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 (1)) were used in the production of this report:

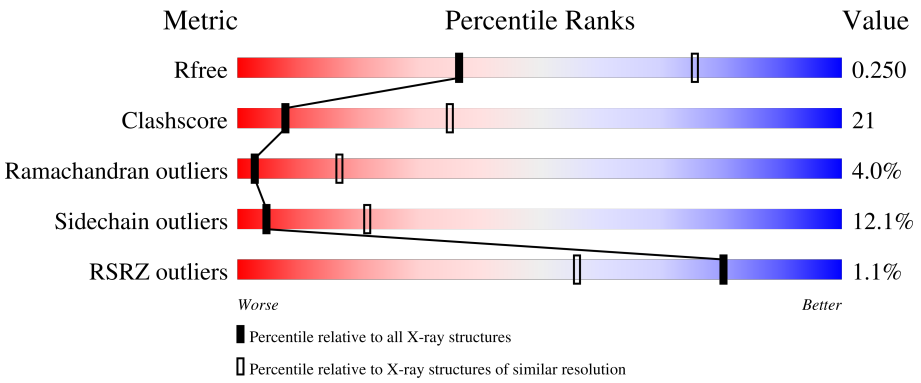
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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	68% 26% 6%
2	BB	231	.% 69% 27% •
2	BP	231	70% 25% 5%
3	AH	232	.% 44% 42% 14%
3	AT	232	2% 45% 44% 11%
3	BC	232	3% 45% 43% 12%
3	BQ	232	2% 45% 43% 12%
4	AI	227	.% 42% 48% 9% •
4	AU	227	3% 44% 46% 9% •
4	BD	227	3% 43% 48% 9% •
4	BR	227	4% 43% 48% 8% •
5	AJ	250	3% 64% 28% 8%
5	AV	250	5% 64% 27% 8%
5	BE	250	7% 62% 29% 8%
5	BS	250	3% 60% 32% 7%
6	AK	234	60% 32% 7%
6	AW	234	63% 30% 7%
6	BF	234	62% 31% 7%
6	BT	234	60% 33% 7%
7	AL	244	70% 28% •
7	AX	244	68% 30% •
7	BG	244	.% 69% 28% •
7	BU	244	67% 31% •
8	AB	196	66% 30% 5%
8	AD	196	67% 28% 6%

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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	2% 60% 35% • •
11	AO	198	2% 64% 32% • •
11	BK	198	2% 64% 31% • •
11	BY	198	2% 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	2% 53% 38% 9%
16	B7	799	.% 51% 39% 10%
17	A6	997	.% 43% 43% 13%
17	A8	997	2% 44% 42% 13%
17	B5	997	3% 44% 42% 12%
17	B8	997	2% 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
			Total	C	N	O	S			
1	AA	243	1921	1221	322	370	8	0	0	0
1	AC	243	1921	1221	322	370	8	0	0	0
1	BA	243	1921	1221	322	370	8	0	0	0
1	BO	243	1921	1221	322	370	8	0	0	0

- Molecule 2 is a protein called Proteasome component Y7.

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

- Molecule 3 is a protein called Proteasome component Y13.

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

- Molecule 4 is a protein called Proteasome component PRE6.

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

- Molecule 5 is a protein called Proteasome component PUP2.

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

- Molecule 6 is a protein called Proteasome component PRE5.

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

- Molecule 7 is a protein called Proteasome component C1.

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

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

- Molecule 8 is a protein called Proteasome component PRE3.

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

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
			Total	C	N	O	S			
9	AM	222	1685	1061	293	324	7	0	0	0
			Total	C	N	O	S			
9	AY	222	1685	1061	293	324	7	0	0	0
			Total	C	N	O	S			
9	BI	222	1685	1061	293	324	7	0	0	0
			Total	C	N	O	S			
9	BW	222	1685	1061	293	324	7	0	0	0

- Molecule 10 is a protein called Proteasome component PUP3.

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

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

- Molecule 11 is a protein called Proteasome component C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	AO	198	1585	1005	269	305	6	0	0	0
11	A1	198	1585	1005	269	305	6	0	0	0
11	BK	198	1585	1005	269	305	6	0	0	0
11	BY	198	1585	1005	269	305	6	0	0	0

- Molecule 12 is a protein called Proteasome component PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	AP	212	1646	1045	282	312	7	0	0	0
12	A2	212	1646	1045	282	312	7	0	0	0
12	BL	212	1646	1045	282	312	7	0	0	0
12	BZ	212	1646	1045	282	312	7	0	0	0

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
			Total	C	N	O	S			
13	AQ	222	1757	1115	303	335	4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	A3	222	1757	1115	303	335	4	0	0	0
13	BM	222	1757	1115	303	335	4	0	0	0
13	B1	222	1757	1115	303	335	4	0	0	0

- Molecule 14 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	AR	233	1824	1154	312	351	7	0	0	0
14	A4	233	1824	1154	312	351	7	0	0	0
14	BN	233	1824	1154	312	351	7	0	0	0
14	B2	233	1824	1154	312	351	7	0	0	0

- Molecule 15 is a protein called Proteasome activator BLM10.

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

- Molecule 16 is a protein called Proteasome activator BLM10.

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

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
			Total	C	N	O	S			
17	A6	997	8070	5211	1339	1484	36	0	0	0
17	A8	997	8070	5211	1339	1484	36	0	0	0
17	B5	997	8070	5211	1339	1484	36	0	0	0
17	B8	997	8070	5211	1339	1484	36	0	0	0

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)

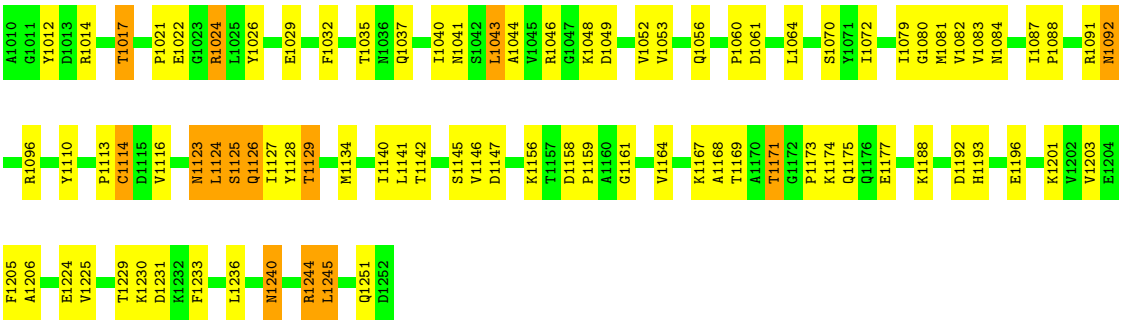
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 67% 28% 5%

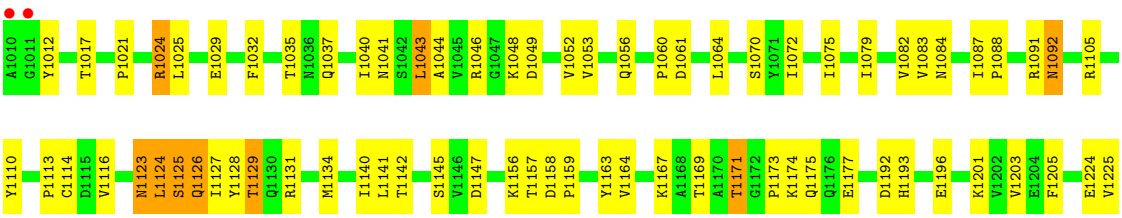
• Molecule 1: Proteasome component C7-alpha

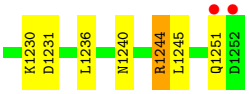
Chain AC: 64% 30% 6%



• Molecule 1: Proteasome component C7-alpha

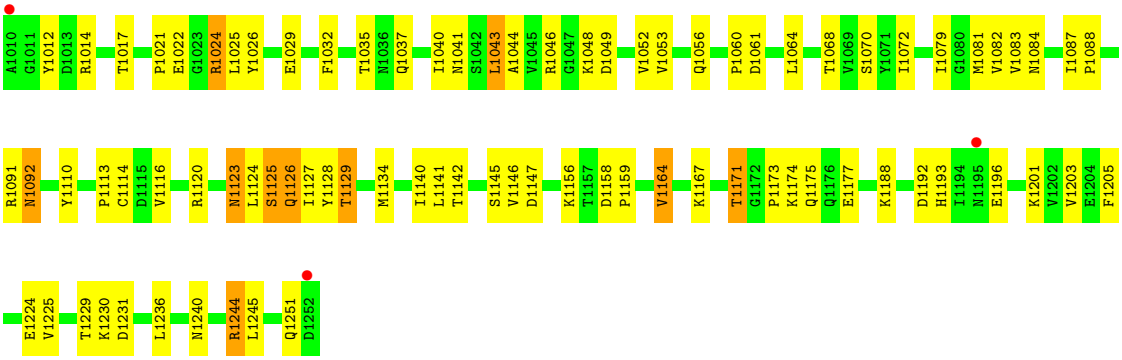
Chain BA: 2% 67% 29%





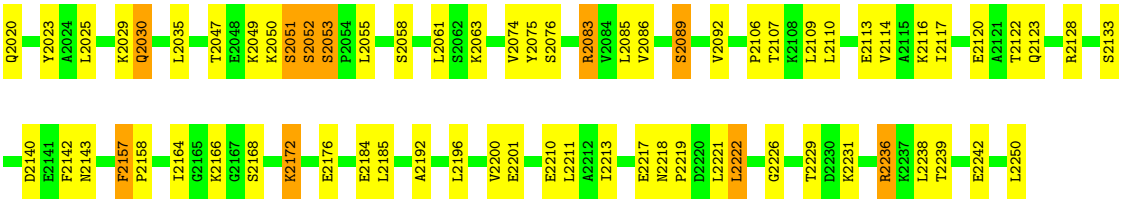
• Molecule 1: Proteasome component C7-alpha

Chain BO:



• Molecule 2: Proteasome component Y7

Chain AG:

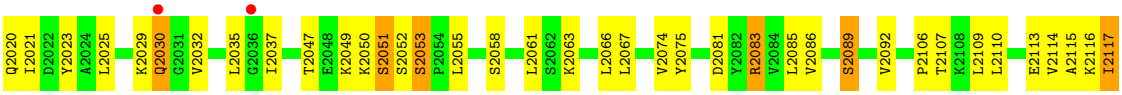


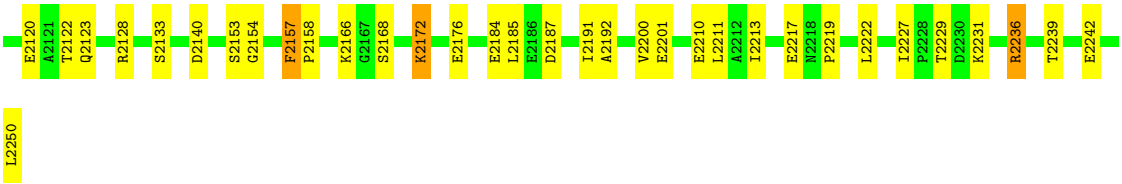
• Molecule 2: Proteasome component Y7

Chain AS:

• Molecule 2: Proteasome component Y7

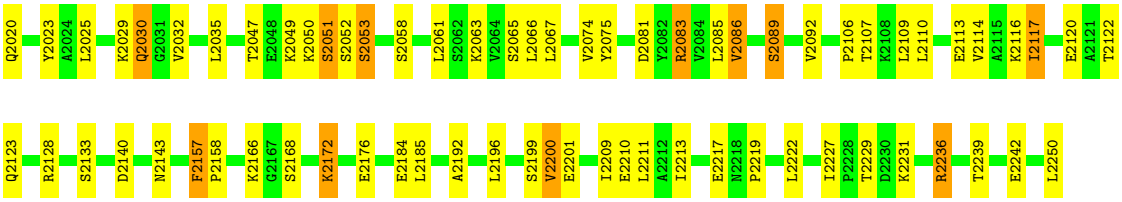
Chain BB:





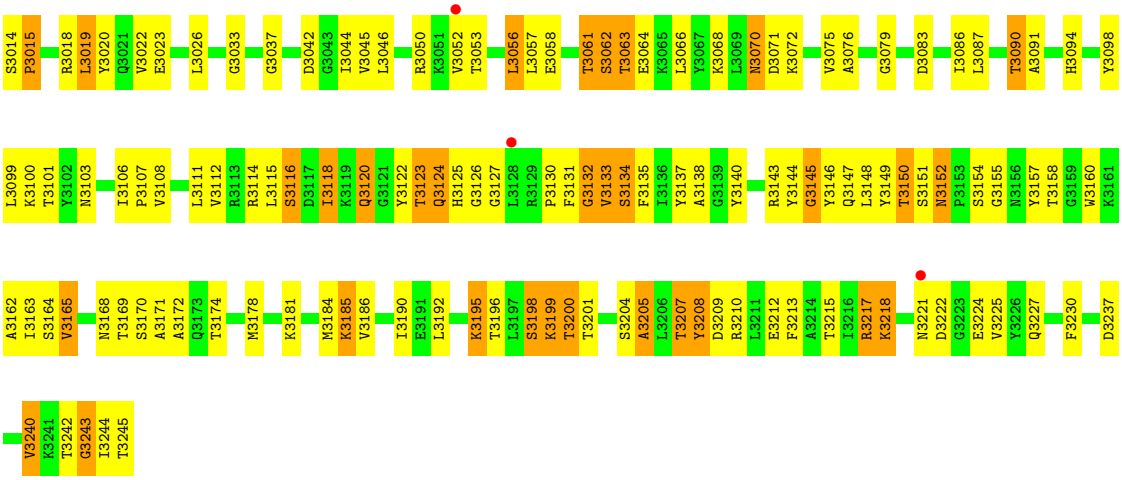
• Molecule 2: Proteasome component Y7

Chain BP:



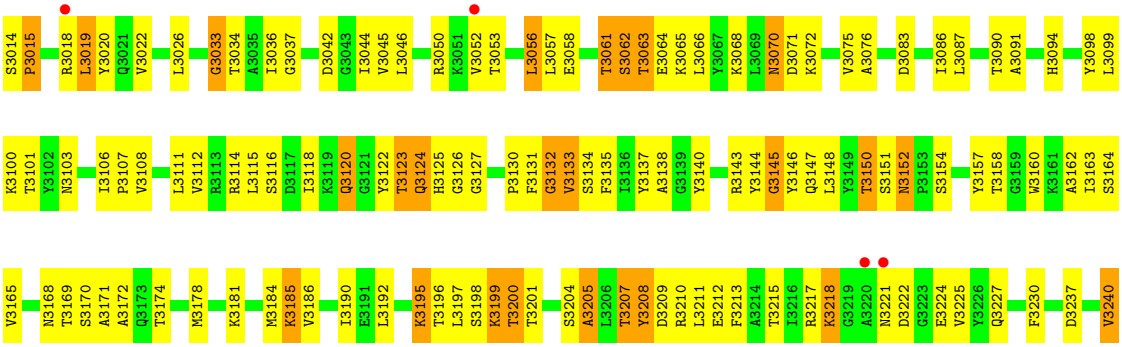
• Molecule 3: Proteasome component Y13

Chain AH:



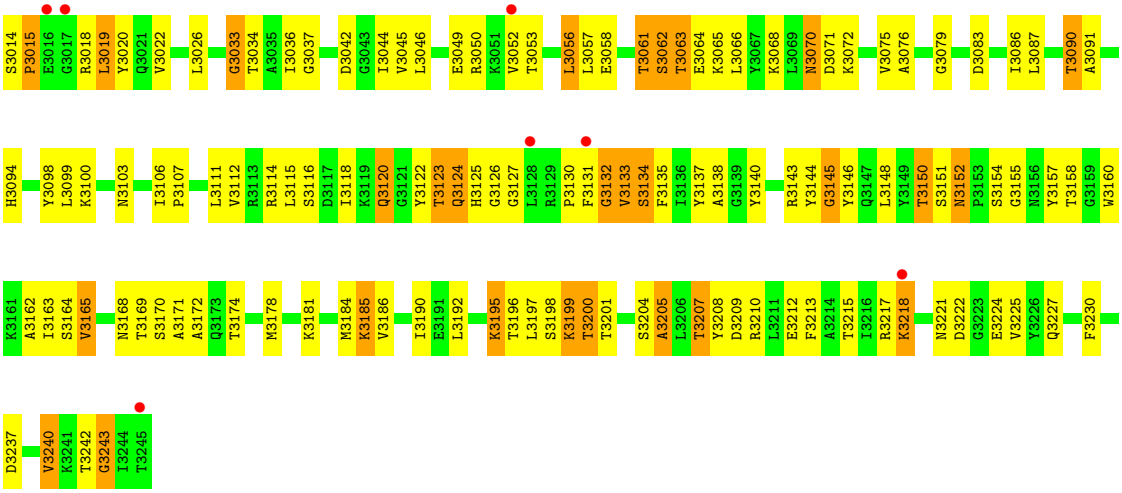
• Molecule 3: Proteasome component Y13

Chain AT:



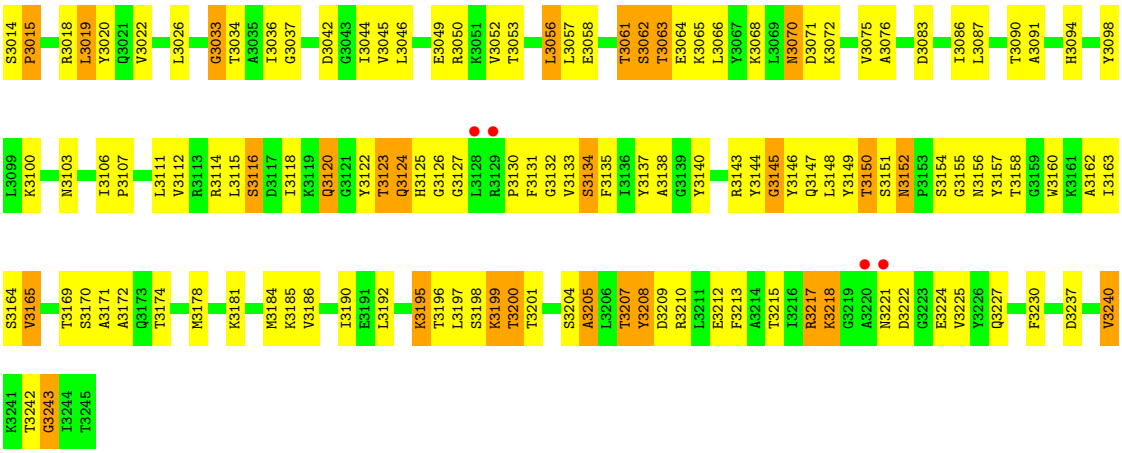
• Molecule 3: Proteasome component Y13

Chain BC:



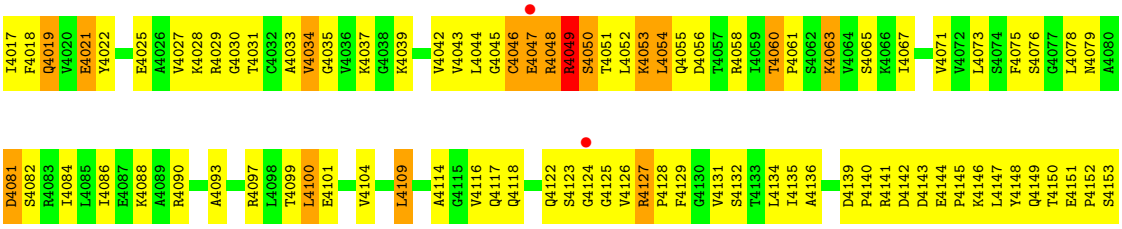
• Molecule 3: Proteasome component Y13

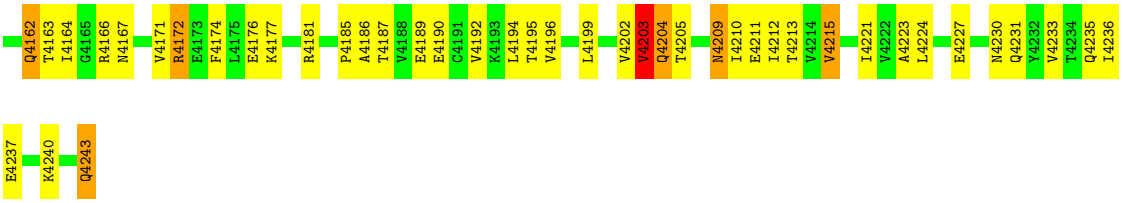
Chain BQ:



• Molecule 4: Proteasome component PRE6

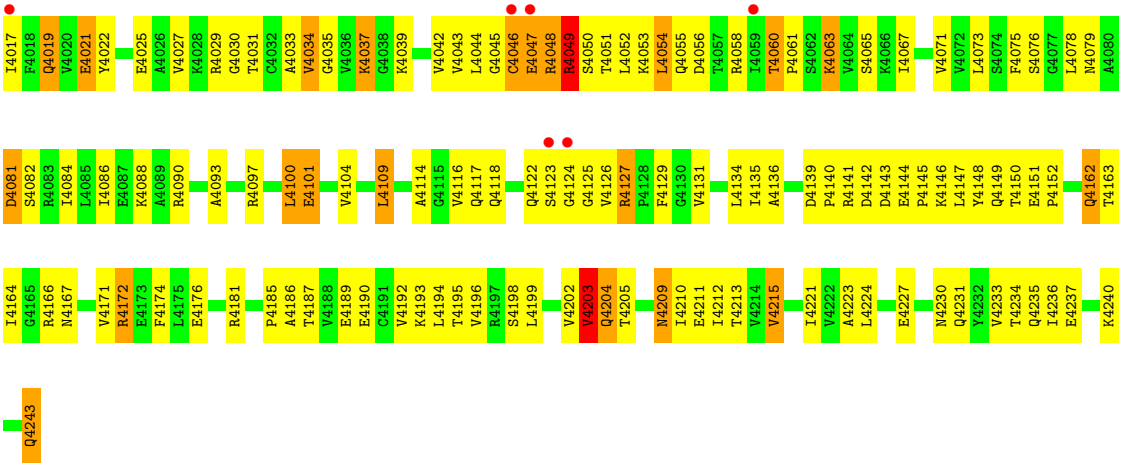
Chain AI:





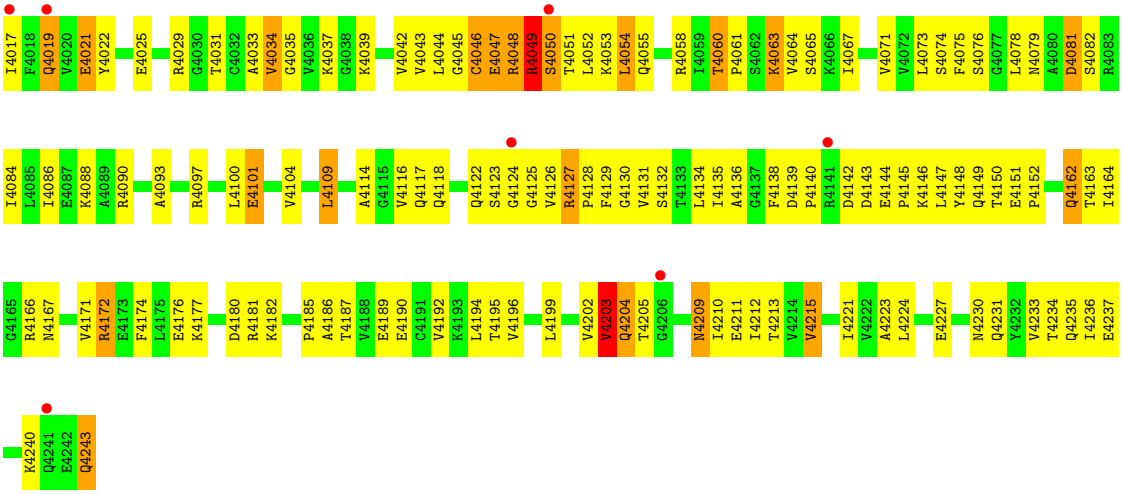
• Molecule 4: Proteasome component PRE6

Chain AU:



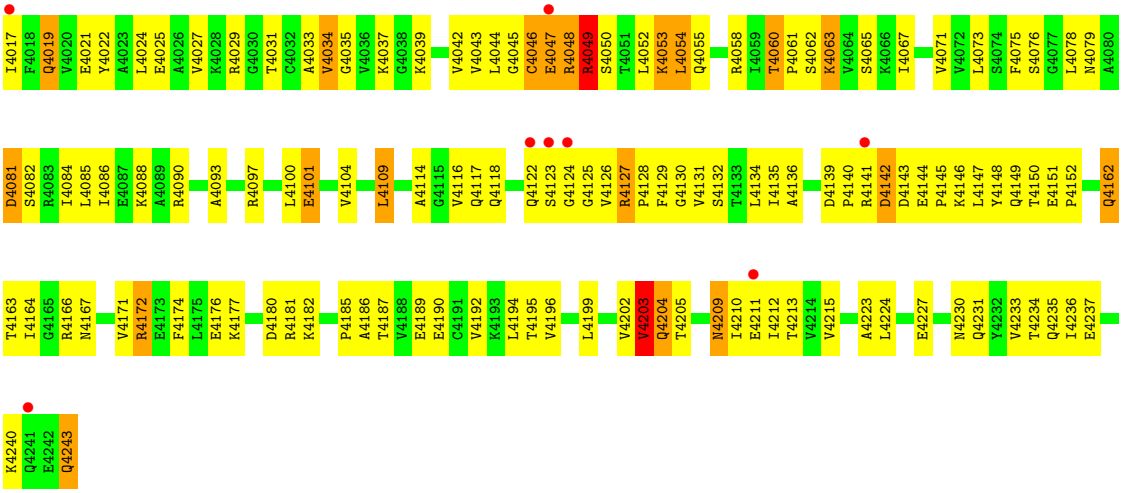
• Molecule 4: Proteasome component PRE6

Chain BD:



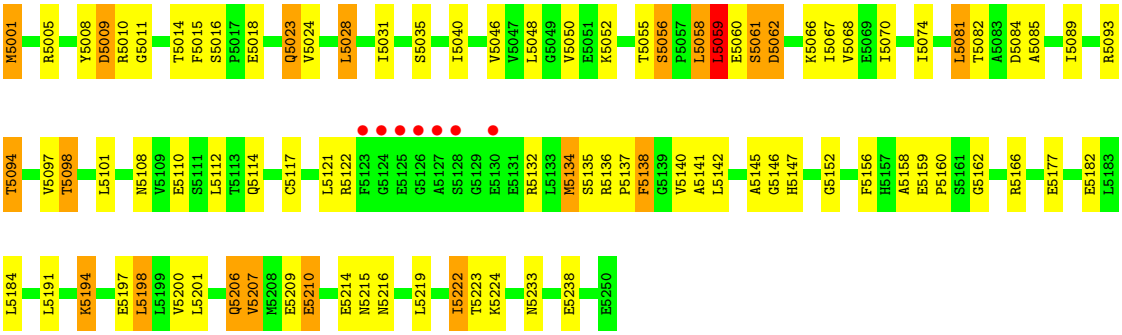
• Molecule 4: Proteasome component PRE6

Chain BR:



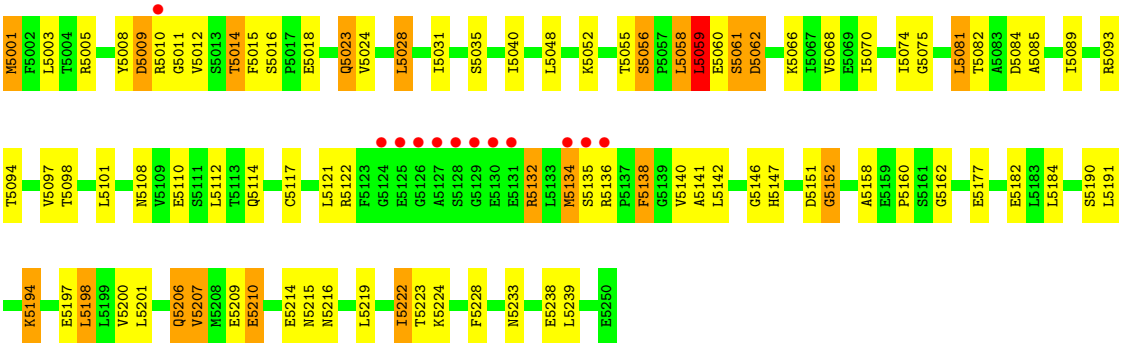
• Molecule 5: Proteasome component PUP2

Chain AJ:



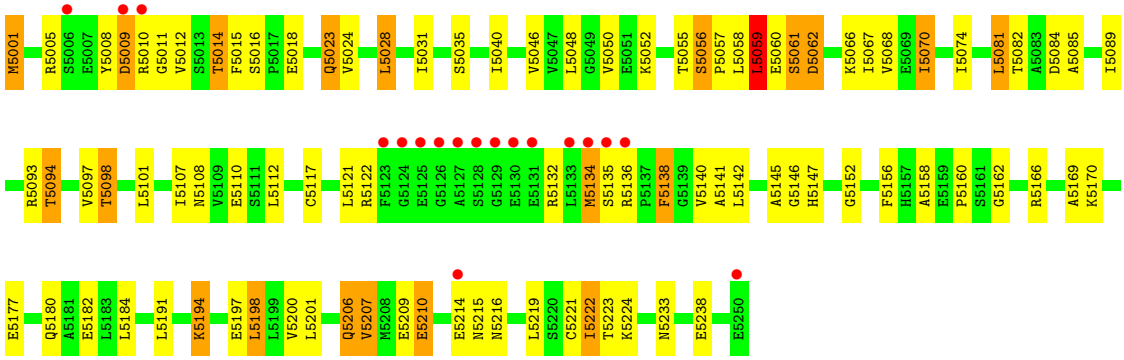
• Molecule 5: Proteasome component PUP2

Chain AV:



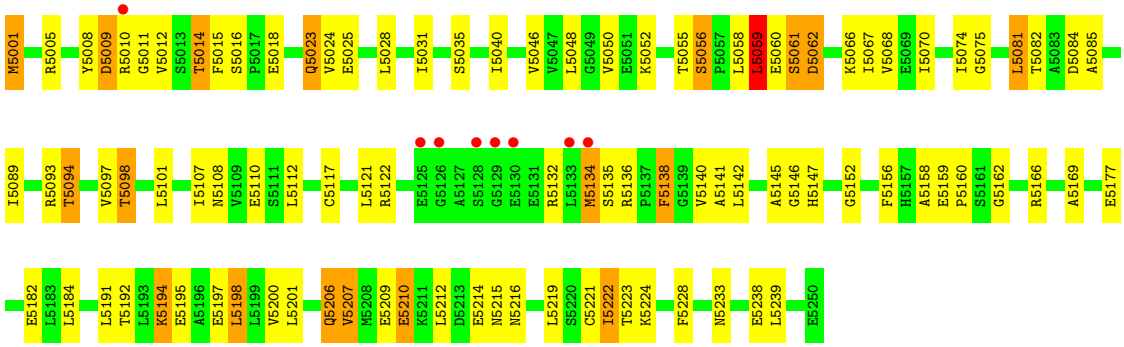
• Molecule 5: Proteasome component PUP2

Chain BE:



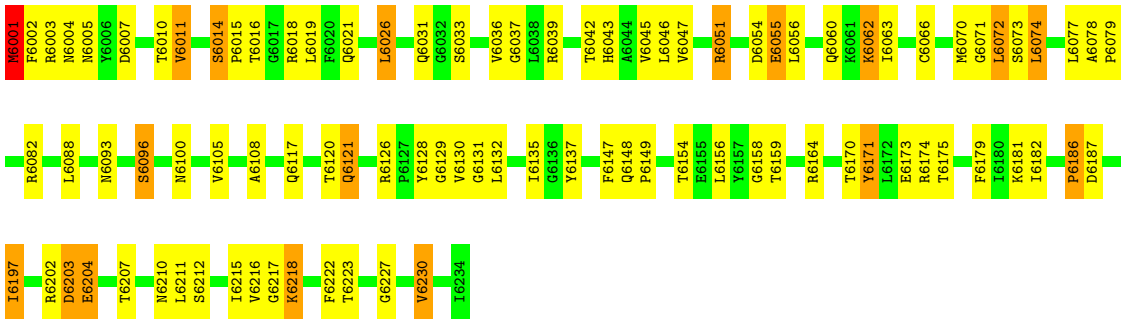
• Molecule 5: Proteasome component PUP2

Chain BS:



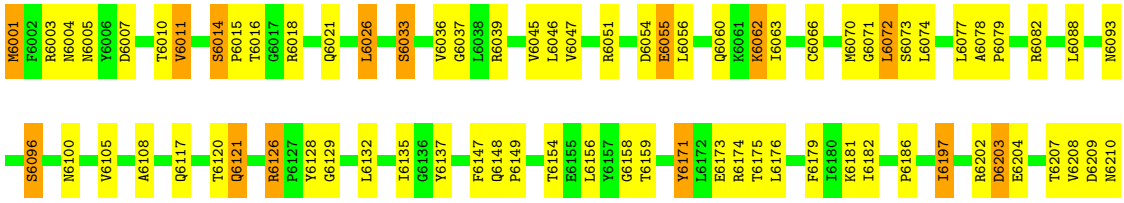
• Molecule 6: Proteasome component PRE5

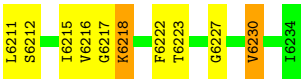
Chain AK:



• Molecule 6: Proteasome component PRE5

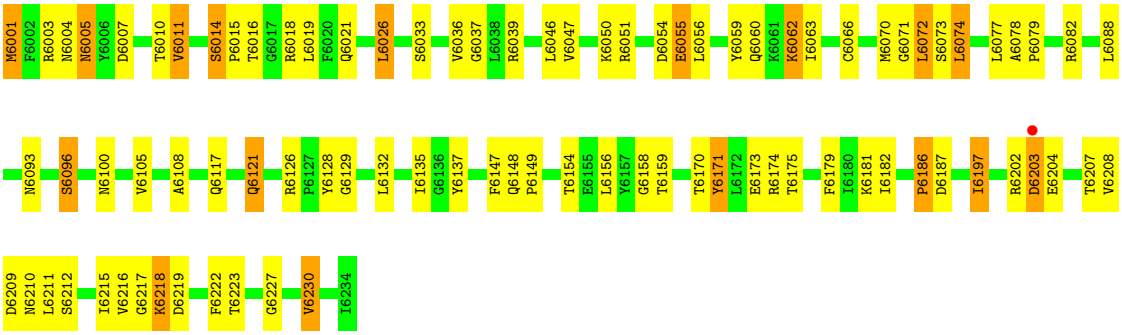
Chain AW:





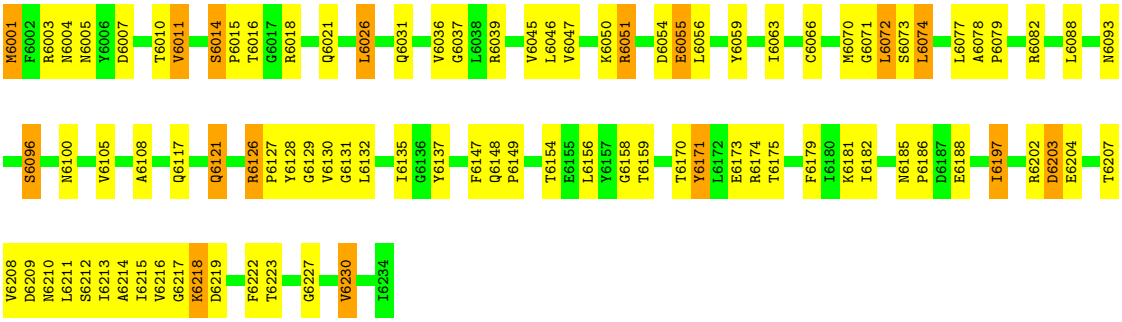
• Molecule 6: Proteasome component PRE5

Chain BF:



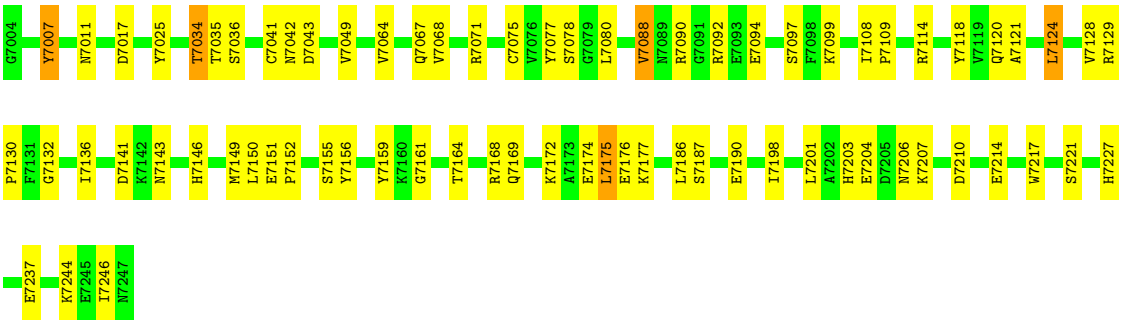
• Molecule 6: Proteasome component PRE5

Chain BT:



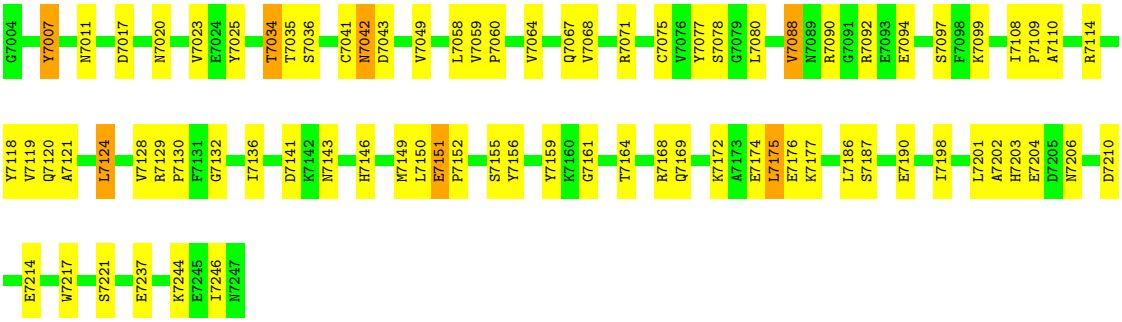
• Molecule 7: Proteasome component C1

Chain AL:



• Molecule 7: Proteasome component C1

Chain AX:

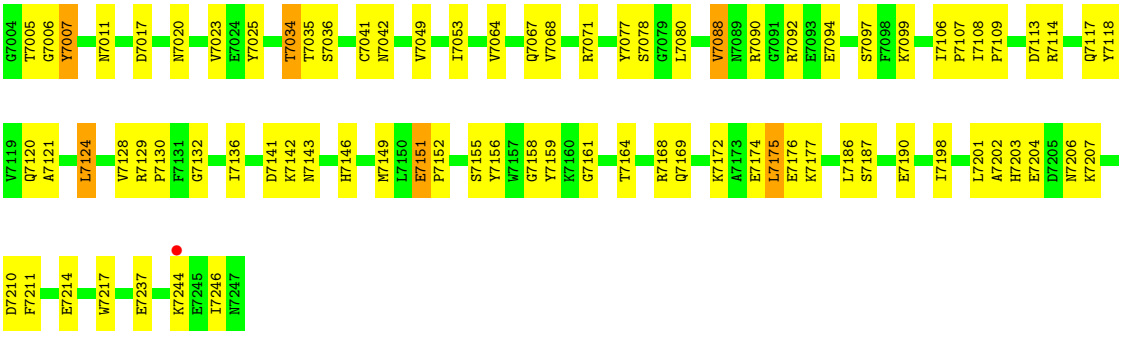


• Molecule 7: Proteasome component C1

Chain BG:

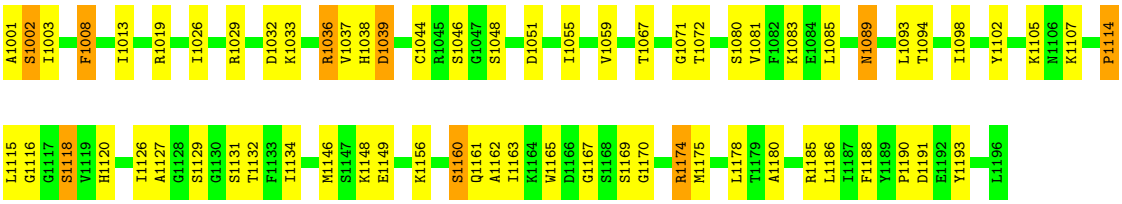
• Molecule 7: Proteasome component C1

Chain BU:



• Molecule 8: Proteasome component PRE3

Chain AB:



• Molecule 8: Proteasome component PRE3

Chain AD: 67% 28% 6%

A1001 S1002 I1003 F1008 A1016 Y1025 R1029 D1032 K1033 R1036 V1037 H1038 D1039 W1042 S1046 G1047 S1048 D1051 I1055 V1059 Q1060 Y1061 H1062 T1067 Y1070 G1071 T1072 P1073 S1080 V1081 F1082 K1083 E1084 L1085 N1089 L1093 T1094 Y1102 K1105 N1106 K1107

I1113 P1114 L1115 S1118 V1119 H1120 I1126 S1129 T1132 F1133 I1134 Y1135 G1136 M1146 S1147 K1148 E1149 K1156 S1160 Q1161 A1162 G1167 S1168 S1169 R1174 M1175 L1178 T1179 A1180 R1185 L1186 I1187 F1188 Y1189 P1190 D1191 E1192 Y1193 L1196

• Molecule 8: Proteasome component PRE3

Chain BH: 68% 27% 6%

A1001 S1002 I1003 F1008 R1029 D1032 K1033 R1036 V1037 H1038 D1039 C1044 R1045 S1046 A1054 I1055 I1058 V1059 T1067 G1071 T1072 P1073 S1080 V1081 F1082 K1083 E1084 L1085 N1089 L1093 I1098 Y1102 K1105 N1106 K1107 P1114 L1115 G1116 G1117 S1118 V1119 H1120 I1126

A1127 G1128 S1129 G1130 S1131 T1132 F1133 I1134 M1146 S1147 K1148 E1149 K1156 S1160 Q1161 A1162 I1163 K1164 W1165 D1166 G1167 S1168 S1169 R1174 M1175 L1178 T1179 A1180 R1185 L1186 I1187 F1188 Y1189 P1190 D1191 E1192 Y1193 L1196

• Molecule 8: Proteasome component PRE3

Chain BV: 68% 27% 5%

A1001 S1002 I1003 F1008 Y1025 R1029 D1032 K1033 L1034 T1035 R1036 V1037 H1038 D1039 C1044 R1045 S1046 G1047 S1048 D1051 I1055 V1059 T1067 G1071 T1072 P1073 V1081 F1082 K1083 E1084 L1085 N1089 L1093 T1094 I1098 Y1102 K1105 N1106 K1107 P1114 L1115 S1118

I1126 A1127 G1128 S1129 G1130 S1131 T1132 F1133 I1134 M1146 S1147 K1148 E1149 K1156 S1160 Q1161 A1162 W1165 D1166 G1167 S1168 S1169 R1174 M1175 L1178 T1179 A1180 R1185 L1186 I1187 F1188 Y1189 P1190 D1191 E1192 Y1193 L1196

• Molecule 9: Proteasome component PUP1

Chain AM: 73% 23% •

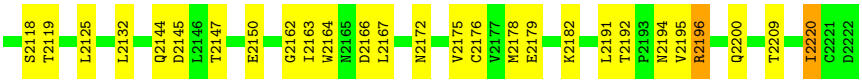
T2001 T2018 T2021 Q2022 G2023 P2024 K2029 N2030 K2033 L2034 S2038 P2039 W2042 A2049 V2055 T2056 Q2057 L2058 I2059 I2063 H2066 S2067 S2071 R2072 V2077 L2080 Y2090 Q2091 G2092 G2102 P2105 F2111 S2112 I2113 S2118 T2119 L2125 Q2144 D2145 L2146

T2147 E2150 Q2160 A2161 G2162 I2163 W2164 N2165 D2166 L2167 N2172 V2175 C2176 V2177 M2178 E2179 K2182 L2191 T2192 P2193 N2194 V2195 R2196 Q2200 T2209 I2220 C2221 D2222

• Molecule 9: Proteasome component PUP1

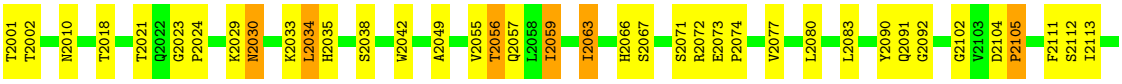
Chain AY: 70% 26% •

T2001 K2007 V2012 T2018 T2021 P2024 K2029 N2030 K2033 L2034 S2038 P2039 W2042 T2048 A2049 V2055 T2056 Q2057 L2058 I2059 I2063 H2066 S2067 S2071 R2072 E2073 P2074 V2077 L2080 Y2090 Q2091 G2092 V2100 A2101 G2102 V2103 D2104 P2105 F2111 S2112 I2113



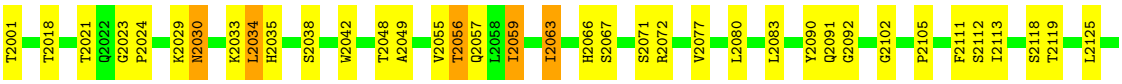
• Molecule 9: Proteasome component PUP1

Chain BI:



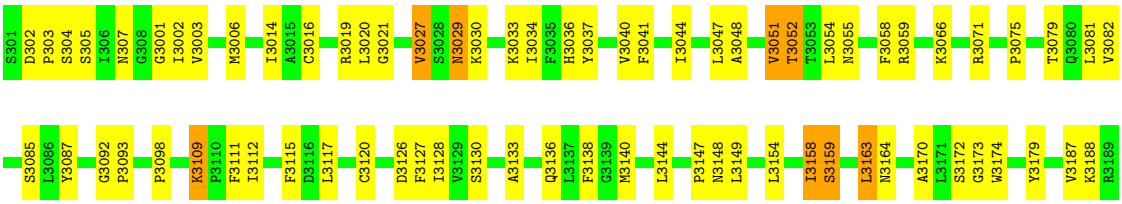
• Molecule 9: Proteasome component PUP1

Chain BW:



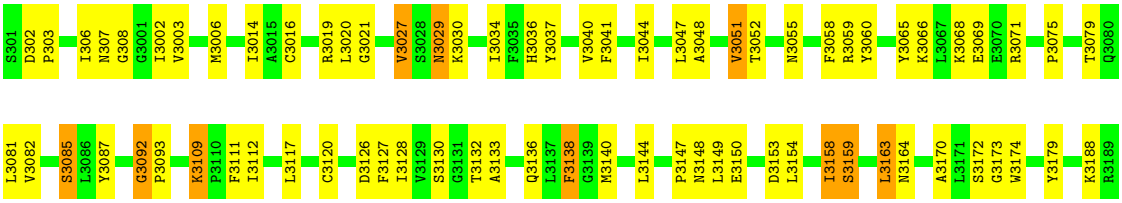
• Molecule 10: Proteasome component PUP3

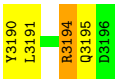
Chain AN:



• Molecule 10: Proteasome component PUP3

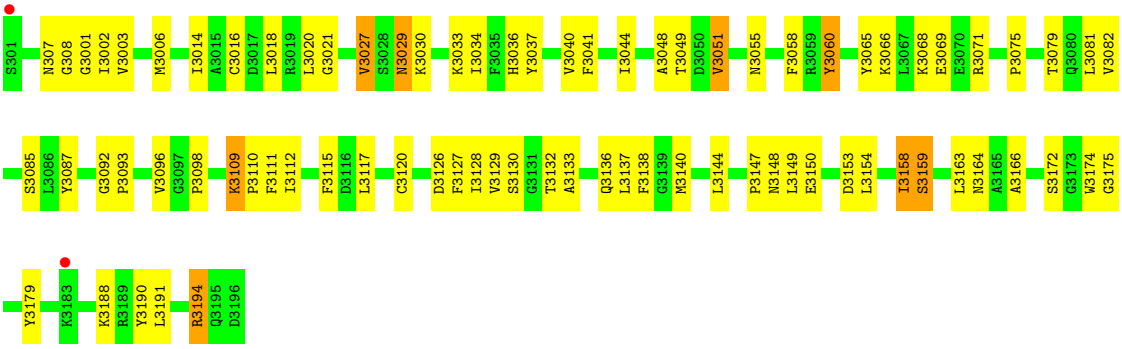
Chain AZ:





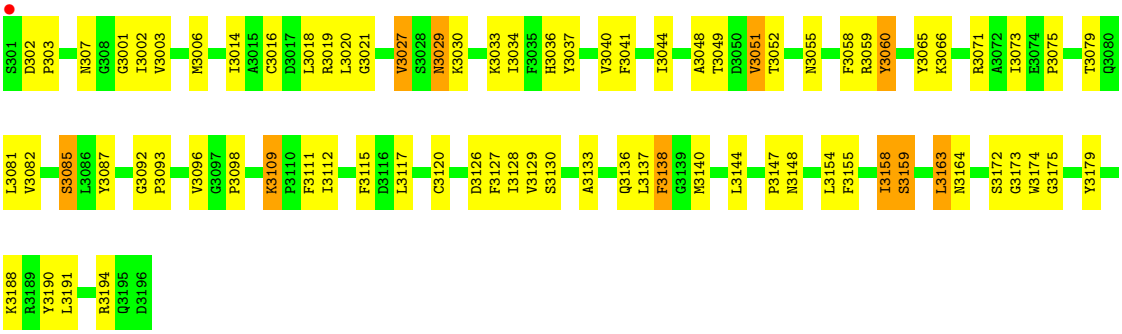
• Molecule 10: Proteasome component PUP3

Chain BJ:



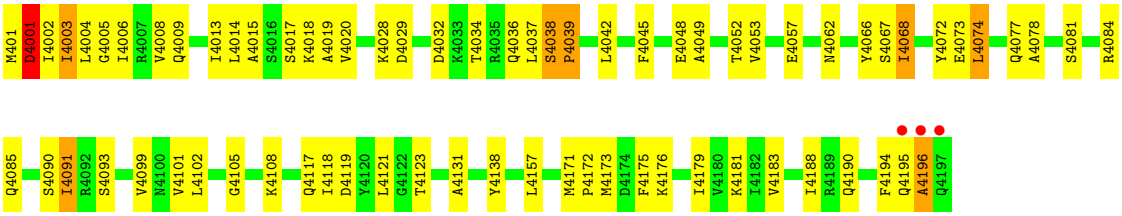
• Molecule 10: Proteasome component PUP3

Chain BX:



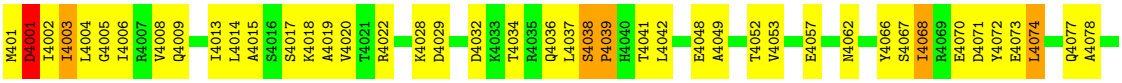
• Molecule 11: Proteasome component C11

Chain AO:



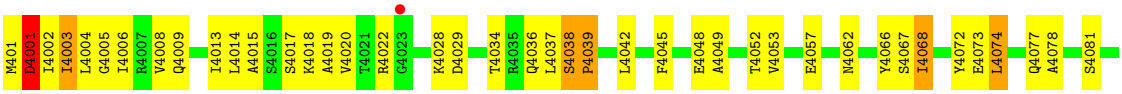
• Molecule 11: Proteasome component C11

Chain A1:



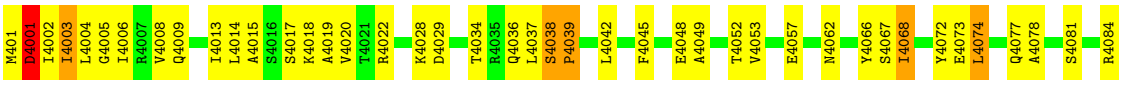
• Molecule 11: Proteasome component C11

Chain BK:



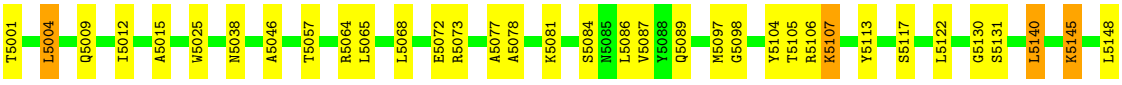
• Molecule 11: Proteasome component C11

Chain BY:



• Molecule 12: Proteasome component PRE2

Chain AP:



• Molecule 12: Proteasome component PRE2

Chain A2:

• Molecule 12: Proteasome component PRE2

Chain BL: 72% 25% •

T5001 L5004 Q5009 I5012 A5015 W5025 A5046 T5057 R5064 L5065 L5068 K5071 E5072 R5073 A5077 A5078 K5081 S5084 N5085 L5086 V5087 Y5088 Q5089 G5098 T5099 M5100 Y5104 T5105 R5106 K5107 Y5113 L5122 V5129 G5130 Q5133 L5140 K5145 L5148

S5149 V5150 E5151 D5152 A5153 L5154 K5158 R5159 S5160 I5161 L5162 A5163 A5164 A5165 G5172 G5173 S5174 L5177 Y5178 H5179 V5180 H5188 H5191 D5192 V5193 G5194 E5195 L5196 V5200 N5208 N5209 G5212

• Molecule 12: Proteasome component PRE2

Chain BZ: 71% 25% •

T5001 L5004 Q5009 I5012 A5015 V5016 D5017 W5025 A5046 T5057 R5064 L5065 L5068 E5072 R5073 A5077 A5078 K5081 S5084 N5085 L5086 V5087 Y5088 Q5089 G5098 Y5104 T5105 R5106 K5107 Y5113 L5122 G5130 S5131 G5132 Q5133 L5140 K5145 L5148 S5149

V5150 E5151 D5152 A5153 L5154 K5158 R5159 S5160 I5161 L5162 A5163 A5164 A5165 G5172 G5173 S5174 V5175 N5176 L5177 Y5178 H5179 V5180 T5181 E5182 H5188 G5189 N5190 H5191 D5192 V5193 G5194 E5195 L5196 V5200 N5208 N5209 G5212

• Molecule 13: Proteasome component C5

Chain AQ: 66% 29% 5%

Q601 F602 N603 P604 Y605 N608 G609 G6001 L6014 D6017 T6018 R6019 N6020 I6021 Y6024 N6027 Y6030 V6034 N6040 I6041 V6042 M6043 V6056 K6057 R6058 N6061 F6068 N6071 D6072 S6076 I6077 N6078 F6094 Y6097 T6100 I6101 I6102 A6103 S6115 F6116 D6117 P6118 V6119

E6123 R6124 E6125 Q6126 C6127 R6128 A6129 S6135 L6136 L6141 D6142 N6143 F6147 Q6150 T6155 N6156 G6157 K6158 V6159 K6160 L6163 K6164 Y6165 L6166 E6170 V6171 I6172 K6173 R6176 T6180 R6185 H6186 I6187 Q6188 V6189 G6190 D6191 L6196 I6197 V6198 T6199 G6202 V6203 K6211 R6212 D6213

• Molecule 13: Proteasome component C5

Chain A3: 62% 35% •

Q601 F602 N603 P604 N608 G609 G6001 T6002 I6003 L6004 E6009 L6014 D6017 T6018 R6019 N6020 I6021 T6022 D6023 Y6024 N6027 Y6030 E6031 P6032 K6033 V6034 N6040 I6041 V6042 M6043 V6056 N6061 W6065 D6069 H6070 N6071 D6072 S6076 I6077 N6078 F6094 T6100 I6101 I6102 A6103 G6104

L6105 K6110 G6111 S6115 F6116 D6117 P6118 V6119 E6123 R6124 E6125 Q6126 C6127 R6128 A6132 A6133 A6134 S6135 L6136 L6141 D6142 N6143 F6147 Q6150 T6155 N6156 G6157 K6158 V6159 K6160 L6163 K6164 Y6165 L6166 E6170 V6171 I6172 K6173 R6176 F6179 T6180 R6185 H6186 I6187 Q6188 V6189 G6190

D6191 G6192 L6193 I6197 V6198 T6199 G6202 V6203 K6211 R6212 D6213

• Molecule 13: Proteasome component C5

Chain BM: 66% 29% 5%

Q601 F602 N603 P604 Y605 N608 G609 G6001 L6004 L6014 D6017 T6018 R6019 N6020 I6021 N6027 Y6030 V6034 N6040 I6041 V6042 M6043 V6056 N6061 W6065 D6069 H6070 N6071 D6072 S6076 I6077 N6078 K6091 F6094 P6095 V6098 H6099 T6100 I6101 I6102 A6103 Y6114 S6115

F6116 D6117 P6118 V6119 E6123 R6124 E6125 Q6126 C6127 R6128 A6132 S6135 L6136 L6141 D6142 N6143 F6147 Q6150 T6155 N6156 G6157 K6158 V6159 K6160 L6163 K6164 Y6165 L6166 E6170 V6171 I6172 K6173 R6176 T6180 R6185 H6186 I6187 Q6188 I6197 V6198 T6199 G6202 V6203 K6211 R6212

D6213

- Molecule 13: Proteasome component C5

Chain B1: 68% 27%

Q601 F602 N603 P604 Y605 N608 L6004 L6014 T6018 R6019 N6020 I6021 N6027 Y6030 V6034 N6040 I6041 V6042 M6043 V6056 N6061 N6071 D6072 S6076 I6077 N6078 F6094 V6098 H6099 T6100 I6101 I6102 A6103 V6113 Y6114 S6115 F6116 D6117 P6118 V6119 E6123 R6124 E6125 Q6126

G6127 R6128 A6132 S6135 L6136 L6141 D6142 N6143 Q6150 T6155 N6156 G6157 K6158 V6159 K6160 L6163 K6164 Y6165 L6166 E6170 V6171 I6172 K6173 R6176 T6180 R6185 H6186 I6187 Q6188 V6189 G6190 D6191 I6197 V6198 T6199 G6202 V6203 L6210 K6211 R6212 D6213

- Molecule 14: Proteasome component PRE4

Chain AR: 62% 31% 6%

T701 Q702 Q703 P704 I705 S7002 Y7008 D7009 N7010 G7011 V7012 L7019 G7020 S7021 Y7022 L7025 L7026 R7027 I7035 N7040 T7041 V7042 I7045 D7051 M7052 I7055 E7056 R7057 L7058 L7059 K7060 D7061 L7062 V7063 T7064 E7065 Y7068 D7074 A7075 E7076 E7077 P7081 L7088 A7089 T7090 V7091 M7092

Y7093 Q7094 R7095 R7096 S7097 P7101 L7102 W7103 A7109 L7119 R7120 Y7121 V7122 N7123 L7124 V7127 T7128 Y7129 S7130 T7133 G7139 N7144 P7145 R7148 K7149 V7150 V7151 D7152 R7153 E7154 S7155 D7156 I7157 P7158 T7161 V7162 Q7163 V7164 E7167 N7171 R7174 V7175 L7176 Y7177 Y7178 R7179 D7180 A7181

S7184 D7193 T7196 G7197 L7198 M7209 K7210 W7211 K7218 G7219 Q7223 K7224 I7225

- Molecule 14: Proteasome component PRE4

Chain A4: 63% 31% 5%

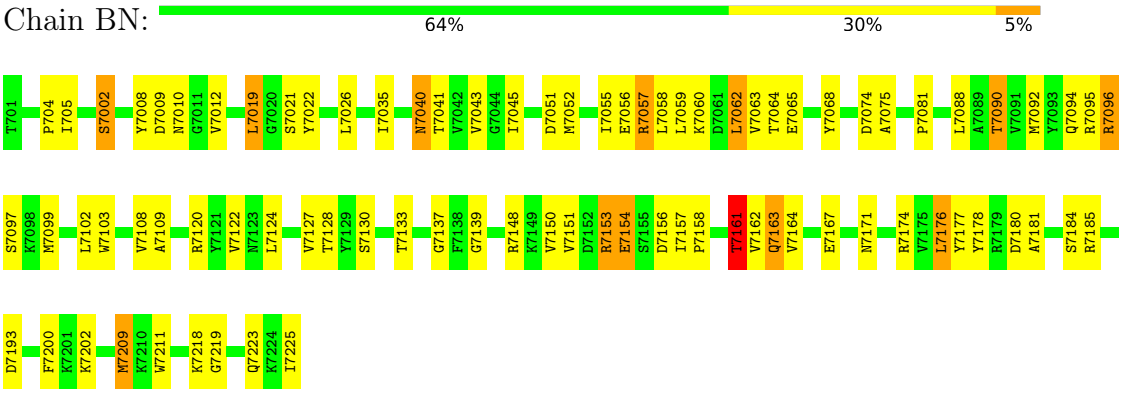
T701 Q702 Q703 P704 I705 V706 T707 G708 T7001 S7002 Y7008 D7009 N7010 G7011 V7012 L7019 G7020 S7021 Y7022 L7026 R7033 L7034 I7035 N7040 T7041 I7045 S7046 D7051 M7052 I7055 E7056 R7057 L7058 L7059 K7060 D7061 L7062 V7063 T7064 E7065 Y7068 D7074 A7075 E7076 E7077 P7081 L7088 A7089

T7090 R7095 R7096 S7097 P7101 L7102 W7103 A7109 L7119 R7120 Y7121 V7122 V7127 T7128 Y7129 S7130 T7133 G7137 F7138 G7139 R7148 K7149 V7150 V7151 D7152 R7153 E7154 S7155 D7156 I7157 P7158 T7161 V7162 Q7163 V7164 E7167 N7171 R7174 V7175 L7176 Y7177 Y7178 R7179 D7180 A7181 S7184

D7193 F7200 K7201 K7202 M7209 K7210 W7211 K7218 G7219 Q7223 K7224 I7225

- Molecule 14: Proteasome component PRE4

Chain BN:

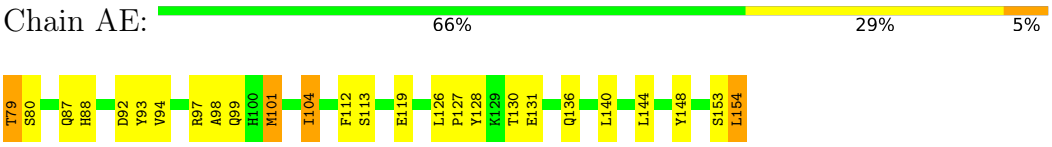


- Molecule 14: Proteasome component PRE4

Chain B2:

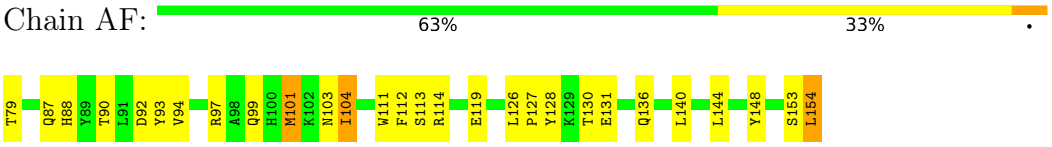
- Molecule 15: Proteasome activator BLM10

Chain AE:



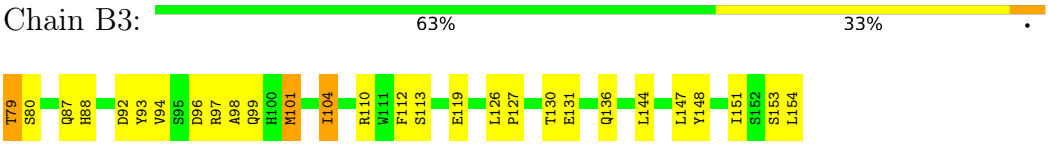
- Molecule 15: Proteasome activator BLM10

Chain AF:



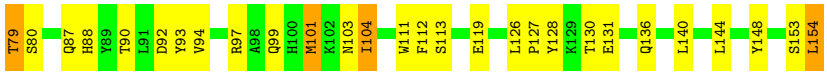
- Molecule 15: Proteasome activator BLM10

Chain B3:



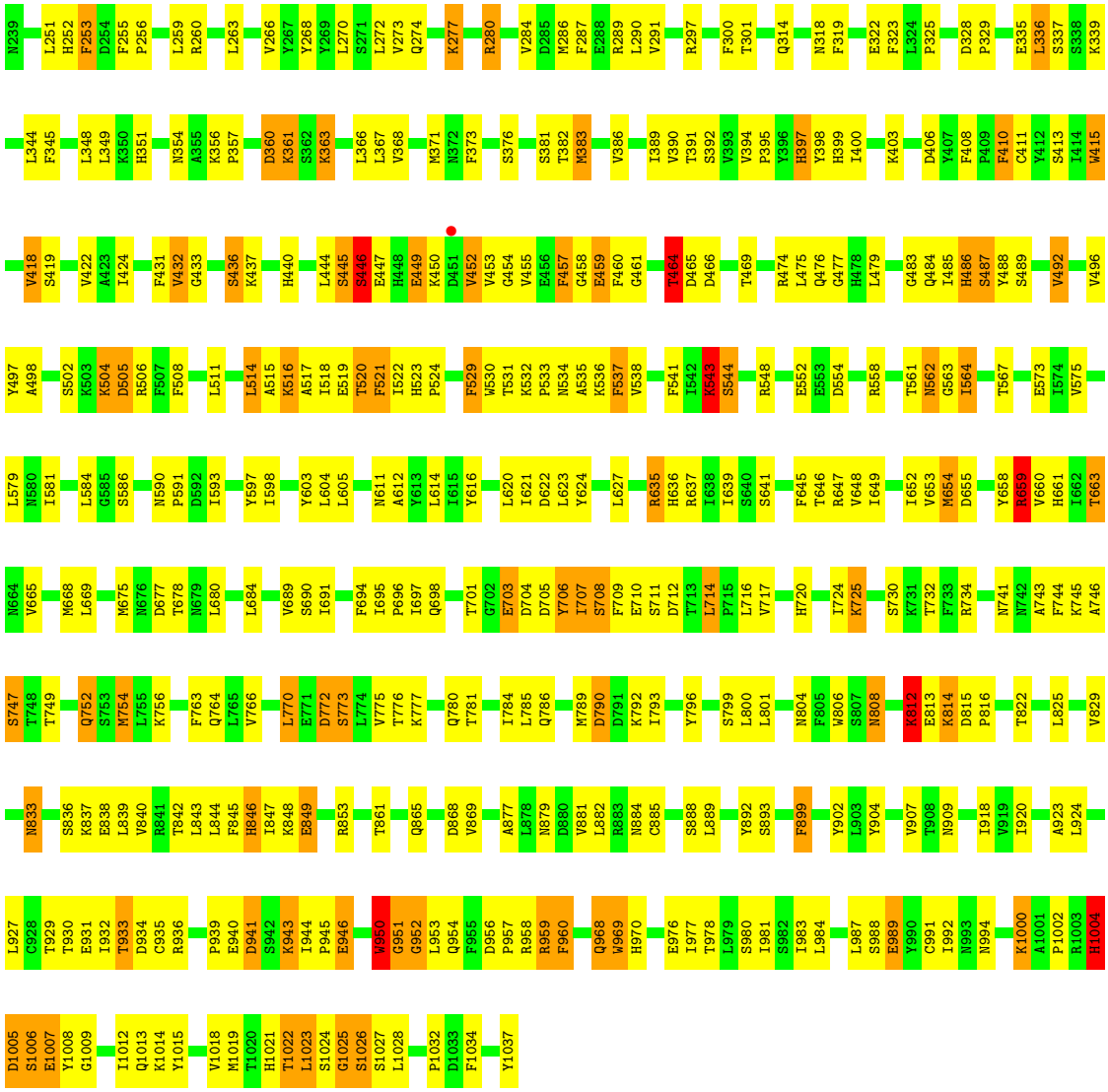
- Molecule 15: Proteasome activator BLM10

Chain B6:



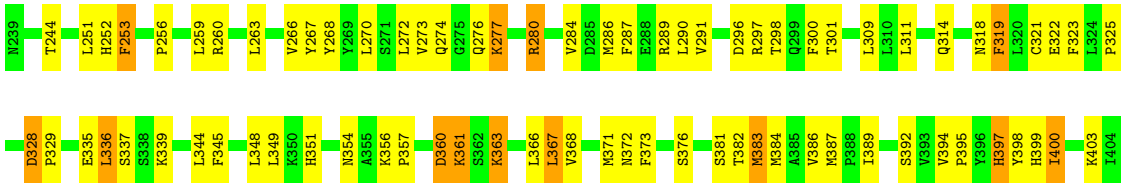
• Molecule 16: Proteasome activator BLM10

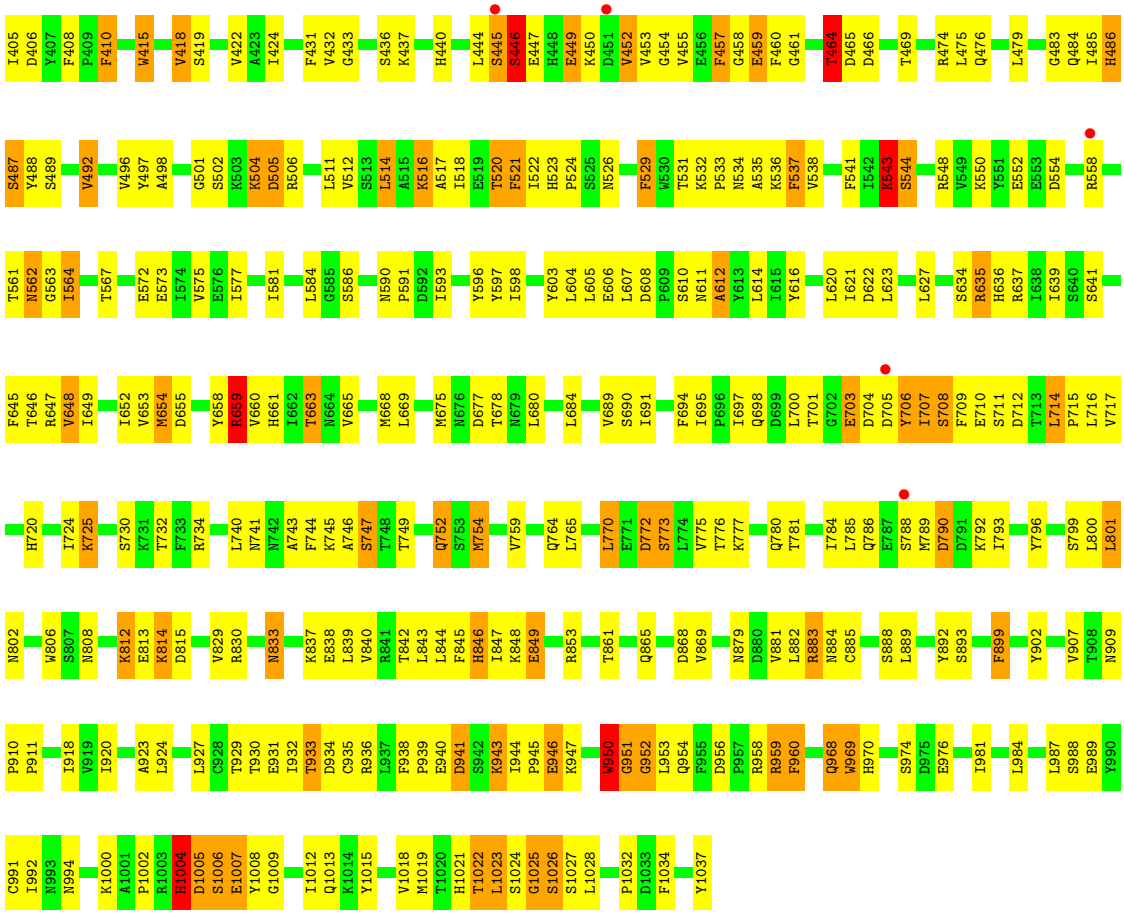
Chain A5:



• Molecule 16: Proteasome activator BLM10

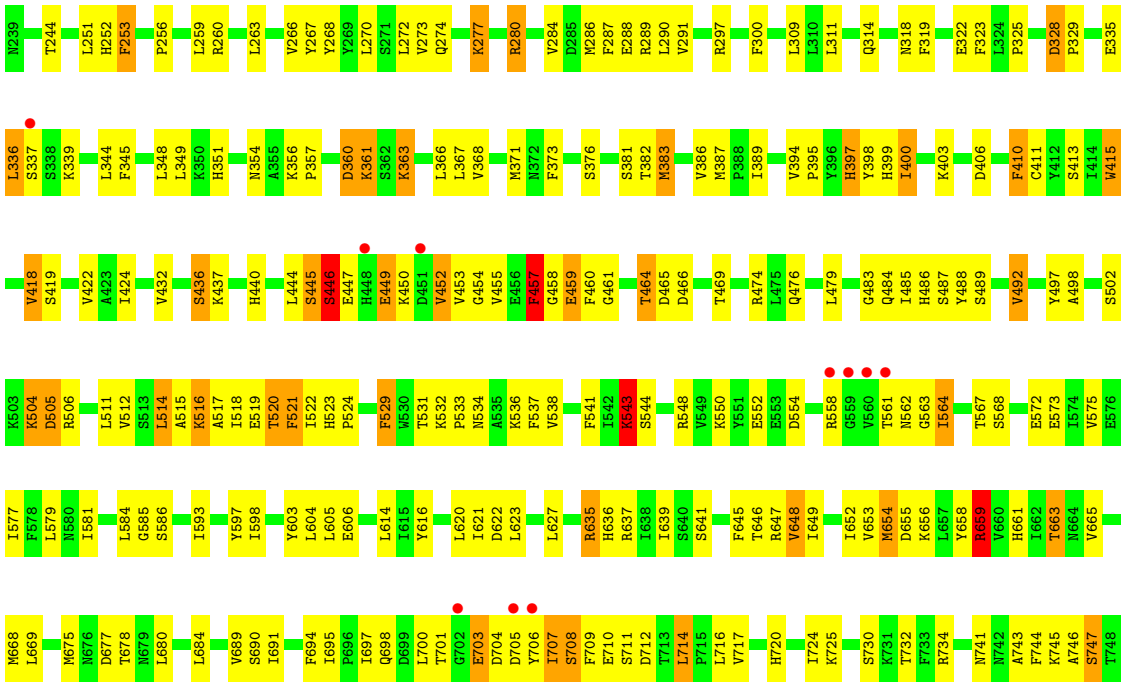
Chain A7:

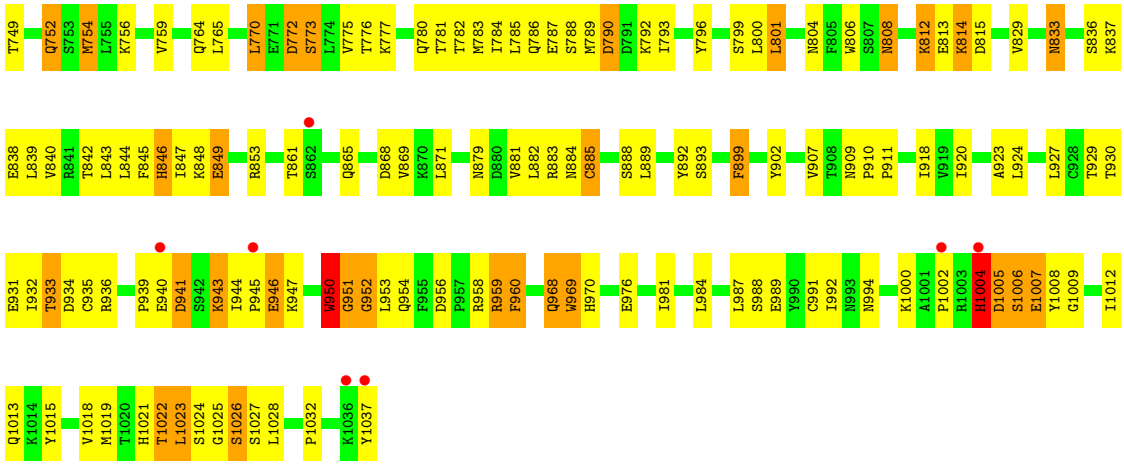




• Molecule 16: Proteasome activator BLM10

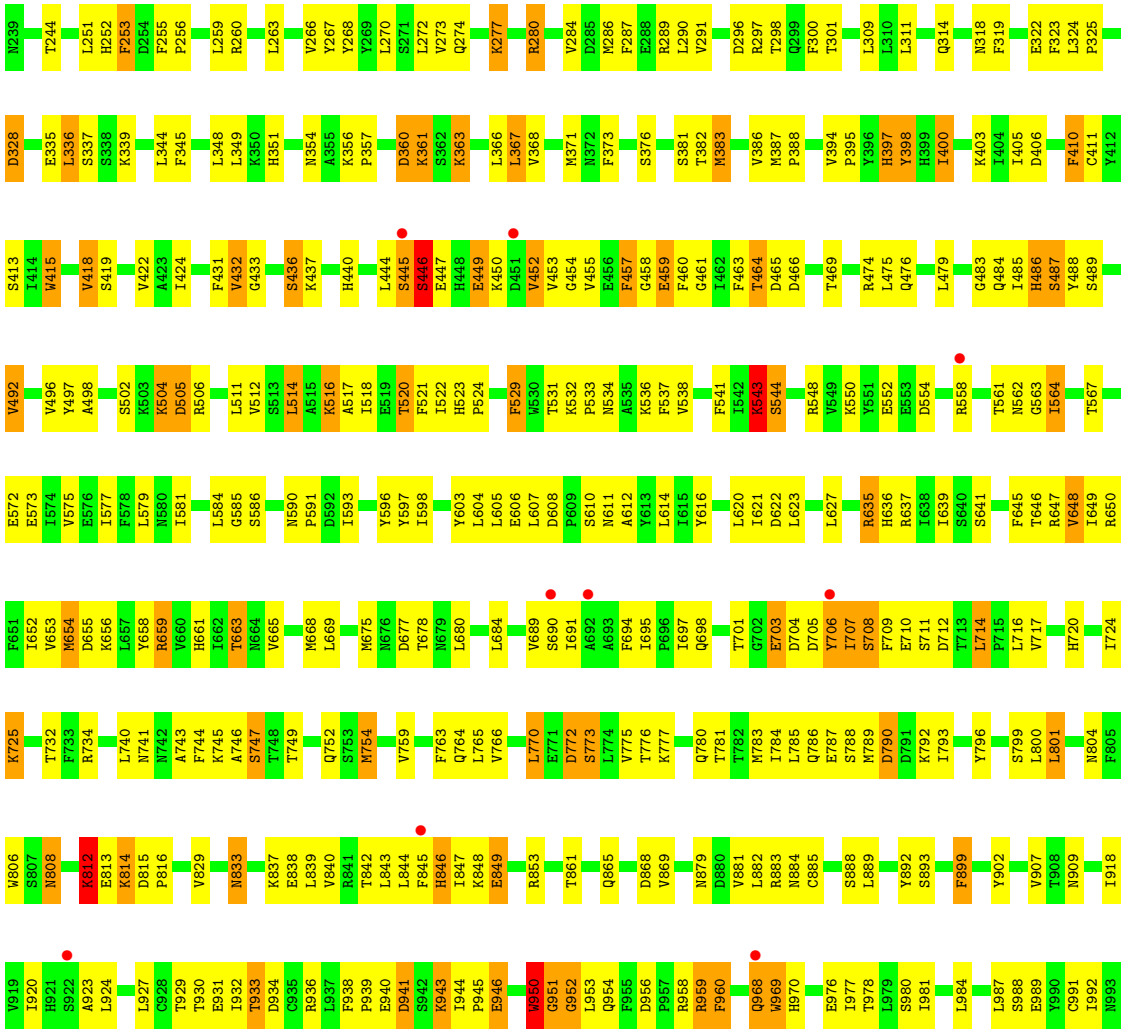
Chain B4:

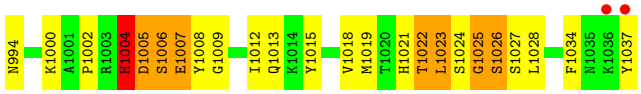




• Molecule 16: Proteasome activator BLM10

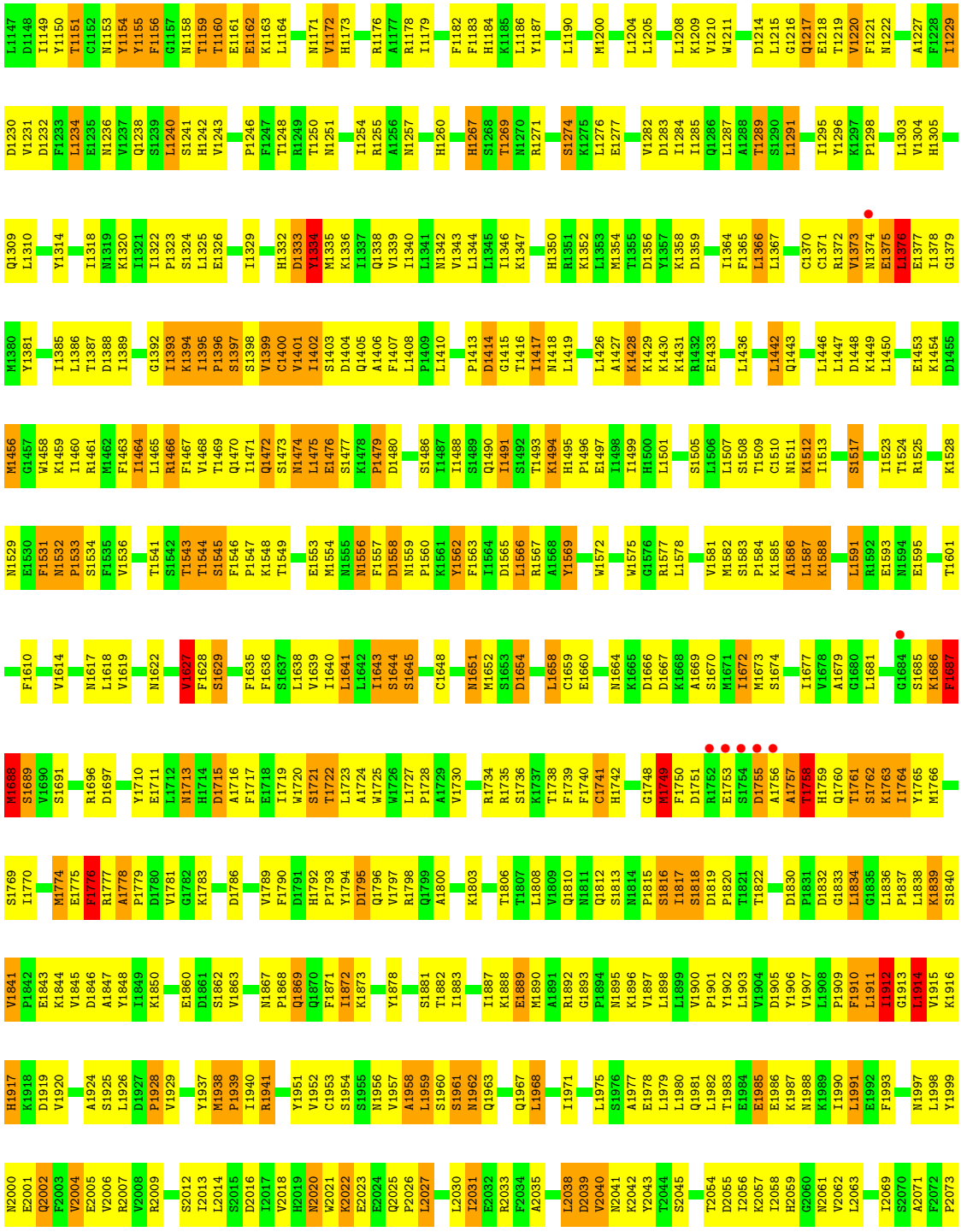
Chain B7:

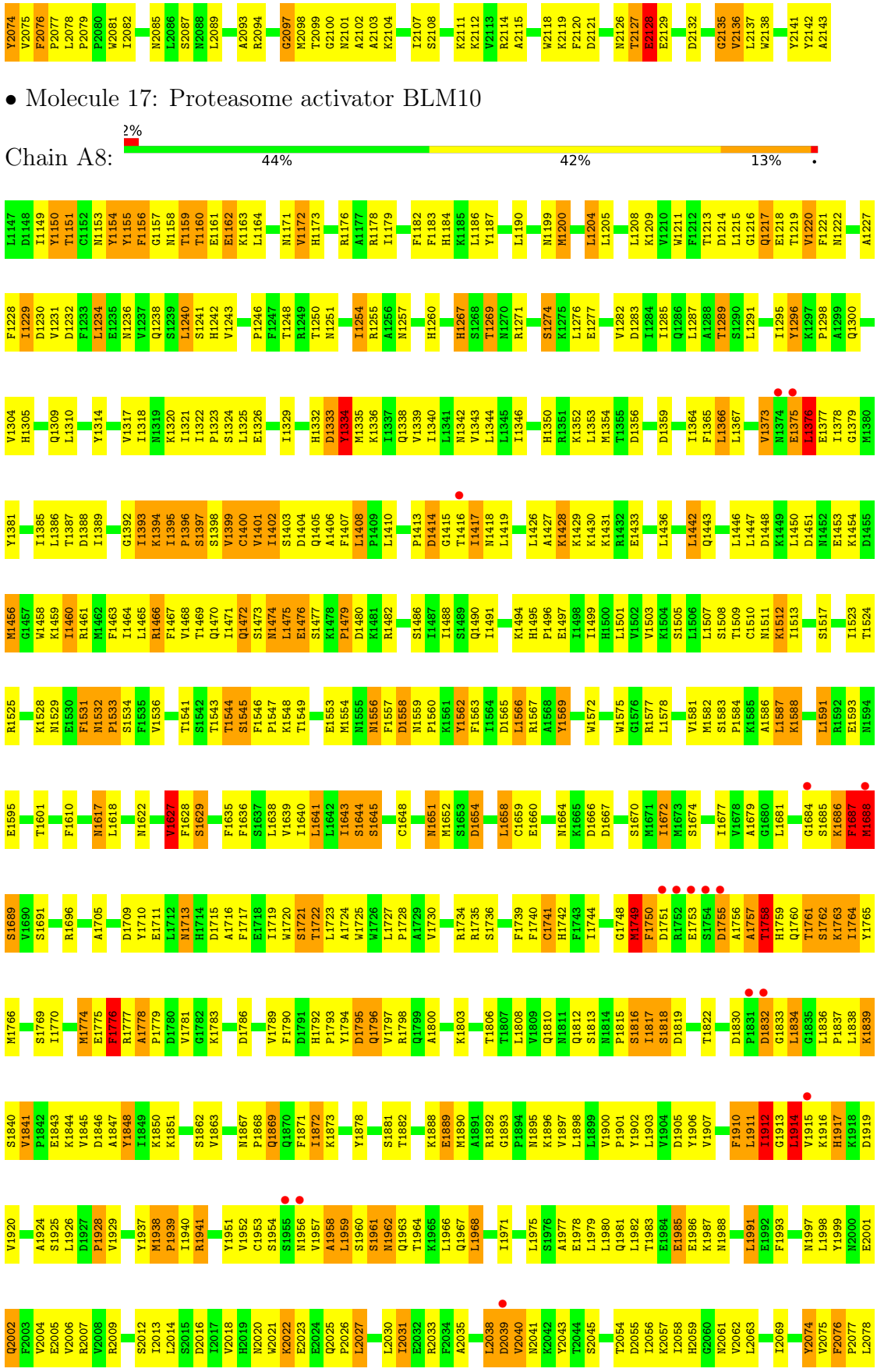


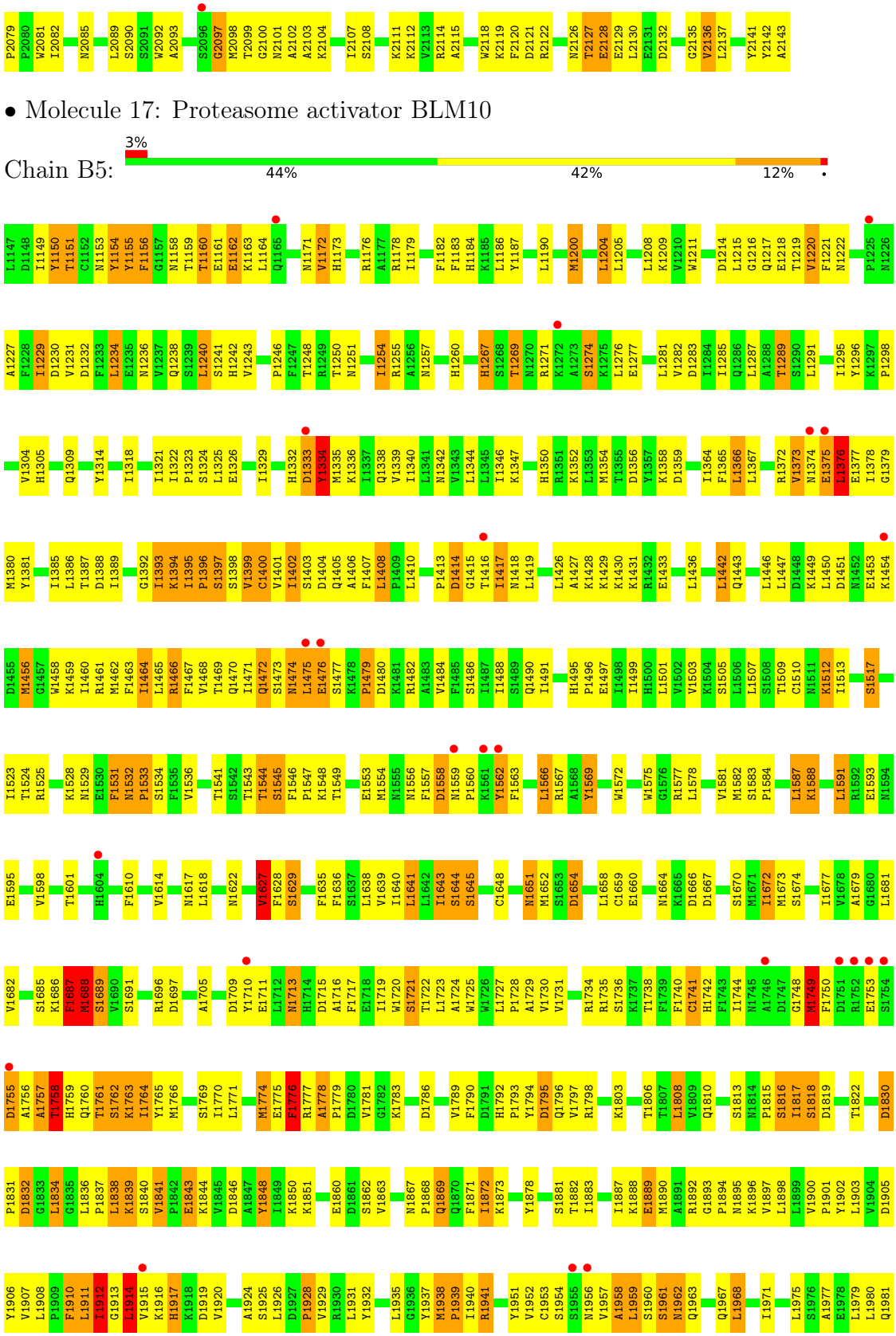


• Molecule 17: Proteasome activator BLM10

Chain A6:

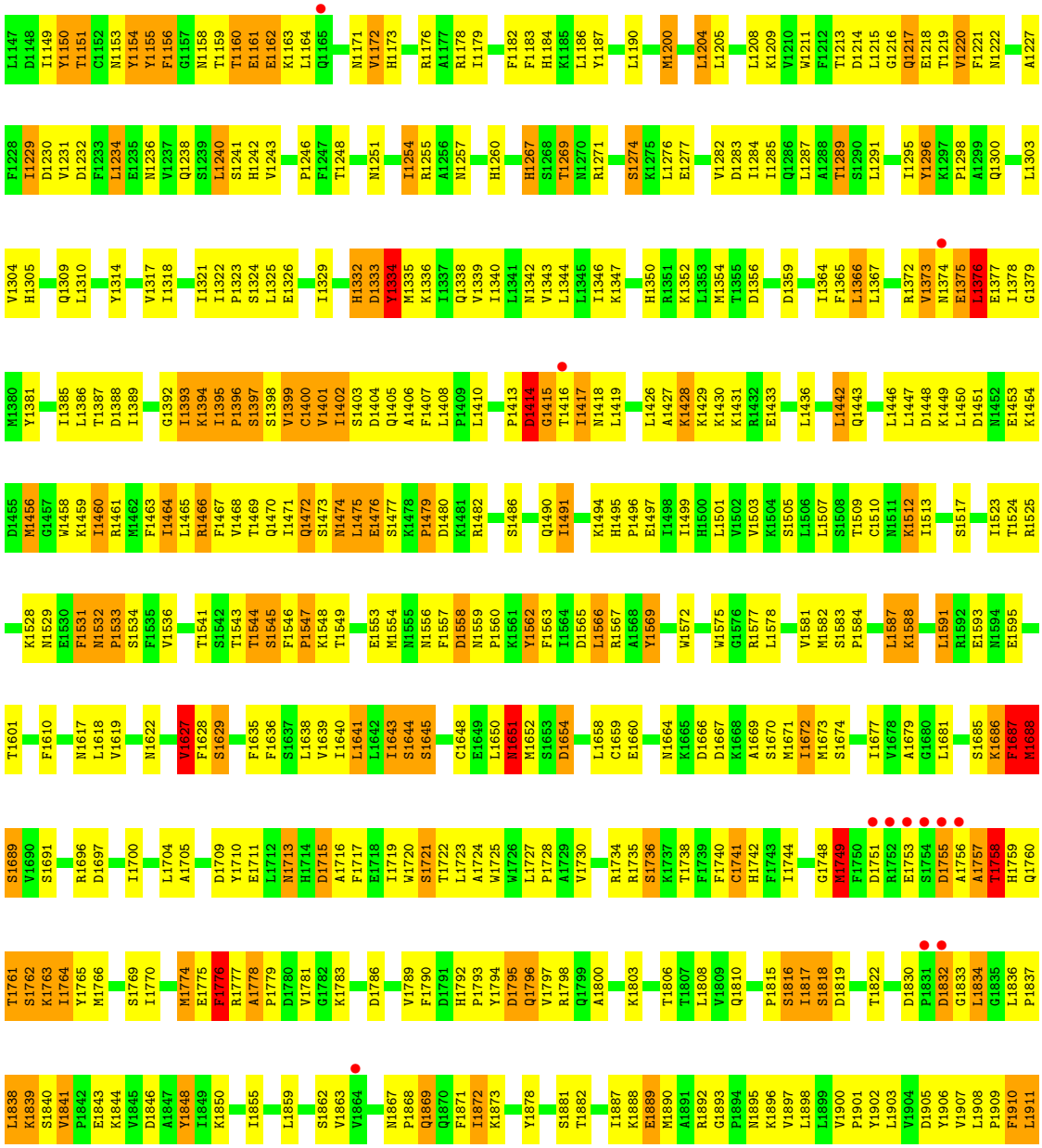


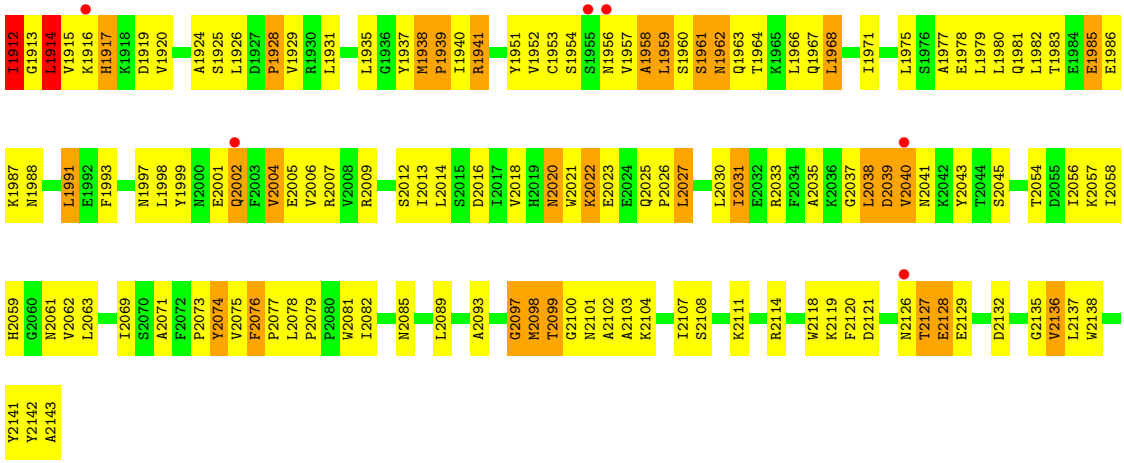

• Molecule 17: Proteasome activator BLM10
Chain A8:
2%
44%
42%
13%


P2079 P2080 W2081 I2082 N2085 L2089 S2090 S2091 W2092 A2093 S2096 G2097 M2098 T2099 G2100 N2101 A2102 A2103 K2104 I2107 S2108 K2111 K2112 V2113 R2114 A2115 W2118 K2119 F2120 D2121 R2122 N2126 T2127 E2128 E2129 L2130 E2131 D2132 G2135 V2136 L2137 Y2141 Y2142 A2143
• Molecule 17: Proteasome activator BLM10
Chain B5:
3%
44%
42%
12%
L1147 D1148 I1149 Y1150 T1151 G1152 N1153 Y1154 Y1155 F1156 G1157 N1158 T1159 T1160 E1161 E1162 K1163 L1164 Q1165 N1171 V1172 H1173 R1176 A1177 R1178 I1179 F1182 F1183 H1184 K1185 L1186 Y1187 L1190 M1200 L1204 L1205 L1208 K1209 V1210 W1211 D1214 L1215 G1216 Q1217 E1218 T1219 V1220 F1221 N1222 P1225 N1226
A1227 F1228 I1229 D1230 V1231 D1232 F1233 L1234 E1235 N1236 V1237 Q1238 S1239 L1240 S1241 H1242 V1243 P1246 F1247 T1248 R1249 T1250 N1251 I1254 R1255 A1256 N1257 H1260 H1267 S1268 T1269 N1270 R1271 K1272 A1273 S1274 K1275 L1276 E1277 L1281 V1282 D1283 I1284 I1285 Q1286 L1287 A1288 T1289 S1290 L1291 I1295 Y1296 K1297 P1298
V1304 H1305 Q1309 Y1314 I1318 I1321 I1322 P1323 S1324 L1325 E1326 I1329 H1332 D1333 Y1334 M1335 K1336 I1337 Q1338 V1339 I1340 L1341 N1342 V1343 L1344 L1345 I1346 K1347 H1350 R1351 K1352 L1353 M1354 T1355 D1356 Y1357 K1358 D1359 I1364 F1365 L1366 L1367 R1372 V1373 N1374 E1375 L1376 E1377 I1378 G1379
M1380 Y1381 I1385 L1386 T1387 D1388 I1389 G1392 I1393 K1394 I1395 P1396 S1397 S1398 V1399 C1400 V1401 I1402 S1403 D1404 Q1405 A1406 F1407 L1408 P1409 L1410 P1413 D1414 G1415 T1416 I1417 N1418 L1419 L1426 A1427 K1428 K1429 K1430 K1431 R1432 E1433 L1436 L1442 Q1443 L1446 L1447 D1448 K1449 L1450 D1451 N1452 E1453 K1454
D1455 M1456 G1457 W1458 K1459 I1460 R1461 M1462 F1463 I1464 L1465 R1466 F1467 V1468 T1469 Q1470 I1471 Q1472 S1473 N1474 L1475 E1476 S1477 K1478 P1479 D1480 K1481 R1482 A1483 V1484 F1485 S1486 I1487 I1488 S1489 Q1490 I1491 H1495 P1496 E1497 I1498 I1499 H1500 L1501 V1502 V1503 K1504 S1505 L1506 L1507 S1508 T1509 C1510 N1511 K1512 I1513 S1517
I1523 T1524 R1525 K1528 N1529 E1530 F1531 N1532 P1533 S1534 F1535 V1536 T1541 S1542 T1543 T1544 S1545 F1546 P1547 K1548 T1549 E1553 M1554 N1555 N1556 F1557 D1558 N1559 P1560 K1561 Y1562 F1563 L1566 R1567 A1568 Y1569 W1572 W1575 G1576 R1577 L1578 V1581 M1582 S1583 P1584 L1587 K1588 L1591 R1592 E1593 N1594
E1595 V1598 T1601 H1604 F1610 V1614 N1617 L1618 N1622 V1627 F1628 S1629 F1635 F1636 S1637 L1638 V1639 I1640 L1641 L1642 I1643 S1644 S1645 C1648 N1651 M1652 S1653 D1654 L1658 C1659 E1660 N1664 K1665 D1666 D1667 S1670 M1671 T1672 M1673 S1674 I1677 V1678 A1679 G1680 L1681
V1682 S1685 K1686 F1687 M1688 S1689 V1690 S1691 R1696 D1697 A1705 D1709 Y1710 E1711 L1712 N1713 H1714 D1715 A1716 F1717 E1718 I1719 W1720 S1721 T1722 L1723 A1724 W1725 W1726 L1727 P1728 A1729 V1730 V1731 R1734 R1735 S1736 K1737 T1738 F1739 F1740 C1741 H1742 F1743 I1744 N1745 A1746 D1747 G1748 M1749 F1750 D1751 R1752 E1753 S1754
D1755 A1756 A1757 T1758 H1759 Q1760 T1761 S1762 K1763 I1764 Y1765 M1766 S1769 I1770 L1771 M1774 E1775 F1776 R1777 A1778 P1779 D1780 V1781 G1782 K1783 D1786 V1789 F1790 D1791 H1792 P1793 Y1794 D1795 Q1796 V1797 R1798 K1803 T1806 T1807 L1808 V1809 Q1810 S1813 N1814 P1815 S1816 I1817 S1818 D1819 T1822 D1830
P1831 D1832 G1833 L1834 G1835 L1836 P1837 L1838 K1839 S1840 V1841 P1842 E1843 K1844 V1845 D1846 A1847 Y1848 I1849 K1850 K1851 E1860 D1861 S1862 V1863 N1867 P1868 Q1869 Q1870 F1871 I1872 K1873 Y1878 S1881 T1882 I1883 I1887 K1888 E1889 M1890 A1891 R1892 G1893 P1894 N1895 K1896 V1897 L1898 L1899 V1900 P1901 Y1902 L1903 V1904 D1905
Y1906 V1907 L1908 P1909 F1910 L1911 I1912 G1913 L1914 V1915 K1916 H1917 K1918 D1919 V1920 A1924 S1925 L1926 D1927 P1928 V1929 R1930 L1931 Y1932 L1935 G1936 Y1937 M1938 P1939 I1940 R1941 Y1951 V1952 C1953 S1954 S1955 N1956 V1957 A1958 L1959 S1960 S1961 N1962 Q1963 Q1967 L1968 I1971 L1975 S1976 A1977 E1978 L1979 L1980 Q1981

• 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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.66	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.