



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:42 PM GMT

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

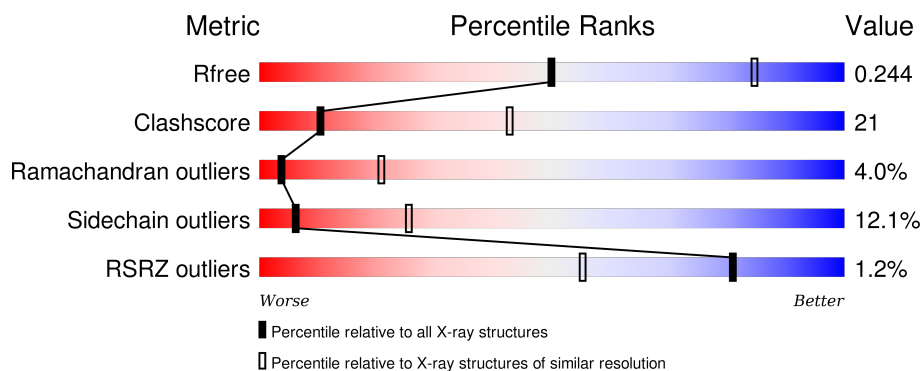
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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







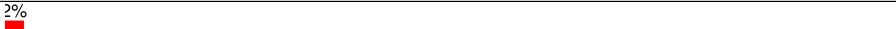
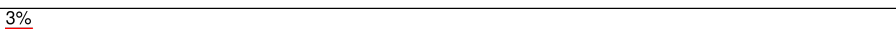
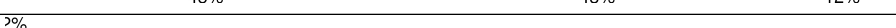



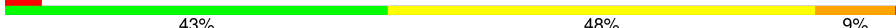
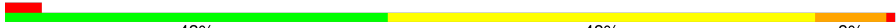












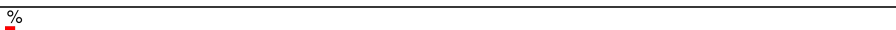
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	<div> <div></div> <div>67%28%5%</div> </div>
1	AC	243	<div> <div></div> <div>64%30%6%</div> </div>
1	BA	243	<div> <div>2%</div> <div>67%29%. .</div> </div>
1	BO	243	<div> <div>2%</div> <div>66%30%. .</div> </div>
2	AG	231	<div> <div></div> <div>70%26%. .</div> </div>


























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










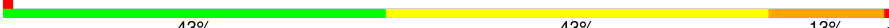
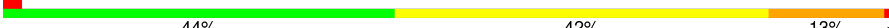


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Mol	Chain	Length	Quality of chain
8	BH	196	
8	BV	196	
9	AM	222	
9	AY	222	
9	BI	222	
9	BW	222	
10	AN	204	
10	AZ	204	
10	BJ	204	
10	BX	204	
11	A1	198	
11	AO	198	
11	BK	198	
11	BY	198	
12	A2	212	
12	AP	212	
12	BL	212	
12	BZ	212	
13	A3	222	
13	AQ	222	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

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Mol	Chain	Length	Quality of chain
14	BN	233	 64% 30% 5%
15	AE	76	 66% 29% 5%
15	AF	76	 63% 33% 4%
15	B3	76	 63% 33% 4%
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

There are 17 unique types of molecules in this entry. The entry contains 158904 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome component C7-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
1	AC	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
1	BA	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
1	BO	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			

- Molecule 2 is a protein called Proteasome component Y7.

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

- Molecule 3 is a protein called Proteasome component Y13.

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

- Molecule 4 is a protein called Proteasome component PRE6.

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

- Molecule 5 is a protein called Proteasome component PUP2.

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

- Molecule 6 is a protein called Proteasome component PRE5.

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

- Molecule 7 is a protein called Proteasome component C1.

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

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

- Molecule 8 is a protein called Proteasome component PRE3.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AB	1001	ALA	-	EXPRESSION TAG	UNP P38624
AD	1001	ALA	-	EXPRESSION TAG	UNP P38624
BH	1001	ALA	-	EXPRESSION TAG	UNP P38624
BV	1001	ALA	-	EXPRESSION TAG	UNP P38624

- Molecule 9 is a protein called Proteasome component PUP1.

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

- Molecule 10 is a protein called Proteasome component PUP3.

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

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

- Molecule 11 is a protein called Proteasome component C11.

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

- Molecule 12 is a protein called Proteasome component PRE2.

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 13 is a protein called Proteasome component C5.

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

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

- Molecule 14 is a protein called Proteasome component PRE4.

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

- Molecule 15 is a protein called Proteasome activator BLM10.

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

- Molecule 16 is a protein called Proteasome activator BLM10.

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

There are 12 discrepancies between the modelled and reference sequences:

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

- Molecule 17 is a protein called Proteasome activator BLM10.

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

There are 16 discrepancies between the modelled and reference sequences:

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

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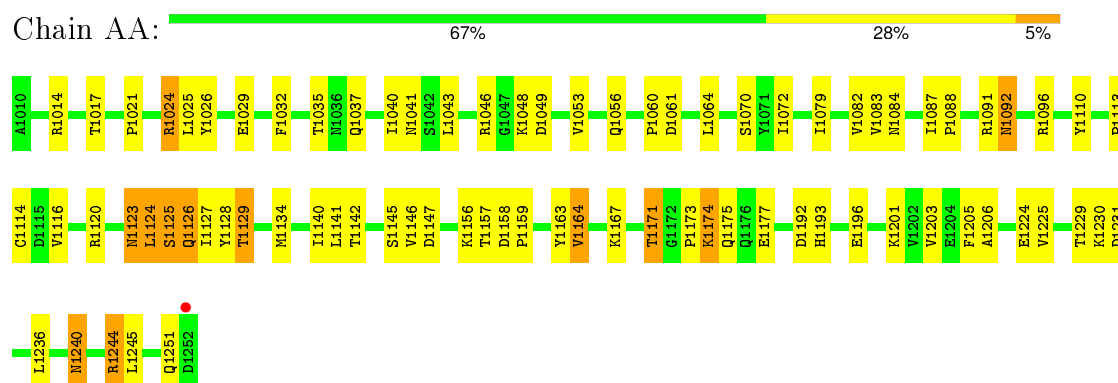
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Chain	Residue	Modelled	Actual	Comment	Reference
B8	1171	ASN	GLN	CONFLICT	UNP P43583
B8	2085	ASN	GLN	CONFLICT	UNP P43583
B8	2101	ASN	GLN	CONFLICT	UNP P43583

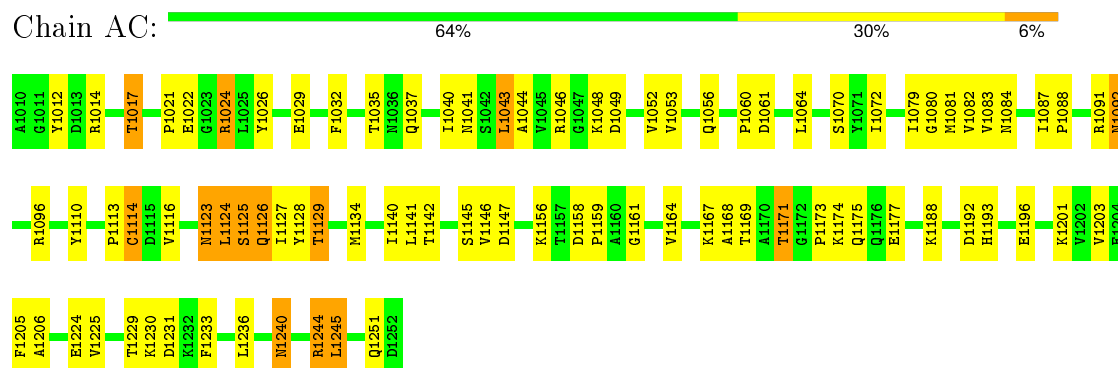
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

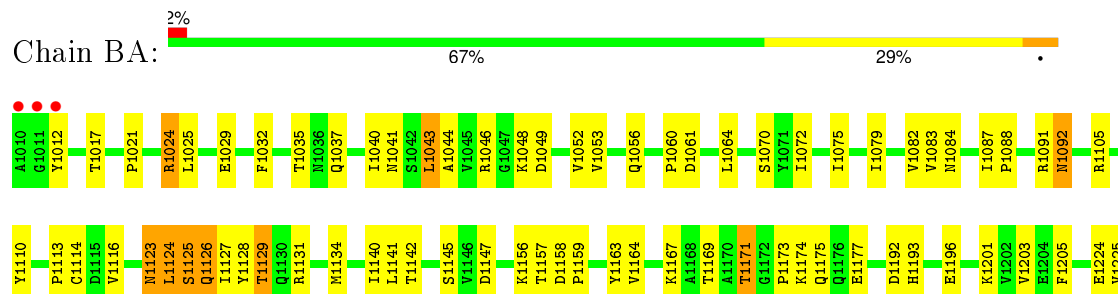
#### • Molecule 1: Proteasome component C7-alpha



#### • Molecule 1: Proteasome component C7-alpha

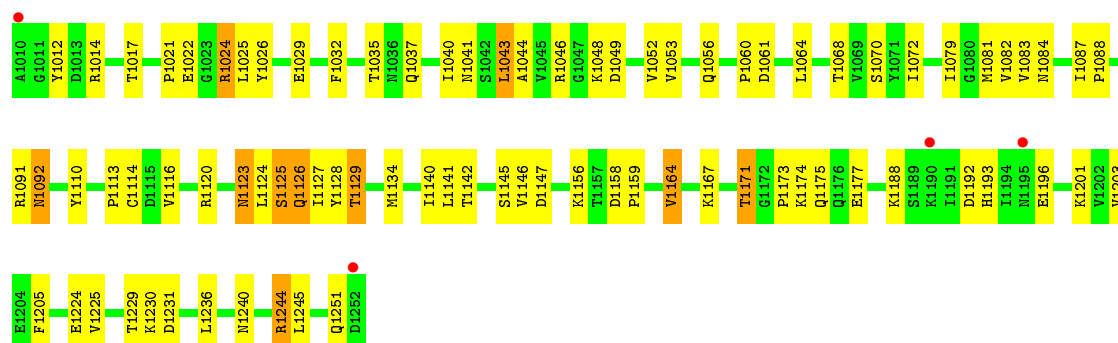


#### • Molecule 1: Proteasome component C7-alpha

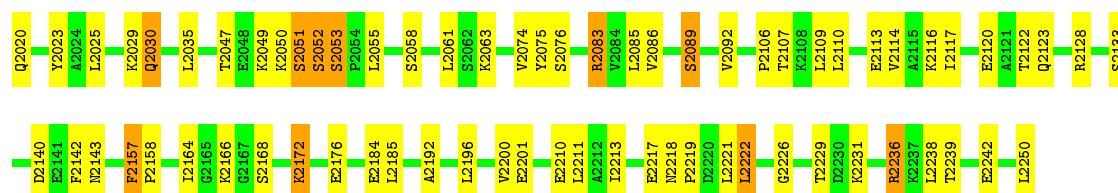




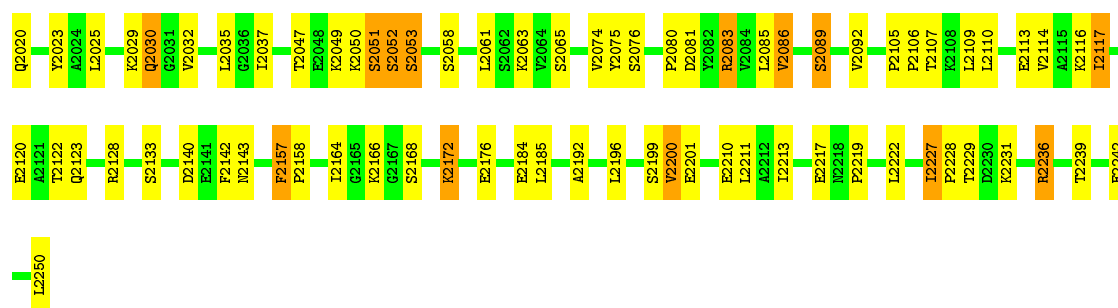
- Molecule 1: Proteasome component C7-alpha



- Molecule 2: Proteasome component Y7

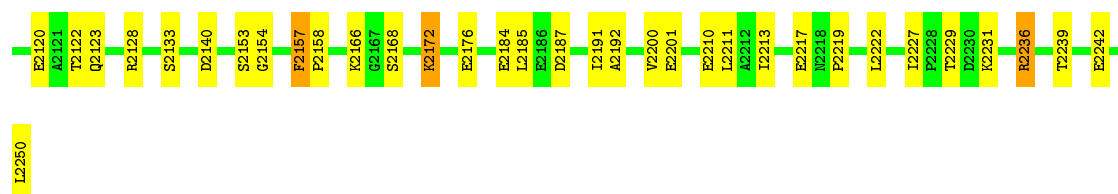


- Molecule 2: Proteasome component Y7



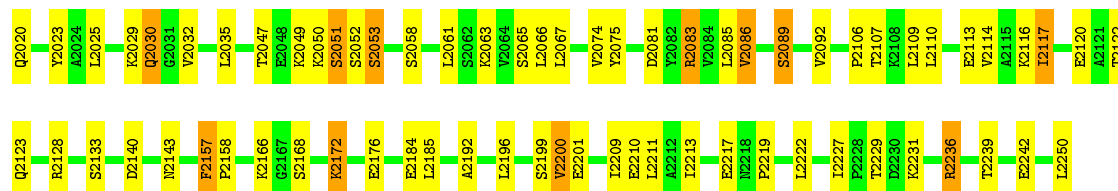
- Molecule 2: Proteasome component Y7





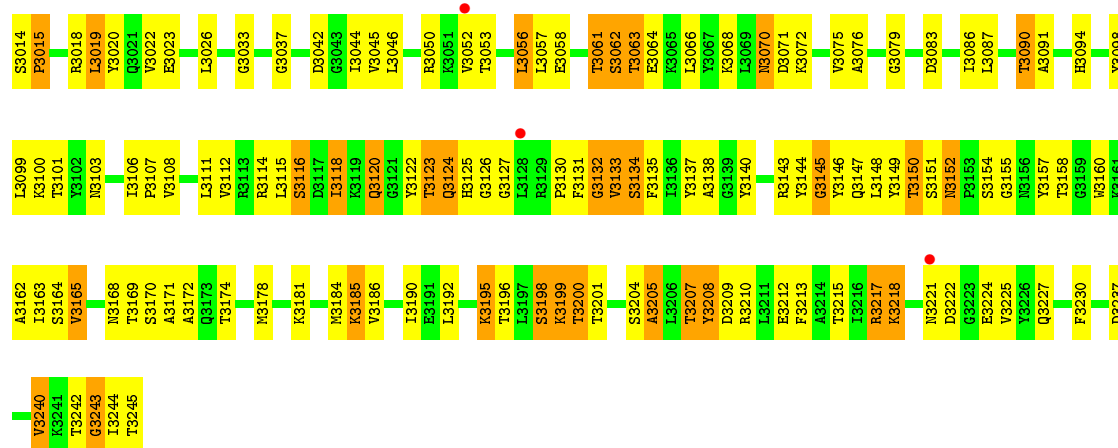
- Molecule 2: Proteasome component Y7

Chain BP: 70% 25% 5%



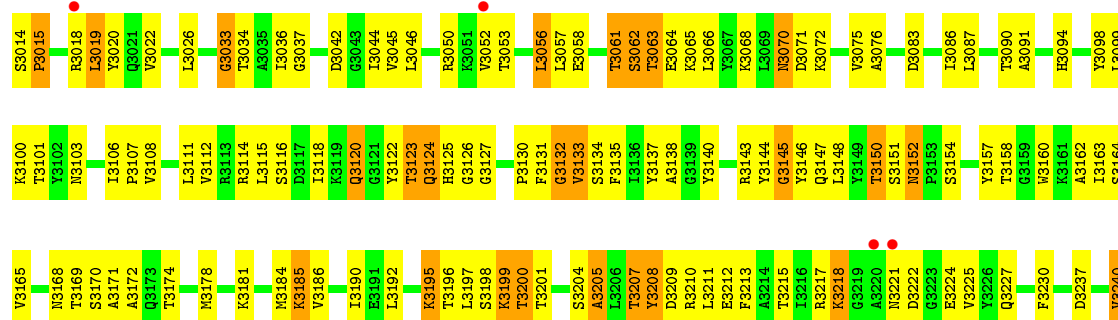
- Molecule 3: Proteasome component Y13

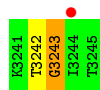
Chain AH: 44% 42% 14%



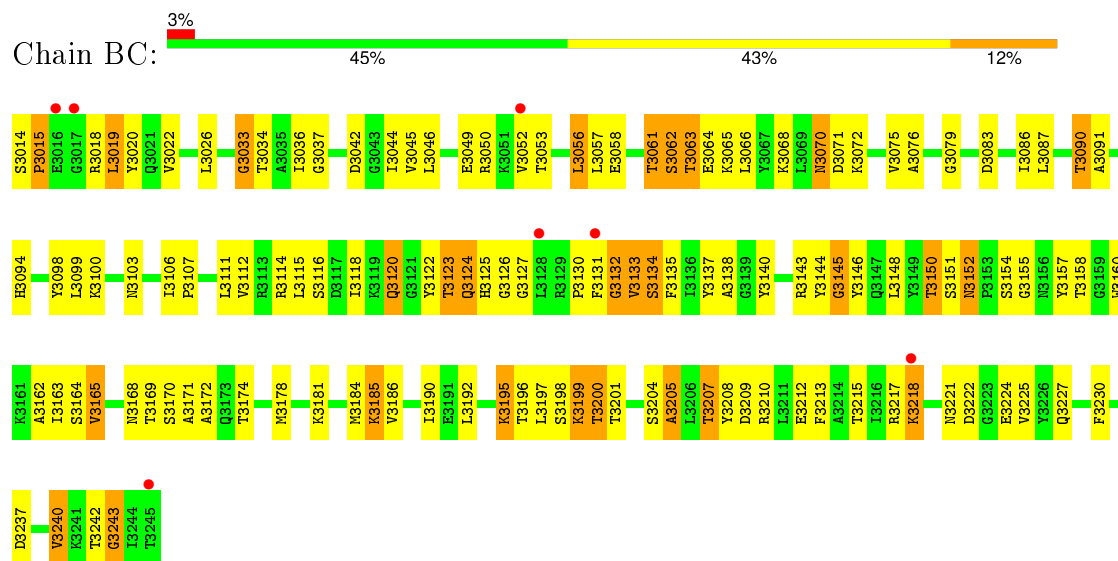
- Molecule 3: Proteasome component Y13

Chain AT: 45% 44% 11%

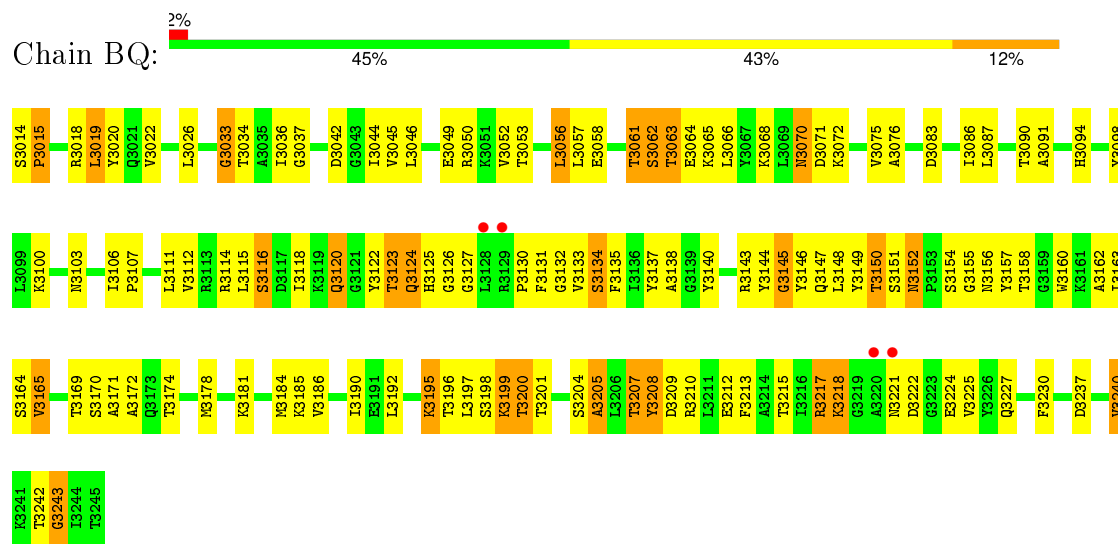




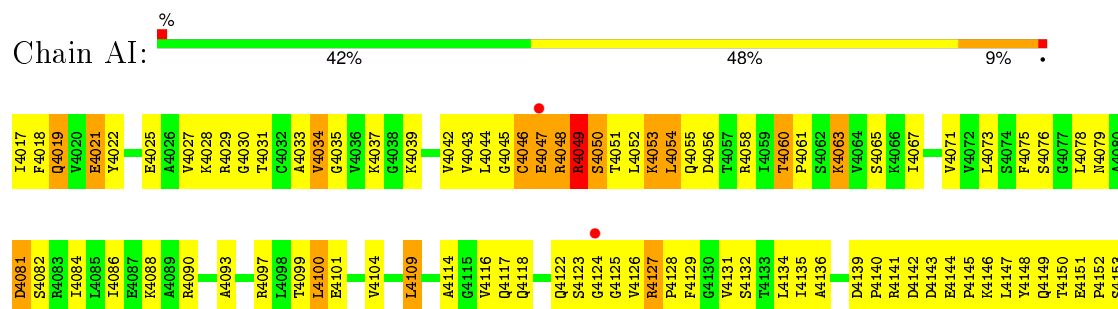
• Molecule 3: Proteasome component Y13



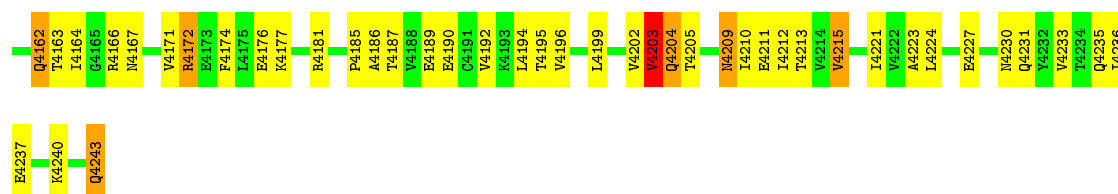
• Molecule 3: Proteasome component Y13



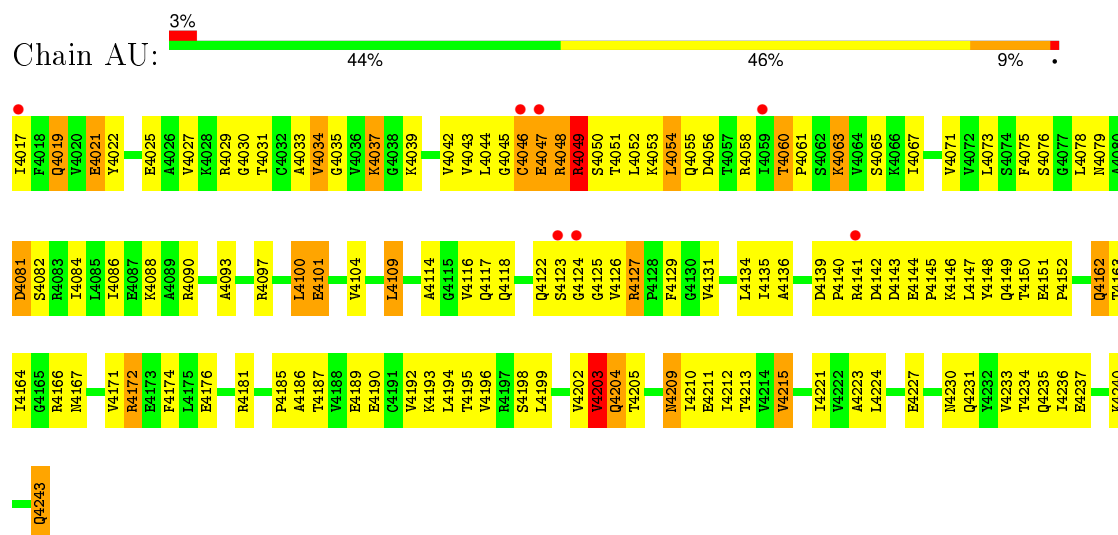
• Molecule 4: Proteasome component PRE6



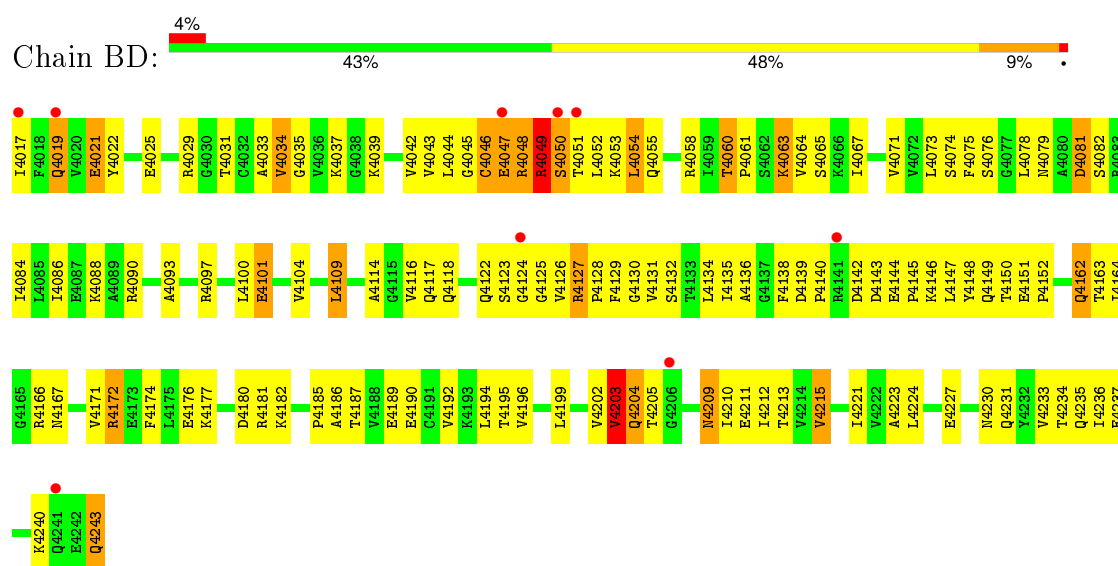




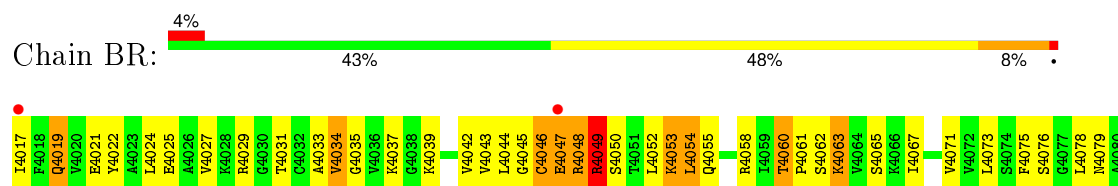
• Molecule 4: Proteasome component PRE6

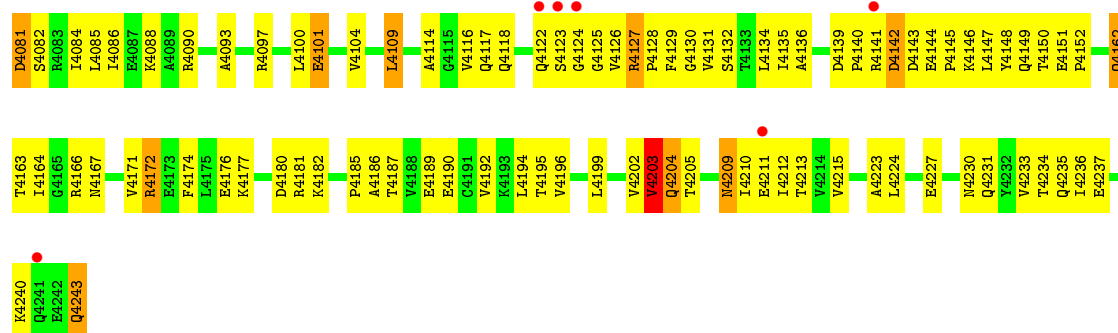


• Molecule 4: Proteasome component PRE6

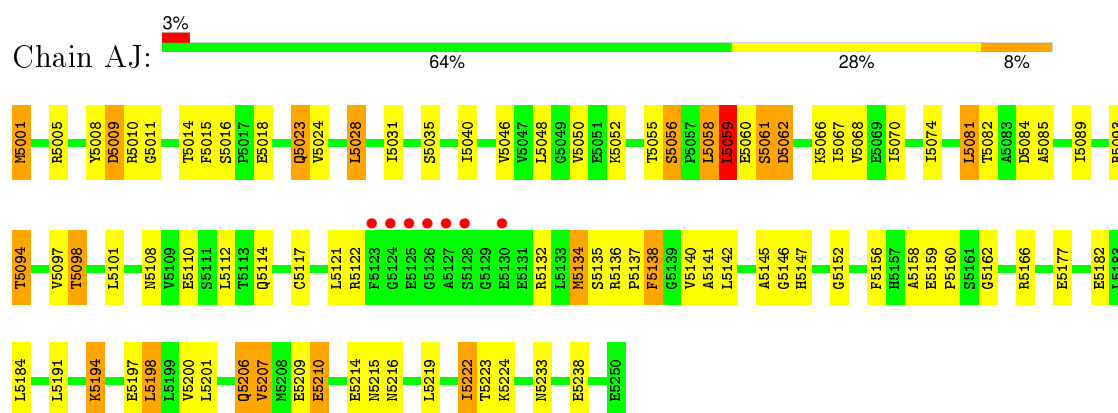


• Molecule 4: Proteasome component PRE6

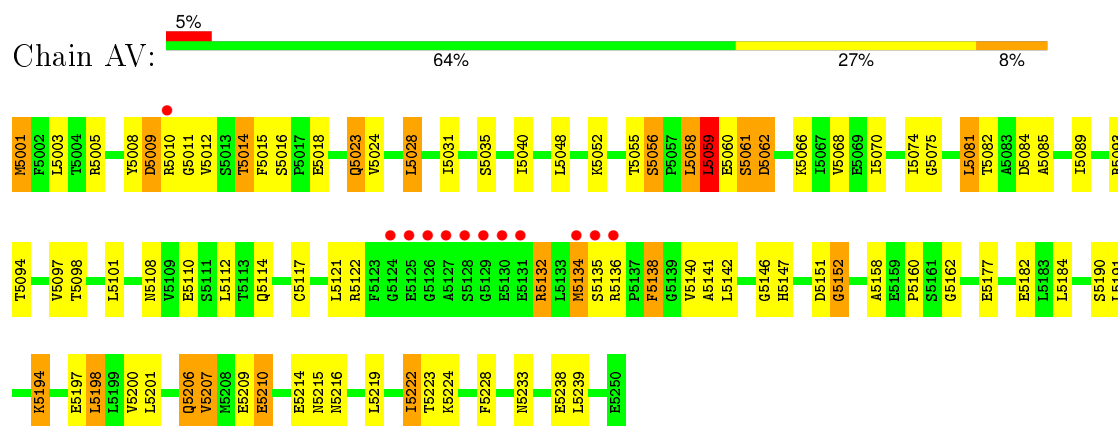




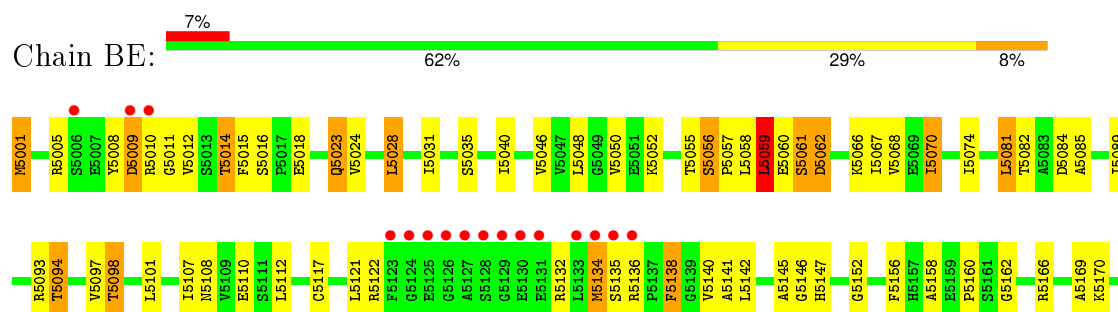
• Molecule 5: Proteasome component PUP2

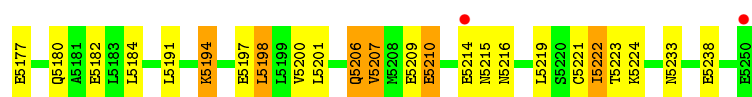


• Molecule 5: Proteasome component PUP2

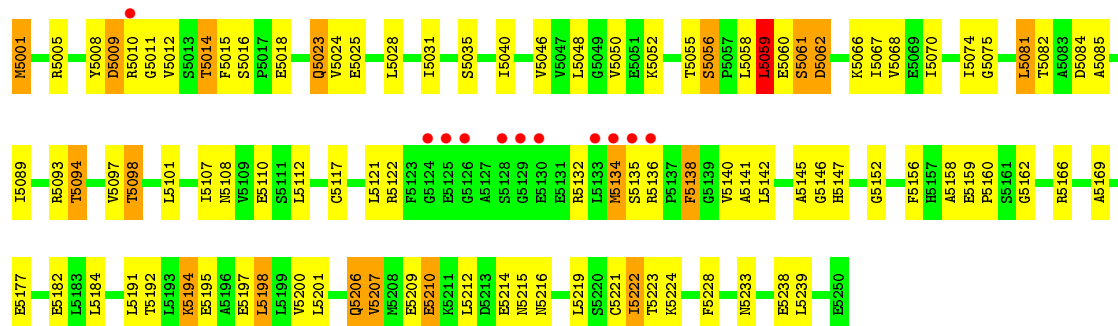


• Molecule 5: Proteasome component PUP2

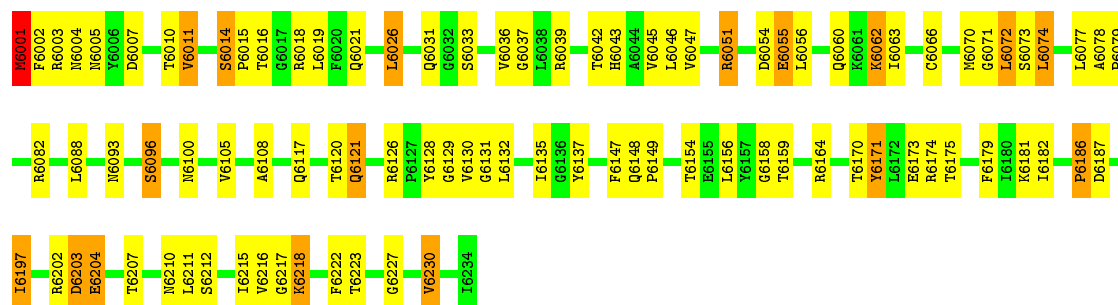




• Molecule 5: Proteasome component PUP2



• Molecule 6: Proteasome component PRE5

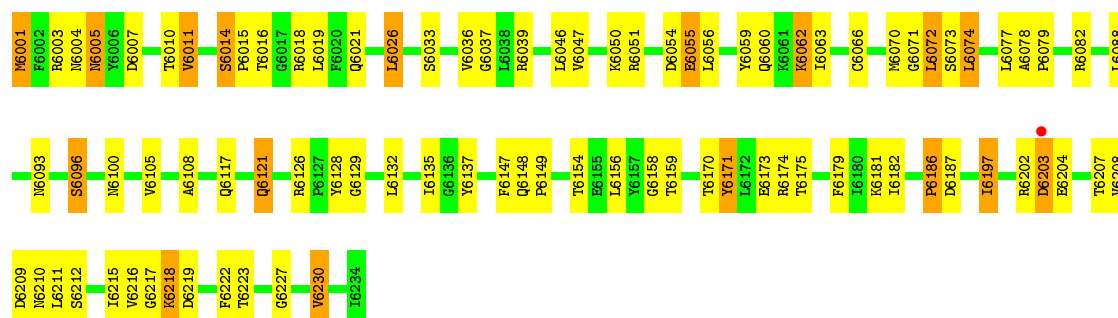


• Molecule 6: Proteasome component PRE5



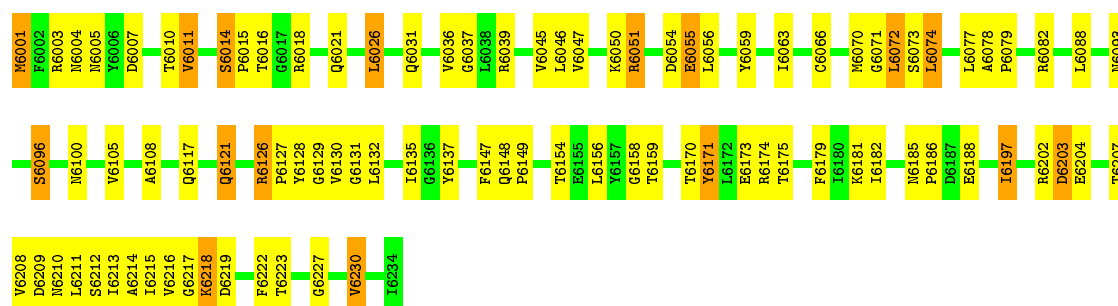
• Molecule 6: Proteasome component PRE5





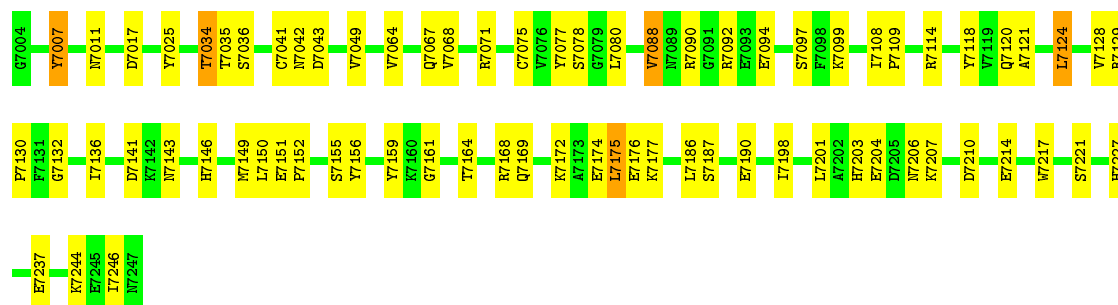
• Molecule 6: Proteasome component PRE5

Chain BT: 60% 33% 7%



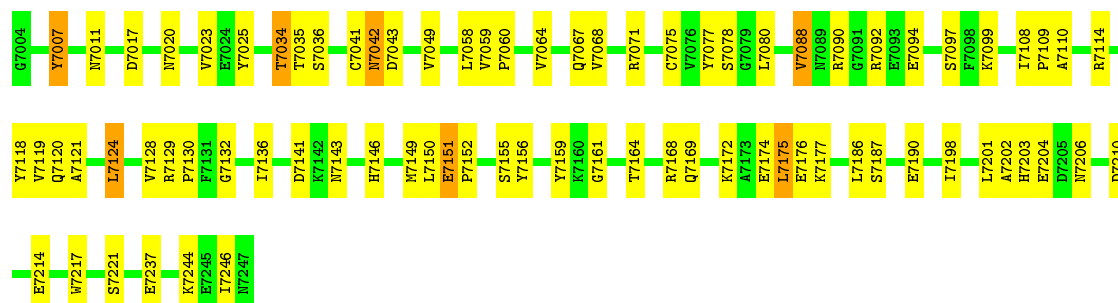
• Molecule 7: Proteasome component C1

Chain AL: 70% 28% 2%

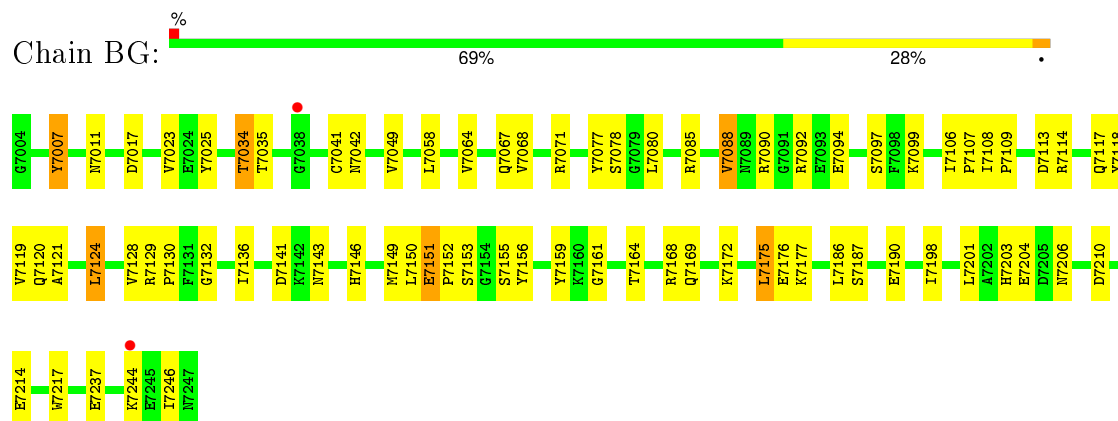


• Molecule 7: Proteasome component C1

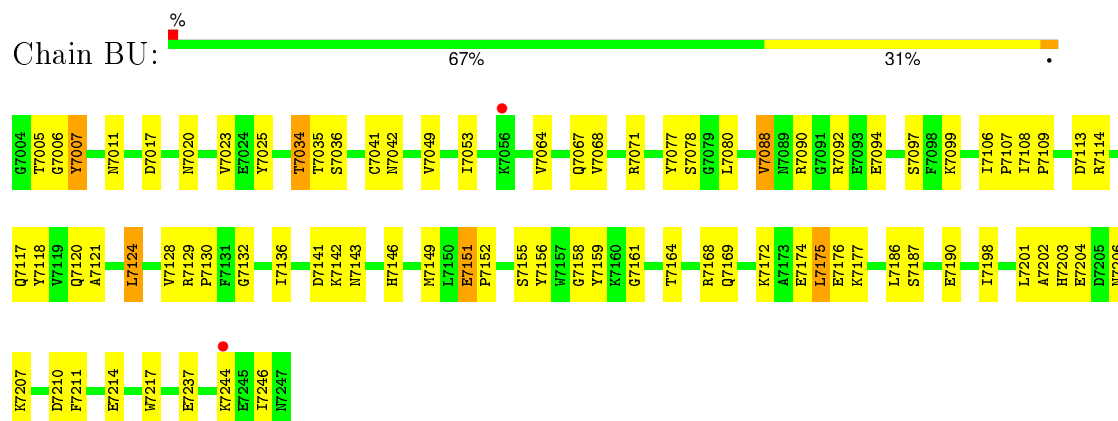
Chain AX: 68% 30% 2%



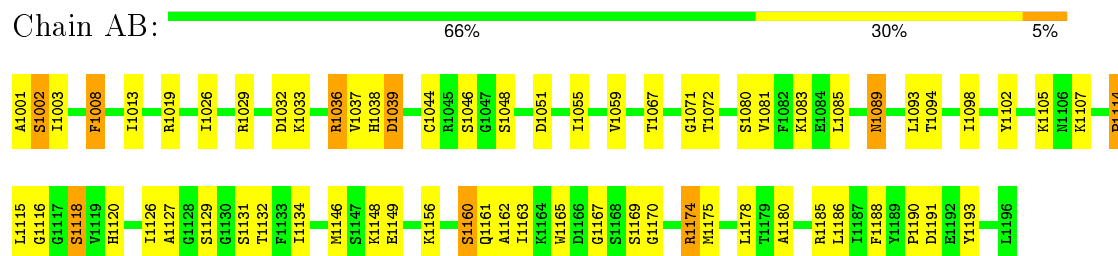
- Molecule 7: Proteasome component C1



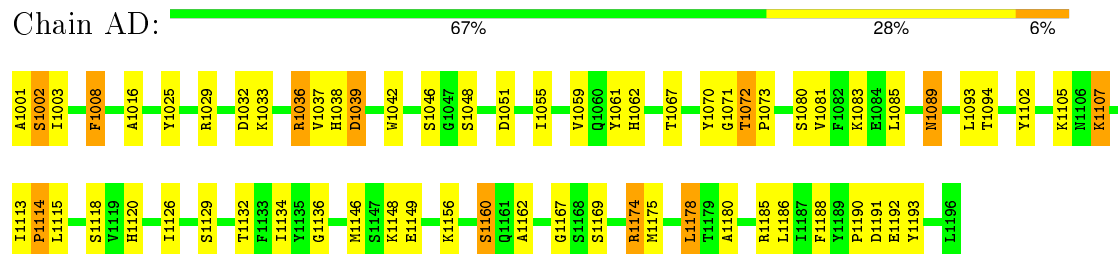
- Molecule 7: Proteasome component C1



- Molecule 8: Proteasome component PRE3

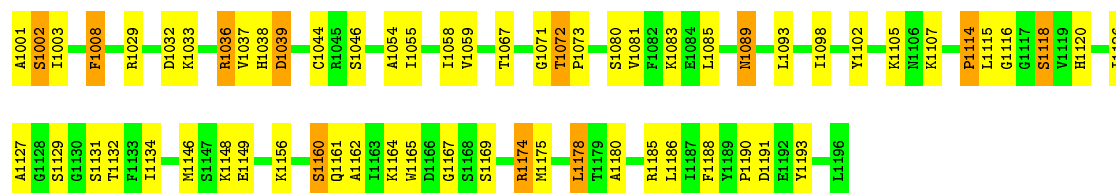


- Molecule 8: Proteasome component PRE3



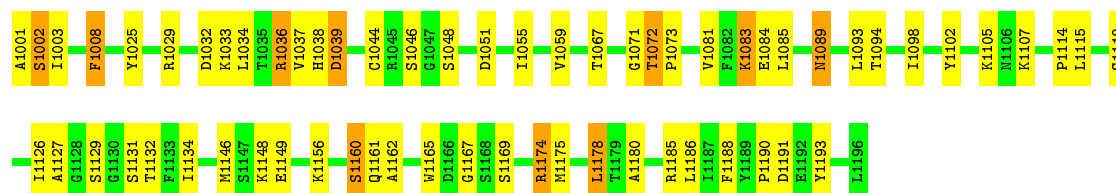
- Molecule 8: Proteasome component PRE3

Chain BH: 



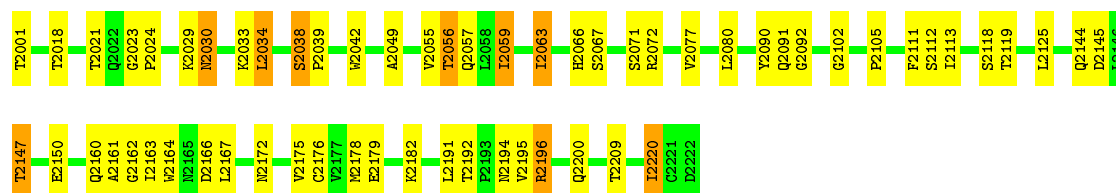
- Molecule 8: Proteasome component PRE3

Chain BV: 



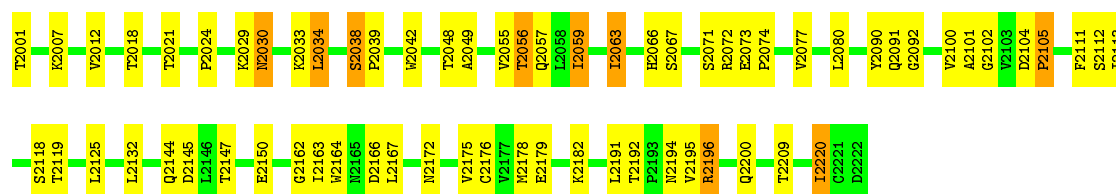
- Molecule 9: Proteasome component PUP1

Chain AM: 



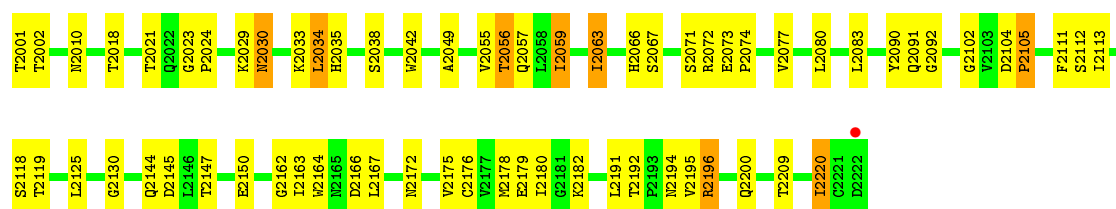
- Molecule 9: Proteasome component PUP1

Chain AY: 

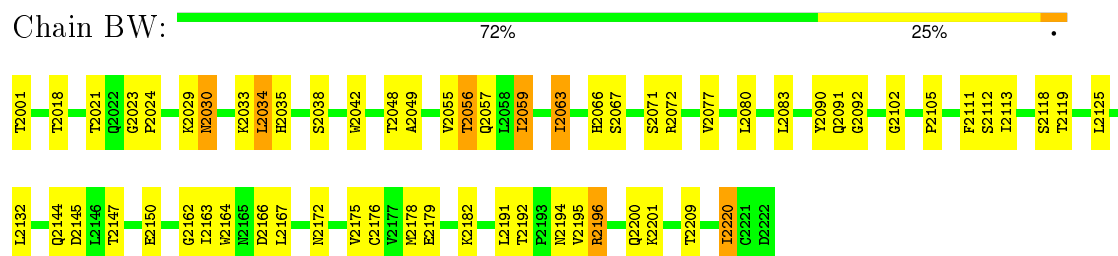


- Molecule 9: Proteasome component PUP1

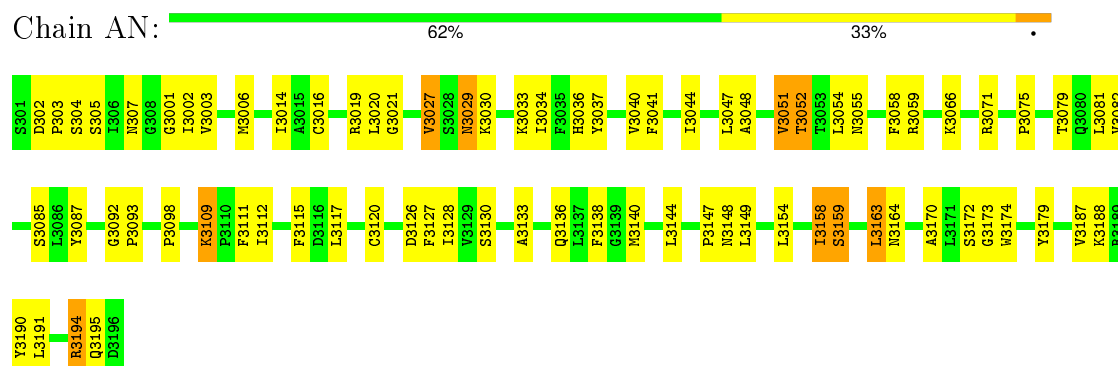
Chain BI: 



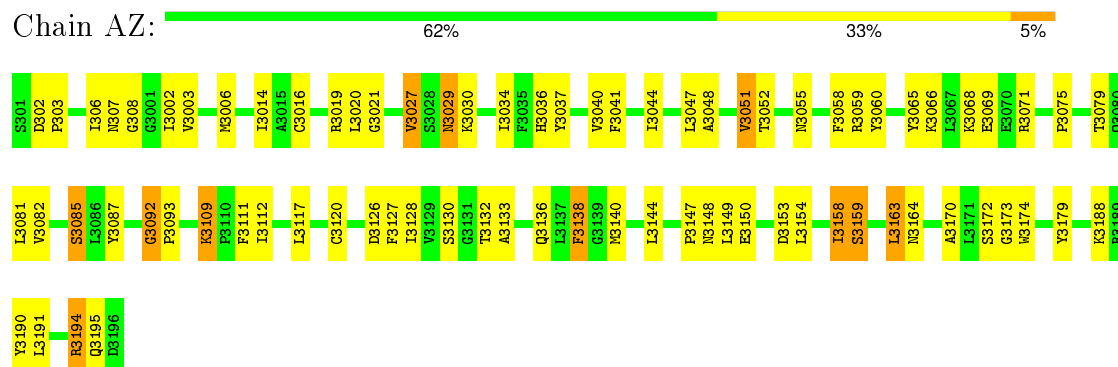
- Molecule 9: Proteasome component PUP1



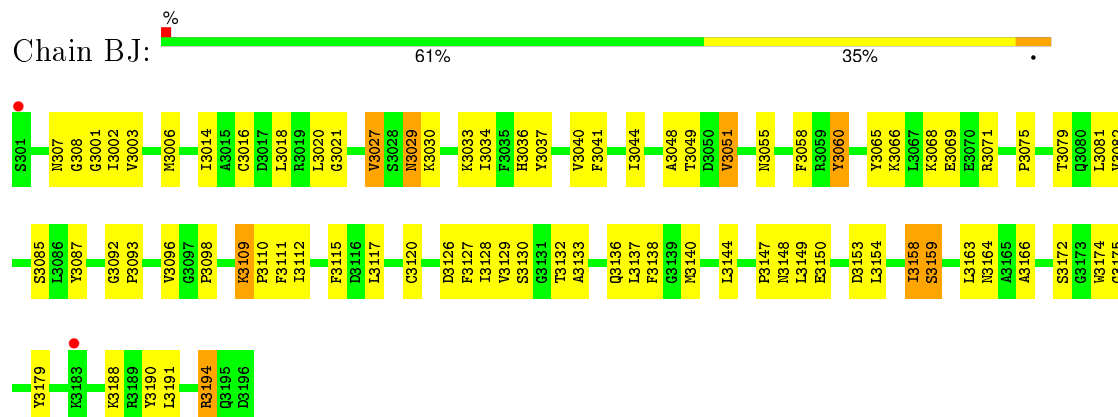
- Molecule 10: Proteasome component PUP3



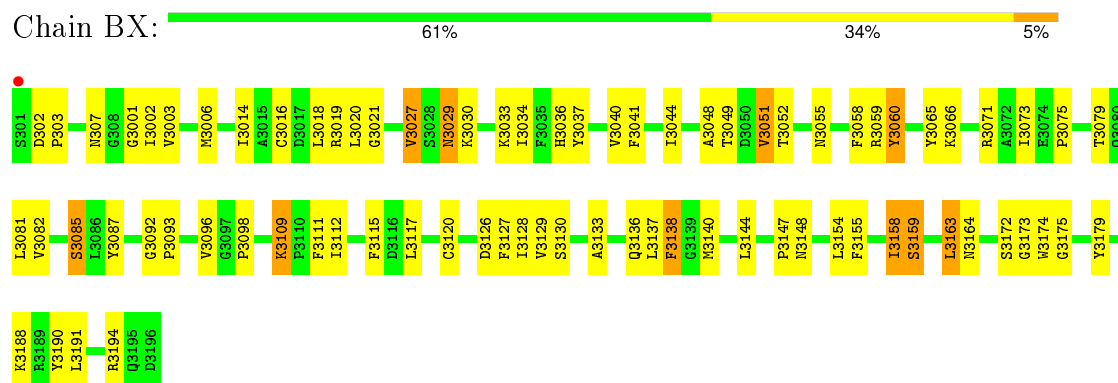
- Molecule 10: Proteasome component PUP3



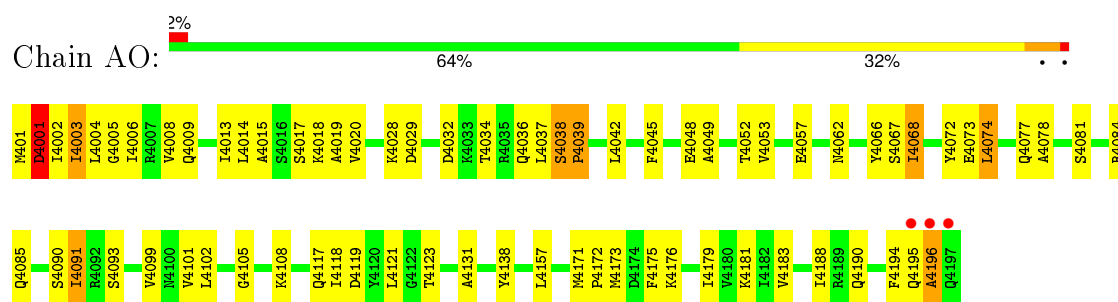
- Molecule 10: Proteasome component PUP3



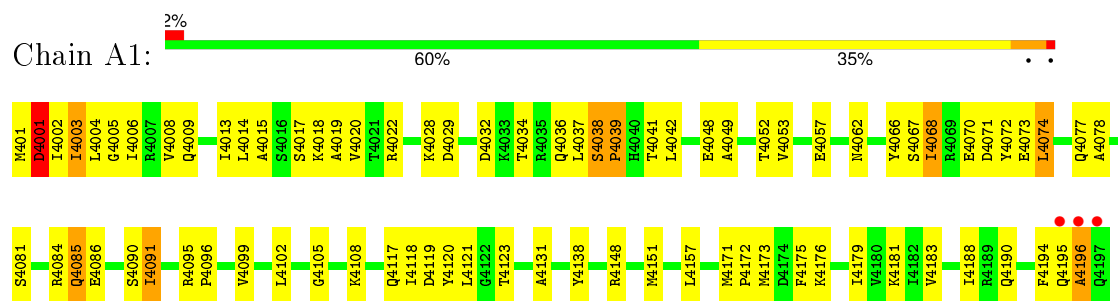
- Molecule 10: Proteasome component PUP3



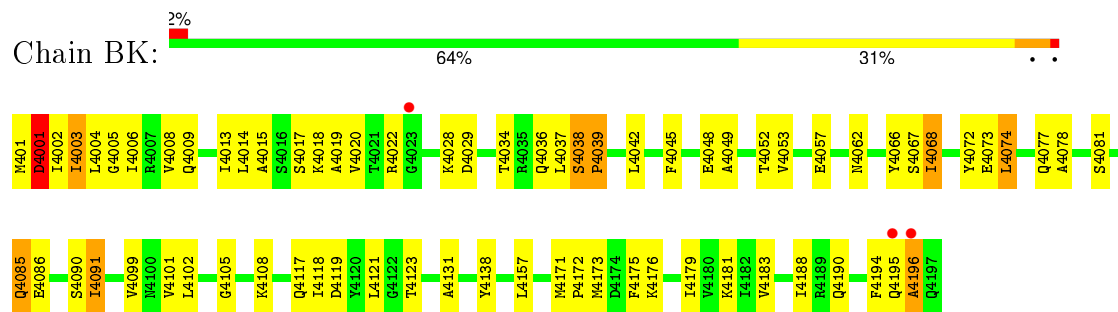
- Molecule 11: Proteasome component C11



- Molecule 11: Proteasome component C11



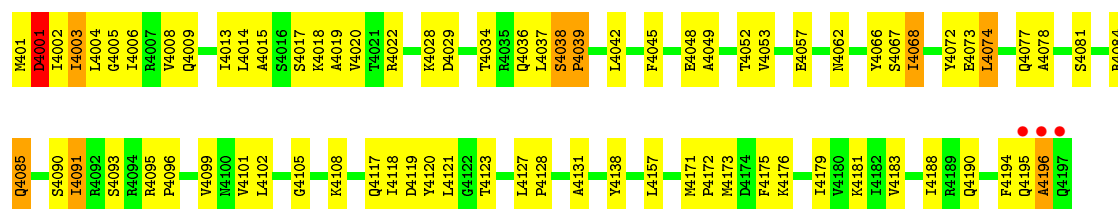
- Molecule 11: Proteasome component C11



- Molecule 11: Proteasome component C11



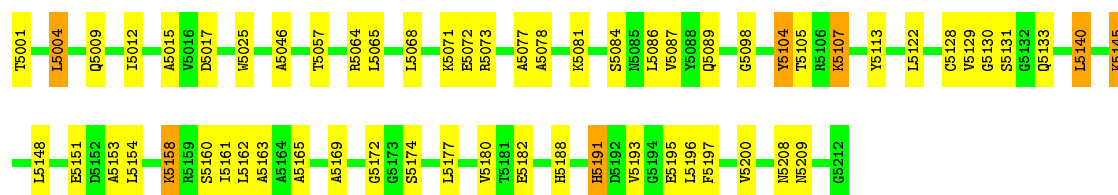




• Molecule 12: Proteasome component PRE2



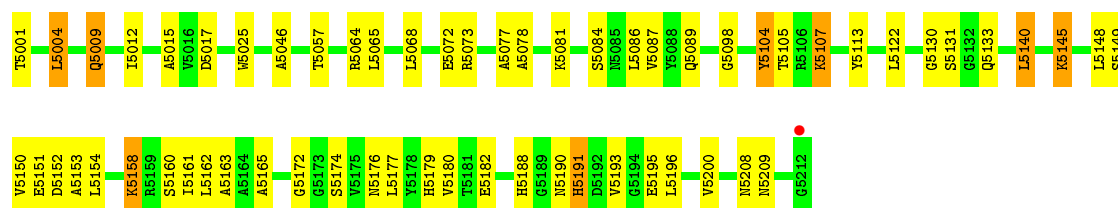
• Molecule 12: Proteasome component PRE2



• Molecule 12: Proteasome component PRE2

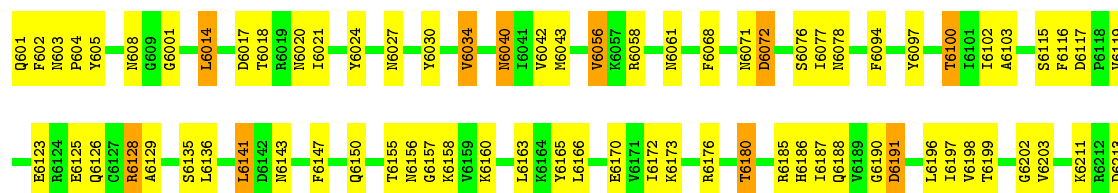


• Molecule 12: Proteasome component PRE2



• Molecule 13: Proteasome component C5

Chain AQ: 



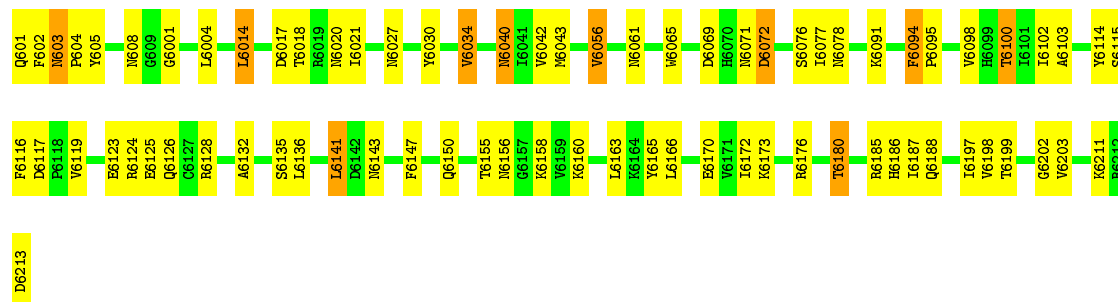
- Molecule 13: Proteasome component C5

Chain A3:  62% 35% 3%



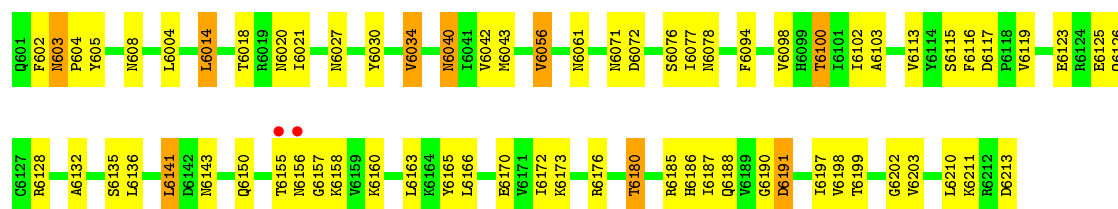
- Molecule 13: Proteasome component C5

Chain BM: 



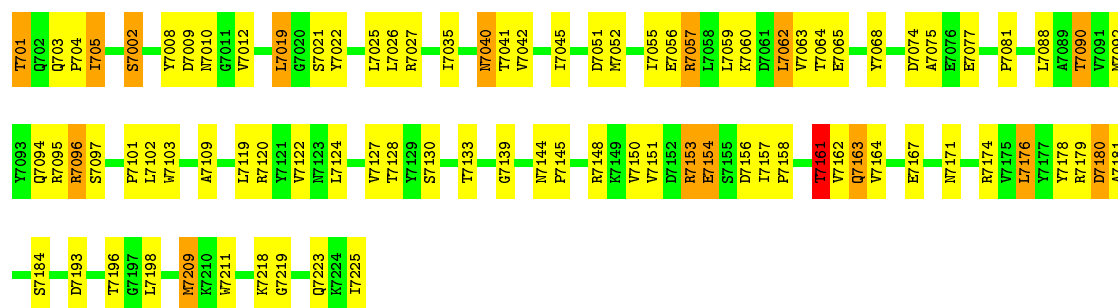
- Molecule 13: Proteasome component C5

Chain B1:  68% 27% .



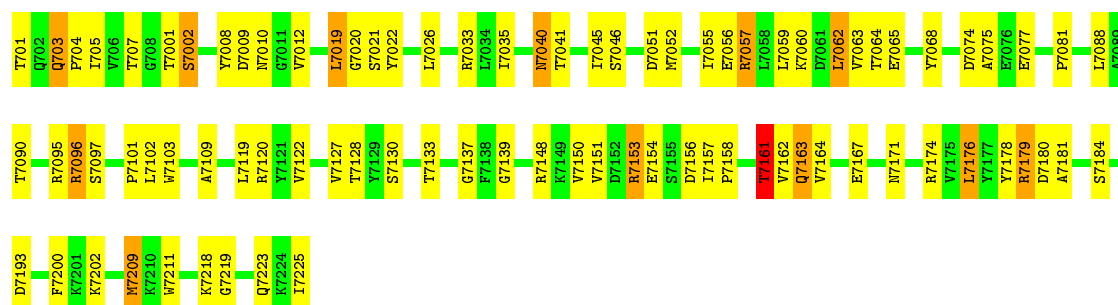
- Molecule 14: Proteasome component PRE4

Chain AR: 



- Molecule 14: Proteasome component PRE4

Chain A4: 63% 31% 5%



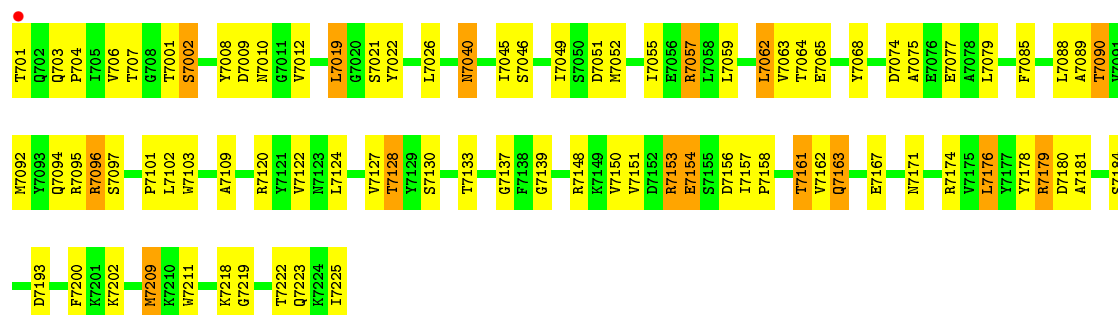
- Molecule 14: Proteasome component PRE4

Chain BN: 64% 30% 5%



- Molecule 14: Proteasome component PRE4

Chain B2: 64% 30% 6%



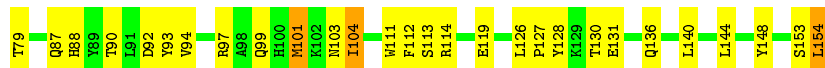
- Molecule 15: Proteasome activator BLM10

Chain AE: 



- Molecule 15: Proteasome activator BLM10

Chain AF: 



- Molecule 15: Proteasome activator BLM10

Chain B3: 



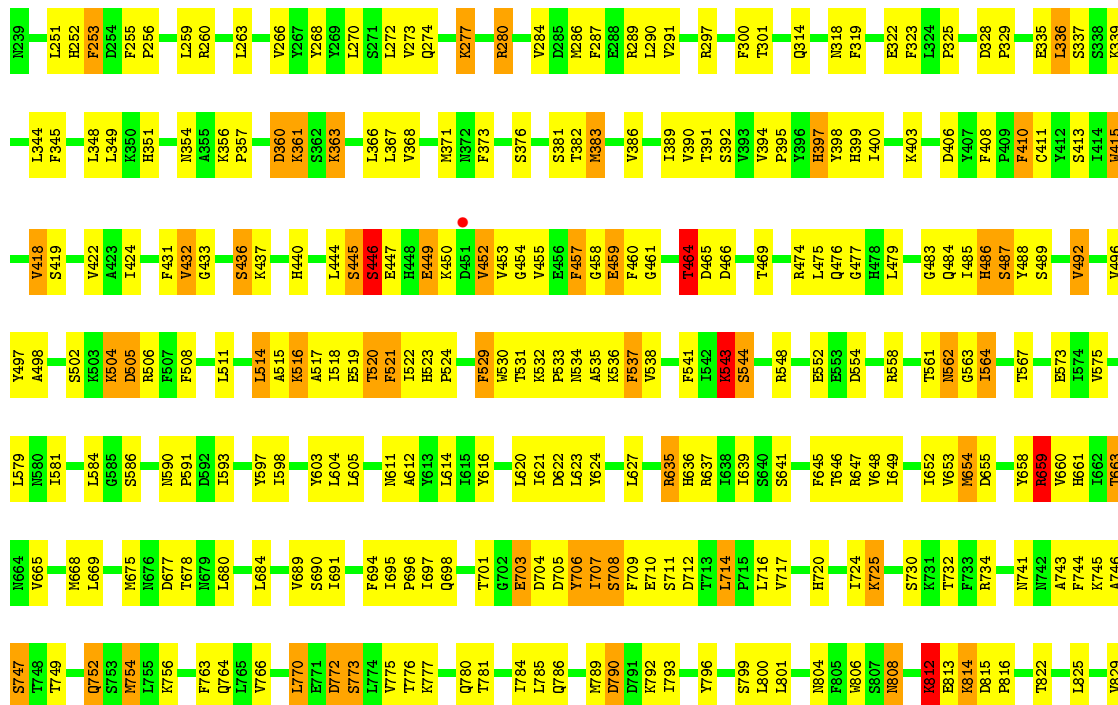
- Molecule 15: Proteasome activator BLM10

Chain B6: 



- Molecule 16: Proteasome activator BLM10

Chain A5: 



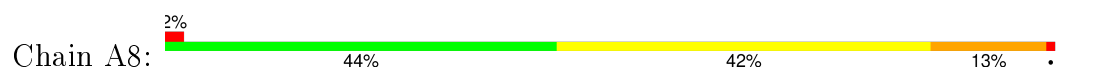






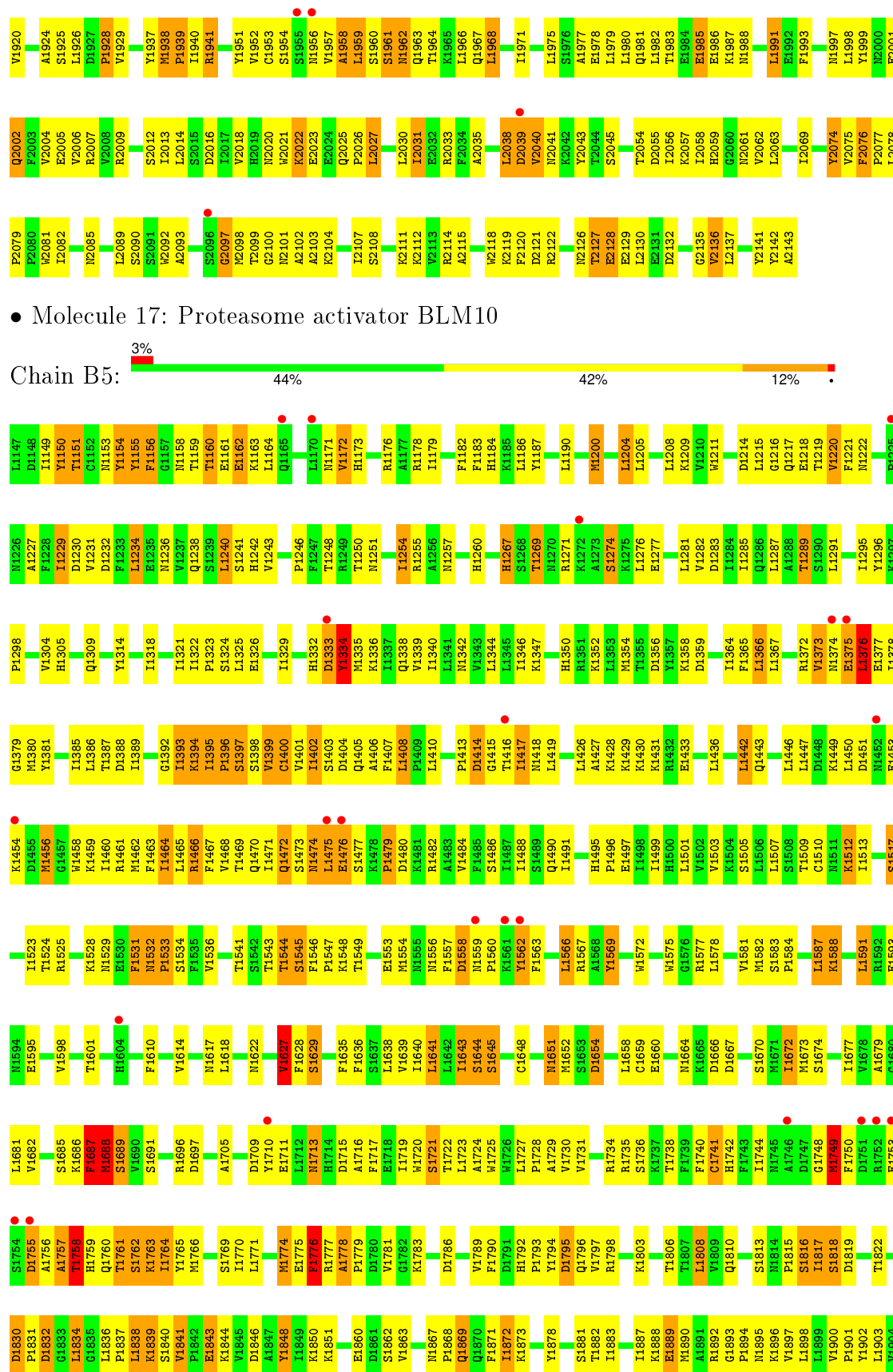
V1841	V1842	V1843	V1844	V1845	V1846	V1847	V1848	V1849	V1850	V1851	V1852	V1853	V1854	V1855	V1856	V1857	V1858	V1859	V1860	V1861	V1862	V1863	V1864	V1865	V1866	V1867	V1868	V1869	V1870	V1871	V1872	V1873	V1874	V1875	V1876	V1877	V1878	V1879	V1880	V1881	V1882	V1883	V1884	V1885	V1886	V1887	V1888	V1889	V1890	V1891	V1892	V1893	V1894	V1895	V1896	V1897	V1898	V1899	V1900	V1901	V1902	V1903	V1904	V1905	V1906	V1907	V1908	V1909	V1910	V1911	V1912	V1913	V1914	V1915	V1916																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
H1917	K1918	D1919	V1920	A1921	V1922	S1923	V1924	V1925	V1926	V1927	V1928	V1929	V1930	V1931	V1932	V1933	V1934	V1935	V1936	V1937	V1938	V1939	V1940	V1941	V1942	V1943	V1944	V1945	V1946	V1947	V1948	V1949	V1950	V1951	V1952	V1953	V1954	V1955	V1956	V1957	V1958	V1959	V1960	V1961	V1962	V1963	V1964	V1965	V1966	V1967	V1968	V1969	V1970	V1971	V1972	V1973	V1974	V1975	V1976	V1977	V1978	V1979	V1980	V1981	V1982	V1983	V1984	V1985	V1986	V1987	V1988	V1989	V1990	V1991	V1992	V1993	V1994	V1995	V1996	V1997	V1998	V1999																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
N2000	E2001	Q2002	F2003	V2004	E2005	V2006	V2007	V2008	V2009	V2010	V2011	V2012	V2013	V2014	V2015	V2016	V2017	V2018	V2019	V2020	V2021	V2022	V2023	V2024	V2025	V2026	V2027	V2028	V2029	V2030	V2031	V2032	V2033	V2034	V2035	V2036	V2037	V2038	V2039	V2040	V2041	V2042	V2043	V2044	V2045	V2046	V2047	V2048	V2049	V2050	V2051	V2052	V2053	V2054	V2055	V2056	V2057	V2058	V2059	V2060	V2061	V2062	V2063	V2064	V2065	V2066	V2067	V2068	V2069	V2070	V2071	V2072	V2073																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
V2074	V2075	V2076	V2077	V2078	V2079	V2080	V2081	V2082	V2083	V2084	V2085	V2086	V2087	V2088	V2089	V2090	V2091	V2092	V2093	V2094	V2095	V2096	V2097	V2098	V2099	V2100	V2101	V2102	V2103	V2104	V2105	V2106	V2107	V2108	V2109	V2110	V2111	V2112	V2113	V2114	V2115	V2116	V2117	V2118	V2119	V2120	V2121	V2122	V2123	V2124	V2125	V2126	V2127	V2128	V2129	V2130	V2131	V2132	V2133	V2134	V2135	V2136	V2137	V2138	V2139	V2140	V2141	V2142	V2143	V2144	V2145	V2146	V2147	V2148	V2149	V2150	V2151	V2152	V2153	V2154	V2155	V2156	V2157	V2158	V2159	V2160	V2161	V2162	V2163	V2164	V2165	V2166	V2167	V2168	V2169	V2170	V2171	V2172	V2173	V2174	V2175	V2176	V2177	V2178	V2179	V2180	V2181	V2182	V2183	V2184	V2185	V2186	V2187	V2188	V2189	V2190	V2191	V2192	V2193	V2194	V2195	V2196	V2197	V2198	V2199	V2200	V2201	V2202	V2203	V2204	V2205	V2206	V2207	V2208	V2209	V2210	V2211	V2212	V2213	V2214	V2215	V2216	V2217	V2218	V2219	V2220	V2221	V2222	V2223	V2224	V2225	V2226	V2227	V2228	V2229	V2230	V2231	V2232	V2233	V2234	V2235	V2236	V2237	V2238	V2239	V2240	V2241	V2242	V2243	V2244	V2245	V2246	V2247	V2248	V2249	V2250	V2251	V2252	V2253	V2254	V2255	V2256	V2257	V2258	V2259	V2260	V2261	V2262	V2263	V2264	V2265	V2266	V2267	V2268	V2269	V2270	V2271	V2272	V2273	V2274	V2275	V2276	V2277	V2278	V2279	V2280	V2281	V2282	V2283	V2284	V2285	V2286	V2287	V2288	V2289	V2290	V2291	V2292	V2293	V2294	V2295	V2296	V2297	V2298	V2299	V2300	V2301	V2302	V2303	V2304	V2305	V2306	V2307	V2308	V2309	V2310	V2311	V2312	V2313	V2314	V2315	V2316	V2317	V2318	V2319	V2320	V2321	V2322	V2323	V2324	V2325	V2326	V2327	V2328	V2329	V2330	V2331	V2332	V2333	V2334	V2335	V2336	V2337	V2338	V2339	V2340	V2341	V2342	V2343	V2344	V2345	V2346	V2347	V2348	V2349	V2350	V2351	V2352	V2353	V2354	V2355	V2356	V2357	V2358	V2359	V2360	V2361	V2362	V2363	V2364	V2365	V2366	V2367	V2368	V2369	V2370	V2371	V2372	V2373	V2374	V2375	V2376	V2377	V2378	V2379	V2380	V2381	V2382	V2383	V2384	V2385	V2386	V2387	V2388	V2389	V2390	V2391	V2392	V2393	V2394	V2395	V2396	V2397	V2398	V2399	V2400	V2401	V2402	V2403	V2404	V2405	V2406	V2407	V2408	V2409	V2410	V2411	V2412	V2413	V2414	V2415	V2416	V2417	V2418	V2419	V2420	V2421	V2422	V2423	V2424	V2425	V2426	V2427	V2428	V2429	V2430	V2431	V2432	V2433	V2434	V2435	V2436	V2437	V2438	V2439	V2440	V2441	V2442	V2443	V2444	V2445	V2446	V2447	V2448	V2449	V2450	V2451	V2452	V2453	V2454	V2455	V2456	V2457	V2458	V2459	V2460	V2461	V2462	V2463	V2464	V2465	V2466	V2467	V2468	V2469	V2470	V2471	V2472	V2473	V2474	V2475	V2476	V2477	V2478	V2479	V2480	V2481	V2482	V2483	V2484	V2485	V2486	V2487	V2488	V2489	V2490	V2491	V2492	V2493	V2494	V2495	V2496	V2497	V2498	V2499	V2500	V2501	V2502	V2503	V2504	V2505	V2506	V2507	V2508	V2509	V2510	V2511	V2512	V2513	V2514	V2515	V2516	V2517	V2518	V2519	V2520	V2521	V2522	V2523	V2524	V2525	V2526	V2527	V2528	V2529	V2530	V2531	V2532	V2533	V2534	V2535	V2536	V2537	V2538	V2539	V2540	V2541	V2542	V2543	V2544	V2545	V2546	V2547	V2548	V2549	V2550	V2551	V2552	V2553	V2554	V2555	V2556	V2557	V2558	V2559	V2560	V2561	V2562	V2563	V2564	V2565	V2566	V2567	V2568	V2569	V2570	V2571	V2572	V2573	V2574	V2575	V2576	V2577	V2578	V2579	V2580	V2581	V2582	V2583	V2584	V2585	V2586	V2587	V2588	V2589	V2590	V2591	V2592	V2593	V2594	V2595	V2596	V2597	V2598	V2599	V2600	V2601	V2602	V2603	V2604	V2605	V2606	V2607	V2608	V2609	V2610	V2611	V2612	V2613	V2614	V2615	V2616	V2617	V2618	V2619	V2620	V2621	V2622	V2623	V2624	V2625	V2626	V2627	V2628	V2629	V2630	V2631	V2632	V2633	V2634	V2635	V2636	V2637	V2638	V2639	V2640	V2641	V2642	V2643	V2644	V2645	V2646	V2647	V2648	V2649	V2650	V2651	V2652	V2653	V2654	V2655	V2656	V2657	V2658	V2659	V2660	V2661	V2662	V2663	V2664	V2665	V2666	V2667	V2668	V2669	V2670	V2671	V2672	V2673	V2674	V2675	V2676	V2677	V2678	V2679	V2680	V2681	V2682	V2683	V2684	V2685	V2686	V2687	V2688	V2689	V2690	V2691	V2692	V2693	V2694	V2695	V2696	V2697	V2698	V2699	V2700	V2701	V2702	V2703	V2704	V2705	V2706	V2707	V2708	V2709	V2710	V2711	V2712	V2713	V2714	V2715	V2716	V2717	V2718	V2719	V2720	V2721	V2722	V2723	V2724	V2725	V2726	V2727	V2728	V2729	V2730	V2731	V2732	V2733	V2734	V2735	V2736	V2737	V2738	V2739	V2740	V2741	V2742	V2743	V2744	V2745	V2746	V2747	V2748	V2749	V2750	V2751	V2752	V2753	V2754	V2755	V2756	V2757	V2758	V2759	V2760	V2761	V2762	V2763	V2764	V2765	V2766	V2767	V2768	V2769	V2770	V2771	V2772	V2773	V2774	V2775	V2776	V2777	V2778	V2779	V2780	V2781	V2782	V2783	V2784	V2785	V2786	V2787	V2788	V2789	V2790	V2791	V2792	V2793	V2794	V2795	V2796	V2797	V2798	V2799	V2800	V2801	V2802	V2803	V2804	V2805	V2806	V2807	V2808	V2809	V2810	V2811	V2812	V2813	V2814	V2815	V2816	V2817	V2818	V2819	V2820	V2821	V2822	V2823	V2824	V2825	V2826	V2827	V2828	V2829	V2830	V2831	V2832	V2833	V2834	V2835	V2836	V2837	V2838	V2839	V2840	V2841	V2842	V2843	V2844	V2845	V2846	V2847	V2848	V2849	V2850	V2851	V2852	V2853	V2854	V2855	V2856	V2857	V2858	V2859	V2860	V2861	V2862	V2863	V2864	V2865	V2866	V2867	V2868	V2869	V2870	V2871	V2872	V2873	V2874	V2875	V2876	V2877	V2878	V2879	V2880	V2881	V2882	V2883	V2884	V2885	V2886	V2887	V2888	V2889	V2890	V2891	V2892	V2893	V2894	V2895	V2896	V2897	V2898	V2899	V2900	V2901	V2902	V2903	V2904	V2905	V2906	V2907	V2908	V2909	V2910	V2911	V2912	V2913	V2914	V2915	V2916	V2917	V2918	V2919	V2920	V2921	V2922	V2923	V2924	V2925	V2926	V2927	V2928	V2929	V2930	V2931	V2932	V2933	V2934	V2935	V2936	V2937	V2938	V2939	V2940	V2941	V2942	V2943	V2944	V2945	V2946	V2947	V2948	V2949	V2950	V2951	V2952	V2953	V2954	V2955	V2956	V2957	V2958	V2959	V2960	V2961	V2962	V2963	V2964	V2965	V2966	V2967	V2968	V2969	V2970	V2971	V2972	V2973	V2974	V2975	V2976	V2977	V2978	V2979	V2980	V2981	V2982	V2983	V2984	V2985	V2986	V2987	V2988	V2989	V2990	V2991	V2992	V2993	V2994	V2995	V2996	V2997	V2998	V2999

• Molecule 17: Proteasome activator BLM10



L1147	D1148	L1149	Y1150	G1151	G1152	N1153	Y1154	Y1155	F1156	G1157	N1158	T1159	T1160	E1161	E1162	K1163	L1164	N1165	N1166	N1167	H1168	H1169	H1170	H1171	H1172	H1173	H1174	H1175	H1176	H1177	H1178	H1179	F1180	F1181	F1182	F1183	H1184	F1185	L1186	Y1187	L1188	L1189	L1190	N1191	N1192	N1193	N1194	N1195	N1196	N1197	N1198	N1199	N1200	L1201	L1202	L1203	L1204	L1205	L1206	L1207	L1208	K1209	V1210	V1211	V1212	T1213	D1214	L1215	Q1216	E1217	E1218	T1219	V1220	F1221	N1222	A1223																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
F1228	I1229	D1230	V1231	D1232	F1233	L1234	E1235	N1236	Q1237	Q1238	S1239	L1240	S1241	H1242	V1243	P1244	P1245	P1246	F1247	T1248	R1249	T1250	N1251	I1252	R1253	R1254	R1255	N1256	N1257	H1258	H1259	H1260	H1261	H1262	H1263	H1264	H1265	H1266	H1267	S1268	T1269	N1270	R1271	S1272	S1273	S1274	R1275	L1276	E1277	V1278	D1279	D1280	I1281	Q1282	Q1283	Q1284	Q1285	Q1286	Q1287	Q1288	Q1289	Q1290	Q1291	Q1292	Q1293	Q1294	Q1295	Q1296	Q1297	Q1298	Q1299	Q1300	Q1301	Q1302	Q1303	Q1304	Q1305	Q1306	Q1307	Q1308	Q1309	Q1310	Q1311	Q1312	Q1313	Q1314	Q1315	Q1316	Q1317	Q1318	Q1319	Q1320	Q1321	Q1322	Q1323	Q1324	Q1325	Q1326	Q1327	Q1328	Q1329	Q1330	Q1331	Q1332	Q1333	Q1334	Q1335	Q1336	Q1337	Q1338	Q1339	Q1340	Q1341	Q1342	Q1343	Q1344	Q1345	Q1346	Q1347	Q1348	Q1349	Q1350	Q1351	Q1352	Q1353	Q1354	Q1355	Q1356	Q1357	Q1358	Q1359	Q1360	Q1361	Q1362	Q1363	Q1364	Q1365	Q1366	Q1367	Q1368	Q1369	Q1370	Q1371	Q1372	Q1373	Q1374	Q1375	Q1376	Q1377	Q1378	Q1379	Q1380	Q1381	Q1382	Q1383	Q1384	Q1385	Q1386	Q1387	Q1388	Q1389	Q1390	Q1391	Q1392	Q1393	Q1394	Q1395	Q1396	Q1397	Q1398	Q1399	Q1400	Q1401	Q1402	Q1403	Q1404	Q1405	Q1406	Q1407	Q1408	Q1409	Q1410	Q1411	Q1412	Q1413	Q1414	Q1415	Q1416	Q1417	Q1418	Q1419	Q1420	Q1421	Q1422	Q1423	Q1424	Q1425	Q1426	Q1427	Q1428	Q1429	Q1430	Q1431	Q1432	Q1433	Q1434	Q1435	Q1436	Q1437	Q1438	Q1439	Q1440	Q1441	Q1442	Q1443	Q1444	Q1445	Q1446	Q1447	Q1448	Q1449	Q1450	Q1451	Q1452	Q1453	Q1454	Q1455	Q1456	Q1457	Q1458	Q1459	Q1460	Q1461	Q1462	Q1463	Q1464	Q1465	Q1466	Q1467	Q1468	Q1469	Q1470	Q1471	Q1472	Q1473	Q1474	Q1475	Q1476	Q1477	Q1478	Q1479	Q1480	Q1481	Q1482	Q1483	Q1484	Q1485	Q1486	Q1487	Q1488	Q1489	Q1490	Q1491	Q1492	Q1493	Q1494	Q1495	Q1496	Q1497	Q1498	Q1499	Q1500	Q1501	Q1502	Q1503	Q1504	Q1505	Q1506	Q1507	Q1508	Q1509	Q1510	Q1511	Q1512	Q1513	Q1514	Q1515	Q1516	Q1517	Q1518	Q1519	Q1520	Q1521	Q1522	Q1523	Q1524	Q1525	Q1526	Q1527	Q1528	Q1529	Q1530	Q1531	Q1532	Q1533	Q1534	Q1535	Q1536	Q1537	Q1538	Q1539	Q1540	Q1541	Q1542	Q1543	Q1544	Q1545	Q1546	Q1547	Q1548	Q1549	Q1550	Q1551	Q1552	Q1553	Q1554	Q1555	Q1556	Q1557	Q1558	Q1559	Q1560	Q1561	Q1562	Q1563	Q1564	Q1565	Q1566	Q1567	Q1568	Q1569	Q1570	Q1571	Q1572	Q1573	Q1574	Q1575	Q1576	Q1577	Q1578	Q1579	Q1580	Q1581	Q1582	Q1583	Q1584	Q1585	Q1586	Q1587	Q1588	Q1589	Q1590	Q1591	Q1592	Q1593	Q1594	Q1595	Q1596	Q1597	Q1598	Q1599	Q1600	Q1601	Q1602	Q1603	Q1604	Q1605	Q1606	Q1607	Q1608	Q1609	Q1610	Q1611	Q1612	Q1613	Q1614	Q1615	Q1616	Q1617	Q1618	Q1619	Q1620	Q1621	Q1622	Q1623	Q1624	Q1625	Q1626	Q1627	Q1628	Q1629	Q1630	Q1631	Q1632	Q1633	Q1634	Q1635	Q1636	Q1637	Q1638	Q1639	Q1640	Q1641	Q1642	Q1643	Q1644	Q1645	Q1646	Q1647	Q1648	Q1649	Q1650	Q1651	Q1652	Q1653	Q1654	Q1655	Q1656	Q1657	Q1658	Q1659	Q1660	Q1661	Q1662	Q1663	Q1664	Q1665	Q1666	Q1667	Q1668	Q1669	Q1670	Q1671	Q1672	Q1673	Q1674	Q1675	Q1676	Q1677	Q1678	Q1679	Q1680	Q1681	Q1682	Q1683	Q1684	Q1685	Q1686	Q1687	Q1688	Q1689	Q1690	Q1691	Q1692	Q1693	Q1694	Q1695	Q1696	Q1697	Q1698	Q1699	Q1700	Q1701	Q1702	Q1703	Q1704	Q1705	Q1706	Q1707	Q1708	Q1709	Q1710	Q1711	Q1712	Q1713	Q1714	Q1715	Q1716	Q1717	Q1718	Q1719	Q1720	Q1721	Q1722	Q1723	Q1724	Q1725	Q1726	Q1727	Q1728	Q1729	Q1730	Q1731	Q1732	Q1733	Q1734	Q1735	Q1736	Q1737	Q1738	Q1739	Q1740	Q1741	Q1742	Q1743	Q1744	Q1745	Q1746	Q1747	Q1748	Q1749	Q1750	Q1751	Q1752	Q1753	Q1754	Q1755	Q1756	Q1757	Q1758	Q1759	Q1760	Q1761	Q1762	Q1763	Q1764	Q1765	Q1766	Q1767	Q1768	Q1769	Q1770	Q1771	Q1772	Q1773	Q1774	Q1775	Q1776	Q1777	Q1778	Q1779	Q1780	Q1781	Q1782	Q1783	Q1784	Q1785	Q1786	Q1787	Q1788	Q1789	Q1790	Q1791	Q1792	Q1793	Q1794	Q1795	Q1796	Q1797	Q1798	Q1799	Q1800	Q1801	Q1802	Q1803	Q1804	Q1805	Q1806	Q1807	Q1808	Q1809	Q1810	Q1811	Q1812	Q1813	Q1814	Q1815	Q1816	Q1817	Q1818	Q1819	Q1820	Q1821	Q1822	Q1823	Q1824	Q1825	Q1826	Q1827	Q1828	Q1829	Q1830	Q1831	Q1832	Q1833	Q1834	Q1835	Q1836	Q1837	Q1838	Q1839	Q1840	Q1841	Q1842	Q1843	Q1844	Q1845	Q1846	Q1847	Q1848	Q1849	Q1850	Q1851	Q1852	Q1853	Q1854	Q1855	Q1856	Q1857	Q1858	Q1859	Q1860	Q1861	Q1862	Q1863	Q1864	Q1865	Q1866	Q1867	Q1868	Q1869	Q1870	Q1871	Q1872	Q1873	Q1874	Q1875	Q1876	Q1877	Q1878	Q1879	Q1880	Q1881	Q1882	Q1883	Q1884	Q1885	Q1886	Q1887	Q1888	Q1889	Q1890	Q1891	Q1892	Q1893	Q1894	Q1895	Q1896	Q1897	Q1898	Q1899	Q1900	Q1901	Q1902	Q1903	Q1904	Q1905	Q1906	Q1907	Q1908	Q1909	Q1910	Q1911	Q1912	Q1913	Q1914	Q1915	Q1916	Q1917	Q1918	Q1919	Q1920	Q1921	Q1922	Q1923	Q1924	Q1925	Q1926	Q1927	Q1928	Q1929	Q1930	Q1931	Q1932	Q1933	Q1934	Q1935	Q1936	Q1937	Q1938	Q1939	Q1940	Q1941	Q1942	Q1943	Q1944	Q1945	Q1946	Q1947	Q1948	Q1949	Q1950	Q1951	Q1952	Q1953	Q1954	Q1955	Q1956	Q1957	Q1958	Q1959	Q1960	Q1961	Q1962	Q1963	Q1964	Q1965	Q1966	Q1967	Q1968	Q1969	Q1970	Q1971	Q1972	Q1973	Q1974	Q1975	Q1976	Q1977	Q1978	Q1979	Q1980	Q1981	Q1982	Q1983	Q1984	Q1985	Q1986	Q1987	Q1988	Q1989	Q1990	Q1991	Q1992	Q1993	Q1994	Q1995	Q1996	Q1997	Q1998	Q1999	Q2000









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.196 , 0.250 0.193 , 0.244	Depositor DCC
$R_{free}$ test set	4957 reflections (1.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.9	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 60.7	EDS
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 495926 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	158904	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	AA	0.60	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(°)	Ideal(°)
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%)	16	56
1	AC	241/243 (99%)	222 (92%)	16 (7%)	3 (1%)	16	56
1	BA	241/243 (99%)	224 (93%)	14 (6%)	3 (1%)	16	56
1	BO	241/243 (99%)	225 (93%)	13 (5%)	3 (1%)	16	56
2	AG	229/231 (99%)	212 (93%)	13 (6%)	4 (2%)	11	46
2	AS	229/231 (99%)	211 (92%)	15 (7%)	3 (1%)	15	53
2	BB	229/231 (99%)	214 (93%)	13 (6%)	2 (1%)	21	64
2	BP	229/231 (99%)	211 (92%)	16 (7%)	2 (1%)	21	64
3	AH	230/232 (99%)	186 (81%)	25 (11%)	19 (8%)	1	5
3	AT	230/232 (99%)	185 (80%)	27 (12%)	18 (8%)	1	6
3	BC	230/232 (99%)	188 (82%)	25 (11%)	17 (7%)	1	6
3	BQ	230/232 (99%)	188 (82%)	24 (10%)	18 (8%)	1	6
4	AI	225/227 (99%)	167 (74%)	45 (20%)	13 (6%)	2	12
4	AU	225/227 (99%)	168 (75%)	43 (19%)	14 (6%)	2	10
4	BD	225/227 (99%)	168 (75%)	44 (20%)	13 (6%)	2	12
4	BR	225/227 (99%)	169 (75%)	42 (19%)	14 (6%)	2	10
5	AJ	248/250 (99%)	215 (87%)	21 (8%)	12 (5%)	3	17
5	AV	248/250 (99%)	214 (86%)	22 (9%)	12 (5%)	3	17
5	BE	248/250 (99%)	216 (87%)	20 (8%)	12 (5%)	3	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	BS	248/250 (99%)	215 (87%)	21 (8%)	12 (5%)	3	17
6	AK	232/234 (99%)	211 (91%)	17 (7%)	4 (2%)	11	46
6	AW	232/234 (99%)	212 (91%)	16 (7%)	4 (2%)	11	46
6	BF	232/234 (99%)	212 (91%)	16 (7%)	4 (2%)	11	46
6	BT	232/234 (99%)	212 (91%)	17 (7%)	3 (1%)	15	53
7	AL	242/244 (99%)	221 (91%)	20 (8%)	1 (0%)	39	80
7	AX	242/244 (99%)	223 (92%)	17 (7%)	2 (1%)	24	66
7	BG	242/244 (99%)	224 (93%)	17 (7%)	1 (0%)	39	80
7	BU	242/244 (99%)	222 (92%)	18 (7%)	2 (1%)	24	66
8	AB	194/196 (99%)	174 (90%)	18 (9%)	2 (1%)	19	61
8	AD	194/196 (99%)	172 (89%)	19 (10%)	3 (2%)	13	50
8	BH	194/196 (99%)	175 (90%)	17 (9%)	2 (1%)	19	61
8	BV	194/196 (99%)	177 (91%)	15 (8%)	2 (1%)	19	61
9	AM	220/222 (99%)	202 (92%)	16 (7%)	2 (1%)	21	64
9	AY	220/222 (99%)	201 (91%)	17 (8%)	2 (1%)	21	64
9	BI	220/222 (99%)	203 (92%)	15 (7%)	2 (1%)	21	64
9	BW	220/222 (99%)	201 (91%)	17 (8%)	2 (1%)	21	64
10	AN	202/204 (99%)	182 (90%)	16 (8%)	4 (2%)	9	41
10	AZ	202/204 (99%)	184 (91%)	16 (8%)	2 (1%)	19	61
10	BJ	202/204 (99%)	187 (93%)	13 (6%)	2 (1%)	19	61
10	BX	202/204 (99%)	184 (91%)	17 (8%)	1 (0%)	34	76
11	A1	196/198 (99%)	175 (89%)	14 (7%)	7 (4%)	4	24
11	AO	196/198 (99%)	176 (90%)	14 (7%)	6 (3%)	5	28
11	BK	196/198 (99%)	175 (89%)	15 (8%)	6 (3%)	5	28
11	BY	196/198 (99%)	175 (89%)	14 (7%)	7 (4%)	4	24
12	A2	210/212 (99%)	190 (90%)	19 (9%)	1 (0%)	34	76
12	AP	210/212 (99%)	191 (91%)	19 (9%)	0	100	100
12	BL	210/212 (99%)	191 (91%)	18 (9%)	1 (0%)	34	76
12	BZ	210/212 (99%)	189 (90%)	21 (10%)	0	100	100
13	A3	220/222 (99%)	203 (92%)	13 (6%)	4 (2%)	11	45
13	AQ	220/222 (99%)	200 (91%)	16 (7%)	4 (2%)	11	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	B1	220/222 (99%)	202 (92%)	14 (6%)	4 (2%)	11	45
13	BM	220/222 (99%)	201 (91%)	17 (8%)	2 (1%)	21	64
14	A4	231/233 (99%)	211 (91%)	16 (7%)	4 (2%)	11	46
14	AR	231/233 (99%)	212 (92%)	16 (7%)	3 (1%)	15	53
14	B2	231/233 (99%)	212 (92%)	16 (7%)	3 (1%)	15	53
14	BN	231/233 (99%)	213 (92%)	15 (6%)	3 (1%)	15	53
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	14
16	A7	797/799 (100%)	640 (80%)	111 (14%)	46 (6%)	2	12
16	B4	797/799 (100%)	651 (82%)	107 (13%)	39 (5%)	3	16
16	B7	797/799 (100%)	639 (80%)	116 (15%)	42 (5%)	2	14
17	A6	995/997 (100%)	782 (79%)	128 (13%)	85 (8%)	1	5
17	A8	995/997 (100%)	775 (78%)	133 (13%)	87 (9%)	1	4
17	B5	995/997 (100%)	780 (78%)	134 (14%)	81 (8%)	1	5
17	B8	995/997 (100%)	776 (78%)	135 (14%)	84 (8%)	1	5
All	All	19944/20080 (99%)	17074 (86%)	2065 (10%)	805 (4%)	4	21

5 of 805 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	207/207 (100%)	187 (90%)	20 (10%)	10	37
1	AC	207/207 (100%)	184 (89%)	23 (11%)	8	29
1	BA	207/207 (100%)	185 (89%)	22 (11%)	8	31
1	BO	207/207 (100%)	185 (89%)	22 (11%)	8	31
2	AG	192/192 (100%)	175 (91%)	17 (9%)	12	42
2	AS	192/192 (100%)	172 (90%)	20 (10%)	9	32
2	BB	192/192 (100%)	172 (90%)	20 (10%)	9	32
2	BP	192/192 (100%)	172 (90%)	20 (10%)	9	32
3	AH	192/192 (100%)	164 (85%)	28 (15%)	4	18
3	AT	192/192 (100%)	164 (85%)	28 (15%)	4	18
3	BC	192/192 (100%)	164 (85%)	28 (15%)	4	18
3	BQ	192/192 (100%)	164 (85%)	28 (15%)	4	18
4	AI	202/202 (100%)	177 (88%)	25 (12%)	6	24
4	AU	202/202 (100%)	176 (87%)	26 (13%)	5	23
4	BD	202/202 (100%)	177 (88%)	25 (12%)	6	24
4	BR	202/202 (100%)	177 (88%)	25 (12%)	6	24
5	AJ	206/206 (100%)	181 (88%)	25 (12%)	6	25
5	AV	206/206 (100%)	181 (88%)	25 (12%)	6	25
5	BE	206/206 (100%)	178 (86%)	28 (14%)	5	20
5	BS	206/206 (100%)	178 (86%)	28 (14%)	5	20
6	AK	193/193 (100%)	166 (86%)	27 (14%)	4	19
6	AW	193/193 (100%)	166 (86%)	27 (14%)	4	19
6	BF	193/193 (100%)	166 (86%)	27 (14%)	4	19
6	BT	193/193 (100%)	168 (87%)	25 (13%)	5	22
7	AL	201/201 (100%)	176 (88%)	25 (12%)	6	24
7	AX	201/201 (100%)	175 (87%)	26 (13%)	5	23
7	BG	201/201 (100%)	175 (87%)	26 (13%)	5	23
7	BU	201/201 (100%)	175 (87%)	26 (13%)	5	23
8	AB	161/161 (100%)	144 (89%)	17 (11%)	8	31
8	AD	161/161 (100%)	145 (90%)	16 (10%)	10	35
8	BH	161/161 (100%)	144 (89%)	17 (11%)	8	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	BV	161/161 (100%)	145 (90%)	16 (10%)	10	35
9	AM	181/181 (100%)	164 (91%)	17 (9%)	11	39
9	AY	181/181 (100%)	164 (91%)	17 (9%)	11	39
9	BI	181/181 (100%)	165 (91%)	16 (9%)	12	42
9	BW	181/181 (100%)	164 (91%)	17 (9%)	11	39
10	AN	172/172 (100%)	158 (92%)	14 (8%)	15	47
10	AZ	172/172 (100%)	155 (90%)	17 (10%)	10	35
10	BJ	172/172 (100%)	158 (92%)	14 (8%)	15	47
10	BX	172/172 (100%)	157 (91%)	15 (9%)	13	43
11	A1	175/175 (100%)	160 (91%)	15 (9%)	13	44
11	AO	175/175 (100%)	161 (92%)	14 (8%)	15	47
11	BK	175/175 (100%)	160 (91%)	15 (9%)	13	44
11	BY	175/175 (100%)	161 (92%)	14 (8%)	15	47
12	A2	169/169 (100%)	152 (90%)	17 (10%)	9	34
12	AP	169/169 (100%)	154 (91%)	15 (9%)	12	42
12	BL	169/169 (100%)	154 (91%)	15 (9%)	12	42
12	BZ	169/169 (100%)	154 (91%)	15 (9%)	12	42
13	A3	185/185 (100%)	166 (90%)	19 (10%)	9	33
13	AQ	185/185 (100%)	164 (89%)	21 (11%)	7	28
13	B1	185/185 (100%)	165 (89%)	20 (11%)	8	30
13	BM	185/185 (100%)	164 (89%)	21 (11%)	7	28
14	A4	199/199 (100%)	176 (88%)	23 (12%)	7	27
14	AR	199/199 (100%)	175 (88%)	24 (12%)	6	25
14	B2	199/199 (100%)	176 (88%)	23 (12%)	7	27
14	BN	199/199 (100%)	178 (89%)	21 (11%)	8	31
15	AE	73/73 (100%)	67 (92%)	6 (8%)	14	46
15	AF	73/73 (100%)	66 (90%)	7 (10%)	10	38
15	B3	73/73 (100%)	66 (90%)	7 (10%)	10	38
15	B6	73/73 (100%)	66 (90%)	7 (10%)	10	38
16	A5	744/744 (100%)	653 (88%)	91 (12%)	6	25
16	A7	744/744 (100%)	651 (88%)	93 (12%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	B4	744/744 (100%)	655 (88%)	89 (12%)	6	26
16	B7	744/744 (100%)	655 (88%)	89 (12%)	6	26
17	A6	909/909 (100%)	774 (85%)	135 (15%)	4	17
17	A8	909/909 (100%)	773 (85%)	136 (15%)	3	17
17	B5	909/909 (100%)	774 (85%)	135 (15%)	4	17
17	B8	909/909 (100%)	771 (85%)	138 (15%)	3	16
All	All	17444/17444 (100%)	15334 (88%)	2110 (12%)	6	25

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

Mol	Chain	Res	Type
17	A8	1397	SER
6	BF	6010	THR
16	B7	833	ASN
17	A8	1627	VAL
1	BA	1164	VAL

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

Mol	Chain	Res	Type
16	A7	780	GLN
4	BD	4243	GLN
15	B6	83	ASN
17	A8	1184	HIS
1	BA	1126	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	243/243 (100%)	-0.66	1 (0%) 93 80	37, 67, 125, 215	0
1	AC	243/243 (100%)	-0.63	0 100 100	52, 87, 139, 216	0
1	BA	243/243 (100%)	-0.24	5 (2%) 67 36	79, 107, 150, 217	0
1	BO	243/243 (100%)	-0.41	4 (1%) 74 47	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%)	-0.31	2 (0%) 85 64	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%)	-0.41	3 (1%) 79 53	56, 113, 176, 219	0
3	AT	232/232 (100%)	-0.24	5 (2%) 65 35	65, 114, 180, 223	0
3	BC	232/232 (100%)	0.01	7 (3%) 54 25	88, 132, 182, 227	0
3	BQ	232/232 (100%)	-0.34	4 (1%) 73 45	81, 123, 180, 227	0
4	AI	227/227 (100%)	-0.31	2 (0%) 85 64	63, 126, 187, 212	0
4	AU	227/227 (100%)	-0.24	7 (3%) 52 24	70, 127, 188, 224	0
4	BD	227/227 (100%)	-0.02	9 (3%) 42 17	89, 137, 193, 222	0
4	BR	227/227 (100%)	-0.12	8 (3%) 48 21	88, 135, 189, 220	0
5	AJ	250/250 (100%)	-0.45	7 (2%) 56 27	60, 99, 188, 246	0
5	AV	250/250 (100%)	-0.20	12 (4%) 34 14	59, 102, 194, 246	0
5	BE	250/250 (100%)	-0.04	18 (7%) 18 7	80, 117, 192, 245	0
5	BS	250/250 (100%)	-0.24	11 (4%) 38 16	82, 115, 191, 246	0
6	AK	234/234 (100%)	-0.67	0 100 100	51, 79, 119, 232	0
6	AW	234/234 (100%)	-0.67	0 100 100	51, 82, 121, 235	0
6	BF	234/234 (100%)	-0.43	1 (0%) 93 80	77, 104, 133, 235	0
6	BT	234/234 (100%)	-0.46	0 100 100	78, 102, 133, 236	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
7	AL	244/244 (100%)	-0.63	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%)	-0.30	2 (0%) 87 67	78, 105, 142, 165	0
7	BU	244/244 (100%)	-0.39	2 (0%) 87 67	72, 101, 143, 163	0
8	AB	196/196 (100%)	-0.78	0 100 100	38, 61, 95, 139	0
8	AD	196/196 (100%)	-0.72	0 100 100	41, 66, 101, 147	0
8	BH	196/196 (100%)	-0.51	0 100 100	71, 94, 119, 155	0
8	BV	196/196 (100%)	-0.45	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%)	-0.45	1 (0%) 91 76	75, 98, 125, 199	0
9	BW	222/222 (100%)	-0.54	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%)	-0.50	2 (0%) 84 60	71, 99, 125, 157	0
10	BX	204/204 (100%)	-0.56	1 (0%) 91 76	69, 90, 118, 162	0
11	A1	198/198 (100%)	-0.68	3 (1%) 76 49	49, 82, 119, 220	0
11	AO	198/198 (100%)	-0.67	3 (1%) 76 49	49, 80, 118, 223	0
11	BK	198/198 (100%)	-0.43	3 (1%) 76 49	76, 102, 130, 225	0
11	BY	198/198 (100%)	-0.51	3 (1%) 76 49	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%)	-0.64	0 100 100	56, 82, 118, 139	0
12	BL	212/212 (100%)	-0.41	1 (0%) 91 76	74, 98, 127, 149	0
12	BZ	212/212 (100%)	-0.59	1 (0%) 91 76	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%)	-0.74	0 100 100	51, 75, 111, 169	0
13	B1	222/222 (100%)	-0.47	2 (0%) 85 64	71, 100, 127, 170	0
13	BM	222/222 (100%)	-0.63	0 100 100	70, 94, 121, 173	0
14	A4	233/233 (100%)	-0.78	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%)	-0.48	1 (0%) 93 80	70, 95, 120, 165	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	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%)	-0.63	0	100	100	73, 107, 139, 145	0
15	B3	76/76 (100%)	-0.11	0	100	100	101, 129, 146, 155	0
15	B6	76/76 (100%)	-0.60	0	100	100	78, 118, 144, 151	0
16	A5	799/799 (100%)	-0.55	1 (0%)	95	90	45, 87, 141, 267	0
16	A7	799/799 (100%)	-0.51	5 (0%)	90	73	54, 95, 144, 267	0
16	B4	799/799 (100%)	-0.22	19 (2%)	62	32	82, 115, 155, 265	0
16	B7	799/799 (100%)	-0.37	11 (1%)	78	51	72, 105, 149, 266	0
17	A6	997/997 (100%)	-0.47	7 (0%)	89	70	55, 107, 166, 261	0
17	A8	997/997 (100%)	-0.42	17 (1%)	73	45	63, 108, 167, 260	0
17	B5	997/997 (100%)	-0.11	28 (2%)	56	27	83, 128, 173, 261	0
17	B8	997/997 (100%)	-0.35	20 (2%)	68	39	77, 114, 170, 261	0
All	All	20080/20080 (100%)	-0.45	239 (1%)	81	55	34, 100, 158, 267	0

The worst 5 of 239 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	B8	1753	GLU	14.5
5	AV	5125	GLU	12.6
17	B8	1754	SER	11.7
17	A8	1755	ASP	10.2
17	B8	1755	ASP	9.9

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.