wwPDB X-ray Structure Validation Summary Report (i)

Feb 22, 2024 – 10:14 AM EST

PDB ID	:	4V7O
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 (i) 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 (i)) were used in the production of this report:

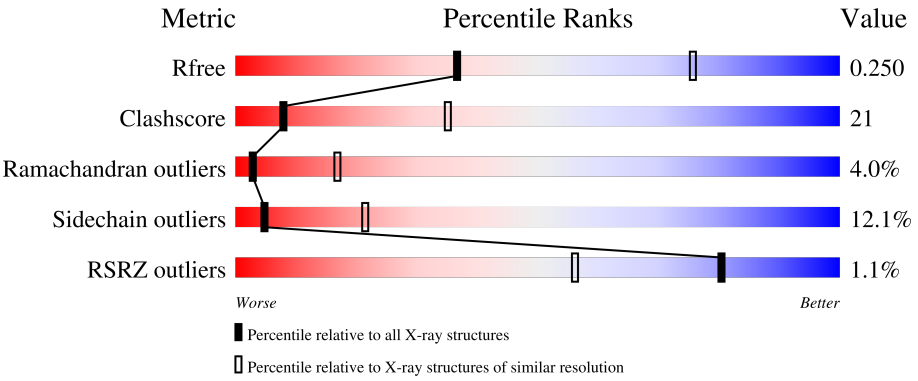
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 <=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	67% 28% 5%
1	AC	243	64% 30% 6%
1	BA	243	2% 67% 29% .
1	BO	243	% 66% 30% .
2	AG	231	70% 26% .

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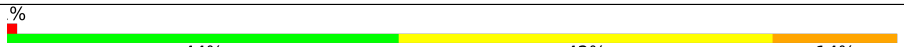
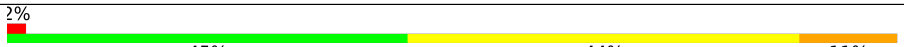
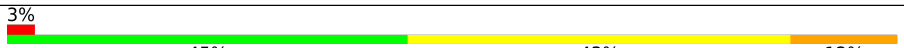
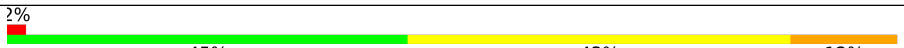
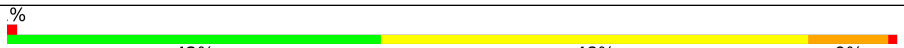
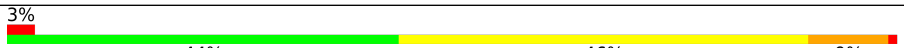
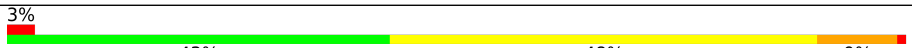
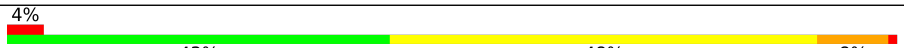
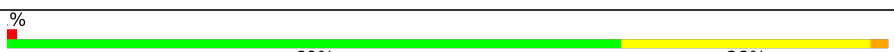
Mol	Chain	Length	Quality of chain
2	AS	231	
2	BB	231	
2	BP	231	
3	AH	232	
3	AT	232	
3	BC	232	
3	BQ	232	
4	AI	227	
4	AU	227	
4	BD	227	
4	BR	227	
5	AJ	250	
5	AV	250	
5	BE	250	
5	BS	250	
6	AK	234	
6	AW	234	
6	BF	234	
6	BT	234	
7	AL	244	
7	AX	244	
7	BG	244	
7	BU	244	
8	AB	196	
8	AD	196	

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Mol	Chain	Length	Quality of chain
8	BH	196	68% 27% 6%
8	BV	196	68% 27% 5%
9	AM	222	73% 23%
9	AY	222	70% 26%
9	BI	222	70% 26%
9	BW	222	72% 25%
10	AN	204	62% 33%
10	AZ	204	62% 33% 5%
10	BJ	204	61% 35%
10	BX	204	61% 34% 5%
11	A1	198	60% 35%
11	AO	198	64% 32%
11	BK	198	64% 31%
11	BY	198	61% 34%
12	A2	212	72% 25%
12	AP	212	69% 27%
12	BL	212	72% 25%
12	BZ	212	71% 25%
13	A3	222	62% 35%
13	AQ	222	66% 29% 5%
13	B1	222	68% 27%
13	BM	222	66% 29% 5%
14	A4	233	63% 31% 5%
14	AR	233	62% 31% 6%
14	B2	233	64% 30% 6%

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Mol	Chain	Length	Quality of chain
14	BN	233	64% 30% 5%
15	AE	76	66% 29% 5%
15	AF	76	63% 33%
15	B3	76	63% 33%
15	B6	76	63% 32% 5%
16	A5	799	52% 38% 9%
16	A7	799	51% 39% 10%
16	B4	799	53% 38% 9%
16	B7	799	51% 39% 10%
17	A6	997	43% 43% 13%
17	A8	997	44% 42% 13%
17	B5	997	44% 42% 12%
17	B8	997	44% 42% 13%

2 Entry composition (i)

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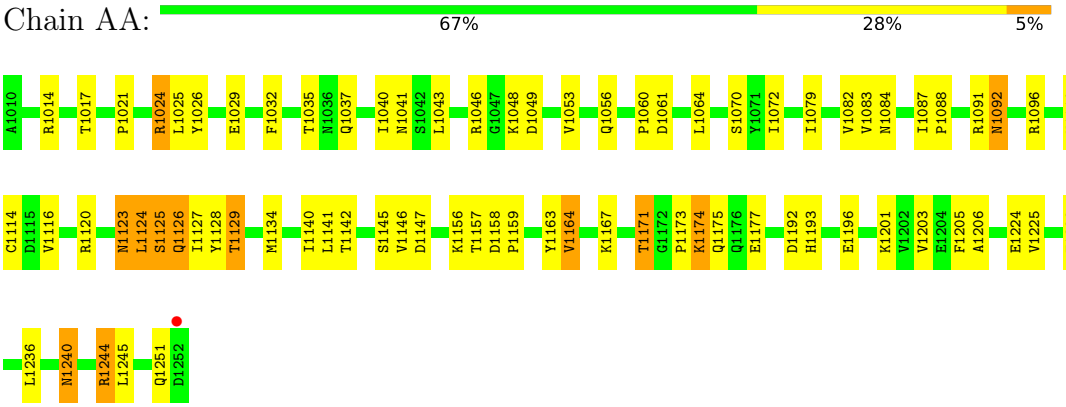
Chain	Residue	Modelled	Actual	Comment	Reference
B8	1171	ASN	GLN	conflict	UNP P43583
B8	2085	ASN	GLN	conflict	UNP P43583
B8	2101	ASN	GLN	conflict	UNP P43583

3 Residue-property plots (i)

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.

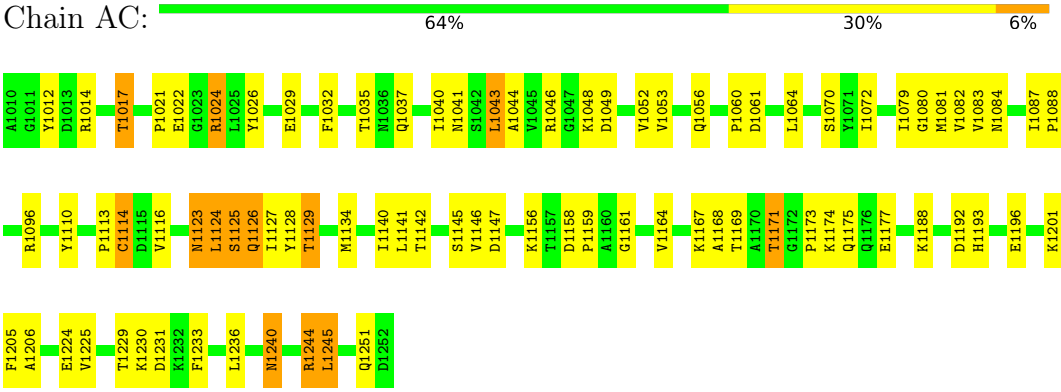
• Molecule 1: Proteasome component C7-alpha

Chain AA:



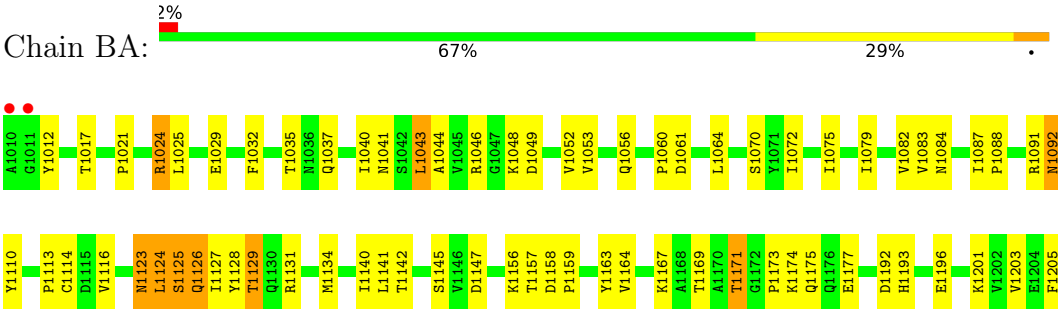
• Molecule 1: Proteasome component C7-alpha

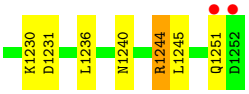
Chain AC:



• Molecule 1: Proteasome component C7-alpha

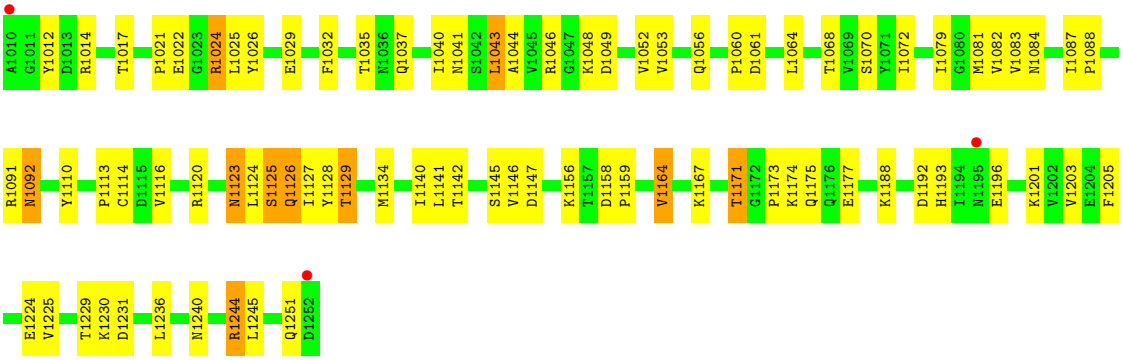
Chain BA:





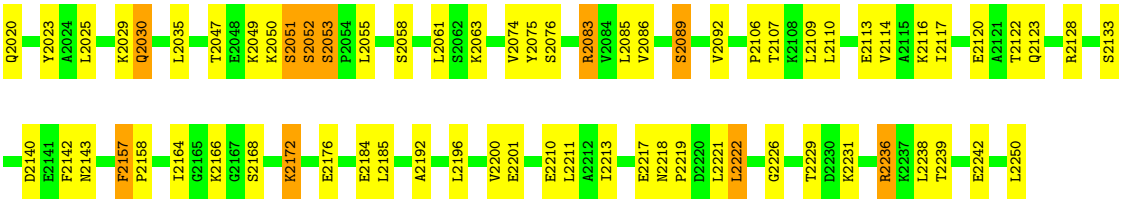
• Molecule 1: Proteasome component C7-alpha

Chain BO:



• Molecule 2: Proteasome component Y7

Chain AG:

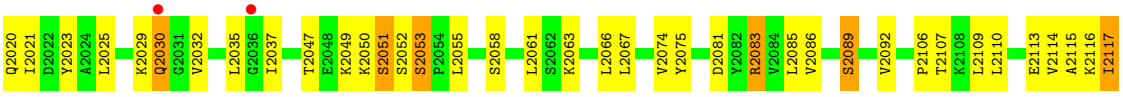


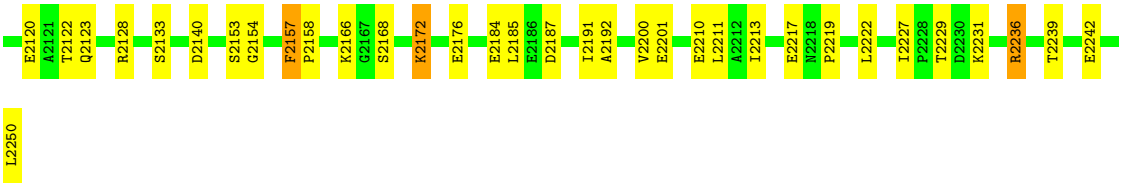
• Molecule 2: Proteasome component Y7

Chain AS:

• Molecule 2: Proteasome component Y7

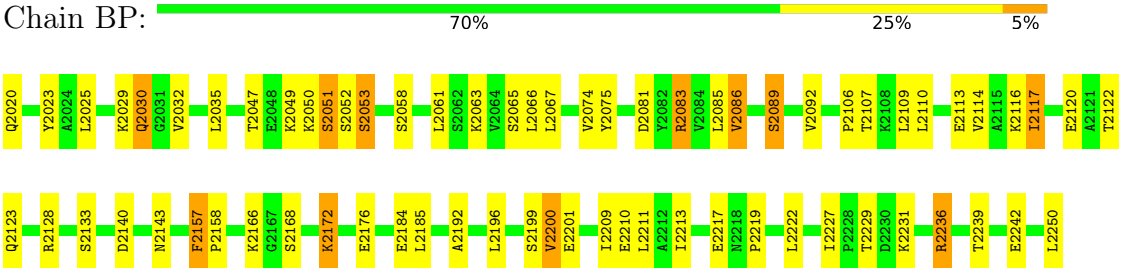
Chain BB:





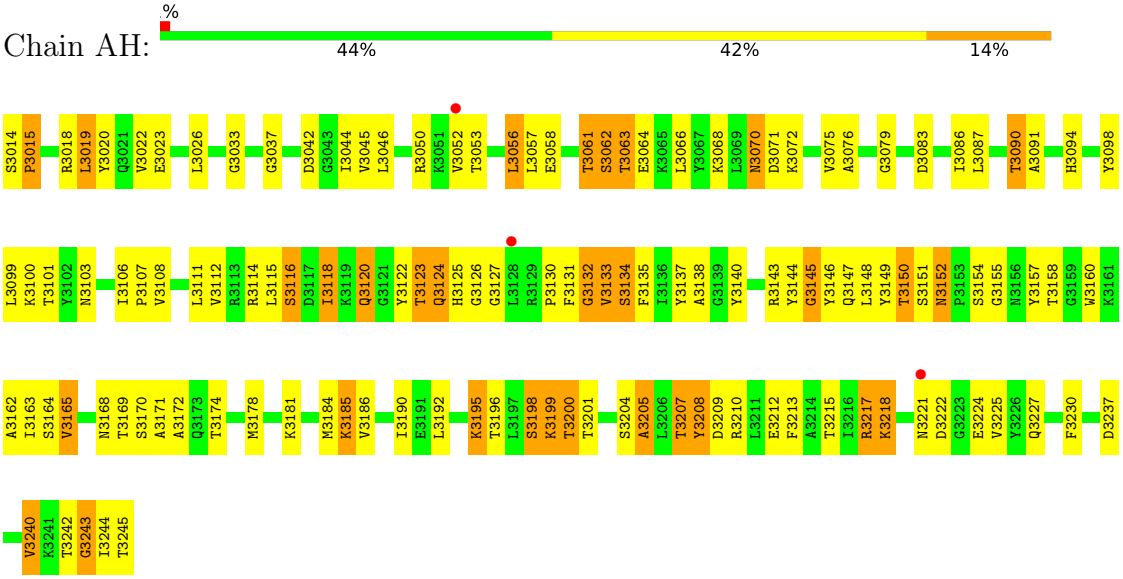
• Molecule 2: Proteasome component Y7

Chain BP:



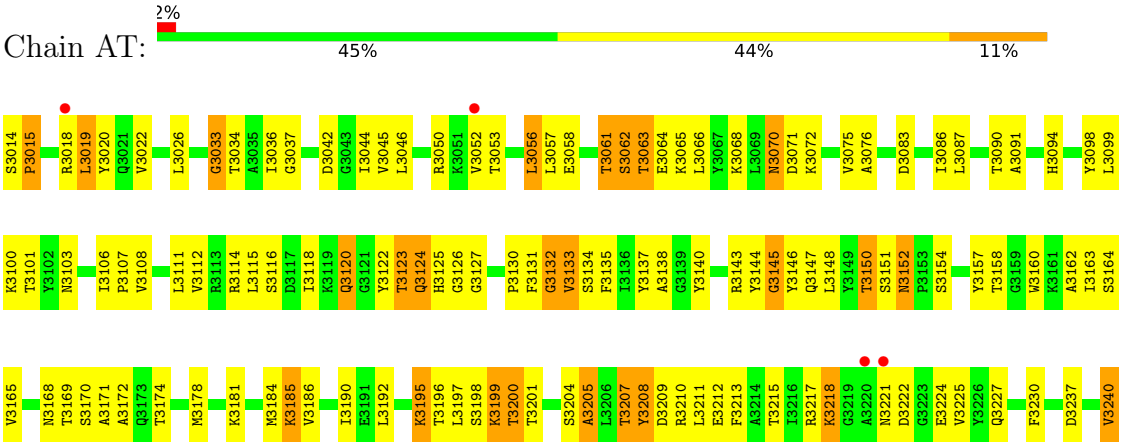
• Molecule 3: Proteasome component Y13

Chain AH:



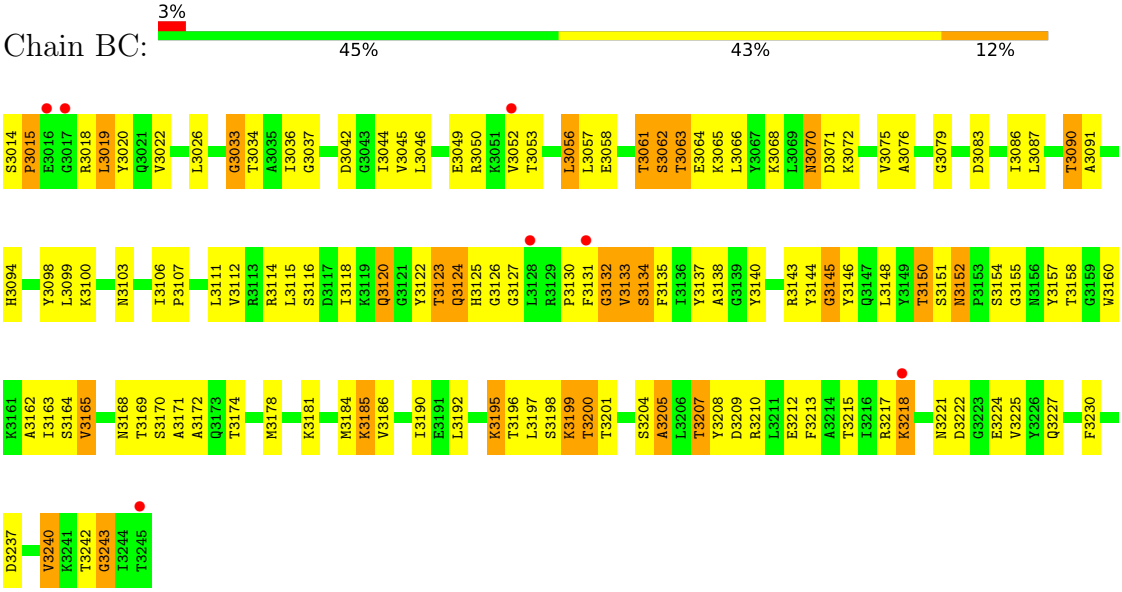
• Molecule 3: Proteasome component Y13

Chain AT:



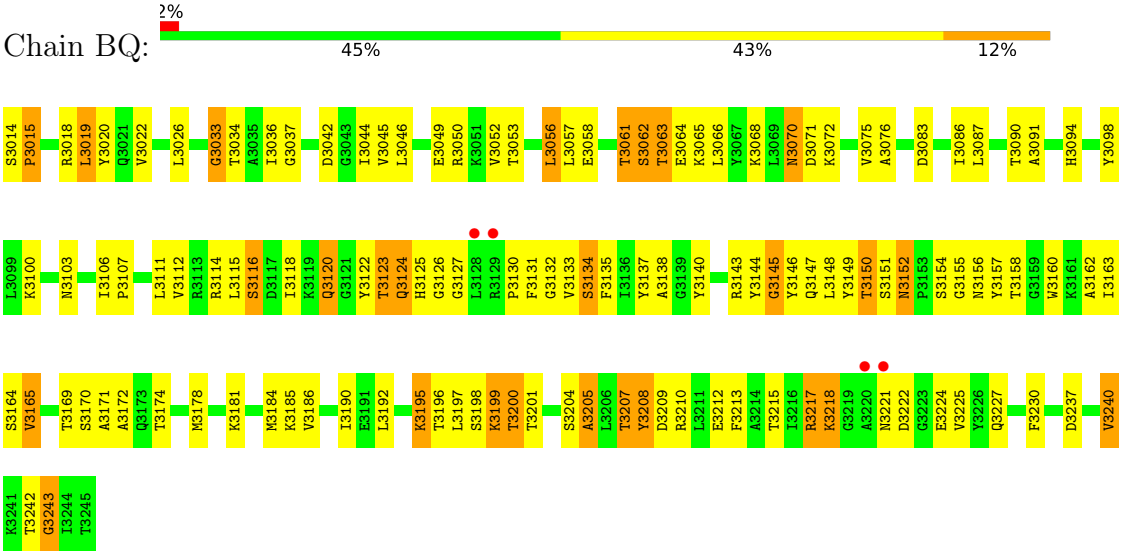
• Molecule 3: Proteasome component Y13

Chain BC:



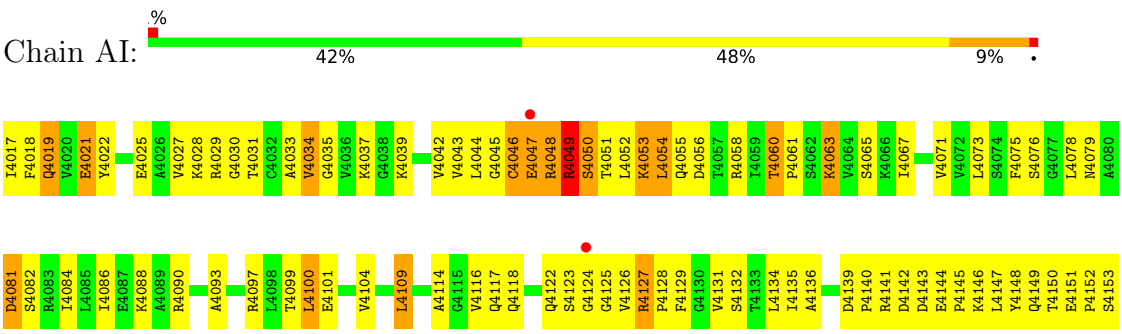
• Molecule 3: Proteasome component Y13

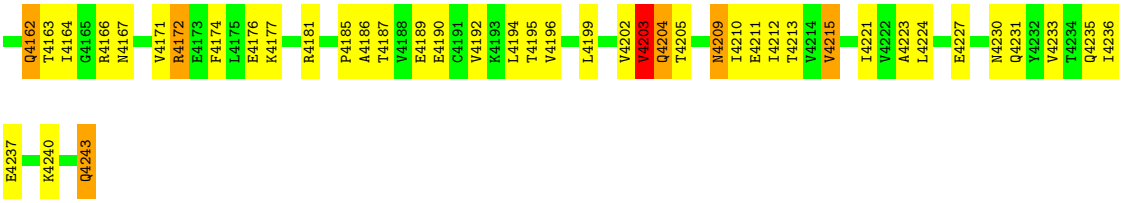
Chain BQ:



• Molecule 4: Proteasome component PRE6

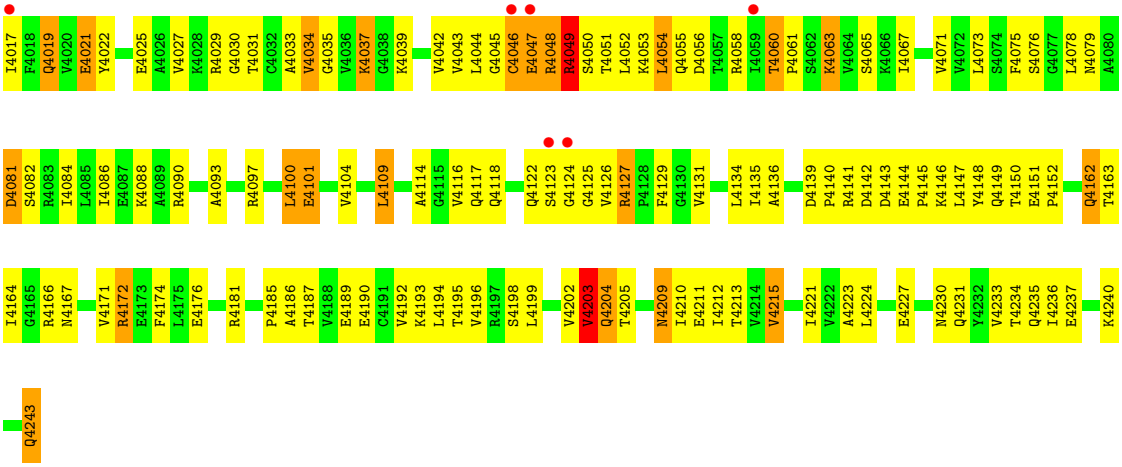
Chain AI:





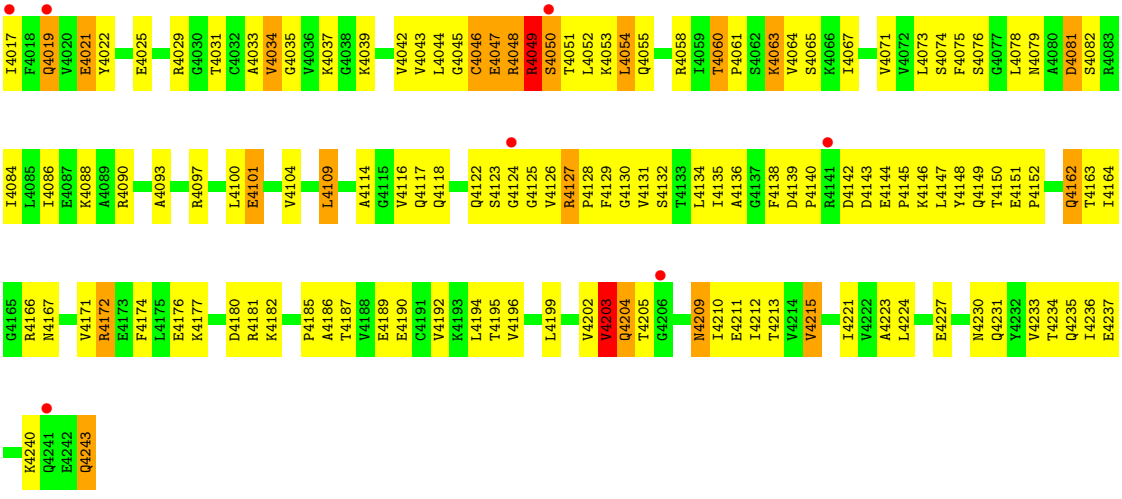
• Molecule 4: Proteasome component PRE6

Chain AU:



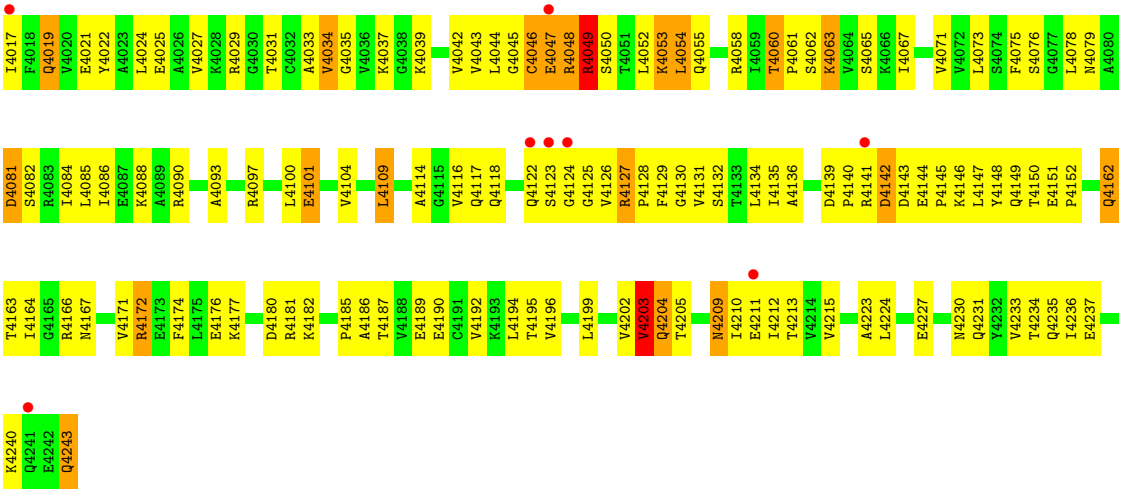
• Molecule 4: Proteasome component PRE6

Chain BD:



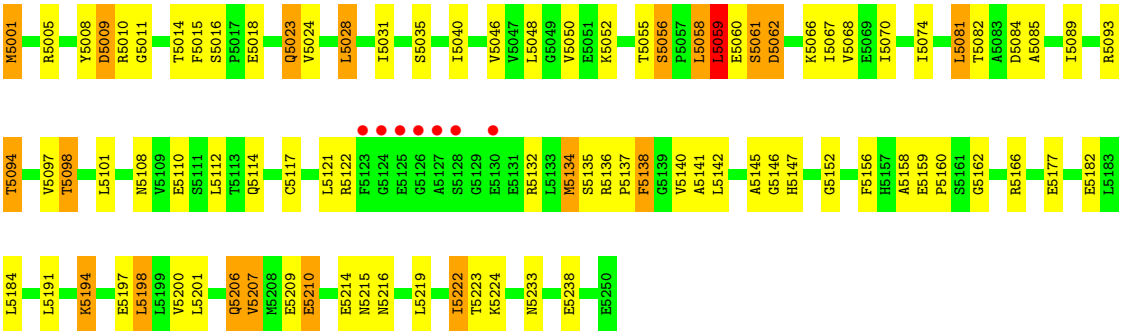
• Molecule 4: Proteasome component PRE6

Chain BR:



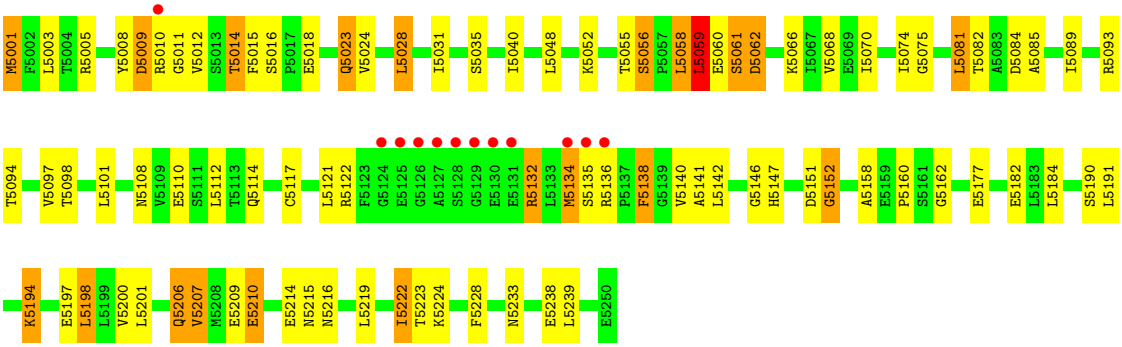
• Molecule 5: Proteasome component PUP2

Chain AJ:



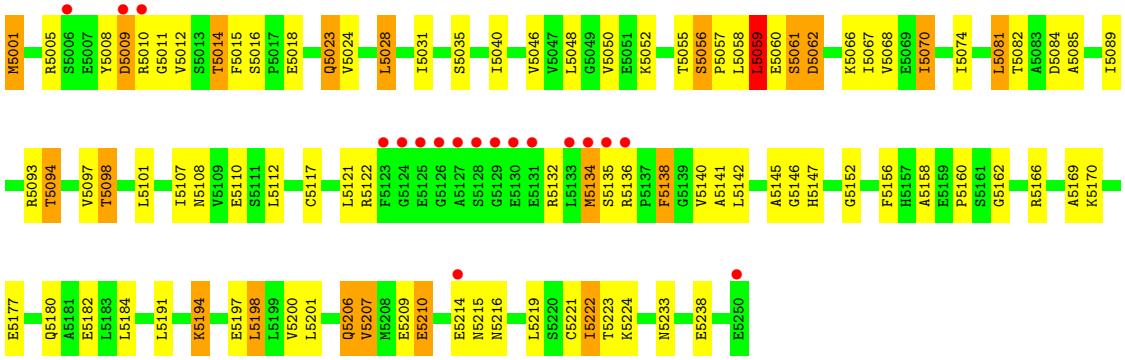
• Molecule 5: Proteasome component PUP2

Chain AV:



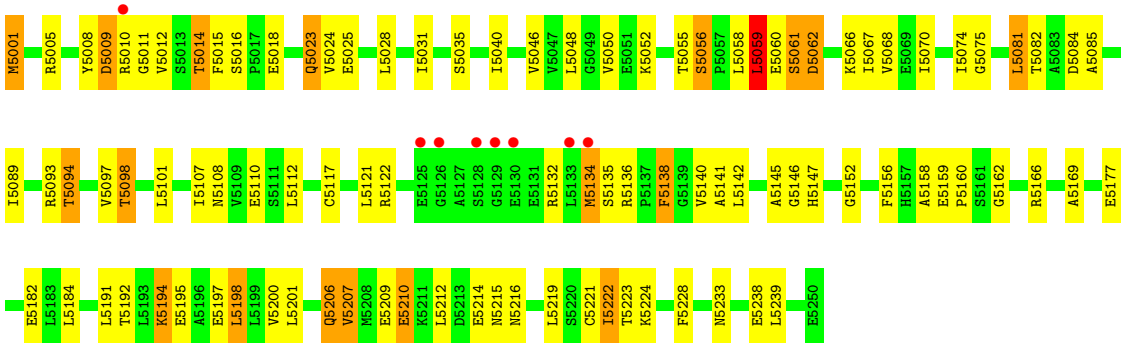
• Molecule 5: Proteasome component PUP2

Chain BE:



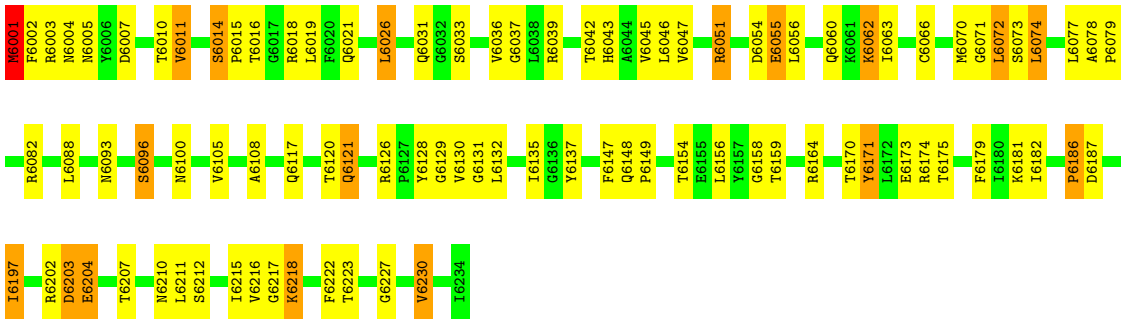
• Molecule 5: Proteasome component PUP2

Chain BS:



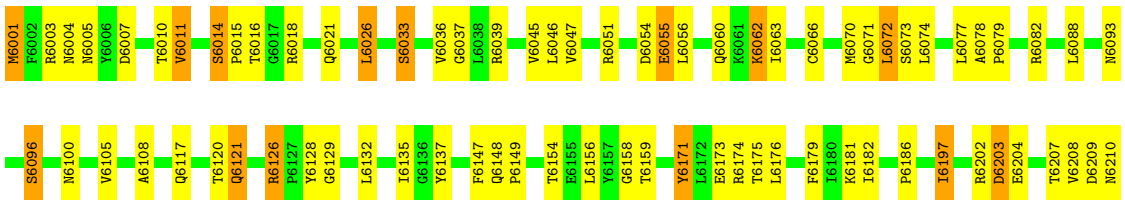
• Molecule 6: Proteasome component PRE5

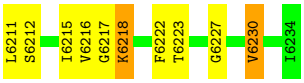
Chain AK:



• Molecule 6: Proteasome component PRE5

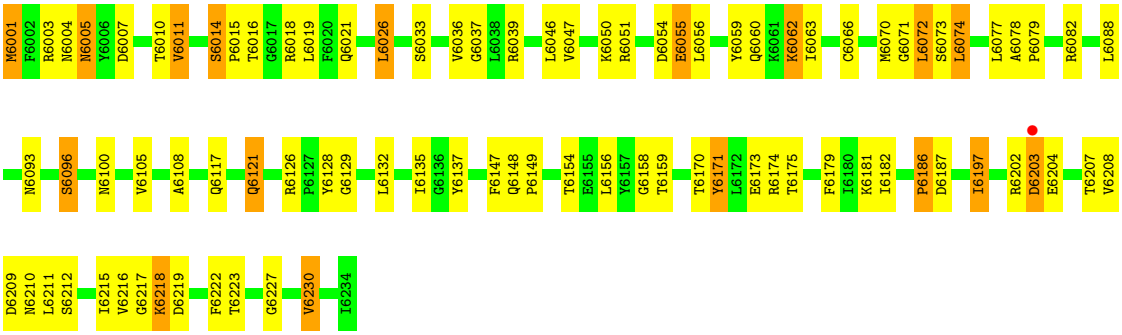
Chain AW:





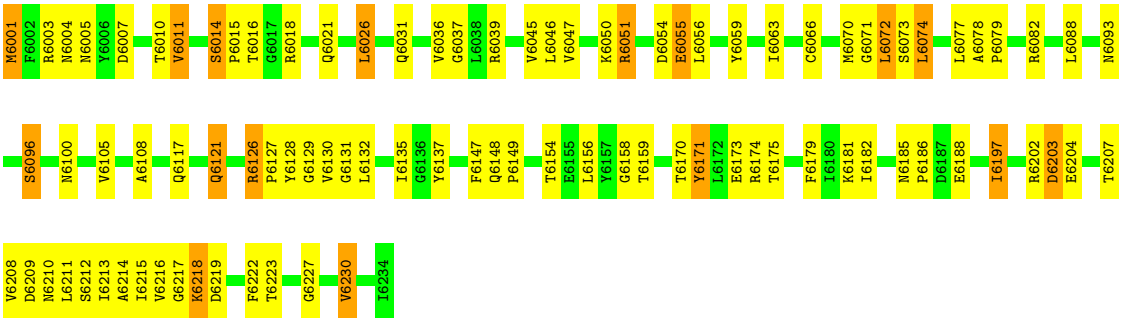
• Molecule 6: Proteasome component PRE5

Chain BF:



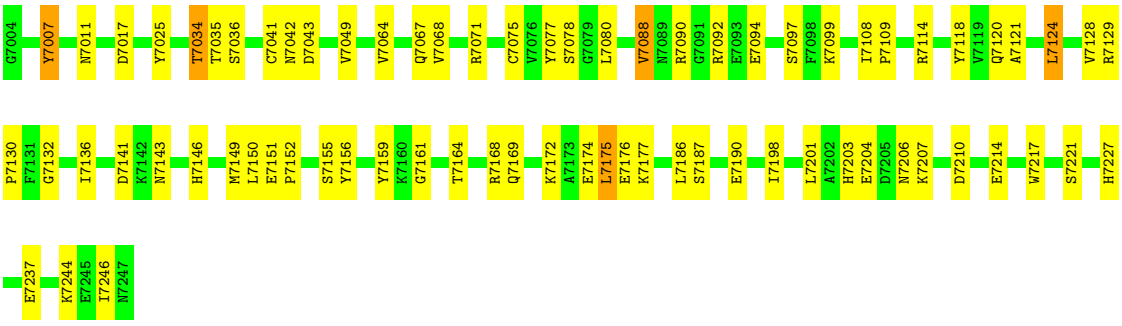
• Molecule 6: Proteasome component PRE5

Chain BT:



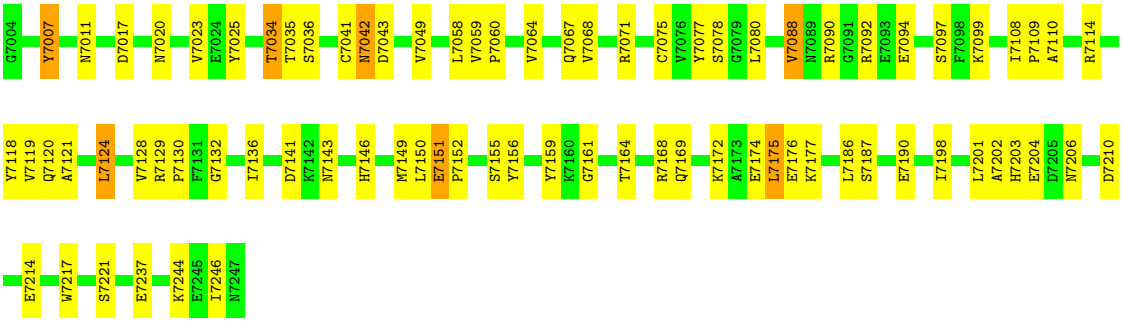
• Molecule 7: Proteasome component C1

Chain AL:



• Molecule 7: Proteasome component C1

Chain AX:

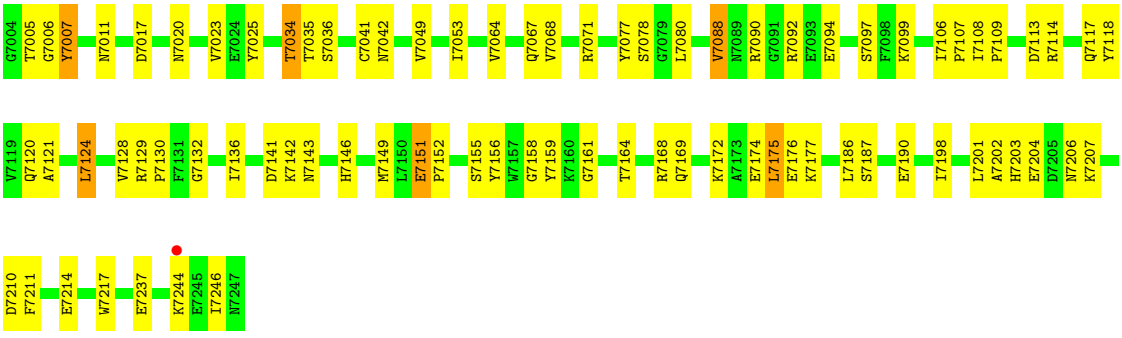


• Molecule 7: Proteasome component C1

Chain BG:

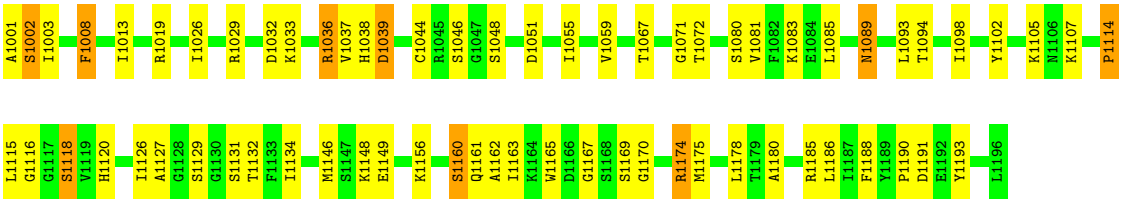
• Molecule 7: Proteasome component C1

Chain BU:



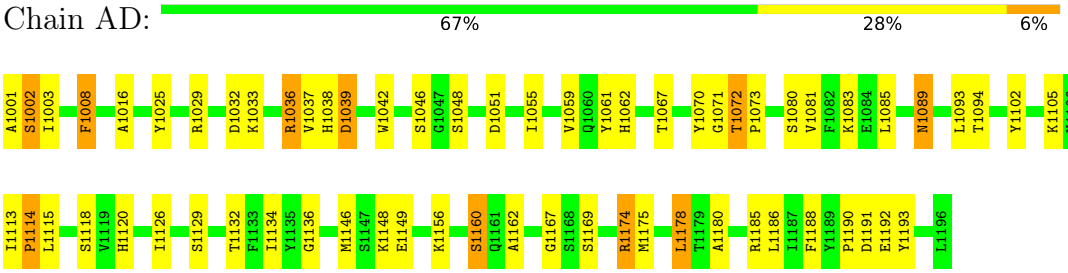
• Molecule 8: Proteasome component PRE3

Chain AB:



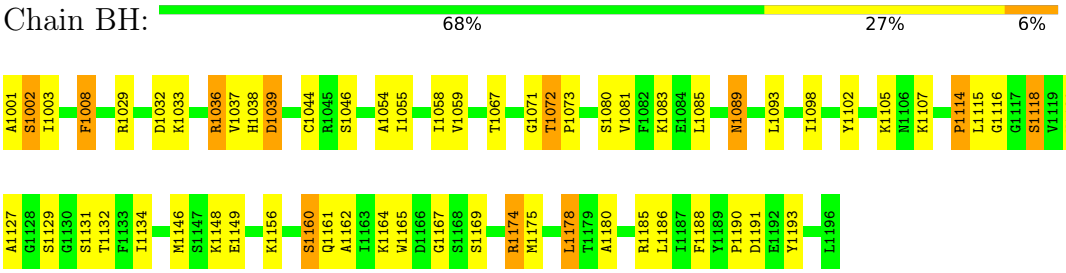
• Molecule 8: Proteasome component PRE3

Chain AD:



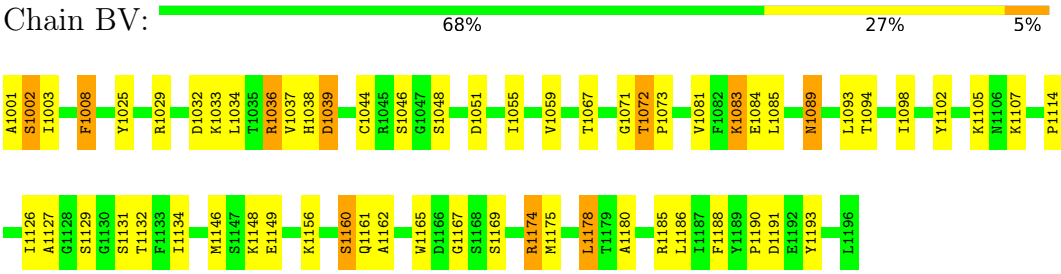
• Molecule 8: Proteasome component PRE3

Chain BH:



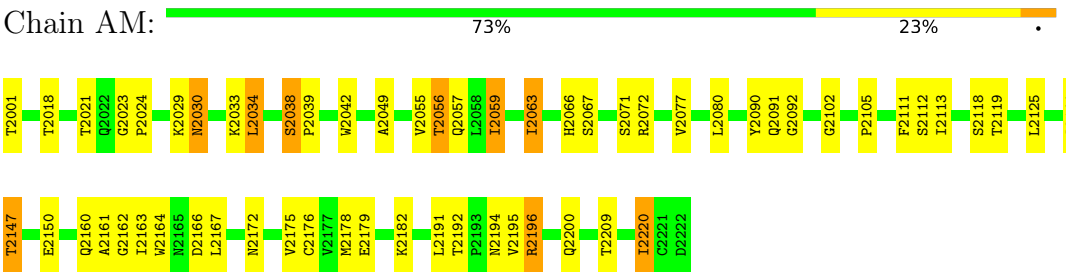
• Molecule 8: Proteasome component PRE3

Chain BV:



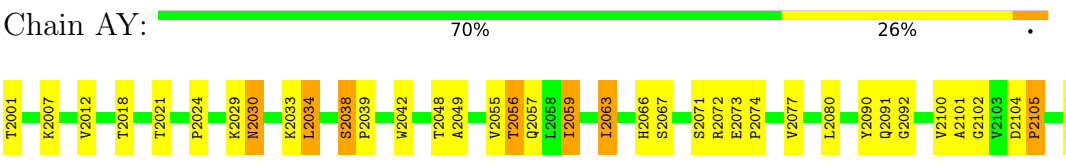
• Molecule 9: Proteasome component PUP1

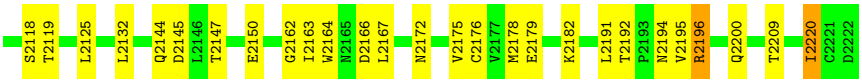
Chain AM:



• Molecule 9: Proteasome component PUP1

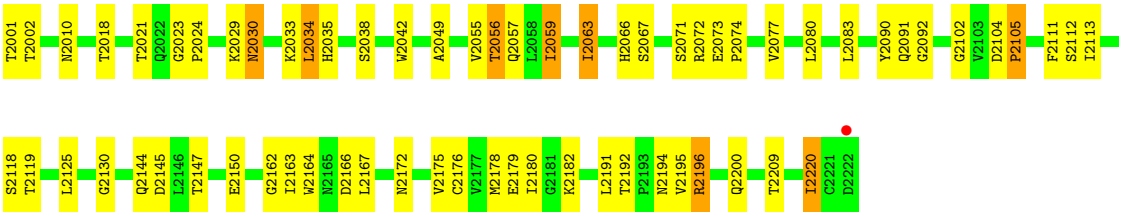
Chain AY:





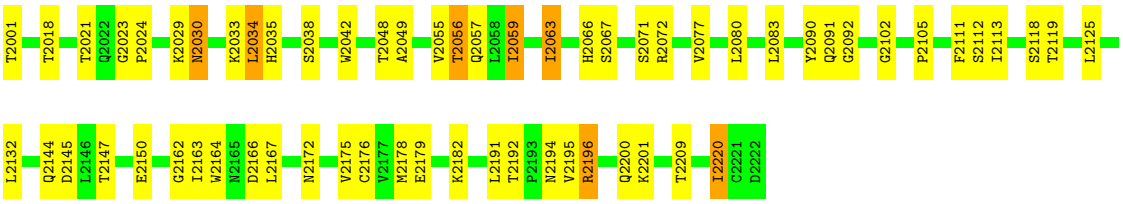
• Molecule 9: Proteasome component PUP1

Chain BI:



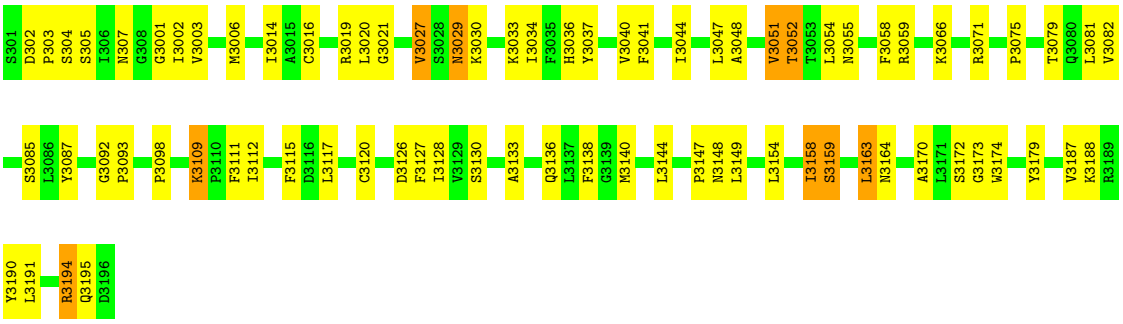
• Molecule 9: Proteasome component PUP1

Chain BW:



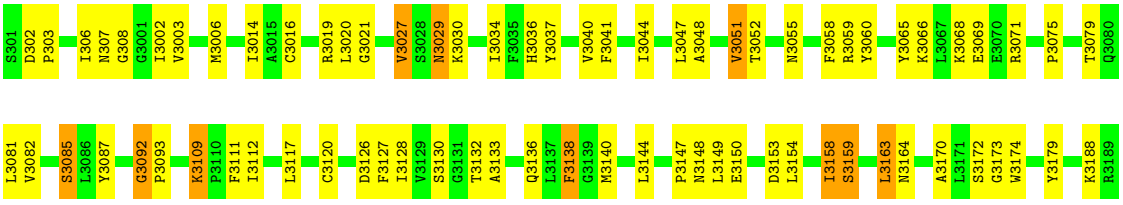
• Molecule 10: Proteasome component PUP3

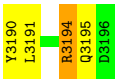
Chain AN:



• Molecule 10: Proteasome component PUP3

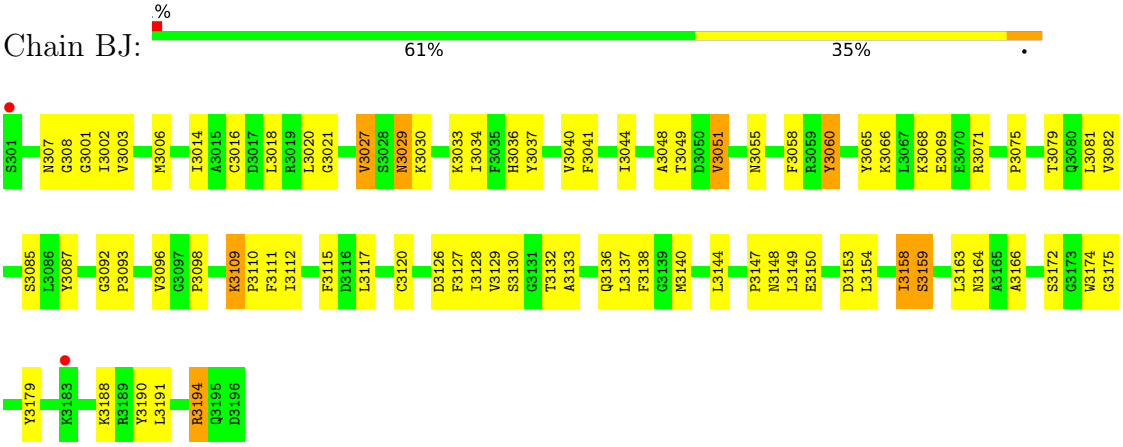
Chain AZ:





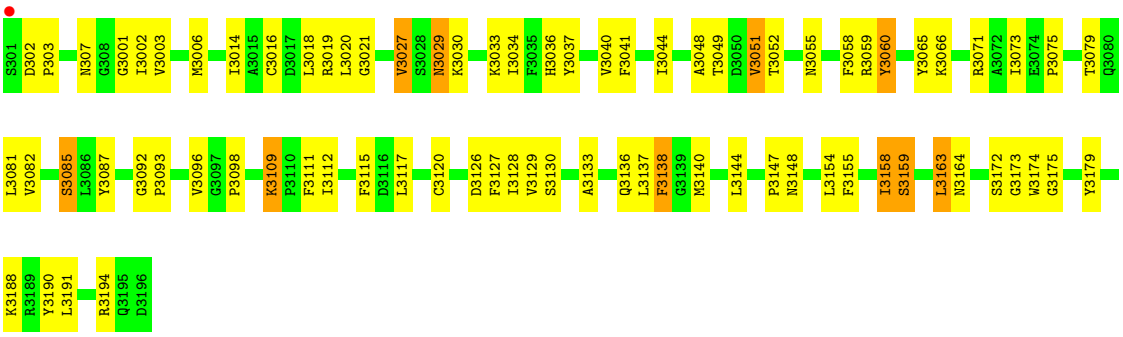
• Molecule 10: Proteasome component PUP3

Chain BJ:



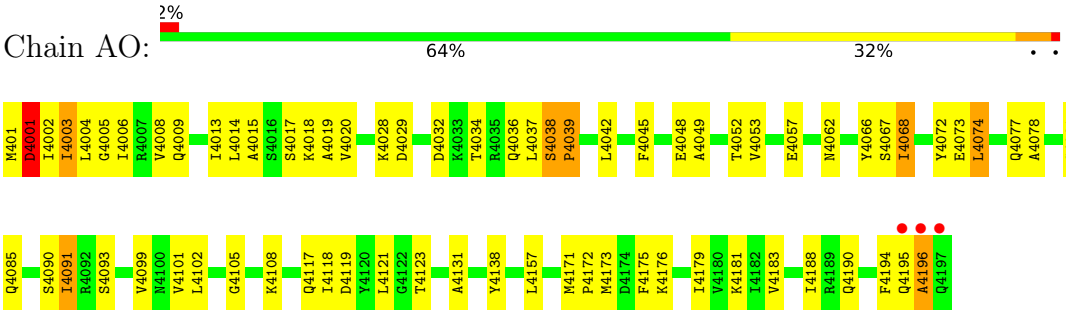
• Molecule 10: Proteasome component PUP3

Chain BX:



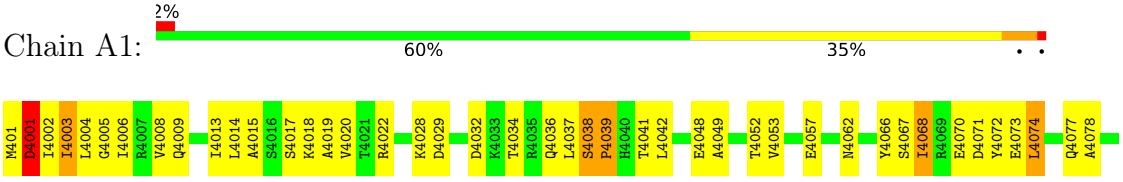
• Molecule 11: Proteasome component C11

Chain AO:



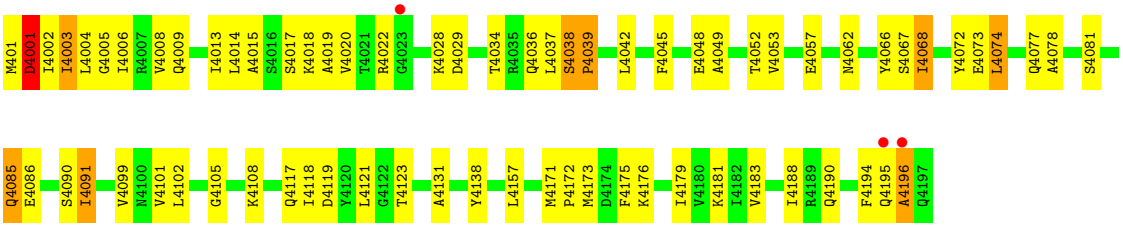
• Molecule 11: Proteasome component C11

Chain A1:



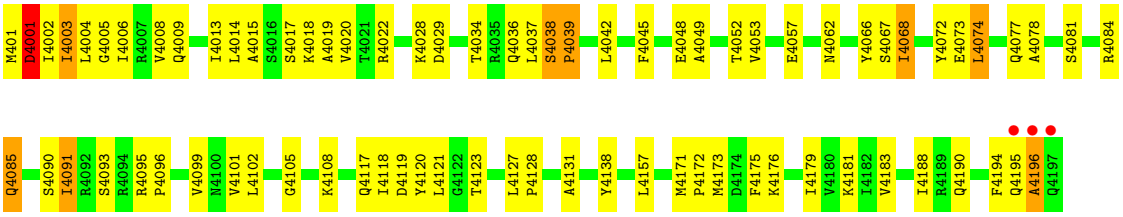
• Molecule 11: Proteasome component C11

Chain BK:



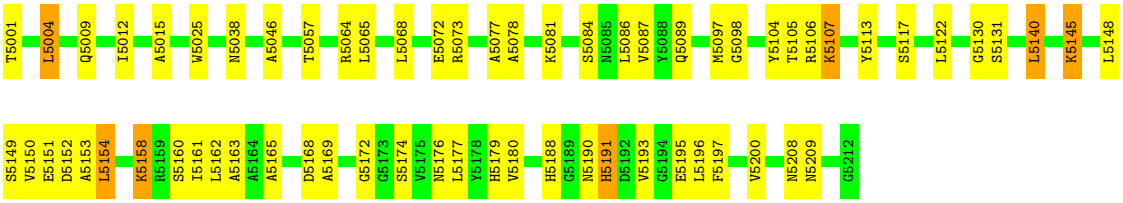
• Molecule 11: Proteasome component C11

Chain BY:



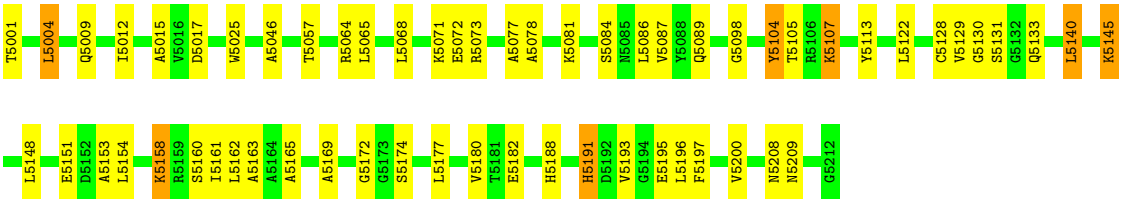
• Molecule 12: Proteasome component PRE2

Chain AP:



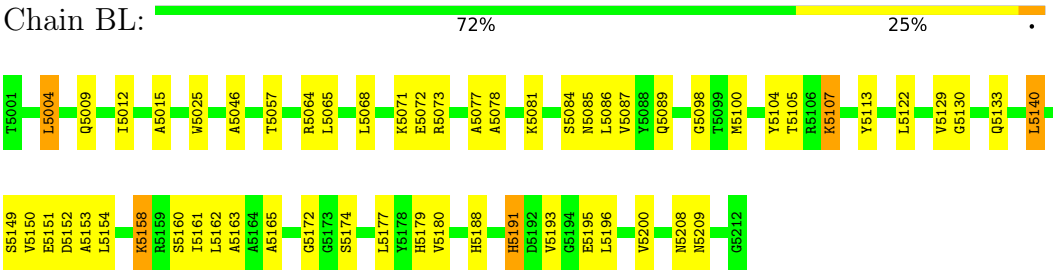
• Molecule 12: Proteasome component PRE2

Chain A2:



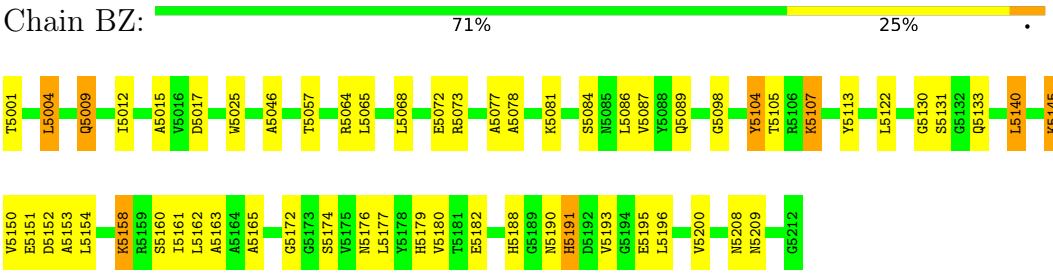
• Molecule 12: Proteasome component PRE2

Chain BL:



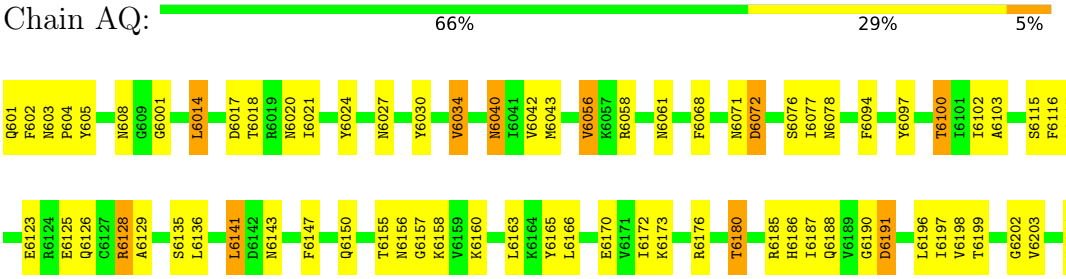
• Molecule 12: Proteasome component PRE2

Chain BZ:



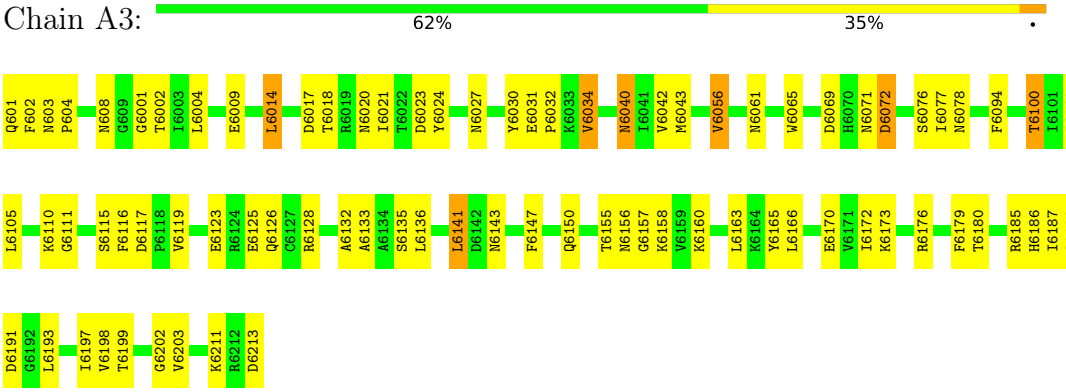
• Molecule 13: Proteasome component C5

Chain AQ:



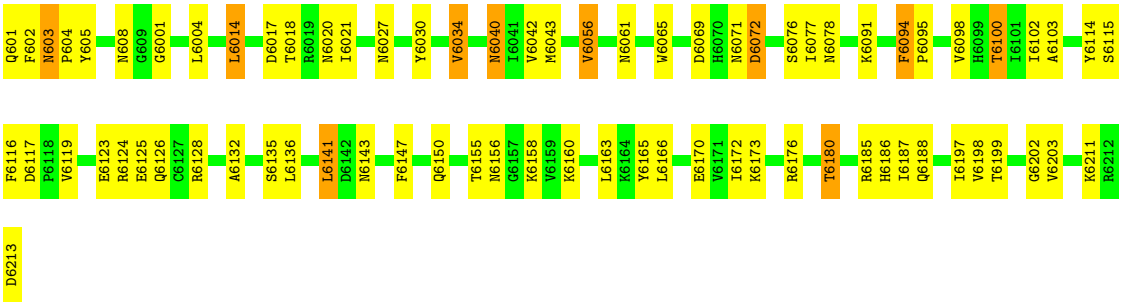
• Molecule 13: Proteasome component C5

Chain A3:



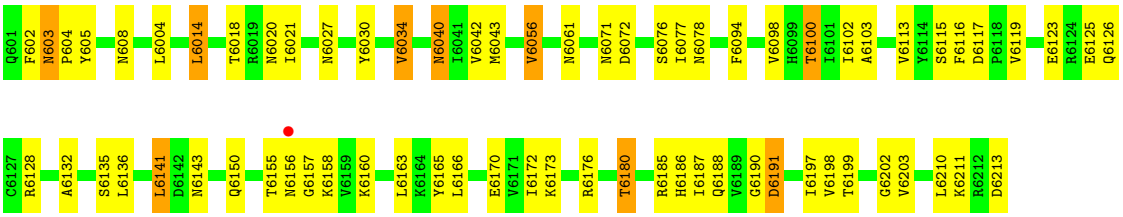
• Molecule 13: Proteasome component C5

Chain BM:



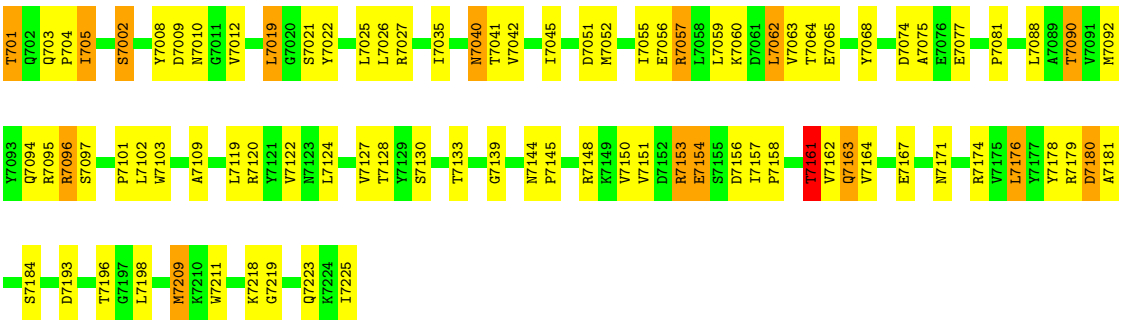
• Molecule 13: Proteasome component C5

Chain B1:



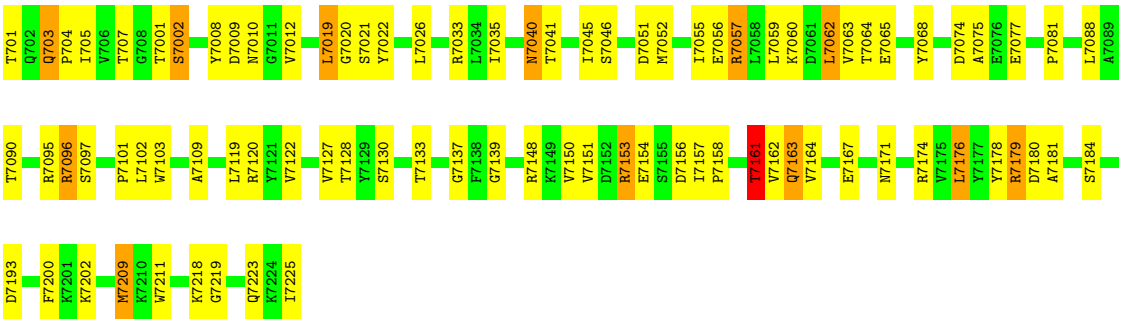
• Molecule 14: Proteasome component PRE4

Chain AR:



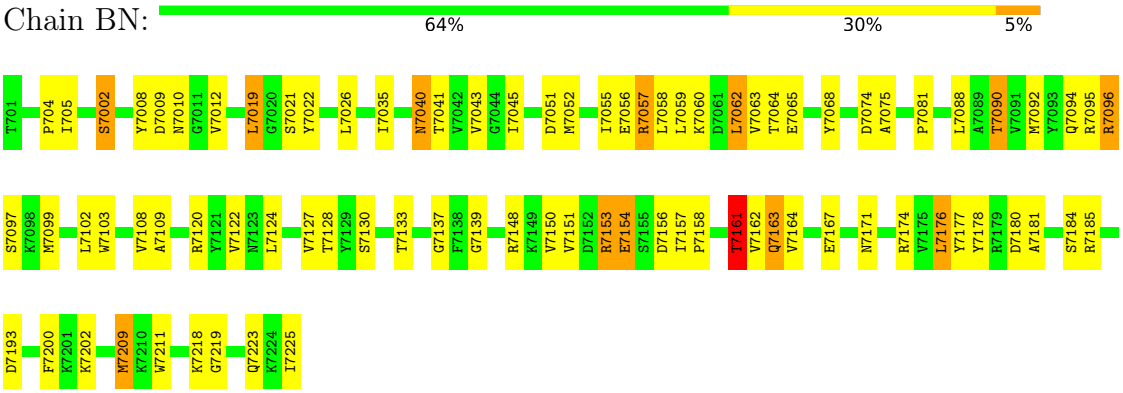
• Molecule 14: Proteasome component PRE4

Chain A4:



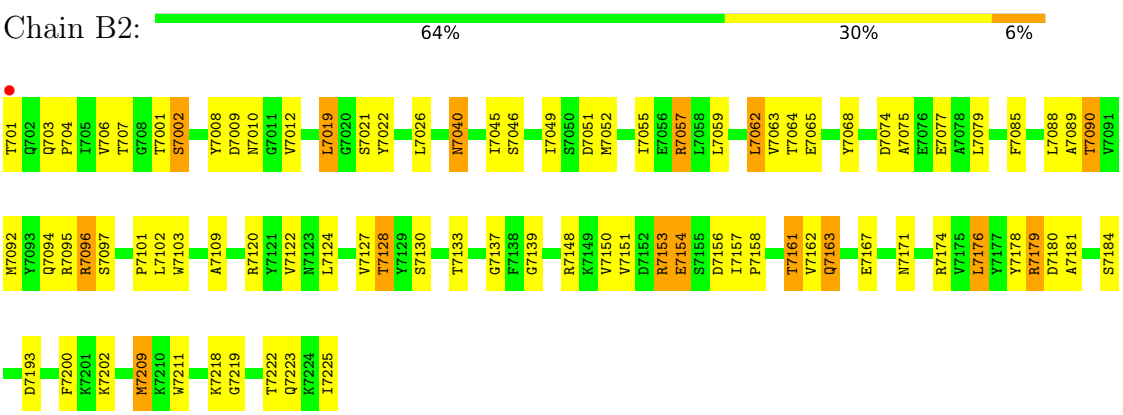
• Molecule 14: Proteasome component PRE4

Chain BN:



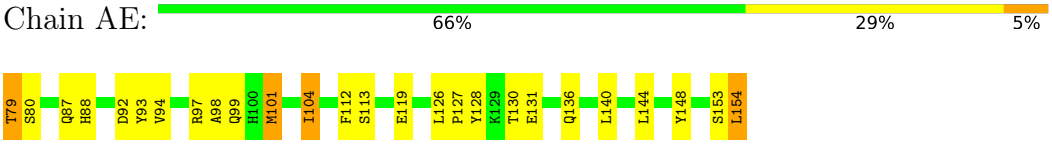
• Molecule 14: Proteasome component PRE4

Chain B2:



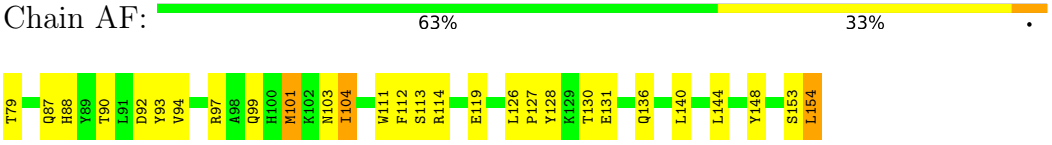
• Molecule 15: Proteasome activator BLM10

Chain AE:



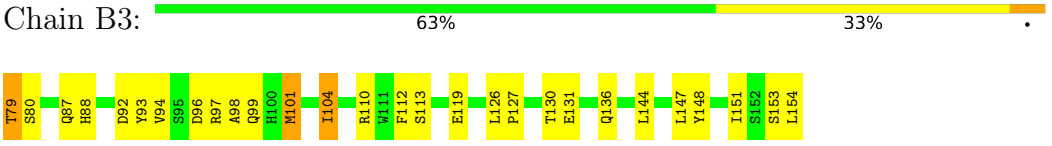
• Molecule 15: Proteasome activator BLM10

Chain AF:



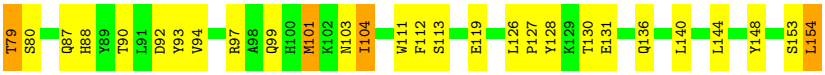
• Molecule 15: Proteasome activator BLM10

Chain B3:



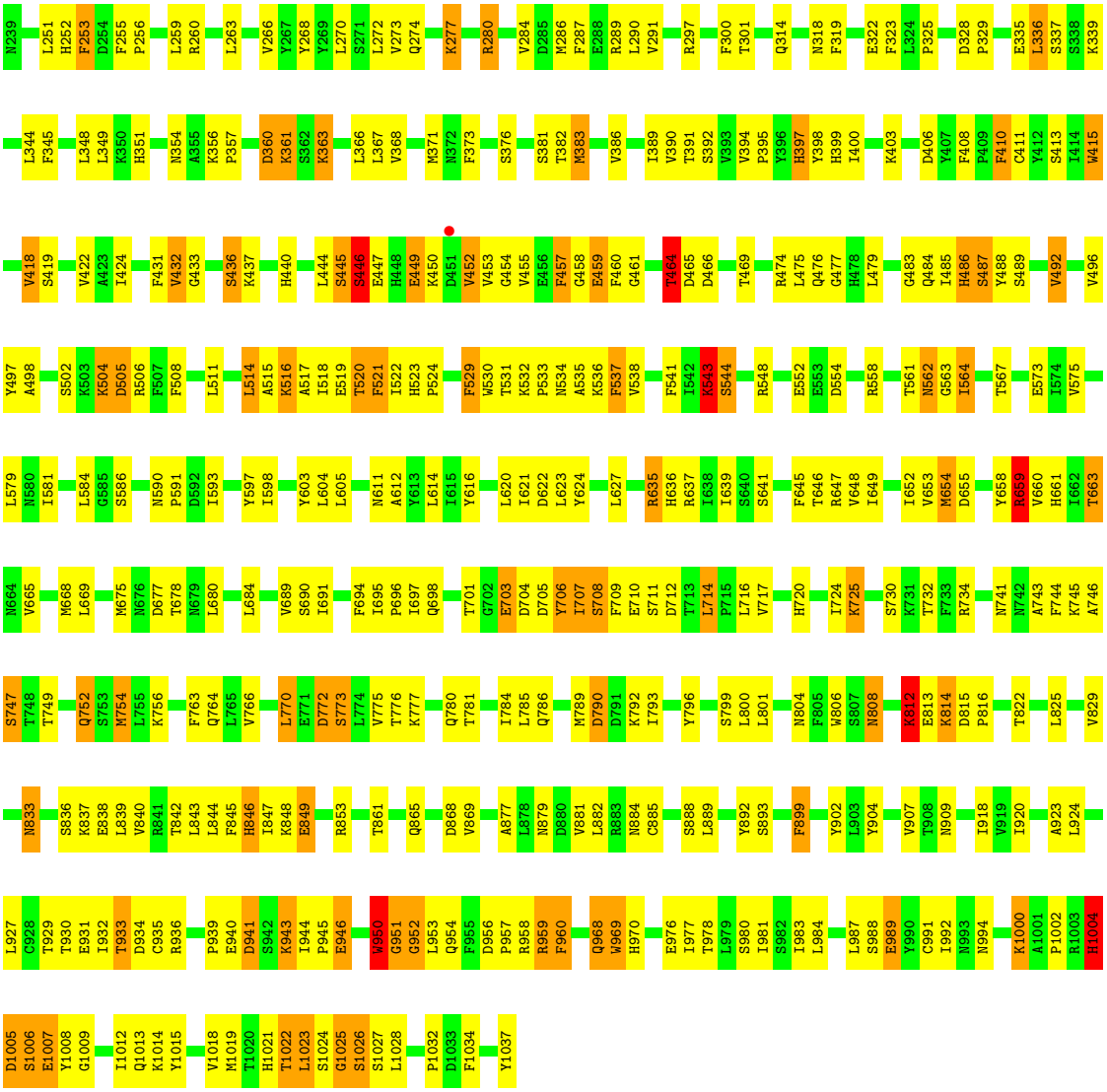
• Molecule 15: Proteasome activator BLM10

Chain B6:



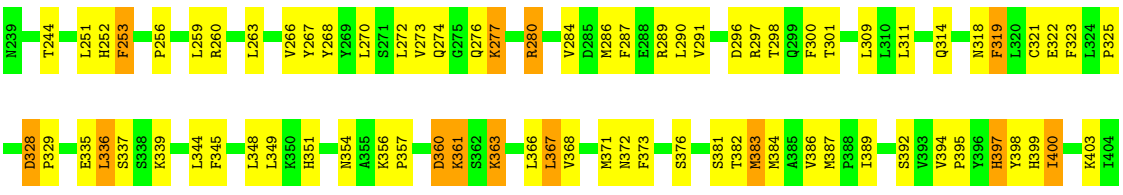
• Molecule 16: Proteasome activator BLM10

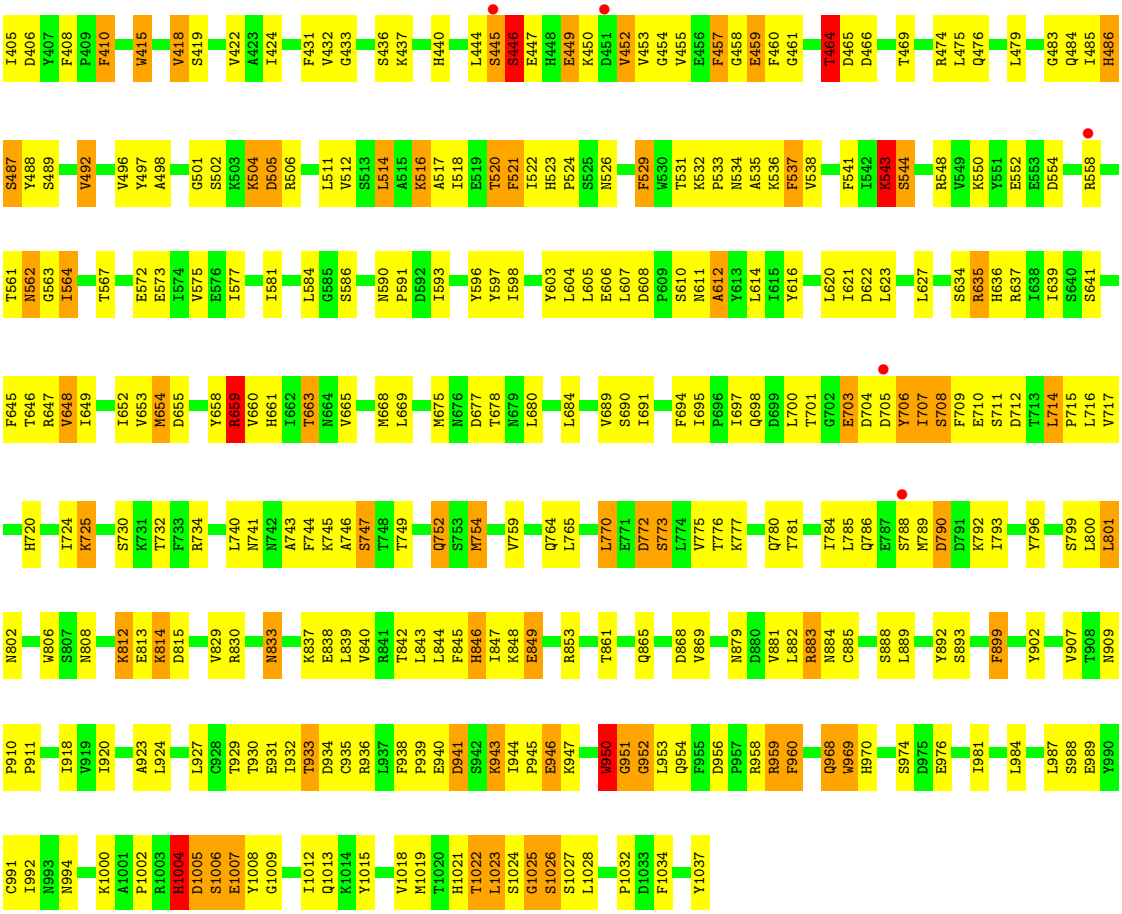
Chain A5:



• Molecule 16: Proteasome activator BLM10

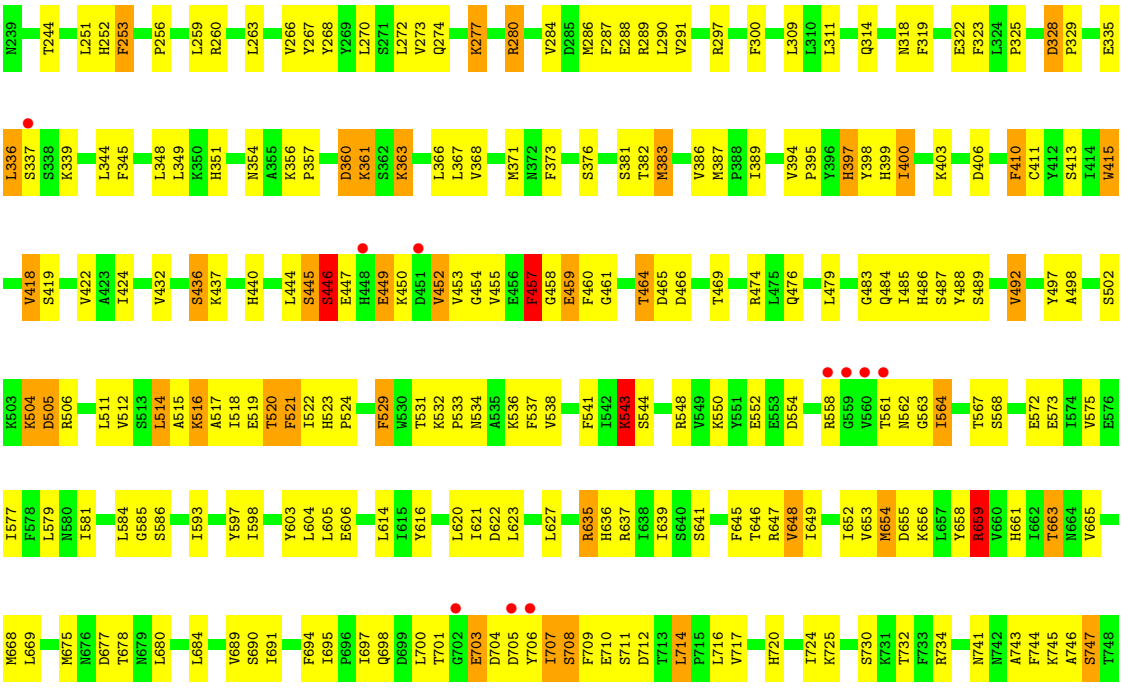
Chain A7:

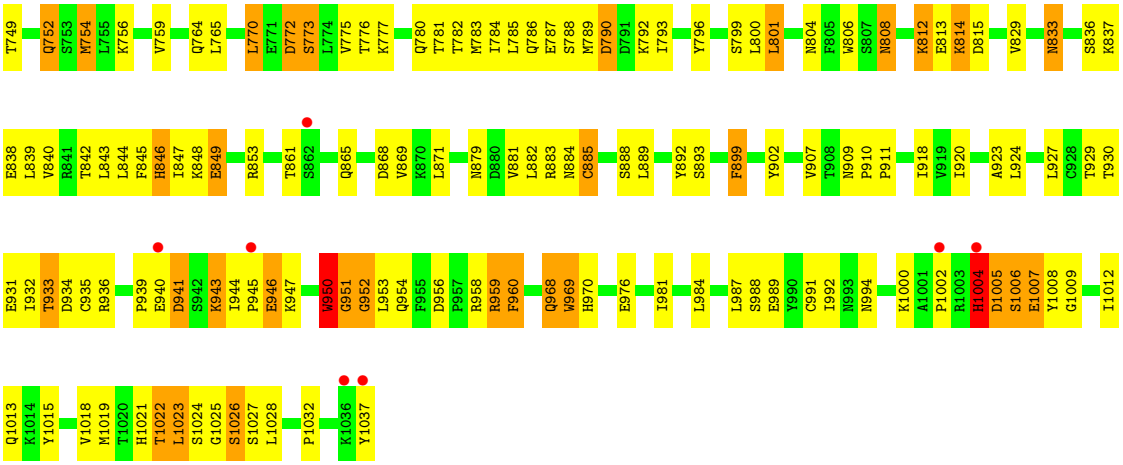




• Molecule 16: Proteasome activator BLM10

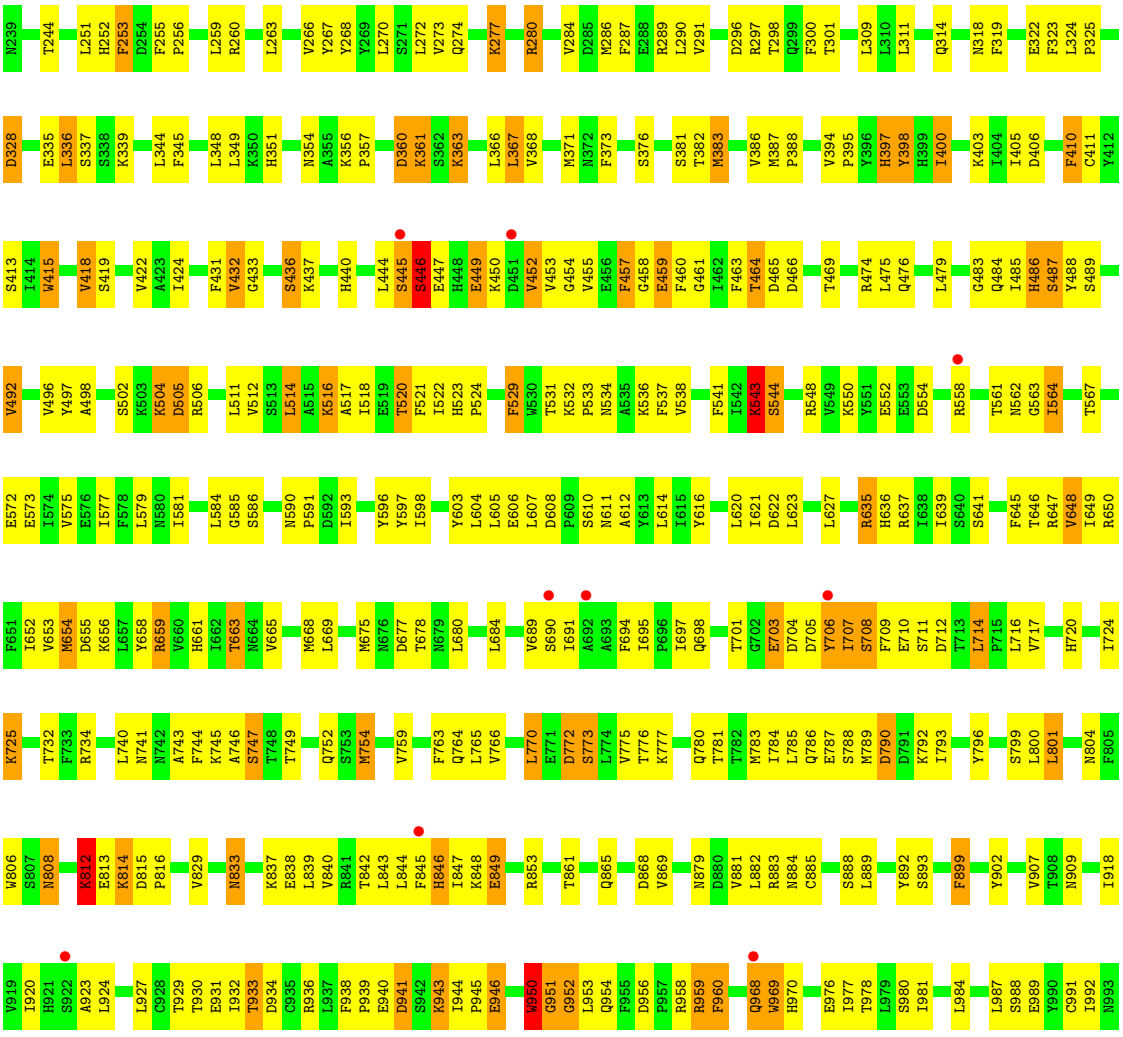
Chain B4:





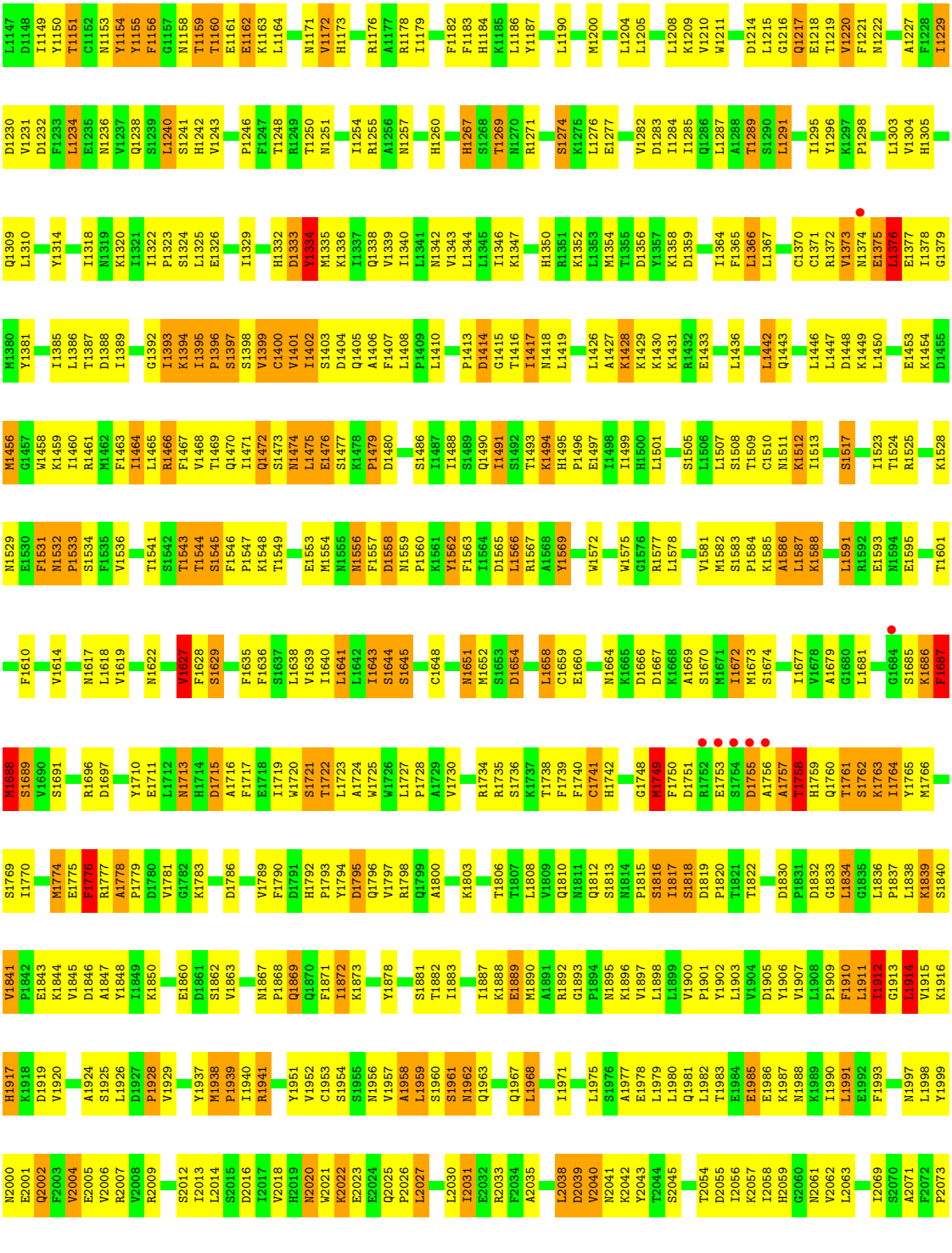
• Molecule 16: Proteasome activator BLM10

Chain B7:



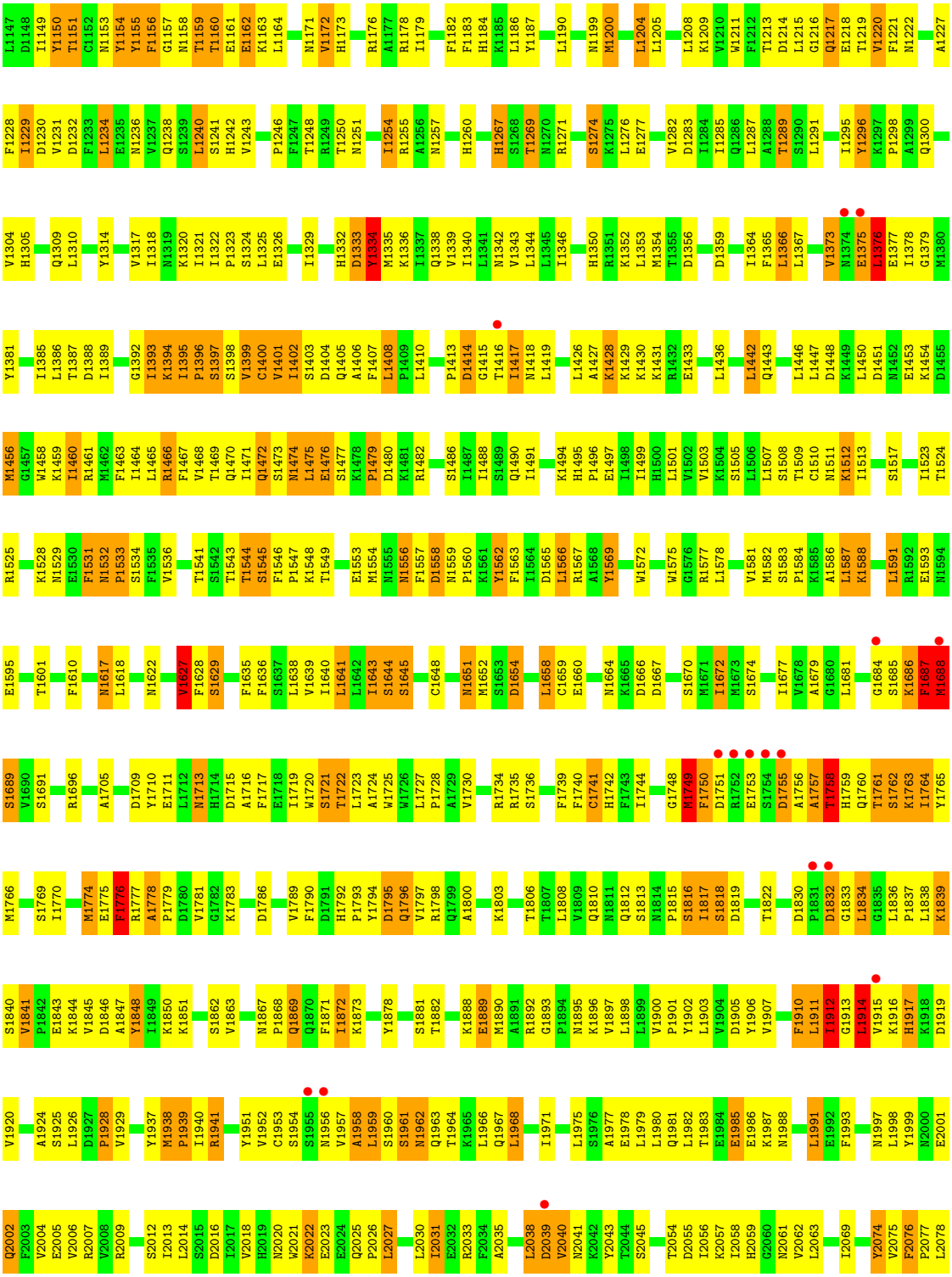
• Molecule 17: Proteasome activator BLM10

Chain A6:



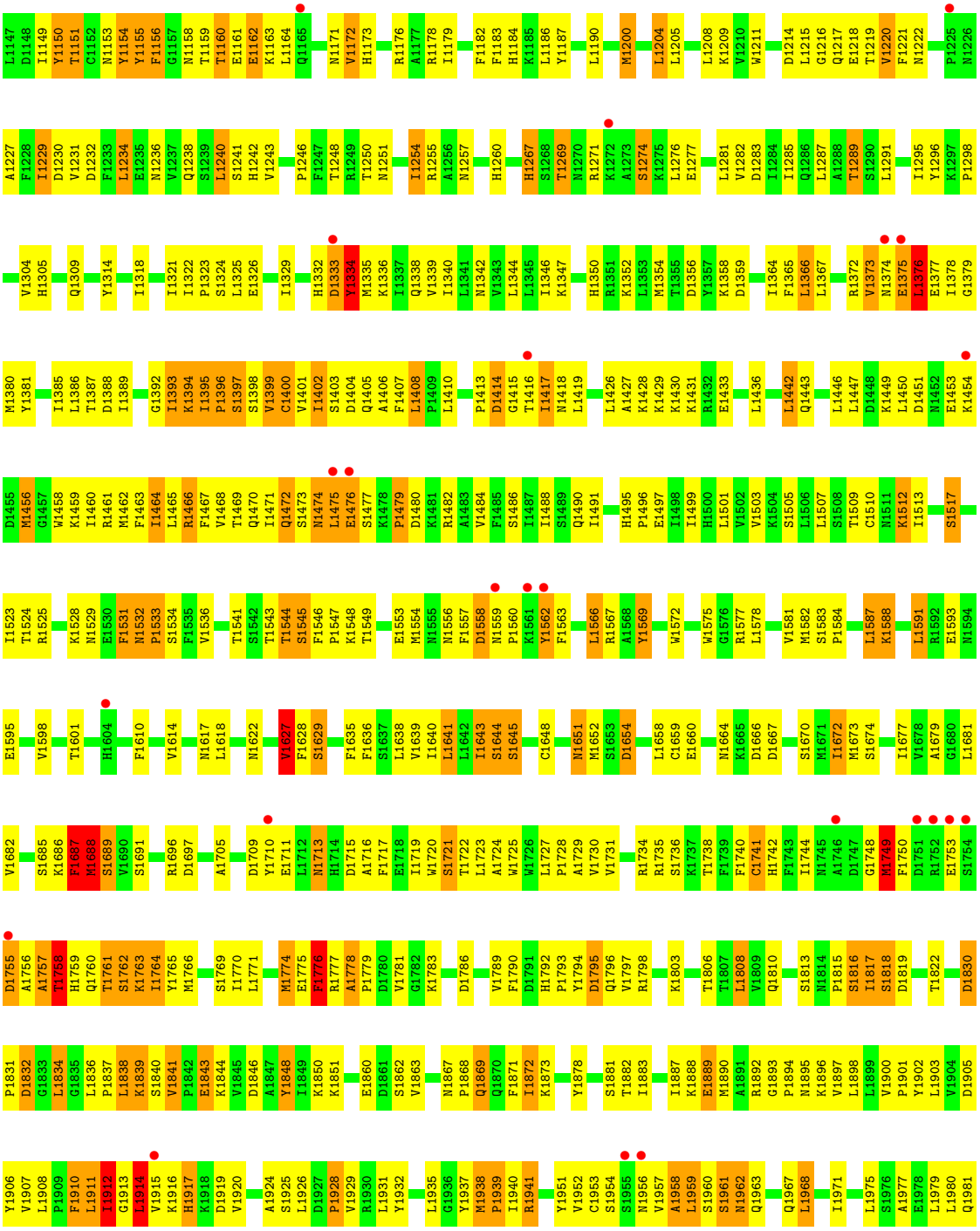
• Molecule 17: Proteasome activator BLM10

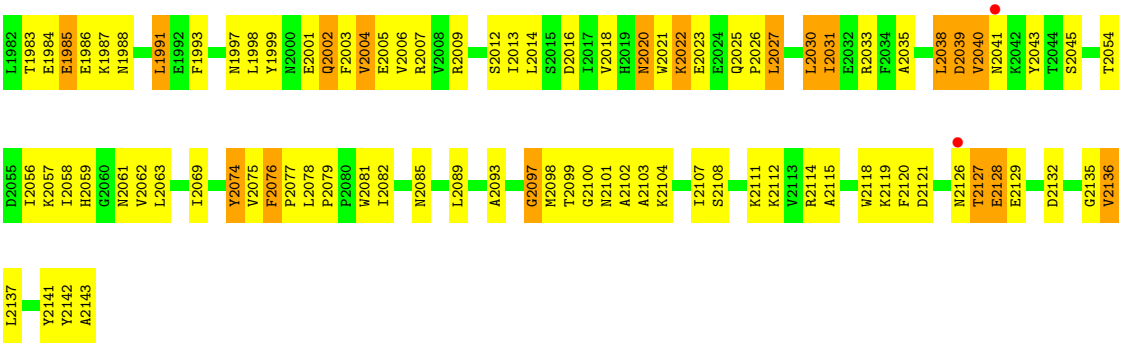
Chain A8:



• Molecule 17: Proteasome activator BLM10

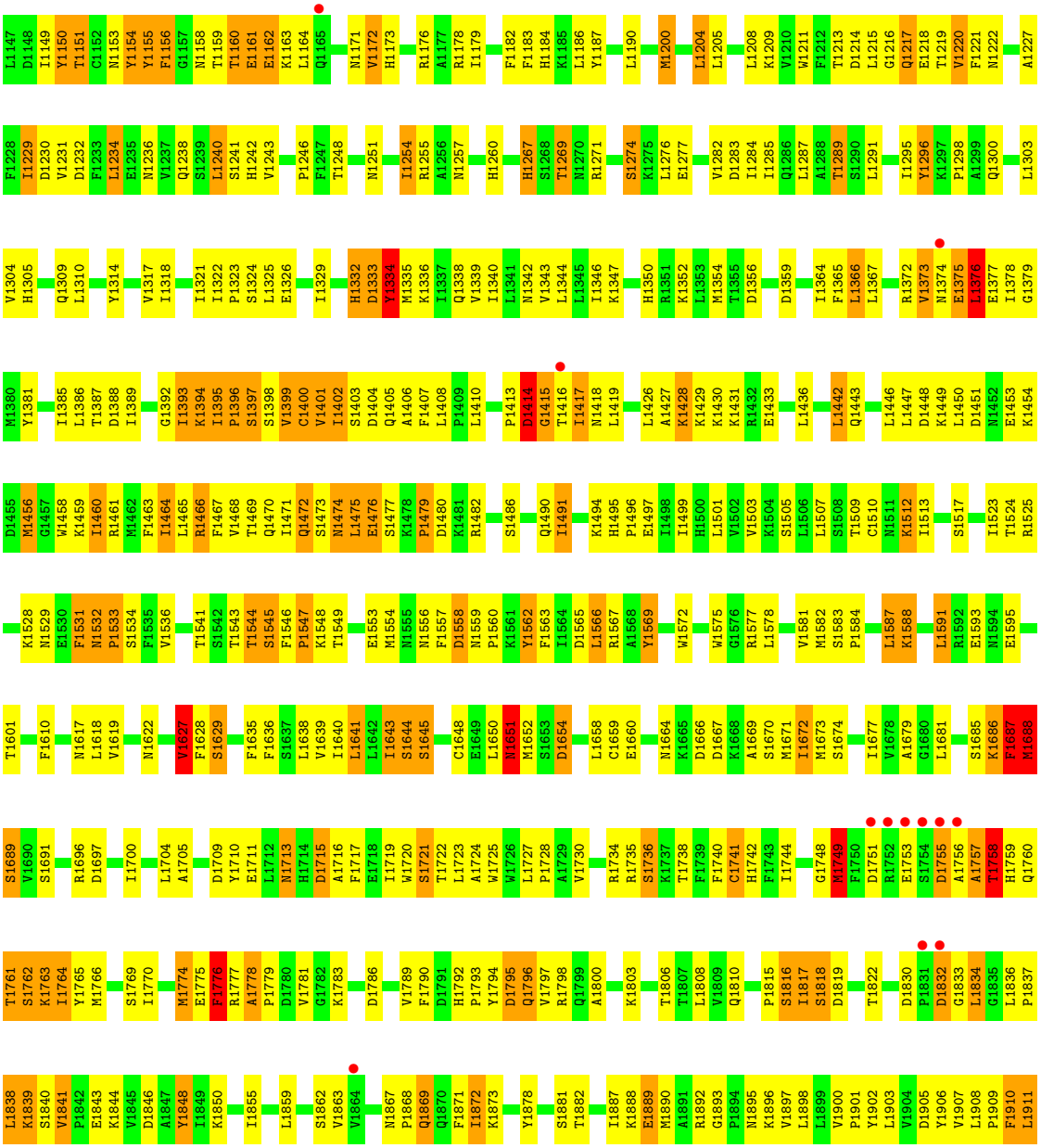
Chain B5:

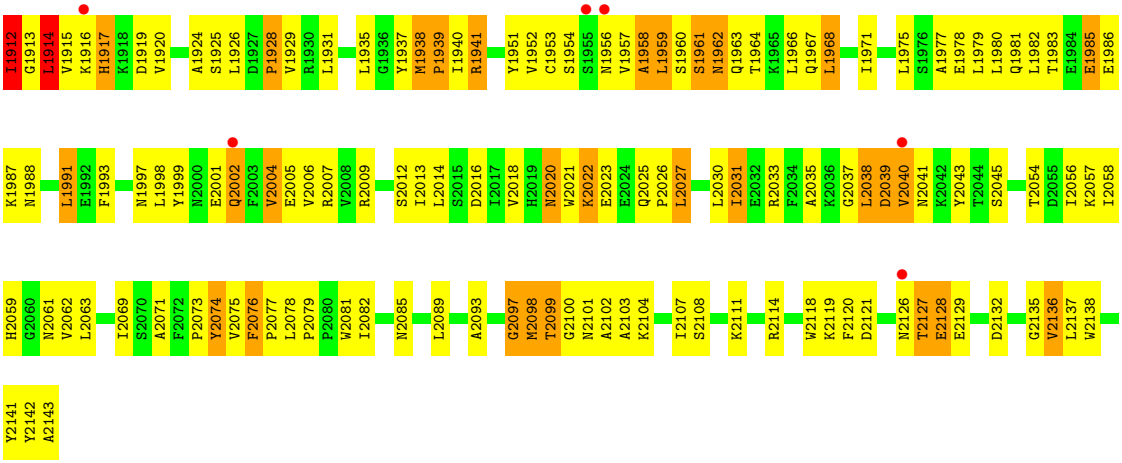




• Molecule 17: Proteasome activator BLM10

Chain B8:




I1912 G1913 L1914 V1915 K1916 H1917 K1918 D1919 V1920 A1924 S1925 L1926 D1927 P1928 V1929 R1930 L1931 L1935 G1936 Y1937 M1938 P1939 I1940 R1941 Y1951 V1952 C1953 S1954 S1955 N1956 V1957 A1958 L1959 S1960 S1961 N1962 Q1963 T1964 K1965 L1966 Q1967 L1968 I1971 L1975 S1976 A1977 E1978 L1979 L1980 Q1981 L1982 T1983 E1984 E1985 E1986
K1987 N1988 L1991 E1992 F1993 N1997 L1998 Y1999 N2000 E2001 Q2002 F2003 V2004 E2005 V2006 R2007 V2008 R2009 S2012 I2013 L2014 S2015 D2016 I2017 V2018 H2019 N2020 W2021 K2022 E2023 E2024 Q2025 P2026 L2027 L2030 I2031 E2032 R2033 F2034 A2035 K2036 G2037 L2038 D2039 V2040 N2041 K2042 Y2043 T2044 S2045 T2054 D2055 I2056 K2057 I2058
H2059 G2060 N2061 V2062 L2063 I2069 S2070 A2071 F2072 P2073 Y2074 V2075 F2076 P2077 L2078 P2079 P2080 W2081 I2082 N2085 L2089 A2093 G2097 M2098 T2099 G2100 N2101 A2102 A2103 K2104 I2107 S2108 K2111 R2114 W2118 K2119 F2120 D2121 N2126 T2127 E2128 E2129 D2132 G2135 V2136 L2137 W2138
Y2141 Y2142 A2143

4 Data and refinement statistics (i)

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 – 3.01	Depositor EDS
% Data completeness (in resolution range)	80.7 (29.99-3.00) 80.7 (29.99-3.01)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 3.00Å)	Xtriage
Refinement program	REFMAC, PHENIX (phenix.refine)	Depositor
R, R_{free}	0.196 , 0.250 0.206 , 0.250	Depositor DCC
R_{free} test set	4965 reflections (1.00%)	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)	0.26 , 60.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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)

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	0.60	0/1959	0.70	0/2652
1	AC	0.48	1/1959 (0.1%)	0.65	0/2652
1	BA	0.46	0/1959	0.62	0/2652
1	BO	0.44	0/1959	0.61	0/2652
2	AG	0.53	0/1802	0.67	2/2440 (0.1%)
2	AS	0.44	0/1802	0.65	1/2440 (0.0%)
2	BB	0.44	0/1802	0.60	1/2440 (0.0%)
2	BP	0.40	0/1802	0.60	1/2440 (0.0%)
3	AH	0.42	0/1831	0.64	0/2479
3	AT	0.41	0/1831	0.63	0/2479
3	BC	0.41	0/1831	0.62	0/2479
3	BQ	0.40	0/1831	0.62	0/2479
4	AI	0.40	0/1808	0.62	1/2446 (0.0%)
4	AU	0.41	0/1808	0.63	1/2446 (0.0%)
4	BD	0.40	0/1808	0.61	0/2446
4	BR	0.40	0/1808	0.61	0/2446
5	AJ	0.46	0/1961	0.64	0/2640
5	AV	0.45	0/1961	0.64	1/2640 (0.0%)
5	BE	0.43	0/1961	0.62	0/2640
5	BS	0.44	0/1961	0.62	0/2640
6	AK	0.55	0/1831	0.71	1/2473 (0.0%)
6	AW	0.54	0/1831	0.70	1/2473 (0.0%)
6	BF	0.46	0/1831	0.63	0/2473
6	BT	0.47	0/1831	0.65	0/2473
7	AL	0.59	1/1936 (0.1%)	0.66	0/2613
7	AX	0.52	1/1936 (0.1%)	0.63	0/2613
7	BG	0.46	0/1936	0.59	0/2613
7	BU	0.45	0/1936	0.60	0/2613
8	AB	0.62	0/1539	0.73	0/2084
8	AD	0.57	0/1539	0.69	0/2084
8	BH	0.48	0/1539	0.63	0/2084
8	BV	0.47	0/1539	0.63	0/2084
9	AM	0.61	0/1716	0.70	0/2326
9	AY	0.55	0/1716	0.70	0/2326

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
9	BI	0.46	0/1716	0.62	0/2326
9	BW	0.44	0/1716	0.63	0/2326
10	AN	0.57	0/1611	0.71	0/2174
10	AZ	0.52	0/1611	0.70	0/2174
10	BJ	0.46	0/1611	0.63	0/2174
10	BX	0.45	0/1611	0.64	0/2174
11	A1	0.46	0/1613	0.64	0/2173
11	AO	0.49	0/1613	0.66	0/2173
11	BK	0.42	0/1613	0.60	0/2173
11	BY	0.43	0/1613	0.60	0/2173
12	A2	0.50	0/1683	0.64	0/2277
12	AP	0.49	0/1683	0.64	0/2277
12	BL	0.44	0/1683	0.61	0/2277
12	BZ	0.43	0/1683	0.60	0/2277
13	A3	0.56	0/1795	0.69	0/2420
13	AQ	0.51	0/1795	0.68	0/2420
13	B1	0.45	0/1795	0.64	0/2420
13	BM	0.45	0/1795	0.63	0/2420
14	A4	0.65	2/1855 (0.1%)	0.78	0/2514
14	AR	0.64	2/1855 (0.1%)	0.78	1/2514 (0.0%)
14	B2	0.51	1/1855 (0.1%)	0.67	0/2514
14	BN	0.49	0/1855	0.68	0/2514
15	AE	0.45	0/660	0.60	1/896 (0.1%)
15	AF	0.44	0/660	0.60	1/896 (0.1%)
15	B3	0.44	0/660	0.56	0/896
15	B6	0.41	0/660	0.60	1/896 (0.1%)
16	A5	0.51	2/6669 (0.0%)	0.67	2/9038 (0.0%)
16	A7	0.48	2/6669 (0.0%)	0.66	3/9038 (0.0%)
16	B4	0.46	1/6669 (0.0%)	0.62	2/9038 (0.0%)
16	B7	0.44	2/6669 (0.0%)	0.63	3/9038 (0.0%)
17	A6	0.47	0/8246	0.68	0/11172
17	A8	0.46	0/8246	0.67	0/11172
17	B5	0.46	0/8246	0.64	0/11172
17	B8	0.44	0/8246	0.65	0/11172
All	All	0.48	15/162060 (0.0%)	0.65	24/219268 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
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 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A5	543	LYS	CD-CE	7.08	1.69	1.51
16	A7	543	LYS	CD-CE	6.55	1.67	1.51
16	A5	543	LYS	CE-NZ	6.46	1.65	1.49
16	A7	543	LYS	CE-NZ	6.43	1.65	1.49
16	B7	543	LYS	CD-CE	6.43	1.67	1.51

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	A5	543	LYS	CD-CE-NZ	9.95	134.59	111.70
16	A7	543	LYS	CD-CE-NZ	8.97	132.32	111.70
16	B7	543	LYS	CD-CE-NZ	8.38	130.98	111.70
16	A7	883	ARG	NE-CZ-NH1	-7.06	116.77	120.30
16	B4	543	LYS	CD-CE-NZ	6.94	127.66	111.70

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	63	0
1	AC	1921	0	1910	68	0
1	BA	1921	0	1910	59	0
1	BO	1921	0	1910	60	0
2	AG	1769	0	1784	51	0
2	AS	1769	0	1784	55	0
2	BB	1769	0	1784	50	0
2	BP	1769	0	1784	51	0
3	AH	1803	0	1802	116	0
3	AT	1803	0	1802	115	0
3	BC	1803	0	1802	105	0
3	BQ	1803	0	1802	110	0
4	AI	1783	0	1804	131	0
4	AU	1783	0	1804	120	0
4	BD	1783	0	1804	120	0
4	BR	1783	0	1804	130	0
5	AJ	1934	0	1905	67	0
5	AV	1934	0	1905	68	1
5	BE	1934	0	1905	69	0
5	BS	1934	0	1905	71	0
6	AK	1803	0	1806	94	0
6	AW	1803	0	1806	82	0
6	BF	1803	0	1806	80	0
6	BT	1803	0	1806	83	0
7	AL	1896	0	1884	45	0
7	AX	1896	0	1884	46	0
7	BG	1896	0	1884	43	0
7	BU	1896	0	1884	46	0
8	AB	1510	0	1476	52	0
8	AD	1510	0	1476	51	0
8	BH	1510	0	1476	49	0
8	BV	1510	0	1476	46	0
9	AM	1685	0	1685	44	0
9	AY	1685	0	1685	54	0
9	BI	1685	0	1685	47	0
9	BW	1685	0	1685	47	0
10	AN	1581	0	1571	55	0
10	AZ	1581	0	1571	60	0
10	BJ	1581	0	1571	61	0
10	BX	1581	0	1571	59	0
11	A1	1585	0	1587	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	AO	1585	0	1587	57	0
11	BK	1585	0	1587	55	0
11	BY	1585	0	1587	58	0
12	A2	1646	0	1592	46	0
12	AP	1646	0	1592	50	0
12	BL	1646	0	1592	43	0
12	BZ	1646	0	1592	49	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	64	0
14	A4	1824	0	1829	67	0
14	AR	1824	0	1829	66	0
14	B2	1824	0	1829	72	0
14	BN	1824	0	1829	62	0
15	AE	642	0	618	28	0
15	AF	642	0	618	30	0
15	B3	642	0	618	27	0
15	B6	642	0	618	27	0
16	A5	6517	0	6442	350	0
16	A7	6517	0	6442	361	1
16	B4	6517	0	6442	324	0
16	B7	6517	0	6442	342	0
17	A6	8070	0	8156	556	0
17	A8	8070	0	8156	549	0
17	B5	8070	0	8156	525	0
17	B8	8070	0	8156	544	0
All	All	158904	0	158236	6805	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 21.

The worst 5 of 6805 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%)	13	48
1	AC	241/243 (99%)	222 (92%)	16 (7%)	3 (1%)	13	48
1	BA	241/243 (99%)	224 (93%)	14 (6%)	3 (1%)	13	48
1	BO	241/243 (99%)	225 (93%)	13 (5%)	3 (1%)	13	48
2	AG	229/231 (99%)	212 (93%)	13 (6%)	4 (2%)	9	39
2	AS	229/231 (99%)	211 (92%)	15 (7%)	3 (1%)	12	45
2	BB	229/231 (99%)	214 (93%)	13 (6%)	2 (1%)	17	55
2	BP	229/231 (99%)	211 (92%)	16 (7%)	2 (1%)	17	55
3	AH	230/232 (99%)	186 (81%)	25 (11%)	19 (8%)	1	4
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	5
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	10
4	AU	225/227 (99%)	168 (75%)	43 (19%)	14 (6%)	1	8
4	BD	225/227 (99%)	168 (75%)	44 (20%)	13 (6%)	1	10
4	BR	225/227 (99%)	169 (75%)	42 (19%)	14 (6%)	1	8
5	AJ	248/250 (99%)	215 (87%)	21 (8%)	12 (5%)	2	13
5	AV	248/250 (99%)	214 (86%)	22 (9%)	12 (5%)	2	13
5	BE	248/250 (99%)	216 (87%)	20 (8%)	12 (5%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	BS	248/250 (99%)	215 (87%)	21 (8%)	12 (5%)	2 13
6	AK	232/234 (99%)	211 (91%)	17 (7%)	4 (2%)	9 39
6	AW	232/234 (99%)	212 (91%)	16 (7%)	4 (2%)	9 39
6	BF	232/234 (99%)	212 (91%)	16 (7%)	4 (2%)	9 39
6	BT	232/234 (99%)	212 (91%)	17 (7%)	3 (1%)	12 45
7	AL	242/244 (99%)	221 (91%)	20 (8%)	1 (0%)	34 72
7	AX	242/244 (99%)	223 (92%)	17 (7%)	2 (1%)	19 57
7	BG	242/244 (99%)	224 (93%)	17 (7%)	1 (0%)	34 72
7	BU	242/244 (99%)	222 (92%)	18 (7%)	2 (1%)	19 57
8	AB	194/196 (99%)	174 (90%)	18 (9%)	2 (1%)	15 53
8	AD	194/196 (99%)	172 (89%)	19 (10%)	3 (2%)	10 42
8	BH	194/196 (99%)	175 (90%)	17 (9%)	2 (1%)	15 53
8	BV	194/196 (99%)	177 (91%)	15 (8%)	2 (1%)	15 53
9	AM	220/222 (99%)	202 (92%)	16 (7%)	2 (1%)	17 55
9	AY	220/222 (99%)	201 (91%)	17 (8%)	2 (1%)	17 55
9	BI	220/222 (99%)	203 (92%)	15 (7%)	2 (1%)	17 55
9	BW	220/222 (99%)	201 (91%)	17 (8%)	2 (1%)	17 55
10	AN	202/204 (99%)	182 (90%)	16 (8%)	4 (2%)	7 34
10	AZ	202/204 (99%)	184 (91%)	16 (8%)	2 (1%)	15 53
10	BJ	202/204 (99%)	187 (93%)	13 (6%)	2 (1%)	15 53
10	BX	202/204 (99%)	184 (91%)	17 (8%)	1 (0%)	29 68
11	A1	196/198 (99%)	175 (89%)	14 (7%)	7 (4%)	3 19
11	AO	196/198 (99%)	176 (90%)	14 (7%)	6 (3%)	4 23
11	BK	196/198 (99%)	175 (89%)	15 (8%)	6 (3%)	4 23
11	BY	196/198 (99%)	175 (89%)	14 (7%)	7 (4%)	3 19
12	A2	210/212 (99%)	190 (90%)	19 (9%)	1 (0%)	29 68
12	AP	210/212 (99%)	191 (91%)	19 (9%)	0	100 100
12	BL	210/212 (99%)	191 (91%)	18 (9%)	1 (0%)	29 68
12	BZ	210/212 (99%)	189 (90%)	21 (10%)	0	100 100
13	A3	220/222 (99%)	203 (92%)	13 (6%)	4 (2%)	8 37
13	AQ	220/222 (99%)	200 (91%)	16 (7%)	4 (2%)	8 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	B1	220/222 (99%)	202 (92%)	14 (6%)	4 (2%)	8 37
13	BM	220/222 (99%)	201 (91%)	17 (8%)	2 (1%)	17 55
14	A4	231/233 (99%)	211 (91%)	16 (7%)	4 (2%)	9 39
14	AR	231/233 (99%)	212 (92%)	16 (7%)	3 (1%)	12 45
14	B2	231/233 (99%)	212 (92%)	16 (7%)	3 (1%)	12 45
14	BN	231/233 (99%)	213 (92%)	15 (6%)	3 (1%)	12 45
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%)	2 11
16	A7	797/799 (100%)	640 (80%)	111 (14%)	46 (6%)	1 10
16	B4	797/799 (100%)	651 (82%)	107 (13%)	39 (5%)	2 13
16	B7	797/799 (100%)	639 (80%)	116 (15%)	42 (5%)	2 11
17	A6	995/997 (100%)	782 (79%)	128 (13%)	85 (8%)	1 4
17	A8	995/997 (100%)	775 (78%)	133 (13%)	87 (9%)	1 3
17	B5	995/997 (100%)	780 (78%)	134 (14%)	81 (8%)	1 4
17	B8	995/997 (100%)	776 (78%)	135 (14%)	84 (8%)	1 4
All	All	19944/20080 (99%)	17074 (86%)	2065 (10%)	805 (4%)	3 17

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 (i)

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%)	187 (90%)	20 (10%)	8	31
1	AC	207/207 (100%)	184 (89%)	23 (11%)	6	25
1	BA	207/207 (100%)	185 (89%)	22 (11%)	6	26
1	BO	207/207 (100%)	185 (89%)	22 (11%)	6	26
2	AG	192/192 (100%)	175 (91%)	17 (9%)	9	35
2	AS	192/192 (100%)	172 (90%)	20 (10%)	7	27
2	BB	192/192 (100%)	172 (90%)	20 (10%)	7	27
2	BP	192/192 (100%)	172 (90%)	20 (10%)	7	27
3	AH	192/192 (100%)	164 (85%)	28 (15%)	3	15
3	AT	192/192 (100%)	164 (85%)	28 (15%)	3	15
3	BC	192/192 (100%)	164 (85%)	28 (15%)	3	15
3	BQ	192/192 (100%)	164 (85%)	28 (15%)	3	15
4	AI	202/202 (100%)	177 (88%)	25 (12%)	4	20
4	AU	202/202 (100%)	176 (87%)	26 (13%)	4	19
4	BD	202/202 (100%)	177 (88%)	25 (12%)	4	20
4	BR	202/202 (100%)	177 (88%)	25 (12%)	4	20
5	AJ	206/206 (100%)	181 (88%)	25 (12%)	5	21
5	AV	206/206 (100%)	181 (88%)	25 (12%)	5	21
5	BE	206/206 (100%)	178 (86%)	28 (14%)	3	17
5	BS	206/206 (100%)	178 (86%)	28 (14%)	3	17
6	AK	193/193 (100%)	166 (86%)	27 (14%)	3	16
6	AW	193/193 (100%)	166 (86%)	27 (14%)	3	16
6	BF	193/193 (100%)	166 (86%)	27 (14%)	3	16
6	BT	193/193 (100%)	168 (87%)	25 (13%)	4	19
7	AL	201/201 (100%)	176 (88%)	25 (12%)	4	20
7	AX	201/201 (100%)	175 (87%)	26 (13%)	4	19
7	BG	201/201 (100%)	175 (87%)	26 (13%)	4	19
7	BU	201/201 (100%)	175 (87%)	26 (13%)	4	19
8	AB	161/161 (100%)	144 (89%)	17 (11%)	6	26
8	AD	161/161 (100%)	145 (90%)	16 (10%)	8	30
8	BH	161/161 (100%)	144 (89%)	17 (11%)	6	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	BV	161/161 (100%)	145 (90%)	16 (10%)	8 30
9	AM	181/181 (100%)	164 (91%)	17 (9%)	8 32
9	AY	181/181 (100%)	164 (91%)	17 (9%)	8 32
9	BI	181/181 (100%)	165 (91%)	16 (9%)	10 36
9	BW	181/181 (100%)	164 (91%)	17 (9%)	8 32
10	AN	172/172 (100%)	158 (92%)	14 (8%)	11 40
10	AZ	172/172 (100%)	155 (90%)	17 (10%)	8 30
10	BJ	172/172 (100%)	158 (92%)	14 (8%)	11 40
10	BX	172/172 (100%)	157 (91%)	15 (9%)	10 37
11	A1	175/175 (100%)	160 (91%)	15 (9%)	10 37
11	AO	175/175 (100%)	161 (92%)	14 (8%)	12 40
11	BK	175/175 (100%)	160 (91%)	15 (9%)	10 37
11	BY	175/175 (100%)	161 (92%)	14 (8%)	12 40
12	A2	169/169 (100%)	152 (90%)	17 (10%)	7 29
12	AP	169/169 (100%)	154 (91%)	15 (9%)	9 35
12	BL	169/169 (100%)	154 (91%)	15 (9%)	9 35
12	BZ	169/169 (100%)	154 (91%)	15 (9%)	9 35
13	A3	185/185 (100%)	166 (90%)	19 (10%)	7 28
13	AQ	185/185 (100%)	164 (89%)	21 (11%)	5 24
13	B1	185/185 (100%)	165 (89%)	20 (11%)	6 26
13	BM	185/185 (100%)	164 (89%)	21 (11%)	5 24
14	A4	199/199 (100%)	176 (88%)	23 (12%)	5 23
14	AR	199/199 (100%)	175 (88%)	24 (12%)	5 21
14	B2	199/199 (100%)	176 (88%)	23 (12%)	5 23
14	BN	199/199 (100%)	178 (89%)	21 (11%)	6 26
15	AE	73/73 (100%)	67 (92%)	6 (8%)	11 39
15	AF	73/73 (100%)	66 (90%)	7 (10%)	8 32
15	B3	73/73 (100%)	66 (90%)	7 (10%)	8 32
15	B6	73/73 (100%)	66 (90%)	7 (10%)	8 32
16	A5	744/744 (100%)	653 (88%)	91 (12%)	5 21
16	A7	744/744 (100%)	651 (88%)	93 (12%)	4 20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	B4	744/744 (100%)	655 (88%)	89 (12%)	5 22
16	B7	744/744 (100%)	655 (88%)	89 (12%)	5 22
17	A6	909/909 (100%)	774 (85%)	135 (15%)	3 14
17	A8	909/909 (100%)	773 (85%)	136 (15%)	3 14
17	B5	909/909 (100%)	774 (85%)	135 (15%)	3 14
17	B8	909/909 (100%)	771 (85%)	138 (15%)	3 14
All	All	17444/17444 (100%)	15334 (88%)	2110 (12%)	5 21

5 of 2110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	B5	1961	SER
16	B7	464	THR
17	B5	1941	ARG
17	B8	1897	VAL
17	A6	1817	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 536 such sidechains are listed below:

Mol	Chain	Res	Type
16	B4	636	HIS
17	B5	1238	GLN
16	B4	611	ASN
17	B8	1309	GLN
16	A5	440	HIS

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 monosaccharides 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, 95^{th} 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%)	-0.66	1 (0%) 92 79	37, 67, 125, 215	0
1	AC	243/243 (100%)	-0.64	0 100 100	52, 87, 139, 216	0
1	BA	243/243 (100%)	-0.26	4 (1%) 72 44	79, 107, 150, 217	0
1	BO	243/243 (100%)	-0.42	3 (1%) 79 54	75, 101, 145, 217	0
2	AG	231/231 (100%)	-0.71	0 100 100	42, 72, 115, 150	0
2	AS	231/231 (100%)	-0.75	0 100 100	54, 86, 122, 161	0
2	BB	231/231 (100%)	-0.32	2 (0%) 84 63	84, 109, 139, 166	0
2	BP	231/231 (100%)	-0.63	0 100 100	69, 98, 129, 164	0
3	AH	232/232 (100%)	-0.42	3 (1%) 77 51	56, 113, 176, 219	0
3	AT	232/232 (100%)	-0.26	4 (1%) 70 41	65, 114, 180, 223	0
3	BC	232/232 (100%)	-0.01	7 (3%) 50 22	88, 132, 182, 227	0
3	BQ	232/232 (100%)	-0.35	4 (1%) 70 41	81, 123, 180, 227	0
4	AI	227/227 (100%)	-0.32	2 (0%) 84 63	63, 126, 187, 212	0
4	AU	227/227 (100%)	-0.26	6 (2%) 56 27	70, 127, 188, 224	0
4	BD	227/227 (100%)	-0.04	7 (3%) 49 21	89, 137, 193, 222	0
4	BR	227/227 (100%)	-0.14	8 (3%) 44 18	88, 135, 189, 220	0
5	AJ	250/250 (100%)	-0.46	7 (2%) 53 25	60, 99, 188, 246	0
5	AV	250/250 (100%)	-0.22	12 (4%) 30 11	59, 102, 194, 246	0
5	BE	250/250 (100%)	-0.06	18 (7%) 15 4	80, 117, 192, 245	0
5	BS	250/250 (100%)	-0.25	8 (3%) 47 20	82, 115, 191, 246	0
6	AK	234/234 (100%)	-0.68	0 100 100	51, 79, 119, 232	0
6	AW	234/234 (100%)	-0.68	0 100 100	51, 82, 121, 235	0
6	BF	234/234 (100%)	-0.45	1 (0%) 92 79	77, 104, 133, 235	0
6	BT	234/234 (100%)	-0.47	0 100 100	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%)	-0.64	0 100 100	41, 72, 122, 153	0
7	AX	244/244 (100%)	-0.69	0 100 100	53, 84, 131, 156	0
7	BG	244/244 (100%)	-0.31	2 (0%) 86 65	78, 105, 142, 165	0
7	BU	244/244 (100%)	-0.40	1 (0%) 92 79	72, 101, 143, 163	0
8	AB	196/196 (100%)	-0.79	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%)	-0.52	0 100 100	71, 94, 119, 155	0
8	BV	196/196 (100%)	-0.46	0 100 100	72, 92, 119, 152	0
9	AM	222/222 (100%)	-0.73	0 100 100	41, 62, 100, 198	0
9	AY	222/222 (100%)	-0.72	0 100 100	48, 74, 107, 195	0
9	BI	222/222 (100%)	-0.46	1 (0%) 91 75	74, 98, 125, 199	0
9	BW	222/222 (100%)	-0.55	0 100 100	73, 93, 119, 197	0
10	AN	204/204 (100%)	-0.68	0 100 100	34, 67, 97, 145	0
10	AZ	204/204 (100%)	-0.73	0 100 100	49, 74, 102, 146	0
10	BJ	204/204 (100%)	-0.52	2 (0%) 82 59	71, 99, 125, 157	0
10	BX	204/204 (100%)	-0.57	1 (0%) 91 75	69, 90, 118, 162	0
11	A1	198/198 (100%)	-0.68	3 (1%) 73 46	49, 82, 119, 220	0
11	AO	198/198 (100%)	-0.67	3 (1%) 73 46	49, 80, 118, 223	0
11	BK	198/198 (100%)	-0.43	3 (1%) 73 46	76, 102, 130, 225	0
11	BY	198/198 (100%)	-0.52	3 (1%) 73 46	69, 99, 128, 223	0
12	A2	212/212 (100%)	-0.72	0 100 100	54, 78, 117, 138	0
12	AP	212/212 (100%)	-0.65	0 100 100	56, 82, 118, 139	0
12	BL	212/212 (100%)	-0.42	0 100 100	74, 98, 127, 149	0
12	BZ	212/212 (100%)	-0.59	0 100 100	66, 100, 129, 150	0
13	A3	222/222 (100%)	-0.75	0 100 100	45, 70, 109, 168	0
13	AQ	222/222 (100%)	-0.75	0 100 100	51, 75, 111, 169	0
13	B1	222/222 (100%)	-0.48	1 (0%) 91 75	71, 100, 127, 170	0
13	BM	222/222 (100%)	-0.64	0 100 100	70, 94, 121, 173	0
14	A4	233/233 (100%)	-0.79	0 100 100	35, 63, 94, 113	0
14	AR	233/233 (100%)	-0.76	0 100 100	43, 65, 96, 115	0
14	B2	233/233 (100%)	-0.49	1 (0%) 92 79	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%)	-0.53	0 100 100	69, 93, 115, 134	0
15	AE	76/76 (100%)	-0.64	0 100 100	71, 103, 142, 147	0
15	AF	76/76 (100%)	-0.64	0 100 100	73, 107, 139, 145	0
15	B3	76/76 (100%)	-0.13	0 100 100	101, 129, 146, 155	0
15	B6	76/76 (100%)	-0.61	0 100 100	78, 118, 144, 151	0
16	A5	799/799 (100%)	-0.56	1 (0%) 95 89	45, 87, 141, 267	0
16	A7	799/799 (100%)	-0.52	5 (0%) 89 72	54, 95, 144, 267	0
16	B4	799/799 (100%)	-0.24	17 (2%) 63 34	82, 115, 155, 265	0
16	B7	799/799 (100%)	-0.38	11 (1%) 75 49	72, 105, 149, 266	0
17	A6	997/997 (100%)	-0.48	7 (0%) 87 69	55, 107, 166, 261	0
17	A8	997/997 (100%)	-0.43	17 (1%) 70 41	63, 108, 167, 260	0
17	B5	997/997 (100%)	-0.12	26 (2%) 56 27	83, 128, 173, 261	0
17	B8	997/997 (100%)	-0.36	18 (1%) 68 40	77, 114, 170, 261	0
All	All	20080/20080 (100%)	-0.46	220 (1%) 80 56	34, 100, 158, 267	0

The worst 5 of 220 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	B8	1753	GLU	14.3
5	AV	5125	GLU	12.1
17	B8	1754	SER	11.5
17	A8	1755	ASP	10.0
17	B8	1755	ASP	9.8

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 monosaccharides 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.