



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 14, 2017 – 10:25 PM EST

PDB ID : 4V7O
Title : Proteasome Activator Complex
Authors : Hill, C.P.; Whitby, F.G.
Deposited on : unknown
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

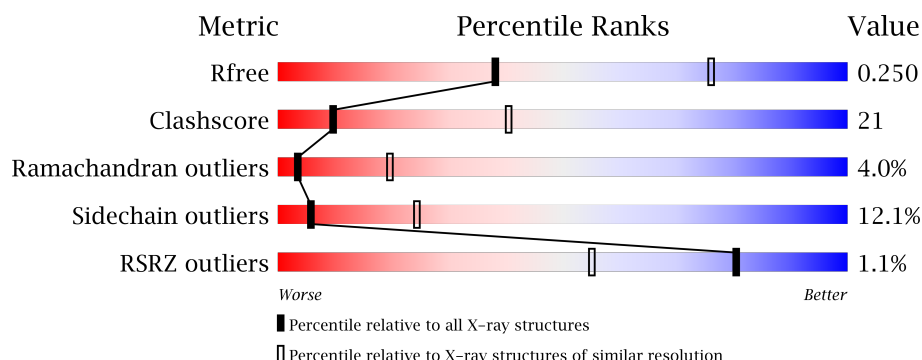
1 Overall quality at a glance

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.






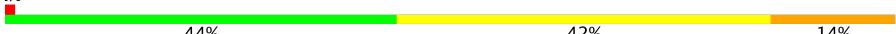

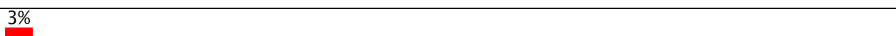
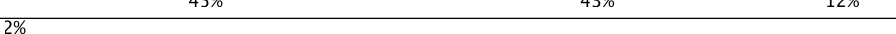

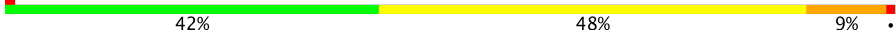


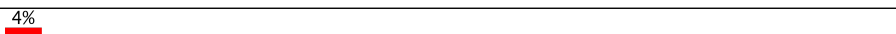
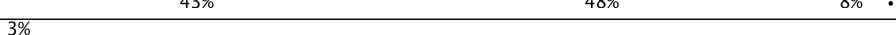












Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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. 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>67%</div> <div>28%</div> <div>5%</div> </div>
1	AC	243	<div> <div>64%</div> <div>30%</div> <div>6%</div> </div>
1	BA	243	<div> <div>2%</div> <div>67%</div> <div>29%</div> <div>.</div> </div>
1	BO	243	<div> <div>.%</div> <div>66%</div> <div>30%</div> <div>.</div> </div>
2	AG	231	<div> <div>70%</div> <div>26%</div> <div>.</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	










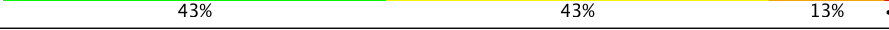



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Mol	Chain	Length	Quality of chain
8	BH	196	
8	BV	196	
9	AM	222	
9	AY	222	
9	BI	222	
9	BW	222	
10	AN	204	
10	AZ	204	
10	BJ	204	
10	BX	204	
11	A1	198	
11	AO	198	
11	BK	198	
11	BY	198	
12	A2	212	
12	AP	212	
12	BL	212	
12	BZ	212	
13	A3	222	
13	AQ	222	
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%•
15	B3	76	 63%33%•
15	B6	76	 63%32%5%
16	A5	799	 52%38%9%•
16	A7	799	 51%39%10%•
16	B4	799	 53%38%9%•
16	B7	799	 51%39%10%•
17	A6	997	 43%43%13%•
17	A8	997	 44%42%13%•
17	B5	997	 44%42%12%•
17	B8	997	 44%42%13%•

2 Entry composition

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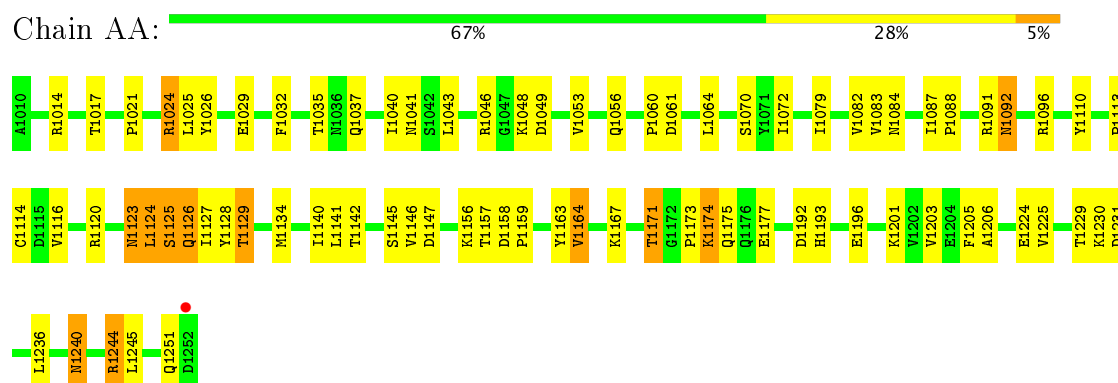
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Chain	Residue	Modelled	Actual	Comment	Reference
B8	1171	ASN	GLN	CONFLICT	UNP P43583
B8	2085	ASN	GLN	CONFLICT	UNP P43583
B8	2101	ASN	GLN	CONFLICT	UNP P43583

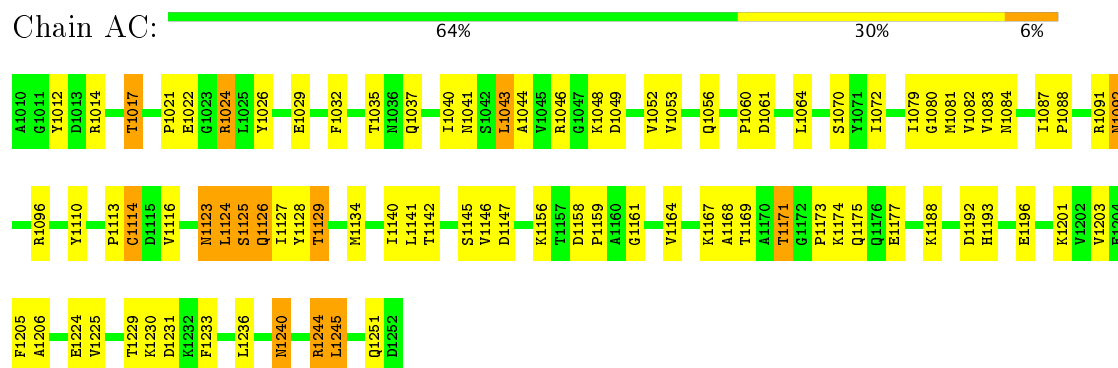
3 Residue-property plots

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

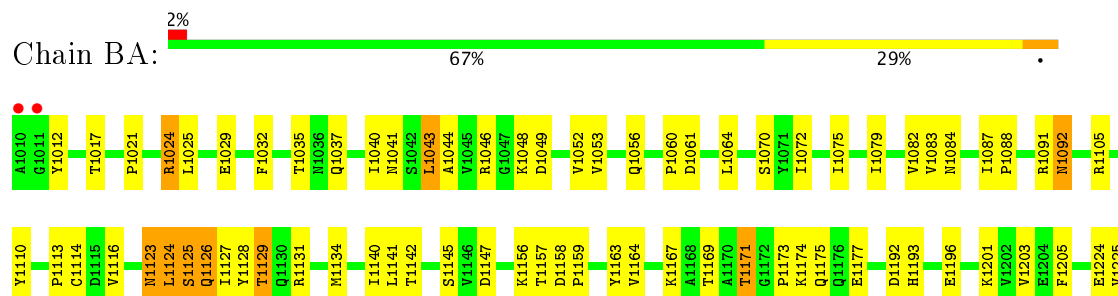
• Molecule 1: Proteasome component C7-alpha



• Molecule 1: Proteasome component C7-alpha



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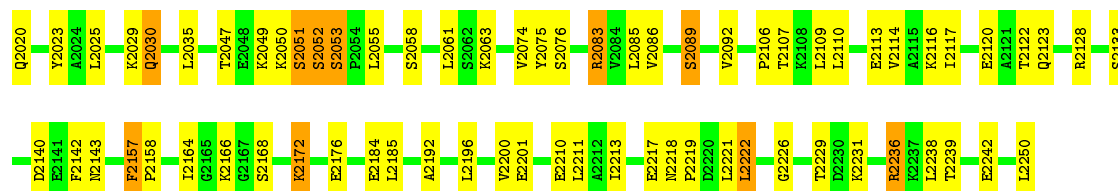




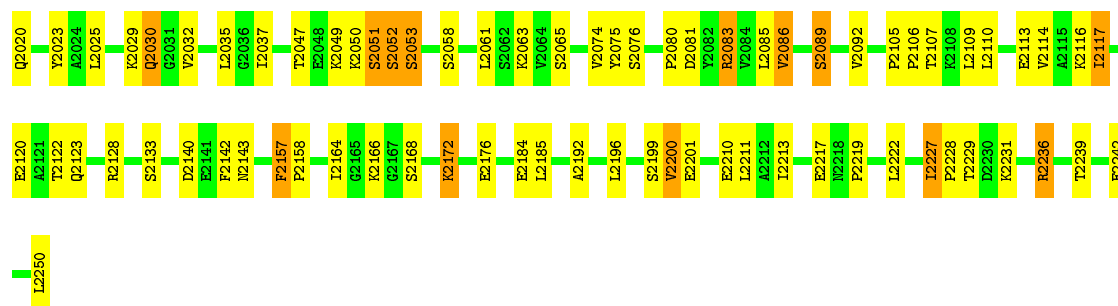
- Molecule 1: Proteasome component C7-alpha



- Molecule 2: Proteasome component Y7

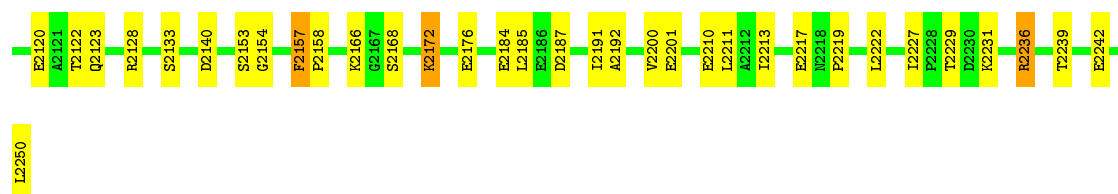


- Molecule 2: Proteasome component Y7



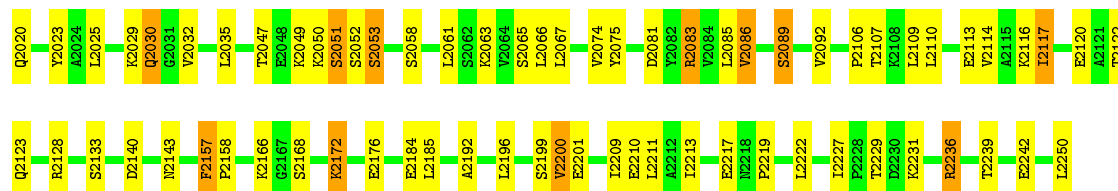
- Molecule 2: Proteasome component Y7





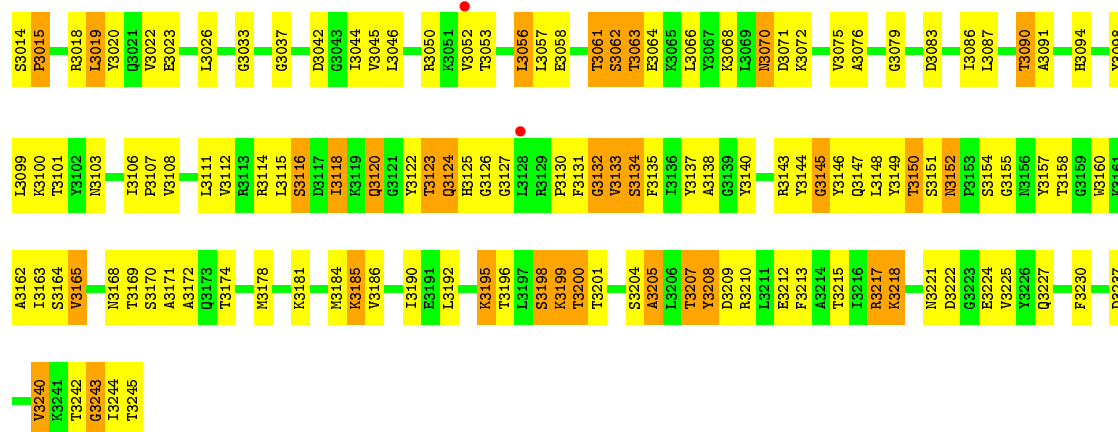
- Molecule 2: Proteasome component Y7

Chain BP: 70% 25% 5%



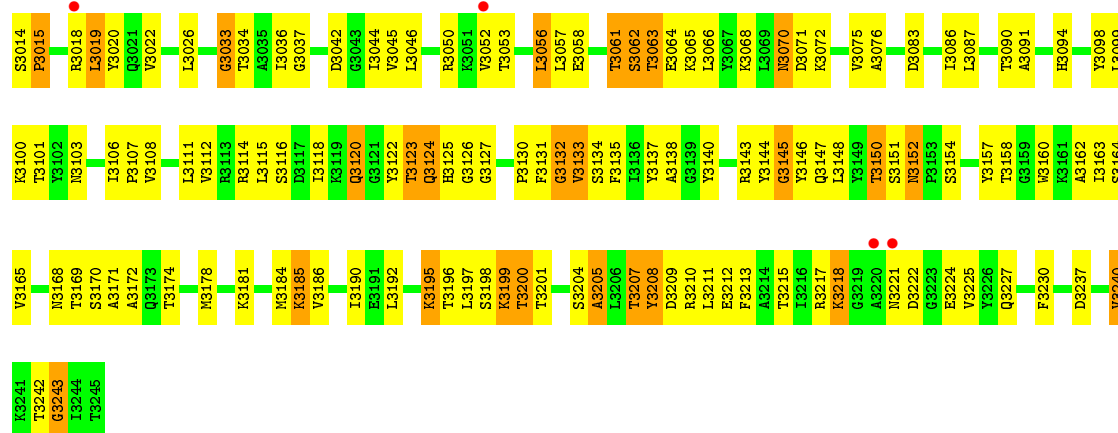
- Molecule 3: Proteasome component Y13

Chain AH: 44% 42% 14%



- Molecule 3: Proteasome component Y13

Chain AT: 45% 44% 11%



Chain BC:

Category	Percentage	Items
Red	3%	S3014, P3015, E3016, G3017, R3018, Y3019, Y3020, Q3021, V3022, L3026, G3033, T3034, A3035, I3036, G3037, D3042, G3043, T3044, V3045, L3046, E3049, R3050, K3051, V3052, T3053, L3056, L3057, E3058, T3061, S3062, T3063, E3064, K3065, L3066, Y3067, K3068, L3069, N3070, D3071, K3072, V3075, A3076, G3079, D3083, T3086, L3087, T3090, A3091
Green	45%	H3094, Y3098, L3099, K3100, N3103, L3106, P3107, L3111, V3112, R3113, K3114, L3115, S3116, D3117, L3118, K3119, G3120, G3121, Y3122, T3123, G3124, H3125, G3126, G3127, L3128, R3129, P3130, F3131, G3132, V3133, S3134, F3135, L3136, T3137, A3138, G3139, Y3140, R3143, Y3144, G3145, Y3146, Q3147, L3148, F3149, T3150, S3151, N3152, P3153, S3154, G3155, N3156, Y3157, G3159, H3160
Yellow	43%	K3161, A3162, I3163, S3164, V3165, N3168, T3169, S3170, A3171, A3172, G3173, T3174, N3178, K3181, M3184, K3185, V3186, L3190, S3191, L3192, K3195, T3196, L3197, S3198, P3199, T3200, T3201, S3204, A3205, L3206, T3207, T3208, D3209, R3210, L3211, E3212, F3213, A3214, T3215, L3216, R3217, K3218, N3221, D3222, G3223, E3224, V3225, L3226, Q3227, F3230
Orange	12%	T3237, V3240, K3241, T3242, G3243, L3244, T3245

Chain BQ:

45% 43% 12%

2%

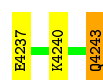
S3014 P3015 R3018 L3019 Y3020 Q3021 V3022 L3026 G3033 T3034 A3035 I3036 G3037 D3042 G3043 I3044 V3045 L3046 E3049 R3050 K3051 V3052 T3053 L3056 L3057 E3058 T3061 S3062 T3063 E3064 K3065 L3066 Y3067 K3068 L3069 N3070 D3071 K3072 V3075 A3076 D3083 I3086 L3087 T3090 A3091 E3094 Y3098

L3099 K3100 M3103 I3106 P3107 L3111 V3112 R3113 R3114 L3115 S3116 D3117 L3118 K3119 Q3120 G3121 Y3122 T3123 Q3124 R3125 K3126 S3127 L3128 R3129 P3130 F3131 G3132 V3133 S3134 F3135 I3136 Y3137 A3138 G3139 Y3140 R3143 Y3144 G3145 Y3146 Q3147 L3148 Y3149 T3150 S3151 N3152 P3153 S3154 G3155 N3156 Y3157 T3158 G3159 K3161 A3162 T3162

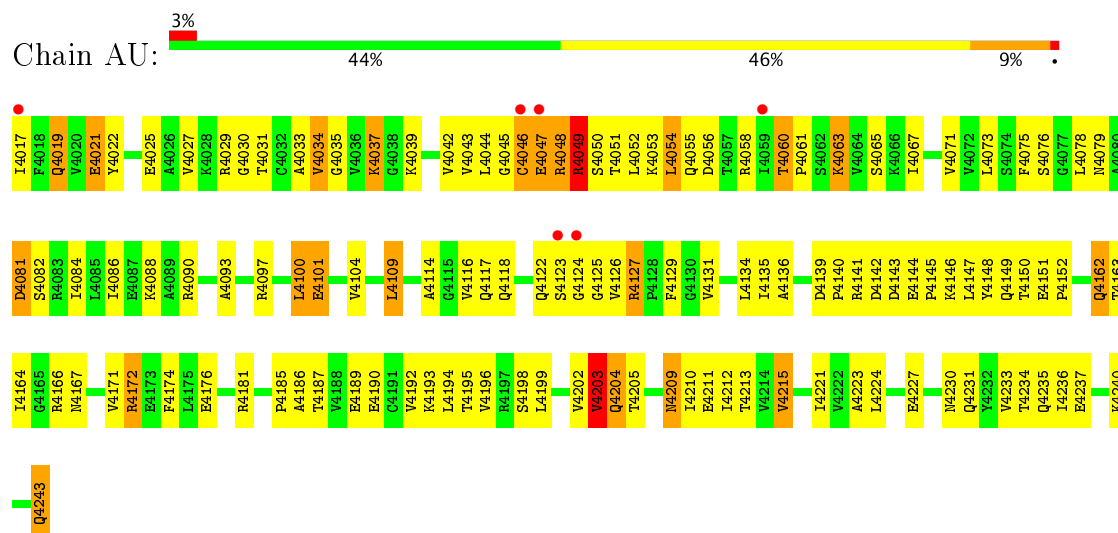
S3164 V3165 T3169 S3170 A3171 A3172 Q3173 T3174 M3178 K3181 M3184 K3185 V3186 I3190 E3191 L3192 K3195 T3196 L3197 S3198 K3199 T3200 T3201 S3204 A3205 L3206 T3207 V3208 D3209 R3210 E3212 F3213 A3214 T3215 L3216 R3217 K3218 G3219 A3220 N3221 D3222 G3223 E3224 V3225 Y3226 Q3227 F3230 D3237 V3240

Chain AI:

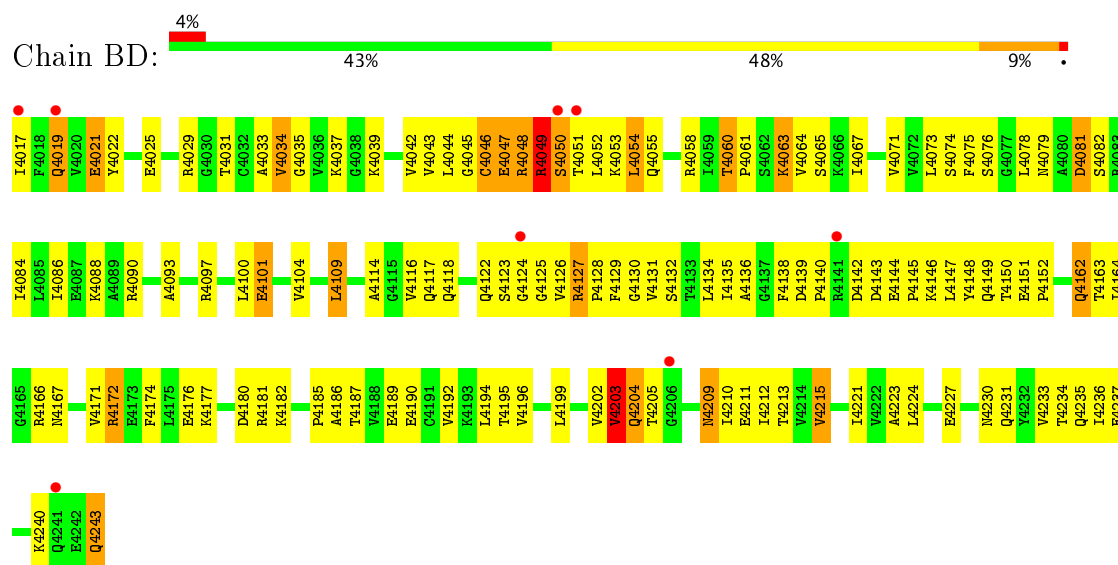
Chain Length	Percentage (%)
T4017	42%
F4018	
Q4019	
V4020	
E4021	
Y4022	
E4025	
V4026	
V4027	
K4028	
R4029	48%
G4030	
T4031	
C4032	
A4033	
Y4034	
G4035	
V4036	
K4037	
G4038	
K4039	9%
V4040	
V4041	
V4042	
V4043	
G4044	
G4045	
C4046	
E4047	
R4048	
R4049	
T4050	
L4051	
L4052	
K4053	
L4054	
Q4055	
D4056	
T4057	
R4058	
L4059	
T4060	
S4061	
S4062	
K4063	
V4064	
S4065	
K4066	
L4067	
V4071	
V4072	
L4073	
S4074	
F4075	
S4076	
G4077	
L4078	
N4079	
S4080	



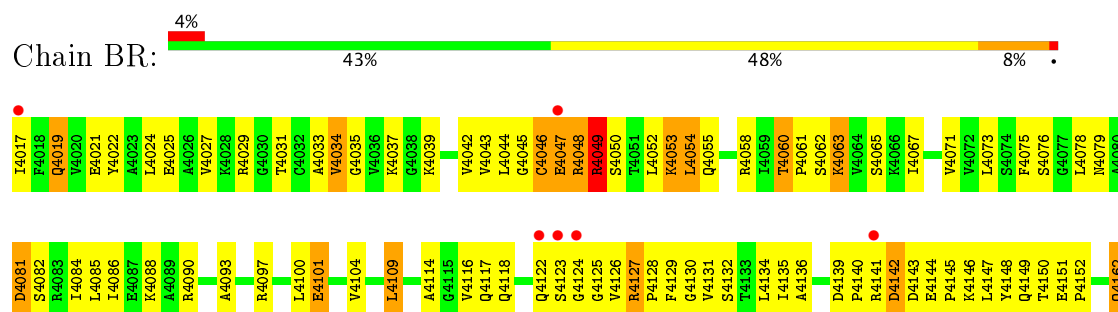
• Molecule 4: Proteasome component PRE6

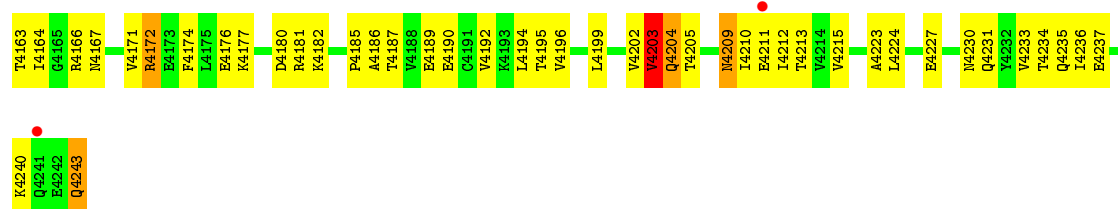


• Molecule 4: Proteasome component PRE6

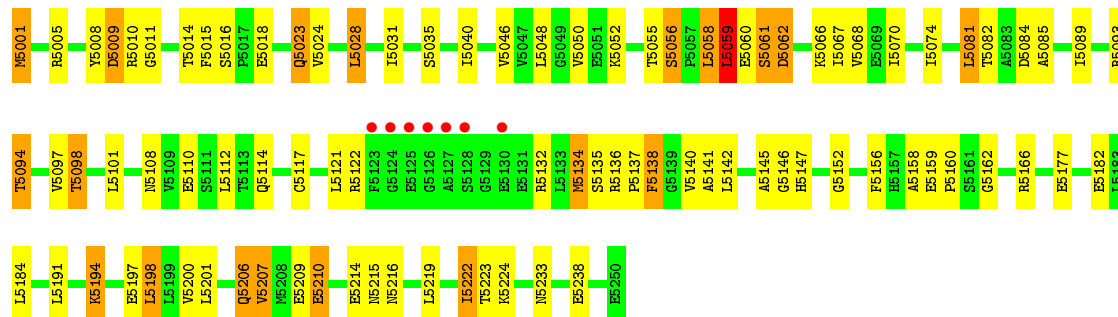


• Molecule 4: Proteasome component PRE6

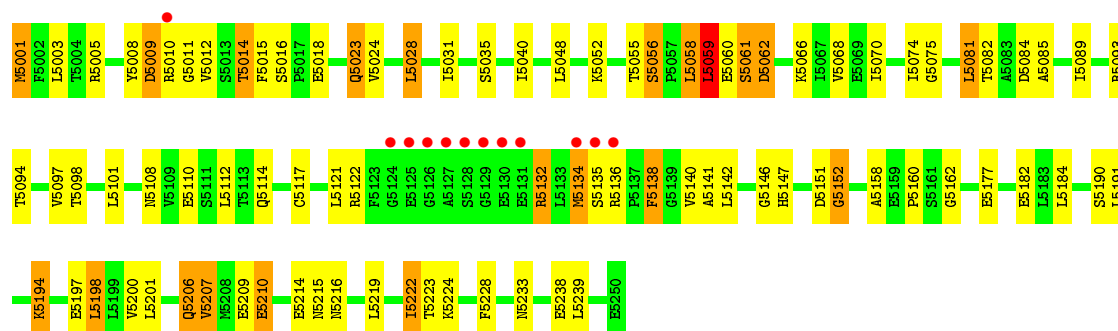




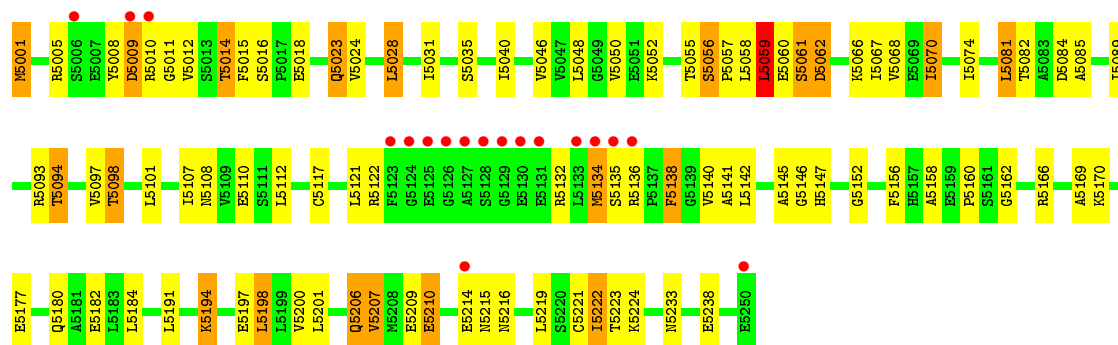
• Molecule 5: Proteasome component PUP2



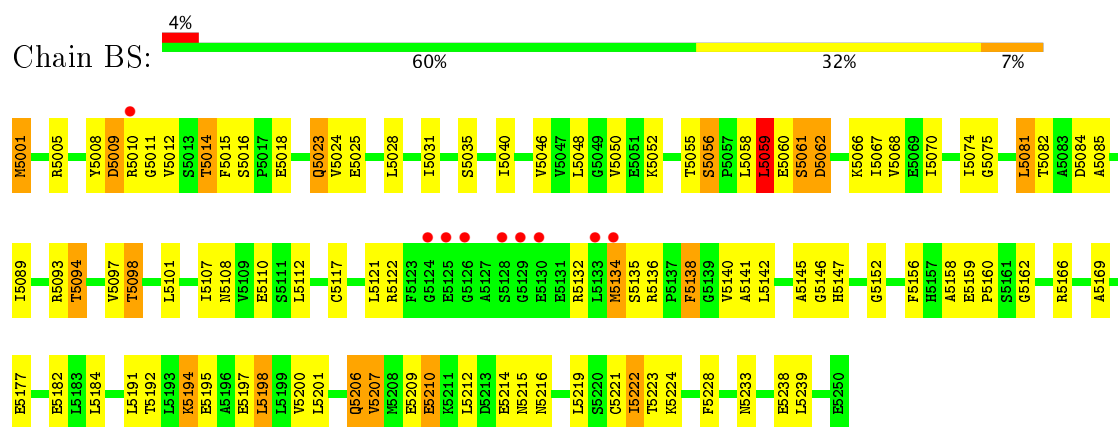
• Molecule 5: Proteasome component PUP2



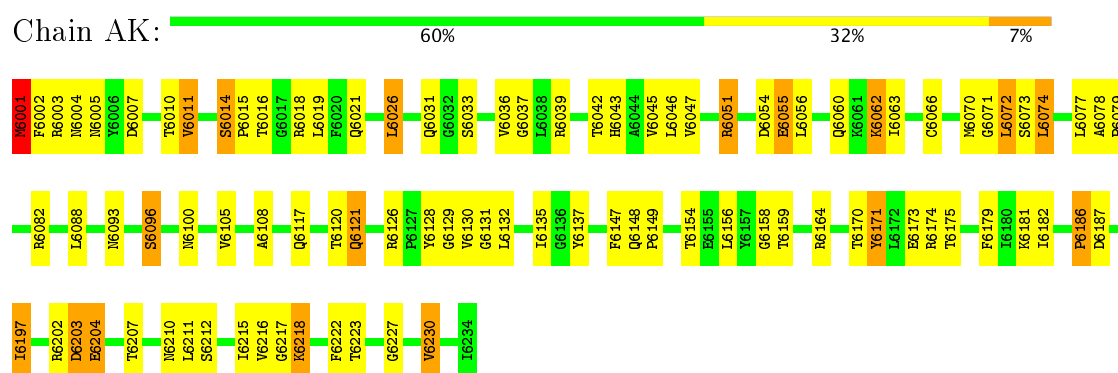
• Molecule 5: Proteasome component PUP2



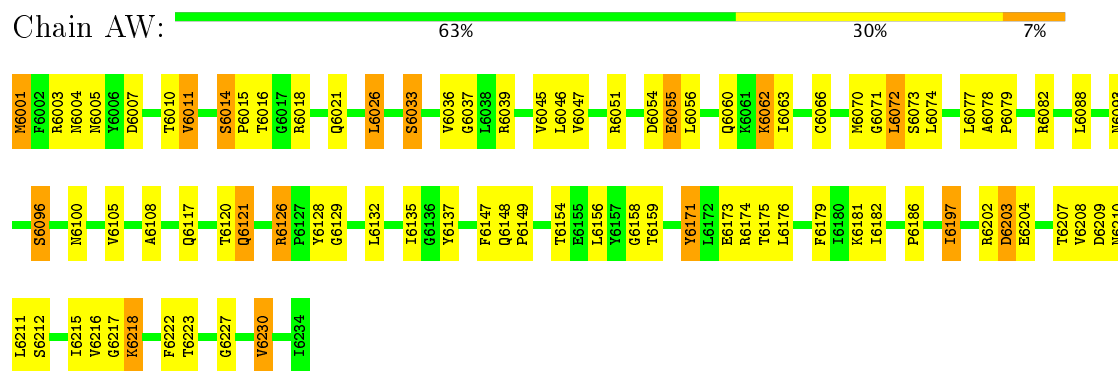
• Molecule 5: Proteasome component PUP2



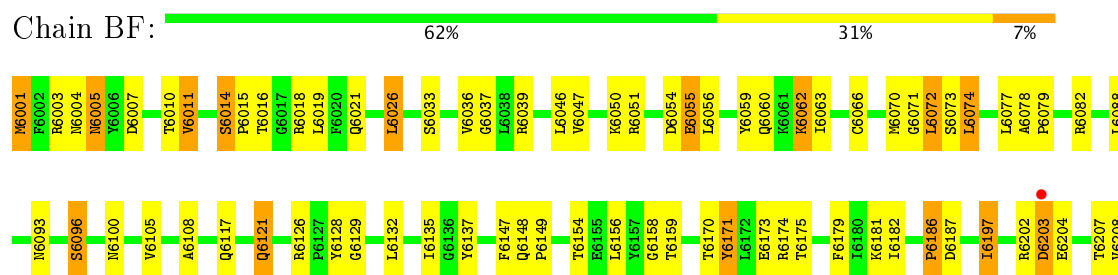
• Molecule 6: Proteasome component PRE5

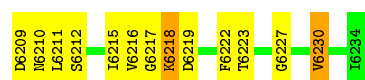


• Molecule 6: Proteasome component PRE5



• Molecule 6: Proteasome component PRE5





• Molecule 6: Proteasome component PRE5

Chain BT: 60% 33% 7%



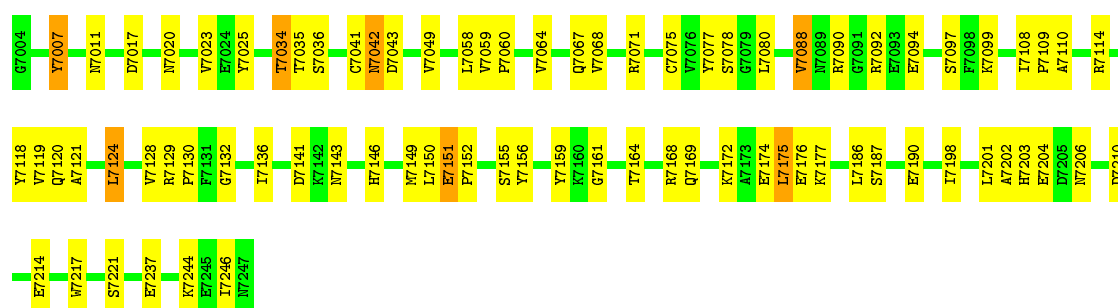
• Molecule 7: Proteasome component C1

Chain AL: 70% 28% .



• Molecule 7: Proteasome component C1

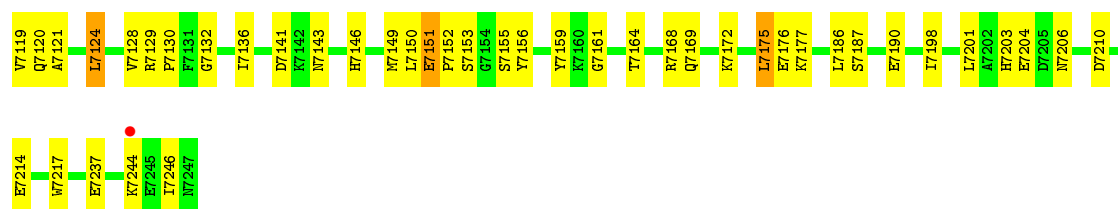
Chain AX: 68% 30% .



• Molecule 7: Proteasome component C1

Chain BG: 69% 28% .





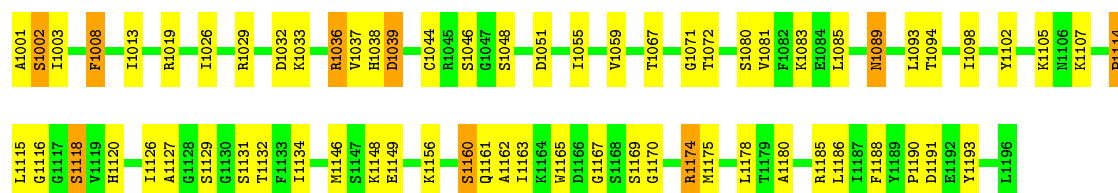
• Molecule 7: Proteasome component C1

Chain BU: 67% 31%



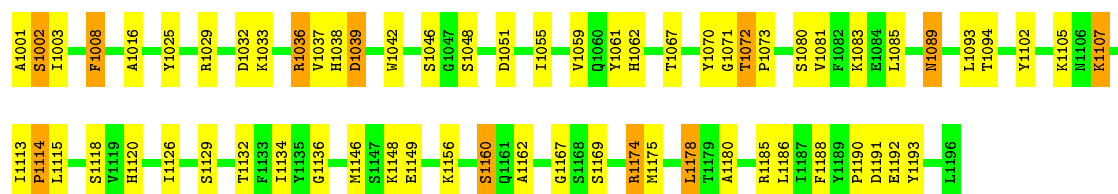
• Molecule 8: Proteasome component PRE3

Chain AB: 66% 30% 5%



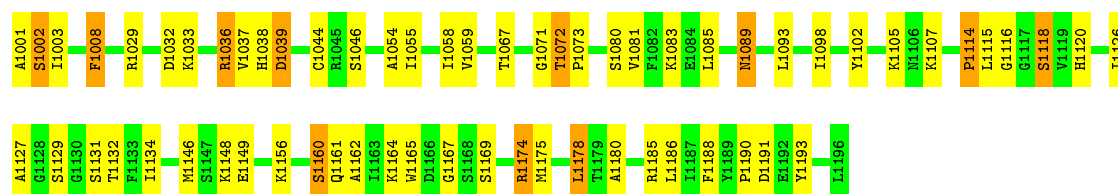
• Molecule 8: Proteasome component PRE3

Chain AD: 67% 28% 6%

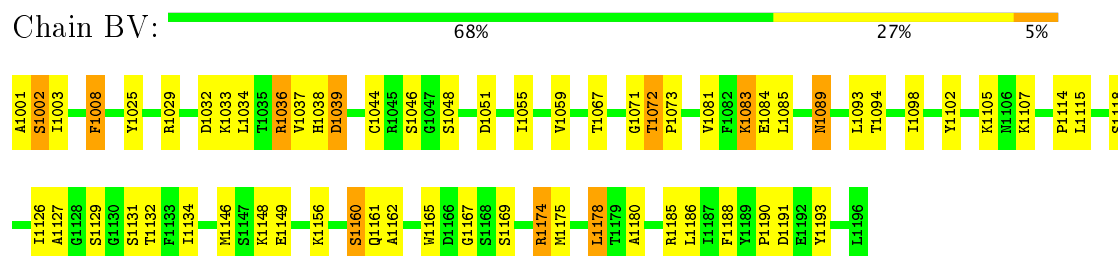


• Molecule 8: Proteasome component PRE3

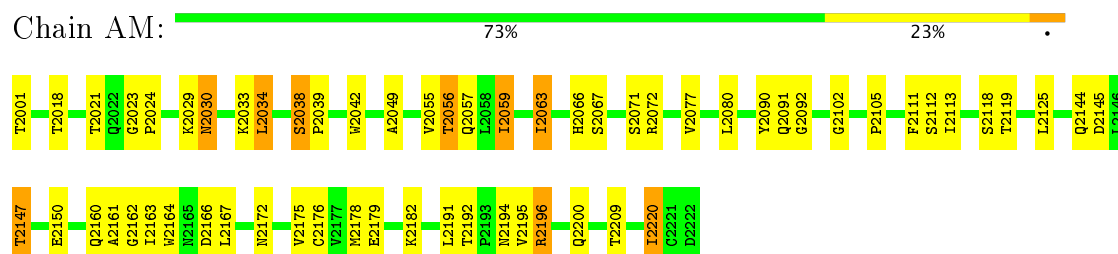
Chain BH: 68% 27% 6%



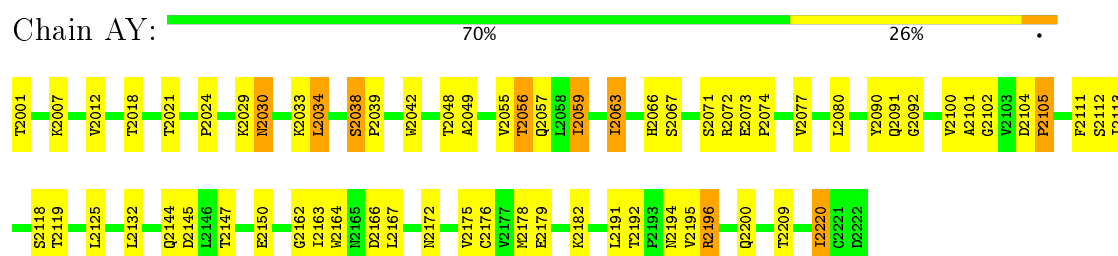
- Molecule 8: Proteasome component PRE3



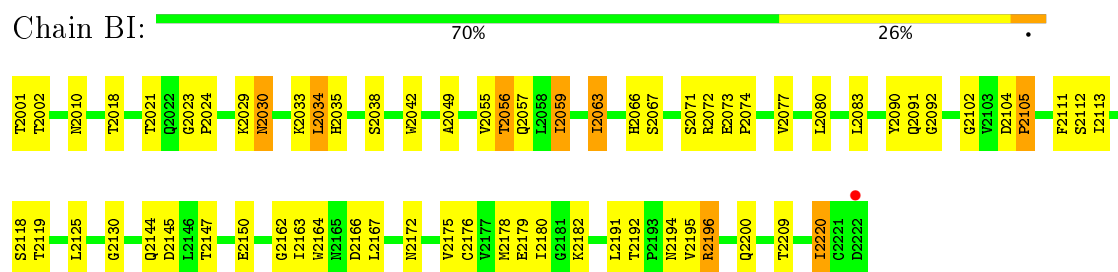
- Molecule 9: Proteasome component PUP1



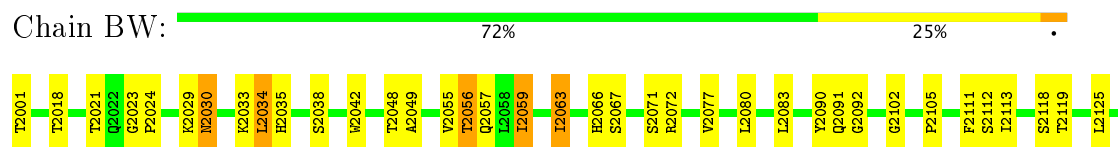
- Molecule 9: Proteasome component PUP1



- Molecule 9: Proteasome component PUP1



- Molecule 9: Proteasome component PUP1

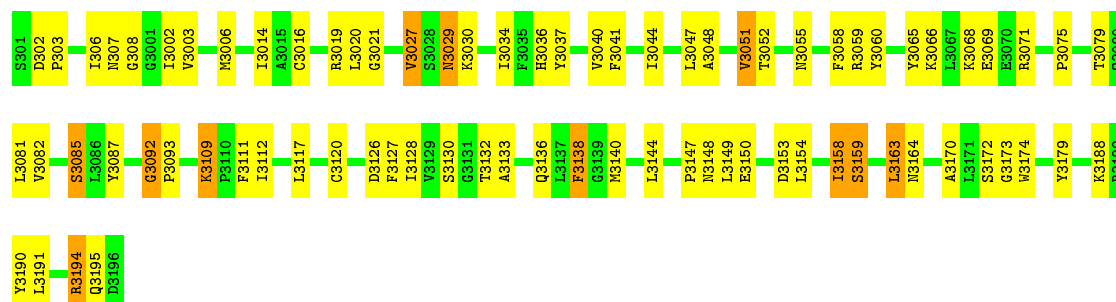




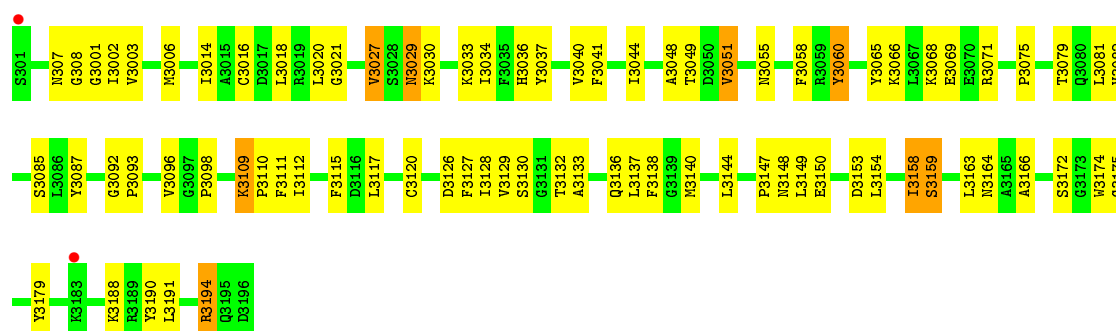
- Molecule 10: Proteasome component PUP3



- Molecule 10: Proteasome component PUP3

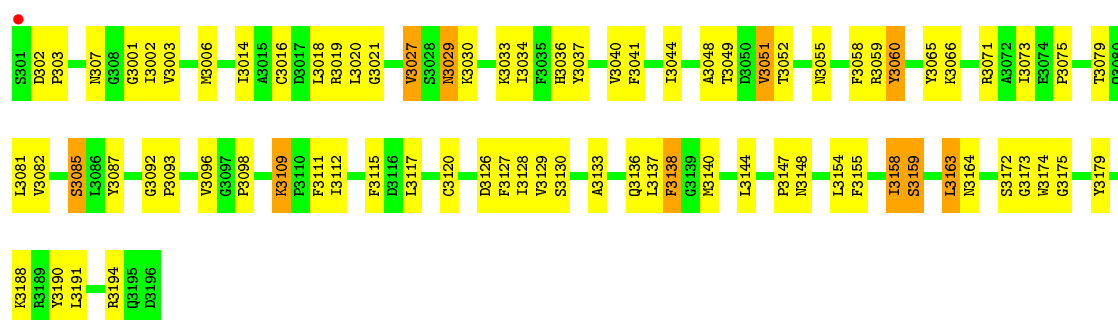


- Molecule 10: Proteasome component PUP3

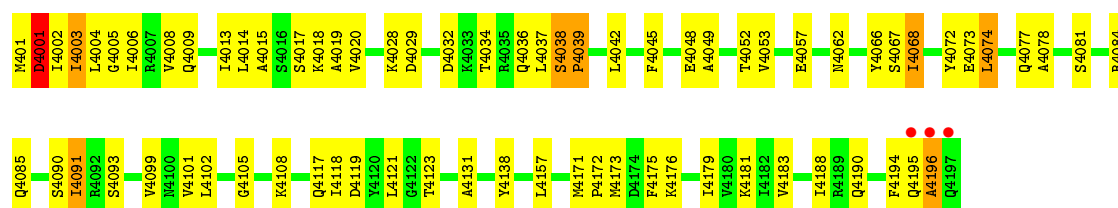


- Molecule 10: Proteasome component PUP3

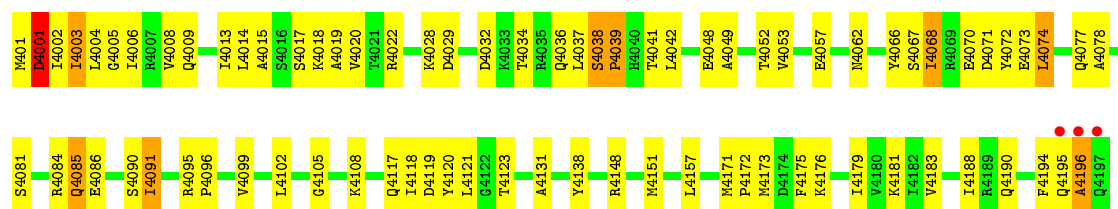




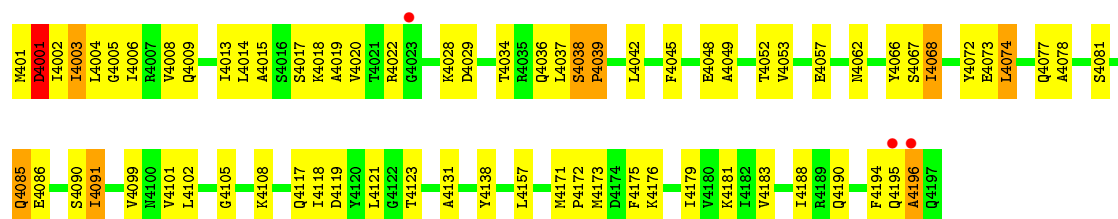
• Molecule 11: Proteasome component C11



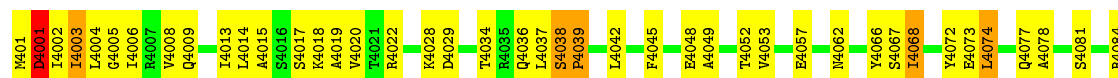
• Molecule 11: Proteasome component C11

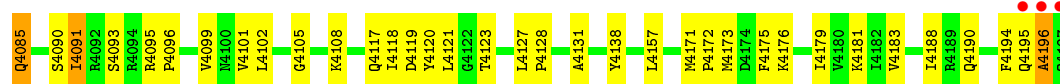


• Molecule 11: Proteasome component C11



• Molecule 11: Proteasome component C11





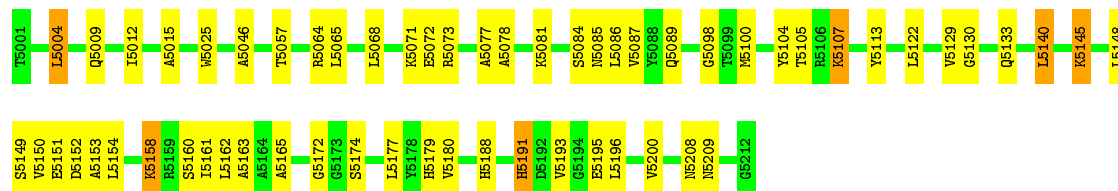
• Molecule 12: Proteasome component PRE2



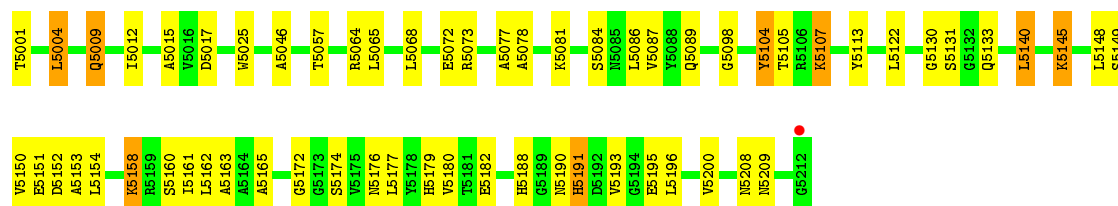
• Molecule 12: Proteasome component PRE2



• Molecule 12: Proteasome component PRE2

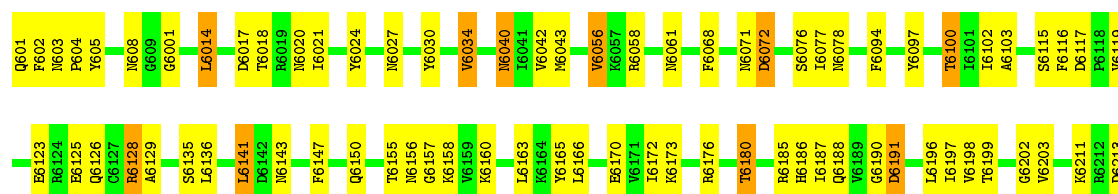


• Molecule 12: Proteasome component PRE2



• Molecule 13: Proteasome component C5





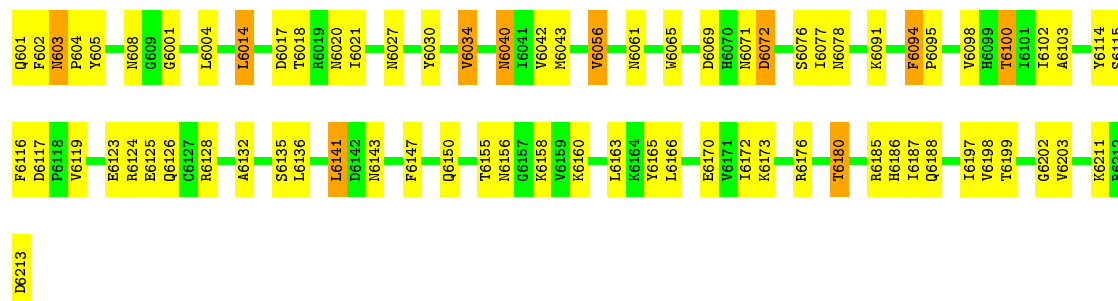
• Molecule 13: Proteasome component C5

Chain A3: 62% 35% .



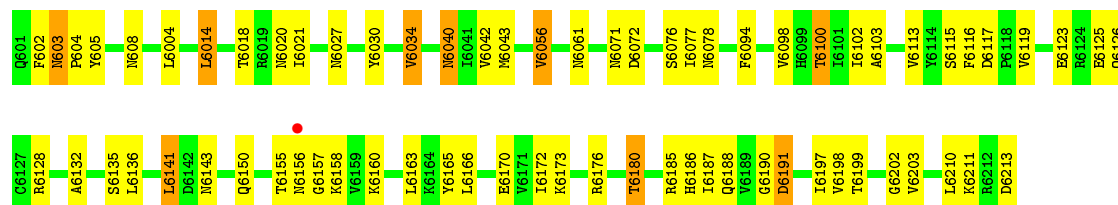
• Molecule 13: Proteasome component C5

Chain BM: 66% 29% 5%



• Molecule 13: Proteasome component C5

Chain B1: 68% 27% .



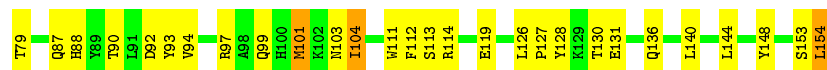
• Molecule 14: Proteasome component PRE4

Chain AR: 62% 31% 6%





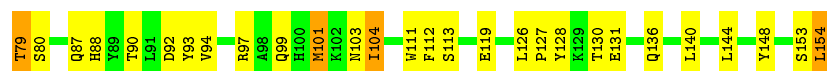
- Molecule 15: Proteasome activator BLM10



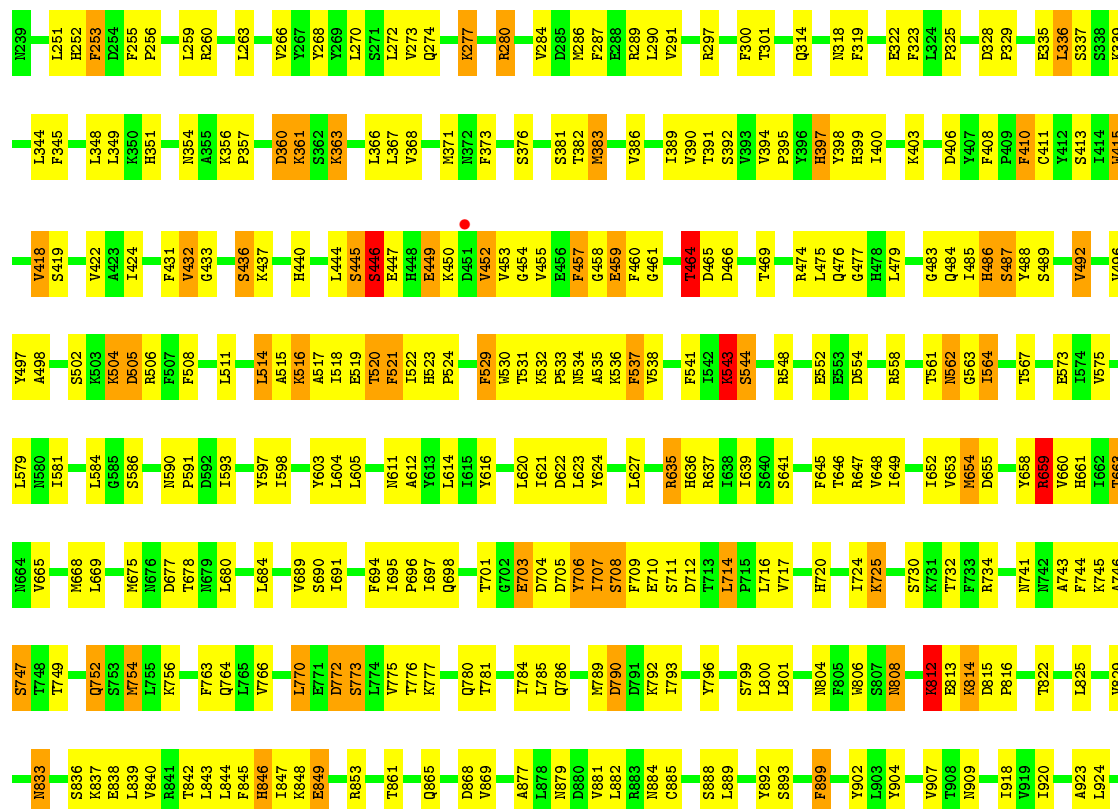
- Molecule 15: Proteasome activator BLM10

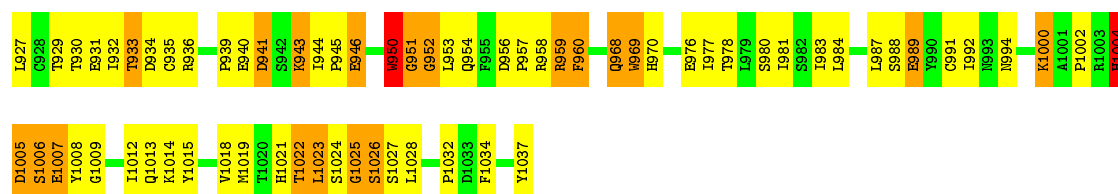


- Molecule 15: Proteasome activator BLM10

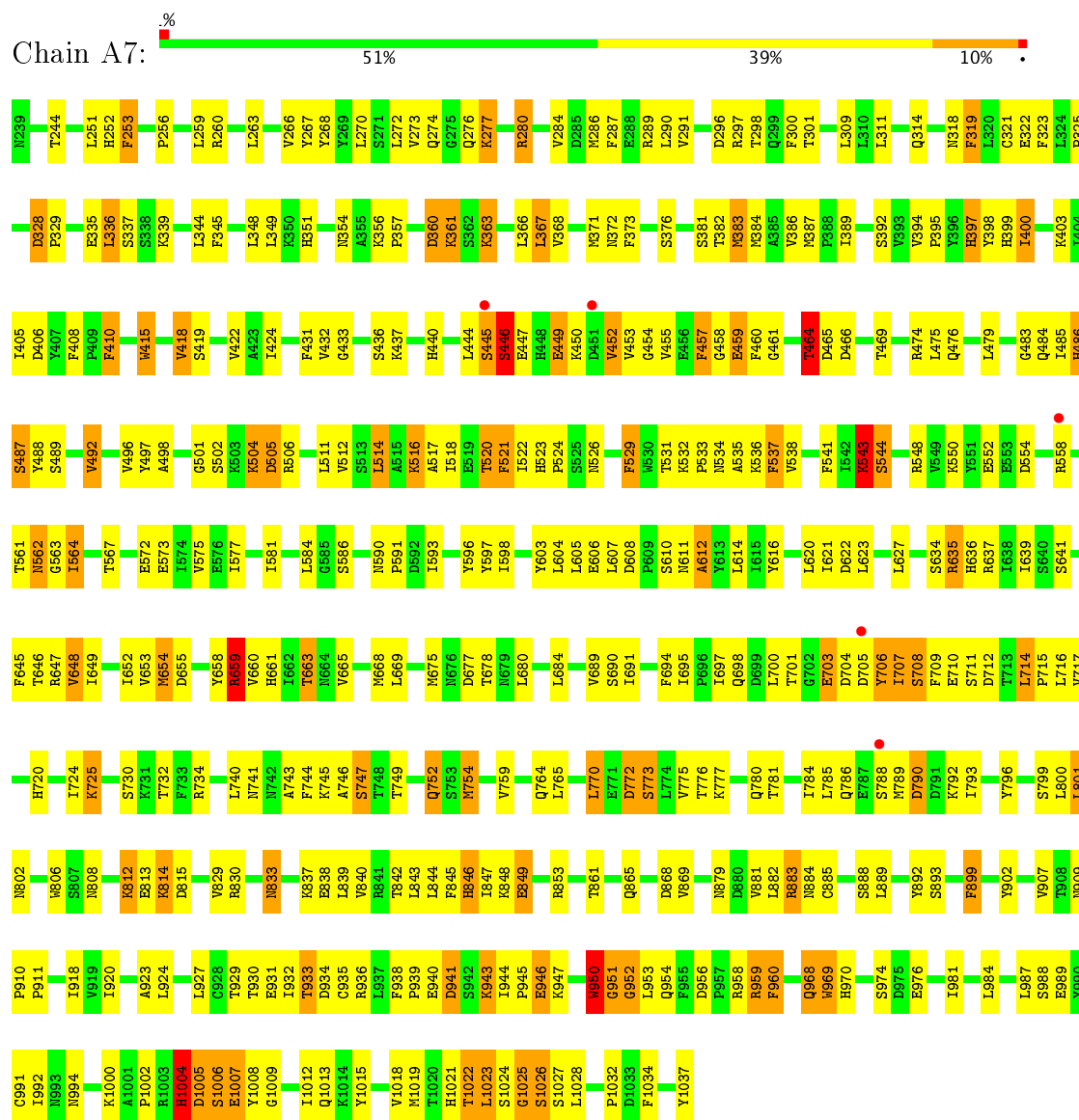


- Molecule 16: Proteasome activator BLM10

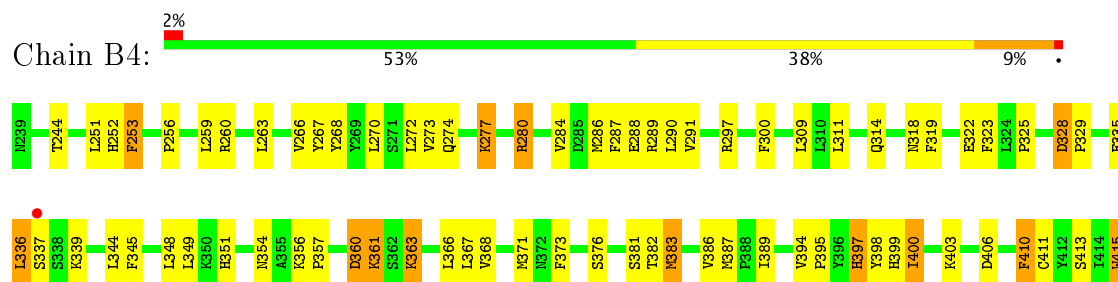




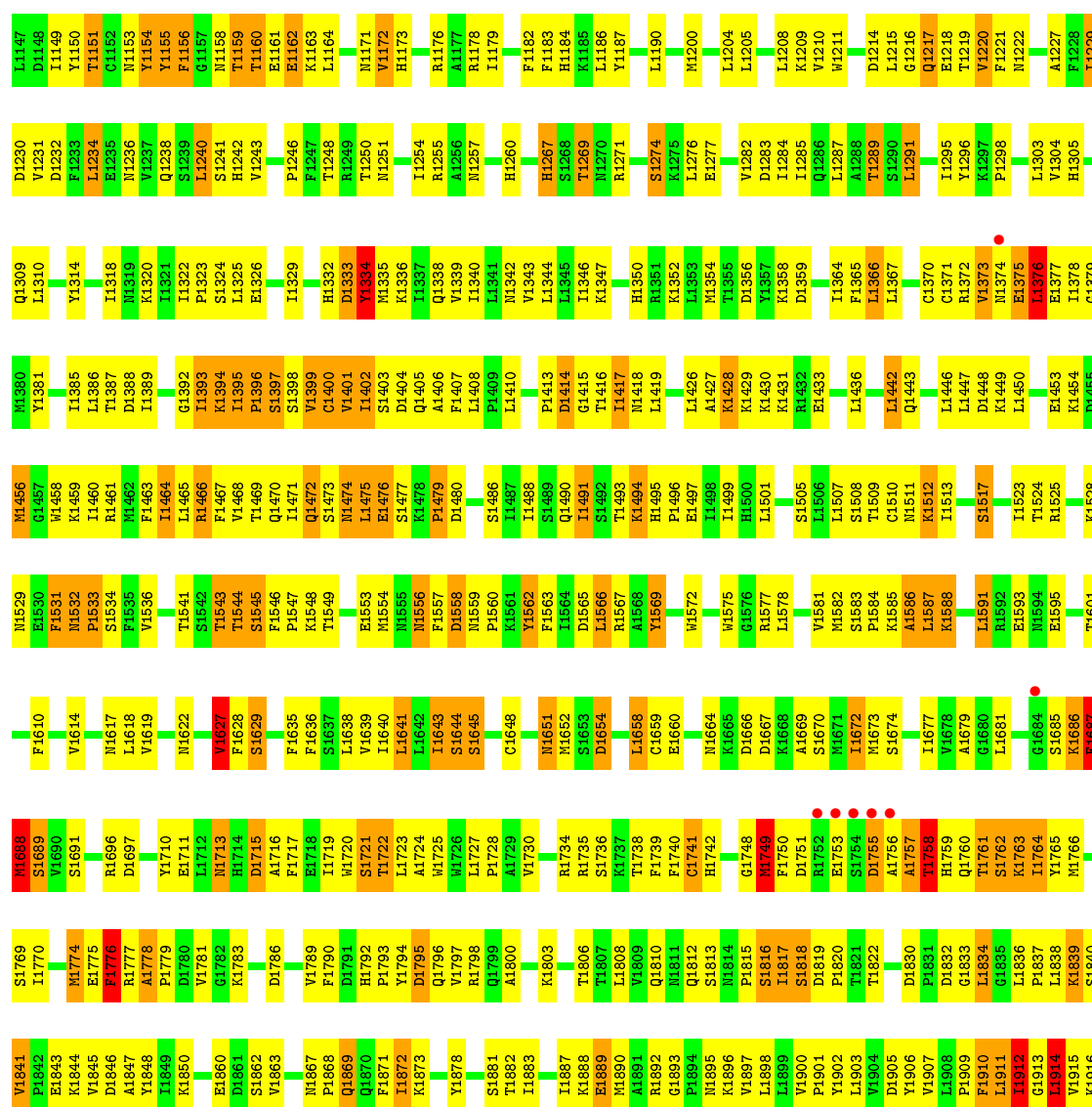
• Molecule 16: Proteasome activator BLM10

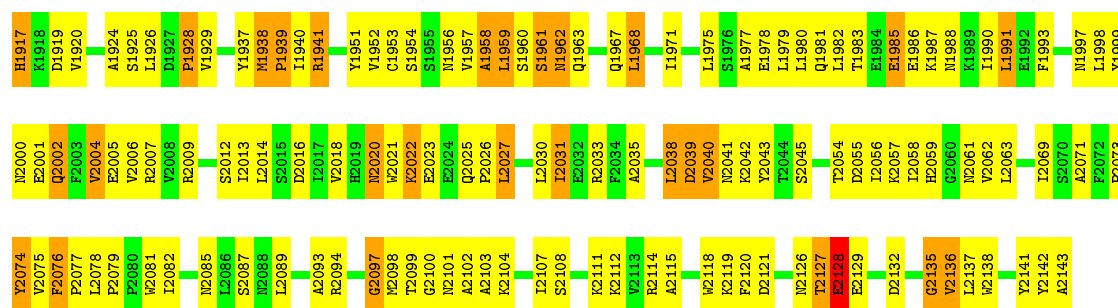


• Molecule 16: Proteasome activator BLM10

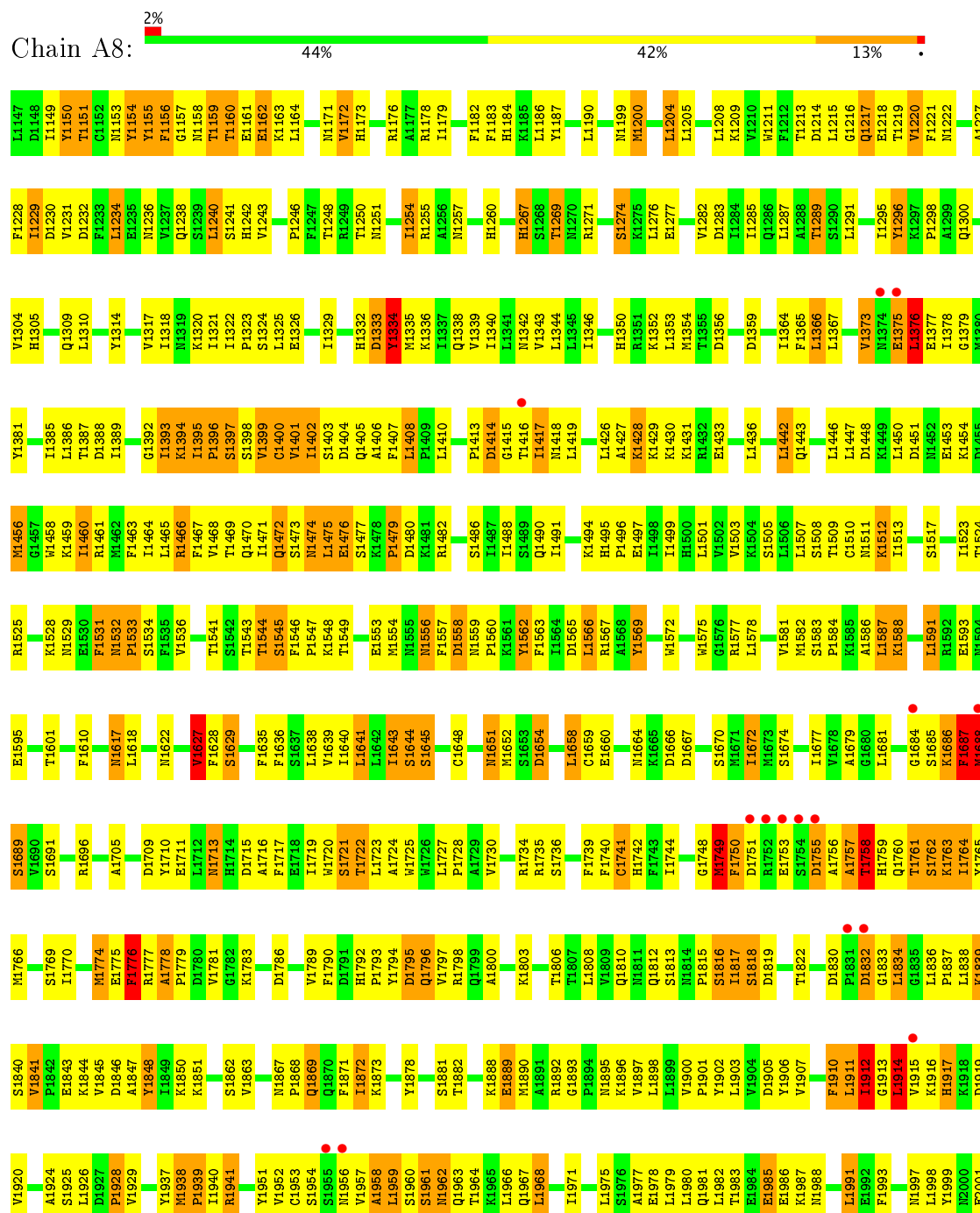


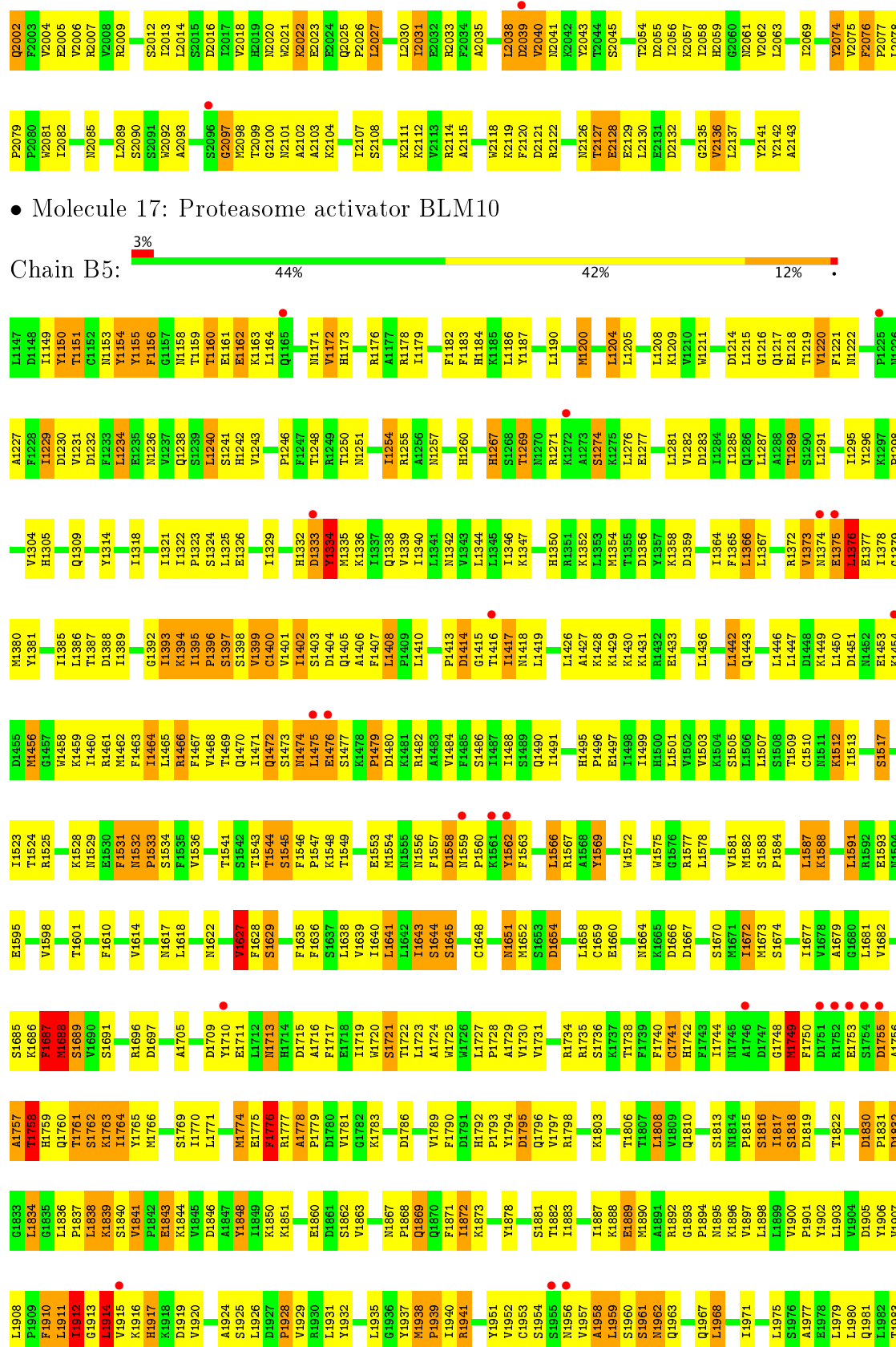






• Molecule 17: Proteasome activator BLM10







● Molecule 17: Proteasome activator BLM10



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	236.12Å 127.74Å 532.67Å 90.00° 102.85° 90.00°	Depositor
Resolution (Å)	29.99 – 3.00 29.99 – 3.01	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	REFMAC, PHENIX (phenix.refine)	Depositor
R, R_{free}	0.196 , 0.250 0.206 , 0.250	Depositor DCC
R_{free} test set	4965 reflections (1.01%)	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 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	158904	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.60	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%)	15	53
1	AC	241/243 (99%)	222 (92%)	16 (7%)	3 (1%)	15	53
1	BA	241/243 (99%)	224 (93%)	14 (6%)	3 (1%)	15	53
1	BO	241/243 (99%)	225 (93%)	13 (5%)	3 (1%)	15	53
2	AG	229/231 (99%)	212 (93%)	13 (6%)	4 (2%)	11	44
2	AS	229/231 (99%)	211 (92%)	15 (7%)	3 (1%)	14	51
2	BB	229/231 (99%)	214 (93%)	13 (6%)	2 (1%)	20	62
2	BP	229/231 (99%)	211 (92%)	16 (7%)	2 (1%)	20	62
3	AH	230/232 (99%)	186 (81%)	25 (11%)	19 (8%)	1	4
3	AT	230/232 (99%)	185 (80%)	27 (12%)	18 (8%)	1	5
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	5
4	AI	225/227 (99%)	167 (74%)	45 (20%)	13 (6%)	2	11
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	11
4	BR	225/227 (99%)	169 (75%)	42 (19%)	14 (6%)	2	10
5	AJ	248/250 (99%)	215 (87%)	21 (8%)	12 (5%)	2	16
5	AV	248/250 (99%)	214 (86%)	22 (9%)	12 (5%)	2	16
5	BE	248/250 (99%)	216 (87%)	20 (8%)	12 (5%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	BS	248/250 (99%)	215 (87%)	21 (8%)	12 (5%)	2	16
6	AK	232/234 (99%)	211 (91%)	17 (7%)	4 (2%)	11	44
6	AW	232/234 (99%)	212 (91%)	16 (7%)	4 (2%)	11	44
6	BF	232/234 (99%)	212 (91%)	16 (7%)	4 (2%)	11	44
6	BT	232/234 (99%)	212 (91%)	17 (7%)	3 (1%)	14	51
7	AL	242/244 (99%)	221 (91%)	20 (8%)	1 (0%)	38	78
7	AX	242/244 (99%)	223 (92%)	17 (7%)	2 (1%)	22	64
7	BG	242/244 (99%)	224 (93%)	17 (7%)	1 (0%)	38	78
7	BU	242/244 (99%)	222 (92%)	18 (7%)	2 (1%)	22	64
8	AB	194/196 (99%)	174 (90%)	18 (9%)	2 (1%)	18	59
8	AD	194/196 (99%)	172 (89%)	19 (10%)	3 (2%)	12	48
8	BH	194/196 (99%)	175 (90%)	17 (9%)	2 (1%)	18	59
8	BV	194/196 (99%)	177 (91%)	15 (8%)	2 (1%)	18	59
9	AM	220/222 (99%)	202 (92%)	16 (7%)	2 (1%)	20	62
9	AY	220/222 (99%)	201 (91%)	17 (8%)	2 (1%)	20	62
9	BI	220/222 (99%)	203 (92%)	15 (7%)	2 (1%)	20	62
9	BW	220/222 (99%)	201 (91%)	17 (8%)	2 (1%)	20	62
10	AN	202/204 (99%)	182 (90%)	16 (8%)	4 (2%)	9	39
10	AZ	202/204 (99%)	184 (91%)	16 (8%)	2 (1%)	18	59
10	BJ	202/204 (99%)	187 (93%)	13 (6%)	2 (1%)	18	59
10	BX	202/204 (99%)	184 (91%)	17 (8%)	1 (0%)	32	74
11	A1	196/198 (99%)	175 (89%)	14 (7%)	7 (4%)	4	22
11	AO	196/198 (99%)	176 (90%)	14 (7%)	6 (3%)	5	26
11	BK	196/198 (99%)	175 (89%)	15 (8%)	6 (3%)	5	26
11	BY	196/198 (99%)	175 (89%)	14 (7%)	7 (4%)	4	22
12	A2	210/212 (99%)	190 (90%)	19 (9%)	1 (0%)	32	74
12	AP	210/212 (99%)	191 (91%)	19 (9%)	0	100	100
12	BL	210/212 (99%)	191 (91%)	18 (9%)	1 (0%)	32	74
12	BZ	210/212 (99%)	189 (90%)	21 (10%)	0	100	100
13	A3	220/222 (99%)	203 (92%)	13 (6%)	4 (2%)	10	43
13	AQ	220/222 (99%)	200 (91%)	16 (7%)	4 (2%)	10	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	B1	220/222 (99%)	202 (92%)	14 (6%)	4 (2%)	10	43
13	BM	220/222 (99%)	201 (91%)	17 (8%)	2 (1%)	20	62
14	A4	231/233 (99%)	211 (91%)	16 (7%)	4 (2%)	11	44
14	AR	231/233 (99%)	212 (92%)	16 (7%)	3 (1%)	14	51
14	B2	231/233 (99%)	212 (92%)	16 (7%)	3 (1%)	14	51
14	BN	231/233 (99%)	213 (92%)	15 (6%)	3 (1%)	14	51
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	13
16	A7	797/799 (100%)	640 (80%)	111 (14%)	46 (6%)	2	11
16	B4	797/799 (100%)	651 (82%)	107 (13%)	39 (5%)	2	15
16	B7	797/799 (100%)	639 (80%)	116 (15%)	42 (5%)	2	13
17	A6	995/997 (100%)	782 (79%)	128 (13%)	85 (8%)	1	4
17	A8	995/997 (100%)	775 (78%)	133 (13%)	87 (9%)	1	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	4
All	All	19944/20080 (99%)	17074 (86%)	2065 (10%)	805 (4%)	3	20

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%)	9	35
1	AC	207/207 (100%)	184 (89%)	23 (11%)	7	28
1	BA	207/207 (100%)	185 (89%)	22 (11%)	8	30
1	BO	207/207 (100%)	185 (89%)	22 (11%)	8	30
2	AG	192/192 (100%)	175 (91%)	17 (9%)	11	40
2	AS	192/192 (100%)	172 (90%)	20 (10%)	8	31
2	BB	192/192 (100%)	172 (90%)	20 (10%)	8	31
2	BP	192/192 (100%)	172 (90%)	20 (10%)	8	31
3	AH	192/192 (100%)	164 (85%)	28 (15%)	3	17
3	AT	192/192 (100%)	164 (85%)	28 (15%)	3	17
3	BC	192/192 (100%)	164 (85%)	28 (15%)	3	17
3	BQ	192/192 (100%)	164 (85%)	28 (15%)	3	17
4	AI	202/202 (100%)	177 (88%)	25 (12%)	5	23
4	AU	202/202 (100%)	176 (87%)	26 (13%)	5	22
4	BD	202/202 (100%)	177 (88%)	25 (12%)	5	23
4	BR	202/202 (100%)	177 (88%)	25 (12%)	5	23
5	AJ	206/206 (100%)	181 (88%)	25 (12%)	6	24
5	AV	206/206 (100%)	181 (88%)	25 (12%)	6	24
5	BE	206/206 (100%)	178 (86%)	28 (14%)	4	19
5	BS	206/206 (100%)	178 (86%)	28 (14%)	4	19
6	AK	193/193 (100%)	166 (86%)	27 (14%)	4	18
6	AW	193/193 (100%)	166 (86%)	27 (14%)	4	18
6	BF	193/193 (100%)	166 (86%)	27 (14%)	4	18
6	BT	193/193 (100%)	168 (87%)	25 (13%)	5	21
7	AL	201/201 (100%)	176 (88%)	25 (12%)	5	23
7	AX	201/201 (100%)	175 (87%)	26 (13%)	5	22
7	BG	201/201 (100%)	175 (87%)	26 (13%)	5	22
7	BU	201/201 (100%)	175 (87%)	26 (13%)	5	22
8	AB	161/161 (100%)	144 (89%)	17 (11%)	8	30
8	AD	161/161 (100%)	145 (90%)	16 (10%)	9	34
8	BH	161/161 (100%)	144 (89%)	17 (11%)	8	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	BV	161/161 (100%)	145 (90%)	16 (10%)	9	34
9	AM	181/181 (100%)	164 (91%)	17 (9%)	10	37
9	AY	181/181 (100%)	164 (91%)	17 (9%)	10	37
9	BI	181/181 (100%)	165 (91%)	16 (9%)	12	41
9	BW	181/181 (100%)	164 (91%)	17 (9%)	10	37
10	AN	172/172 (100%)	158 (92%)	14 (8%)	14	45
10	AZ	172/172 (100%)	155 (90%)	17 (10%)	9	34
10	BJ	172/172 (100%)	158 (92%)	14 (8%)	14	45
10	BX	172/172 (100%)	157 (91%)	15 (9%)	12	41
11	A1	175/175 (100%)	160 (91%)	15 (9%)	12	42
11	AO	175/175 (100%)	161 (92%)	14 (8%)	14	45
11	BK	175/175 (100%)	160 (91%)	15 (9%)	12	42
11	BY	175/175 (100%)	161 (92%)	14 (8%)	14	45
12	A2	169/169 (100%)	152 (90%)	17 (10%)	9	33
12	AP	169/169 (100%)	154 (91%)	15 (9%)	11	40
12	BL	169/169 (100%)	154 (91%)	15 (9%)	11	40
12	BZ	169/169 (100%)	154 (91%)	15 (9%)	11	40
13	A3	185/185 (100%)	166 (90%)	19 (10%)	8	31
13	AQ	185/185 (100%)	164 (89%)	21 (11%)	7	27
13	B1	185/185 (100%)	165 (89%)	20 (11%)	7	29
13	BM	185/185 (100%)	164 (89%)	21 (11%)	7	27
14	A4	199/199 (100%)	176 (88%)	23 (12%)	6	26
14	AR	199/199 (100%)	175 (88%)	24 (12%)	6	24
14	B2	199/199 (100%)	176 (88%)	23 (12%)	6	26
14	BN	199/199 (100%)	178 (89%)	21 (11%)	8	30
15	AE	73/73 (100%)	67 (92%)	6 (8%)	13	44
15	AF	73/73 (100%)	66 (90%)	7 (10%)	10	36
15	B3	73/73 (100%)	66 (90%)	7 (10%)	10	36
15	B6	73/73 (100%)	66 (90%)	7 (10%)	10	36
16	A5	744/744 (100%)	653 (88%)	91 (12%)	6	24
16	A7	744/744 (100%)	651 (88%)	93 (12%)	5	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	B4	744/744 (100%)	655 (88%)	89 (12%)	6	25
16	B7	744/744 (100%)	655 (88%)	89 (12%)	6	25
17	A6	909/909 (100%)	774 (85%)	135 (15%)	3	16
17	A8	909/909 (100%)	773 (85%)	136 (15%)	3	16
17	B5	909/909 (100%)	774 (85%)	135 (15%)	3	16
17	B8	909/909 (100%)	771 (85%)	138 (15%)	3	16
All	All	17444/17444 (100%)	15334 (88%)	2110 (12%)	6	24

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, 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%)	-0.67	1 (0%) 92 77	37, 67, 125, 215	0
1	AC	243/243 (100%)	-0.64	0 100 100	52, 87, 139, 216	0
1	BA	243/243 (100%)	-0.26	4 (1%) 72 44	79, 107, 150, 217	0
1	BO	243/243 (100%)	-0.43	3 (1%) 79 53	75, 101, 145, 217	0
2	AG	231/231 (100%)	-0.72	0 100 100	42, 72, 115, 150	0
2	AS	231/231 (100%)	-0.75	0 100 100	54, 86, 122, 161	0
2	BB	231/231 (100%)	-0.32	2 (0%) 84 61	84, 109, 139, 166	0
2	BP	231/231 (100%)	-0.64	0 100 100	69, 98, 129, 164	0
3	AH	232/232 (100%)	-0.43	2 (0%) 84 61	56, 113, 176, 219	0
3	AT	232/232 (100%)	-0.26	4 (1%) 70 42	65, 114, 180, 223	0
3	BC	232/232 (100%)	-0.02	7 (3%) 51 23	88, 132, 182, 227	0
3	BQ	232/232 (100%)	-0.35	4 (1%) 70 42	81, 123, 180, 227	0
4	AI	227/227 (100%)	-0.33	2 (0%) 84 61	63, 126, 187, 212	0
4	AU	227/227 (100%)	-0.26	6 (2%) 56 27	70, 127, 188, 224	0
4	BD	227/227 (100%)	-0.04	8 (3%) 44 19	89, 137, 193, 222	0
4	BR	227/227 (100%)	-0.14	8 (3%) 44 19	88, 135, 189, 220	0
5	AJ	250/250 (100%)	-0.46	7 (2%) 53 25	60, 99, 188, 246	0
5	AV	250/250 (100%)	-0.22	12 (4%) 31 12	59, 102, 194, 246	0
5	BE	250/250 (100%)	-0.07	18 (7%) 16 6	80, 117, 192, 245	0
5	BS	250/250 (100%)	-0.26	9 (3%) 43 18	82, 115, 191, 246	0
6	AK	234/234 (100%)	-0.68	0 100 100	51, 79, 119, 232	0
6	AW	234/234 (100%)	-0.68	0 100 100	51, 82, 121, 235	0
6	BF	234/234 (100%)	-0.45	1 (0%) 92 77	77, 104, 133, 235	0
6	BT	234/234 (100%)	-0.47	0 100 100	78, 102, 133, 236	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
7	AL	244/244 (100%)	-0.64	0	100	100	41, 72, 122, 153	0
7	AX	244/244 (100%)	-0.70	0	100	100	53, 84, 131, 156	0
7	BG	244/244 (100%)	-0.32	2 (0%)	86	64	78, 105, 142, 165	0
7	BU	244/244 (100%)	-0.41	1 (0%)	92	77	72, 101, 143, 163	0
8	AB	196/196 (100%)	-0.79	0	100	100	38, 61, 95, 139	0
8	AD	196/196 (100%)	-0.73	0	100	100	41, 66, 101, 147	0
8	BH	196/196 (100%)	-0.52	0	100	100	71, 94, 119, 155	0
8	BV	196/196 (100%)	-0.46	0	100	100	72, 92, 119, 152	0
9	AM	222/222 (100%)	-0.73	0	100	100	41, 62, 100, 198	0
9	AY	222/222 (100%)	-0.72	0	100	100	48, 74, 107, 195	0
9	BI	222/222 (100%)	-0.46	1 (0%)	90	74	75, 98, 125, 199	0
9	BW	222/222 (100%)	-0.55	0	100	100	73, 93, 119, 197	0
10	AN	204/204 (100%)	-0.68	0	100	100	34, 67, 97, 145	0
10	AZ	204/204 (100%)	-0.73	0	100	100	49, 74, 102, 146	0
10	BJ	204/204 (100%)	-0.52	2 (0%)	82	58	71, 99, 125, 157	0
10	BX	204/204 (100%)	-0.57	1 (0%)	90	74	69, 90, 118, 162	0
11	A1	198/198 (100%)	-0.68	3 (1%)	74	47	49, 82, 119, 220	0
11	AO	198/198 (100%)	-0.68	3 (1%)	74	47	49, 80, 118, 223	0
11	BK	198/198 (100%)	-0.44	3 (1%)	74	47	76, 102, 130, 225	0
11	BY	198/198 (100%)	-0.52	3 (1%)	74	47	69, 99, 128, 223	0
12	A2	212/212 (100%)	-0.73	0	100	100	54, 78, 117, 138	0
12	AP	212/212 (100%)	-0.65	0	100	100	56, 82, 118, 139	0
12	BL	212/212 (100%)	-0.43	0	100	100	74, 98, 127, 149	0
12	BZ	212/212 (100%)	-0.60	1 (0%)	90	74	66, 100, 129, 150	0
13	A3	222/222 (100%)	-0.76	0	100	100	45, 70, 109, 168	0
13	AQ	222/222 (100%)	-0.75	0	100	100	51, 75, 111, 169	0
13	B1	222/222 (100%)	-0.48	1 (0%)	90	74	71, 100, 127, 170	0
13	BM	222/222 (100%)	-0.64	0	100	100	70, 94, 121, 173	0
14	A4	233/233 (100%)	-0.79	0	100	100	35, 63, 94, 113	0
14	AR	233/233 (100%)	-0.77	0	100	100	43, 65, 96, 115	0
14	B2	233/233 (100%)	-0.49	1 (0%)	92	77	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%)	-0.54	0	100	100	69, 93, 115, 134	0
15	AE	76/76 (100%)	-0.65	0	100	100	71, 103, 142, 147	0
15	AF	76/76 (100%)	-0.64	0	100	100	73, 107, 139, 145	0
15	B3	76/76 (100%)	-0.13	0	100	100	101, 129, 146, 155	0
15	B6	76/76 (100%)	-0.61	0	100	100	78, 118, 144, 151	0
16	A5	799/799 (100%)	-0.57	1 (0%)	95	88	45, 87, 141, 267	0
16	A7	799/799 (100%)	-0.52	5 (0%)	89	71	54, 95, 144, 267	0
16	B4	799/799 (100%)	-0.24	15 (1%)	67	37	82, 115, 155, 265	0
16	B7	799/799 (100%)	-0.38	11 (1%)	75	49	72, 105, 149, 266	0
17	A6	997/997 (100%)	-0.48	7 (0%)	87	67	55, 107, 166, 261	0
17	A8	997/997 (100%)	-0.43	17 (1%)	70	42	63, 108, 167, 260	0
17	B5	997/997 (100%)	-0.13	25 (2%)	58	29	83, 128, 173, 261	0
17	B8	997/997 (100%)	-0.36	17 (1%)	70	42	77, 114, 170, 261	0
All	All	20080/20080 (100%)	-0.47	218 (1%)	80	55	34, 100, 158, 267	0

The worst 5 of 218 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	B8	1753	GLU	14.2
5	AV	5125	GLU	12.4
17	B8	1754	SER	11.4
17	A8	1755	ASP	10.0
17	B8	1755	ASP	9.7

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.