300	361	3			
3	BC	232	Total	C	N	O	S	0	0	0
			1803	1139	300	361	3			
3	BQ	232	Total	C	N	O	S	0	0	0
			1803	1139	300	361	3			

- Molecule 4 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AI	227	Total	C	N	O	S	0	0	0
			1783	1113	312	354	4			
4	AU	227	Total	C	N	O	S	0	0	0
			1783	1113	312	354	4			
4	BD	227	Total	C	N	O	S	0	0	0
			1783	1113	312	354	4			
4	BR	227	Total	C	N	O	S	0	0	0
			1783	1113	312	354	4			

- Molecule 5 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AJ	250	Total	C	N	O	S	0	0	0
			1934	1209	325	392	8			
5	AV	250	Total	C	N	O	S	0	0	0
			1934	1209	325	392	8			
5	BE	250	Total	C	N	O	S	0	0	0
			1934	1209	325	392	8			
5	BS	250	Total	C	N	O	S	0	0	0
			1934	1209	325	392	8			

- Molecule 6 is a protein called Proteasome component PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AK	234	Total	C	N	O	S	0	0	0
			1803	1134	313	351	5			
6	AW	234	Total	C	N	O	S	0	0	0
			1803	1134	313	351	5			
6	BF	234	Total	C	N	O	S	0	0	0
			1803	1134	313	351	5			
6	BT	234	Total	C	N	O	S	0	0	0
			1803	1134	313	351	5			

- Molecule 7 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AL	244	Total	C	N	O	S	0	0	0
			1896	1205	329	358	4			
7	AX	244	Total	C	N	O	S	0	0	0
			1896	1205	329	358	4			
7	BG	244	Total	C	N	O	S	0	0	0
			1896	1205	329	358	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	BU	244	Total	C	N	O	S	0	0	0
			1896	1205	329	358	4			

- Molecule 8 is a protein called Proteasome component PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AB	196	Total	C	N	O	S	0	0	0
			1510	954	250	299	7			
8	AD	196	Total	C	N	O	S	0	0	0
			1510	954	250	299	7			
8	BH	196	Total	C	N	O	S	0	0	0
			1510	954	250	299	7			
8	BV	196	Total	C	N	O	S	0	0	0
			1510	954	250	299	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AB	1001	ALA	-	expression tag	UNP P38624
AD	1001	ALA	-	expression tag	UNP P38624
BH	1001	ALA	-	expression tag	UNP P38624
BV	1001	ALA	-	expression tag	UNP P38624

- Molecule 9 is a protein called Proteasome component PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AM	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			
9	AY	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			
9	BI	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			
9	BW	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			

- Molecule 10 is a protein called Proteasome component PUP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AN	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
10	AZ	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	BJ	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
10	BX	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	AO	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			
11	A1	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			
11	BK	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			
11	BY	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	AP	212	Total	C	N	O	S	0	0	0
			1646	1045	282	312	7			
12	A2	212	Total	C	N	O	S	0	0	0
			1646	1045	282	312	7			
12	BL	212	Total	C	N	O	S	0	0	0
			1646	1045	282	312	7			
12	BZ	212	Total	C	N	O	S	0	0	0
			1646	1045	282	312	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AP	5033	ARG	LYS	conflict	UNP P30656
A2	5033	ARG	LYS	conflict	UNP P30656
BL	5033	ARG	LYS	conflict	UNP P30656
BZ	5033	ARG	LYS	conflict	UNP P30656

- Molecule 13 is a protein called Proteasome component C5.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	A3	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
13	BM	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
13	B1	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	AR	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
14	A4	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
14	BN	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
14	B2	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 15 is a protein called Proteasome activator BLM10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AE	76	Total	C	N	O	S	0	0	0
			642	411	109	120	2			
15	AF	76	Total	C	N	O	S	0	0	0
			642	411	109	120	2			
15	B3	76	Total	C	N	O	S	0	0	0
			642	411	109	120	2			
15	B6	76	Total	C	N	O	S	0	0	0
			642	411	109	120	2			

- Molecule 16 is a protein called Proteasome activator BLM10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	A5	799	Total	C	N	O	S	0	0	0
			6517	4191	1074	1220	32			
16	A7	799	Total	C	N	O	S	0	0	0
			6517	4191	1074	1220	32			
16	B4	799	Total	C	N	O	S	0	0	0
			6517	4191	1074	1220	32			
16	B7	799	Total	C	N	O	S	0	0	0
			6517	4191	1074	1220	32			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A5	299	GLN	ASN	conflict	UNP P43583
A5	802	ASN	GLN	conflict	UNP P43583
A5	884	ASN	GLN	conflict	UNP P43583
A7	299	GLN	ASN	conflict	UNP P43583
A7	802	ASN	GLN	conflict	UNP P43583
A7	884	ASN	GLN	conflict	UNP P43583
B4	299	GLN	ASN	conflict	UNP P43583
B4	802	ASN	GLN	conflict	UNP P43583
B4	884	ASN	GLN	conflict	UNP P43583
B7	299	GLN	ASN	conflict	UNP P43583
B7	802	ASN	GLN	conflict	UNP P43583
B7	884	ASN	GLN	conflict	UNP P43583

- Molecule 17 is a protein called Proteasome activator BLM10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	A6	997	Total	C	N	O	S	0	0	0
			8070	5211	1339	1484	36			
17	A8	997	Total	C	N	O	S	0	0	0
			8070	5211	1339	1484	36			
17	B5	997	Total	C	N	O	S	0	0	0
			8070	5211	1339	1484	36			
17	B8	997	Total	C	N	O	S	0	0	0
			8070	5211	1339	1484	36			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A6	1168	ASN	GLN	conflict	UNP P43583
A6	1171	ASN	GLN	conflict	UNP P43583
A6	2085	ASN	GLN	conflict	UNP P43583
A6	2101	ASN	GLN	conflict	UNP P43583
A8	1168	ASN	GLN	conflict	UNP P43583
A8	1171	ASN	GLN	conflict	UNP P43583
A8	2085	ASN	GLN	conflict	UNP P43583
A8	2101	ASN	GLN	conflict	UNP P43583
B5	1168	ASN	GLN	conflict	UNP P43583
B5	1171	ASN	GLN	conflict	UNP P43583
B5	2085	ASN	GLN	conflict	UNP P43583
B5	2101	ASN	GLN	conflict	UNP P43583
B8	1168	ASN	GLN	conflict	UNP P43583

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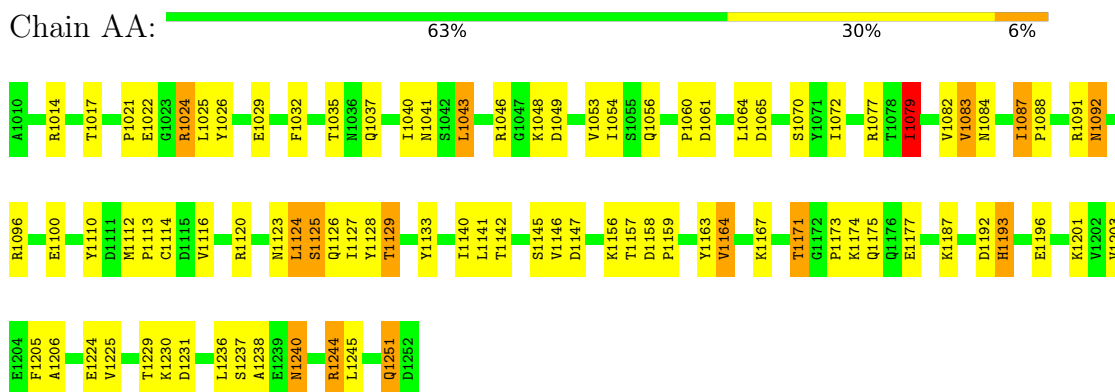
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Chain	Residue	Modelled	Actual	Comment	Reference
B8	1171	ASN	GLN	conflict	UNP P43583
B8	2085	ASN	GLN	conflict	UNP P43583
B8	2101	ASN	GLN	conflict	UNP P43583

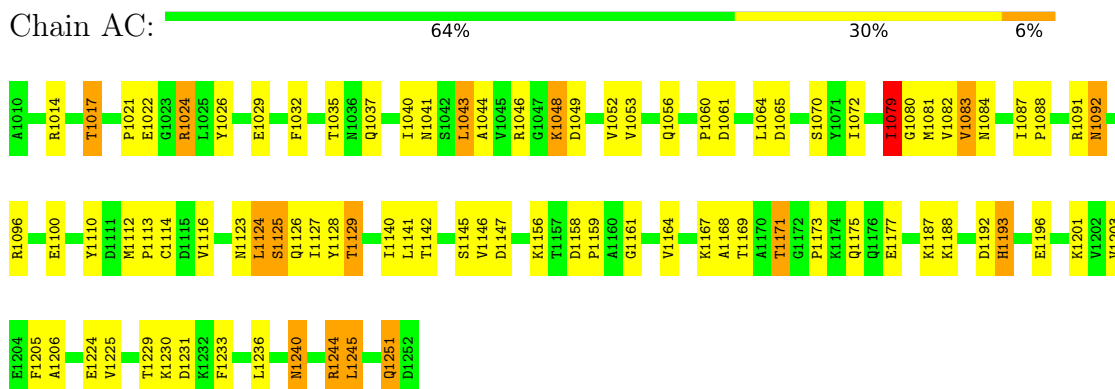
3 Residue-property plots

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.

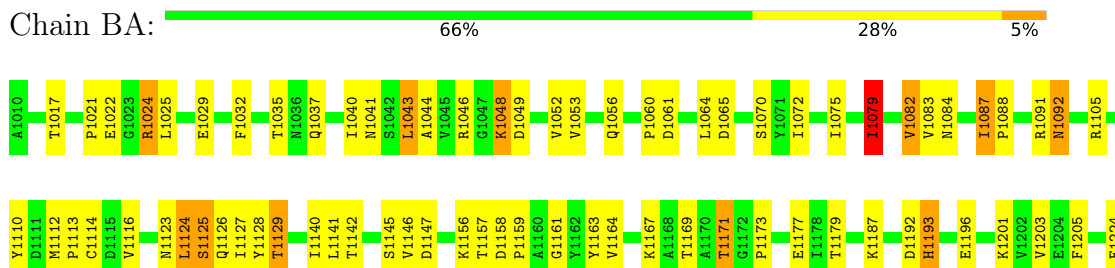
- Molecule 1: Proteasome component C7-alpha



- Molecule 1: Proteasome component C7-alpha



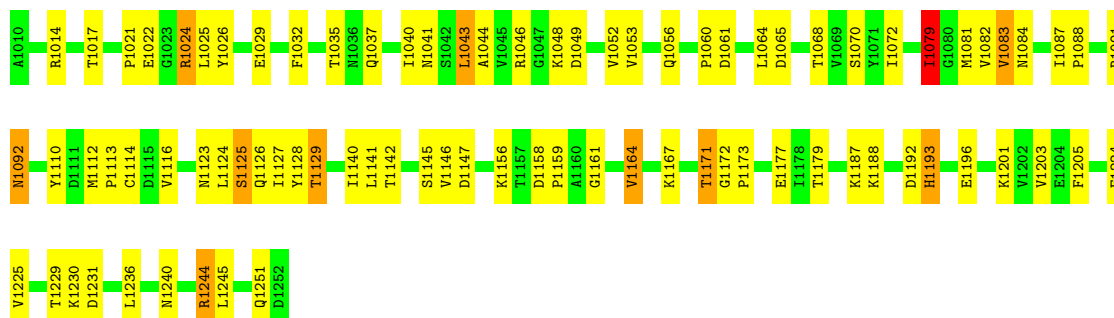
- Molecule 1: Proteasome component C7-alpha





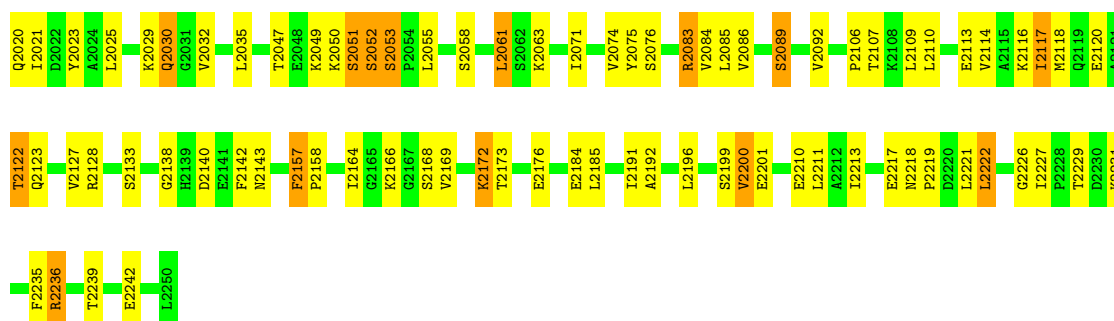
• Molecule 1: Proteasome component C7-alpha

Chain BO: 65% 30%



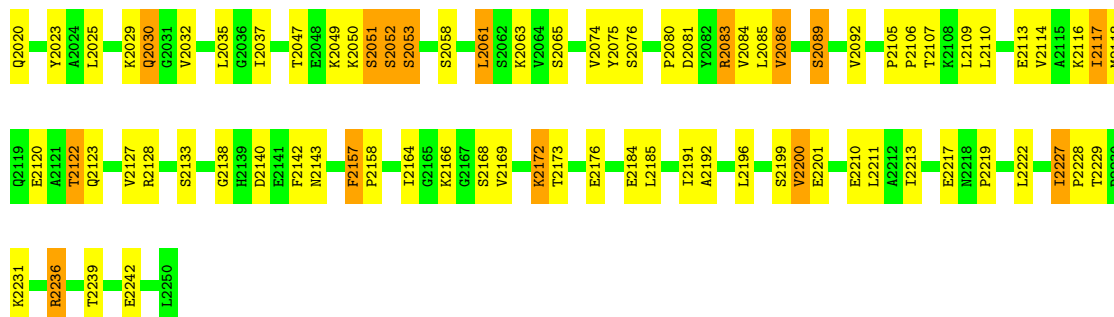
• Molecule 2: Proteasome component Y7

Chain AG: 65% 29% 6%



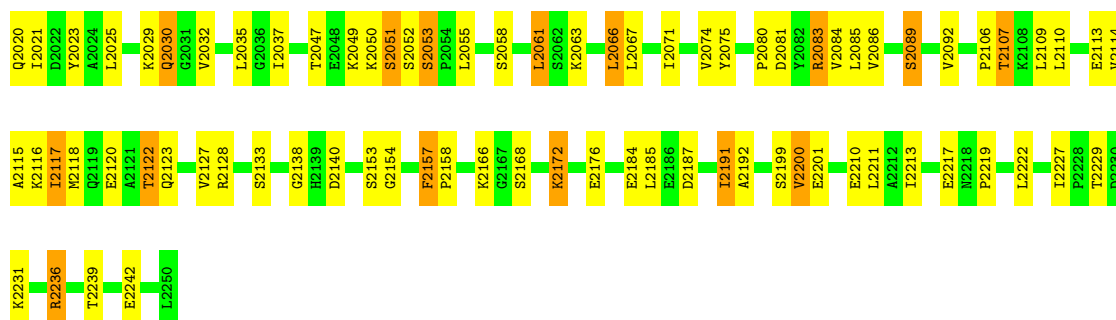
• Molecule 2: Proteasome component Y7

Chain AS: 66% 28% 6%



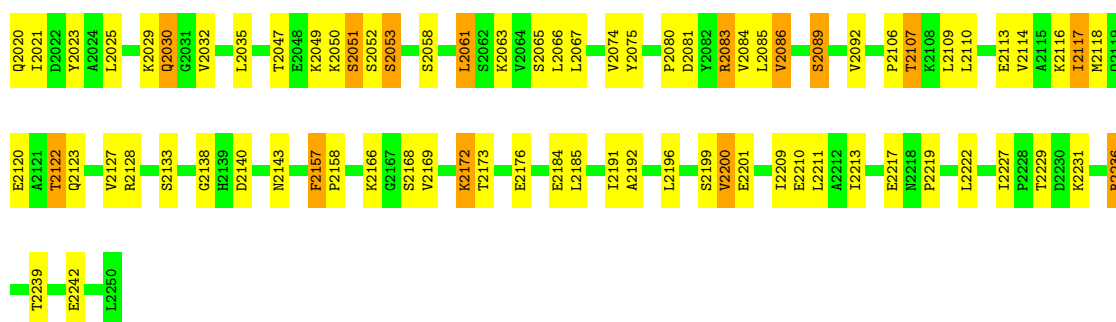
• Molecule 2: Proteasome component Y7

Chain BB: 66% 27% 6%



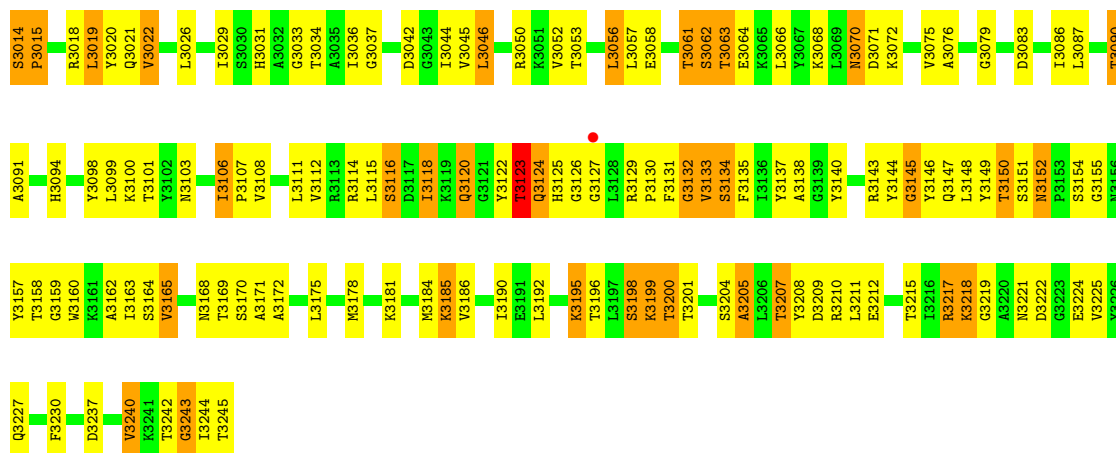
• Molecule 2: Proteasome component Y7

Chain BP: 67% 27% 6%



• Molecule 3: Proteasome component Y13

Chain AH: 41% 44% 15%



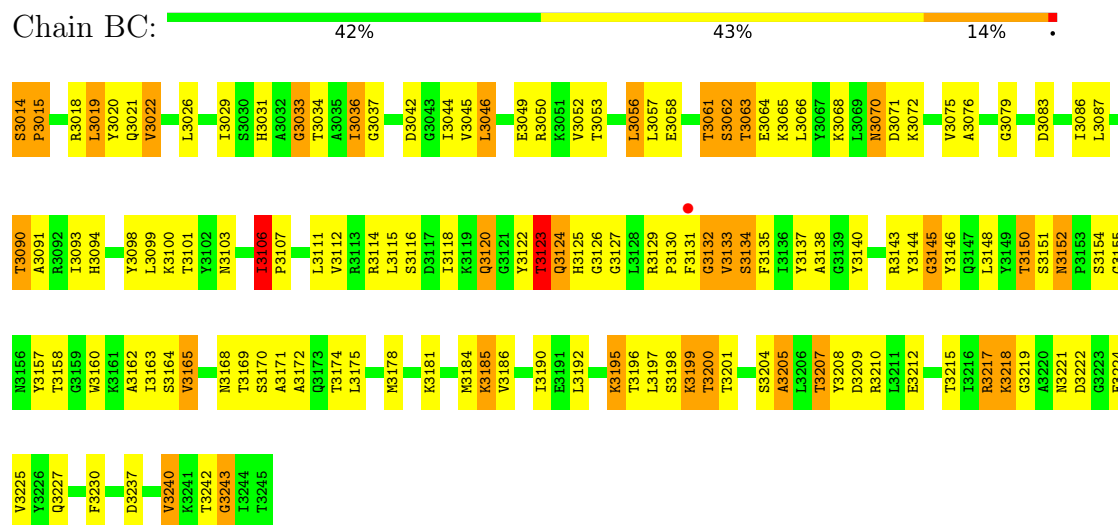
• Molecule 3: Proteasome component Y13

Chain AT: 41% 45% 14%

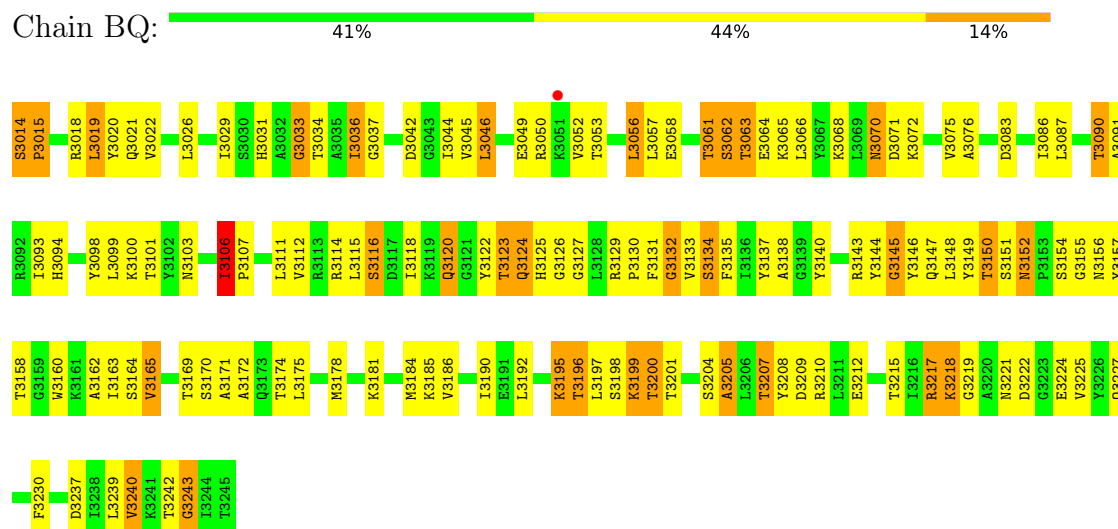




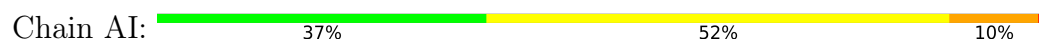
• Molecule 3: Proteasome component Y13

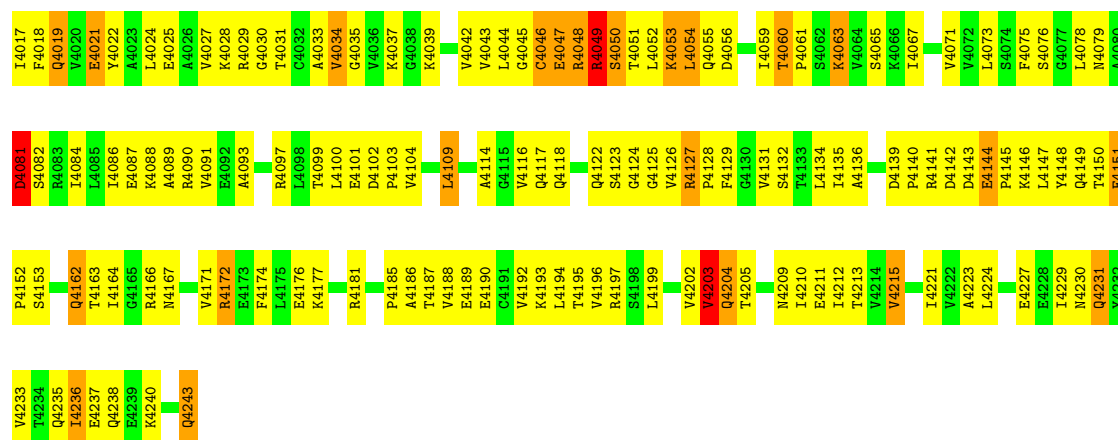


• Molecule 3: Proteasome component Y13

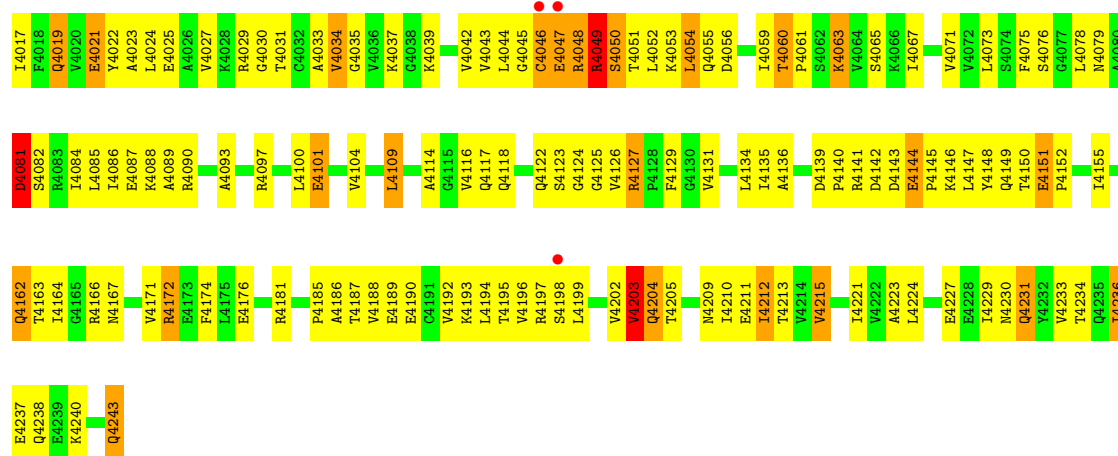


• Molecule 4: Proteasome component PRE6

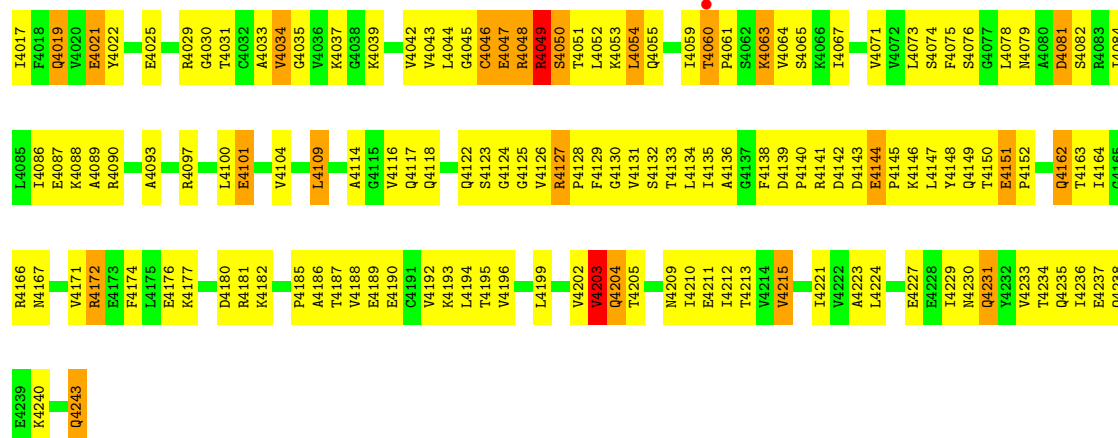




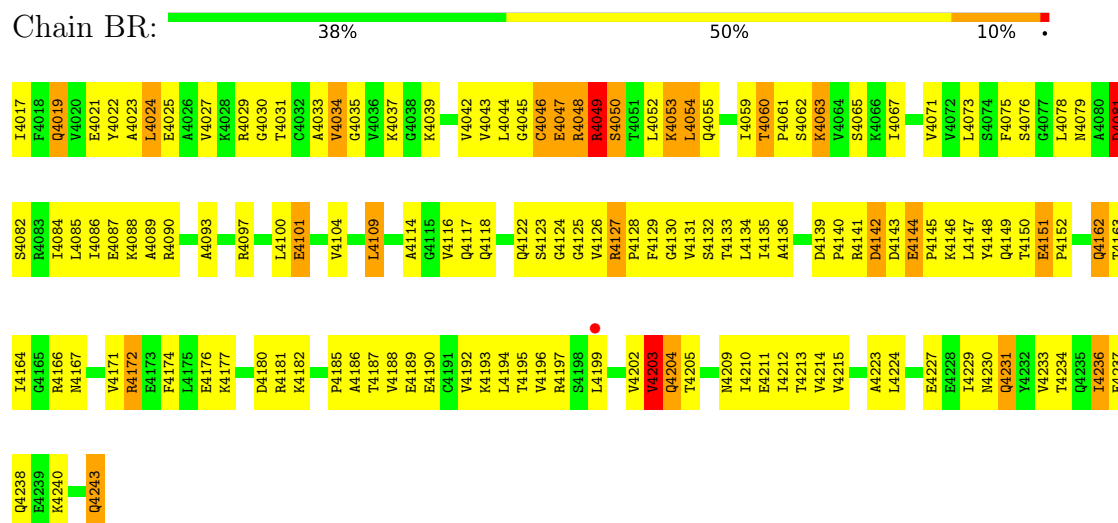
• Molecule 4: Proteasome component PRE6



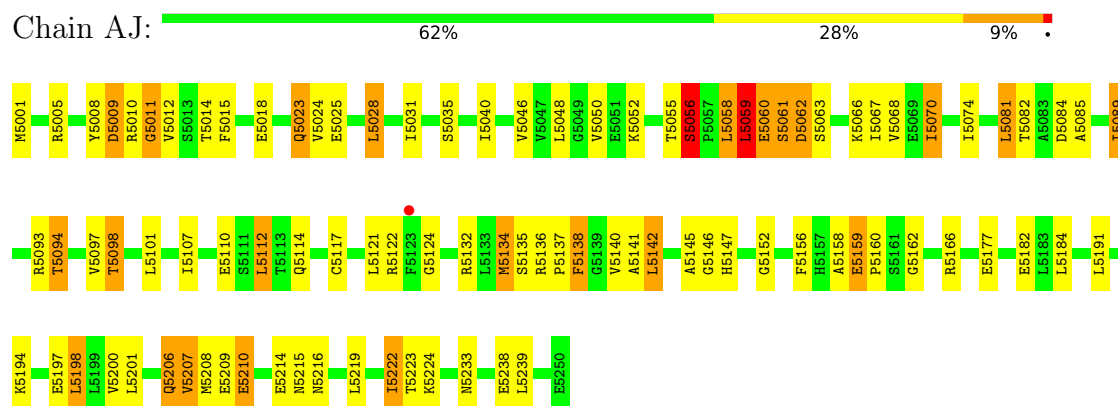
• Molecule 4: Proteasome component PRE6



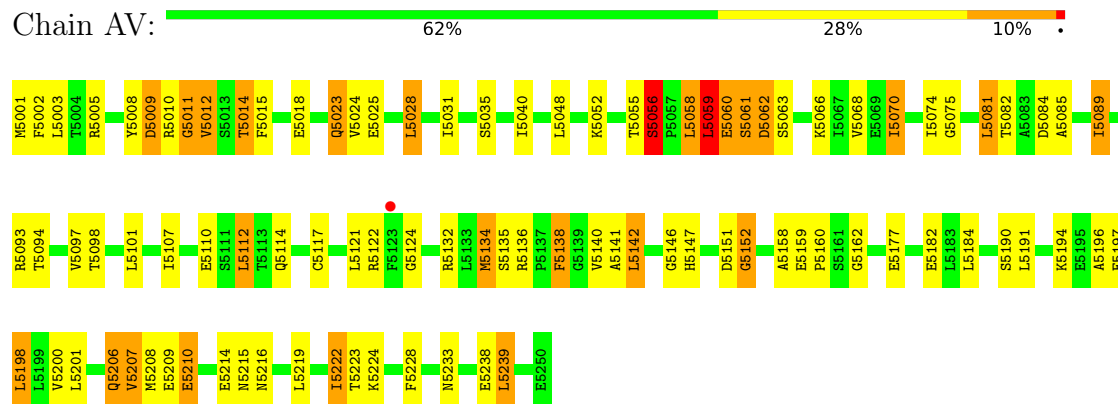
• Molecule 4: Proteasome component PRE6



• Molecule 5: Proteasome component PUP2

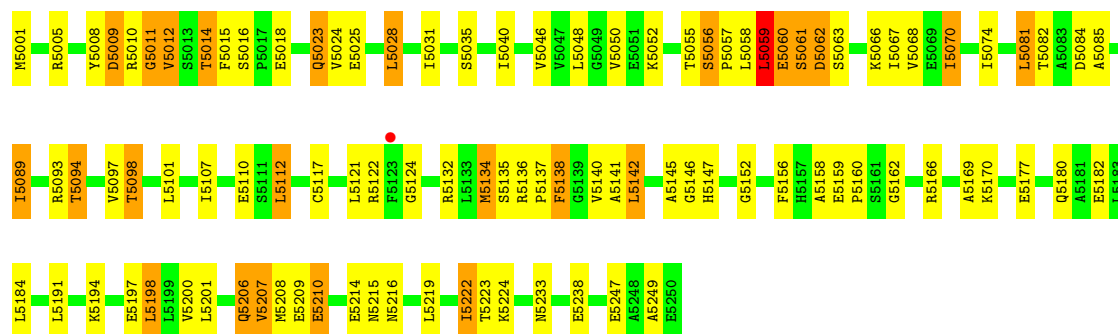


• Molecule 5: Proteasome component PUP2

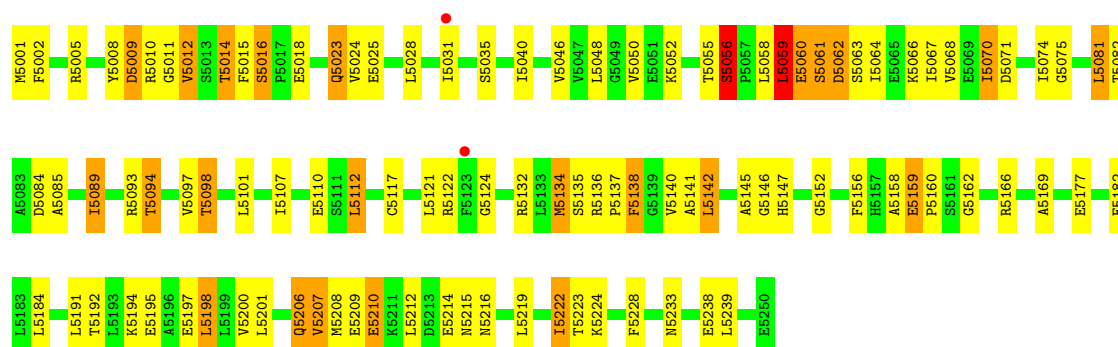


• Molecule 5: Proteasome component PUP2

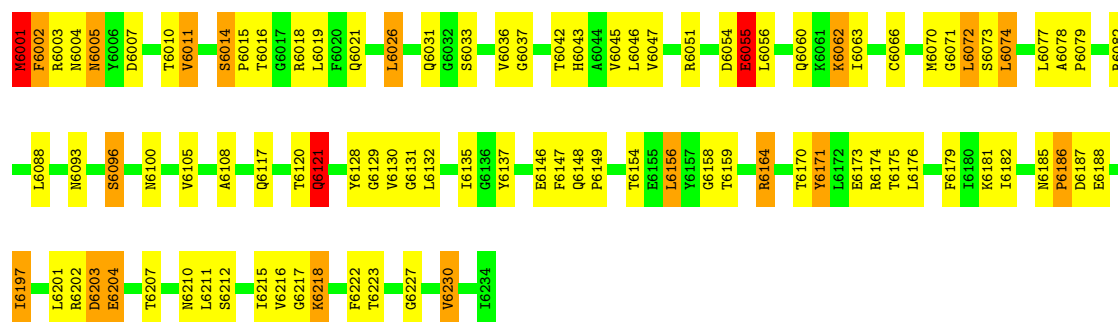




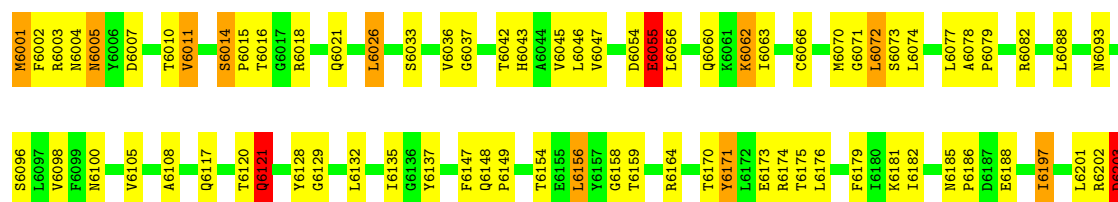
• Molecule 5: Proteasome component PUP2



• Molecule 6: Proteasome component PRE5



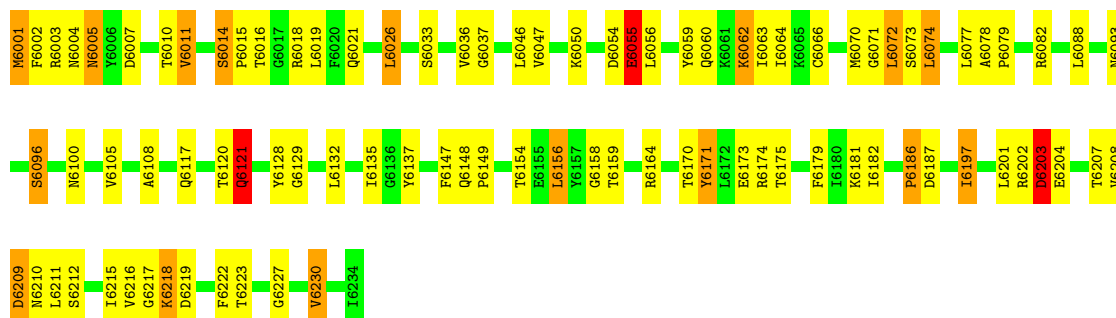
• Molecule 6: Proteasome component PRE5





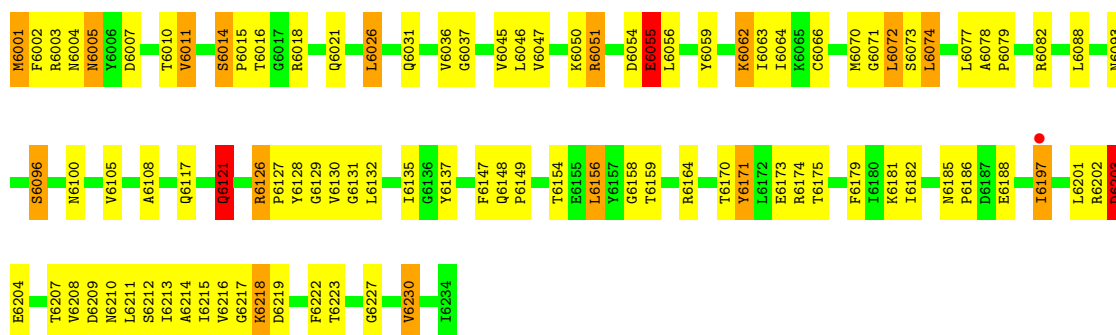
• Molecule 6: Proteasome component PRE5

Chain BF: 61% 31% 7% .



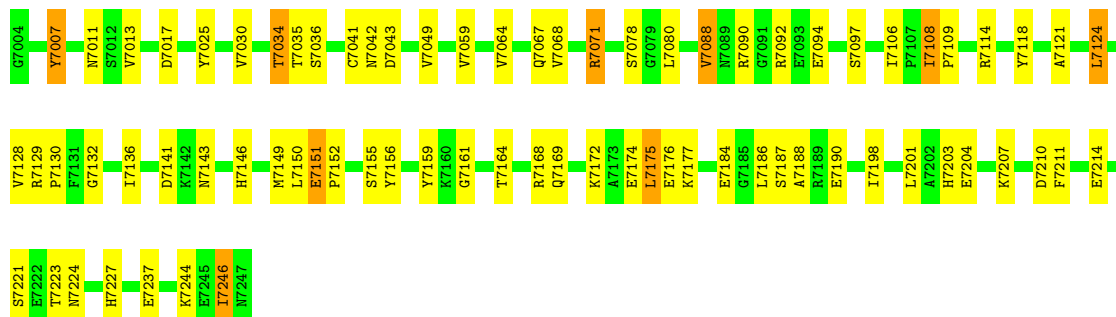
• Molecule 6: Proteasome component PRE5

Chain BT: 59% 33% 7% .



• Molecule 7: Proteasome component C1

Chain AL: 69% 27% .



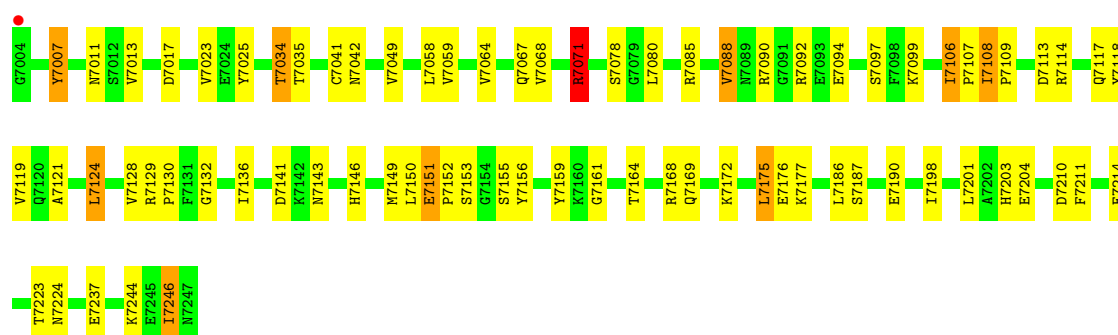
• Molecule 7: Proteasome component C1

Chain AX: 67% 29% .



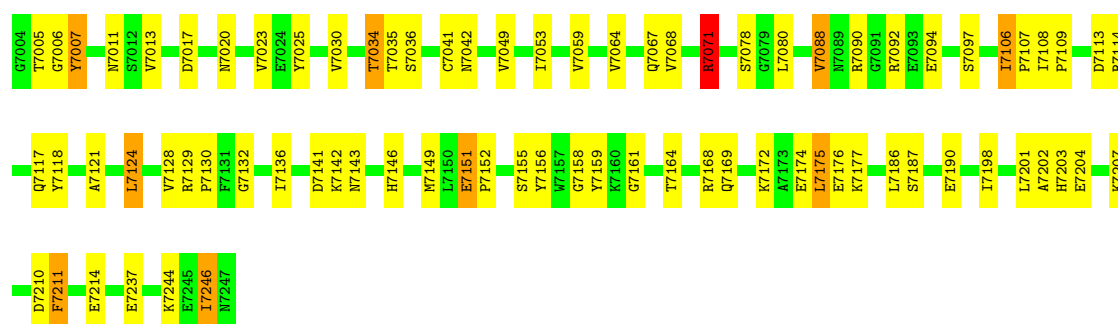
• Molecule 7: Proteasome component C1

Chain BG: 69% 27% .



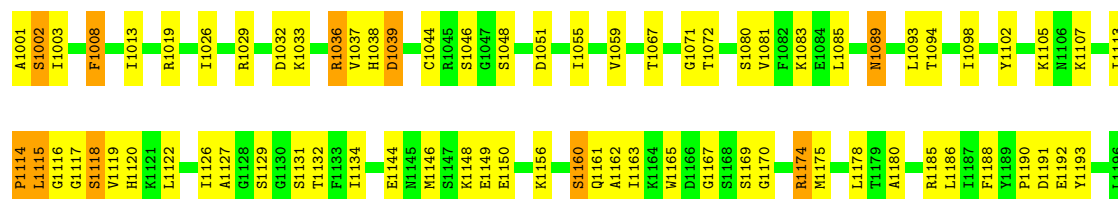
• Molecule 7: Proteasome component C1

Chain BU: 68% 28% .



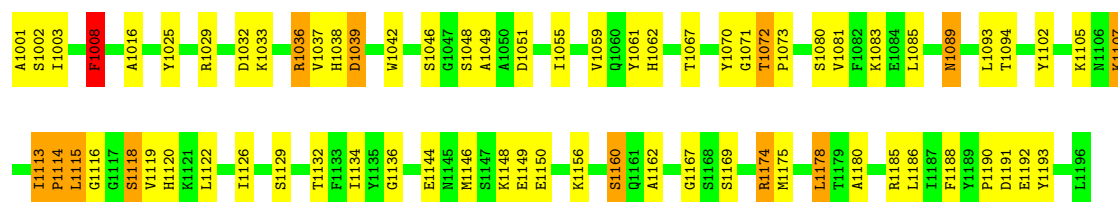
• Molecule 8: Proteasome component PRE3

Chain AB: 62% 33% 5%



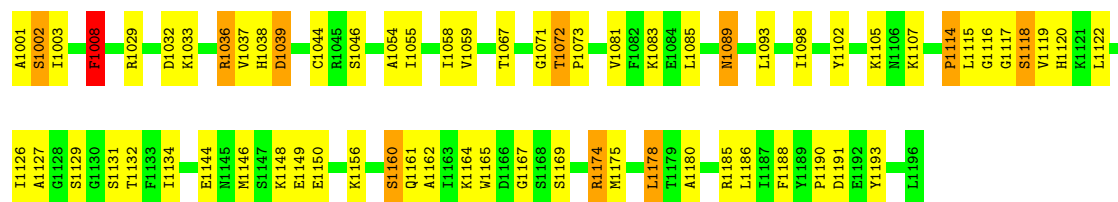
• Molecule 8: Proteasome component PRE3

Chain AD:  64% 30% 6% •



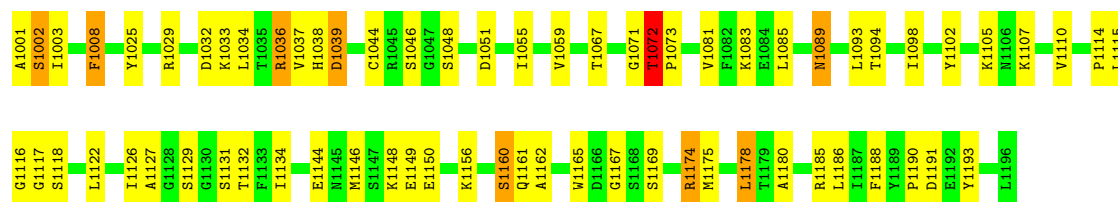
• Molecule 8: Proteasome component PRE3

Chain BH:  66% 29% 5% •



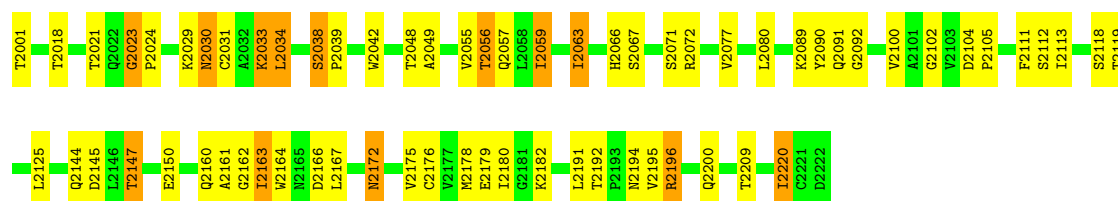
• Molecule 8: Proteasome component PRE3

Chain BV:  65% 30% • •



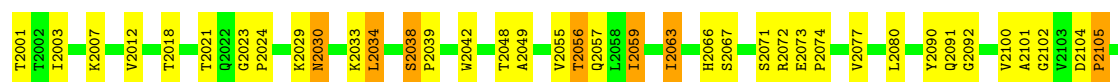
• Molecule 9: Proteasome component PUP1

Chain AM:  70% 24% 6%



• Molecule 9: Proteasome component PUP1

Chain AY:  68% 27% 5%

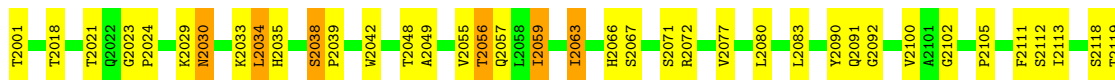




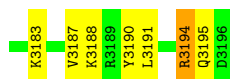
• Molecule 9: Proteasome component PUP1



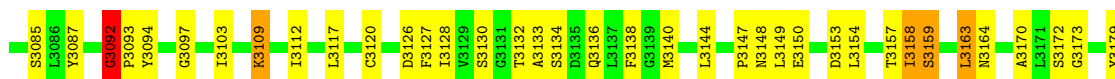
• Molecule 9: Proteasome component PUP1



• Molecule 10: Proteasome component PUP3



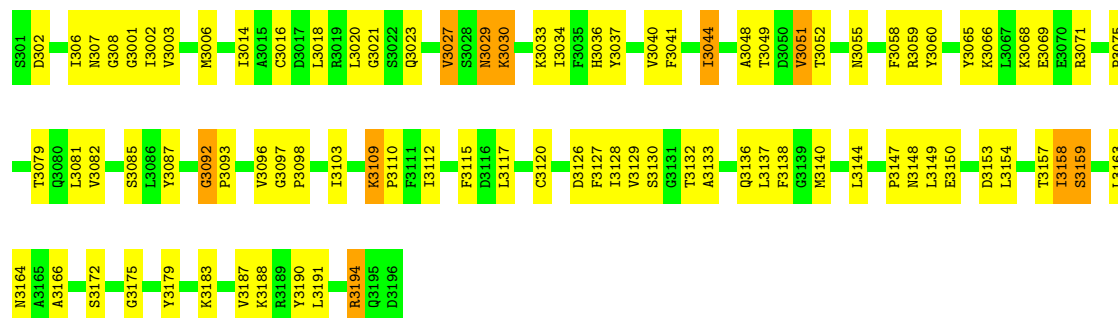
• Molecule 10: Proteasome component PUP3





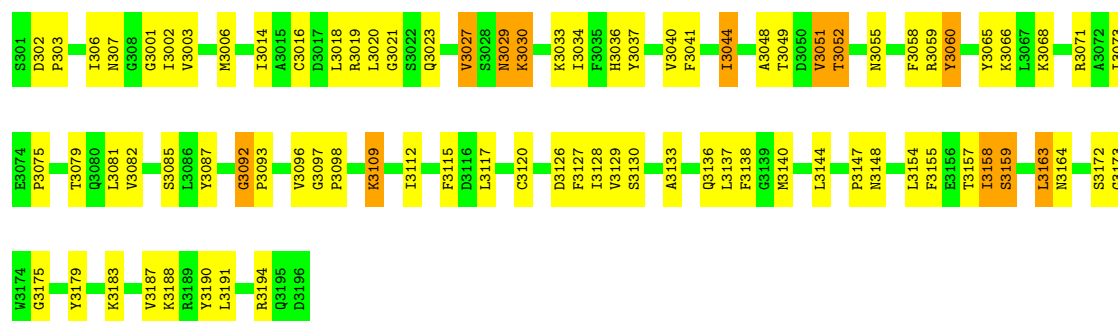
• Molecule 10: Proteasome component PUP3

Chain BJ: 57% 38% 5%



• Molecule 10: Proteasome component PUP3

Chain BX: 59% 35% 6%



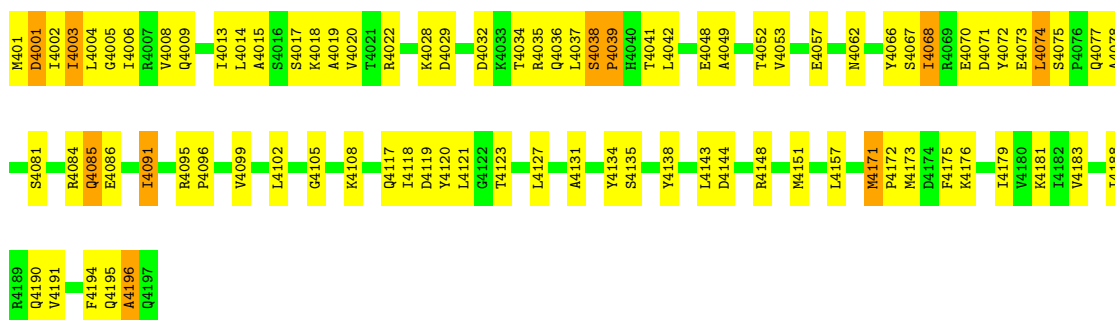
• Molecule 11: Proteasome component C11

Chain AO: 59% 36% 5%



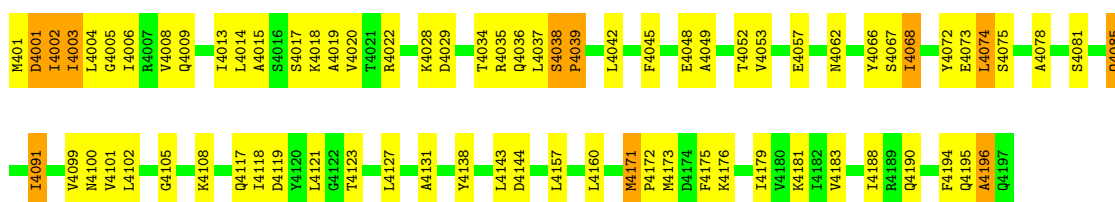
• Molecule 11: Proteasome component C11

Chain A1: 57% 38% 5%



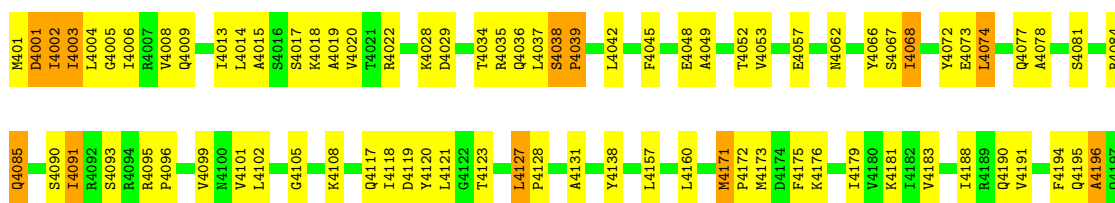
• Molecule 11: Proteasome component C11

Chain BK: 62% 32% 6%



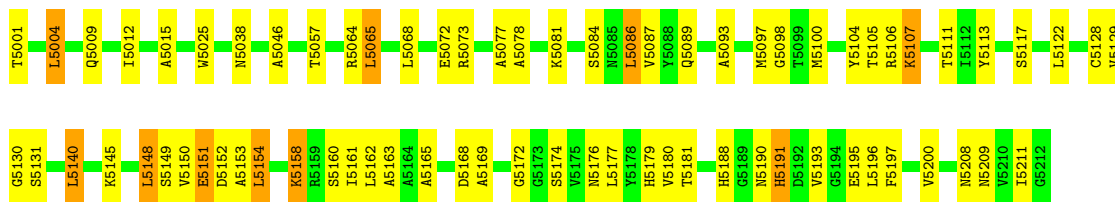
• Molecule 11: Proteasome component C11

Chain BY: 60% 34% 6%



• Molecule 12: Proteasome component PRE2

Chain AP: 66% 29% 5%



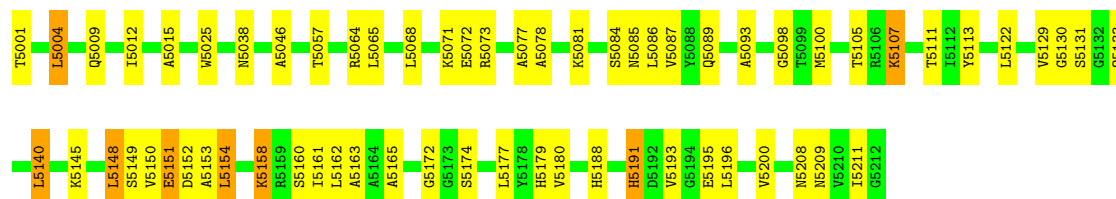
• Molecule 12: Proteasome component PRE2

Chain A2: 69% 27% 4%

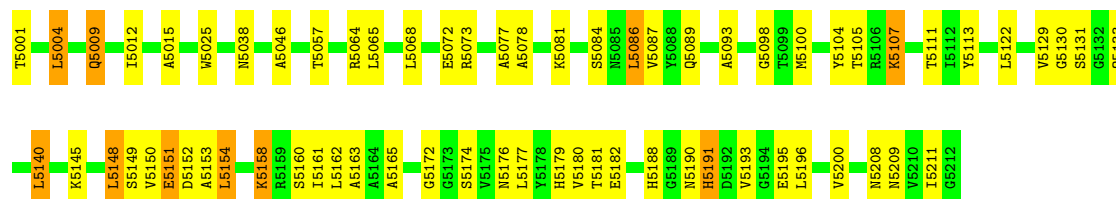




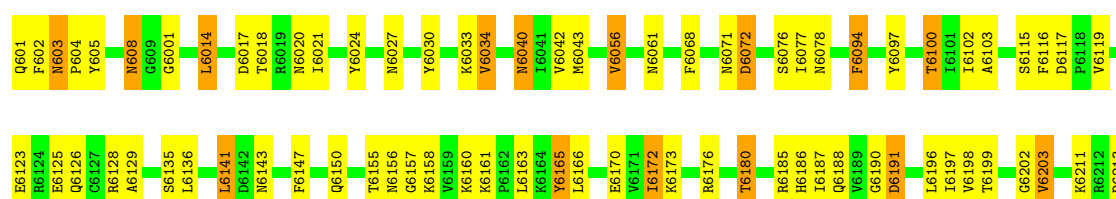
• Molecule 12: Proteasome component PRE2



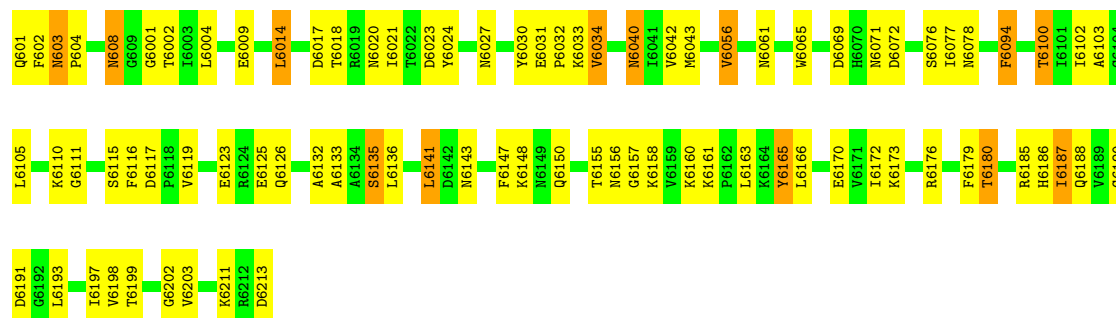
• Molecule 12: Proteasome component PRE2



• Molecule 13: Proteasome component C5



• Molecule 13: Proteasome component C5



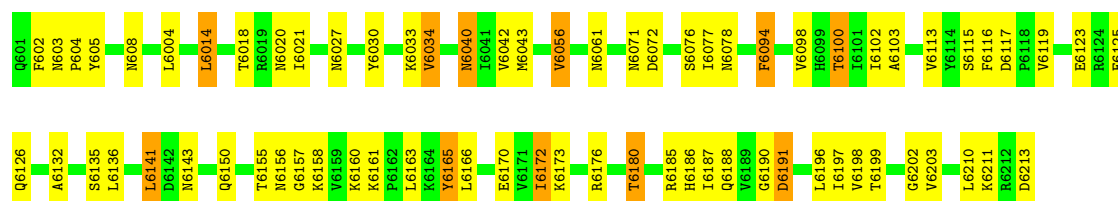
• Molecule 13: Proteasome component C5

Chain BM:  65% 30% 5%



• Molecule 13: Proteasome component C5

Chain B1:  68% 27% 5%



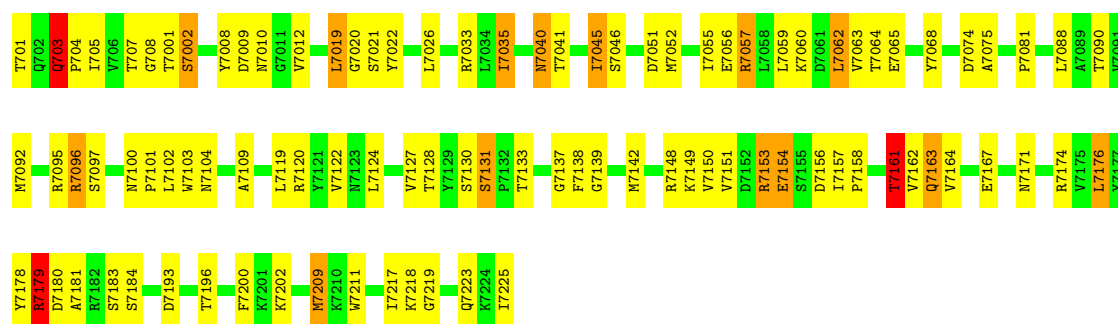
• Molecule 14: Proteasome component PRE4

Chain AR:  59% 33% 7%

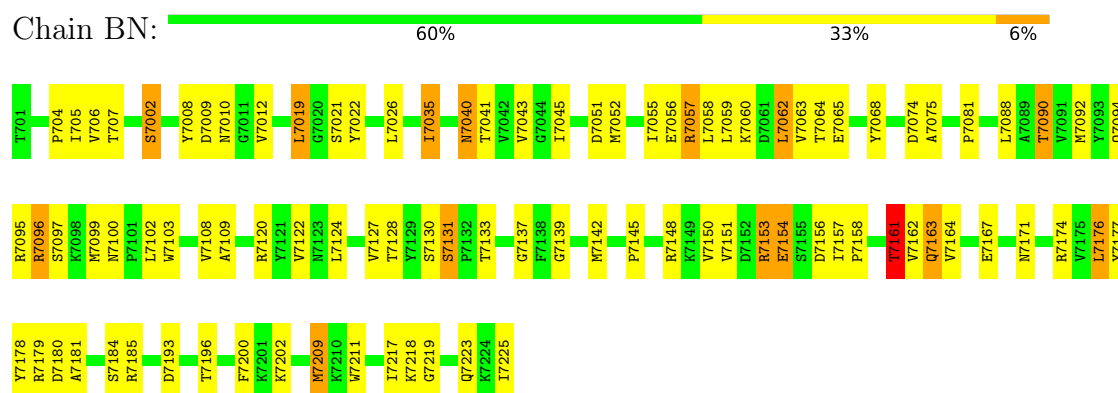


• Molecule 14: Proteasome component PRE4

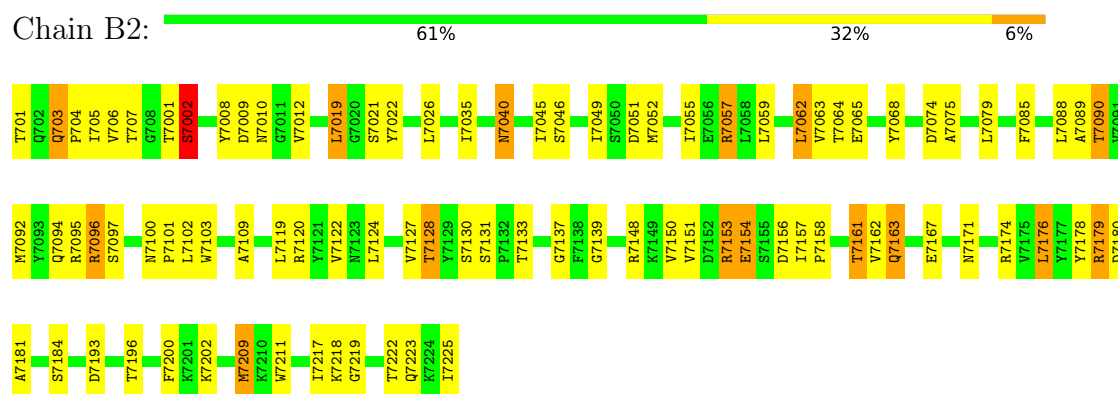
Chain A4:  58% 34% 6%



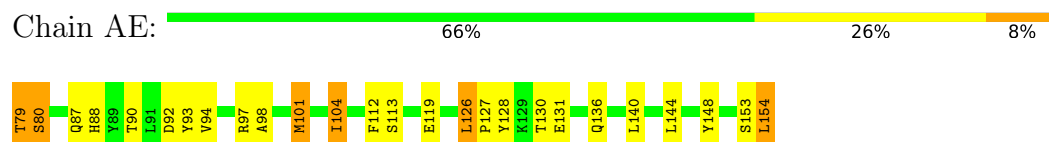
- Molecule 14: Proteasome component PRE4



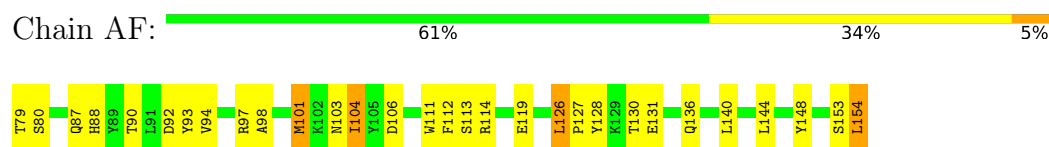
- Molecule 14: Proteasome component PRE4



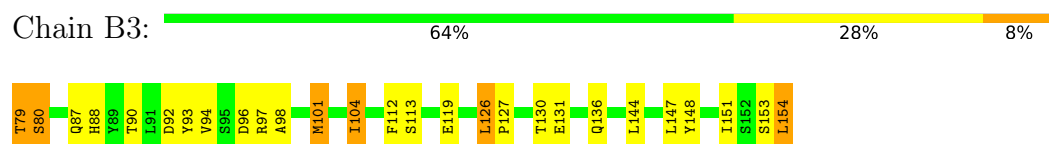
- Molecule 15: Proteasome activator BLM10



- Molecule 15: Proteasome activator BLM10



- Molecule 15: Proteasome activator BLM10



- Molecule 15: Proteasome activator BLM10

Response	Percentage
Yes, the U.S. is a democracy	61%
No, the U.S. is not a democracy	33%
Don't know	7%

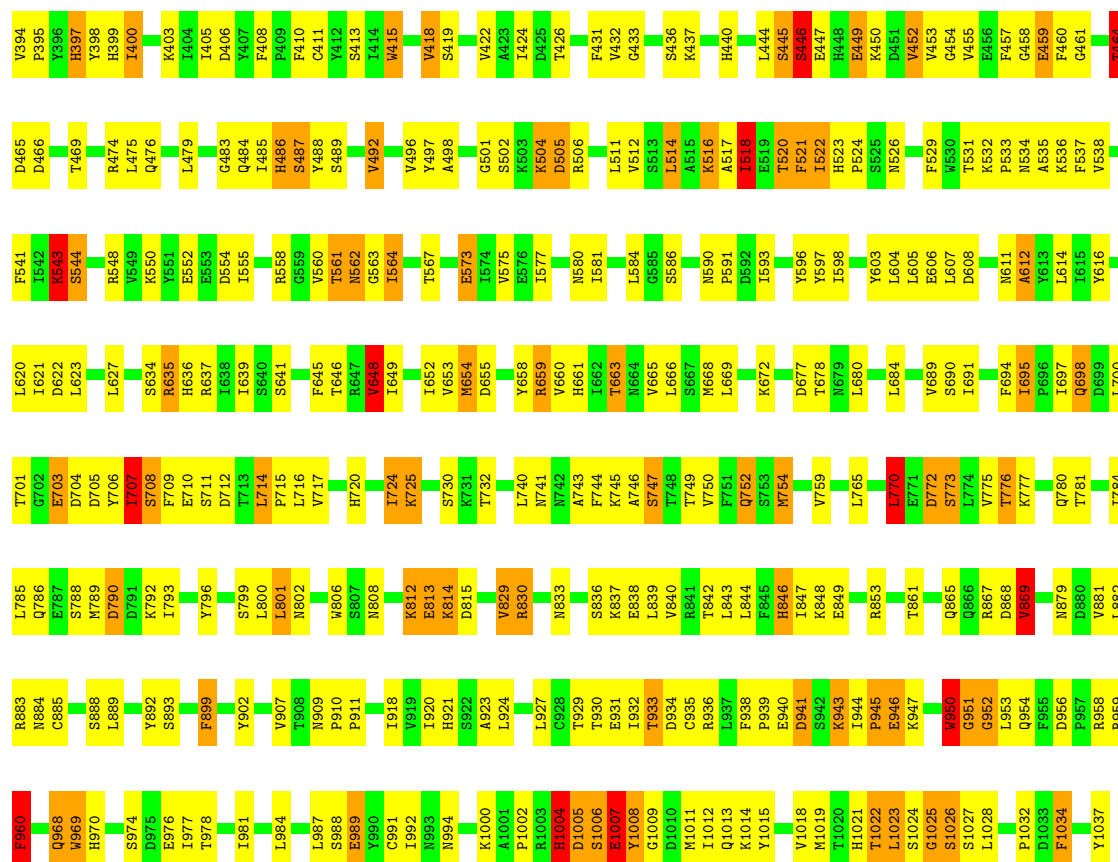


Response	Percentage
Doing a good job	49%
Not doing a good job	40%
Don't know	10%

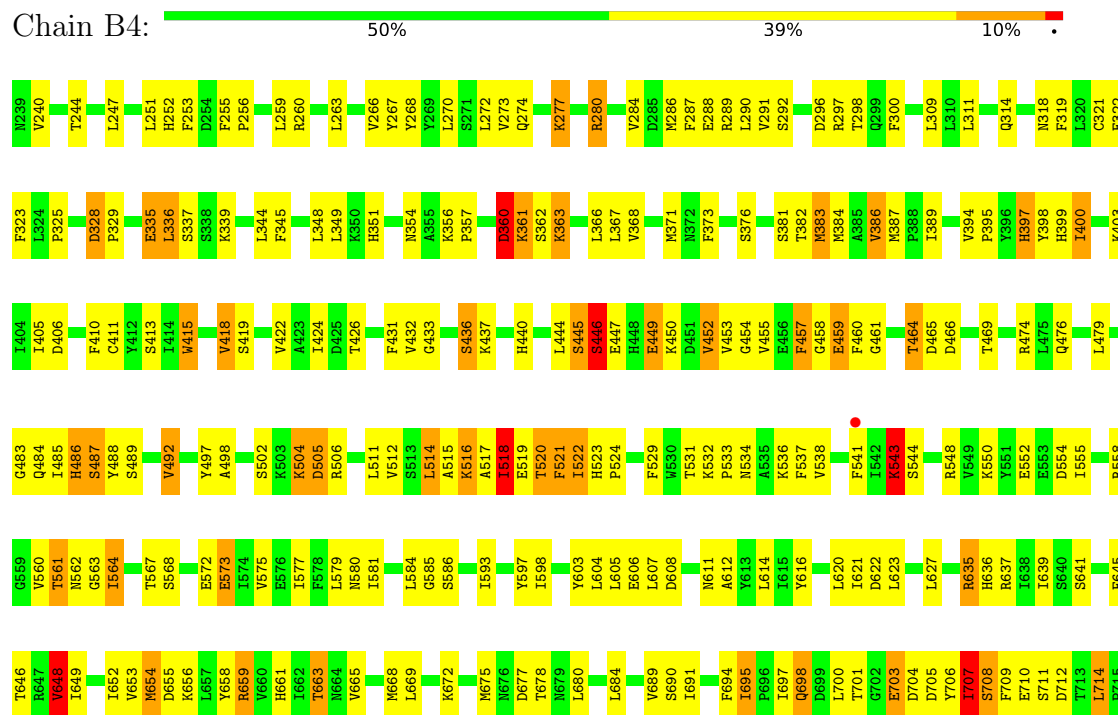


Response	Percentage
Yes	48%
No	40%
Don't know	10%





• Molecule 16: Proteasome activator BLM10



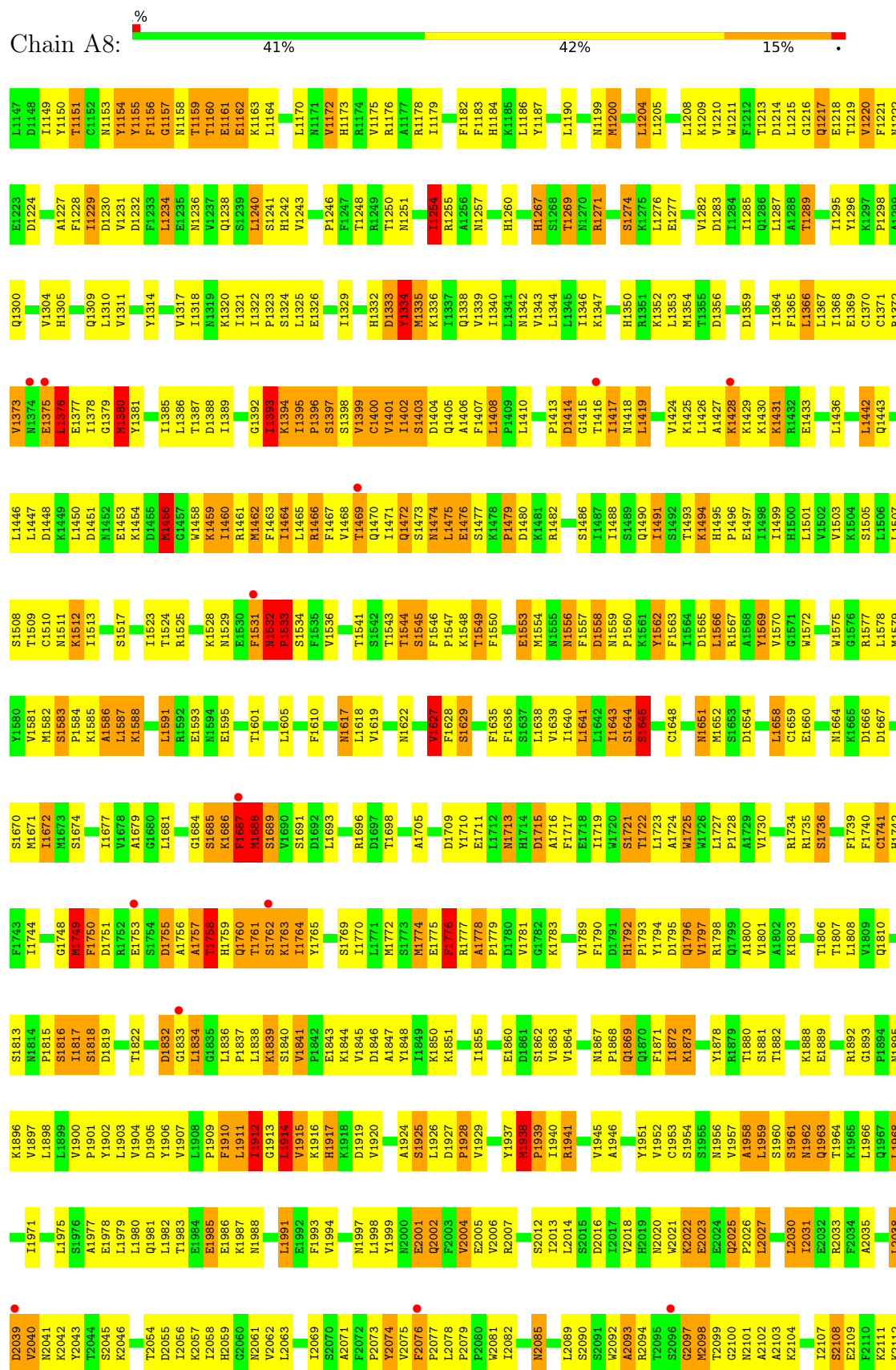


Chain A6:



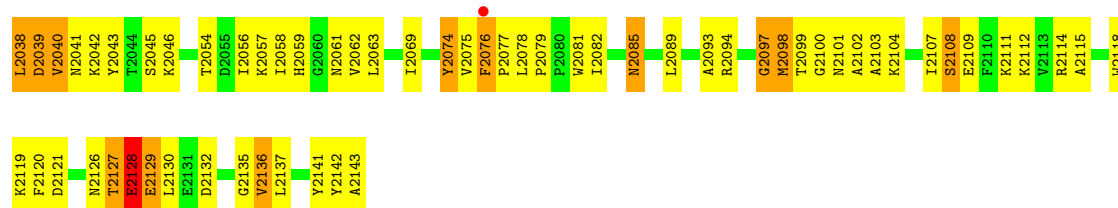
T2127	E2128	E2129	L2130	E2131	D2132	G2135	L2136	L2137	W2138		Y2141	A2142	A2143		T2054	D2055	L2056	K2057	L2058	H2059	G2060	N2061	V2062	L2063		L2069	S2070	A2071	F2072	T2073	Y2074	V2075	F2076	T2077	L2078	T2079	P2080	W2081	L2082	W2085	L2089	S2090	S2091	W2092	A2093	R2094	G2097	K2098	T2099	G2100	N2101	A2102	A2103	K2104	L2107	S2108	E2109	F2110	K2111	V2112	N2114	A2115		W2118	L2119	F2120	D2121		W2126																																																																																																																																																																																																																																																																																																																																																																																																																																											
L1982	T1983	E1984	E1985	L1986	K1987	L1911	L1912	K1899	G1913	L1914	V1915	K1916	H1917	F1993	V1994	N1997	L1998	Y1999	N2000	E2001	Q2002	F2003	V2004	E2005	V2006	R2007	S2012	I2013	L2014	S2015	S2016	S2017	N2019	G2097	N2098	T2099	G2100	N2101	A2102	A2103	K2104	L2107	S2108	E2109	F2110	K2111	V2112	N2114	A2115		W2118	L2119	F2120	D2121		W2126																																																																																																																																																																																																																																																																																																																																																																																																																																																								
Y1906	V1907	L1908	P1909	F1910	L1911	L1912	K1899	G1913	L1914	V1915	K1916	H1917	F1993	V1994	N1997	L1998	Y1999	N2000	E2001	Q2002	F2003	V2004	E2005	V2006	R2007	S2012	I2013	L2014	S2015	S2016	S2017	N2019	G2097	N2098	T2099	G2100	N2101	A2102	A2103	K2104	L2107	S2108	E2109	F2110	K2111	V2112	N2114	A2115		W2118	L2119	F2120	D2121		W2126																																																																																																																																																																																																																																																																																																																																																																																																																																																									
G1833	L1834	G1835	L1836	P1837	L1838	K1839	S1840	I1841	E1842	P1843	L1844	V1845	D1846	A1847	Y1848	I1849	K1850	S1855	E1860	D1861	S1862	V1863	V1864	N1867	P1868	Q1869	Q1870	F1871	L1872	K1873	Y1878	L1879	T1880	S1881	L1882	I1883	L1887	K1888	E1889	R1892	G1893	P1894	N1895	K1896	L1897	L1898	L1899	V1900	P1901	A1902	L1903	V1904	D1905	L1982																																																																																																																																																																																																																																																																																																																																																																																																																																																										
A1756	A1757	T1758	G1759	Q1760	T1761	S1685	S1762	K1763	I1764	Y1765	M1766		S1769	I1691	L1692	L1693	D1696	D1697	T1698	Y1710	L1711	L1712	H1713	D1714	D1715	A1716	F1717	E1718	I1719	L1720	S1721	L1722	A1724	W1725	V1726	L1727	P1728	A1729	V1730	R1734	R1735	S1736	K1737	T1738	F1739	C1740	C1741	H1742	G1748	R1749	S1750	D1751	R1752	E1753	S1754	D1755	L1982																																																																																																																																																																																																																																																																																																																																																																																																																																																							
L1591	R1592	E1593	M1594	E1595	T1601	L1605	S1606	F1607	V1608	V1609	L1614	M1617	L1618	V1619	N1622	V1627	F1628	S1629	F1635	F1636	S1637	L1638	V1639	I1640	L1641	L1642	L1643	L1644	L1645	L1646	L1647	L1648	L1649	N1650	N1651	M1652	S1653	D1654	L1658	C1659	E1660	N1664	K1665	D1666	K1668	M1669	S1670	M1671	I1672	L1673	S1674	D1675	L1982																																																																																																																																																																																																																																																																																																																																																																																																																																																											
T1524	R1525	K1528	M1529	E1530	F1531	N1532	P1533	S1534	F1535	V1536	T1541	S1542	T1543	T1544	S1545	F1546	P1547	K1548	T1549	F1550	E1553	M1554	N1555	M1556	F1557	D1558	N1559	P1560	K1561	T1562	F1563	L1564	D1565	L1566	L1567	A1568	Y1569	V1570	G1571	W1572	W1575	G1576	L1577	L1578	M1579	Y1580	M1582	S1583	M1584	K1585	A1586	L1587	K1588	L1982																																																																																																																																																																																																																																																																																																																																																																																																																																																										
I1378	G1379	M1380	Y1381	I1385	L1386	T1387	D1388	I1389		G1392	T1393	K1394	L1395	P1396	S1397	S1398	V1399	C1400	V1401	L1402	S1403	D1404	Q1405	E1406	F1407	L1408	P1409	L1410	P1413	D1414	G1415	T1416	I1417	L1418	L1419	V1424	K1425	L1426	A1427	K1428	K1429	K1430	K1431	R1432	E1433	L1436	L1442	Q1443	L1446	L1447	D1448	K1449	L1450	L1982																																																																																																																																																																																																																																																																																																																																																																																																																																																										
L1310	V1311	Y1314	L1318	M1319	L1320	L1321	L1322	P1323	S1324	L1325	L1326	L1329	H1332	D1333	Y1334	M1335	K1336	I1337	Q1338	V1339	A1340	L1341	L1342	L1343	L1344	L1345	L1346	K1347	L1348	L1349	H1350	R1351	K1352	M1353	L1354	K1355	D1356	V1357	K1358	D1359	I1364	F1365	L1366	L1367	L1368	L1369	C1370	C1371	R1372	L1373	M1374	L1375	E1377	L1982																																																																																																																																																																																																																																																																																																																																																																																																																																																										
D1230	V1231	D1232	F1233	L1234	E1235	N1236	Q1237	Q1238	S1239	L1240	S1241	H1242	V1243	P1246	F1247	T1248	R1249	T1250	N1251	I1252	I1253	I1254	R1255	A1256	N1257	H1260	H1267	S1268	T1269	N1270	R1271	S1274	K1275	L1276	E1277	V1282	D1283	I1284	A1285	Q1286	L1287	A1288	T1289	S1290	L1291	I1295	I1298	P1298	L1303	V1304	H1305	Q1309	L1982																																																																																																																																																																																																																																																																																																																																																																																																																																																											
L1147	D1148	L1149	T1150	T1151	G1152	N1153	L1154	F1155	G1157	N1158	T1159	T1160	E1161	E1162	K1163	L1164																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																

● Molecule 17: Proteasome activator BLM10

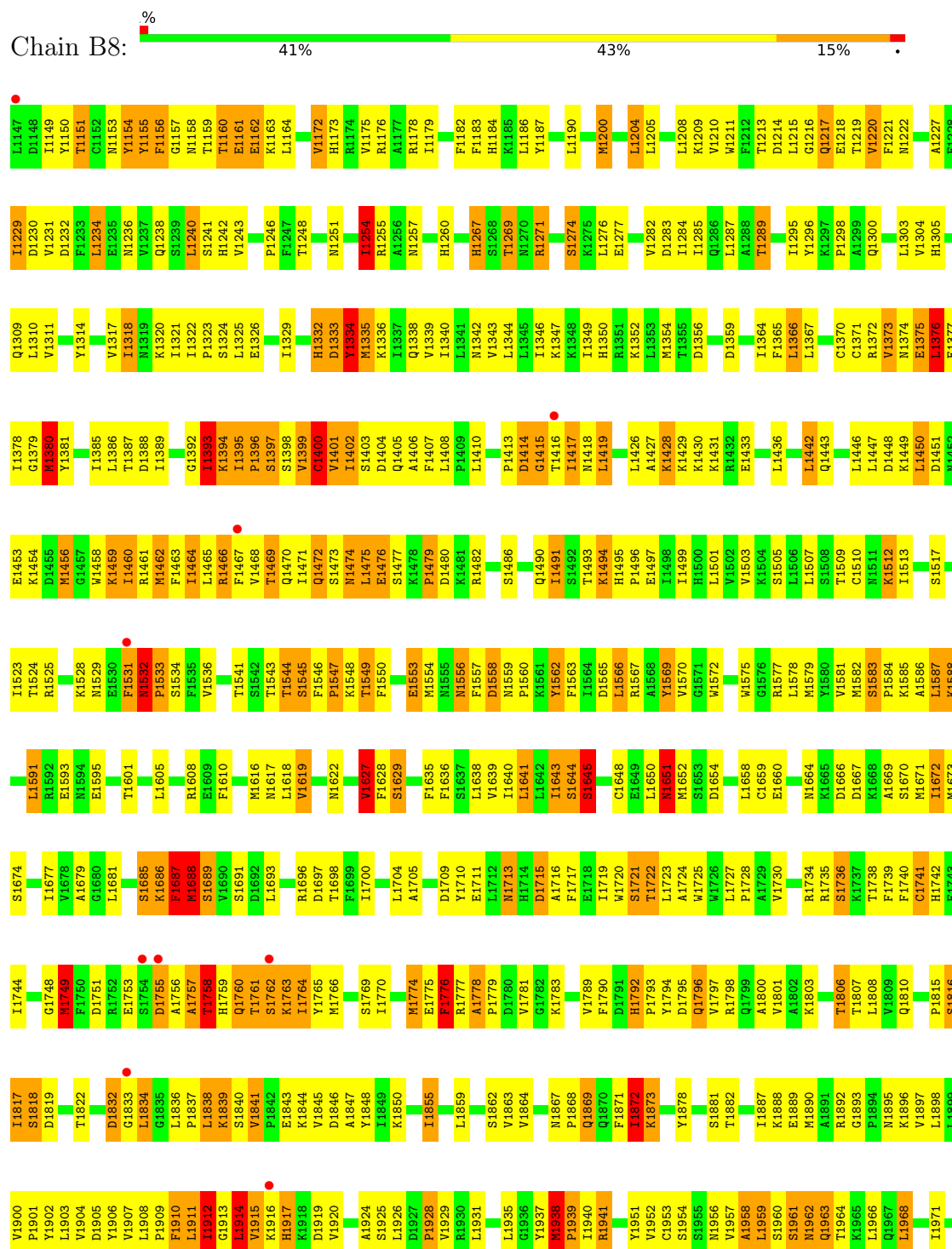


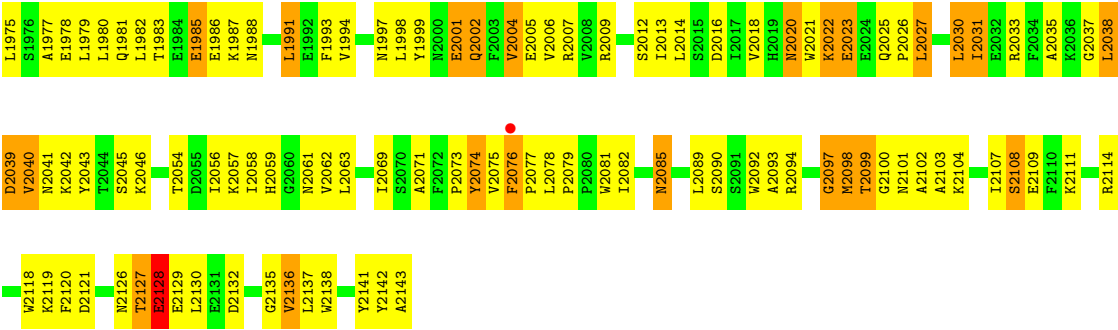
Chain B5: %





• Molecule 17: Proteasome activator BLM10





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	236.12Å 127.74Å 532.67Å 90.00° 102.85° 90.00°	Depositor
Resolution (Å)	29.99 – 3.00 29.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	80.7 (29.99-3.00) 80.6 (29.99-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 3.00Å)	Xtriage
Refinement program	REFMAC, PHENIX (phenix.refine)	Depositor
R, R_{free}	0.196 , 0.250 0.205 , 0.249	Depositor DCC
R_{free} test set	4965 reflections (0.81%)	wwPDB-VP
Wilson B-factor (Å ²)	67.9	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 68.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	158904	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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 ⓘ

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 >5	RMSZ	# Z >5
1	AA	0.78	0/1959	1.06	10/2652 (0.4%)
1	AC	0.61	0/1959	0.98	9/2652 (0.3%)
1	BA	0.55	0/1959	0.97	8/2652 (0.3%)
1	BO	0.55	0/1959	0.96	9/2652 (0.3%)
2	AG	0.71	0/1802	0.95	3/2440 (0.1%)
2	AS	0.58	0/1802	0.91	1/2440 (0.0%)
2	BB	0.52	0/1802	0.89	2/2440 (0.1%)
2	BP	0.50	0/1802	0.89	2/2440 (0.1%)
3	AH	0.56	0/1831	1.02	8/2479 (0.3%)
3	AT	0.56	0/1831	1.01	7/2479 (0.3%)
3	BC	0.51	0/1831	1.00	7/2479 (0.3%)
3	BQ	0.52	0/1831	0.99	6/2479 (0.2%)
4	AI	0.53	0/1808	0.97	8/2446 (0.3%)
4	AU	0.53	0/1808	0.96	8/2446 (0.3%)
4	BD	0.51	0/1808	0.95	7/2446 (0.3%)
4	BR	0.50	0/1808	0.94	8/2446 (0.3%)
5	AJ	0.60	0/1961	0.95	8/2640 (0.3%)
5	AV	0.58	0/1961	0.95	9/2640 (0.3%)
5	BE	0.53	0/1961	0.92	5/2640 (0.2%)
5	BS	0.53	0/1961	0.93	10/2640 (0.4%)
6	AK	0.71	0/1831	0.98	5/2473 (0.2%)
6	AW	0.70	1/1831 (0.1%)	0.96	5/2473 (0.2%)
6	BF	0.56	0/1831	0.92	4/2473 (0.2%)
6	BT	0.57	0/1831	0.91	5/2473 (0.2%)
7	AL	0.74	1/1936 (0.1%)	1.01	7/2613 (0.3%)
7	AX	0.64	0/1936	0.98	8/2613 (0.3%)
7	BG	0.54	0/1936	0.95	9/2613 (0.3%)
7	BU	0.54	0/1936	0.96	8/2613 (0.3%)
8	AB	0.80	0/1539	1.01	5/2084 (0.2%)
8	AD	0.72	0/1539	0.99	6/2084 (0.3%)
8	BH	0.58	0/1539	0.92	4/2084 (0.2%)
8	BV	0.57	0/1539	0.94	6/2084 (0.3%)
9	AM	0.78	0/1716	1.00	8/2326 (0.3%)
9	AY	0.68	0/1716	0.98	3/2326 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	BI	0.55	0/1716	0.93	4/2326 (0.2%)
9	BW	0.54	0/1716	0.93	1/2326 (0.0%)
10	AN	0.70	0/1611	1.08	9/2174 (0.4%)
10	AZ	0.64	0/1611	1.03	6/2174 (0.3%)
10	BJ	0.56	0/1611	0.98	9/2174 (0.4%)
10	BX	0.55	0/1611	0.96	5/2174 (0.2%)
11	A1	0.59	0/1613	0.98	7/2173 (0.3%)
11	AO	0.63	0/1613	1.00	10/2173 (0.5%)
11	BK	0.52	0/1613	0.95	7/2173 (0.3%)
11	BY	0.54	0/1613	0.96	6/2173 (0.3%)
12	A2	0.63	0/1683	0.91	1/2277 (0.0%)
12	AP	0.62	0/1683	0.92	1/2277 (0.0%)
12	BL	0.51	0/1683	0.90	1/2277 (0.0%)
12	BZ	0.50	0/1683	0.89	1/2277 (0.0%)
13	A3	0.71	0/1795	1.06	10/2420 (0.4%)
13	AQ	0.67	0/1795	1.06	11/2420 (0.5%)
13	B1	0.55	0/1795	0.98	6/2420 (0.2%)
13	BM	0.57	0/1795	1.00	8/2420 (0.3%)
14	A4	0.81	0/1855	1.10	12/2514 (0.5%)
14	AR	0.77	0/1855	1.09	8/2514 (0.3%)
14	B2	0.61	0/1855	0.98	5/2514 (0.2%)
14	BN	0.59	0/1855	0.98	5/2514 (0.2%)
15	AE	0.55	0/660	0.94	3/896 (0.3%)
15	AF	0.56	0/660	0.95	5/896 (0.6%)
15	B3	0.53	0/660	0.89	3/896 (0.3%)
15	B6	0.50	0/660	0.93	2/896 (0.2%)
16	A5	0.66	3/6669 (0.0%)	0.97	15/9038 (0.2%)
16	A7	0.60	3/6669 (0.0%)	0.95	16/9038 (0.2%)
16	B4	0.55	1/6669 (0.0%)	0.93	14/9038 (0.2%)
16	B7	0.54	0/6669	0.93	16/9038 (0.2%)
17	A6	0.61	1/8246 (0.0%)	1.01	29/11172 (0.3%)
17	A8	0.60	1/8246 (0.0%)	1.00	37/11172 (0.3%)
17	B5	0.55	0/8246	0.97	26/11172 (0.2%)
17	B8	0.55	1/8246 (0.0%)	0.98	29/11172 (0.3%)
All	All	0.60	12/162060 (0.0%)	0.97	546/219268 (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
16	A5	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	A7	0	1
16	B4	0	1
16	B7	0	1
17	A6	0	1
17	A8	0	1
17	B5	0	1
17	B8	0	2
All	All	0	10

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A5	518	ILE	CA-CB	6.22	1.62	1.54
7	AL	7108	ILE	CA-CB	-6.20	1.51	1.54
16	B4	518	ILE	CA-CB	5.83	1.62	1.54
17	A6	1460	ILE	CA-CB	5.67	1.62	1.54
6	AW	6216	VAL	CA-CB	-5.54	1.51	1.55

The worst 5 of 546 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AH	3014	SER	CA-C-N	12.66	135.67	119.84
3	AH	3014	SER	C-N-CA	12.66	135.67	119.84
3	BQ	3014	SER	CA-C-N	12.47	135.43	119.84
3	BQ	3014	SER	C-N-CA	12.47	135.43	119.84
3	BC	3014	SER	CA-C-N	12.46	135.42	119.84

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	A5	1000	LYS	Peptide
16	A5	486	HIS	Peptide
17	A6	1587	LEU	Peptide
16	A7	486	HIS	Peptide
17	A8	1587	LEU	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	1921	0	1910	64	0
1	AC	1921	0	1910	68	0
1	BA	1921	0	1910	61	0
1	BO	1921	0	1910	62	0
2	AG	1769	0	1784	54	0
2	AS	1769	0	1784	59	0
2	BB	1769	0	1784	57	0
2	BP	1769	0	1784	56	0
3	AH	1803	0	1802	125	0
3	AT	1803	0	1802	129	0
3	BC	1803	0	1802	113	0
3	BQ	1803	0	1802	117	0
4	AI	1783	0	1804	138	0
4	AU	1783	0	1804	130	0
4	BD	1783	0	1804	126	0
4	BR	1783	0	1804	138	0
5	AJ	1934	0	1905	73	0
5	AV	1934	0	1905	72	1
5	BE	1934	0	1905	76	0
5	BS	1934	0	1905	77	0
6	AK	1803	0	1806	96	0
6	AW	1803	0	1806	86	0
6	BF	1803	0	1806	81	0
6	BT	1803	0	1806	85	0
7	AL	1896	0	1884	47	0
7	AX	1896	0	1884	49	0
7	BG	1896	0	1884	45	0
7	BU	1896	0	1884	46	0
8	AB	1510	0	1476	55	0
8	AD	1510	0	1476	54	0
8	BH	1510	0	1476	50	0
8	BV	1510	0	1476	47	0
9	AM	1685	0	1685	45	0
9	AY	1685	0	1685	55	0
9	BI	1685	0	1685	49	0
9	BW	1685	0	1685	50	0
10	AN	1581	0	1571	55	0
10	AZ	1581	0	1571	62	0
10	BJ	1581	0	1571	61	0
10	BX	1581	0	1571	57	0
11	A1	1585	0	1587	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	AO	1585	0	1587	62	0
11	BK	1585	0	1587	58	0
11	BY	1585	0	1587	59	0
12	A2	1646	0	1592	51	0
12	AP	1646	0	1592	54	0
12	BL	1646	0	1592	47	0
12	BZ	1646	0	1592	54	0
13	A3	1757	0	1708	68	0
13	AQ	1757	0	1708	68	0
13	B1	1757	0	1708	71	0
13	BM	1757	0	1708	65	0
14	A4	1824	0	1829	71	0
14	AR	1824	0	1829	70	0
14	B2	1824	0	1829	75	0
14	BN	1824	0	1829	65	0
15	AE	642	0	618	27	0
15	AF	642	0	618	31	0
15	B3	642	0	618	29	0
15	B6	642	0	618	30	0
16	A5	6517	0	6442	378	0
16	A7	6517	0	6442	382	1
16	B4	6517	0	6442	348	0
16	B7	6517	0	6442	369	0
17	A6	8070	0	8156	592	0
17	A8	8070	0	8156	597	0
17	B5	8070	0	8156	563	0
17	B8	8070	0	8156	585	0
All	All	158904	0	158236	7255	1

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 23.

The worst 5 of 7255 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)
11:A1:401:MET:HA	11:A1:4001:ASP:HB2	1.17	1.17
17:B8:1396:PRO:HA	17:B8:1475:LEU:HD22	1.28	1.13
17:A8:1396:PRO:HA	17:A8:1475:LEU:HD22	1.31	1.12
3:AH:3070:ASN:ND2	3:AH:3072:LYS:H	1.48	1.11
3:BQ:3070:ASN:ND2	3:BQ:3072:LYS:H	1.47	1.11

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AV:5190:SER:OG	16:A7:1000:LYS:NZ[1_565]	2.18	0.02

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	AA	241/243 (99%)	221 (92%)	17 (7%)	3 (1%)	10	40
1	AC	241/243 (99%)	222 (92%)	16 (7%)	3 (1%)	10	40
1	BA	241/243 (99%)	224 (93%)	14 (6%)	3 (1%)	10	40
1	BO	241/243 (99%)	225 (93%)	13 (5%)	3 (1%)	10	40
2	AG	229/231 (99%)	212 (93%)	13 (6%)	4 (2%)	7	32
2	AS	229/231 (99%)	211 (92%)	15 (7%)	3 (1%)	9	38
2	BB	229/231 (99%)	214 (93%)	13 (6%)	2 (1%)	14	48
2	BP	229/231 (99%)	211 (92%)	16 (7%)	2 (1%)	14	48
3	AH	230/232 (99%)	186 (81%)	25 (11%)	19 (8%)	0	3
3	AT	230/232 (99%)	185 (80%)	27 (12%)	18 (8%)	1	4
3	BC	230/232 (99%)	188 (82%)	25 (11%)	17 (7%)	1	4
3	BQ	230/232 (99%)	188 (82%)	24 (10%)	18 (8%)	1	4
4	AI	225/227 (99%)	167 (74%)	45 (20%)	13 (6%)	1	8
4	AU	225/227 (99%)	168 (75%)	43 (19%)	14 (6%)	1	6
4	BD	225/227 (99%)	168 (75%)	44 (20%)	13 (6%)	1	8
4	BR	225/227 (99%)	169 (75%)	42 (19%)	14 (6%)	1	6
5	AJ	248/250 (99%)	215 (87%)	21 (8%)	12 (5%)	2	11
5	AV	248/250 (99%)	214 (86%)	22 (9%)	12 (5%)	2	11
5	BE	248/250 (99%)	216 (87%)	20 (8%)	12 (5%)	2	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	BS	248/250 (99%)	215 (87%)	21 (8%)	12 (5%)	2	11
6	AK	232/234 (99%)	211 (91%)	17 (7%)	4 (2%)	7	32
6	AW	232/234 (99%)	212 (91%)	16 (7%)	4 (2%)	7	32
6	BF	232/234 (99%)	212 (91%)	16 (7%)	4 (2%)	7	32
6	BT	232/234 (99%)	212 (91%)	17 (7%)	3 (1%)	9	38
7	AL	242/244 (99%)	221 (91%)	20 (8%)	1 (0%)	30	65
7	AX	242/244 (99%)	223 (92%)	17 (7%)	2 (1%)	16	50
7	BG	242/244 (99%)	224 (93%)	17 (7%)	1 (0%)	30	65
7	BU	242/244 (99%)	222 (92%)	18 (7%)	2 (1%)	16	50
8	AB	194/196 (99%)	174 (90%)	18 (9%)	2 (1%)	12	45
8	AD	194/196 (99%)	172 (89%)	19 (10%)	3 (2%)	8	35
8	BH	194/196 (99%)	175 (90%)	17 (9%)	2 (1%)	12	45
8	BV	194/196 (99%)	177 (91%)	15 (8%)	2 (1%)	12	45
9	AM	220/222 (99%)	202 (92%)	16 (7%)	2 (1%)	14	48
9	AY	220/222 (99%)	201 (91%)	17 (8%)	2 (1%)	14	48
9	BI	220/222 (99%)	203 (92%)	15 (7%)	2 (1%)	14	48
9	BW	220/222 (99%)	201 (91%)	17 (8%)	2 (1%)	14	48
10	AN	202/204 (99%)	182 (90%)	16 (8%)	4 (2%)	6	28
10	AZ	202/204 (99%)	184 (91%)	16 (8%)	2 (1%)	12	45
10	BJ	202/204 (99%)	187 (93%)	13 (6%)	2 (1%)	12	45
10	BX	202/204 (99%)	184 (91%)	17 (8%)	1 (0%)	24	60
11	A1	196/198 (99%)	175 (89%)	14 (7%)	7 (4%)	2	16
11	AO	196/198 (99%)	176 (90%)	14 (7%)	6 (3%)	3	19
11	BK	196/198 (99%)	175 (89%)	15 (8%)	6 (3%)	3	19
11	BY	196/198 (99%)	175 (89%)	14 (7%)	7 (4%)	2	16
12	A2	210/212 (99%)	190 (90%)	19 (9%)	1 (0%)	24	60
12	AP	210/212 (99%)	191 (91%)	19 (9%)	0	100	100
12	BL	210/212 (99%)	191 (91%)	18 (9%)	1 (0%)	24	60
12	BZ	210/212 (99%)	189 (90%)	21 (10%)	0	100	100
13	A3	220/222 (99%)	203 (92%)	13 (6%)	4 (2%)	6	31
13	AQ	220/222 (99%)	200 (91%)	16 (7%)	4 (2%)	6	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	B1	220/222 (99%)	202 (92%)	14 (6%)	4 (2%)	6	31
13	BM	220/222 (99%)	201 (91%)	17 (8%)	2 (1%)	14	48
14	A4	231/233 (99%)	211 (91%)	16 (7%)	4 (2%)	7	32
14	AR	231/233 (99%)	212 (92%)	16 (7%)	3 (1%)	9	38
14	B2	231/233 (99%)	212 (92%)	16 (7%)	3 (1%)	9	38
14	BN	231/233 (99%)	213 (92%)	15 (6%)	3 (1%)	9	38
15	AE	74/76 (97%)	67 (90%)	7 (10%)	0	100	100
15	AF	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
15	B3	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
15	B6	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
16	A5	797/799 (100%)	646 (81%)	109 (14%)	42 (5%)	1	9
16	A7	797/799 (100%)	640 (80%)	111 (14%)	46 (6%)	1	8
16	B4	797/799 (100%)	651 (82%)	107 (13%)	39 (5%)	1	10
16	B7	797/799 (100%)	639 (80%)	116 (15%)	42 (5%)	1	9
17	A6	995/997 (100%)	782 (79%)	128 (13%)	85 (8%)	0	3
17	A8	995/997 (100%)	775 (78%)	133 (13%)	87 (9%)	0	3
17	B5	995/997 (100%)	780 (78%)	134 (14%)	81 (8%)	1	3
17	B8	995/997 (100%)	776 (78%)	135 (14%)	84 (8%)	0	3
All	All	19944/20080 (99%)	17074 (86%)	2065 (10%)	805 (4%)	2	14

5 of 805 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AH	3130	PRO
3	AH	3145	GLY
3	AH	3200	THR
3	AH	3243	GLY
4	AI	4050	SER

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	AA	207/207 (100%)	184 (89%)	23 (11%)	6	25
1	AC	207/207 (100%)	186 (90%)	21 (10%)	7	29
1	BA	207/207 (100%)	186 (90%)	21 (10%)	7	29
1	BO	207/207 (100%)	188 (91%)	19 (9%)	8	33
2	AG	192/192 (100%)	165 (86%)	27 (14%)	3	16
2	AS	192/192 (100%)	165 (86%)	27 (14%)	3	16
2	BB	192/192 (100%)	166 (86%)	26 (14%)	4	18
2	BP	192/192 (100%)	165 (86%)	27 (14%)	3	16
3	AH	192/192 (100%)	160 (83%)	32 (17%)	2	12
3	AT	192/192 (100%)	161 (84%)	31 (16%)	2	12
3	BC	192/192 (100%)	158 (82%)	34 (18%)	2	10
3	BQ	192/192 (100%)	158 (82%)	34 (18%)	2	10
4	AI	202/202 (100%)	175 (87%)	27 (13%)	4	18
4	AU	202/202 (100%)	175 (87%)	27 (13%)	4	18
4	BD	202/202 (100%)	177 (88%)	25 (12%)	4	20
4	BR	202/202 (100%)	175 (87%)	27 (13%)	4	18
5	AJ	206/206 (100%)	177 (86%)	29 (14%)	3	16
5	AV	206/206 (100%)	177 (86%)	29 (14%)	3	16
5	BE	206/206 (100%)	176 (85%)	30 (15%)	3	15
5	BS	206/206 (100%)	176 (85%)	30 (15%)	3	15
6	AK	193/193 (100%)	165 (86%)	28 (14%)	3	15
6	AW	193/193 (100%)	165 (86%)	28 (14%)	3	15
6	BF	193/193 (100%)	163 (84%)	30 (16%)	2	13
6	BT	193/193 (100%)	163 (84%)	30 (16%)	2	13
7	AL	201/201 (100%)	178 (89%)	23 (11%)	5	24
7	AX	201/201 (100%)	178 (89%)	23 (11%)	5	24
7	BG	201/201 (100%)	178 (89%)	23 (11%)	5	24
7	BU	201/201 (100%)	178 (89%)	23 (11%)	5	24
8	AB	161/161 (100%)	141 (88%)	20 (12%)	4	20
8	AD	161/161 (100%)	142 (88%)	19 (12%)	5	22
8	BH	161/161 (100%)	143 (89%)	18 (11%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	BV	161/161 (100%)	144 (89%)	17 (11%)	6	27
9	AM	181/181 (100%)	161 (89%)	20 (11%)	6	25
9	AY	181/181 (100%)	160 (88%)	21 (12%)	5	23
9	BI	181/181 (100%)	161 (89%)	20 (11%)	6	25
9	BW	181/181 (100%)	162 (90%)	19 (10%)	6	27
10	AN	172/172 (100%)	153 (89%)	19 (11%)	6	25
10	AZ	172/172 (100%)	154 (90%)	18 (10%)	6	27
10	BJ	172/172 (100%)	153 (89%)	19 (11%)	6	25
10	BX	172/172 (100%)	152 (88%)	20 (12%)	5	23
11	A1	175/175 (100%)	162 (93%)	13 (7%)	13	42
11	AO	175/175 (100%)	161 (92%)	14 (8%)	11	38
11	BK	175/175 (100%)	161 (92%)	14 (8%)	11	38
11	BY	175/175 (100%)	161 (92%)	14 (8%)	11	38
12	A2	169/169 (100%)	150 (89%)	19 (11%)	6	24
12	AP	169/169 (100%)	149 (88%)	20 (12%)	5	22
12	BL	169/169 (100%)	152 (90%)	17 (10%)	7	29
12	BZ	169/169 (100%)	151 (89%)	18 (11%)	6	26
13	A3	185/185 (100%)	165 (89%)	20 (11%)	6	26
13	AQ	185/185 (100%)	165 (89%)	20 (11%)	6	26
13	B1	185/185 (100%)	165 (89%)	20 (11%)	6	26
13	BM	185/185 (100%)	165 (89%)	20 (11%)	6	26
14	A4	199/199 (100%)	172 (86%)	27 (14%)	3	17
14	AR	199/199 (100%)	173 (87%)	26 (13%)	4	19
14	B2	199/199 (100%)	172 (86%)	27 (14%)	3	17
14	BN	199/199 (100%)	173 (87%)	26 (13%)	4	19
15	AE	73/73 (100%)	66 (90%)	7 (10%)	8	31
15	AF	73/73 (100%)	66 (90%)	7 (10%)	8	31
15	B3	73/73 (100%)	66 (90%)	7 (10%)	8	31
15	B6	73/73 (100%)	66 (90%)	7 (10%)	8	31
16	A5	744/744 (100%)	644 (87%)	100 (13%)	4	18
16	A7	744/744 (100%)	644 (87%)	100 (13%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	B4	744/744 (100%)	642 (86%)	102 (14%)	3	17
16	B7	744/744 (100%)	646 (87%)	98 (13%)	4	18
17	A6	909/909 (100%)	757 (83%)	152 (17%)	2	12
17	A8	909/909 (100%)	758 (83%)	151 (17%)	2	12
17	B5	909/909 (100%)	758 (83%)	151 (17%)	2	12
17	B8	909/909 (100%)	757 (83%)	152 (17%)	2	12
All	All	17444/17444 (100%)	15111 (87%)	2333 (13%)	4	18

5 of 2333 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	B4	502	SER
17	B8	1872	ILE
16	B4	869	VAL
16	B4	489	SER
15	B6	104	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 612 such sidechains are listed below:

Mol	Chain	Res	Type
7	BU	7011	ASN
16	B7	539	HIS
9	BW	2030	ASN
6	BT	6210	ASN
16	B4	351	HIS

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 oligosaccharides 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.

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	AA	243/243 (100%)	-0.45	0 100 100	37, 67, 125, 215	0
1	AC	243/243 (100%)	-0.55	0 100 100	52, 87, 139, 216	0
1	BA	243/243 (100%)	-0.02	0 100 100	79, 107, 150, 217	0
1	BO	243/243 (100%)	-0.35	0 100 100	75, 101, 145, 217	0
2	AG	231/231 (100%)	-0.60	0 100 100	42, 72, 115, 150	0
2	AS	231/231 (100%)	-0.62	0 100 100	54, 86, 122, 161	0
2	BB	231/231 (100%)	-0.10	0 100 100	84, 109, 139, 166	0
2	BP	231/231 (100%)	-0.54	0 100 100	69, 98, 129, 164	0
3	AH	232/232 (100%)	-0.14	1 (0%) 88 76	56, 113, 176, 219	0
3	AT	232/232 (100%)	-0.26	0 100 100	65, 114, 180, 223	0
3	BC	232/232 (100%)	-0.05	1 (0%) 88 76	88, 132, 182, 227	0
3	BQ	232/232 (100%)	-0.13	1 (0%) 88 76	81, 123, 180, 227	0
4	AI	227/227 (100%)	-0.17	0 100 100	63, 126, 187, 212	0
4	AU	227/227 (100%)	-0.06	3 (1%) 75 53	70, 127, 188, 224	0
4	BD	227/227 (100%)	-0.08	1 (0%) 88 76	89, 137, 193, 222	0
4	BR	227/227 (100%)	-0.07	1 (0%) 88 76	88, 135, 189, 220	0
5	AJ	250/250 (100%)	-0.37	1 (0%) 88 76	60, 99, 188, 246	0
5	AV	250/250 (100%)	-0.30	1 (0%) 88 76	59, 102, 194, 246	0
5	BE	250/250 (100%)	-0.11	1 (0%) 88 76	80, 117, 192, 245	0
5	BS	250/250 (100%)	-0.18	2 (0%) 82 64	82, 115, 191, 246	0
6	AK	234/234 (100%)	-0.60	0 100 100	51, 79, 119, 232	0
6	AW	234/234 (100%)	-0.53	0 100 100	51, 82, 121, 235	0
6	BF	234/234 (100%)	-0.22	0 100 100	77, 104, 133, 235	0
6	BT	234/234 (100%)	-0.11	1 (0%) 88 76	78, 102, 133, 236	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
7	AL	244/244 (100%)	-0.51	0	100	100	41, 72, 122, 153	0
7	AX	244/244 (100%)	-0.60	1 (0%)	88	76	53, 84, 131, 156	0
7	BG	244/244 (100%)	-0.09	1 (0%)	88	76	78, 105, 142, 165	0
7	BU	244/244 (100%)	-0.15	0	100	100	72, 101, 143, 163	0
8	AB	196/196 (100%)	-0.72	0	100	100	38, 61, 95, 139	0
8	AD	196/196 (100%)	-0.73	0	100	100	41, 66, 101, 147	0
8	BH	196/196 (100%)	-0.25	0	100	100	71, 94, 119, 155	0
8	BV	196/196 (100%)	-0.16	0	100	100	72, 92, 119, 152	0
9	AM	222/222 (100%)	-0.67	0	100	100	41, 62, 100, 198	0
9	AY	222/222 (100%)	-0.70	0	100	100	48, 74, 107, 195	0
9	BI	222/222 (100%)	-0.10	0	100	100	74, 98, 125, 199	0
9	BW	222/222 (100%)	-0.46	0	100	100	73, 93, 119, 197	0
10	AN	204/204 (100%)	-0.69	0	100	100	34, 67, 97, 145	0
10	AZ	204/204 (100%)	-0.70	0	100	100	49, 74, 102, 146	0
10	BJ	204/204 (100%)	-0.33	0	100	100	71, 99, 125, 157	0
10	BX	204/204 (100%)	-0.48	0	100	100	69, 90, 118, 162	0
11	A1	198/198 (100%)	-0.66	0	100	100	49, 82, 119, 220	0
11	AO	198/198 (100%)	-0.61	0	100	100	49, 80, 118, 223	0
11	BK	198/198 (100%)	-0.49	0	100	100	76, 102, 130, 225	0
11	BY	198/198 (100%)	-0.48	0	100	100	69, 99, 128, 223	0
12	A2	212/212 (100%)	-0.63	0	100	100	54, 78, 117, 138	0
12	AP	212/212 (100%)	-0.64	0	100	100	56, 82, 118, 139	0
12	BL	212/212 (100%)	-0.41	0	100	100	74, 98, 127, 149	0
12	BZ	212/212 (100%)	-0.50	0	100	100	66, 100, 129, 150	0
13	A3	222/222 (100%)	-0.67	0	100	100	45, 70, 109, 168	0
13	AQ	222/222 (100%)	-0.74	0	100	100	51, 75, 111, 169	0
13	B1	222/222 (100%)	-0.33	0	100	100	71, 100, 127, 170	0
13	BM	222/222 (100%)	-0.46	0	100	100	70, 94, 121, 173	0
14	A4	233/233 (100%)	-0.72	0	100	100	35, 63, 94, 113	0
14	AR	233/233 (100%)	-0.72	1 (0%)	88	76	43, 65, 96, 115	0
14	B2	233/233 (100%)	-0.10	0	100	100	70, 95, 120, 165	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
14	BN	233/233 (100%)	-0.42	0 100 100	69, 93, 115, 134	0
15	AE	76/76 (100%)	-0.37	0 100 100	71, 103, 142, 147	0
15	AF	76/76 (100%)	-0.37	0 100 100	73, 107, 139, 145	0
15	B3	76/76 (100%)	-0.01	0 100 100	101, 129, 146, 155	0
15	B6	76/76 (100%)	-0.29	0 100 100	78, 118, 144, 151	0
16	A5	799/799 (100%)	-0.44	1 (0%) 92 86	45, 87, 141, 267	0
16	A7	799/799 (100%)	-0.43	0 100 100	54, 95, 144, 267	0
16	B4	799/799 (100%)	-0.07	1 (0%) 92 86	82, 115, 155, 265	0
16	B7	799/799 (100%)	-0.30	1 (0%) 92 86	72, 105, 149, 266	0
17	A6	997/997 (100%)	-0.23	4 (0%) 88 76	55, 107, 166, 261	0
17	A8	997/997 (100%)	-0.21	13 (1%) 75 53	63, 108, 167, 260	0
17	B5	997/997 (100%)	0.01	6 (0%) 85 69	83, 128, 173, 261	0
17	B8	997/997 (100%)	-0.19	10 (1%) 79 59	77, 114, 170, 261	0
All	All	20080/20080 (100%)	-0.33	53 (0%) 90 79	34, 100, 158, 267	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	B8	1416	THR	6.1
17	A8	1416	THR	4.8
17	B5	2076	PHE	3.8
17	A8	2096	SER	3.6
17	A8	2076	PHE	3.4

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

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.