



wwPDB X-ray Structure Validation Summary Report

Jul 23, 2014 – 08:38 AM EDT

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 validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

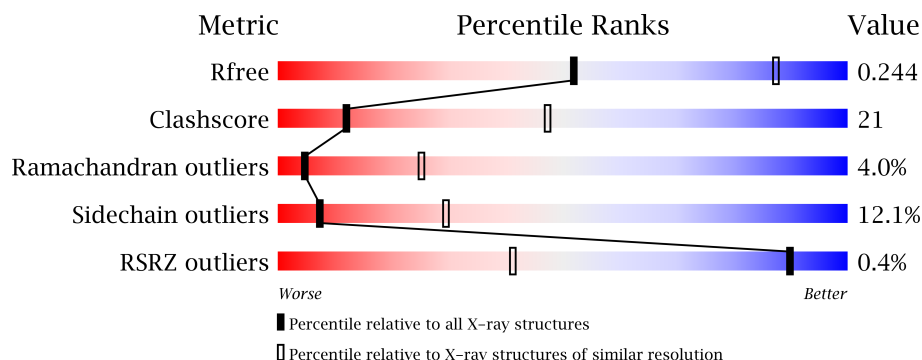
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	243	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	AC	243	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	BA	243	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	BO	243	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
2	AG	231	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
2	AS	231	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
2	BB	231	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
2	BP	231	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
3	AH	232	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
3	AT	232	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
3	BC	232	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
3	BQ	232	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
4	AI	227	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
4	AU	227	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>









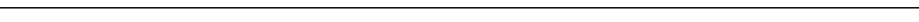

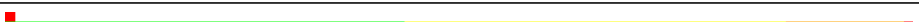

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Mol	Chain	Length	Quality of chain
4	BD	227	
4	BR	227	
5	AJ	250	
5	AV	250	
5	BE	250	
5	BS	250	
6	AK	234	
6	AW	234	
6	BF	234	
6	BT	234	
7	AL	244	
7	AX	244	
7	BG	244	
7	BU	244	
8	AB	196	
8	AD	196	
8	BH	196	
8	BV	196	
9	AM	222	
9	AY	222	
9	BI	222	
9	BW	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	
14	BN	233	

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Mol	Chain	Length	Quality of chain
15	AE	76	
15	AF	76	
15	B3	76	
15	B6	76	
16	A5	799	
16	A7	799	
16	B4	799	
16	B7	799	
17	A6	997	
17	A8	997	
17	B5	997	
17	B8	997	

2 Entry composition

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

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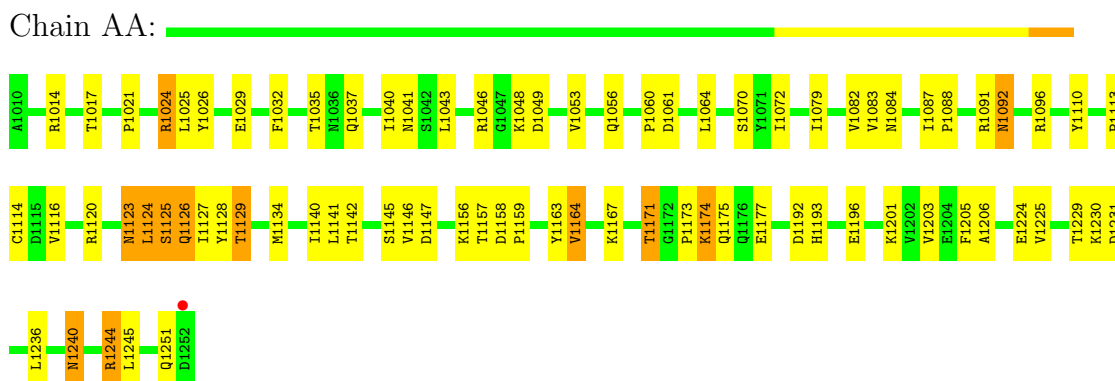
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Chain	Residue	Modelled	Actual	Comment	Reference
B8	1171	ASN	GLN	CONFLICT	UNP P43583
B8	2085	ASN	GLN	CONFLICT	UNP P43583
B8	2101	ASN	GLN	CONFLICT	UNP P43583

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.

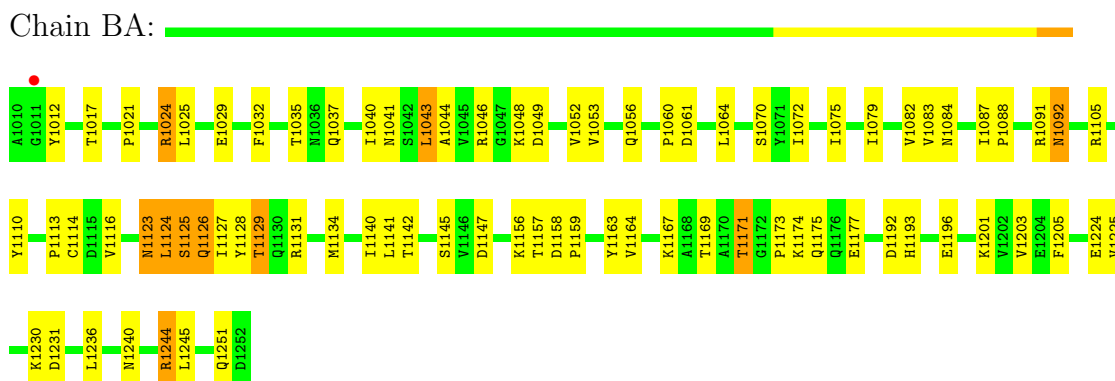
- Molecule 1: Proteasome component C7-alpha



- Molecule 1: Proteasome component C7-alpha

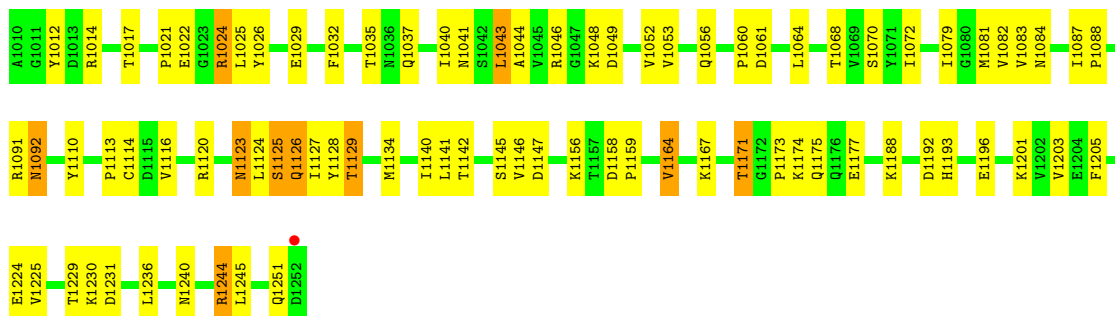


- Molecule 1: Proteasome component C7-alpha



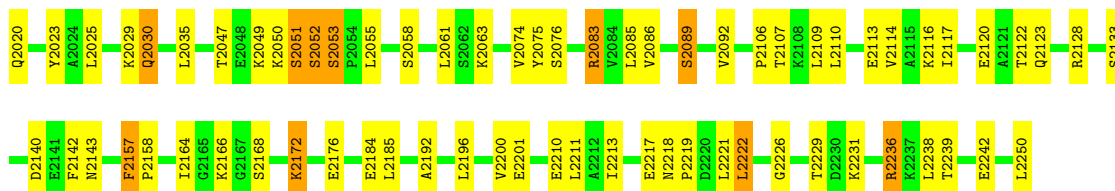
- Molecule 1: Proteasome component C7-alpha

Chain BO:



- Molecule 2: Proteasome component Y7

Chain AG:



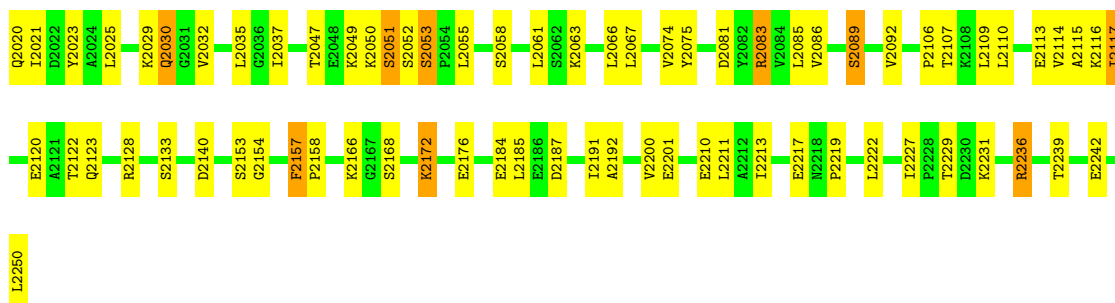
- Molecule 2: Proteasome component Y7

Chain AS:



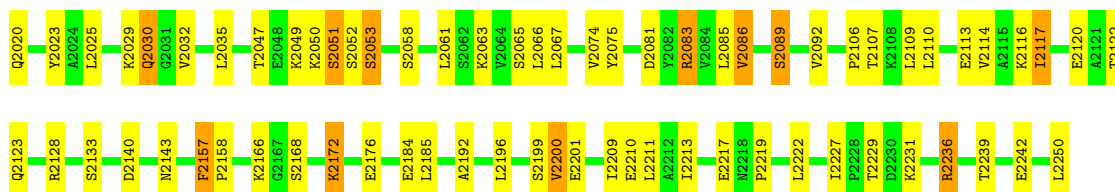
- Molecule 2: Proteasome component Y7

Chain BB:



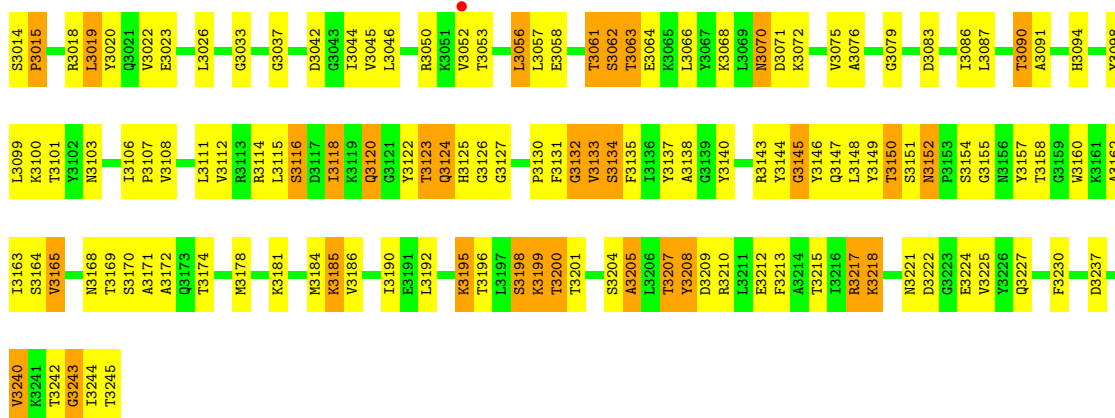
- Molecule 2: Proteasome component Y7

Chain BP:



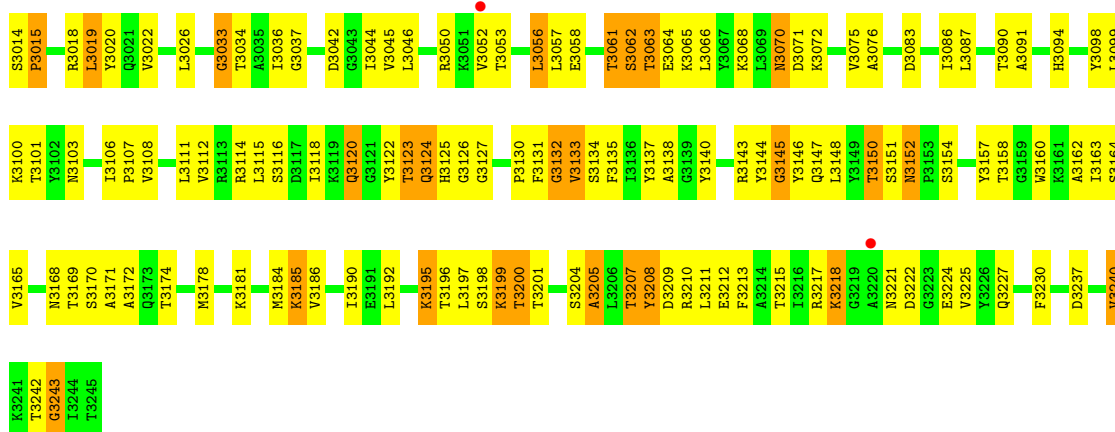
• Molecule 3: Proteasome component Y13

Chain AH:



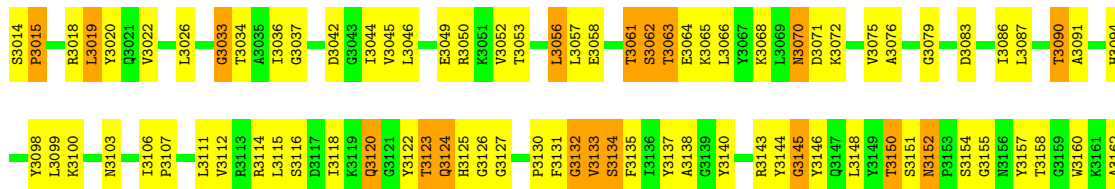
• Molecule 3: Proteasome component Y13

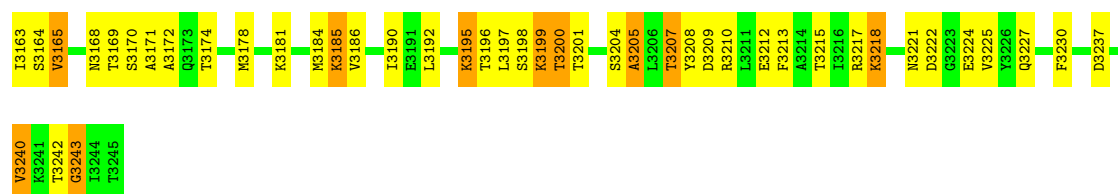
Chain AT:



• Molecule 3: Proteasome component Y13

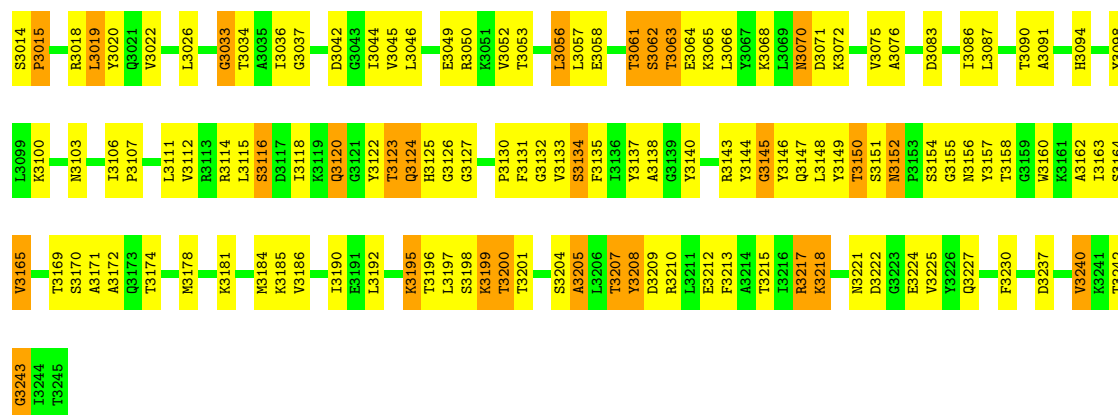
Chain BC:





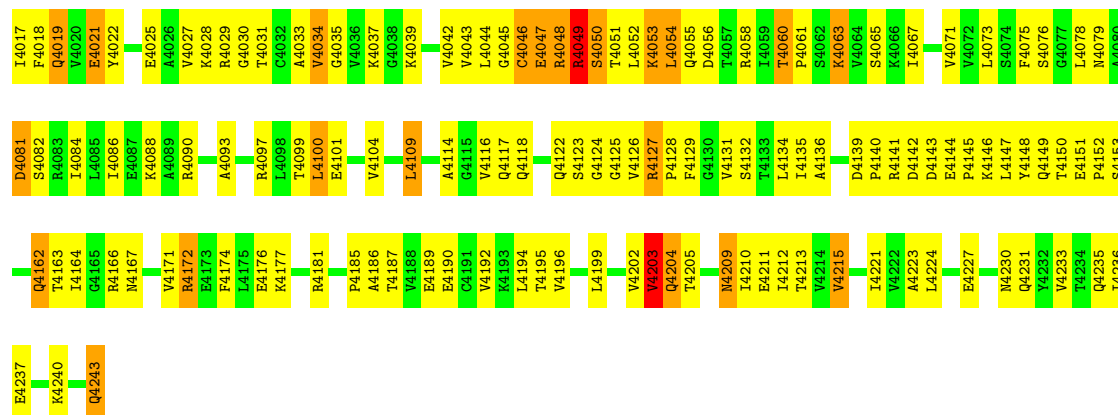
• Molecule 3: Proteasome component Y13

Chain BQ:



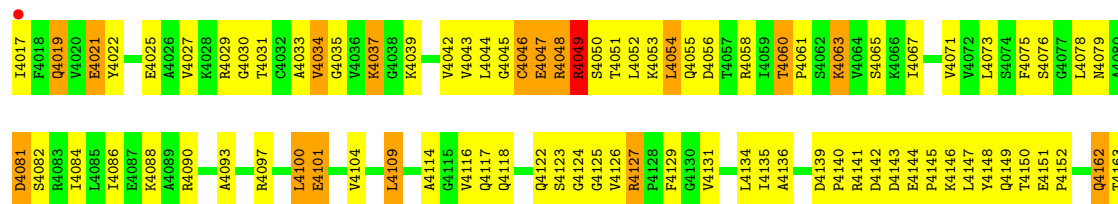
• Molecule 4: Proteasome component PRE6

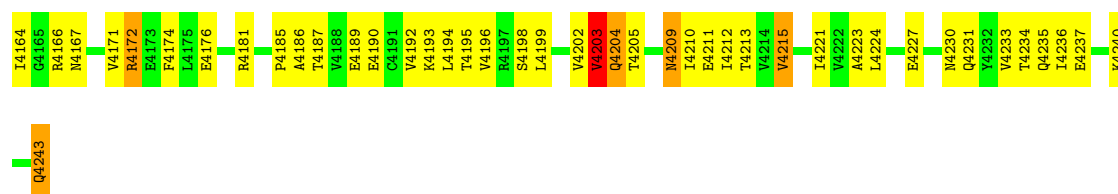
Chain AI:



• Molecule 4: Proteasome component PRE6

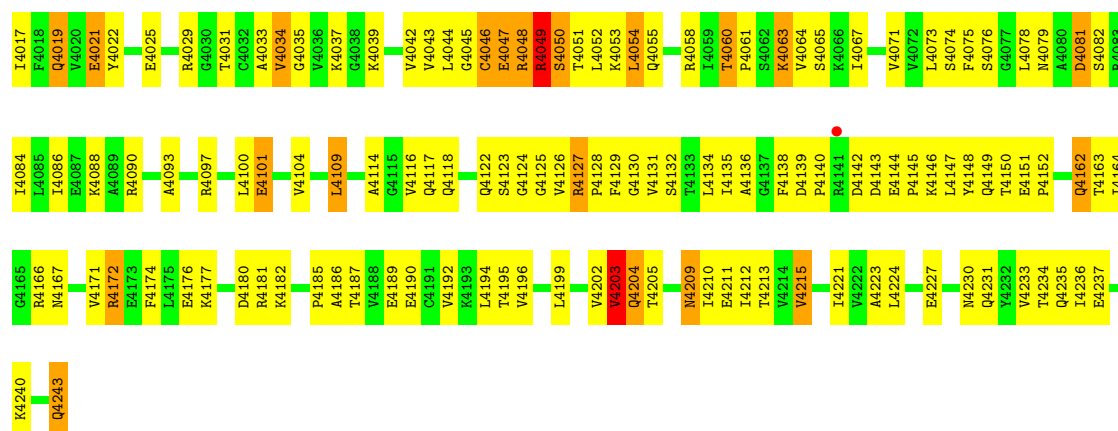
Chain AU:





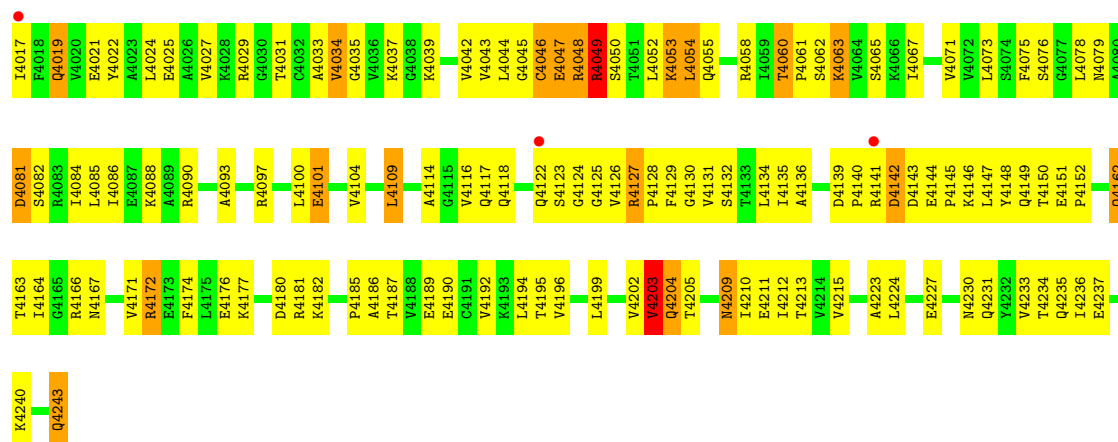
• Molecule 4: Proteasome component PRE6

Chain BD:



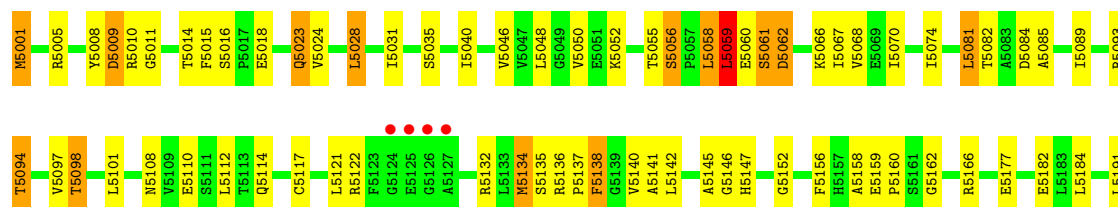
• Molecule 4: Proteasome component PRE6

Chain BR:



• Molecule 5: Proteasome component PUP2

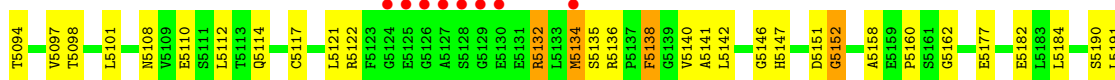
Chain AJ:





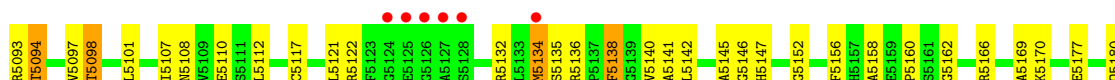
• Molecule 5: Proteasome component PUP2

Chain AV:



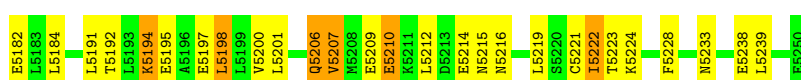
• Molecule 5: Proteasome component PUP2

Chain BE:



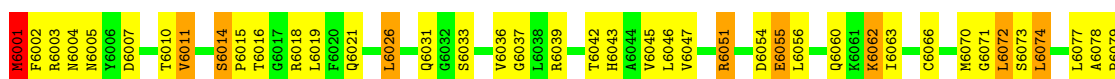
• Molecule 5: Proteasome component PUP2

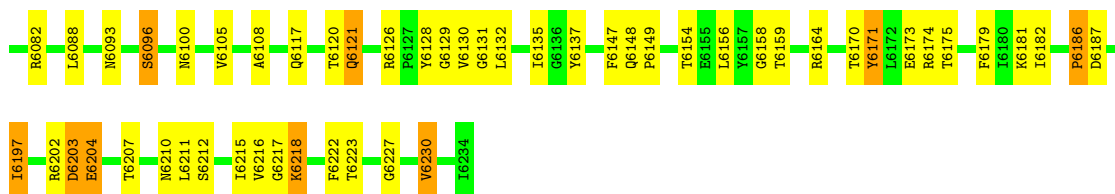
Chain BS:



• Molecule 6: Proteasome component PRE5

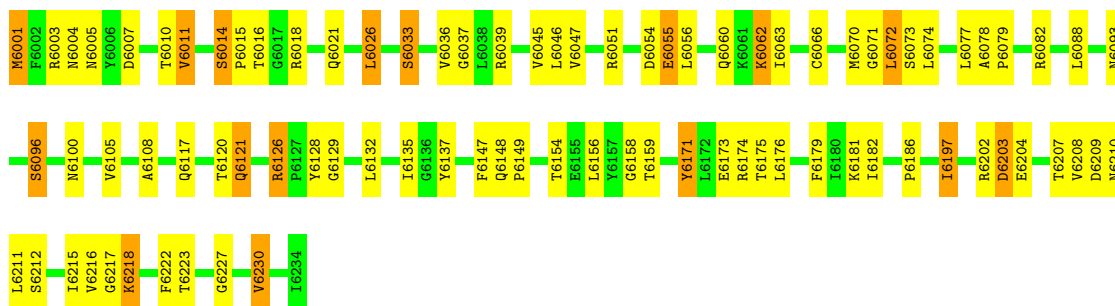
Chain AK:





- Molecule 6: Proteasome component PRE5

Chain AW:



- Molecule 6: Proteasome component PRE5

Chain BF:



- Molecule 6: Proteasome component PRE5

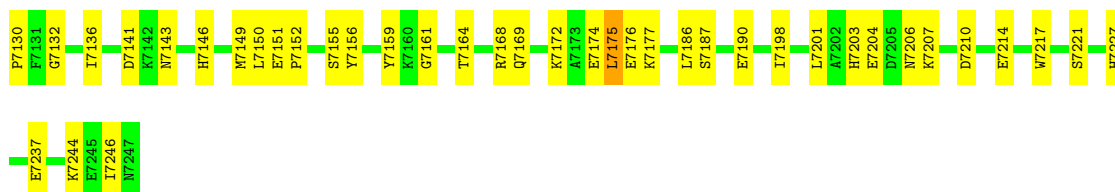
Chain BT:



- Molecule 7: Proteasome component C1

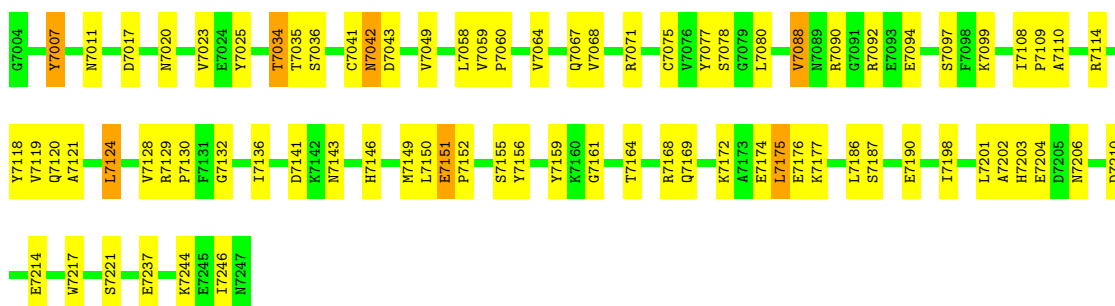
Chain AL:





- Molecule 7: Proteasome component C1

Chain AX:



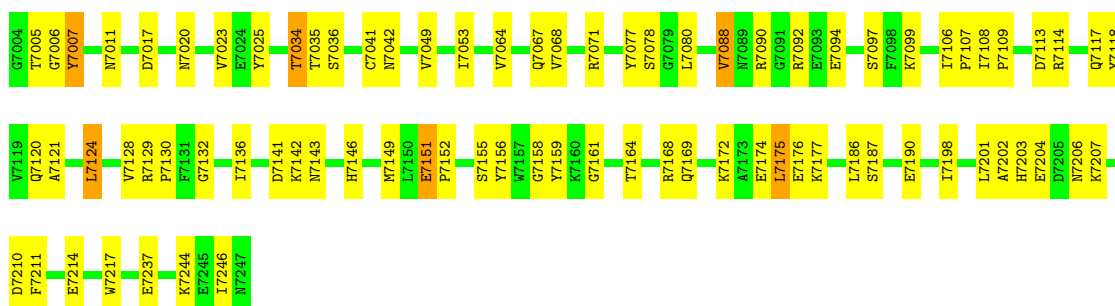
- Molecule 7: Proteasome component C1

Chain BG:



- Molecule 7: Proteasome component C1

Chain BU:



- Molecule 8: Proteasome component PRE3

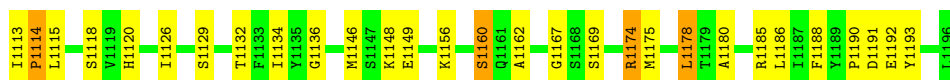
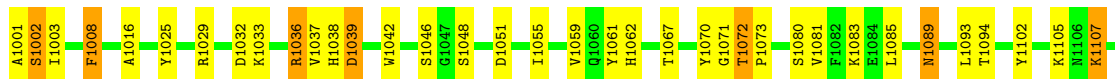
Chain AB:





- Molecule 8: Proteasome component PRE3

Chain AD:



- Molecule 8: Proteasome component PRE3

Chain BH:



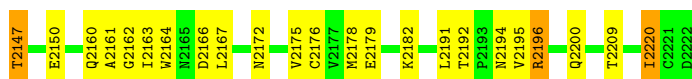
- Molecule 8: Proteasome component PRE3

Chain BV:



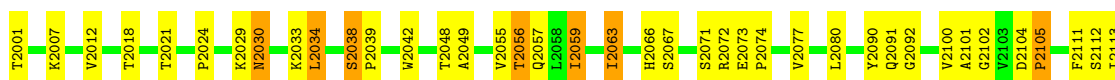
- Molecule 9: Proteasome component PUP1

Chain AM:



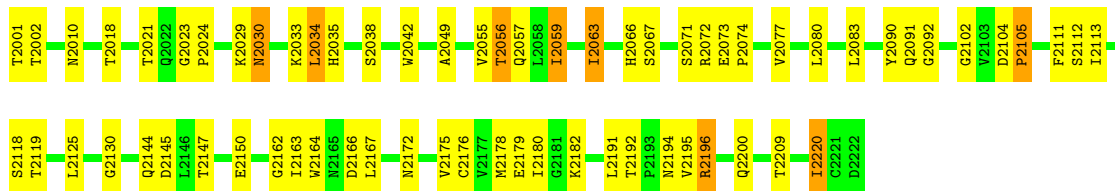
- Molecule 9: Proteasome component PUP1

Chain AY:



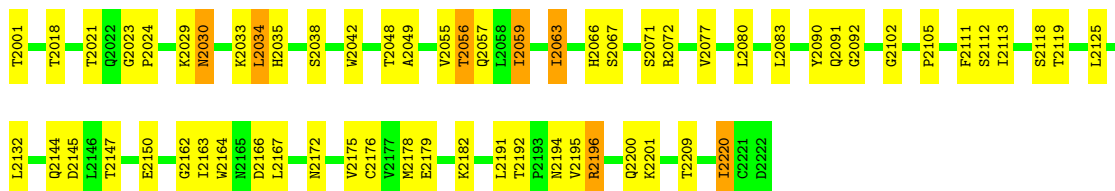
- Molecule 9: Proteasome component PUP1

Chain BI:



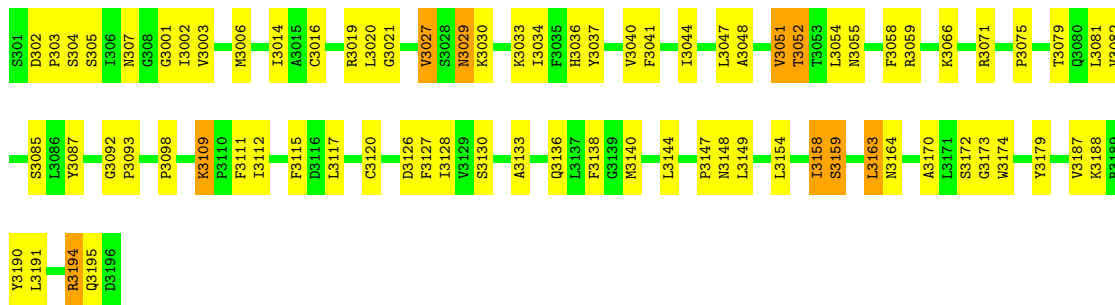
- Molecule 9: Proteasome component PUP1

Chain BW:



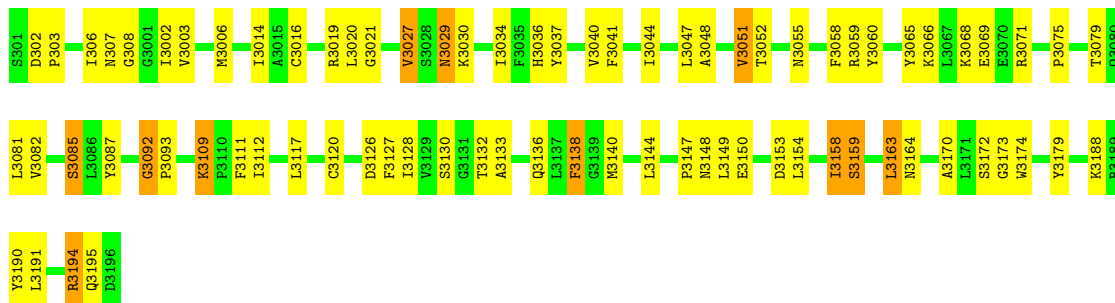
- Molecule 10: Proteasome component PUP3

Chain AN:



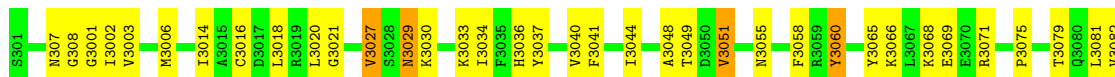
- Molecule 10: Proteasome component PUP3

Chain AZ:



- Molecule 10: Proteasome component PUP3

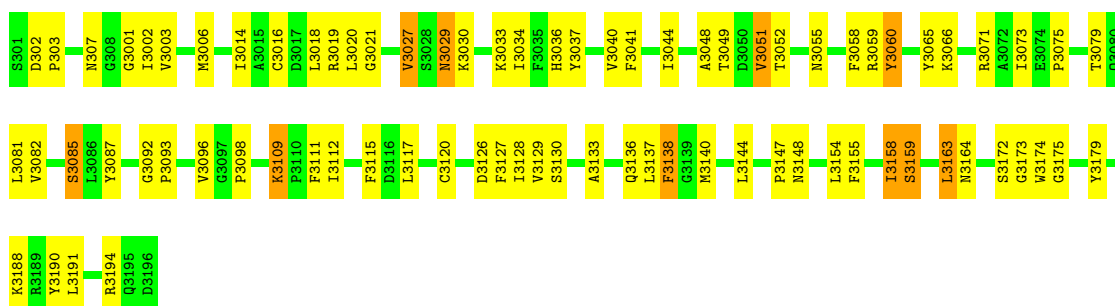
Chain BJ:





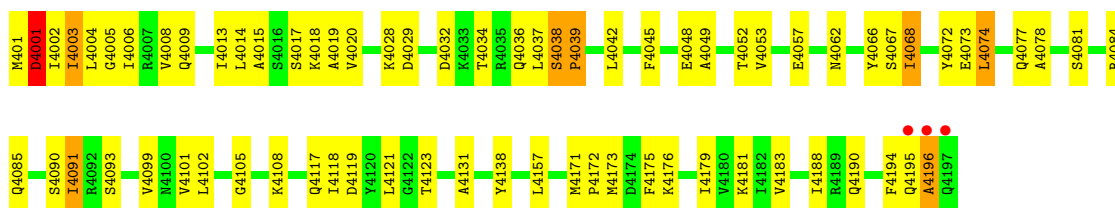
• Molecule 10: Proteasome component PUP3

Chain BX:



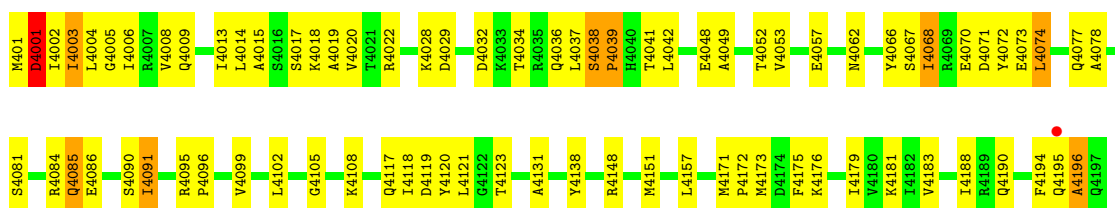
• Molecule 11: Proteasome component C11

Chain AO:



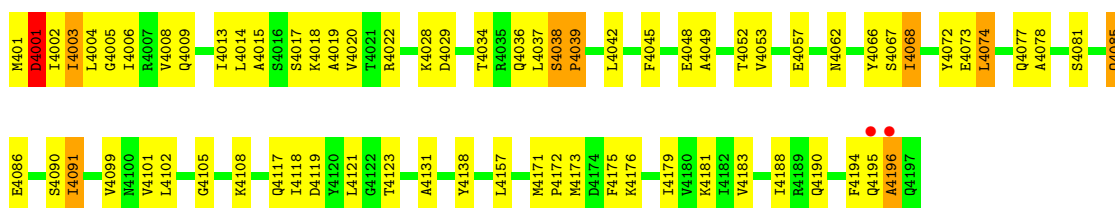
• Molecule 11: Proteasome component C11

Chain A1:



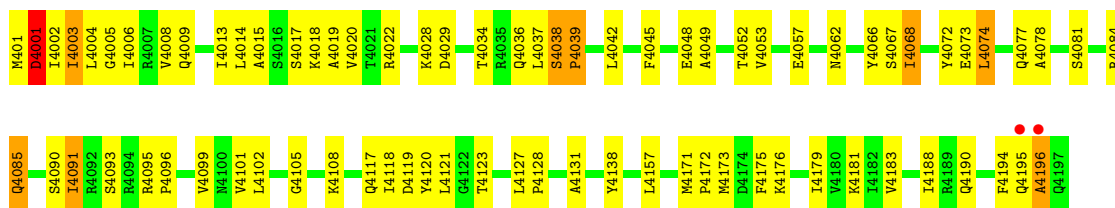
• Molecule 11: Proteasome component C11

Chain BK:



• Molecule 11: Proteasome component C11

Chain BY:



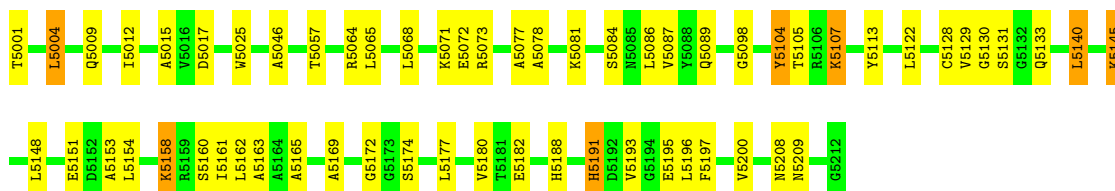
- Molecule 12: Proteasome component PRE2

Chain AP:



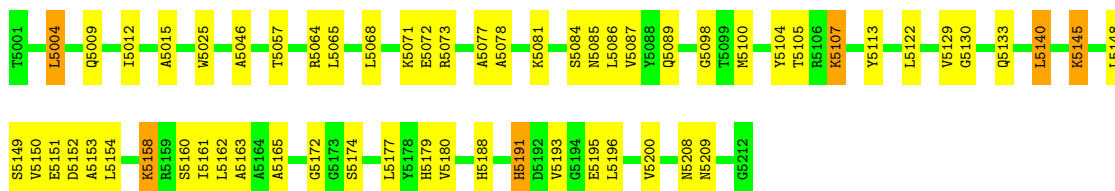
- Molecule 12: Proteasome component PRE2

Chain A2:



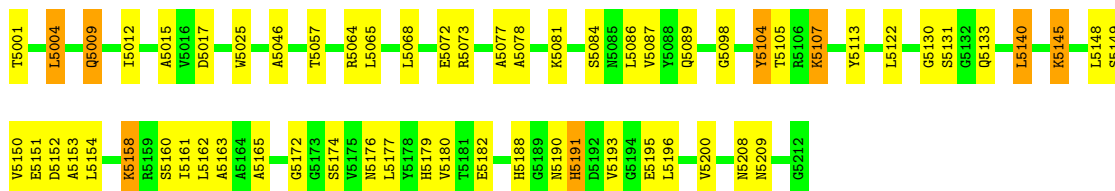
- Molecule 12: Proteasome component PRE2

Chain BL:



- Molecule 12: Proteasome component PRE2

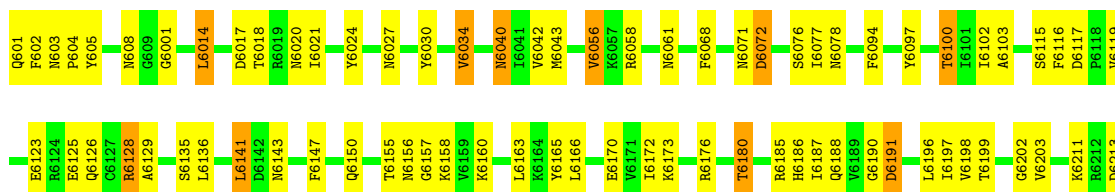
Chain BZ:



- Molecule 13: Proteasome component C5

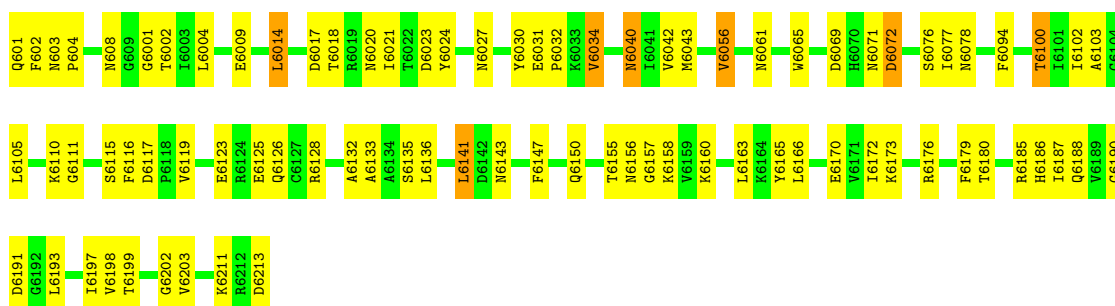
Chain AQ:





• Molecule 13: Proteasome component C5

Chain A3:



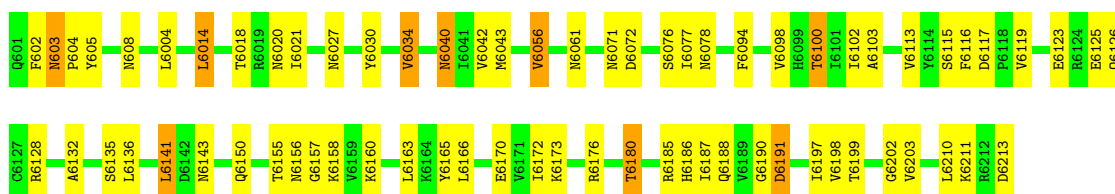
• Molecule 13: Proteasome component C5

Chain BM:



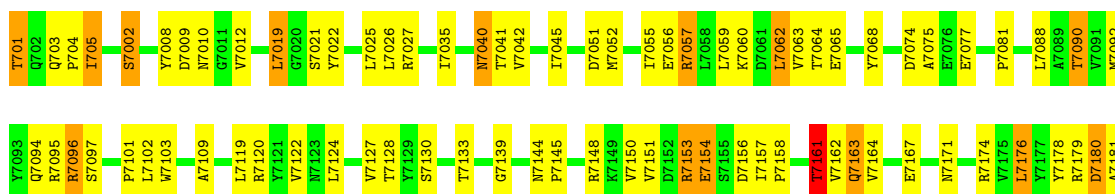
• Molecule 13: Proteasome component C5

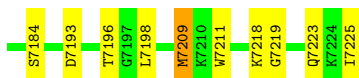
Chain B1:



• Molecule 14: Proteasome component PRE4

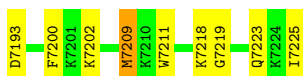
Chain AR:





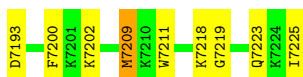
- Molecule 14: Proteasome component PRE4

Chain A4:



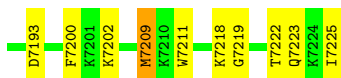
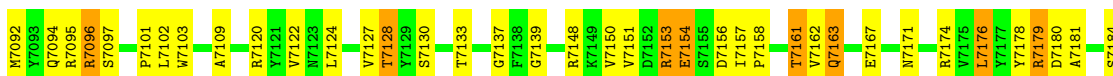
- Molecule 14: Proteasome component PRE4

Chain BN:



- Molecule 14: Proteasome component PRE4

Chain B2:



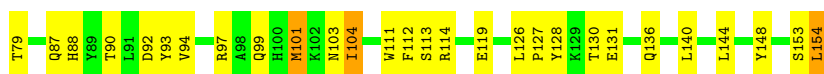
- Molecule 15: Proteasome activator BLM10

Chain AE:



- Molecule 15: Proteasome activator BLM10

Chain AF:



• Molecule 15: Proteasome activator BLM10

Chain B3:



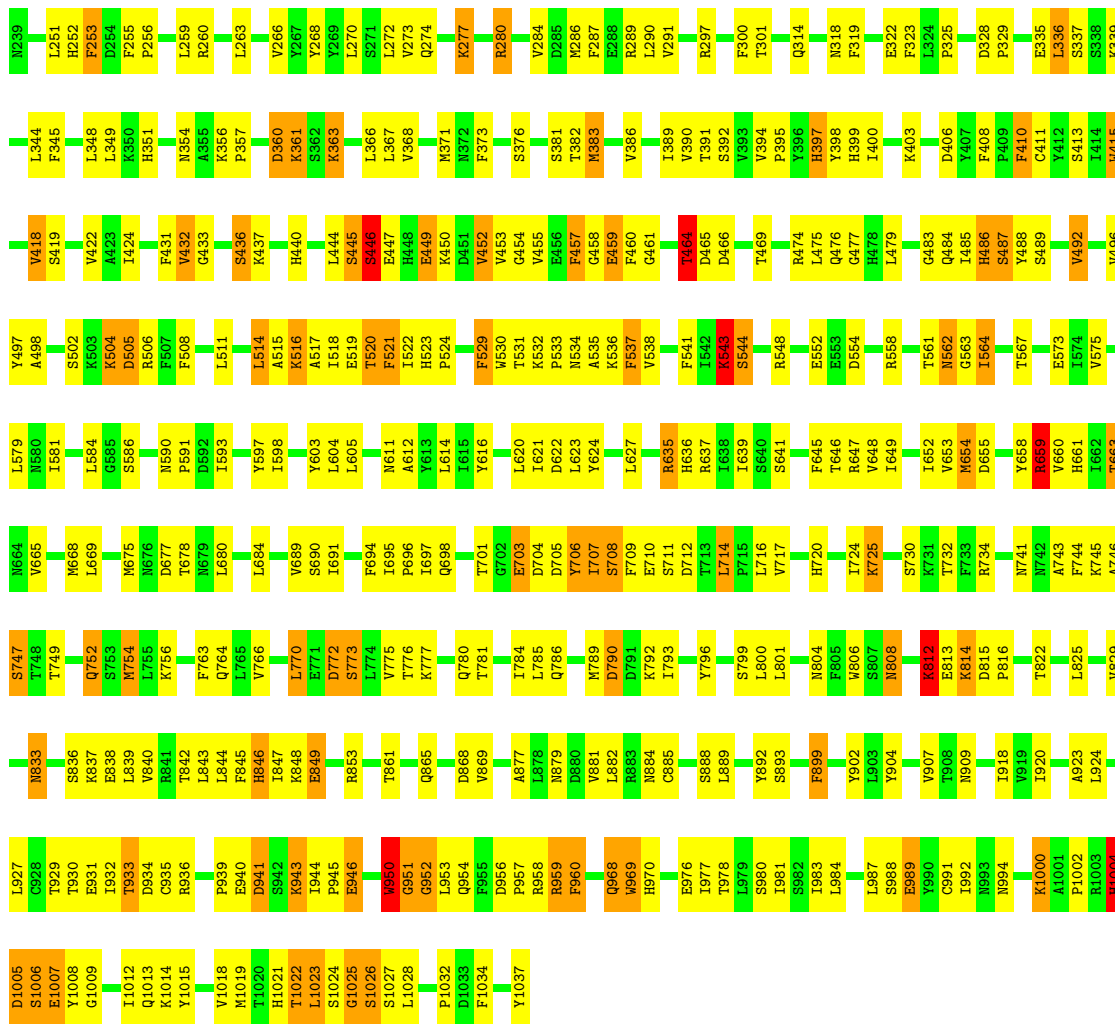
• Molecule 15: Proteasome activator BLM10

Chain B6:



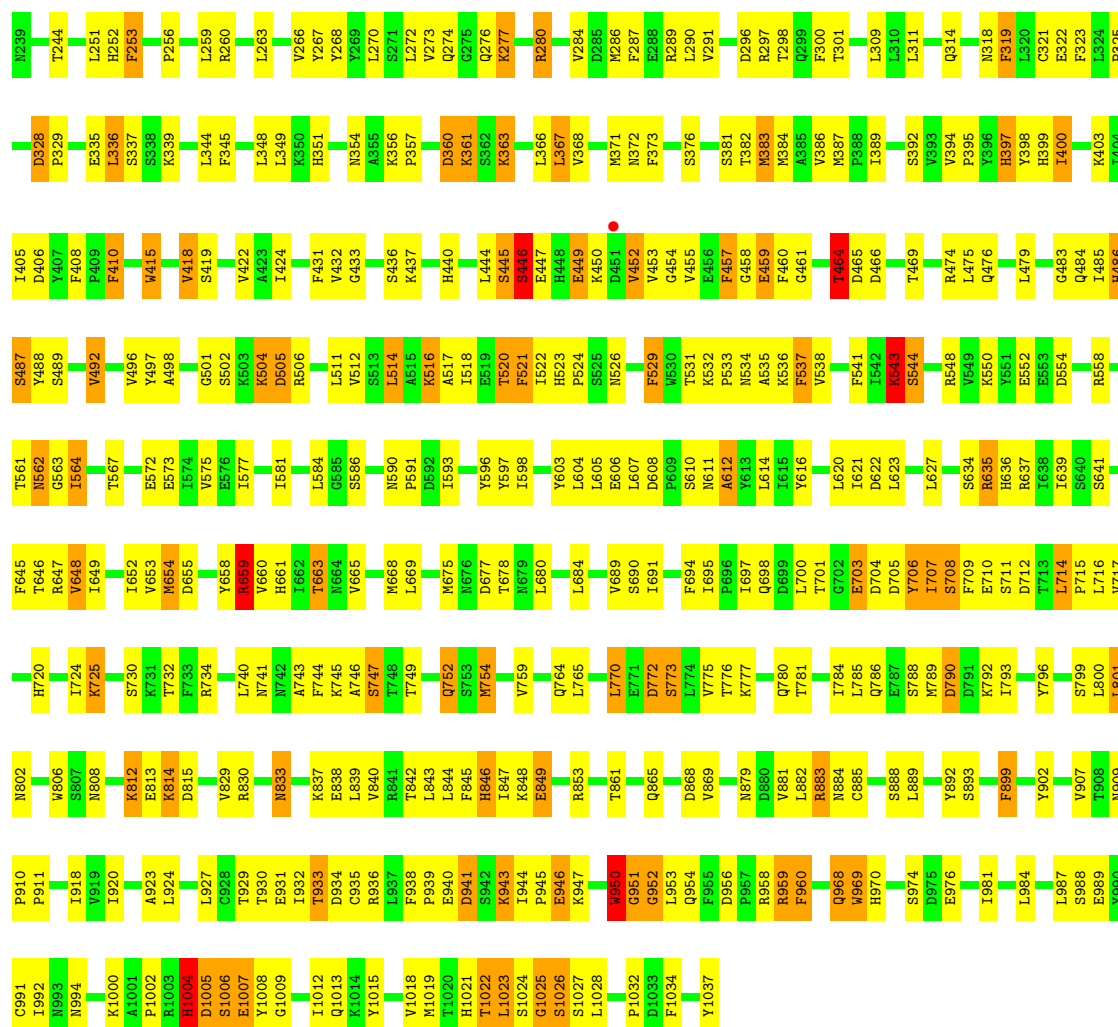
• Molecule 16: Proteasome activator BLM10

Chain A5:



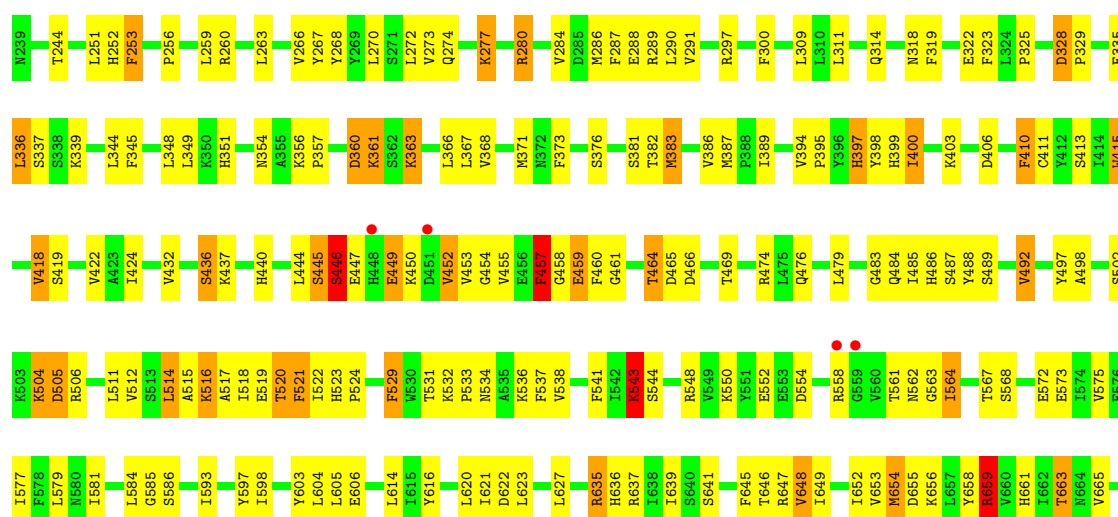
• Molecule 16: Proteasome activator BLM10

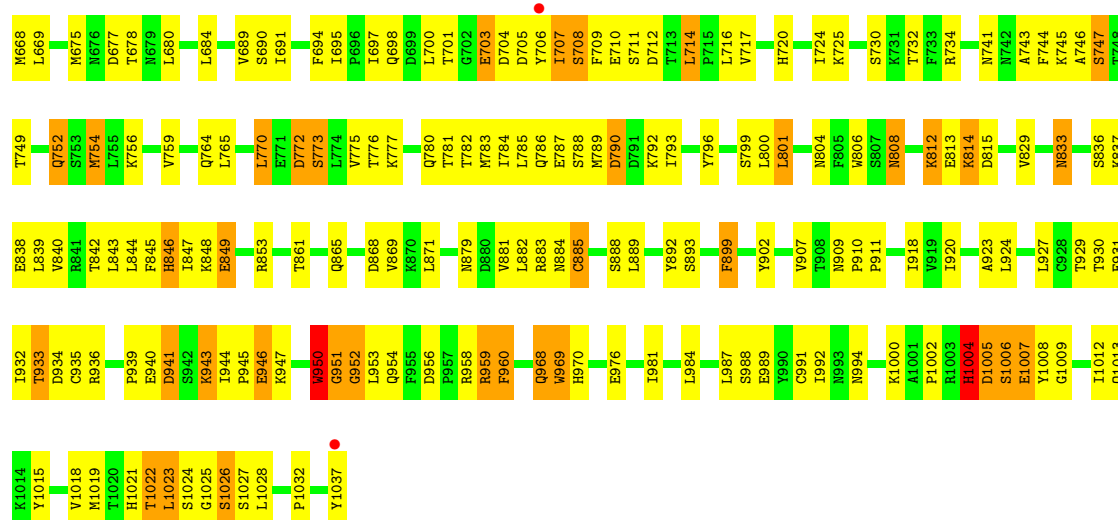
Chain A7:



● Molecule 16: Proteasome activator BLM10

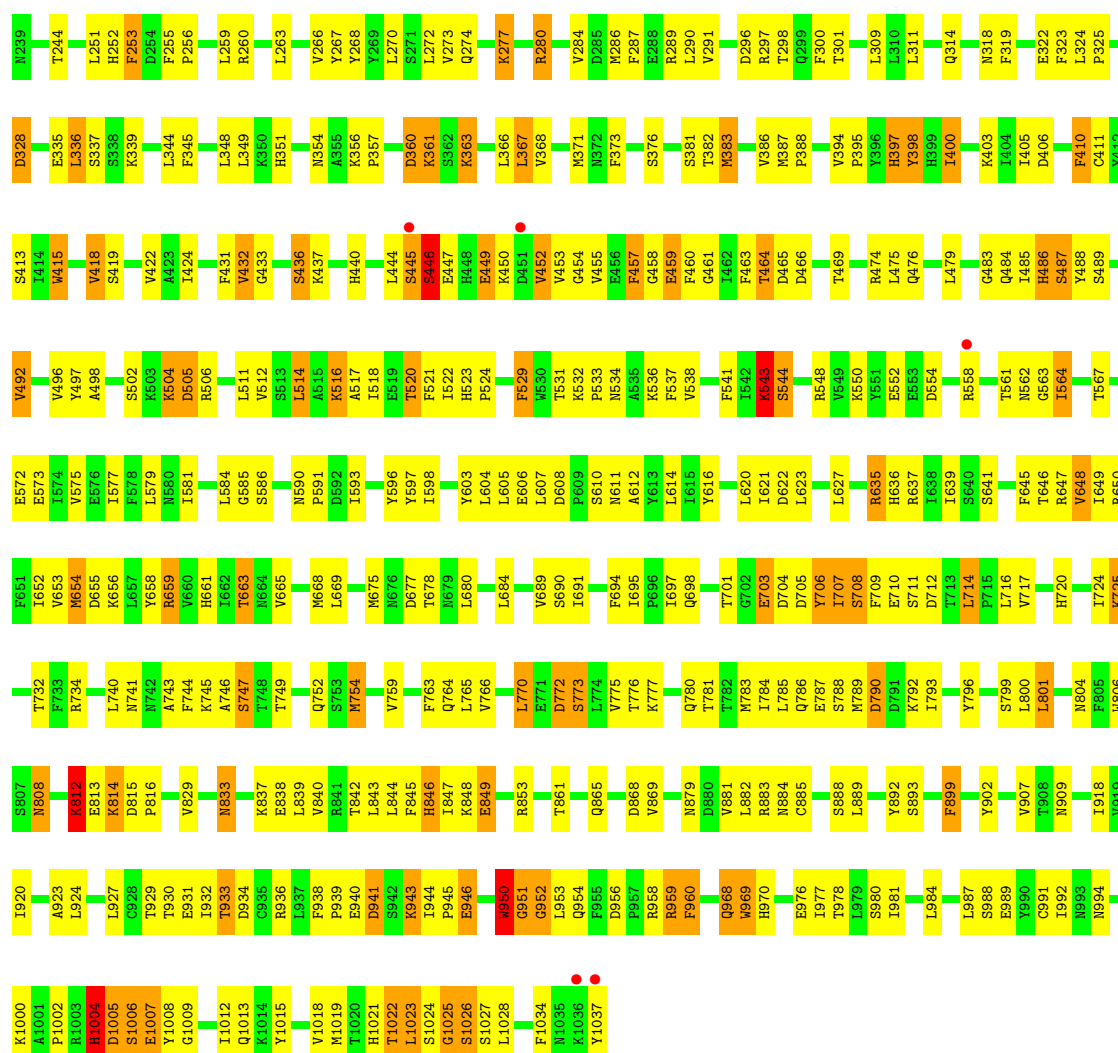
Chain B4:



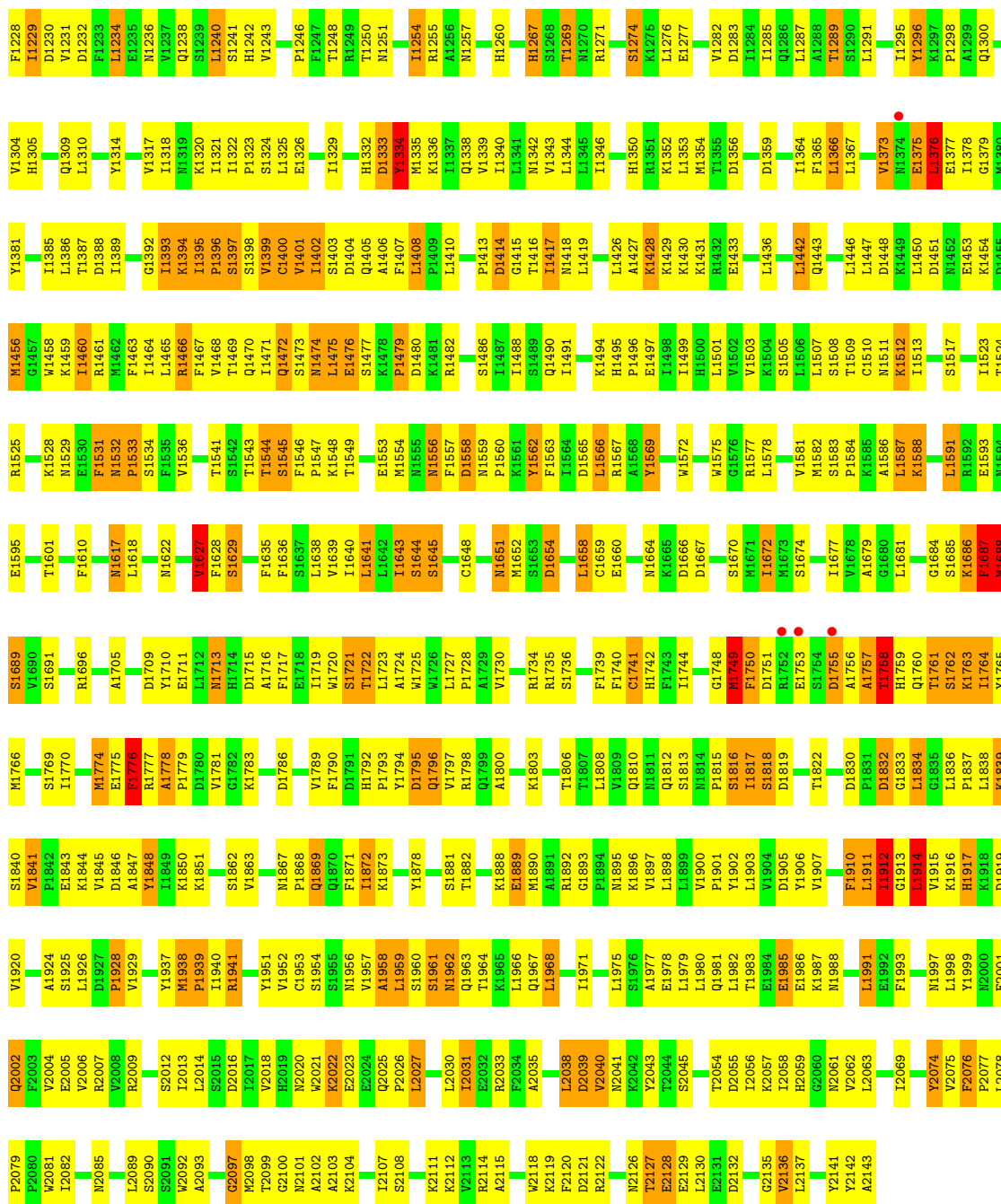


• Molecule 16: Proteasome activator BLM10

Chain B7:

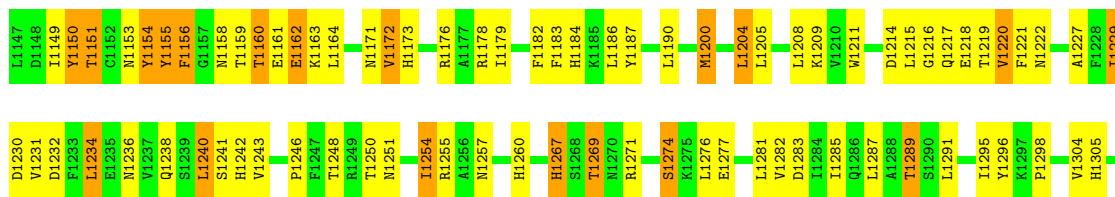


• Molecule 17: Proteasome activator BLM10



● Molecule 17: Proteasome activator BLM10

Chain B5:





A2143	N2061	L1991	L1914	K1839	S1762	V1690	K1528	M1456	Y1381
V2062	L2063	F1993	V1915	S1840	K1763	S1691	M1529	G1457	L1385
L2069			K1916	V1841	I1764		E1530	K1458	L1386
S2070			H1917	F1842	Y1765	R1696	F1531	K1459	T1387
A2071			K1918	E1843	M1766	D1697	P1532	L1460	D1388
F2072			D1919	K1844		I1700	S1534	R1461	I1389
L1998			V1920	Y1845	S1769		F1535	M1462	
Y1999				D1846	I1770		V1536	F1463	G1392
S2000			A1924	A1847		L1704		I1464	I1393
E2001			S1925	E1775	M1774	A1705		L1465	K1394
Q2002			L1926	E1776			T1541	R1466	I1395
F2003			D1927	S1776		D1709	S1542	F1467	P1396
Y2004			K1928	R1777		Y1710	T1543	V1468	S1397
E2005			V1929	A1778		E1711	T1544	T1469	
P2006			L1859	P1779		L1712	S1545	Q1470	S1398
R2007						M1713	F1546	I1471	V1399
V2008						K1714	P1547	Q1472	C1400
R2009			L1935	S1862	G1782	D1715	K1548	S1473	V1401
			G1936	V1863	K1783	A1716	T1549	I1402	I1402
S2012			Y1937		D1786	F1717		L1475	S1403
L2013			M1938	M1867		E1718	E1553	E1476	L1404
L2014			P1939	P1868		I1719	M1559	E1478	Q1405
S2015			T1940	Q1869		W1720	M1554	S1477	A1406
D2016			R1941	Q1870		S1721	M1556	P1479	F1407
L2017				F1871	D1791	T1722	F1557	D1480	L1408
V2018			Y1951	I1872	H1792	L1723	D1558	K1481	F1409
H2019			C1952	K1873	P1793	A1724	M1559	R1482	L1410
N2020			S1954	Y1878	Y1794	W1725	P1560	S1486	D1413
W2021			S1954		D1795	W1726	K1561		D1414
K2022			L1956	S1881	Q1796	L1727	Y1562	Q1490	G1415
E2023			V1957	T1882	V1797	P1728	F1563	I1491	T1416
Z2024			A1958		Q1799	A1729	D1564		I1417
Q2025			S1960		A1800	V1730	D1565	K1494	N1418
P2026			S1962	I1887	K1803		A1568	H1495	L1419
L2027			N1961	E1888		R1734		P1496	
L2030			Q1963	M1890		R1735	Y1569	E1497	L1426
E2032			T1964	A1891	T1806	K1737		I1498	A1427
F2034			L1966	R1892	T1807	T1738	W1572	I1499	K1428
A2035			Q1967	L1893	T1808	F1739		H1500	K1429
K2036			L1968	P1894	V1809	F1740	W1575	L1501	K1430
G2037				N1895	Q1810	C1741	G1576	V1502	K1431
L2038				K1896		H1742	R1577	V1503	R1432
D2039				V1897	P1815	F1743	L1578	K1504	E1433
V2040				L1898	S1816	M1744		S1505	
N2041				L1899	I1817		V1581	L1506	L1436
K2042			S1976	V1900	S1818	G1748	M1582	L1507	
Y2043			A1977	P1901	D1819	M1749	S1583	T1508	L1442
Z2044			E1978	Y1902		F1750	P1584	T1509	Q1443
S2045			L1979	L1903	T1822	D1751		C1510	
T2054			L1980	V1904		R1752	L1587	M1511	L1446
L2055			Q1981	D1905	D1830	E1753	K1589	L1512	L1447
Z2056			L1982	Y1906	P1831	S1754		I1513	L1448
K2057			T1983	V1907	D1832	F1755	L1591		K1449
H2058			F1984	L1908	G1833	A1756	R1592	S1517	L1450
Y2141			E1985	P1909	L1834		E1593		D1451
Y2142			E1986	F1910	G1835	S1685	M1594	M1452	
			K1987	L1911	L1836	K1686	E1595	T1523	E1453
			M1988	I1912	P1837	F1687		T1524	K1454
				G1913	L1838	T1761		R1525	D1455

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	236.12Å 127.74Å 532.67Å 90.00° 102.85° 90.00°	Depositor
Resolution (Å)	29.99 – 3.00 29.99 – 3.01	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	67.9	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 31.1	EDS
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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 Close contacts ⓘ

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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	BX	1581	0	1571	59	0
11	A1	1585	0	1587	58	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

The worst 5 of 6805 close contacts within the same asymmetric unit are listed below.

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

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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%)	19	64
1	AC	241/243 (99%)	222 (92%)	16 (7%)	3 (1%)	19	64
1	BA	241/243 (99%)	224 (93%)	14 (6%)	3 (1%)	19	64
1	BO	241/243 (99%)	225 (93%)	13 (5%)	3 (1%)	19	64
2	AG	229/231 (99%)	212 (93%)	13 (6%)	4 (2%)	14	54
2	AS	229/231 (99%)	211 (92%)	15 (7%)	3 (1%)	18	62
2	BB	229/231 (99%)	214 (93%)	13 (6%)	2 (1%)	25	73
2	BP	229/231 (99%)	211 (92%)	16 (7%)	2 (1%)	25	73
3	AH	230/232 (99%)	186 (81%)	25 (11%)	19 (8%)	1	6
3	AT	230/232 (99%)	185 (80%)	27 (12%)	18 (8%)	1	7
3	BC	230/232 (99%)	188 (82%)	25 (11%)	17 (7%)	2	8
3	BQ	230/232 (99%)	188 (82%)	24 (10%)	18 (8%)	1	7
4	AI	225/227 (99%)	167 (74%)	45 (20%)	13 (6%)	3	15
4	AU	225/227 (99%)	168 (75%)	43 (19%)	14 (6%)	2	13
4	BD	225/227 (99%)	168 (75%)	44 (20%)	13 (6%)	3	15
4	BR	225/227 (99%)	169 (75%)	42 (19%)	14 (6%)	2	13
5	AJ	248/250 (99%)	215 (87%)	21 (8%)	12 (5%)	4	20
5	AV	248/250 (99%)	214 (86%)	22 (9%)	12 (5%)	4	20
5	BE	248/250 (99%)	216 (87%)	20 (8%)	12 (5%)	4	20
5	BS	248/250 (99%)	215 (87%)	21 (8%)	12 (5%)	4	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	AK	232/234 (99%)	211 (91%)	17 (7%)	4 (2%)	14	54
6	AW	232/234 (99%)	212 (91%)	16 (7%)	4 (2%)	14	54
6	BF	232/234 (99%)	212 (91%)	16 (7%)	4 (2%)	14	54
6	BT	232/234 (99%)	212 (91%)	17 (7%)	3 (1%)	18	62
7	AL	242/244 (99%)	221 (91%)	20 (8%)	1 (0%)	43	87
7	AX	242/244 (99%)	223 (92%)	17 (7%)	2 (1%)	27	76
7	BG	242/244 (99%)	224 (93%)	17 (7%)	1 (0%)	43	87
7	BU	242/244 (99%)	222 (92%)	18 (7%)	2 (1%)	27	76
8	AB	194/196 (99%)	174 (90%)	18 (9%)	2 (1%)	22	70
8	AD	194/196 (99%)	172 (89%)	19 (10%)	3 (2%)	15	58
8	BH	194/196 (99%)	175 (90%)	17 (9%)	2 (1%)	22	70
8	BV	194/196 (99%)	177 (91%)	15 (8%)	2 (1%)	22	70
9	AM	220/222 (99%)	202 (92%)	16 (7%)	2 (1%)	25	73
9	AY	220/222 (99%)	201 (91%)	17 (8%)	2 (1%)	25	73
9	BI	220/222 (99%)	203 (92%)	15 (7%)	2 (1%)	25	73
9	BW	220/222 (99%)	201 (91%)	17 (8%)	2 (1%)	25	73
10	AN	202/204 (99%)	182 (90%)	16 (8%)	4 (2%)	11	48
10	AZ	202/204 (99%)	184 (91%)	16 (8%)	2 (1%)	22	70
10	BJ	202/204 (99%)	187 (93%)	13 (6%)	2 (1%)	22	70
10	BX	202/204 (99%)	184 (91%)	17 (8%)	1 (0%)	38	84
11	A1	196/198 (99%)	175 (89%)	14 (7%)	7 (4%)	5	29
11	AO	196/198 (99%)	176 (90%)	14 (7%)	6 (3%)	7	34
11	BK	196/198 (99%)	175 (89%)	15 (8%)	6 (3%)	7	34
11	BY	196/198 (99%)	175 (89%)	14 (7%)	7 (4%)	5	29
12	A2	210/212 (99%)	190 (90%)	19 (9%)	1 (0%)	38	84
12	AP	210/212 (99%)	191 (91%)	19 (9%)	0	100	100
12	BL	210/212 (99%)	191 (91%)	18 (9%)	1 (0%)	38	84
12	BZ	210/212 (99%)	189 (90%)	21 (10%)	0	100	100
13	A3	220/222 (99%)	203 (92%)	13 (6%)	4 (2%)	13	53
13	AQ	220/222 (99%)	200 (91%)	16 (7%)	4 (2%)	13	53
13	B1	220/222 (99%)	202 (92%)	14 (6%)	4 (2%)	13	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	BM	220/222 (99%)	201 (91%)	17 (8%)	2 (1%)	25	73
14	A4	231/233 (99%)	211 (91%)	16 (7%)	4 (2%)	14	54
14	AR	231/233 (99%)	212 (92%)	16 (7%)	3 (1%)	18	62
14	B2	231/233 (99%)	212 (92%)	16 (7%)	3 (1%)	18	62
14	BN	231/233 (99%)	213 (92%)	15 (6%)	3 (1%)	18	62
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%)	3	18
16	A7	797/799 (100%)	640 (80%)	111 (14%)	46 (6%)	3	15
16	B4	797/799 (100%)	651 (82%)	107 (13%)	39 (5%)	3	20
16	B7	797/799 (100%)	639 (80%)	116 (15%)	42 (5%)	3	18
17	A6	995/997 (100%)	782 (79%)	128 (13%)	85 (8%)	1	6
17	A8	995/997 (100%)	775 (78%)	133 (13%)	87 (9%)	1	5
17	B5	995/997 (100%)	780 (78%)	134 (14%)	81 (8%)	1	7
17	B8	995/997 (100%)	776 (78%)	135 (14%)	84 (8%)	1	6
All	All	19944/20080 (99%)	17074 (86%)	2065 (10%)	805 (4%)	5	25

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%)	12	42
1	AC	207/207 (100%)	184 (89%)	23 (11%)	9	34
1	BA	207/207 (100%)	185 (89%)	22 (11%)	10	36
1	BO	207/207 (100%)	185 (89%)	22 (11%)	10	36
2	AG	192/192 (100%)	175 (91%)	17 (9%)	14	48
2	AS	192/192 (100%)	172 (90%)	20 (10%)	10	37
2	BB	192/192 (100%)	172 (90%)	20 (10%)	10	37
2	BP	192/192 (100%)	172 (90%)	20 (10%)	10	37
3	AH	192/192 (100%)	164 (85%)	28 (15%)	5	21
3	AT	192/192 (100%)	164 (85%)	28 (15%)	5	21
3	BC	192/192 (100%)	164 (85%)	28 (15%)	5	21
3	BQ	192/192 (100%)	164 (85%)	28 (15%)	5	21
4	AI	202/202 (100%)	177 (88%)	25 (12%)	7	28
4	AU	202/202 (100%)	176 (87%)	26 (13%)	6	26
4	BD	202/202 (100%)	177 (88%)	25 (12%)	7	28
4	BR	202/202 (100%)	177 (88%)	25 (12%)	7	28
5	AJ	206/206 (100%)	181 (88%)	25 (12%)	7	29
5	AV	206/206 (100%)	181 (88%)	25 (12%)	7	29
5	BE	206/206 (100%)	178 (86%)	28 (14%)	5	24
5	BS	206/206 (100%)	178 (86%)	28 (14%)	5	24
6	AK	193/193 (100%)	166 (86%)	27 (14%)	5	23
6	AW	193/193 (100%)	166 (86%)	27 (14%)	5	23
6	BF	193/193 (100%)	166 (86%)	27 (14%)	5	23
6	BT	193/193 (100%)	168 (87%)	25 (13%)	6	26
7	AL	201/201 (100%)	176 (88%)	25 (12%)	7	28
7	AX	201/201 (100%)	175 (87%)	26 (13%)	6	26
7	BG	201/201 (100%)	175 (87%)	26 (13%)	6	26
7	BU	201/201 (100%)	175 (87%)	26 (13%)	6	26
8	AB	161/161 (100%)	144 (89%)	17 (11%)	10	36
8	AD	161/161 (100%)	145 (90%)	16 (10%)	11	40
8	BH	161/161 (100%)	144 (89%)	17 (11%)	10	36
8	BV	161/161 (100%)	145 (90%)	16 (10%)	11	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	AM	181/181 (100%)	164 (91%)	17 (9%)	13	44
9	AY	181/181 (100%)	164 (91%)	17 (9%)	13	44
9	BI	181/181 (100%)	165 (91%)	16 (9%)	14	48
9	BW	181/181 (100%)	164 (91%)	17 (9%)	13	44
10	AN	172/172 (100%)	158 (92%)	14 (8%)	17	53
10	AZ	172/172 (100%)	155 (90%)	17 (10%)	11	40
10	BJ	172/172 (100%)	158 (92%)	14 (8%)	17	53
10	BX	172/172 (100%)	157 (91%)	15 (9%)	15	49
11	A1	175/175 (100%)	160 (91%)	15 (9%)	15	50
11	AO	175/175 (100%)	161 (92%)	14 (8%)	17	53
11	BK	175/175 (100%)	160 (91%)	15 (9%)	15	50
11	BY	175/175 (100%)	161 (92%)	14 (8%)	17	53
12	A2	169/169 (100%)	152 (90%)	17 (10%)	11	39
12	AP	169/169 (100%)	154 (91%)	15 (9%)	14	48
12	BL	169/169 (100%)	154 (91%)	15 (9%)	14	48
12	BZ	169/169 (100%)	154 (91%)	15 (9%)	14	48
13	A3	185/185 (100%)	166 (90%)	19 (10%)	10	38
13	AQ	185/185 (100%)	164 (89%)	21 (11%)	8	33
13	B1	185/185 (100%)	165 (89%)	20 (11%)	9	35
13	BM	185/185 (100%)	164 (89%)	21 (11%)	8	33
14	A4	199/199 (100%)	176 (88%)	23 (12%)	8	31
14	AR	199/199 (100%)	175 (88%)	24 (12%)	7	29
14	B2	199/199 (100%)	176 (88%)	23 (12%)	8	31
14	BN	199/199 (100%)	178 (89%)	21 (11%)	10	36
15	AE	73/73 (100%)	67 (92%)	6 (8%)	17	52
15	AF	73/73 (100%)	66 (90%)	7 (10%)	12	43
15	B3	73/73 (100%)	66 (90%)	7 (10%)	12	43
15	B6	73/73 (100%)	66 (90%)	7 (10%)	12	43
16	A5	744/744 (100%)	653 (88%)	91 (12%)	7	29
16	A7	744/744 (100%)	651 (88%)	93 (12%)	7	28
16	B4	744/744 (100%)	655 (88%)	89 (12%)	7	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	B7	744/744 (100%)	655 (88%)	89 (12%)	7	30
17	A6	909/909 (100%)	774 (85%)	135 (15%)	4	20
17	A8	909/909 (100%)	773 (85%)	136 (15%)	4	20
17	B5	909/909 (100%)	774 (85%)	135 (15%)	4	20
17	B8	909/909 (100%)	771 (85%)	138 (15%)	4	20
All	All	17444/17444 (100%)	15334 (88%)	2110 (12%)	7	29

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 chains 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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	243/243 (100%)	-0.45	1 (0%) 90 41	37, 67, 125, 215	0
1	AC	243/243 (100%)	-0.43	0 100 100	52, 87, 139, 216	0
1	BA	243/243 (100%)	-0.21	1 (0%) 90 41	79, 107, 150, 217	0
1	BO	243/243 (100%)	-0.29	1 (0%) 90 41	75, 101, 145, 217	0
2	AG	231/231 (100%)	-0.48	0 100 100	42, 72, 115, 150	0
2	AS	231/231 (100%)	-0.50	0 100 100	54, 86, 122, 161	0
2	BB	231/231 (100%)	-0.24	0 100 100	84, 109, 139, 166	0
2	BP	231/231 (100%)	-0.42	0 100 100	69, 98, 129, 164	0
3	AH	232/232 (100%)	-0.30	1 (0%) 90 41	56, 113, 176, 219	0
3	AT	232/232 (100%)	-0.21	2 (0%) 81 24	65, 114, 180, 223	0
3	BC	232/232 (100%)	-0.05	0 100 100	88, 132, 182, 227	0
3	BQ	232/232 (100%)	-0.25	0 100 100	81, 123, 180, 227	0
4	AI	227/227 (100%)	-0.21	0 100 100	63, 126, 187, 212	0
4	AU	227/227 (100%)	-0.19	1 (0%) 90 41	70, 127, 188, 224	0
4	BD	227/227 (100%)	-0.05	1 (0%) 90 41	89, 137, 193, 222	0
4	BR	227/227 (100%)	-0.14	3 (1%) 74 19	88, 135, 189, 220	0
5	AJ	250/250 (100%)	-0.30	4 (1%) 68 16	60, 99, 188, 246	0
5	AV	250/250 (100%)	-0.18	8 (3%) 45 9	59, 102, 194, 246	0
5	BE	250/250 (100%)	-0.07	7 (2%) 50 10	80, 117, 192, 245	0
5	BS	250/250 (100%)	-0.16	5 (2%) 62 12	82, 115, 191, 246	0
6	AK	234/234 (100%)	-0.44	0 100 100	51, 79, 119, 232	0
6	AW	234/234 (100%)	-0.45	0 100 100	51, 82, 121, 235	0
6	BF	234/234 (100%)	-0.32	1 (0%) 90 41	77, 104, 133, 235	0
6	BT	234/234 (100%)	-0.32	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%)	-0.44	0 100 100	41, 72, 122, 153	0
7	AX	244/244 (100%)	-0.46	0 100 100	53, 84, 131, 156	0
7	BG	244/244 (100%)	-0.26	0 100 100	78, 105, 142, 165	0
7	BU	244/244 (100%)	-0.27	0 100 100	72, 101, 143, 163	0
8	AB	196/196 (100%)	-0.53	0 100 100	38, 61, 95, 139	0
8	AD	196/196 (100%)	-0.49	0 100 100	41, 66, 101, 147	0
8	BH	196/196 (100%)	-0.34	0 100 100	71, 94, 119, 155	0
8	BV	196/196 (100%)	-0.32	0 100 100	72, 92, 119, 152	0
9	AM	222/222 (100%)	-0.47	0 100 100	41, 62, 100, 198	0
9	AY	222/222 (100%)	-0.48	0 100 100	48, 74, 107, 195	0
9	BI	222/222 (100%)	-0.29	0 100 100	75, 98, 125, 199	0
9	BW	222/222 (100%)	-0.37	0 100 100	73, 93, 119, 197	0
10	AN	204/204 (100%)	-0.46	0 100 100	34, 67, 97, 145	0
10	AZ	204/204 (100%)	-0.50	0 100 100	49, 74, 102, 146	0
10	BJ	204/204 (100%)	-0.36	0 100 100	71, 99, 125, 157	0
10	BX	204/204 (100%)	-0.39	0 100 100	69, 90, 118, 162	0
11	A1	198/198 (100%)	-0.45	1 (0%) 88 36	49, 82, 119, 220	0
11	AO	198/198 (100%)	-0.44	3 (1%) 70 16	49, 80, 118, 223	0
11	BK	198/198 (100%)	-0.30	2 (1%) 79 22	76, 102, 130, 225	0
11	BY	198/198 (100%)	-0.37	2 (1%) 79 22	69, 99, 128, 223	0
12	A2	212/212 (100%)	-0.46	0 100 100	54, 78, 117, 138	0
12	AP	212/212 (100%)	-0.42	0 100 100	56, 82, 118, 139	0
12	BL	212/212 (100%)	-0.28	0 100 100	74, 98, 127, 149	0
12	BZ	212/212 (100%)	-0.38	0 100 100	66, 100, 129, 150	0
13	A3	222/222 (100%)	-0.50	0 100 100	45, 70, 109, 168	0
13	AQ	222/222 (100%)	-0.50	0 100 100	51, 75, 111, 169	0
13	B1	222/222 (100%)	-0.32	0 100 100	71, 100, 127, 170	0
13	BM	222/222 (100%)	-0.41	0 100 100	70, 94, 121, 173	0
14	A4	233/233 (100%)	-0.52	0 100 100	35, 63, 94, 113	0
14	AR	233/233 (100%)	-0.51	0 100 100	43, 65, 96, 115	0
14	B2	233/233 (100%)	-0.33	1 (0%) 90 41	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%)	-0.35	0 100 100	69, 93, 115, 134	0
15	AE	76/76 (100%)	-0.42	0 100 100	71, 103, 142, 147	0
15	AF	76/76 (100%)	-0.44	0 100 100	73, 107, 139, 145	0
15	B3	76/76 (100%)	-0.12	0 100 100	101, 129, 146, 155	0
15	B6	76/76 (100%)	-0.43	0 100 100	78, 118, 144, 151	0
16	A5	799/799 (100%)	-0.39	0 100 100	45, 87, 141, 267	0
16	A7	799/799 (100%)	-0.36	1 (0%) 93 63	54, 95, 144, 267	0
16	B4	799/799 (100%)	-0.19	6 (0%) 83 26	82, 115, 155, 265	0
16	B7	799/799 (100%)	-0.27	5 (0%) 86 32	72, 105, 149, 266	0
17	A6	997/997 (100%)	-0.33	5 (0%) 88 36	55, 107, 166, 261	0
17	A8	997/997 (100%)	-0.31	4 (0%) 90 41	63, 108, 167, 260	0
17	B5	997/997 (100%)	-0.12	7 (0%) 84 28	83, 128, 173, 261	0
17	B8	997/997 (100%)	-0.25	6 (0%) 86 32	77, 114, 170, 261	0
All	All	20080/20080 (100%)	-0.32	79 (0%) 90 41	34, 100, 158, 267	0

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	B8	1753	GLU	10.8
17	B8	1752	ARG	8.8
5	AV	5125	GLU	8.0
17	A6	1753	GLU	6.6
5	AJ	5127	ALA	6.3

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.