



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:30 PM UTC

PDB ID : 3HF9 / pdb_00003hf9
Title : Crystal Structure of Mycobacterium Tuberculosis Proteasome open-gate mutant modified by inhibitor GL1
Authors : Li, D.; Li, H.
Deposited on : 2009-05-11
Resolution : 2.88 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

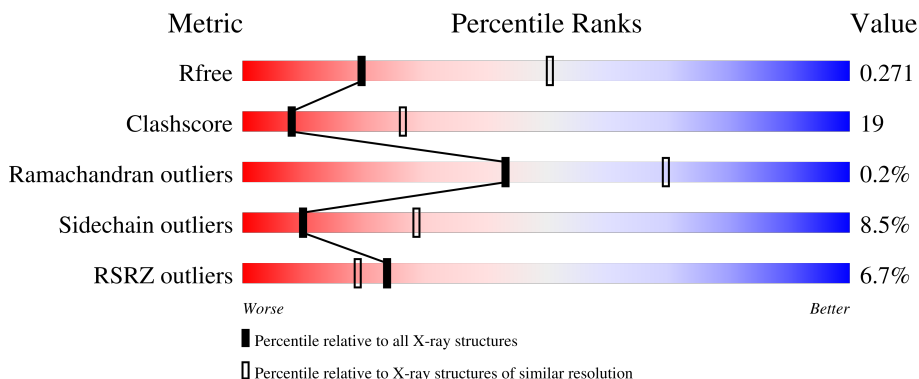
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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}	180053	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1	240	10% 55% 32% • 12%
1	3	240	4% 58% 25% • 12%
1	A	240	4% 45% 37% 6% 12%
1	B	240	• 50% 30% 8% 12%
1	D	240	31% 42% 39% 7% 12%

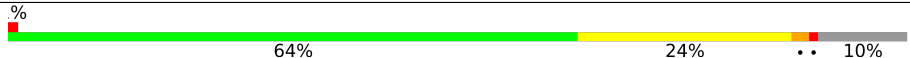
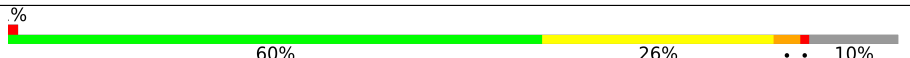
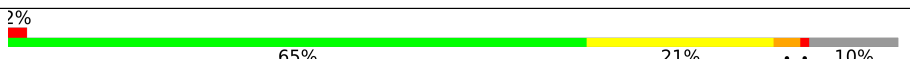
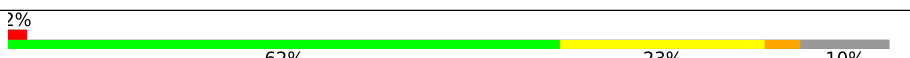
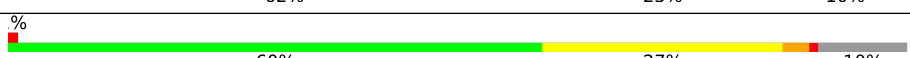
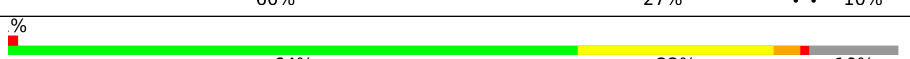
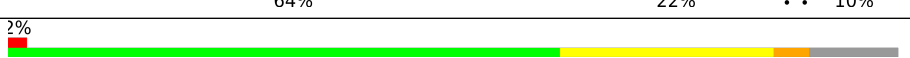
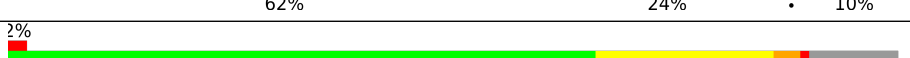
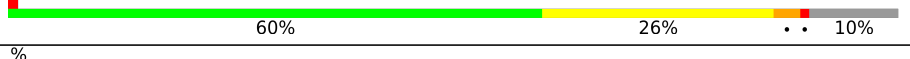
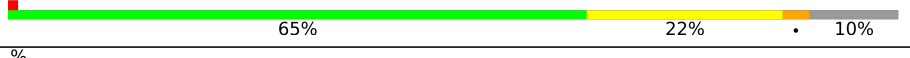
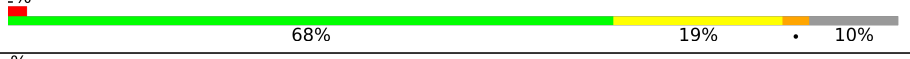
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Mol	Chain	Length	Quality of chain
1	F	240	
1	I	240	
1	K	240	
1	M	240	
1	O	240	
1	Q	240	
1	S	240	
1	U	240	
1	W	240	
1	Y	240	
1	a	240	
1	b	240	
1	d	240	
1	f	240	
1	i	240	
1	k	240	
1	m	240	
1	o	240	
1	q	240	
1	s	240	
1	u	240	
1	w	240	
1	y	240	
2	2	240	
2	4	240	

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Mol	Chain	Length	Quality of chain
2	C	240	
2	E	240	
2	G	240	
2	H	240	
2	J	240	
2	L	240	
2	N	240	
2	P	240	
2	R	240	
2	T	240	
2	V	240	
2	X	240	
2	Z	240	
2	c	240	
2	e	240	
2	g	240	
2	h	240	
2	j	240	
2	l	240	
2	n	240	
2	p	240	
2	r	240	
2	t	240	
2	v	240	
2	x	240	

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Mol	Chain	Length	Quality of chain
2	z	240	 A horizontal bar chart showing the quality of chain. The bar is divided into segments representing different quality metrics. The segments are labeled with percentages: 62%, 25%, and 10%. The bar starts with a small red segment, followed by a large green segment (62%), a yellow segment (25%), and a small grey segment (10%).

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OZT	2	1	-	-	X	-
2	OZT	4	301	-	-	X	-
2	OZT	E	1	-	-	X	-
2	OZT	H	1	-	-	X	-
2	OZT	L	1	-	-	X	-
2	OZT	X	1	-	-	X	-
2	OZT	g	301	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 90443 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 (Alpha subunit) PrcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	B	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	D	210	Total	C	N	O	S	0	0	0
			1625	1017	298	307	3			
1	F	193	Total	C	N	O	S	0	0	0
			1490	939	267	282	2			
1	I	212	Total	C	N	O	S	0	0	0
			1640	1028	300	309	3			
1	K	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	M	205	Total	C	N	O	S	0	0	0
			1589	995	292	299	3			
1	O	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	Q	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	S	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	U	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	W	193	Total	C	N	O	S	0	0	0
			1487	936	267	282	2			
1	Y	210	Total	C	N	O	S	0	0	0
			1625	1017	298	307	3			
1	1	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	a	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	b	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	d	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	f	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	i	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	k	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	m	208	Total	C	N	O	S	0	0	0
			1612	1008	296	305	3			
1	o	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	q	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	s	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	u	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	w	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	y	211	Total	C	N	O	S	0	0	0
			1633	1023	299	308	3			
1	3	210	Total	C	N	O	S	0	0	0
			1625	1017	298	307	3			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	initiating methionine	UNP O33244
B	9	MET	-	initiating methionine	UNP O33244
D	9	MET	-	initiating methionine	UNP O33244
F	9	MET	-	initiating methionine	UNP O33244
I	9	MET	-	initiating methionine	UNP O33244
K	9	MET	-	initiating methionine	UNP O33244
M	9	MET	-	initiating methionine	UNP O33244
O	9	MET	-	initiating methionine	UNP O33244
Q	9	MET	-	initiating methionine	UNP O33244
S	9	MET	-	initiating methionine	UNP O33244
U	9	MET	-	initiating methionine	UNP O33244
W	9	MET	-	initiating methionine	UNP O33244
Y	9	MET	-	initiating methionine	UNP O33244
1	9	MET	-	initiating methionine	UNP O33244
a	309	MET	-	initiating methionine	UNP O33244

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Chain	Residue	Modelled	Actual	Comment	Reference
b	309	MET	-	initiating methionine	UNP O33244
d	309	MET	-	initiating methionine	UNP O33244
f	309	MET	-	initiating methionine	UNP O33244
i	309	MET	-	initiating methionine	UNP O33244
k	309	MET	-	initiating methionine	UNP O33244
m	309	MET	-	initiating methionine	UNP O33244
o	309	MET	-	initiating methionine	UNP O33244
q	309	MET	-	initiating methionine	UNP O33244
s	309	MET	-	initiating methionine	UNP O33244
u	309	MET	-	initiating methionine	UNP O33244
w	309	MET	-	initiating methionine	UNP O33244
y	309	MET	-	initiating methionine	UNP O33244
3	309	MET	-	initiating methionine	UNP O33244

- Molecule 2 is a protein called Proteasome (Beta subunit) PrcB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	C	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	E	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	G	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	J	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	L	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	N	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	P	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	R	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	T	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	V	218	Total	C	N	O	S	0	0	0
			1610	1009	277	320	4			
2	X	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	Z	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	h	214	Total	C	N	O	S	0	0	0
			1588	995	273	316	4			
2	c	215	Total	C	N	O	S	0	0	0
			1596	1001	274	317	4			
2	e	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	g	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	j	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	l	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	n	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	p	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	r	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	t	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	v	219	Total	C	N	O	S	0	0	0
			1615	1012	278	321	4			
2	x	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	z	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			
2	4	217	Total	C	N	O	S	0	0	0
			1606	1007	276	319	4			

There are 196 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	OZT	-	insertion	UNP O33245
H	235	HIS	-	expression tag	UNP O33245
H	236	HIS	-	expression tag	UNP O33245
H	237	HIS	-	expression tag	UNP O33245
H	238	HIS	-	expression tag	UNP O33245
H	239	HIS	-	expression tag	UNP O33245
H	240	HIS	-	expression tag	UNP O33245
C	1	OZT	-	insertion	UNP O33245
C	235	HIS	-	expression tag	UNP O33245

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Chain	Residue	Modelled	Actual	Comment	Reference
C	236	HIS	-	expression tag	UNP O33245
C	237	HIS	-	expression tag	UNP O33245
C	238	HIS	-	expression tag	UNP O33245
C	239	HIS	-	expression tag	UNP O33245
C	240	HIS	-	expression tag	UNP O33245
E	1	OZT	-	insertion	UNP O33245
E	235	HIS	-	expression tag	UNP O33245
E	236	HIS	-	expression tag	UNP O33245
E	237	HIS	-	expression tag	UNP O33245
E	238	HIS	-	expression tag	UNP O33245
E	239	HIS	-	expression tag	UNP O33245
E	240	HIS	-	expression tag	UNP O33245
G	1	OZT	-	insertion	UNP O33245
G	235	HIS	-	expression tag	UNP O33245
G	236	HIS	-	expression tag	UNP O33245
G	237	HIS	-	expression tag	UNP O33245
G	238	HIS	-	expression tag	UNP O33245
G	239	HIS	-	expression tag	UNP O33245
G	240	HIS	-	expression tag	UNP O33245
J	1	OZT	-	insertion	UNP O33245
J	235	HIS	-	expression tag	UNP O33245
J	236	HIS	-	expression tag	UNP O33245
J	237	HIS	-	expression tag	UNP O33245
J	238	HIS	-	expression tag	UNP O33245
J	239	HIS	-	expression tag	UNP O33245
J	240	HIS	-	expression tag	UNP O33245
L	1	OZT	-	insertion	UNP O33245
L	235	HIS	-	expression tag	UNP O33245
L	236	HIS	-	expression tag	UNP O33245
L	237	HIS	-	expression tag	UNP O33245
L	238	HIS	-	expression tag	UNP O33245
L	239	HIS	-	expression tag	UNP O33245
L	240	HIS	-	expression tag	UNP O33245
N	1	OZT	-	insertion	UNP O33245
N	235	HIS	-	expression tag	UNP O33245
N	236	HIS	-	expression tag	UNP O33245
N	237	HIS	-	expression tag	UNP O33245
N	238	HIS	-	expression tag	UNP O33245
N	239	HIS	-	expression tag	UNP O33245
N	240	HIS	-	expression tag	UNP O33245
P	1	OZT	-	insertion	UNP O33245
P	235	HIS	-	expression tag	UNP O33245

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Chain	Residue	Modelled	Actual	Comment	Reference
P	236	HIS	-	expression tag	UNP O33245
P	237	HIS	-	expression tag	UNP O33245
P	238	HIS	-	expression tag	UNP O33245
P	239	HIS	-	expression tag	UNP O33245
P	240	HIS	-	expression tag	UNP O33245
R	1	OZT	-	insertion	UNP O33245
R	235	HIS	-	expression tag	UNP O33245
R	236	HIS	-	expression tag	UNP O33245
R	237	HIS	-	expression tag	UNP O33245
R	238	HIS	-	expression tag	UNP O33245
R	239	HIS	-	expression tag	UNP O33245
R	240	HIS	-	expression tag	UNP O33245
T	1	OZT	-	insertion	UNP O33245
T	235	HIS	-	expression tag	UNP O33245
T	236	HIS	-	expression tag	UNP O33245
T	237	HIS	-	expression tag	UNP O33245
T	238	HIS	-	expression tag	UNP O33245
T	239	HIS	-	expression tag	UNP O33245
T	240	HIS	-	expression tag	UNP O33245
V	1	OZT	-	insertion	UNP O33245
V	235	HIS	-	expression tag	UNP O33245
V	236	HIS	-	expression tag	UNP O33245
V	237	HIS	-	expression tag	UNP O33245
V	238	HIS	-	expression tag	UNP O33245
V	239	HIS	-	expression tag	UNP O33245
V	240	HIS	-	expression tag	UNP O33245
X	1	OZT	-	insertion	UNP O33245
X	235	HIS	-	expression tag	UNP O33245
X	236	HIS	-	expression tag	UNP O33245
X	237	HIS	-	expression tag	UNP O33245
X	238	HIS	-	expression tag	UNP O33245
X	239	HIS	-	expression tag	UNP O33245
X	240	HIS	-	expression tag	UNP O33245
Z	1	OZT	-	insertion	UNP O33245
Z	235	HIS	-	expression tag	UNP O33245
Z	236	HIS	-	expression tag	UNP O33245
Z	237	HIS	-	expression tag	UNP O33245
Z	238	HIS	-	expression tag	UNP O33245
Z	239	HIS	-	expression tag	UNP O33245
Z	240	HIS	-	expression tag	UNP O33245
2	1	OZT	-	insertion	UNP O33245
2	235	HIS	-	expression tag	UNP O33245

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Chain	Residue	Modelled	Actual	Comment	Reference
2	236	HIS	-	expression tag	UNP O33245
2	237	HIS	-	expression tag	UNP O33245
2	238	HIS	-	expression tag	UNP O33245
2	239	HIS	-	expression tag	UNP O33245
2	240	HIS	-	expression tag	UNP O33245
h	301	OZT	-	insertion	UNP O33245
h	535	HIS	-	expression tag	UNP O33245
h	536	HIS	-	expression tag	UNP O33245
h	537	HIS	-	expression tag	UNP O33245
h	538	HIS	-	expression tag	UNP O33245
h	539	HIS	-	expression tag	UNP O33245
h	540	HIS	-	expression tag	UNP O33245
c	301	OZT	-	insertion	UNP O33245
c	535	HIS	-	expression tag	UNP O33245
c	536	HIS	-	expression tag	UNP O33245
c	537	HIS	-	expression tag	UNP O33245
c	538	HIS	-	expression tag	UNP O33245
c	539	HIS	-	expression tag	UNP O33245
c	540	HIS	-	expression tag	UNP O33245
e	301	OZT	-	insertion	UNP O33245
e	535	HIS	-	expression tag	UNP O33245
e	536	HIS	-	expression tag	UNP O33245
e	537	HIS	-	expression tag	UNP O33245
e	538	HIS	-	expression tag	UNP O33245
e	539	HIS	-	expression tag	UNP O33245
e	540	HIS	-	expression tag	UNP O33245
g	301	OZT	-	insertion	UNP O33245
g	535	HIS	-	expression tag	UNP O33245
g	536	HIS	-	expression tag	UNP O33245
g	537	HIS	-	expression tag	UNP O33245
g	538	HIS	-	expression tag	UNP O33245
g	539	HIS	-	expression tag	UNP O33245
g	540	HIS	-	expression tag	UNP O33245
j	301	OZT	-	insertion	UNP O33245
j	535	HIS	-	expression tag	UNP O33245
j	536	HIS	-	expression tag	UNP O33245
j	537	HIS	-	expression tag	UNP O33245
j	538	HIS	-	expression tag	UNP O33245
j	539	HIS	-	expression tag	UNP O33245
j	540	HIS	-	expression tag	UNP O33245
l	301	OZT	-	insertion	UNP O33245
l	535	HIS	-	expression tag	UNP O33245

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Chain	Residue	Modelled	Actual	Comment	Reference
l	536	HIS	-	expression tag	UNP O33245
l	537	HIS	-	expression tag	UNP O33245
l	538	HIS	-	expression tag	UNP O33245
l	539	HIS	-	expression tag	UNP O33245
l	540	HIS	-	expression tag	UNP O33245
n	301	OZT	-	insertion	UNP O33245
n	535	HIS	-	expression tag	UNP O33245
n	536	HIS	-	expression tag	UNP O33245
n	537	HIS	-	expression tag	UNP O33245
n	538	HIS	-	expression tag	UNP O33245
n	539	HIS	-	expression tag	UNP O33245
n	540	HIS	-	expression tag	UNP O33245
p	301	OZT	-	insertion	UNP O33245
p	535	HIS	-	expression tag	UNP O33245
p	536	HIS	-	expression tag	UNP O33245
p	537	HIS	-	expression tag	UNP O33245
p	538	HIS	-	expression tag	UNP O33245
p	539	HIS	-	expression tag	UNP O33245
p	540	HIS	-	expression tag	UNP O33245
r	301	OZT	-	insertion	UNP O33245
r	535	HIS	-	expression tag	UNP O33245
r	536	HIS	-	expression tag	UNP O33245
r	537	HIS	-	expression tag	UNP O33245
r	538	HIS	-	expression tag	UNP O33245
r	539	HIS	-	expression tag	UNP O33245
r	540	HIS	-	expression tag	UNP O33245
t	301	OZT	-	insertion	UNP O33245
t	535	HIS	-	expression tag	UNP O33245
t	536	HIS	-	expression tag	UNP O33245
t	537	HIS	-	expression tag	UNP O33245
t	538	HIS	-	expression tag	UNP O33245
t	539	HIS	-	expression tag	UNP O33245
t	540	HIS	-	expression tag	UNP O33245
v	301	OZT	-	insertion	UNP O33245
v	535	HIS	-	expression tag	UNP O33245
v	536	HIS	-	expression tag	UNP O33245
v	537	HIS	-	expression tag	UNP O33245
v	538	HIS	-	expression tag	UNP O33245
v	539	HIS	-	expression tag	UNP O33245
v	540	HIS	-	expression tag	UNP O33245
x	301	OZT	-	insertion	UNP O33245
x	535	HIS	-	expression tag	UNP O33245

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Chain	Residue	Modelled	Actual	Comment	Reference
x	536	HIS	-	expression tag	UNP O33245
x	537	HIS	-	expression tag	UNP O33245
x	538	HIS	-	expression tag	UNP O33245
x	539	HIS	-	expression tag	UNP O33245
x	540	HIS	-	expression tag	UNP O33245
z	301	OZT	-	insertion	UNP O33245
z	535	HIS	-	expression tag	UNP O33245
z	536	HIS	-	expression tag	UNP O33245
z	537	HIS	-	expression tag	UNP O33245
z	538	HIS	-	expression tag	UNP O33245
z	539	HIS	-	expression tag	UNP O33245
z	540	HIS	-	expression tag	UNP O33245
4	301	OZT	-	insertion	UNP O33245
4	535	HIS	-	expression tag	UNP O33245
4	536	HIS	-	expression tag	UNP O33245
4	537	HIS	-	expression tag	UNP O33245
4	538	HIS	-	expression tag	UNP O33245
4	539	HIS	-	expression tag	UNP O33245
4	540	HIS	-	expression tag	UNP O33245

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total O 2 2	0	0
3	B	2	Total O 2 2	0	0
3	F	3	Total O 3 3	0	0
3	I	4	Total O 4 4	0	0
3	K	3	Total O 3 3	0	0
3	M	1	Total O 1 1	0	0
3	O	3	Total O 3 3	0	0
3	S	2	Total O 2 2	0	0
3	U	1	Total O 1 1	0	0
3	1	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	a	5	Total O 5 5	0	0
3	b	3	Total O 3 3	0	0
3	d	2	Total O 2 2	0	0
3	f	1	Total O 1 1	0	0
3	i	1	Total O 1 1	0	0
3	k	2	Total O 2 2	0	0
3	o	1	Total O 1 1	0	0
3	q	1	Total O 1 1	0	0
3	s	2	Total O 2 2	0	0
3	u	2	Total O 2 2	0	0
3	w	4	Total O 4 4	0	0
3	y	2	Total O 2 2	0	0
3	3	5	Total O 5 5	0	0
3	H	1	Total O 1 1	0	0
3	E	4	Total O 4 4	0	0
3	G	2	Total O 2 2	0	0
3	J	2	Total O 2 2	0	0
3	L	1	Total O 1 1	0	0
3	N	6	Total O 6 6	0	0
3	P	4	Total O 4 4	0	0
3	R	3	Total O 3 3	0	0

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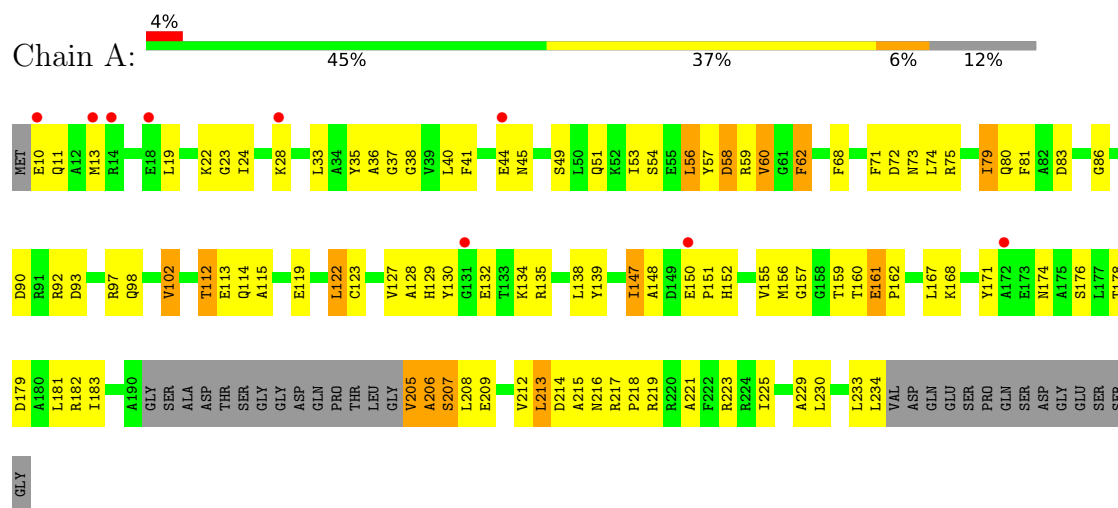
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	T	1	Total 1	O 1	0	0
3	V	6	Total 6	O 6	0	0
3	X	4	Total 4	O 4	0	0
3	2	1	Total 1	O 1	0	0
3	h	3	Total 3	O 3	0	0
3	c	6	Total 6	O 6	0	0
3	e	5	Total 5	O 5	0	0
3	g	3	Total 3	O 3	0	0
3	j	3	Total 3	O 3	0	0
3	l	3	Total 3	O 3	0	0
3	n	2	Total 2	O 2	0	0
3	p	2	Total 2	O 2	0	0
3	r	2	Total 2	O 2	0	0
3	t	2	Total 2	O 2	0	0
3	v	4	Total 4	O 4	0	0
3	x	1	Total 1	O 1	0	0
3	z	4	Total 4	O 4	0	0
3	4	7	Total 7	O 7	0	0

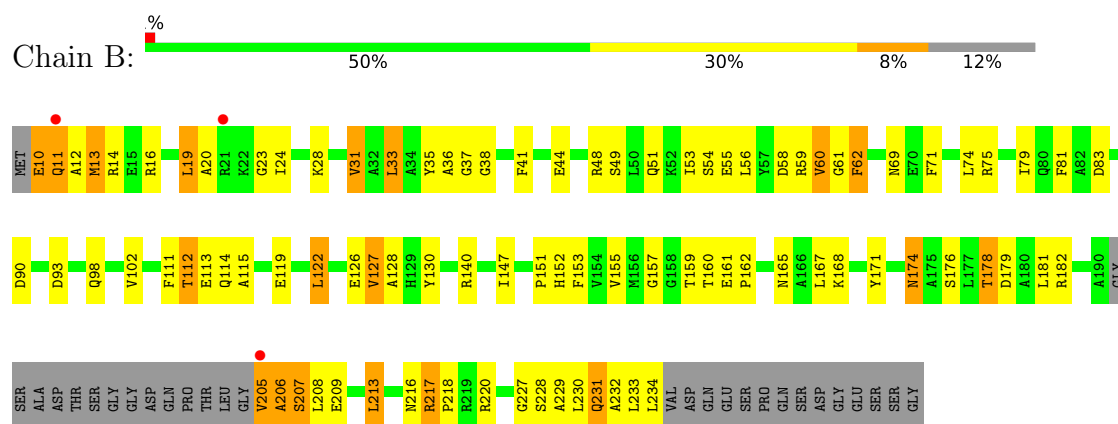
3 Residue-property plots

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

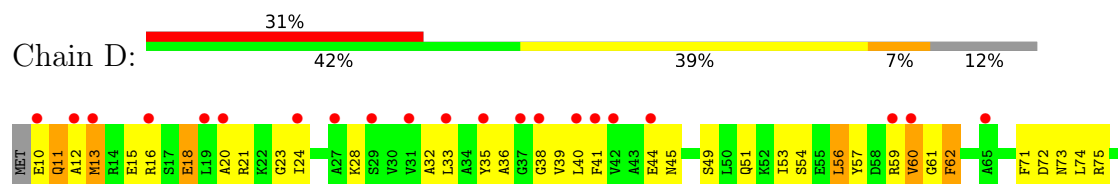
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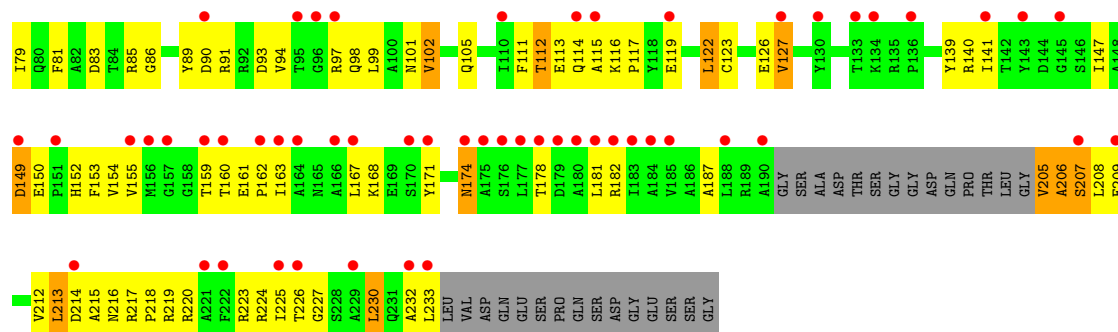


• Molecule 1: Proteasome (Alpha subunit) PrcA

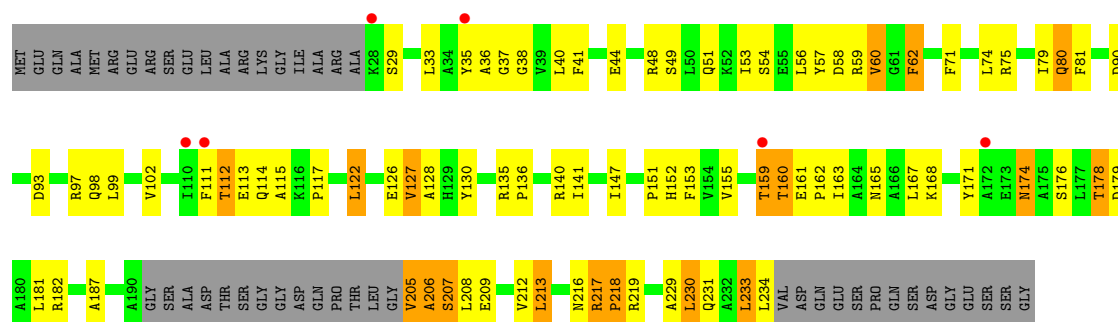
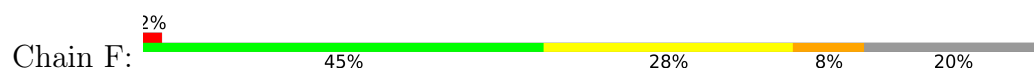


• Molecule 1: Proteasome (Alpha subunit) PrcA

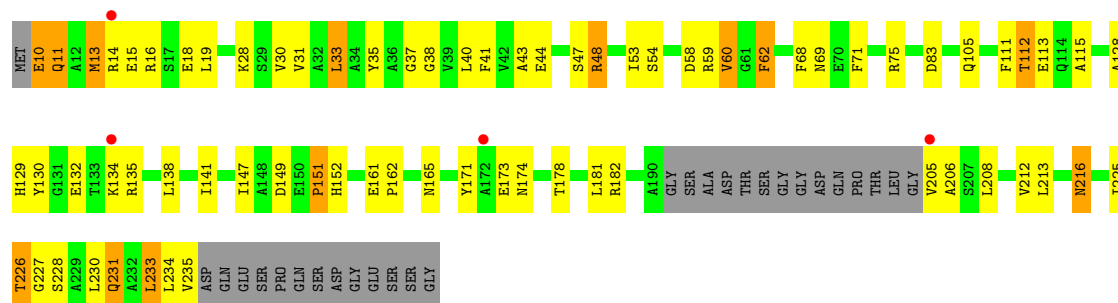




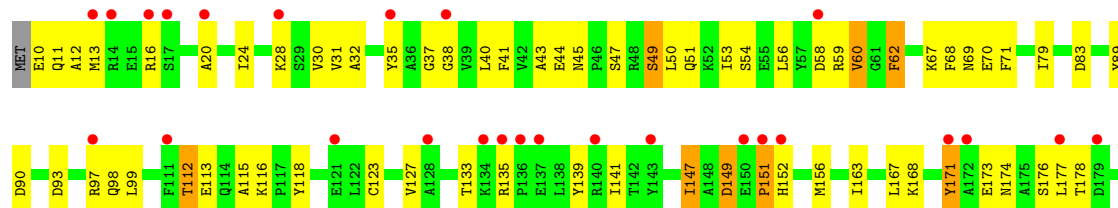
• Molecule 1: Proteasome (Alpha subunit) PrcA



• Molecule 1: Proteasome (Alpha subunit) PrcA

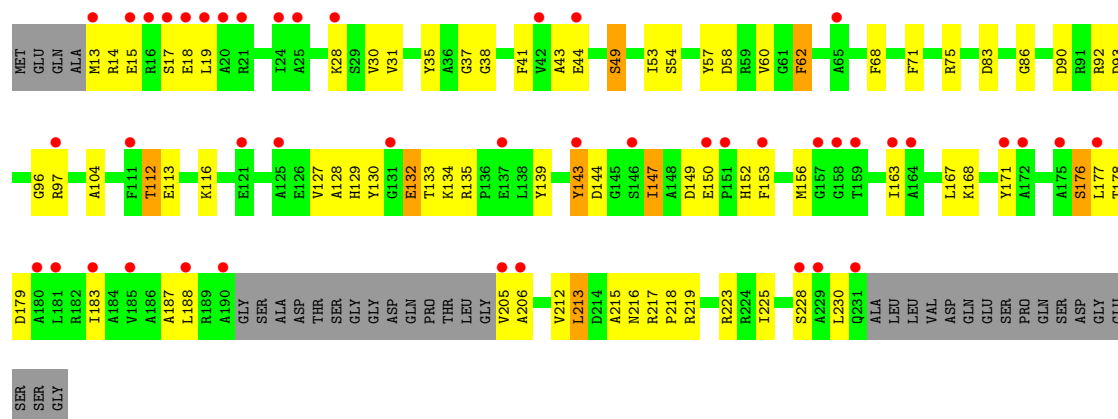


• Molecule 1: Proteasome (Alpha subunit) PrcA

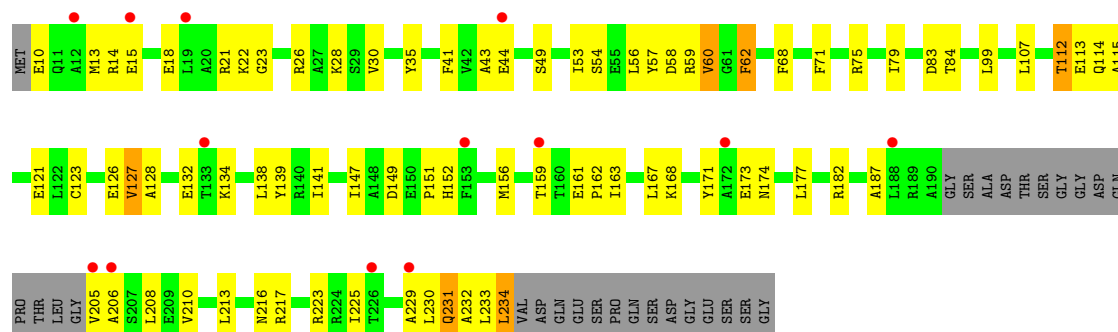




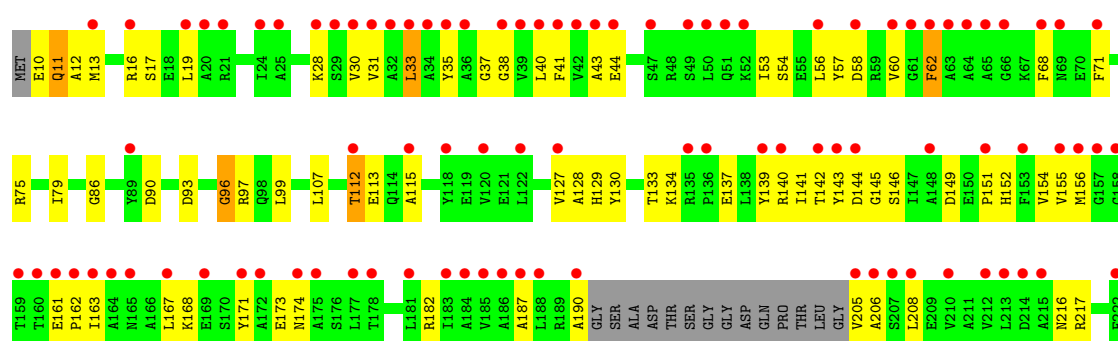
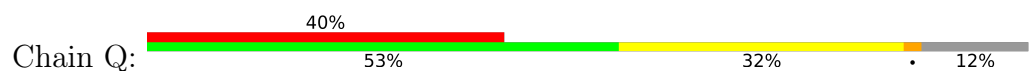
● Molecule 1: Proteasome (Alpha subunit) PrcA

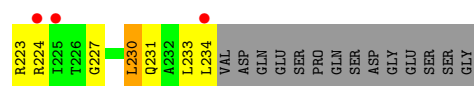


● Molecule 1: Proteasome (Alpha subunit) PrcA

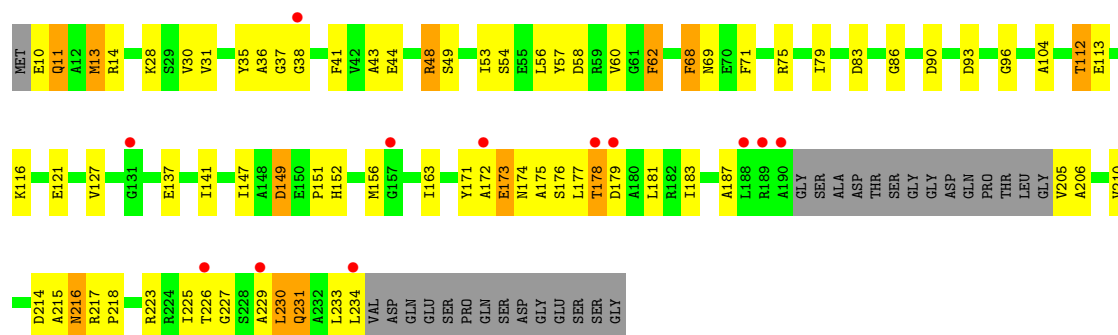


● Molecule 1: Proteasome (Alpha subunit) PrcA

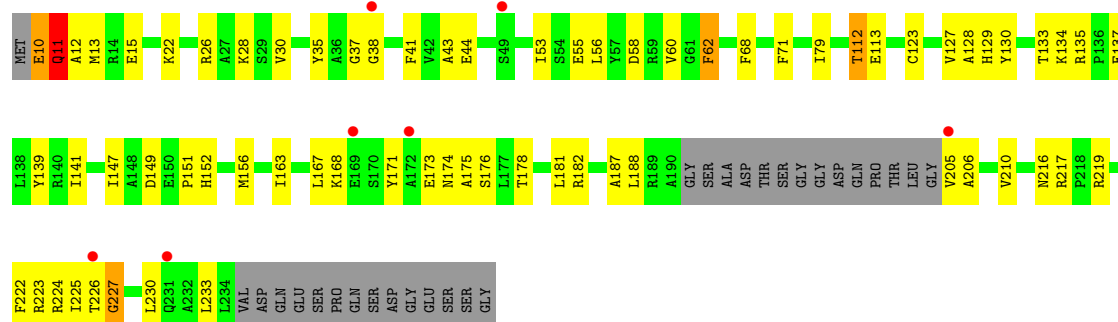




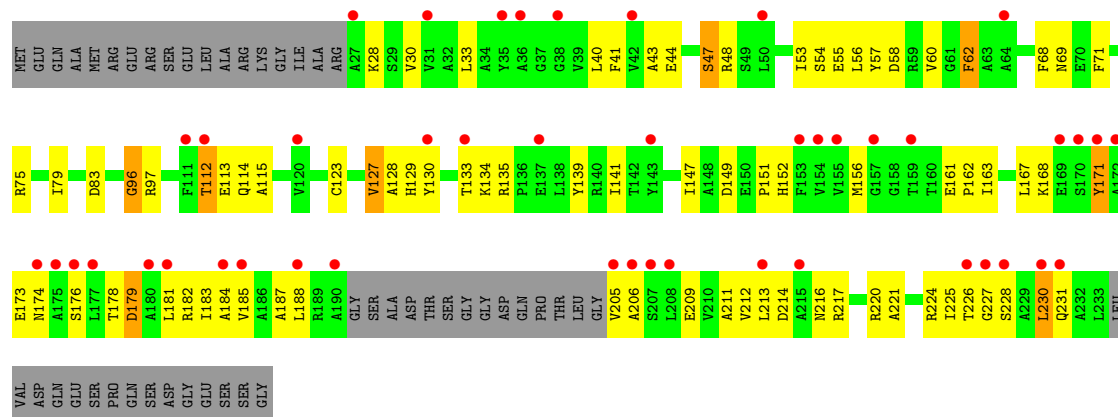
• Molecule 1: Proteasome (Alpha subunit) PrcA



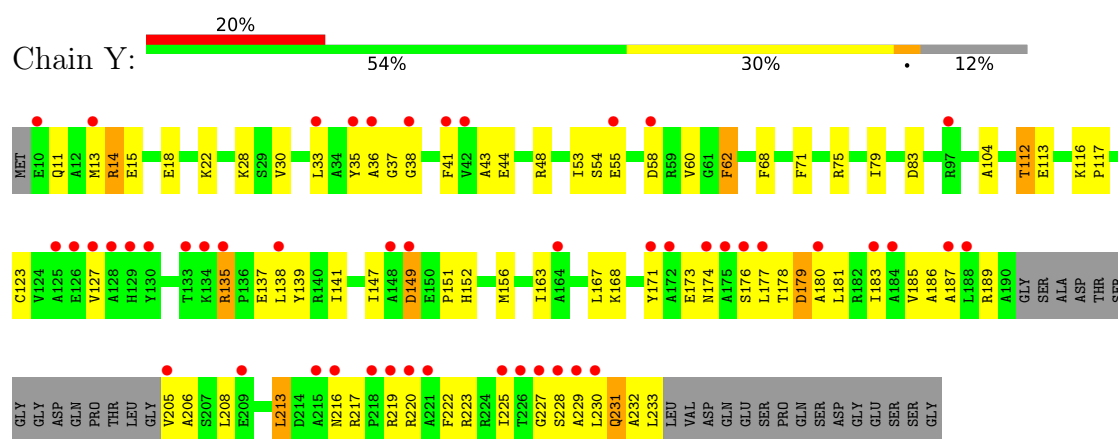
• Molecule 1: Proteasome (Alpha subunit) PrcA



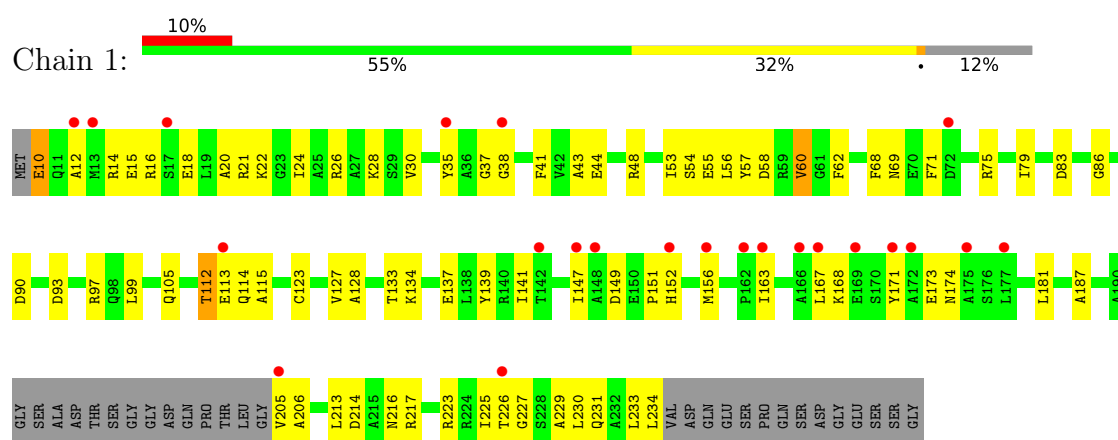
• Molecule 1: Proteasome (Alpha subunit) PrcA



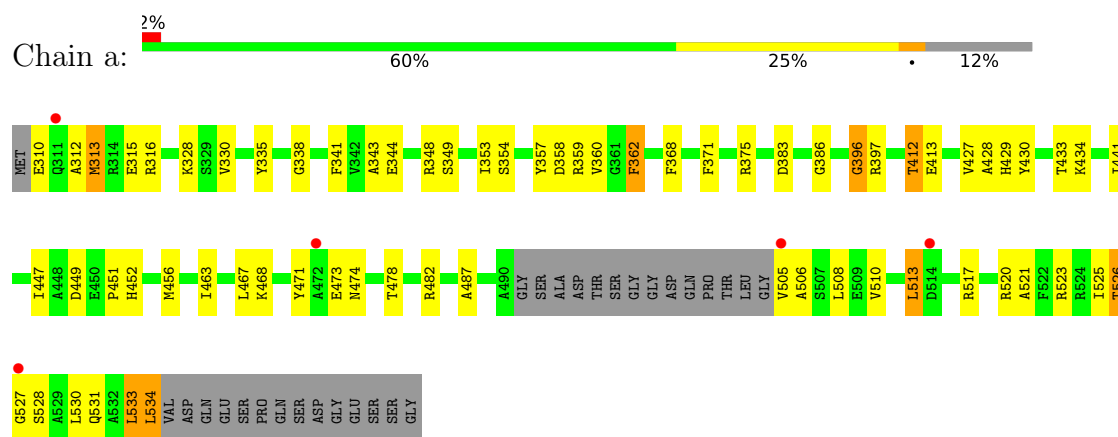
• Molecule 1: Proteasome (Alpha subunit) PrcA



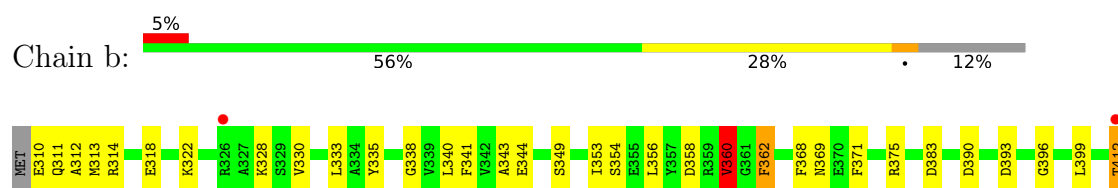
• Molecule 1: Proteasome (Alpha subunit) PrcA

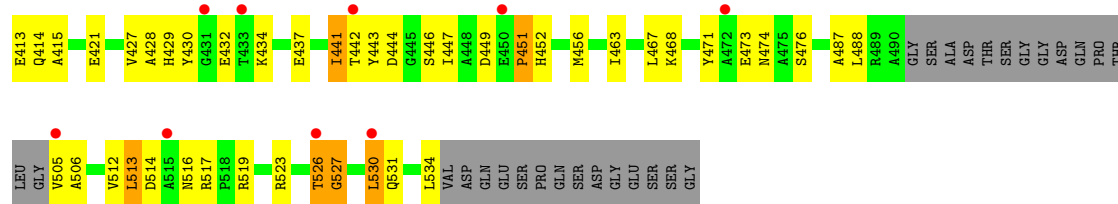


• Molecule 1: Proteasome (Alpha subunit) PrcA

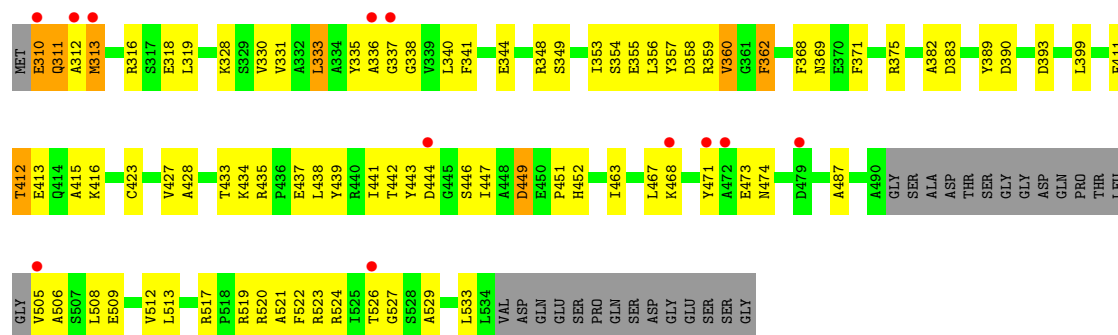


• Molecule 1: Proteasome (Alpha subunit) PrcA

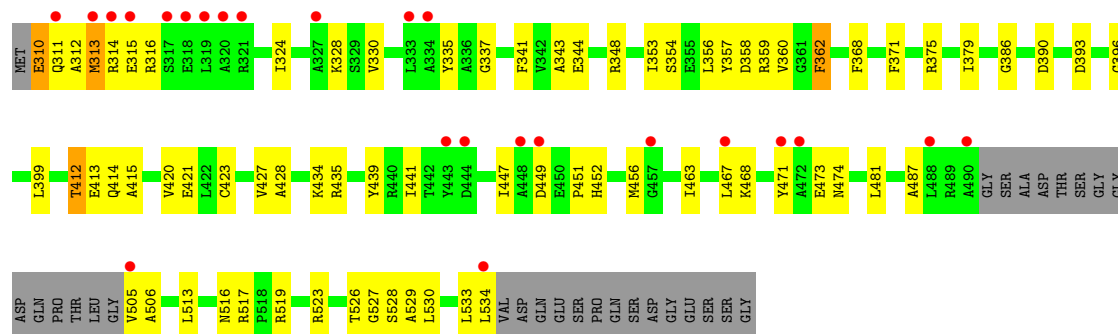




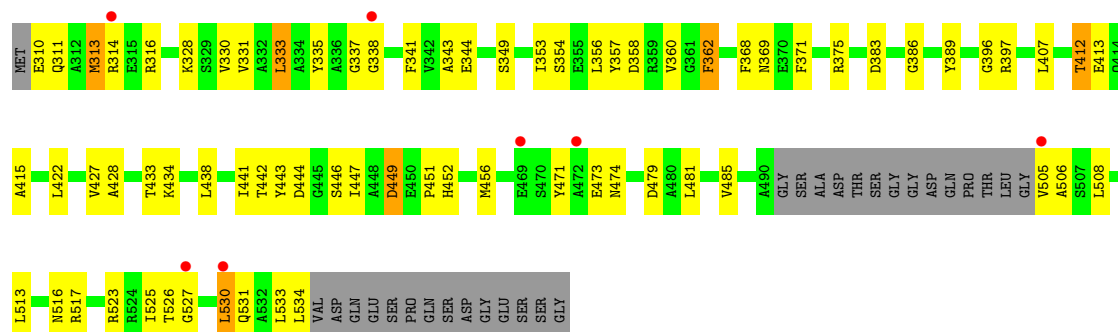
• Molecule 1: Proteasome (Alpha subunit) PrCA



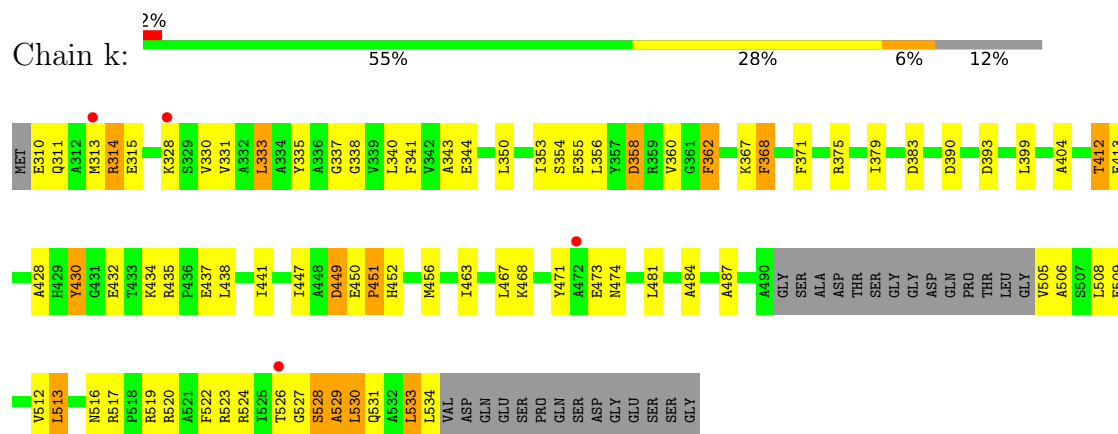
• Molecule 1: Proteasome (Alpha subunit) PrCA



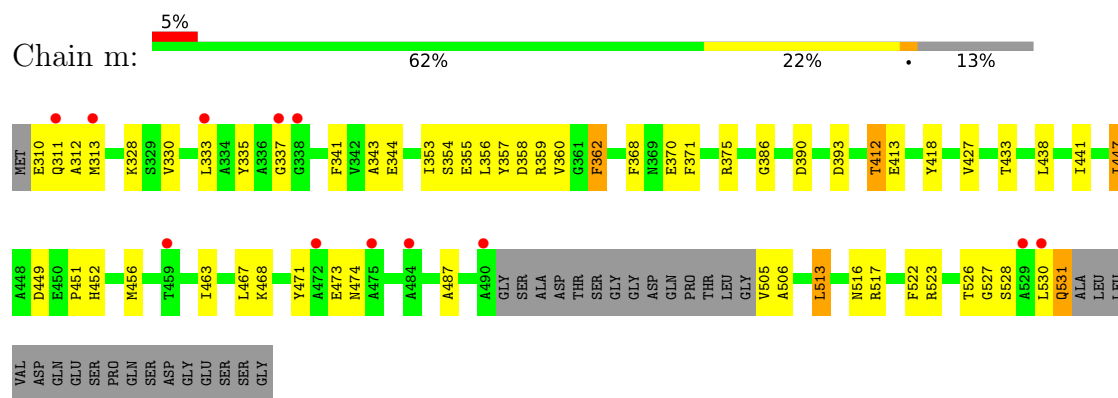
• Molecule 1: Proteasome (Alpha subunit) PrCA



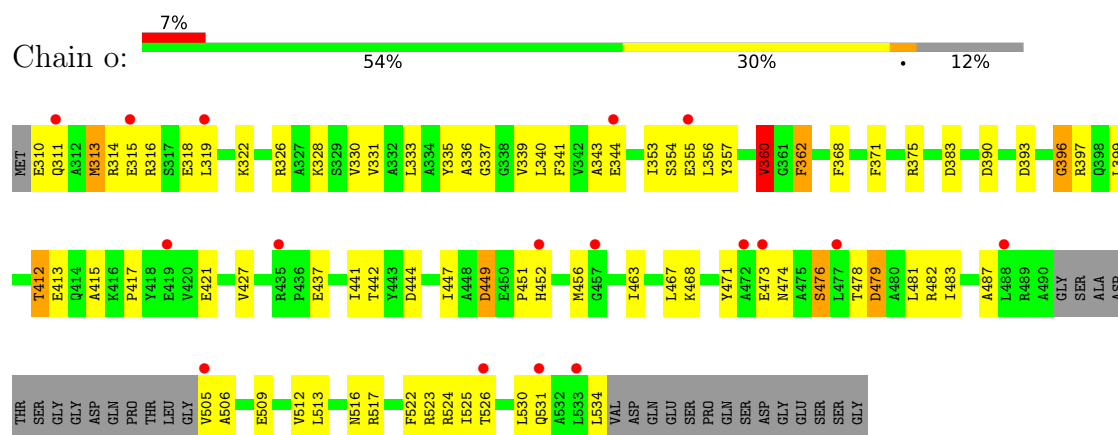
• Molecule 1: Proteasome (Alpha subunit) PrcA



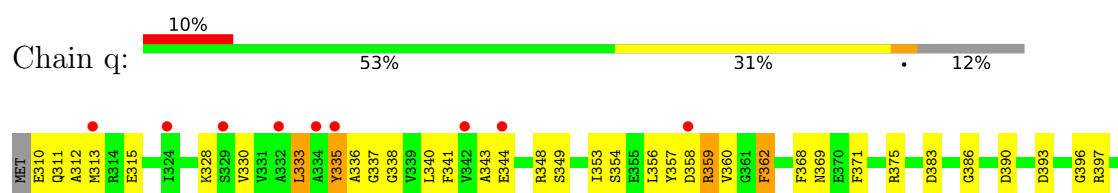
• Molecule 1: Proteasome (Alpha subunit) PrcA

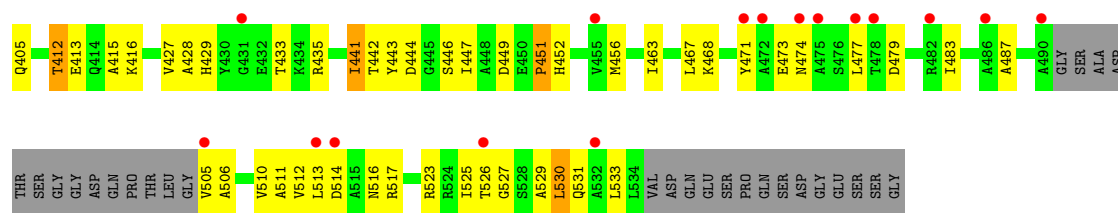


• Molecule 1: Proteasome (Alpha subunit) PrcA

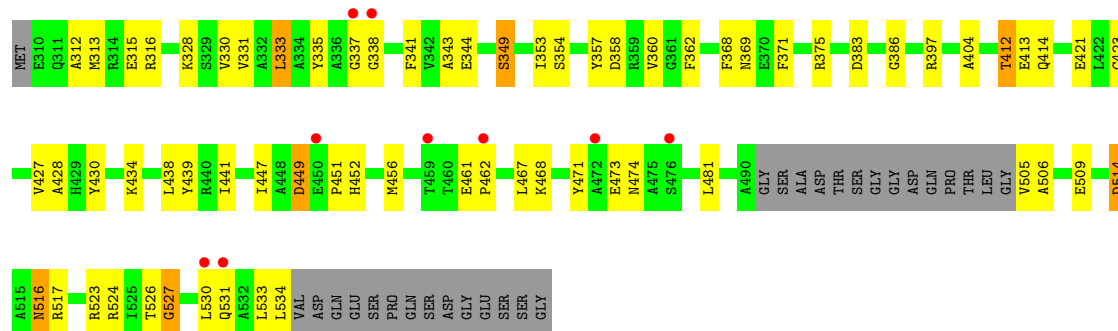


• Molecule 1: Proteasome (Alpha subunit) PrcA

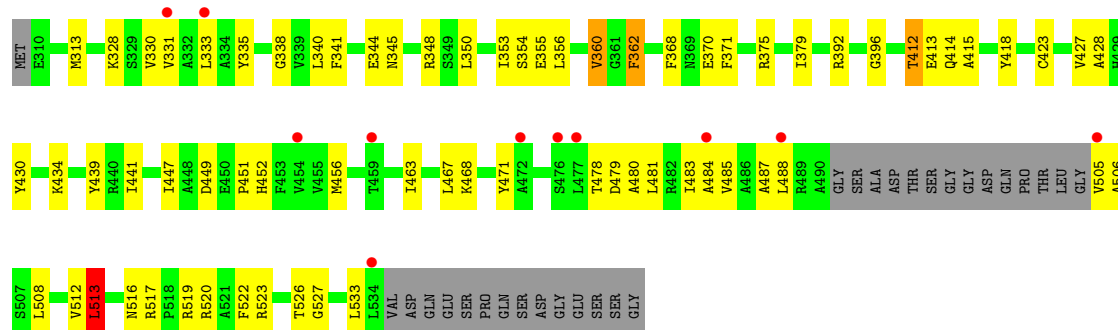




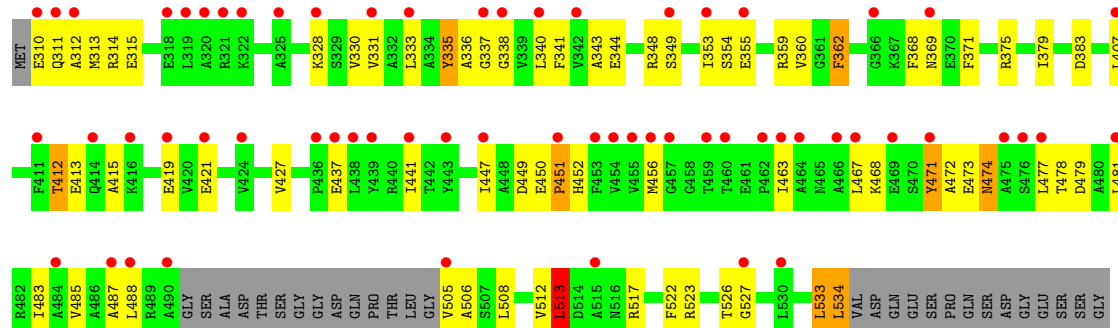
• Molecule 1: Proteasome (Alpha subunit) PrcA



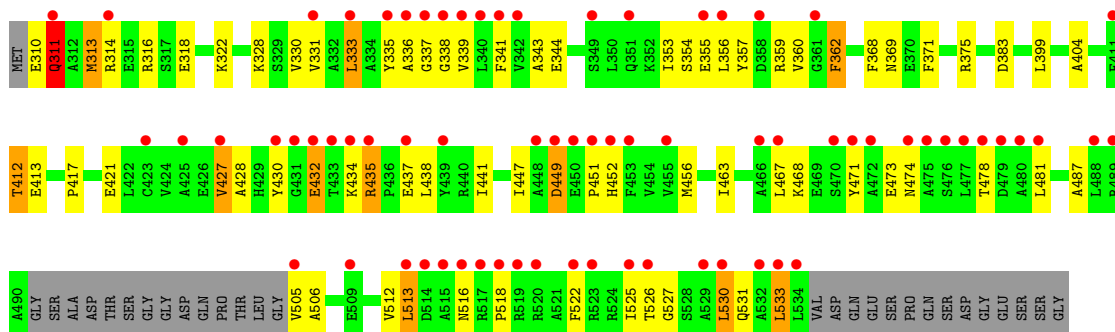
• Molecule 1: Proteasome (Alpha subunit) PrcA



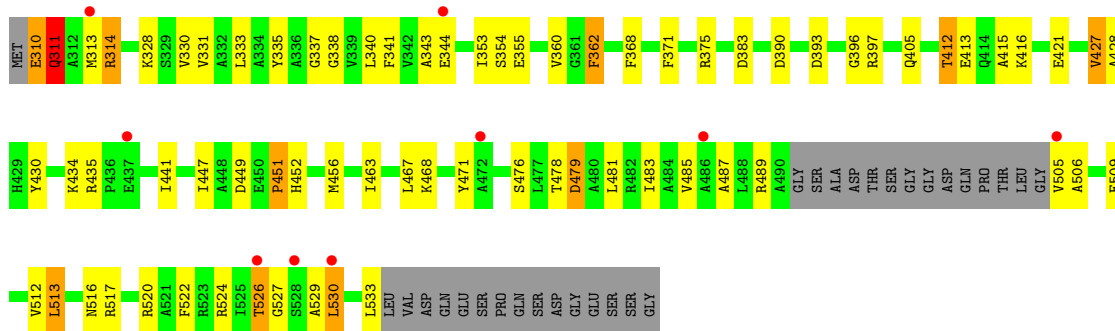
• Molecule 1: Proteasome (Alpha subunit) PrcA



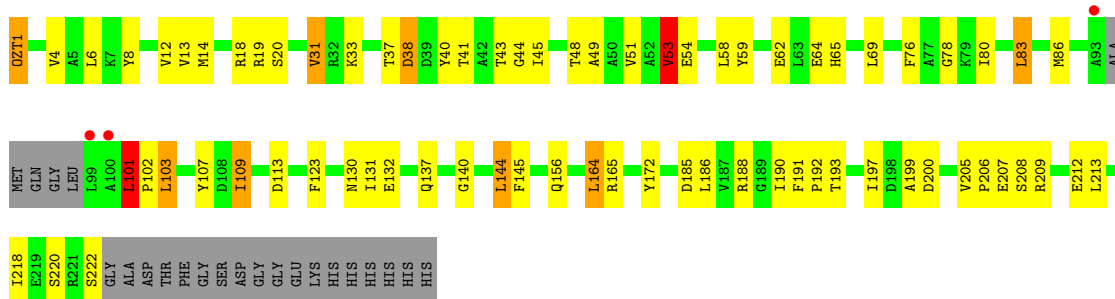
Chain y:



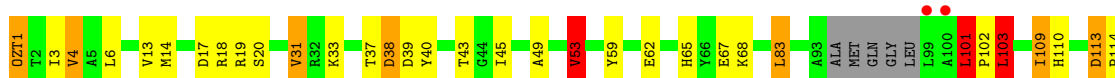
Chain 3: 4% 58% 25% 12%

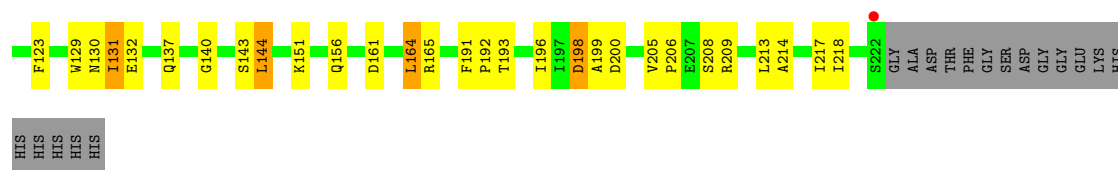


Chain H: %

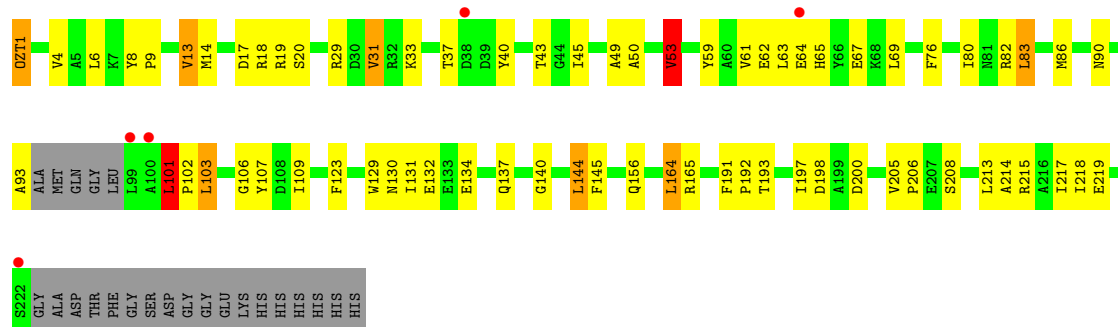


Chain C: %

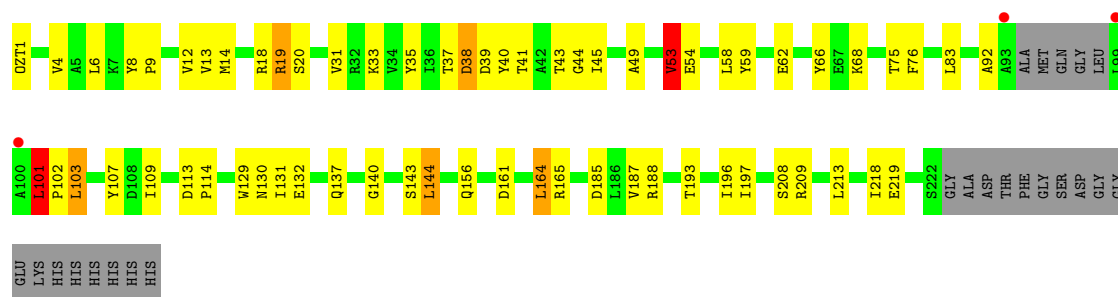




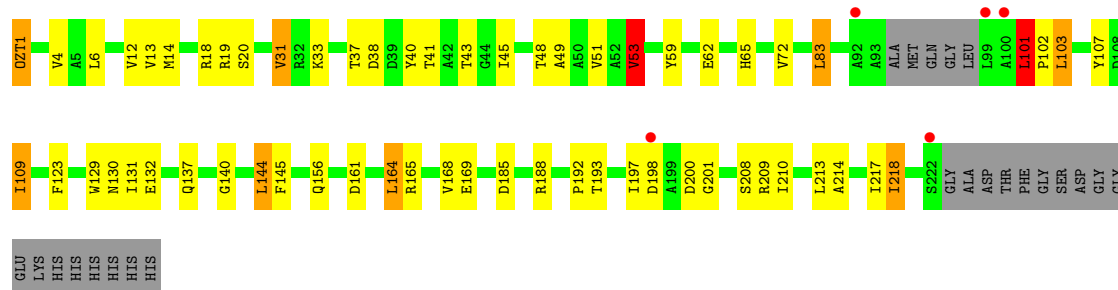
• Molecule 2: Proteasome (Beta subunit) PrcB



• Molecule 2: Proteasome (Beta subunit) PrcB



• Molecule 2: Proteasome (Beta subunit) PrcB

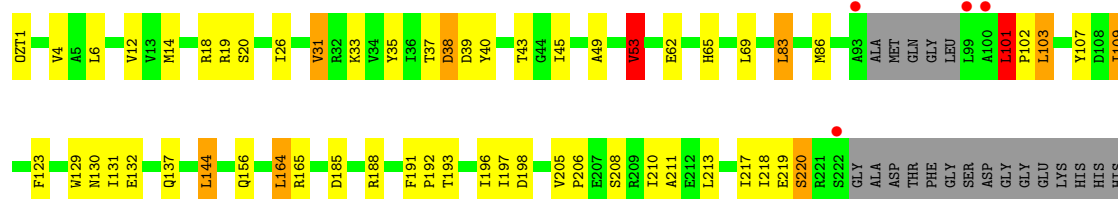


• Molecule 2: Proteasome (Beta subunit) PrcB

ASP
GLY
GLY
GLY
LYS
HIS
HIS
HIS
HIS
HIS

• Molecule 2: Proteasome (Beta subunit) PrcB

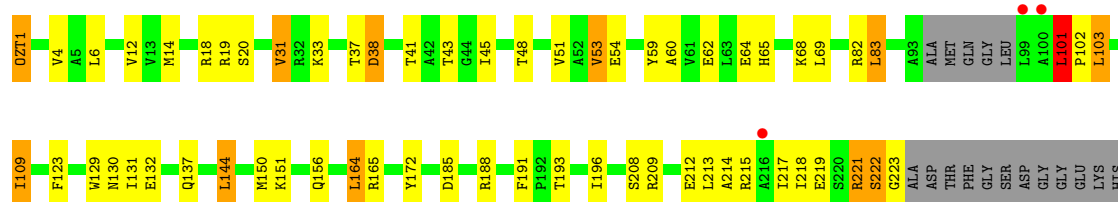
Chain T:  2% 66% 20% 10%



HIS
HIS
HIS

• Molecule 2: Proteasome (Beta subunit) PrcB

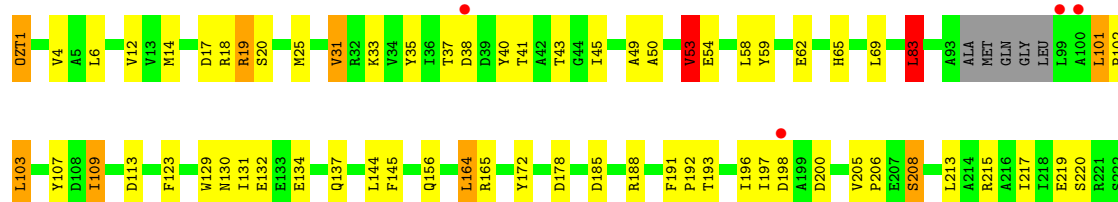
Chain V:  65% 21% 5% 9%



HIS
HIS
HIS
HIS
HIS

• Molecule 2: Proteasome (Beta subunit) PrcB

Chain X:  63% 23% 10%

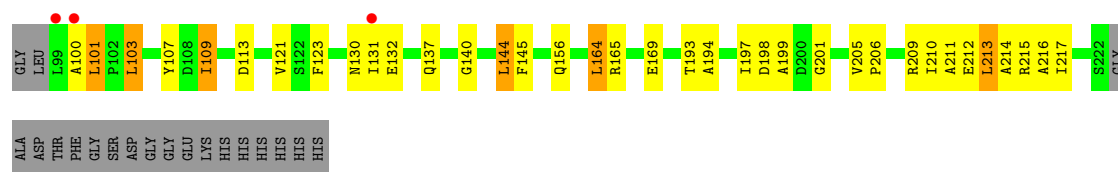


GLY
ALA
ASP
THR
PHE
GLY
SER
ASP
GLY
GLY
GLU
LYS
HIS
HIS
HIS
HIS
HIS

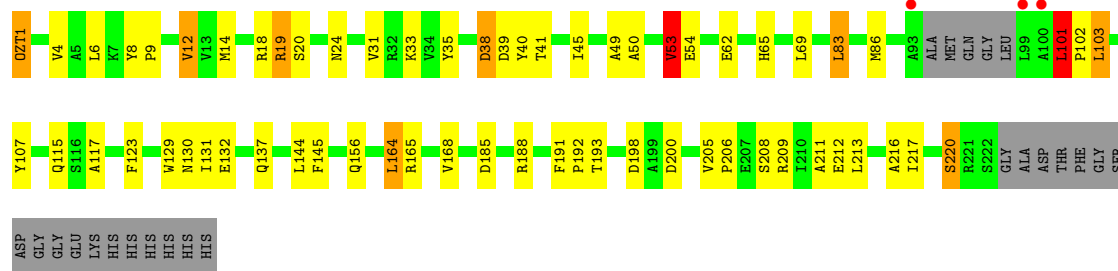
• Molecule 2: Proteasome (Beta subunit) PrcB

Chain Z:  62% 24% 10%

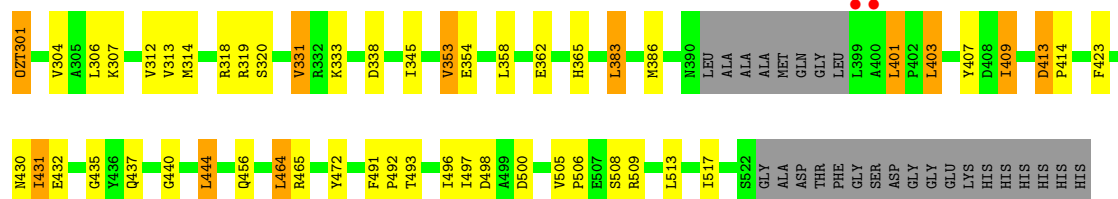




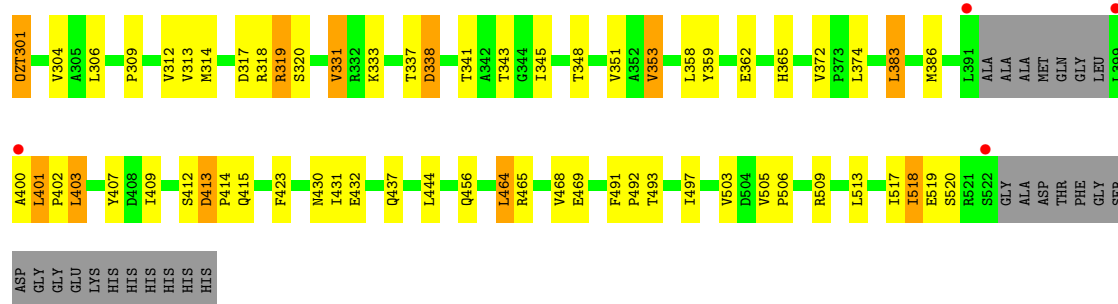
• Molecule 2: Proteasome (Beta subunit) PrcB



• Molecule 2: Proteasome (Beta subunit) PrcB

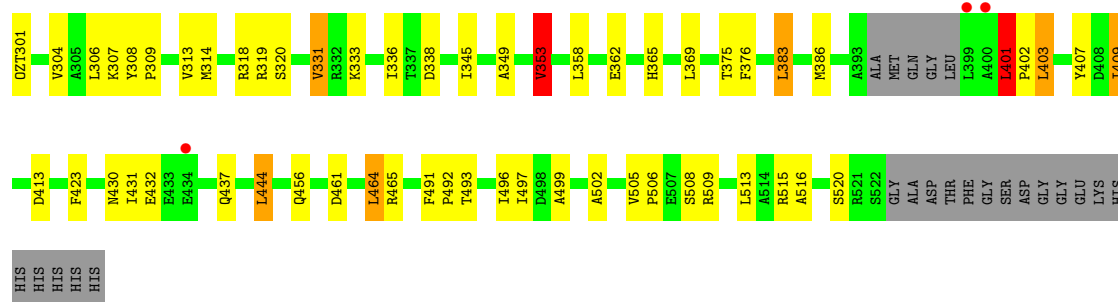


• Molecule 2: Proteasome (Beta subunit) PrcB

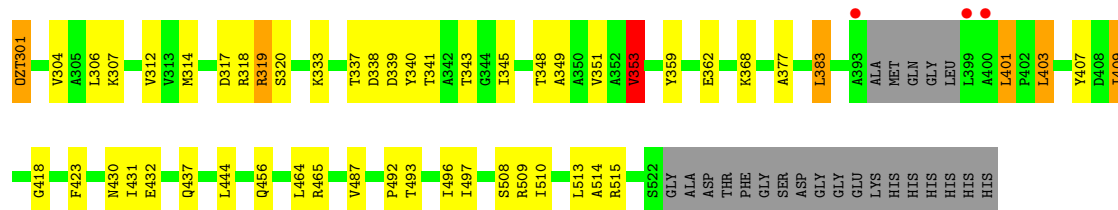


• Molecule 2: Proteasome (Beta subunit) PrcB

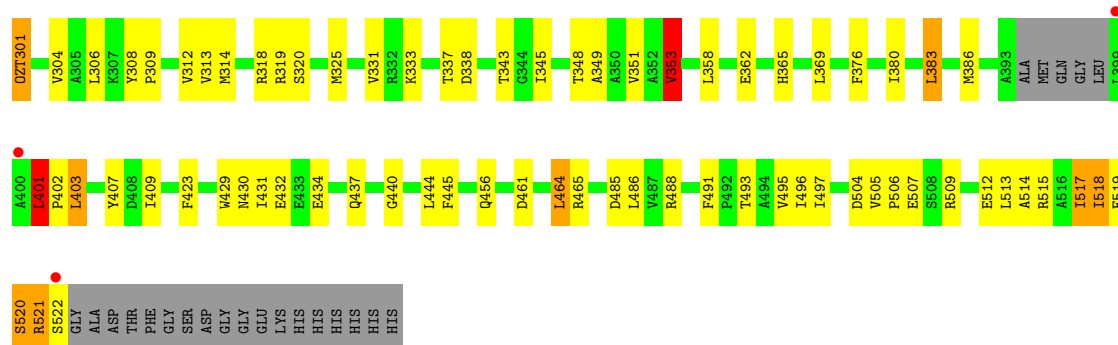




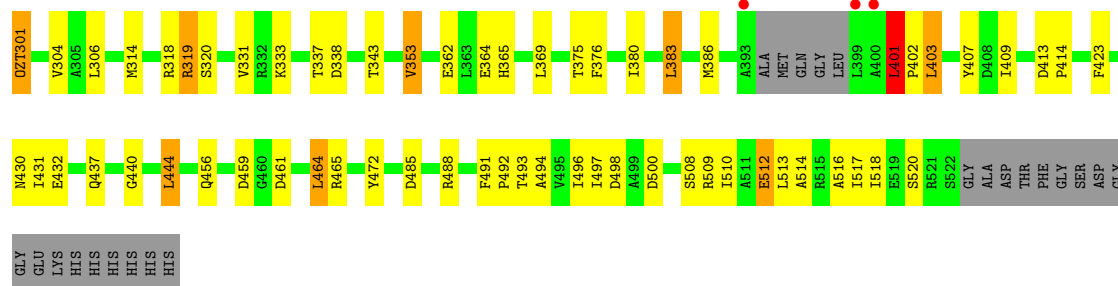
• Molecule 2: Proteasome (Beta subunit) PrcB



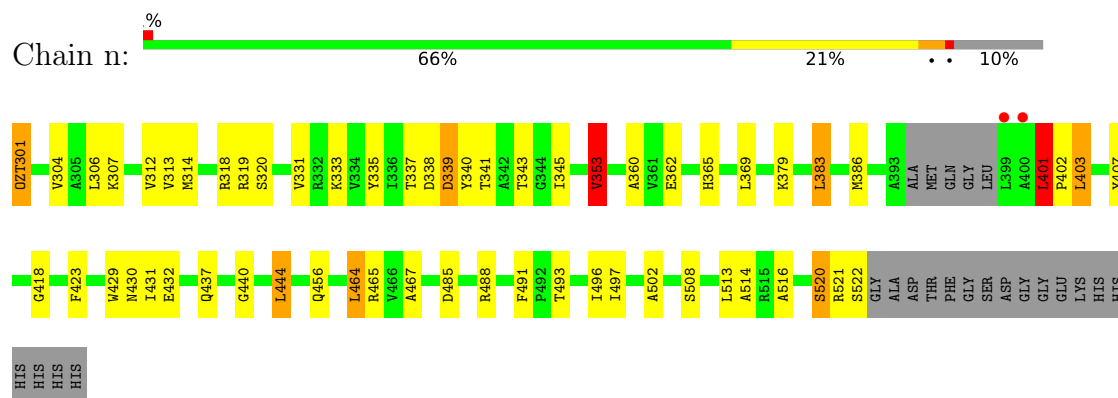
• Molecule 2: Proteasome (Beta subunit) PrcB



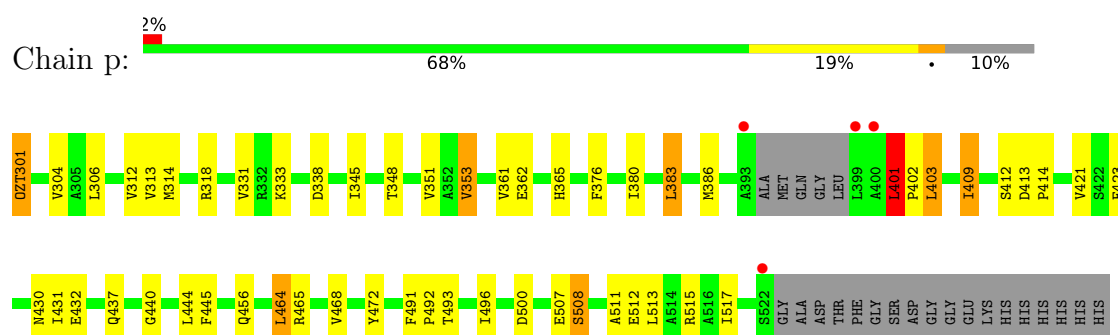
• Molecule 2: Proteasome (Beta subunit) PrcB



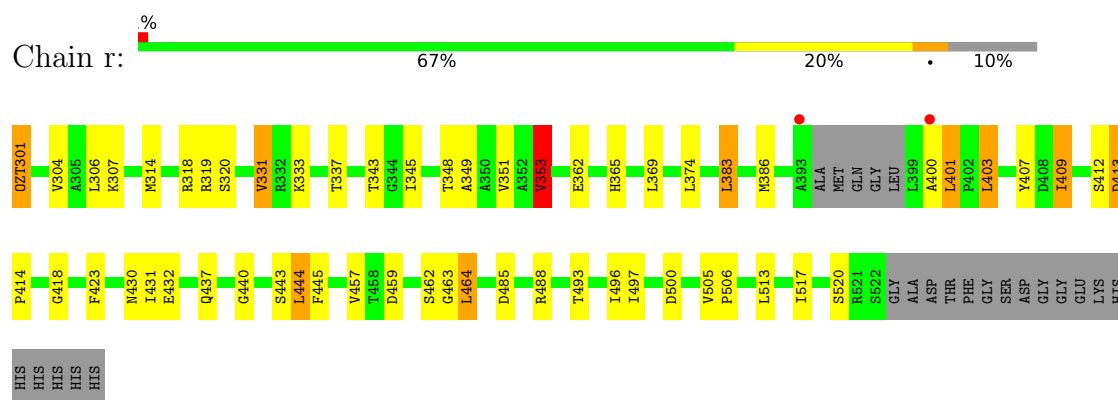
• Molecule 2: Proteasome (Beta subunit) PrcB



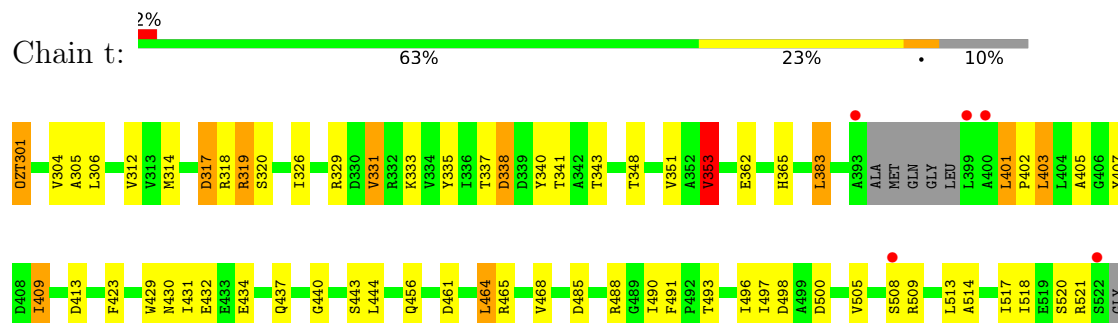
• Molecule 2: Proteasome (Beta subunit) PrcB



• Molecule 2: Proteasome (Beta subunit) PrcB

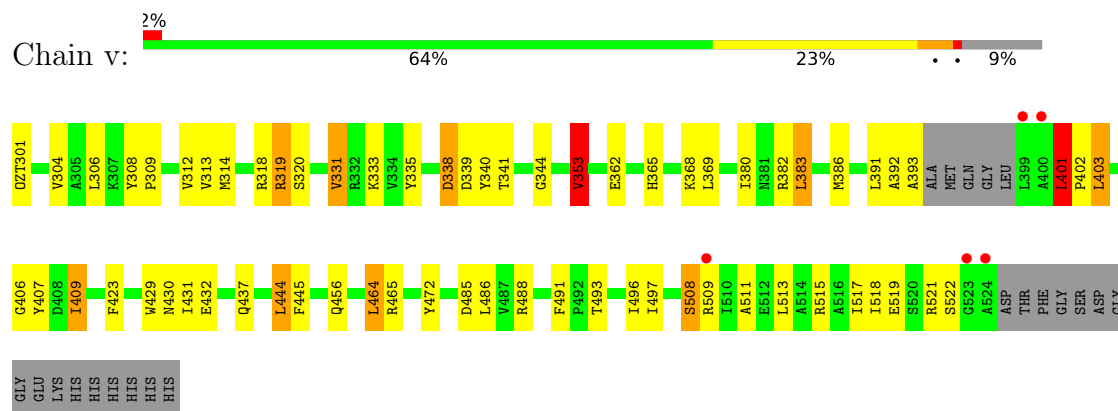


• Molecule 2: Proteasome (Beta subunit) PrcB

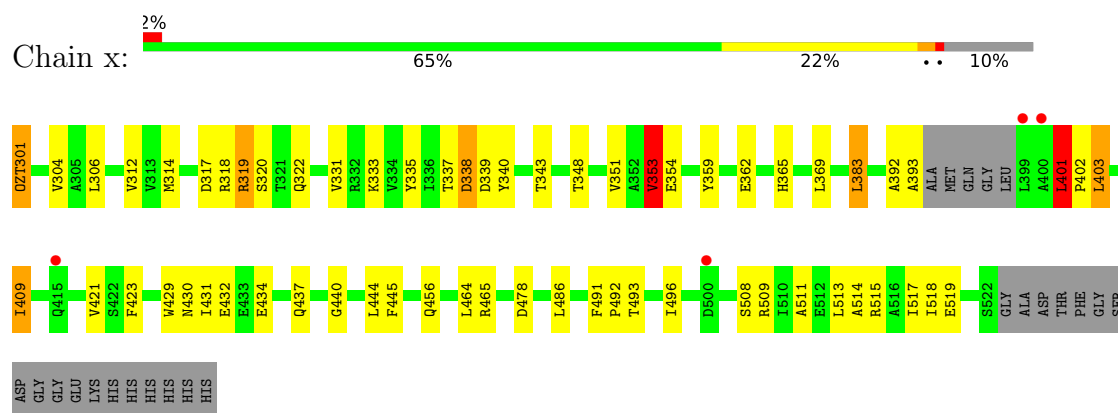


ALA
ASP
THR
PHE
GLY
SER
ASP
GLY
GLY
LYS
LYS
HIS
HIS
HIS
HIS
HIS

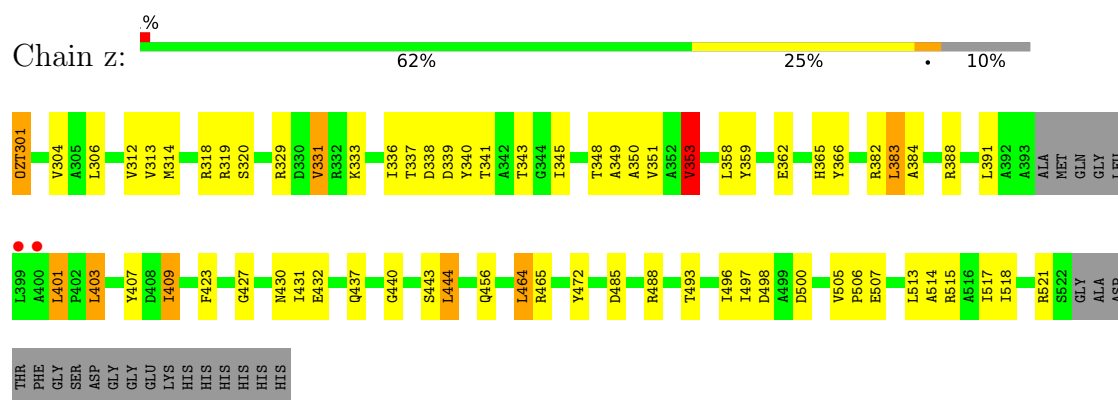
• Molecule 2: Proteasome (Beta subunit) PrcB



• Molecule 2: Proteasome (Beta subunit) PrcB

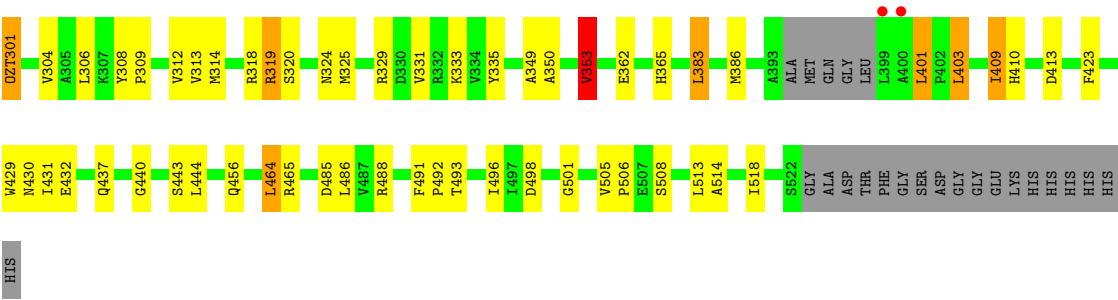


• Molecule 2: Proteasome (Beta subunit) PrcB



• Molecule 2: Proteasome (Beta subunit) PrcB





HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.58Å 209.62Å 284.93Å 90.00° 102.01° 90.00°	Depositor
Resolution (Å)	25.12 – 2.88 25.12 – 2.88	Depositor EDS
% Data completeness (in resolution range)	88.6 (25.12-2.88) 88.5 (25.12-2.88)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine), CNS	Depositor
R, R_{free}	0.217 , 0.267 0.231 , 0.271	Depositor DCC
R_{free} test set	13598 reflections (4.39%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	90443	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.88 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2193e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OZT

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	1	0.66	0/1657	0.94	3/2238 (0.1%)
1	3	0.66	0/1649	0.95	7/2227 (0.3%)
1	A	0.73	1/1657 (0.1%)	1.04	9/2238 (0.4%)
1	B	0.79	1/1657 (0.1%)	1.07	5/2238 (0.2%)
1	D	0.56	0/1649	0.97	5/2227 (0.2%)
1	F	0.73	0/1514	1.02	3/2050 (0.1%)
1	I	0.65	0/1664	1.00	6/2248 (0.3%)
1	K	0.63	0/1657	1.03	10/2238 (0.4%)
1	M	0.60	0/1613	0.98	7/2178 (0.3%)
1	O	0.68	0/1657	0.96	4/2238 (0.2%)
1	Q	0.56	0/1657	0.94	5/2238 (0.2%)
1	S	0.67	0/1657	0.96	8/2238 (0.4%)
1	U	0.63	0/1657	0.94	3/2238 (0.1%)
1	W	0.54	0/1511	0.96	7/2046 (0.3%)
1	Y	0.62	0/1649	0.97	5/2227 (0.2%)
1	a	0.72	0/1657	0.93	3/2238 (0.1%)
1	b	0.73	0/1657	0.99	6/2238 (0.3%)
1	d	0.58	0/1657	0.93	3/2238 (0.1%)
1	f	0.60	0/1657	0.86	2/2238 (0.1%)
1	i	0.69	0/1657	0.97	2/2238 (0.1%)
1	k	0.64	0/1657	0.99	7/2238 (0.3%)
1	m	0.60	0/1636	0.93	3/2209 (0.1%)
1	o	0.63	0/1657	0.93	4/2238 (0.2%)
1	q	0.59	0/1657	0.93	4/2238 (0.2%)
1	s	0.67	0/1657	0.94	2/2238 (0.1%)
1	u	0.62	0/1657	0.95	3/2238 (0.1%)
1	w	0.57	0/1657	0.93	3/2238 (0.1%)
1	y	0.58	0/1657	0.96	4/2238 (0.2%)
2	2	0.86	0/1620	1.01	4/2196 (0.2%)
2	4	0.85	0/1620	0.99	5/2196 (0.2%)
2	C	0.74	0/1620	0.97	7/2196 (0.3%)
2	E	0.72	0/1620	0.97	4/2196 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	G	0.87	0/1620	0.99	5/2196 (0.2%)
2	H	0.83	1/1620 (0.1%)	1.02	8/2196 (0.4%)
2	J	0.73	1/1620 (0.1%)	0.94	5/2196 (0.2%)
2	L	0.83	0/1620	0.96	5/2196 (0.2%)
2	N	0.93	2/1620 (0.1%)	1.07	8/2196 (0.4%)
2	P	0.99	2/1620 (0.1%)	1.06	9/2196 (0.4%)
2	R	0.70	0/1620	0.95	4/2196 (0.2%)
2	T	0.82	0/1620	1.01	4/2196 (0.2%)
2	V	0.92	1/1624 (0.1%)	1.03	4/2201 (0.2%)
2	X	0.86	0/1620	1.01	7/2196 (0.3%)
2	Z	0.75	0/1620	0.99	7/2196 (0.3%)
2	c	0.77	0/1610	0.99	6/2182 (0.3%)
2	e	0.79	0/1620	1.03	7/2196 (0.3%)
2	g	0.87	1/1620 (0.1%)	0.98	3/2196 (0.1%)
2	h	0.87	0/1602	1.03	7/2171 (0.3%)
2	j	0.76	0/1620	0.96	5/2196 (0.2%)
2	l	0.86	0/1620	1.03	5/2196 (0.2%)
2	n	0.89	2/1620 (0.1%)	1.02	3/2196 (0.1%)
2	p	0.94	1/1620 (0.1%)	1.00	4/2196 (0.2%)
2	r	0.75	0/1620	0.98	6/2196 (0.3%)
2	t	0.79	0/1620	0.94	5/2196 (0.2%)
2	v	0.90	1/1629 (0.1%)	1.04	6/2208 (0.3%)
2	x	0.81	1/1620 (0.1%)	0.99	5/2196 (0.2%)
2	z	0.68	0/1620	0.95	5/2196 (0.2%)
All	All	0.74	15/91370 (0.0%)	0.98	286/123638 (0.2%)

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	LYS	C-N	-7.40	1.24	1.33
2	V	60	ALA	CA-CB	-6.23	1.43	1.53
2	p	361	VAL	CA-CB	-6.11	1.46	1.54
2	H	190	ILE	CA-CB	-5.89	1.47	1.54
2	g	377	ALA	CA-CB	-5.74	1.44	1.53

The worst 5 of 286 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	11	GLN	N-CA-C	-12.39	97.26	112.38
2	J	218	ILE	N-CA-C	10.06	120.07	110.42
1	K	226	THR	N-CA-C	10.00	122.18	111.28
1	I	228	SER	N-CA-C	-9.67	100.72	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	k	528	SER	N-CA-C	-9.59	101.36	112.87

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	1	1633	0	1633	70	0
1	3	1625	0	1622	68	0
1	A	1633	0	1633	106	0
1	B	1633	0	1633	87	0
1	D	1625	0	1622	145	0
1	F	1490	0	1483	84	0
1	I	1640	0	1642	90	0
1	K	1633	0	1633	80	0
1	M	1589	0	1587	86	0
1	O	1633	0	1633	56	0
1	Q	1633	0	1633	97	0
1	S	1633	0	1633	103	0
1	U	1633	0	1633	58	0
1	W	1487	0	1477	70	0
1	Y	1625	0	1622	109	0
1	a	1633	0	1633	70	0
1	b	1633	0	1633	72	0
1	d	1633	0	1633	84	0
1	f	1633	0	1633	65	0
1	i	1633	0	1633	72	0
1	k	1633	0	1633	80	0
1	m	1612	0	1606	48	0
1	o	1633	0	1633	78	0
1	q	1633	0	1633	91	0
1	s	1633	0	1633	82	0
1	u	1633	0	1633	68	0
1	w	1633	0	1633	110	0
1	y	1633	0	1633	124	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2	1606	0	1593	48	0
2	4	1606	0	1593	43	0
2	C	1606	0	1593	48	0
2	E	1606	0	1593	71	0
2	G	1606	0	1593	49	0
2	H	1606	0	1593	61	0
2	J	1606	0	1593	49	0
2	L	1606	0	1593	57	0
2	N	1606	0	1593	49	0
2	P	1606	0	1593	40	0
2	R	1606	0	1593	72	0
2	T	1606	0	1593	47	0
2	V	1610	0	1596	65	0
2	X	1606	0	1593	58	0
2	Z	1606	0	1593	60	0
2	c	1596	0	1583	56	0
2	e	1606	0	1593	36	0
2	g	1606	0	1593	50	0
2	h	1588	0	1572	36	0
2	j	1606	0	1593	58	0
2	l	1606	0	1593	45	0
2	n	1606	0	1593	35	0
2	p	1606	0	1593	37	0
2	r	1606	0	1593	49	0
2	t	1606	0	1593	57	0
2	v	1615	0	1601	51	0
2	x	1606	0	1593	43	0
2	z	1606	0	1593	61	0
3	1	3	0	0	1	0
3	2	1	0	0	0	0
3	3	5	0	0	2	0
3	4	7	0	0	1	0
3	A	2	0	0	2	0
3	B	2	0	0	1	0
3	E	4	0	0	2	0
3	F	3	0	0	2	0
3	G	2	0	0	1	0
3	H	1	0	0	1	0
3	I	4	0	0	3	0
3	J	2	0	0	0	0
3	K	3	0	0	4	0
3	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	1	0	0	1	0
3	N	6	0	0	4	0
3	O	3	0	0	1	0
3	P	4	0	0	0	0
3	R	3	0	0	2	0
3	S	2	0	0	0	0
3	T	1	0	0	1	0
3	U	1	0	0	0	0
3	V	6	0	0	0	0
3	X	4	0	0	0	0
3	a	5	0	0	2	0
3	b	3	0	0	0	0
3	c	6	0	0	0	0
3	d	2	0	0	0	0
3	e	5	0	0	3	0
3	f	1	0	0	0	0
3	g	3	0	0	0	0
3	h	3	0	0	3	0
3	i	1	0	0	0	0
3	j	3	0	0	0	0
3	k	2	0	0	1	0
3	l	3	0	0	1	0
3	n	2	0	0	1	0
3	o	1	0	0	0	0
3	p	2	0	0	0	0
3	q	1	0	0	1	0
3	r	2	0	0	0	0
3	s	2	0	0	0	0
3	t	2	0	0	0	0
3	u	2	0	0	3	0
3	v	4	0	0	0	0
3	w	4	0	0	2	0
3	x	1	0	0	0	0
3	y	2	0	0	0	0
3	z	4	0	0	1	0
All	All	90443	0	89905	3512	0

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 19.

The worst 5 of 3512 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)
1:D:13:MET:N	1:D:13:MET:HE3	1.40	1.36
1:D:35:TYR:CE2	1:D:40:LEU:HB2	1.65	1.32
1:a:313:MET:HA	1:a:313:MET:CE	1.63	1.26
1:M:35:TYR:CE1	1:M:37:GLY:HA3	1.68	1.26
1:S:230:LEU:HD23	1:S:230:LEU:C	1.51	1.25

There are no symmetry-related clashes.

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	1	207/240 (86%)	193 (93%)	13 (6%)	1 (0%)	24	51
1	3	206/240 (86%)	196 (95%)	9 (4%)	1 (0%)	24	51
1	A	207/240 (86%)	189 (91%)	18 (9%)	0	100	100
1	B	207/240 (86%)	187 (90%)	19 (9%)	1 (0%)	24	51
1	D	206/240 (86%)	185 (90%)	21 (10%)	0	100	100
1	F	189/240 (79%)	170 (90%)	18 (10%)	1 (0%)	24	51
1	I	208/240 (87%)	199 (96%)	8 (4%)	1 (0%)	24	51
1	K	207/240 (86%)	196 (95%)	10 (5%)	1 (0%)	24	51
1	M	201/240 (84%)	190 (94%)	11 (6%)	0	100	100
1	O	207/240 (86%)	197 (95%)	9 (4%)	1 (0%)	24	51
1	Q	207/240 (86%)	194 (94%)	12 (6%)	1 (0%)	24	51
1	S	207/240 (86%)	194 (94%)	12 (6%)	1 (0%)	24	51
1	U	207/240 (86%)	194 (94%)	12 (6%)	1 (0%)	24	51
1	W	189/240 (79%)	175 (93%)	13 (7%)	1 (0%)	24	51
1	Y	206/240 (86%)	196 (95%)	9 (4%)	1 (0%)	24	51
1	a	207/240 (86%)	197 (95%)	9 (4%)	1 (0%)	24	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b	207/240 (86%)	193 (93%)	13 (6%)	1 (0%)	24	51
1	d	207/240 (86%)	196 (95%)	10 (5%)	1 (0%)	24	51
1	f	207/240 (86%)	190 (92%)	16 (8%)	1 (0%)	24	51
1	i	207/240 (86%)	195 (94%)	11 (5%)	1 (0%)	24	51
1	k	207/240 (86%)	199 (96%)	7 (3%)	1 (0%)	24	51
1	m	204/240 (85%)	190 (93%)	13 (6%)	1 (0%)	24	51
1	o	207/240 (86%)	194 (94%)	12 (6%)	1 (0%)	24	51
1	q	207/240 (86%)	194 (94%)	12 (6%)	1 (0%)	24	51
1	s	207/240 (86%)	196 (95%)	10 (5%)	1 (0%)	24	51
1	u	207/240 (86%)	198 (96%)	8 (4%)	1 (0%)	24	51
1	w	207/240 (86%)	197 (95%)	9 (4%)	1 (0%)	24	51
1	y	207/240 (86%)	197 (95%)	9 (4%)	1 (0%)	24	51
2	2	213/240 (89%)	208 (98%)	5 (2%)	0	100	100
2	4	213/240 (89%)	211 (99%)	2 (1%)	0	100	100
2	C	213/240 (89%)	212 (100%)	1 (0%)	0	100	100
2	E	213/240 (89%)	212 (100%)	1 (0%)	0	100	100
2	G	213/240 (89%)	209 (98%)	4 (2%)	0	100	100
2	H	213/240 (89%)	210 (99%)	3 (1%)	0	100	100
2	J	213/240 (89%)	211 (99%)	2 (1%)	0	100	100
2	L	213/240 (89%)	207 (97%)	6 (3%)	0	100	100
2	N	213/240 (89%)	210 (99%)	3 (1%)	0	100	100
2	P	213/240 (89%)	208 (98%)	5 (2%)	0	100	100
2	R	213/240 (89%)	209 (98%)	4 (2%)	0	100	100
2	T	213/240 (89%)	208 (98%)	5 (2%)	0	100	100
2	V	214/240 (89%)	209 (98%)	5 (2%)	0	100	100
2	X	213/240 (89%)	209 (98%)	4 (2%)	0	100	100
2	Z	213/240 (89%)	208 (98%)	5 (2%)	0	100	100
2	c	211/240 (88%)	205 (97%)	6 (3%)	0	100	100
2	e	213/240 (89%)	209 (98%)	4 (2%)	0	100	100
2	g	213/240 (89%)	206 (97%)	7 (3%)	0	100	100
2	h	210/240 (88%)	207 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	j	213/240 (89%)	207 (97%)	5 (2%)	1 (0%)	24	51
2	l	213/240 (89%)	209 (98%)	4 (2%)	0	100	100
2	n	213/240 (89%)	207 (97%)	6 (3%)	0	100	100
2	p	213/240 (89%)	205 (96%)	8 (4%)	0	100	100
2	r	213/240 (89%)	208 (98%)	5 (2%)	0	100	100
2	t	213/240 (89%)	211 (99%)	2 (1%)	0	100	100
2	v	215/240 (90%)	212 (99%)	3 (1%)	0	100	100
2	x	213/240 (89%)	209 (98%)	4 (2%)	0	100	100
2	z	213/240 (89%)	211 (99%)	2 (1%)	0	100	100
All	All	11711/13440 (87%)	11238 (96%)	447 (4%)	26 (0%)	43	70

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	151	PRO
1	F	151	PRO
1	I	151	PRO
1	b	451	PRO
1	o	451	PRO

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	1	162/184 (88%)	152 (94%)	10 (6%)	16	43
1	3	161/184 (88%)	147 (91%)	14 (9%)	9	27
1	A	162/184 (88%)	148 (91%)	14 (9%)	10	28
1	B	162/184 (88%)	140 (86%)	22 (14%)	3	10
1	D	161/184 (88%)	141 (88%)	20 (12%)	4	13
1	F	149/184 (81%)	129 (87%)	20 (13%)	4	11
1	I	163/184 (89%)	147 (90%)	16 (10%)	7	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	162/184 (88%)	149 (92%)	13 (8%)	11	31
1	M	158/184 (86%)	148 (94%)	10 (6%)	16	42
1	O	162/184 (88%)	151 (93%)	11 (7%)	14	39
1	Q	162/184 (88%)	150 (93%)	12 (7%)	13	35
1	S	162/184 (88%)	148 (91%)	14 (9%)	10	28
1	U	162/184 (88%)	149 (92%)	13 (8%)	11	31
1	W	148/184 (80%)	137 (93%)	11 (7%)	13	35
1	Y	161/184 (88%)	147 (91%)	14 (9%)	9	27
1	a	162/184 (88%)	148 (91%)	14 (9%)	10	28
1	b	162/184 (88%)	149 (92%)	13 (8%)	11	31
1	d	162/184 (88%)	148 (91%)	14 (9%)	10	28
1	f	162/184 (88%)	150 (93%)	12 (7%)	13	35
1	i	162/184 (88%)	149 (92%)	13 (8%)	11	31
1	k	162/184 (88%)	148 (91%)	14 (9%)	10	28
1	m	160/184 (87%)	149 (93%)	11 (7%)	14	38
1	o	162/184 (88%)	151 (93%)	11 (7%)	14	39
1	q	162/184 (88%)	146 (90%)	16 (10%)	7	22
1	s	162/184 (88%)	151 (93%)	11 (7%)	14	39
1	u	162/184 (88%)	153 (94%)	9 (6%)	19	47
1	w	162/184 (88%)	149 (92%)	13 (8%)	11	31
1	y	162/184 (88%)	147 (91%)	15 (9%)	8	25
2	2	161/177 (91%)	147 (91%)	14 (9%)	9	27
2	4	161/177 (91%)	149 (92%)	12 (8%)	12	34
2	C	161/177 (91%)	148 (92%)	13 (8%)	11	30
2	E	161/177 (91%)	150 (93%)	11 (7%)	14	39
2	G	161/177 (91%)	147 (91%)	14 (9%)	9	27
2	H	161/177 (91%)	144 (89%)	17 (11%)	6	19
2	J	161/177 (91%)	150 (93%)	11 (7%)	14	39
2	L	161/177 (91%)	143 (89%)	18 (11%)	6	17
2	N	161/177 (91%)	146 (91%)	15 (9%)	8	25
2	P	161/177 (91%)	147 (91%)	14 (9%)	9	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	R	161/177 (91%)	146 (91%)	15 (9%)	8	25
2	T	161/177 (91%)	146 (91%)	15 (9%)	8	25
2	V	161/177 (91%)	146 (91%)	15 (9%)	8	25
2	X	161/177 (91%)	148 (92%)	13 (8%)	11	30
2	Z	161/177 (91%)	150 (93%)	11 (7%)	14	39
2	c	161/177 (91%)	145 (90%)	16 (10%)	7	22
2	e	161/177 (91%)	149 (92%)	12 (8%)	12	34
2	g	161/177 (91%)	147 (91%)	14 (9%)	9	27
2	h	160/177 (90%)	145 (91%)	15 (9%)	8	24
2	j	161/177 (91%)	148 (92%)	13 (8%)	11	30
2	l	161/177 (91%)	147 (91%)	14 (9%)	9	27
2	n	161/177 (91%)	147 (91%)	14 (9%)	9	27
2	p	161/177 (91%)	148 (92%)	13 (8%)	11	30
2	r	161/177 (91%)	150 (93%)	11 (7%)	14	39
2	t	161/177 (91%)	146 (91%)	15 (9%)	8	25
2	v	161/177 (91%)	147 (91%)	14 (9%)	9	27
2	x	161/177 (91%)	146 (91%)	15 (9%)	8	25
2	z	161/177 (91%)	151 (94%)	10 (6%)	16	43
All	All	9008/10108 (89%)	8244 (92%)	764 (8%)	10	28

5 of 764 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	220	SER
2	2	208	SER
2	N	207	GLU
2	L	210	ILE
2	T	208	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 162 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	130	ASN
2	l	430	ASN
2	P	130	ASN

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Mol	Chain	Res	Type
2	2	65	HIS
2	r	430	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

28 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OZT	T	1	2	6,9,10	2.75	2 (33%)	9,12,14	2.34	3 (33%)
2	OZT	h	301	2	6,9,10	3.08	2 (33%)	9,12,14	2.41	4 (44%)
2	OZT	X	1	2	6,9,10	3.02	2 (33%)	9,12,14	2.58	4 (44%)
2	OZT	L	1	2	6,9,10	2.74	2 (33%)	9,12,14	2.46	5 (55%)
2	OZT	N	1	2	6,9,10	2.91	2 (33%)	9,12,14	2.28	4 (44%)
2	OZT	z	301	2	6,9,10	3.37	2 (33%)	9,12,14	2.45	3 (33%)
2	OZT	E	1	2	6,9,10	3.28	2 (33%)	9,12,14	2.68	5 (55%)
2	OZT	l	301	2	6,9,10	2.81	2 (33%)	9,12,14	2.51	4 (44%)
2	OZT	t	301	2	6,9,10	2.83	2 (33%)	9,12,14	2.20	4 (44%)
2	OZT	Z	1	2	6,9,10	2.92	2 (33%)	9,12,14	1.72	3 (33%)
2	OZT	g	301	2	6,9,10	2.84	2 (33%)	9,12,14	2.72	4 (44%)
2	OZT	r	301	2	6,9,10	3.00	2 (33%)	9,12,14	2.60	4 (44%)
2	OZT	C	1	2	6,9,10	3.18	2 (33%)	9,12,14	1.77	2 (22%)
2	OZT	2	1	2	6,9,10	2.83	2 (33%)	9,12,14	2.21	3 (33%)
2	OZT	c	301	2	6,9,10	3.04	2 (33%)	9,12,14	2.19	5 (55%)
2	OZT	n	301	2	6,9,10	3.31	2 (33%)	9,12,14	2.25	4 (44%)
2	OZT	v	301	2	6,9,10	3.25	2 (33%)	9,12,14	2.87	3 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OZT	p	301	2	6,9,10	3.20	2 (33%)	9,12,14	2.85	5 (55%)
2	OZT	x	301	2	6,9,10	3.40	2 (33%)	9,12,14	2.36	4 (44%)
2	OZT	4	301	2	6,9,10	3.32	2 (33%)	9,12,14	2.83	5 (55%)
2	OZT	R	1	2	6,9,10	3.25	2 (33%)	9,12,14	3.02	5 (55%)
2	OZT	G	1	2	6,9,10	2.95	2 (33%)	9,12,14	2.32	3 (33%)
2	OZT	e	301	2	6,9,10	3.13	2 (33%)	9,12,14	2.06	4 (44%)
2	OZT	J	1	2	6,9,10	3.16	2 (33%)	9,12,14	2.36	3 (33%)
2	OZT	V	1	2	6,9,10	3.12	2 (33%)	9,12,14	1.96	3 (33%)
2	OZT	j	301	2	6,9,10	2.99	2 (33%)	9,12,14	1.82	5 (55%)
2	OZT	H	1	2	6,9,10	3.30	2 (33%)	9,12,14	2.69	4 (44%)
2	OZT	P	1	2	6,9,10	2.80	2 (33%)	9,12,14	2.66	4 (44%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OZT	T	1	2	-	0/1/14/16	0/1/1/1
2	OZT	h	301	2	-	0/1/14/16	0/1/1/1
2	OZT	X	1	2	-	0/1/14/16	0/1/1/1
2	OZT	L	1	2	-	0/1/14/16	0/1/1/1
2	OZT	N	1	2	-	0/1/14/16	0/1/1/1
2	OZT	z	301	2	-	0/1/14/16	0/1/1/1
2	OZT	E	1	2	-	0/1/14/16	0/1/1/1
2	OZT	l	301	2	-	0/1/14/16	0/1/1/1
2	OZT	t	301	2	-	1/1/14/16	0/1/1/1
2	OZT	Z	1	2	-	0/1/14/16	0/1/1/1
2	OZT	g	301	2	-	0/1/14/16	0/1/1/1
2	OZT	r	301	2	-	0/1/14/16	0/1/1/1
2	OZT	C	1	2	-	0/1/14/16	0/1/1/1
2	OZT	2	1	2	-	1/1/14/16	0/1/1/1
2	OZT	c	301	2	-	0/1/14/16	0/1/1/1
2	OZT	n	301	2	-	1/1/14/16	0/1/1/1
2	OZT	v	301	2	-	0/1/14/16	0/1/1/1
2	OZT	p	301	2	-	0/1/14/16	0/1/1/1
2	OZT	x	301	2	-	0/1/14/16	0/1/1/1
2	OZT	4	301	2	-	1/1/14/16	0/1/1/1
2	OZT	R	1	2	-	1/1/14/16	0/1/1/1
2	OZT	G	1	2	-	0/1/14/16	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OZT	e	301	2	-	0/1/14/16	0/1/1/1
2	OZT	J	1	2	-	0/1/14/16	0/1/1/1
2	OZT	V	1	2	-	0/1/14/16	0/1/1/1
2	OZT	j	301	2	-	0/1/14/16	0/1/1/1
2	OZT	H	1	2	-	0/1/14/16	0/1/1/1
2	OZT	P	1	2	-	0/1/14/16	0/1/1/1

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	x	301	OZT	O1-C5	7.69	1.46	1.36
2	z	301	OZT	O1-C5	7.68	1.46	1.36
2	n	301	OZT	O1-C5	7.63	1.46	1.36
2	E	1	OZT	O1-C5	7.49	1.46	1.36
2	4	301	OZT	O1-C5	7.47	1.46	1.36

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4	301	OZT	C2-O1-C5	-5.91	101.57	110.33
2	r	301	OZT	C2-CA-C	-5.81	106.08	114.16
2	H	1	OZT	CA-N-C5	-5.77	103.83	112.75
2	J	1	OZT	O1-C2-C7	-5.65	101.34	108.68
2	v	301	OZT	C2-CA-C	-5.17	106.98	114.16

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	R	1	OZT	O-C-CA-C2
2	t	301	OZT	O-C-CA-C2
2	2	1	OZT	O-C-CA-C2
2	n	301	OZT	O-C-CA-C2
2	4	301	OZT	O-C-CA-C2

There are no ring outliers.

23 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	h	301	OZT	2	0
2	X	1	OZT	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	1	OZT	4	0
2	N	1	OZT	2	0
2	z	301	OZT	1	0
2	E	1	OZT	4	0
2	l	301	OZT	1	0
2	t	301	OZT	1	0
2	Z	1	OZT	1	0
2	g	301	OZT	11	0
2	r	301	OZT	1	0
2	C	1	OZT	2	0
2	2	1	OZT	6	0
2	c	301	OZT	1	0
2	n	301	OZT	1	0
2	p	301	OZT	1	0
2	x	301	OZT	2	0
2	4	301	OZT	5	0
2	J	1	OZT	1	0
2	V	1	OZT	3	0
2	j	301	OZT	1	0
2	H	1	OZT	8	0
2	P	1	OZT	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	1	211/240 (87%)	0.75	23 (10%) 10 9	19, 76, 123, 148	0
1	3	210/240 (87%)	0.49	9 (4%) 40 32	26, 72, 119, 146	0
1	A	211/240 (87%)	0.41	9 (4%) 40 32	20, 58, 105, 155	0
1	B	211/240 (87%)	0.14	3 (1%) 73 66	16, 48, 93, 141	0
1	D	210/240 (87%)	1.78	75 (35%) 1 1	36, 98, 148, 167	0
1	F	193/240 (80%)	0.30	6 (3%) 51 42	21, 55, 103, 136	0
1	I	212/240 (88%)	0.40	4 (1%) 66 58	23, 55, 101, 116	0
1	K	211/240 (87%)	1.12	31 (14%) 6 4	30, 74, 114, 166	0
1	M	205/240 (85%)	1.27	45 (21%) 2 2	27, 82, 142, 204	0
1	O	211/240 (87%)	0.50	13 (6%) 26 20	15, 67, 114, 137	0
1	Q	211/240 (87%)	2.00	97 (45%) 0 0	52, 111, 152, 185	0
1	S	211/240 (87%)	0.59	12 (5%) 29 23	23, 64, 113, 134	0
1	U	211/240 (87%)	0.60	7 (3%) 49 40	11, 69, 117, 140	0
1	W	193/240 (80%)	1.40	45 (23%) 2 2	31, 89, 134, 158	0
1	Y	210/240 (87%)	1.30	49 (23%) 2 2	29, 80, 125, 142	0
1	a	211/240 (87%)	0.34	5 (2%) 59 50	21, 61, 114, 153	0
1	b	211/240 (87%)	0.47	11 (5%) 33 26	20, 61, 110, 129	0
1	d	211/240 (87%)	0.68	12 (5%) 29 23	25, 76, 124, 160	0
1	f	211/240 (87%)	0.89	24 (11%) 10 8	25, 80, 124, 150	0
1	i	211/240 (87%)	0.37	7 (3%) 49 40	18, 56, 105, 131	0
1	k	211/240 (87%)	0.37	4 (1%) 66 58	20, 58, 105, 159	0
1	m	208/240 (86%)	0.70	12 (5%) 29 22	21, 76, 124, 159	0
1	o	211/240 (87%)	0.73	17 (8%) 18 15	22, 74, 123, 158	0
1	q	211/240 (87%)	1.15	25 (11%) 9 8	36, 88, 132, 152	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	s	211/240 (87%)	0.48	9 (4%)	40 32	16, 64, 108, 133	0
1	u	211/240 (87%)	0.71	11 (5%)	33 26	21, 76, 117, 138	0
1	w	211/240 (87%)	1.57	62 (29%)	1 1	41, 96, 138, 187	0
1	y	211/240 (87%)	1.51	71 (33%)	1 1	41, 83, 126, 145	0
2	2	216/240 (90%)	-0.21	3 (1%)	73 66	16, 38, 90, 124	0
2	4	216/240 (90%)	-0.11	2 (0%)	81 75	15, 42, 88, 112	0
2	C	216/240 (90%)	0.17	3 (1%)	73 66	19, 51, 92, 122	0
2	E	216/240 (90%)	0.35	5 (2%)	61 52	16, 55, 92, 154	0
2	G	216/240 (90%)	-0.17	3 (1%)	73 66	14, 41, 86, 149	0
2	H	216/240 (90%)	0.08	3 (1%)	73 66	21, 47, 89, 125	0
2	J	216/240 (90%)	0.20	5 (2%)	61 52	21, 51, 94, 143	0
2	L	216/240 (90%)	0.15	4 (1%)	66 58	21, 45, 86, 140	0
2	N	216/240 (90%)	-0.21	2 (0%)	81 75	16, 33, 76, 114	0
2	P	216/240 (90%)	-0.27	2 (0%)	81 75	13, 34, 77, 121	0
2	R	216/240 (90%)	0.59	6 (2%)	55 46	26, 62, 100, 135	0
2	T	216/240 (90%)	0.01	4 (1%)	66 58	14, 42, 90, 114	0
2	V	217/240 (90%)	-0.32	3 (1%)	73 66	11, 32, 80, 126	0
2	X	216/240 (90%)	0.07	4 (1%)	66 58	22, 42, 85, 119	0
2	Z	216/240 (90%)	0.44	6 (2%)	55 46	28, 55, 100, 145	0
2	c	214/240 (89%)	-0.01	4 (1%)	66 58	20, 45, 83, 130	0
2	e	216/240 (90%)	0.05	3 (1%)	73 66	18, 46, 90, 122	0
2	g	216/240 (90%)	0.01	3 (1%)	73 66	21, 46, 89, 152	0
2	h	213/240 (88%)	-0.20	2 (0%)	81 75	14, 39, 75, 119	0
2	j	216/240 (90%)	0.03	3 (1%)	73 66	15, 47, 88, 127	0
2	l	216/240 (90%)	-0.07	3 (1%)	73 66	18, 39, 84, 128	0
2	n	216/240 (90%)	-0.20	2 (0%)	81 75	13, 38, 87, 120	0
2	p	216/240 (90%)	-0.31	4 (1%)	66 58	13, 33, 73, 140	0
2	r	216/240 (90%)	0.19	2 (0%)	81 75	21, 50, 93, 124	0
2	t	216/240 (90%)	0.07	5 (2%)	61 52	18, 48, 90, 121	0
2	v	218/240 (90%)	-0.21	5 (2%)	61 52	13, 36, 85, 123	0
2	x	216/240 (90%)	0.08	4 (1%)	66 58	24, 45, 92, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	z	216/240 (90%)	0.09	2 (0%) 81 75	22, 49, 98, 130	0
All	All	11907/13440 (88%)	0.41	795 (6%) 24 19	11, 56, 117, 204	0

The worst 5 of 795 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	177	LEU	6.0
1	k	472	ALA	5.7
1	M	19	LEU	5.1
1	D	35	TYR	4.9
1	w	443	TYR	4.8

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	OZT	R	1	9/10	0.91	0.11	18,44,69,87	0
2	OZT	c	301	9/10	0.91	0.13	39,63,87,89	0
2	OZT	E	1	9/10	0.92	0.11	37,49,92,109	0
2	OZT	l	301	9/10	0.93	0.12	24,38,76,81	0
2	OZT	e	301	9/10	0.94	0.10	26,57,76,88	0
2	OZT	r	301	9/10	0.94	0.09	23,32,68,69	0
2	OZT	t	301	9/10	0.94	0.10	28,37,51,63	0
2	OZT	z	301	9/10	0.94	0.08	26,36,64,66	0
2	OZT	J	1	9/10	0.95	0.08	22,28,50,52	0
2	OZT	L	1	9/10	0.95	0.10	30,51,75,78	0
2	OZT	x	301	9/10	0.95	0.07	26,34,49,61	0
2	OZT	C	1	9/10	0.95	0.09	26,53,60,67	0
2	OZT	4	301	9/10	0.95	0.09	11,23,37,60	0
2	OZT	V	1	9/10	0.96	0.08	18,39,47,73	0
2	OZT	v	301	9/10	0.96	0.09	26,50,58,58	0
2	OZT	g	301	9/10	0.96	0.09	21,28,60,70	0
2	OZT	X	1	9/10	0.96	0.08	5,31,53,62	0
2	OZT	T	1	9/10	0.96	0.07	15,22,49,54	0
2	OZT	Z	1	9/10	0.97	0.07	7,30,54,97	0
2	OZT	n	301	9/10	0.97	0.07	3,38,52,53	0
2	OZT	p	301	9/10	0.97	0.07	14,42,57,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	OZT	2	1	9/10	0.97	0.07	10,20,43,65	0
2	OZT	h	301	9/10	0.97	0.07	14,36,46,49	0
2	OZT	N	1	9/10	0.97	0.06	3,25,42,54	0
2	OZT	P	1	9/10	0.97	0.07	10,26,35,48	0
2	OZT	H	1	9/10	0.97	0.07	0,26,62,100	0
2	OZT	j	301	9/10	0.97	0.07	6,46,65,76	0
2	OZT	G	1	9/10	0.98	0.06	18,32,46,66	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.